Title word cross-reference

\( (N - 1) \) [ACD\textsuperscript{+}13a, ACD\textsuperscript{+}13b]. \( (n = 2, 3, 4) \) [VSP19]. \( (\sigma^3, \lambda^3) \) [TR12]. 
\( (\sigma^3, \lambda^5) \) [TR12]. + [CXW14, GTK10, NMLD13]. 0 [UD12]. 1 
[MG15, TS15b, YZLZ18]. \( 1 - n \) [CYG\textsuperscript{+}15]. 10 [AC11b, TS15b]. 13 
[GYGW12, SIT18]. 15 [AC11b]. 17 [GZZ12]. 18 [LW16]. 2 [CWT\textsuperscript{+}12, 
CBDS19, GSS13, MSBF16, MH10, SJD14, WvRSM14, YDL\textsuperscript{+}10, YZLZ18]. 20 
[AC11b, LYL16, YVEI\textsuperscript{+}17]. 24 [TS15b]. 3 
[AARP17, CM16, DVVP14, GMMH\textsuperscript{+}16, GSS13, GPK12, GBG\textsuperscript{+}19, HSW\textsuperscript{+}19, 
LTT16, MG15, MA16, MYT\textsuperscript{+}14, MP19b, MSSP17, PSS14, Pop18, RVCFF13, 
TS15b, VVMY18, YLL11, YZLZ18, dLvNC18b]. 4 
[AFSW16, GWJJ12, ZTH\textsuperscript{+}15]. 4d [Hil13]. 4f [Hua16]. 4 \times 1 [LGKS17]. 4 \times 4 
[SH14]. 5 [APY\textsuperscript{+}16, LZH16, WFL\textsuperscript{+}19, YLL11]. 5\textsuperscript{12} [MKH15]. 6 
[MCAY15, Rab12, TSZQ12]. 6\textsuperscript{2} [MKH15]. 6\textsuperscript{3} [MKH15]. 6\textsuperscript{4} [MKH15]. 7 \times 7 
[UGK18]. 8 [CSC\textsuperscript{+}18, TN12]. 8 \times 2 [LGKS17]. [2 + 2] [LXFC17]. [5 + 1]
\[ \text{CAT}^{+13}, \text{JXSW15}, \text{MCK17a}, \text{TDKT10}. \] \( f^{\text{n}} \) \([\text{BBG}^{+18b}]\).
\( \gamma \)
\[ \text{BTZ}^{+11}, \text{DBG11}, \text{YLCX10}. \] \( J \) \([\text{KNP}^{+12}, \text{LZH}^{+11}]\). \( k \) \([\text{Hug14}, \text{YS15}]\).
\( \kappa \)
\[ \text{YSRSS10}. \] \( \lambda \) \([\text{BH15}]\), \( \lambda^{3} \) \([\text{SLT14}]\), \( \lambda^{N} \) \([\text{XHL16}]\). \( \leftrightarrow \) \([\text{RSK}^{+15}]\).
\( \text{M} \)
\[ \text{ATIP18}, \text{AM19a}, \text{LLX}^{+19}, \text{MP19b}, \text{YLT}^{+19}, \text{NMH19}. \] \( m = 1, 2 \) \([\text{SIT18}]\).
\( n = 2 \) \([\text{TS15b}]\). \( m = 2, 3 \) \([\text{TS15b}]\). \( M^{+} \) \([\text{ATIP18}]\).
\( \mu \) \([\text{RHPWS13}]\).
\text{N} \[ \text{AARP17}, \text{HPT17}, \text{JSW10}, \text{KYCL11}, \text{KYKR15}, \text{KSK11}, \text{LHL}^{+10}, \text{LXZ}^{+10}, \text{MB16}, \text{PH17}, \text{PM18b}, \text{QZM11}, \text{RF15}, \text{YLZ}^{+10}, \text{ZYY}^{+10a}, \text{ZBP11}, \text{dSdLBN17}, \text{BLBC}^{+13}, \text{BS10b}, \text{HCBI11}, \text{JLH}^{+14}, \text{LLX}^{+19}, \text{LXFC17}, \text{OKY18}, \text{RRF11}, \text{SLY}^{+19}, \text{TCGT18}, \text{TT18}. \] \( n + m = 4 \) \([\text{XhD15}]\). \( n + m = 3 \)
\([\text{GT10}]\).
\( n = 0 \) \([\text{MCAY15}]\). \( n = 1 \)
\[ \text{GWJJ12}, \text{Rab12}, \text{RVCFF13}, \text{TN12}, \text{TSQ12}, \text{YLL11}, \text{TS15b}. \] \( n = 1, 2 \)
\[ \text{ABB}^{+12}, \text{ABB}^{+13}. \] \( n = 10 \) \([\text{TS15b}]\).
\( n = 12 \) \([\text{YVEI}^{+17}]\). \( n = 2 \)
\[ \text{WYGW12}, \text{TS15b}. \] \( n = 3 \) \([\text{SIT18}]\).
\( n = 4 \) \([\text{GZZ12}, \text{TS15b}]\). \( n = 5 \) \([\text{AC11b}]\).
\( n \leq 20 \) \([\text{ASS10}]\).
\( n \leq 25 \) \([\text{Tak11}]\).
\( n \leq 55 \) \([\text{Tak10}]\).
\( N \log N \) \([\text{AO10}]\), \( O(N) \)
\([\text{BSL1}1] \).
\( p \) \([\text{HNN}^{+17}, \text{MCK17b}]\).
\( \pi \)
\[ \text{AH10}, \text{BLBC}^{+13}, \text{BSF18}, \text{CLFRO18}, \text{CKL}^{+11}, \text{DLMH12}, \text{GNC}^{+18}, \text{GZM16}, \text{HSZ}^{+11}, \text{KV14}, \text{KDS17}, \text{MUN}^{+19}, \text{MVKS10}, \text{MIS}^{+15}, \text{OOK11}, \text{PM18a}, \text{RF15}, \text{SSG15}, \text{SDF12}, \text{SWW}^{+19}, \text{YJN}^{+11}, \text{Zha11}, \text{ZZMW19}. \] \( \pi \) \( \cdots \)
\[ \text{YZZ}^{+17}. \] \( \pi \cdots \pi \) \([\text{CCCLCGRO14}]\).
\( pK_{a} \) \([\text{BA11}, \text{CPK19}]\).
\( \Psi \) \([\text{Lüc14}]\).
\( q = 0, \pm 1, -2 \) \([\text{XhD15}]\).
\( r_{m}^{2} \) \([\text{RCM}^{+13b}]\).
\( \rightarrow \)
\[ \text{CK10}, \text{Chu10}, \text{GTK10}, \text{H211}, \text{HBL12}, \text{LWD13}, \text{NMLD13}. \]
\( S_{1} \) \([\text{KKL}^{+13}]\).
\( \sigma \)
\[ \text{DPSL16}, \text{GZM16}, \text{LZL}^{+15b}, \text{PM18a}. \]
\( \sigma_{\pi} \) \([\text{CZY11}, \text{YWZ14}]\).
\( \Lambda^{A} \)
\([\text{MCLD10}]\).
\( \times \) \([\text{SRS14}]\).
\( \rightarrow \) \([\text{CSNCS}^{+18}, \text{SB19}, \text{XCLZ19}]\).
\( v = 0 \) \([\text{LWD13}]\).
\( X \)
\[ \text{AM19a}, \text{Sak18}, \text{UT15}. \]
\( x = 1 \) \([\text{CWT}^{+12}, \text{LZTV10}]\).
\( Y \) \([\text{UT15}]\).

-1 \([\text{DLvNC18a}]\).
-5 \([\text{LL10c}]\).
-A \([\text{YJN}^{+11}]\).
-acceptor \([\text{MIS}^{+15}]\).
-Ace \([\text{LHL}^{+10}]\).
-acetals \([\text{YZL}^{+15}]\).
-Acetate \([\text{BHP19}]\).
-Aceto- \([\text{SJD14}]\).
-acetyl- \([\text{ZBP11}]\).
-acetylation \([\text{LHL}^{+10}]\).
-adrenergic \([\text{LLHM16}, \text{VKC10}]\).
-AI \([\text{YR13}]\).
-alkenoyl \([\text{YZL}^{+15}]\).
-alumina \([\text{SH14}]\).
-amination \([\text{YZ17}]\).
-amino \([\text{ZKH}^{+10}]\).
-aminopolyoxycarboxylate \([\text{CMD13}]\).
-arene \([\text{ZCK}^{+16}]\).
-atomic \([\text{XJSW15}]\).
-ATPase \([\text{II10}]\).
-azacrown-5 \([\text{ZYY}^{+10a}]\).
-barrel \([\text{yOaCG10}, \text{WXL}^{+12}]\).
-based \([\text{BPE16}, \text{EBK13}, \text{EP15}, \text{EB18}, \text{LFB14}, \text{MP19a}, \text{PBE16}]\).
-benzaldehyde \([\text{Lu11}]\).
-bipyridyl \([\text{KPL15}]\).
-block \([\text{CAT}^{+13}, \text{MCK17b}, \text{TDKT10}]\).
-bound \([\text{CKL}^{+11}]\).
-bound \([\text{XSW13}]\).
-butane \([\text{TCGT18}]\).
-butanol \([\text{BS10b}]\).
-butene \([\text{MSBF16}, \text{WvRSM14}]\).
-butyl- \([\text{MG15}]\).
-butylbenzene \([\text{HCB11}]\).
-carboxylates \([\text{AARP17}]\).
-carrabiose \([\text{YRSS10}]\).
-catalyst \([\text{SSD19}]\).
-catalyzed \([\text{YXZZ17}]\).
-cation \([\text{MUN}^{+19}]\).
-chloridophenylacetohydroxamate \([\text{CBDS19}]\).
-conjugated \([\text{BLBC}^{+13}]\).
-coumaric \([\text{HNN}^{+17}]\).
-couplings \([\text{LZH}^{+11}]\).
-Cu \([\text{NGAS17}]\).
-curcumin \([\text{AMK11}]\).
-cyclodextrin \([\text{DBG11}]\).
-dimensional \([\text{MB16}]\).
-dimethylaminophenyl \([\text{YLZ}^{+10}]\).
-effect \([\text{RWR}^{+13}]\).
-electron \([\text{KTK17}, \text{LW16}, \text{LYL16}, \text{HPT17}, \text{PHT17}]\).
-erythrose \([\text{SM17}]\).
-expanded \([\text{MLQ}^{+12}]\).
-\textbf{F12a} \([\text{MLCD11}]\).
-form \([\text{GWX}^{+12}]\).
-glucosamine


0 [KKH19].


7 [ADF+10, CD19, MBR+15]. 7-azaindole [YYT12]. 7-diphenylamino-9
7-tetraene [ABDGN12]. 7.0 [GLW19].

8 [AAC+16]. 8-formyl-7-hydroxycoumarin [LZHH11]. 8-naphthoquinone [HWW19]. 8R [BG13].

8-naphthoquinone [HWW19]. 8R [BG13].


9H-9-borafluorenes [ZQ14].

= [ATP18, ATIP18, ASS+17, AM19a, AM19b, CXS10, EPH+15, GPK+16, GN18, JLA+14, JJAB16, JJJ16, LDJ+10, LLL+11, JJJ16, Li14a, Li14b, LGW12, LLX+19, LZSM19, LCWW10, LWD13, MP19b, MCK17a, MCK17b, OKY18, PGS+15, PMG+16, Rab12, RDT14, SPS+12, Sak18, SLIB12, TLDG+12, TFQ+11, TT18, TG12b, UT15, WWKS16, XhD15, YW12, YLT+19, YS13, YHCS11, ZYLL12, ZLLL12, ZLX+19].


ability [LLL+10, PGS+15, RTS+13]. above [MK17]. Absolute [Gri13, HLW+17, KB11b, KYB13, VED10]. absorbing [NPG+18]. Absorption [RS17a, ZLL+10, DMD+18, FD13, HNN+17, KB16, LLBO12, LX11, LXZ+10, MKK+19, PMC+17, PMT10, PDG+16, SGDT10, TYN15, TZ12, Tsi14, WWD14, ZTH+15, ZDX11, QCR12]. abstraction [AAMD+11, BS10b, CSXZ17, GY12, JCG+10, LJW+11b, PNE18, WLHZ12, dCRN18]. Ac [SNKS10]. ACCDB [MP19c]. Accelerated [MFEM15, MFEM16, SH19a, YKNN19, AGB13, BDTP11, CVT+11, CF18, DWC17, GBL+11, HEMCZE+14, HAP+12, KV13, LL11, MLN+18, REV+17, YLX14, YSG12, ZC14, ZLL+13]. accelerates [HS17b]. Accelerating [HASR+12, HB19, LZ12, YWJ+16, HP10a]. Acceleration [BK+S11, ON14, SOM+13, UTM11, WSGN11, OOT15]. accelerator [SBV10]. accelerators [KK17a]. acceptance [BB11b, KB11c, NDW15, dRBO13]. acceptor [EHT19, Gil11, Lu11, MSV16, MBS+15, SB19, ZSTRS+18, ZZL19]. acceptor-bridge-donor [ZSTRS+18]. acceptors [KKK+19, uLhY11, TZ12]. accessibility [HPL+18, LHL+10]. accessible [FZY+12, WXL+12, WBF17]. Accessing [JZZM14]. accompanying [HSN14]. according [GM17, LPE+10, YZZ16]. account [EPH+13, Tsi18]. Accounting [XML+15, HH11, MBC11]. Accuracy [ASW19, DBM+15, FCE15, FKY+13, LLH17, BPB11, GRAR+14, HWLW11, KSR+16, LZ12, LDZW17, MLG18, NTNY15, yOaCG10, RS13, RVCFF13, Rob13, TO10, VVW+18, ZYS+10, AIM+18, Gil11, SDIP18]. Accurate [BS16b, BS18, CX10, CSXZ17, EFOD13, FLMI11, IN13, KG15, LAC+13, LLH11, LVL+10, MK13b, MFR+11, NWW17, Pol13, PVJ10, Sch12, SRR16, SY11, ZSB+16, ZSY+17, TH13, VSP19, WL14, YB16, ZWLX11, ZYL12, ZLLL12, ZLX+19].
ZWX19, AF14, ABS⁺19, BS10a, BPM15, Ben17, CCLP12, CSGOA17, CRZ⁺18, DKE⁺17, GA13, GBW⁺14, GWZX12, HRC13, KKH18, LC17b, LZZ14, MAK⁺14, ME10, MFR⁺17, NH16, yOTn16, dIRL11, RB13a, RCR⁺16, RDDS10, RR14, SH15, SS16b, VAMS14, VDVR14, VRKT19, WX⁺12, WJG⁺13, WX12, XSSL11, YOMT14, dVZ17, dSAI13].

Accurately [Bow16, LFB14, MA16, Zha12b].

ACE [WCDM11, LHL⁺10].

acetaldehyde [AS11, AAMD⁺11].

acetals [YZL⁺15].

acetamides [JSW10].

Acetate [BHP19].

acetic [KSNT19].

Aceto [SJD14].

acetohydroxyacid [XLY10].

acetonitrile [KT18, RS14].

acetyl [ZBP11, ZP13].

acetylacetone [SJWE10].

acetylation [FHK⁺12, IMK⁺16, LHL⁺10].

acetylcholine [SRA17].

acetylene [GRCL12, HSY⁺11, LT13, Tak10].

achieve [PH17, RAR⁺11].

Achieving [SLY⁺19, NNK⁺16].

Achim [Spr10].

acid [BLG11, CYY⁺17, CC18b, CM16, CB11d, FD14, FZL⁺15, Fel10, FP17b, FCE15, GRL⁺11, HNN⁺17, HG15, HCP15, KSNT19, KLS10, KML10, LBC⁺12, LXL⁺11, LF12, LP11b, LPM17, MSL10, MRO17, NH⁺10, OXW16, PHHD13, PG18, SIS10, SZBM13, SGG⁺18, SW12, SV11, TKCN19, TL16, VMP17, WC14, WG12, XN17, ZSB⁺11, ZWP11, ZHHX11, dSH19].

acid-arsenic [KSNT19].

acid-catalyzed [CYY⁺17].

acid-phosphoric [KSNT19].

acid-water [TL16].

acid/base [VMP17].

acidic [APY⁺16, TCC⁺18, YDX16].

acidities [ALK⁺15].

acidity [CRZ⁺18, CPK12].

Acids [WBKS19, BSG⁺18b, CCCLCGRO14, DKE⁺17, EHSPT16, FCE15, GREA11, RSL16, SCF⁺19, SST⁺18, XLY10, ZKH⁺10].

ACP [STM⁺15, SJ16].

across [AAC⁺16, GMPB12, MGS⁺16].

acylate [LZL⁺16].

act [LC10].

acting [BT18].

Actinide [SVLK18, RST⁺13].

action [XLY12].

activated [CV12, FWS⁺18, KSR17, ZG19].

Activation [Niz13, AALCM11, DR11, DSM⁺11, FB12, KMT⁺19, LSL⁺19, MRR11, MBGF15, PG18, SH19b, TM18, TS15a, WC11, XLY10, YXZ17].

activation-strain [FB12].

activator [BM12].

active [AIGP15, BHE⁺18, Cas13, DAP⁺18, DPF⁺12, EB18, LHZ10, NH19, PDG⁺16, SCSW13, SC18b, XTN18].

active-site [DAP⁺18].

active-space [NH19, PDG⁺16, XTN18].

actives [EOO⁺16].

activities [AHK⁺19].

activity [BPC13, DXL⁺10, GA13, GHL17, GFP17, MJLY14a, RCM⁺13b, SLY⁺10, TD10, TTB⁺11, YB13, Zsa10, ZDW18].

acute [TTL⁺12].

acyclic [NMH19, ZKH⁺10].

acyl [PS10].

adamantane [EHSPT16].

adamantane-based [EHSPT16].

Adapted [ELKE19, FF11, SS15, TH13, YKH15].

Adaptive [SK14, KEMP17, LZS⁺17, AOW11, BGR13, DSK17, FHMB15, HDM⁺15, LL19a, MJ14, MBFP15, MJG⁺15, OZ14, PN13, SNS13, WTD⁺19, WMW⁺10].

Adaptive-numerical-bias [KEMP17].

adaptively [ER18, SR18].

adcluster [IN13].

Adding [PFAS⁺19, XHLH16, Zha12b].

addition [FWB14, KSO⁺19, KS13b, NG14].

Additive [XVA⁺16, DPNM11, HM13, TSR⁺16, VHA⁺10, VMP17].

additivity [VRKT19, ZRL⁺15].

address [LG14].

Addressing [MMH19, cCVG⁺14].

alignment
[BF15, HRK+10, HKRS11, HS11, MJM+15, RP15, RHJ11, Ran12]. alignments [CYI+10, Ran13]. aliphatic [CROB16, SB10]. Alkali [YHCS11, Ano11, AM19a, DDM+15, JHM+09, JHM+11, THP+15, ZWY+10a].

alkali-metal [ZWY+10a]. Alkalides [WXS+12]. Alkaline-earth [WD10]. alkane [JGS+17, ZSTI14]. Alkaline [XZ11, Ano11, JHM+09, JHM+11, WP+15].

alkoxy-catalyzed [WFL+19]. alkyl [Den12, RMGB11]. All-atom [SM14b, CS14, DPNM11, HM13, JYC+16, KT18, LZZ14, MZZ11, OCW+15, VHA+10]. all-atomistic [FPH+19]. All-electron [KKA+18, PGdO+16].


alkoxy-catalyzed [WFL+19]. alkyl [Den12, RMGB11]. alkylthiols [FVP14]. alkyn [WWTI19]. alkaline [Jor17, YXZZ17]. Alkali [YHCS11, Ano11, AM19a, DDM+15, JHM+09, JHM+11, WP+15].

alkali-metal [ZWY+10a]. Alkalides [WXS+12]. Alkaline-earth [WD10]. alkane [JGS+17, ZSTI14]. Alkaline [XZ11, Ano11, JHM+09, JHM+11, WP+15].

alkoxy-catalyzed [WFL+19]. alkyl [Den12, RMGB11]. All-atom [SM14b, CS14, DPNM11, HM13, JYC+16, KT18, LZZ14, MZZ11, OCW+15, VHA+10]. all-atomistic [FPH+19]. All-electron [KKA+18, PGdO+16].

amyloid- [IO13b], amyloid-beta [LH11], analog [JBAM11], analogs [DCHL12, LP11b, SISK10, VM11, WBT10], analogue [PGW+17], analogues [LPS+13, NK19, SGWA17, VVBL17, VM19, WS12, YLL11].

analyses [BSF18, CBD510, KASH14, KP11, PZBA13, SKGB13, VVJ15, XWW+11].

Analysis [BMD19, CDM+15, ELKE19, HAI+16, JCGM18, KKGW19, LL19a, MOS12, SZL19, svLK18, Spr18, XFG+16, AKMT11, AST+16, ASL+11, ARRC15, AAB+19, AS18, Ano15-58, AM19a, AM19b, BK15, BL19, BH14, BSSP+13, BBG+18b, CLFR018, CMM18, CAF+13, CEB015, CCC+11, CAT+13, CH14, DMJ17, DDP+18, DHF+11, DJD12, DBK17, DJS+18, DCS15, DN19, ESD18, EHSPT16, EB18, Fer17, FB12, FHW+11, FHK+12, GVP+10, GLW13a, GLW13b, GNDA+12, dCGCRN19, GCP+13, Han11, HSX+19, HCD+10, HPSK12, HHT+13a, HHT+13b, HGW18, HDHL15a, HDHL15b, HDHL15c, HHWL17, Hug12, IY18, Jan16, JHH+13, JJJW+14, JZZM14, JCX10, JLS18, KG13, KYG+15, LSL+19, LBC+19, LL13a, LCPS13, LMZ+11b, LFM12, LAHS16, LGKS17, MLG18, MTD13, MJ14, MT19b, Mez10, MADWB11, MCLD10, MGS+16, MCK17b, NK19, NH19].

Analysis [NIIT15, NS17, OXBW16, OC14, PTK11, PSP15, PRyi+17, Ptb+15, PPUBGD10, PS14, RDT14, RSGS18, RC18, REL17, RLG14, SFM+18, SLY+10, SBB10, SFR+11, SHF18, SSGS15, SEJ+18, SB18, Sndk16, SSi13c, SB19, SPR+13, SH18b, SSP+19b, SH19b, Tyn15, TCB16, TD10, TTB+10, TS10b, UKS11, VBMA13, WNP+16, WWW19, Wei12a, Wei12b, WDKT19, XFG+15, YK13, YNH+17, Yes12, Yes15, ZCS+15, ZBB16, ZH12, ZZZ+19, ZCWX18, dSH19, vSGP10, JCHT18, ZSB+11].

Analytic [Boz18, MTD13, NF18, SZX13a, SZX13b, TSH+19, My17b].

Analytical [CCR18, CCB15, HNWF07, HNWF12, HH17, LBGS16, SFG+17, WOH18, CHC+13, FBY+17, GNR19, HHIa, KN17, KTSW11, MK13a, Popn11, Pop18, ZWF15].

Analyzing [BGS+19, BD11, MRB14, BCP+10, HPT17, LZS+17, PHT17, SWA13, WES13].

anapole [ZPP+16].

anatase [HRL11].

and/or [KB10, Pog10].

androstenedione [VCM15].

angle [CKP10, GBFD12, XML+15].

angle-dependent [CKP10].

angles [BKLA13, EJ13, FZY+12, GREA11, KTK17, LDH+14, OZ14, YZ16].

angular [BBG+18b, ENKK+17].

anharmonic [Kow11, SSWX14].

anhydrase [SSP+13].

anhydrides [RB12].

aniline [PLP+16].

Anion [TT18, CG15, KSN19, LCI0, uLhY11, LCC18, SC18a, SDF12].

Anionic [BHP19, AM19a, AM19b, GZZ12, GWPJ11, HPL13, JCP14, QZ10b, ZYR+15].

anionic-water [JCP14].

anions [PVS12, RDT14, RJS17, ZFY+10b, ZYL+12].

anisotropic [Ano10a, CAT+13, EPH+13, ENKK+17, NLP+16, SLX+15, SN10].

anisotropy [BP18, CGP12, LPLB16, ZLZ14].

ANN [XWW+11, ZDW18].

ANN-based [ZDW18].

annealing
[RHJ11, SHMO11, SHL*11, ZC14, LMZ11a]. annihilation [BL12].
annulated [RS17a]. anode [GNI18, YZLZi9]. Anomerization [SM17].
anoma-rzirconocene/borate [OSA19]. ansatz [Bou14, WGA18]. answer
[SJWE10, Tan19]. ant [ZsA10]. antagonists [LLL+10]. anthrax [JAH+17].
Anti [WFZ+18, ZsA10]. Anti-Electrostatic [WFZ+18]. anti-HIV-1
[ZsA10]. antiaromatic [TDKT10]. antibiotics [PG15]. antibody [UNT16].
anticancer [AJA+19, SZZ+18]. Anticooperativity [TDT19].
antiferromagnetic [ZB18]. Antiferromagnetically [SZL19]. antigen
[JAH+17]. antimicrobials [PPUBGD10]. antioxidant [GAI13, ZDW18].
antiparasitic [PPUBGD10]. antisense [ICS+12, ICS+13].
antitrypanosomal [PSdPE+10]. antitubercular [TD10]. AO [YOPB16].
AOFORCE [vW11]. APBS [UHH+11]. API [LAS+14, ZW18]. AppA
Application [AFBR17, BAMR13, BPE16, DAG19, GCCM15, HTS15, LDG+15, MBA11, MTS+19, MH10, OL13, PAK15, RVP+11, SMP17a, SRS14, SCI7, SDL14, SMM+18, Tak18, VKTRJ15, WH11, WFS19, ZsA10, vSGP10, CSAdOM17, CJPTC18, DGP14, Elki6, GLB16, GFG11, GWC16, HYSF19, IUK+11, KTO19, KFY+13, Ks18, KSK11, LLHM16, LP11a, LLL+10, LLLC11, LGRic1c, MDTD13, MdOdQ18, PFR13, RZG+13, RCM+13b, SDMP18, SN16a, SLX+15, SYH12, VV14, VKC10, WCDM11, You10, AFPI13, BD11, CZNA11, Fer13h, Fer13a, FCOGM12, GAI13, HYUS11, KUDG12, MCC11, Pet11, PW12, SPZP19, TSZQ12]. Applications [KGHC15, LCPS13, LCA17, Spr18, APK14, CGP11, EVR18, Fel10, GBFD12, HZY+10, HCD+10, IO13b, KK0+16, uLHy11, LJR+12, MG11, NS18, SSM15, SGM+13, ISP+10].
applied [BLG11, CTP13, GKR13, KKR+13, LTT16, PM18b, Ray13, RKG11, ZS7SM10]. Applying [KBI1a, ZSLL17, CC11]. Approach [Coo19, NNT+19, VSP19, ACD+13b, BPE16, BBG+18a, BVH17, BGR13, CCLP12, CRZ+18, CHC+13, CXS10, DK11, DGP14, DVVP14, DFF+15, DHE+12, FRSA14, Fer17, FNSF+11, FCCP17, FD16, FSD+18, dCGR19, GPE13, GZ14, GH16a, HRC13, HDH12, HNN+17, HBBY10, HZSS17, ITY+19, JCCX10, KV12, KV13, KHM19, KT19, KId19, KSK11, KT10, KSHP+19, KKH+19, KKH18, LLTC12, LH1a4, LG14, MZZ11, Man19b, MGWR12, ME10, Mor15, NSK18, NB19, NLL19, NNO16, OT12, PRP15, PMC+17, PSPE+10, PH10b, PBE16, PPUBGD10, PLP+16, RKG10, RB12, RVP+11, SLT14, Szd1B9, SEF+16, SH11b, SY16a, St15, SLLL13, SHG+16, SM17, TO19, TAG16, TSR+16, VVLG17, WFS19, XZ11, YKO+11, ZSLL17, ZLW10, AIM+18, GFG11, ACD+13a]. approach-an [KKH18]. approaches [BP18, BH13, CME11, DBM+17, ECZWD17, HBI+17, IT19, LSH+11, RLDJ17, RSR15, VLB+10, YJ11, ZDT18]. Appropriate [LZL13]. Approximate [Gav12, KV12, KV13, RP15, RZ16, SM14a, HH16a]. approximation [AO10, Boz18, Cas13, HH17, Kid19, Sch12, WHM10, WDKT19, YD17, YN15].


Based [ZYL†12, ZGZ19, ZT14, dCLFGL13, dSVdM†16, dVZ17, FAS†18, NKJ16, WTD†19, ZDW18, dLvNC18a, dLvNC18b]. Based-on [CDS16].

Bases [WBKS19, CWZB10, KASH14, LRVM18, MSLS10, SC18b, SBW12, WGA18, ZLL†10, Zha12a, ZBMZH15]. Basic [CMvG10, WLF19]. Basin [JLH†14, RDRC16]. Basin-hopping [JLH†14]. Basins [SBN13a, dLC18a, SBN13b]. Basis [B LF14, BRLS08, BRLS12, PHK14, WGA18, ZLL†10, Zha12a, ZBMZH15].


C [LdSRR16, LTR18, LAHS16, LLD17, LCWW10, LWD13, MLQ12, MCK17a, MCK17b, NDK18, PMG16, RLA11, Sak18, SKMS13, STS10, SBW12, Tak11, UT15, WCY11, WWKS16, YZZ17, ZYG14, ZLY16, ZLX19, BS16a, VAMS14, AM19a, Ben17, BWKW10a, BS16b, BH13, CG12, ED15, FL15, GWT17, GMSV14, GZ12, HJ13, HS16, IMK16, JLS10, LJW19, KV14, KMT19, KP10, LFB14, LLJ17, LDH14, MSV16, MH11, MSCP19, Niz13, OPR16, PTK11, Pic14, PZBA13, RWR13, SNDK16, TFQ10, TFQ11, TS15a, TKCN19, VAR12, VED10, WKC10a, W10, WWT19, W11, WTH16, Yes12, Yes15, YDGZ15, ZZZ19].


caging [DPB12]. calbindin [TJR19, PNG10]. calcium [Pla11, PD12, TJR19].

calcium-binding [TJR19]. calcium-induced [PD12]. Calculate

[GH16b, BCSCJ13, BACSCJ10, HDK12, PSC11, SK17, Yap11, YFH19].
calculated [CHP11, GY10, KJDB12, MJLV14a, MR11, NMLD13, SKMS13, Yan11, YA018].
calculating [CPZ19, Hei18, PNI13, SK12, WNP16, WWD14, CPK12, CXD19, EFS16, EDP11, HAI16, OK16, SM16a, WTYT17, dRBO13].

Calculation [Fer13b, Fer13a, HQSZ19, KSH13, KPG18, MY17a, MMJ10, MS15, SH11b, SOD11, SOvG12, AC11a, Bac12, BW11a, BK17b, BD11, BL12, CPR18, CCR18, CHG16, CG15, CX10, DKE17, DSX11, FD14, FGM11, FPH19, GRE11, GGM16, H111, JIS13, KHN16, KN17, KB16, KDB13, KNR18, LFN1, LLW12, LZW11, MYT14, MLC13, MS12, NYN17, NH19, NMR19, NFDP13, PDMT10, PAK15, Pic14, PW12, RO14b, RZ16, RB12, RRK16, SBV10, SH18a, SLIB12, SCSW13, SACdG14, SMM17, SR11, UT15, VVV15a, VVG13, WLLH18, WLF19, WDHZ13, ZHS18, ZZL10b, ZLLL12, ZGZC19, HH10].

Calculations [HBI17, HWB19, Jia19, MP19b, SR19, THI19, AR10, AAC16, BE12, BLL13, BS10a, BTMS12, BH15, Bou14, BS18, BG12, BLZ13, CR14, CCJ10, CS17, CCKK16, CBDS19, CMvG10, CXS10, CHK10, CKG18, DGH11, DSV19, DGSVGM19, EFAC13, EK17, EWK13, EP12, EB12,
EBK13, EB18, FAA15, FRC18, FA18, FE14, GRARO$^+$14, GA18, GMO16, HASR$^+$12, HYL$^+$11, HS14a, HB14, HSH15, Hel13, HG10, HG13, HBL12, HYUS11, HGW18, Ibr17, IMS18, ISM18, JCG$^+$11, KK17a, KB10, KKN11, KGHK12, KMS$^+$19, KKR$^+$13, KERY$^+$16, KFT18, KCPMG12, KKL$^+$13, KSH$^+$17, KKH18, LEdOLdV17, LRVM18, LOB18, LMZ11a, LCH10, LYT$^+$13, LCA17, LvG13b, LCK$^+$18, LCM$^+$14, Lun12, MK17, MK19, MUGNVJ$^+$18, MLN$^+$18, MCLD10, MEH18, MCK17a, MCK17b, NWW17, NZM18, NLL19, NH19, PLAG11, SHL$^+$13, SPZP18a, CKT13, LCB10, TCPPC14, Zha12b].

calculations [OLA15, OOT15, OZLSBH12, PBLdS12, PTK11, PHK14, POB13, PBBP11, PDG$^+$16, PN13, PGW$^+$17, RAR$^+$11, RLZ$^+$18, RHT$^+$15, RLD12, RR11, REV$^+$17, RI10, RK15, SH15, SRSL015, SP13, SPHF$^+$18, SS16b, SCW11, SWPR11, SRS14, SMP17b, SDMS13, SHB17, SKTT11, SPZP18b, SPZP19, TLD$^+$12, TNY18, TS10a, TN19b, UHH$^+$18, VLA$^+$10, VKAM12, VKNT16, VHR16, VFRAR16, VMP17, VI17, WC13, WSZW15, WHK$^+$12, WTH$^+$16, WGA18, WXY14, XYW$^+$14, YWJ$^+$16, YD17, YN15, YJ19, ZRCC11, ZLT13, ZLZ14, ZWMM10, ZH12, MSPC19, NQB19].
calibrate [dCLFGL13].
calibration [VVLG17].
call [ZPF14].
can [ZPF14].
Can [ASMS10, IMSR18, KV15b, LZW$^+$11, NH19, PLAG11, SHL$^+$13, SPZP18a, CIKT13, LCB10, TCPPC14, Zha12b].

canada [Fel10].
cancer [NS10, WC11].
Canepa [LHMM11].
cannabinoid [ILKR11].
Canonical [CP15, HH11, JSD$^+$11, PLH16].
capacity [KOP$^+$14, PGC12, WKCl0a, WKLC12].
capability [LC10].
capabilities [AAC$^+$16].
capacity [KOP$^+$14, PGC12, WKCl0a, WKLC12].
capillary [NFPD13].
caps [WDS$^+$19].
capture [GLZ17, SMD18].
car [DL19, KCK$^+$15].
carbon [JLLW19, SC17, AJA$^+$19, AS15a, AAMR18, ASL$^+$11, BPE16, CME11, DI11, Den12, DC13, Fom13, FTR15, GSSMM15, GPK$^+$16, GBS$^+$17, GZZ12, JWO15, KGHK12, KV14, KPH$^+$19, KHE$^+$19, KGJZ19, LPS16, LL10c, LT14, LK16b, MSY19, OCW$^+$15, RHN10, RRK16, Sie18, TSR$^+$16, VS14, WYL$^+$15, WDZN16, YZN13, YZZ$^+$17, ZYW$^+$16, ZLY$^+$16, ZWF15, OSI$^+$19].
carbon-beryllium [CME11].
carbon-carbon [KGJZ19].
carbon-germanium [GSM15].
carbonate [ZSWL12].
carbondioxide [Sea10].
carbonic [SSP$^+$14].
carbons [MKB$^+$13, RVB$^+$12].
carbonyl [BH19, CZH12, CROB16, TS10b, ZBMZH15].
carbonylation [MRC$^+$18].
carbonyls [SSX\textsuperscript{+14}]. carboranes [HJ13]. carboxybetaine [DQ16].
carboxylates [AARP17, RVM19]. carboxylation [CKG18, DGSVGVM19].
carboxylic [LPMT17, RB12, dSH19]. card [SR11]. Carlo [LHMM11, NQB19, Aou16, BFH\textsuperscript{+13}, CLK11, CG12, CTP13, CAP17, DMN15, FFA14, GP12, GPM17, HFSO12, Hes19, HMM10, HYUS11, HQC16, HHHY10, HJJ\textsuperscript{+13}, LPK16, LMZ11a, LZ12, MS16, MBRC16, MOS12, NDW15, OPBR17, PSS14, PS13, Pon10, PHH\textsuperscript{+12}, RHNN10, RdA12, SCOJ13, SAGC16, SMRM\textsuperscript{+17}, SSP19a, SE14, SE14, YO19, ZLM\textsuperscript{+15}, ZW17]. Carlo/Brownian [DMN15]. Carlo/molecular [RdA12].
carotenoids [PVAM16]. carrabiose [YSRSS10]. carrier [SFDE16]. carriers [GMASBF\textsuperscript{+16}, UGK18]. Cartesian [REH13, FHMB15, AlQ19, Elk16].
caryolene [ONTTL16]. caryolene-forming [ONTTL16]. CAS [KMS\textsuperscript{+19}, MH11]. cascade [HS17b, ONTTL16, ZZWT12]. cascaded [LZL\textsuperscript{+15a}]. Case [BMD19, Alg17, ASMS10, AM19a, AM19b, BM12, BG13, CCLP12, CB11c, DSB\textsuperscript{+19}, DOM\textsuperscript{+11}, DS12a, EFOD13, EOA\textsuperscript{+11}, GH10, GKR13, GpdC\textsuperscript{+16}, HSH15, KB13, LAPAS11, LP11a, LT13, MIS\textsuperscript{+15}, OME16, PG18, PVAM16, Ray13, RVM19, Rod13, RKG11, RCM\textsuperscript{+13b}, RJS17, SRF\textsuperscript{+17}, SC18a, SPZP18b, TLA10, VKNT16, WDS\textsuperscript{+19}, ZTH\textsuperscript{+15}, RAR\textsuperscript{+11}]. cases [GREA11]. CASPT2 [LWGZ15, SGWA17, VFRAR16, WGA18]. Cassandra [SMRM\textsuperscript{+17}]. CASSCF [KSHP\textsuperscript{+19}, KKL\textsuperscript{+13}, LWGZ15, NH19, SGWA17]. CASSCF/CASPT2 [LWGZ15]. CASSCF/MC [KKL\textsuperscript{+13}].
CASSCF/MC-XQDPT2 [KKL\textsuperscript{+13}]. CAST [GBW\textsuperscript{+14}]. catalysis [Can10, Can11, EvRC\textsuperscript{+18}, GSMZ19, KK19, LHMM11, MG14, RNS19, WFL\textsuperscript{+19}]. catalyst [BEM14, DK19, DSHLM18, LLC17, OSA19, RLZ\textsuperscript{+18}, WWT19, YZ15b, ZSWL12, ZX19, dSdDar10, SSD19]. catalysts [AHK\textsuperscript{+19}, BEPM14, GSMZ19, JJB16, MPJ\textsuperscript{+19}, NJX\textsuperscript{+10}, WJX\textsuperscript{+10}].
Catalytic [YMY\textsuperscript{+19}, AKH\textsuperscript{+19}, GHL17, GA19, KV15b, ONTTL16, SJD14, SLY\textsuperscript{+10}, SOY12, TM18, UKS11, WZQW10, dSdDar10]. catalyzed [AS11, BF19b, CYY\textsuperscript{+17}, CJC10, CPL11, HPT16a, HDB15, JJL16, KSO\textsuperscript{+19}, KB13, KT12, MRC\textsuperscript{+18}, MG15, MTS\textsuperscript{+19}, QLYL10, TLA10, Ts17, VCM15, WCWW11, WFL\textsuperscript{+19}, WWT19, WXY14, XLYZ10, YXZZ17, YZ17, YZLZ18, dSdDar10, dSdLBN17, dCDP15]. catastrophic [ABDGN12, GND\textsuperscript{+12}]. catechol [PBLdS12]. catechol-O-methyltransferase [PBLdS12]. Catenanes [LAHS16].
cathepsin [ETLS17]. cathode [SMIN\textsuperscript{+19}]. cation [CCCLCGRO14, CGPP11, DLMH12, DDM\textsuperscript{+15}, MUN\textsuperscript{+19}, RMGB11, SSGS15, ZYL\textsuperscript{+12}].
Cationic [HJ13, SC18a, WJX\textsuperscript{+10}]. Cations [ND19, SB19, CCI18b, KGR\textsuperscript{+16}, LCL\textsuperscript{+10}, LSRR16, LLR18, PVS12, SB\textsuperscript{+17}, Tac17, THP\textsuperscript{+15}, ZWY\textsuperscript{+10a}, ZWS\textsuperscript{+10}]. cations/nucleobases [CC18b]. caused [GDV17]. caveolin [PGI19]. caveolin-1 [PGI19]. cavitation [CC18a]. cavities [HRB\textsuperscript{+17}, ZSB\textsuperscript{+16}]. cavities/vacancies [HRB\textsuperscript{+17}]. cavity [KD18, ZWS\textsuperscript{+10}]. CAVS [SDZ17]. CB [BTMS12, CC18a, ILKR11]. CBS [KG15]. CBS-QB3 [KG15]. CC [Gil11, LTLC12]. CC2 [SGWA17].
CC3 [LZ14]. ccCA [RJWW12]. CCSD
PL14, PTB+15, RSSG18, RO14b, Rez19, Ric16, REL17, SPS+12, SDF+18, SSGS15, SmIN+19, SMP17a, SFLG+17, SLC+17, TN10, TKNN10, UT15, UGK18, VPR10, VAR12, VL17b, WCT+11, WWCL15, YKO+11, YWZ14, YLZ+10, YJ17, YFH+19, ZDZM13, ZZL19, dSH19, dLC17. charge-assisted [SSGS15]. charge-inverted [UT15, YJ17]. Charge-transfer [JM11, ANH+11, EAC13, YLZ+10]. charge-transport [HLWD15].

charged [BK13, KD10, MRO17, NPP13, RJS17, Tsi14]. Charges [WFZ+18, CCB15, IM17, JMLL13, LRM18, RB13a, SN15, TBSM12, VSA11, Yan14, ZBG11].


Chemical [dCDP15, Chu10]. chemical-bonding [MDTD13]. Chemically [BS10b]. Chemistry [Ano10b, Ano15-59, Cam19, HJG09, KKGW19, Spr10, ZLX+19, Ali11, BRP+12, BGR13, CBH14, CD19, DDM+15, FLM11, GHV17, HSN+18, IGK16, JBB+11, KTNN10, LBC+19, LK16a, MP19c, OZLSBH12, PNP+16, PPUBG10, RZG+13, Rez16, REL+14, TKNN10, TF15, UDK+18, VVP12, VV14, WDY13, ZVY+15, GS16, MEFM16, XFG+16].

concentration [IPAA11], concept [GRL+11, GRL+12, dSVdM+16].
conceptual [DDP+18, vS18], concerted [HL10], concurrent [HS14b].
condensation [KNE11a, XLYZ10], condensed [BGL+18, BG17, HRB+17, 
MK+19, RSLML12, VKAM12, dSdS12a, dSdS12b]. condensed-matter 
[BGL+18], condensed-phase [MKK+19], condition 
[AA18, IKN13, MTvG12, TTC+18, YAO18]. conditional [BMPML+13].
conditions [AA18, BRGN12, KB14a, MO15, MO17, NO16, SSP19a, SIE15, 
SKMS13, TCPPC14, VECT12]. CONDON 
[SvLK18, CHC+13, MCLD10, MLCD11]. conducting [SV11]. conduction 
[KJ10]. conductivity [ASL+11]. Conductor 
[KB14b, GRN19, KD18, SDF+17]. Conductor-like 
[KB14b, GRN19, KD18, SDF+17]. conductors [MRB14, NFI+16]. cone 
[BKLA13]. confidence [KSM17]. Configuration 
[KKGW19, SS13a, Cas13, CTP13, CAP17, EK17, FF11, FA18, GA14, GP11a, 
HPT17, HBL12, LCB10, MT19b, MIS+15, MCP18, ZRCC11].
configurational [RO14a, WTD+19, WDHZ13]. Confined 
[NS15, CCR18, CDB10, FTR15, Vyb15, Vyb16]. Confinement 
[CC18a, DCG18b, TM16]. Confining [WRG+17]. conformation 
[AST+16, CR19, EJ13, FBvdB18, GKJ+19, PVJ10, SEF+16].
conformation-dependent [PVJ10]. Conformational 
[CDM+15, ETLS17, KRTB10, LGL11, LTA+11, MO17, OGL10, vRWGS17, 
AD10, BLKP12, BD11, ČMD13, DPSL16, DPNM11, DSHLM18, FCD10, 
FCOGM12, GDV17, GO13, GBSE11, HTS15, HYNS19, HDL+17, HKNH18, 
HCD+10, IMK+16, ISK14, JLS18, KB10, KNE11a, KGM12, LLHM16, LC17b, 
NMF+14, Pet11, PKIC11, PLH16, PVSS2, PS14, RSL16, SBT17, SIE11, 
SEM12, SDMS13, TJB12, VZ14, YZ16, YBS19, Yon16].
conformational-space [AD10]. conformationally [AFPI13, CP15].
conformations [CC12b, DJ13, ESD18, LC16, LZZ14, NR11, OCL11, PGI19, 
PH10a, RVP+11, ZC14, DKV18]. Conformers 
[SS+18, BHF+18, DBG11, HH10, HH11, LG11, MS17, TCGNT18, VP19].
congested [MvBD18]. conjugate [MSV16]. Conjugated 
[RVB+12, BLBG+13, HDHL15a, HDHL15b, HDHL15c, JYS+12, RSSG18, 
YJN+11, JCHT18]. conjugating [JDW+19]. conjunction 
[CGA19, LBH+11, NCI13, RKG10]. connected 
[ACD+13a, ACD+13b, NR11, XTN18]. connection [Lüe14]. connections 
[CDC19]. Connectivity [ISP+10, ZYS+10]. Conquer 
[NN19, YKNN19, BRP+12, BGR13, KKN11, KFT18, NYH+17, NN18, 
NNK+16, WX12, YN15]. consensus [DMJ17, SRA17, PLV+11].
consequences [KG15], conservation [MB16], conserved [JDW+19].
Conserving [PH17], considerable [LLD17]. Consideration [Fom11], 
considerations [SBGP18]. Considering [CSEMB+16]. considers [YBS19].
Consistent 
[LOB18, MKO+13, POB13, BKŠ+11, BY11, BK17b, DK11, GBVA11, Hili13, 
HKR+14, JSXH16, KT10, KFT18, LBH+11, LCW12, ON14, OLPB19, Reiz19,
SPS$^{+12}$, SMP$^{17b}$, SCSW$^{13}$, TYN$^{15}$, VGV$^{+11}$, YN$^{15}$, ZBG$^{11}$, BLKP$^{12}$].

**consistently** [IM$^{17}$]. **consolidate** [BK$^{17c}$]. **constant**

[AB$^{16a}$, CS$^{14}$, IN$^{19}$, KSK$^{11}$, KNP$^{+12}$, KB$^{19}$, MK$^{17}$, MK$^{19}$, PLFS$^{18}$, PS$^{13}$, RAGL$^{11}$, Sak$^{18}$, STM$^{17}$, Vor$^{12}$, WOH$^{16}$, WOH$^{18}$, dACP$^{12}$].

**constant-distance** [dACP$^{12}$]. **constants** [AAMD$^{+11}$, CBH$^{14}$, CPK$^{12}$, DSD$^{+11}$, ECZWD$^{17}$, FD$^{14}$, GAI$^{13}$, GKR$^{13}$, MG$^{11}$, OZLSBH$^{12}$, Ray$^{13}$, RSG$^{14}$, RK$^{G11}$, Ru$^{i11}$, RRK$^{16}$, SSC$^{+19}$, SPHF$^{+18}$, SH$^{18a}$, SACdG$^{14}$, TTR$^{+12}$, Tsi$^{14}$, WL$^{14}$, XWW$^{+11}$, YS$^{13}$, ZZL$^{+10b}$, ZLLL$^{12}$]. **Constrained** [SLG$^{15}$, GREAI$^{11}$, GA$^{12}$, VBV$^{13b}$, WBN$^{+13}$].

**Constraint** [HNyH$^{19}$]. **constraints** [KB$^{11a}$, OPBR$^{17}$, OZ$^{S}^{+13}$]. **construct** [HH$^{10}$]. **constructed** [HDL$^{+17}$, Tsi$^{19}$, ZLY$^{+16}$].

**Constructing** [Che$^{17}$, LLH$^{+19}$, HS$^{16b}$, LG$^{11}$, SWA$^{13}$]. **Construction** [FZL$^{+19}$, AGR$^{11b}$, JCP$^{C11}$, KD$^{18}$, KSR$^{17}$, LZX$^{16}$, UIW$^{+10}$, WWD$^{14}$, YD$^{17}$]. **contact** [DB$^{K17}$, LL$^{19b}$, MK$^{13a}$]. **contact-assisted** [LL$^{19b}$].

**contacting** [Mau$^{14}$]. **contacts** [CCCLCGRO$^{14}$, Ham$^{11}$, Kri$^{10}$, PRP$^{15}$, SNDK$^{16}$]. **containing** [AKMY$^{B18}$, ACD$^{+13a}$, ACD$^{+13b}$, DT$^{19}$, DGL$^{+13}$, GP$^{12}$, GPdC$^{+16}$, HDPM$^{14}$, KLN$^{12}$, KGJ$^{Z19}$, LDZW$^{17}$, MUGNVJ$^{+18}$, VDVR$^{14}$, YHVM$^{12}$, YDX$^{16}$, ZZL$^{+12}$, ZM$^{10}$, MSCP$^{19}$]. **contaminated** [YR$^{13}$].

**content** [CGBK$^{13}$, GWPJ$^{11}$]. **Contents** [Ano$^{16-115}$, Ano$^{16-121}$, Ano$^{16-122}$, Ano$^{16-123}$, Ano$^{16-124}$, Ano$^{16-125}$, Ano$^{16-126}$, Ano$^{16-128}$, Ano$^{16-116}$, Ano$^{16-117}$, Ano$^{16-118}$, Ano$^{16-119}$, Ano$^{16-120}$]. **context** [CBG$^{16}$].

**continuation** [PJ$^{13}$]. **Continuous** [Dry$^{14}$, LPLA$^{13}$, PZBA$^{13}$, BS$^{19}$, FGM$^{11}$, LBGS$^{16}$]. **Continuum** [CCR$^{18}$, JJJ$^{16}$, ND$^{19}$, ALRM$^{18}$, Cam$^{15}$, CZY$^{11}$, GRN$^{19}$, HZSS$^{17}$, ISO$^{+13}$, LFN$^{+10}$, MCUJ$^{15}$, SK$^{12}$, SK$^{17}$, TNG$^{+10}$, WC$^{13}$, WRFH$^{10}$, XZ$^{11}$]. **Contracted** [FC$^{18}$, SM$^{18}$]. **Contraction** [Hes$^{19}$, HSN$^{14}$, STM$^{17}$].

**contractions** [KK$^{17a}$]. **Contrasting** [TS$^{15a}$]. **contribution** [Pro$^{16}$].

**Contributions** [JJH$^{+13}$, ARRC$^{15}$, BCNH$^{+11}$, CGR$^{16}$, CPN$^{+17}$, ENKK$^{+17}$, WS$^{10}$]. **control** [B$^{VY}^{+12}$, DPAB$^{16}$, He$^{l13}$, HH$^{16b}$, KFT$^{18}$, LPL$^{B16}$, SR$^{10}$, XYW$^{+14}$, ZQ$^{14}$].

**Controlled** [PGK$^{+19}$]. **Controlled-advancement** [PGK$^{+19}$]. **Controlling** [FWB$^{14}$, NPG$^{+18}$, SS$^{19}$]. **convective** [SBN$^{13a}$, SBN$^{13b}$].

**cooperative** [DBG$^{11}$, WFL$^{+19}$]. **convex** [CLFRO$^{18}$, GWW$^{19}$]. **convolution** [SZTSM$^{10}$]. **convolutional** [LHO$^{17}$].

**coordinate** [DK$^{17}$, AFSW$^{16}$, JSW$^{10}$, KPH$^{+19}$, SM$^{16a}$]. **coordinate** [AMGB$^{10}$, HSN$^{14}$, He$^{l13}$, LL$^{15}$, LL$^{13a}$, MS$^{10}$, WBN$^{+13}$]. **coordinated** [Sak$^{18}$]. **Coordinates** [AlQ$^{19}$, BK$^{15}$, LWK$^{+14}$, MK$^{19}$, NCV$^{10}$, PH$^{10a}$, Sch$^{13}$, VBV$^{13b}$, You$^{10}$, ZT$^{14}$]. **Coordination** [LBC$^{+19}$, ASMS$^{10}$, AHK$^{+19}$, CRC$^{13}$, GBPC$^{C19}$, HS$^{16b}$, HH$^{18}$, KLZ$^{+18}$, KJ$^{10}$, Mor$^{15}$, SB$^{19}$].
copolymerization [DSHLM18]. copper
[JRSHP14, KKPT11, SBC+11, SIT18, SPR+13, WC14, ASMS10, BSG+18b, CPK12, HRJ+14, HGHP14, HRJ+15, XWSW13]. coprocessors [WS13].

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[Ano16-89, Ano16-94, Ano16-95, Ano16-96, Ano16-97, Ano16-98, Ano16-99, Ano16-100, Ano16-101, Ano16-102, Ano16-90, Ano16-91, Ano16-92, Ano16-93].


Coriolis [LWD13, Wu10]. Corrected [SG13, AG12, BLBG+13, CLFRO18, CR14, GEG11, Han11, KSH13, KSS13, MMS16, Rui11, SHL+18, ST13, SPH11, SH19a, ST15, VCL18]. correcting [vS18]. Correction
[ND19, DAG19, HGHP14, NLP+16, OLPB19, RR12, SMG11, TSH+19]. corrections [JKS+16, KB10, KLN12, LCM+14, MGWR12, PTK11, RJPB12, RRK16, SJJ+15, SSA+17, TG12a, VL17a]. correctly [ASMS10]. correlate [MJLV14a]. correlated [BWKW10a, BKWK10b, EK17, GA12, HKN16, LCM+14, MGWR12, OOK11, RLD12, SJC11, WWU12, WWD14]. correlating [TZCK18, SNKS10]. Correlation
[ASL+11, CKB17, ELKE19, RLA18, SN16b, VSP19, Vyb16, CSKH15, CSHK16, ESM+12, FRSA14, Hll13, HGCCGR+16, HG10, KSH13, KN1P+12, LBH+11, LKZ18, MKGA10, NYH+17, NLL19, OAN15a, PBT+15, SH18a, SPH11, SH19a, VL17a, WFS19, ZPP+16]. correlations [AHK+19, CSKH16, Hei18, SB10, TTB+10]. corresponding [PG14, RvL11].

Corrigendum
[PDG+16, BLDK+13, BYE+16, CBP14, Gil11, LCM+14, SRR16, TF15].
cost-effective [LCM+14]. cost-efficient [CBP14]. Could
[EPH+13, EPH+15, TIA10]. Coulomb
[FED17, GC18, IO13a, JKS+16, LMR14]. Coulombic [DPAB16]. coundaric
[HHN+17]. coundaric [MS11, ZDX11]. count [KTK17]. counterintuitive
[WDS+19]. Counterpoise [SMGB11, LCM+14]. Counting [QZ10a, RNP13].
couple [IYK11, Tsi17]. Coupled [DAB16, Höf14, SZL19, VV14, ACD+13a, ACD+13b, BYE+16, CAT+13, EV18, FYZ+12, GA18, HKN18, HN1K19, HDM+15, HGCCGR+16, ILKR11, IYK11, JIL+14, KT19, Les19, MC12, PGS+15, RKDM14, SB14, SH18b, SM17, TX19, TX18, XBSS19].

Coupled-cluster [Höf14, VV14, BYE+16, HGCCGR+16, Les19, MC12, PGS+15, TX19, TX18]. coupled-cluster/Kohn [VY14].
coupled-electron [SB14]. Coupling [NNT+19, AMQ+14, BLZ+13, FD16,
32
GP11a, KSK11, KNP+ 12, KKA+ 18, Kos16, KKH18, LLB+ 12, LSH+ 11,
LWD13, MG11, MCP18, PLFS18, PS17, Rui11, RRK16, SPHF+ 18, SH18a,
SACdG14, Wu10, YB11, ZTH+ 15, ZLZ14, ZYvIZ14, GA19]. couplings
[CSEMB+ 16, LK11, LZH+ 11, YFH+ 19, ZB18, dVAG16]. covalency [HS14a].
Covalent
[WBT10, FCCP17, HAI+ 16, KAR12, MŘ17, OZS+ 13, RS13, SFA17].
CovalentDock [OZS+ 13]. covalently [CZNA11]. Cover
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**Cover**
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crown/ammonium [AvKSP16]. CrWO [WMW11]. cryo [MKM +17].

cryo-EM [MKM +17]. cryptands [EHT19]. CRYSPLOT [BPC19]. Crystal [FDCJG18, Kri10, VM11, ASL +11, BCSCJ +13, BCJC +14, Elk16, GMG +10, HB14, HJ10, MCAC +16, NHF +10, NTNY15, SPZP18b, VMV19, OPB +12, CPR18].

crystalline [BPC19, DOM +11, DCOD13, DLSD13, DB12, EP12, EFOD13, GKB +10, GS12, RB10, TNI +19a, WGN +16, WGLG +16, XP13, ZRCC11, ZSWL12].

cu-O [ZRCC11]. Cu-ZSM-5 [Mor15]. Cu2II [WGLG +16]. Cuby [Rez16].


curcumin [AMK11]. Curie [WMW11]. curing [LPMT17, PPH +14].

Current [ATM18, NS17, ABM +15, ATIP18, BL19, FNSF +11, GWT +17, HBLCCG15, PCLL11, PL18, PZM15, Vik11]. current-density [Vik11].

currents [CPN +17, RVB +12]. Curvature [LPLS16, RR12, NW17].
SFG$^{+17}$, SHL$^{+18}$, Sea10, SCW11, SDM$^{+16}$, SEF$^{+16}$, SE14, SH14, ST13, SHL$^{+13}$, SPR$^{+13}$, SZX13a, SZX13b, SMM15a, SMM15b, SMM$^{+18}$, SKTT11, SZZS16, STS15, SK11, TLDG$^{+12}$, TN10, VGV$^{+11}$. density [VAR12, VECT12, VV14, Vik11, VI17, VED10, VHS$^{+19}$, Vyb16, WKC10a, WHL$^{+10}$, WGL$^{+11}$, WCWW11, WWU12, WWCL15, WHX$^{+10}$, WL14, WTH$^{+16}$, XYW$^{+14}$, YLZ$^{+10}$, YS13, Yu12b, ZTH$^{+15}$, ZXS$^{+10}$, ZSWL12, ZKE$^{+17}$, ZDX11, ZLHH14, ZCWX18, ZGS$^{+10}$, dSD12b, dSDLBNB17, dLC17, dLvNC18a, CDM10, FAS$^{+18}$, VV19]. density-based [LZS$^{+17}$]. density-density [DSAS19, SS16a]. density-fitting [Boz18, Hil13]. Density-Functional [YKNN19, Oht16, CHG$^{+16}$, HNWF07, HNWF12, IM17, JCP14, KZZ$^{+16}$, MFR$^{+17}$, NF17, NN18, NO16, NNK$^{+16}$, Rez19, RHPWS13, SPS$^{+12}$, VED10]. density-peaks [LZS$^{+17}$]. deoxy [VM11]. deoxyribonucleoside [XVN17]. deoxyribonucleosides [RJWW12]. dependant [PNG10]. Dependence [CFM$^{+19}$, BRLS08, BRLS12, ELP19, FE14, GZZ12, KKO$^{+16}$, KGM12, Lar12, LPE$^{+10}$, LLTC12, MP17b, PZA15, PBE16, PS10, SGPJS$^{+17}$, SY16b, AD10, MGWR12]. Dependences [NNT$^{+19}$, SMM$^{+18}$]. dependency [DKT13, PHDH13]. Dependent [YKNN19, AALCM11, BS16a, CHG$^{+16}$, CP15, CKP10, DP15, EPD$^{+10}$, GTK10, HNWF07, HNWF12, HG10, HYUS11, JYS$^{+12}$, KS18, KCPMG12, LPLS16, LZ12, LZGS11, Mat10, NS10, PAK17, PPJ14, PVJ10, RHPWS13, REL17, SY16a, SFBT17, Vik11, WHL$^{+10}$, WHX$^{+10}$, YLZ$^{+10}$, ZXS$^{+10}$, ZDX11]. depending [Lin18]. depolarized [KKK$^{+19}$]. deposition [SE14]. depth [DDP$^{+18}$]. derivates [UGK18]. derivation [SCMA$^{+17}$, VVV$^{+15}$b]. derivative [MY17b, TPL$^{+10}$].

Derivatives [KTSW11, CWHH11, CZH12, CBTZ16, CROB16, GRN19, HSZ$^{+11}$, JS17a, JYS$^{+12}$, KG11, KPL15, LWGZ15, LWWG12, MFR$^{+11}$, MIS$^{+15}$, NS10, NF18, PC14, RBV$^{+12}$, RFN15, REH13, SBR13, SZX13a, SVJ15, VVJ15, VVY18, VSD10, WGL$^{+11}$, WRG$^{+17}$, WDP$^{+12}$, ZsA10, ZZ12, ZZWX11]. derive [RVP$^{+11}$]. derived [CIKT13, GMMH$^{+16}$, KSR$^{+16}$, LRVM18, LZGS11, MUGNVJ$^{+18}$, MCLD10, OSS10, PLZ17, REL17, SOYC12, SE14, TBSM12]. Deriving [CCYL11].

descent [MS16]. describe [LCK$^{+18}$, RHRC16, RS13]. described [BM12, CCB15, KDS17]. Describing [MKGA10, CGA19, DAP$^{+18}$, JCP14, JBSQG11, MY17b, VBD11].

Description [FD16, MR17, Rez19, SWW$^{+19}$, BBG$^{+18a}$, BD12, BE16, Cam15, CRZ$^{+18}$, LAM19, LZZC13, MFR$^{+11}$, PM13, PLH16, PVAM16, RVM19, SRF$^{+17}$, SSA$^{+17}$, TKNN10, WvRSM14, WL14]. descriptor [DFP$^{+15}$, MA16, PRYI$^{+17}$, TMJ15, WMW$^{+10}$, Yap11]. descriptor-based [DFP$^{+15}$]. Descriptors [ELKE19, STF$^{+19}$, CBD19, FCI$^{+10}$, FZL$^{+15}$, GJMPAM$^{+14}$, MdOdQ18, MCF$^{+18}$, MH10, NK16, PKIC11, RB13b, SIT18, TTB$^{+10}$, Wei12b, YLCX10, Yap11, YDX16, ZWX16]. Design [LI19, LLX$^{+19}$, LCM16, Spr18, SCSM19, Tak14, TZ12, VBD11, AM10, AFBR17, BAMR13, BEPM14, BPC13, CBP14, DPB$^{+12}$, DPOS16, DGL$^{+13}$,
diabetic [RGVC$^{+19}$, YFH$^{+19}$, DHOG$^{+13}$]. diabetes [PC$^{11}$]. Diagnosis [MC$^{12}$, TDK$^{+10}$]. diagonal [BMBJ$^{+11}$, KTK$^{+17}$, WZ$^{+19}$]. diagonalization [BK$^{+8}$, HKR$^{+14}$]. diagonalization-free [BK$^{+8}$, HKR$^{+14}$]. diagram [OV$^{+14}$, VED$^{+10}$, ZY$^{+14}$]. diagrammatic [WWD$^{+14}$, YD$^{+17}$]. diameter [AS$^{+15a}$, KGHK$^{+12}$]. diamond [JWO$^{+15}$, WGN$^{+16}$, WGLG$^{+16}$, ZSL$^{+11}$]. diamond-like [ZSL$^{+11}$]. dianion [DP$^{+11}$, GRD$^{+10}$, YZGS$^{+14a}$]. diarylalkyl [NS$^{+10}$]. diarylalkyl-imidazole [NS$^{+10}$]. diarylalkyl-triazole [NS$^{+10}$]. Diarylbibenzofuranone [SFA$^{+17}$]. diaryldichalcogenides [ZWGO$^{+16}$]. diastereoselectivity [AARP$^{+17}$]. Diatomic [ATM$^{+18}$, KKA$^{+18}$, LS$^{+11b}$, Tsi$^{+14}$, WDKT$^{+19}$]. diatropic [CPN$^{+17}$.] dicarbide [Kop$^{+16}$, Kop$^{+18}$]. dicationic [GC$^{+18}$]. dichalcogenides [FZL$^{+19}$]. dichloropentacene [ZYG$^{+15}$]. dichroism [HNHR$^{+13}$, SEJ$^{+18}$, ˇSB$^{+13}$, ˇSB$^{+15}$]. Dickerson [IPAA$^{+11}$]. dicopper [RHPWS$^{+13}$]. dielectric [DOM$^{+11}$, DSF$^{+17}$, JLCA$^{+17}$, KCPMG$^{+12}$, PS$^{+13}$, WXL$^{+17}$, YHW$^{+17}$]. Diels [BJSI$^{+12}$, CC$^{+18a}$, FB$^{+14a}$, GND$^{+12}$, LZH$^{+16}$, ORZ$^{+11}$, ST$^{+13}$, dSV$^{+16}$]. difference [LLH$^{+17}$, WL$^{+10}$, Yon$^{+16}$, ZRCC$^{+11}$]. difference-dedicated [ZRCC$^{+11}$]. differences [BVC$^{+13}$, GO$^{+13}$, HDL$^{+17}$, KHWB$^{+17}$, LGL$^{+11}$, PM$^{+18a}$]. Different [PH$^{+15}$, BRGN$^{+12}$, Dil$^{+15}$, DLC$^{+18b}$, FZL$^{+15}$, GO$^{+13}$, GR$^{+11}$, GFPSD$^{+17}$, GMPB$^{+12}$, Kar$^{+17}$, KB$^{+19}$, MCS$^{+11}$, MC$^{+12}$, MPA$^{+12}$, NMLD$^{+13}$, NOKJ$^{+16}$, RHNN$^{+10}$, Rao$^{+11}$, SLP$^{+12}$, SIG$^{+15}$, TTC$^{+18}$, TSNC$^{+17}$, UT$^{+15}$, VVY$^{+18}$, ZR$^{+10}$]. Differential [HHT$^{+13a}$, HHT$^{+13b}$, CJL$^{+13}$, MY$^{+17a}$, MY$^{+17b}$, WDKT$^{+19}$]. Difficult [RJS$^{+15}$, VDVR$^{+14}$]. Diffusion [NQB$^{+19}$, CPZ$^{+19}$, CPV$^{+12}$, CC$^{+12a}$, GC$^{+11}$, KB$^{+19}$, RSLS$^{+13}$, ZW$^{+17}$, WH$^{+11}$]. diffusional [BPLL$^{+12}$, FBvdB$^{+18}$, FZL$^{+19}$, KTY$^{+17}$, KRSC$^{+12}$, KTO$^{+13}$, MB$^{+16}$, PJ$^{+13}$, SG$^{+10a}$, SHL$^{+19}$, TYN$^{+15}$, TCX$^{+13}$, TKC$^{+11}$, XCLZ$^{+19}$, YZLZ$^{+19}$, ZWX$^{+16}$]. different [LLH$^{+17}$, WL$^{+10}$, Yon$^{+16}$, ZRCC$^{+11}$]. differences [BVC$^{+13}$, GO$^{+13}$, HDL$^{+17}$, KHWB$^{+17}$, LGL$^{+11}$, PM$^{+18a}$]. Dimer [BPPS$^{+19}$, LWL$^{+16}$, ZQH$^{+19}$, ARRC$^{+15}$, ANH$^{+11}$, BPPS$^{+17}$, CBTZ$^{+16}$, FCL$^{+10}$, FMNC$^{+11}$, JT$^{+18}$, KCB$^{+12}$, LC$^{+10}$, Nav$^{+18}$, PD$^{+11}$, SKY$^{+11}$, Tac$^{+17}$, WWKS$^{+16}$, YCGA$^{+10}$]. Dimeric [VL$^{+19}$, PS$^{+14}$]. dimerization [DS$^{+11}$, Kar$^{+12}$, TNI$^{+19a}$, TLA$^{+10}$, WJX$^{+10}$]. dimerization/oligomerization [KAR$^{+12}$]. dimers [AM$^{+19a}$, BCNH$^{+11}$, BWKW$^{+10a}$, BWKW$^{+10b}$, CLFRO$^{+18}$, CK$^{+10}$, DT$^{+19}$, JKS$^{+16}$, LJW$^{+11a}$,
Dimetallic [ZYG+14], dimethyl [GC11, KPH+19, WLC12, ZSWL12], dimethylacridine [FWS+18], dimethylaminoazobenzene [KP10], dimethylaminophenyl [YLZ+10], dimethylnitrosamine [FFA14], dinitrophenol [MIS+15], Dinuclear [SCSM19, ITY+19, OSS10, QLYL10], diodes [FWS+18, ZGZ19], diorganotin [CBDS19], dioxane [GM17], dioxetanone [RSLML12, dSdS12a, dSdS12b], Dioxide [SC17, KPH+19, Kop17b, QZ10b], dioxygen [DSM+11], dioxygenase [DGH+11], diphenyl [GKR13, Ray13, RKG11], diphenylamino [FWS+18], diplatinum [KT12], Dipoles [Ali18, Cam19, GH16b, LIRL+16, ZBG11, AS15b, B LBG+13, DHOG13, GH16a, HBKL10, IY18, KCB+12, LHHW14, MNNK10a, MNNK10b, PC14, Yan11, dSH19], dippened [IN13], Dirac [JKS+16], diradical [HWB19, VSH19, YSSB12, ZB18], dipeptides [KH16, LIRL+16, RSL16], diphenylalanine [KLN16], diphenylamino [FWS+18], diphenylalkane [KLN16], diphenylamine [KP10], diphosphonlitrosamine [FFA14], dinitrophenol [MIS+15],...
[CSXZ17, SZX13a, SZX13b, ZWLX11, ZWX19]. **Douglas** [YS13]. **DOX** [RCR+16]. **DPO** [WGL+11]. **DPPC** [LBDP12, vRWGS17]. **DPT** [BH13, BZH14]. **Dramatic** [MLY+13]. **dramatically** [CSC+18]. **Draw** [LBB+15]. **drawback** [BRGN12]. **Driven** [IPAA11].

[BSL11, BG17, DMS+11, GA19, HXM+16, KC13b, LZL+13, LLL+12, REL17].

**Driving** [YZLZ18, RN17, YZ17]. **Droplet** [SJSS19]. **Drude** [ALRM18, LRvdSM15, LM18a, Ric16, SM14b, ZM10, HLEM18]. **Drug** [GSHM10, MBA14, AJA+19, FLM11, GMASBF16, HSW+19, Ibr11, ISP+10, PC11, PVJ10, VHA+10, Won18]. **drug-like** [VHA+10].

**DSiCl** [LX11].

**DSPMP** [FZL+15].

**DsRed.M1** [SGDT10].

**DSS** [GZM11].

**DSSCs** [ZSTRS+18].

**DTTO** [MCAG+16].

**dual** [JCG+10, MA16, TMJ15].

**Duncanson** [Bac12].

**Durandal** [BSZ+12]. **during** [GBPCC19, GNDA+12, LBC+12, MJLV14a, MJLV14b, OSA19, PNG10, RSKG14, dCDP15].

**dyad** [KP10].

**dyads** [KCK+15].

**Dye** [MP19a, ACS12, JYS+12, SLP+12].

**dye-aggregates** [ACS12, JYS+12, LLL+15a, SLP+12, YJN+11].

**dye-sensitizer** [YJN+11].

**Dyes** [FAS+18, DBM+17, NPG+18, VAA14, WJG+13, YJN+11, ZSTRS+18].

**dyes*** [FA18]. **Dynamic** [LKL10, SFA17, SBZ19, VP19, TNYN16, AKK+16, BS10a, BMB13, CVT+11, ESM+12, GBL+11, Hel13, MR14, NYN17, OPR16, VOR12, WSFS19, PBDW11].

**dynamical** [ALH+10, EFOD13, Ham11, VVMY18, VPR10].

**dynamically** [HS17a]. **Dynamics** [AIM+18, BHF+18, BHB19, CPV+12, JK13, MFEM16, NNT+19, NN19, AASP18, AJA+19, AALCM11, AG11, AS15a, Aki16, ASL+11, ABD11, APK14, AB16a, ALH+10, BHBI2, BSL11, BDTP11, BJSI12, BW15, BF17, BMBJ11, Bow16, BEL+11, CTR13, CS14, CH16, CCOH14, CCW+10, CHKR10, DASA15, DGH+11, DMN15, DSD+11, DZT11, DJS+18, DLZ15, DDM+15, DL19, EP10, EK15, EPH+13, ETLS17, EFOD13, EvRC+18, Fon13, FBEM11, FPH+19, GBL+11, GDV17, GR11, GKB+19, GWZ15, GWC14, GGM+12, GPdC+16, GP11b, GC11, HZ11, HS17b, HKNH18, HHHK19, HHC+10, HP10b, HPT17, HPDK12, HJ10, HHWL17, HLEM18, HRID16, HC14, IUK+11, ISK14, IN19, IM17, III10, IPAA11, JIS13, JA10, JBSQG11, JCG+10, JAH+17, JLS18, JWST10, JMS14, JS17b, JND+19, KT19, K17, KCH+15, KVQ+10, KUDG12, KSN19].

**dynamics** [KGHC15, KCC+18, KDB13, KB14a, KNE11a, KERY+16, KLOS10, KJM+17, Kop19b, KSR+16, KG13, KZP+18a, KN18, KV15a, KVR10, LL15, Lar12, LWK+14, LH11, LJR+12, LLI13a, LRvdSM15, LCH10, LQC+13, LMI+14, LPE+10, LLTC12, LZS+17, LPLB16, LLL12, LDPD12, MBT14, MMH19, MSY19, Man19b, MKS+12, MSC+10, MJ14, MN15, MCRL17, MLN+18, MFEM15, MADWB11, MKM+17, MB16, MHR11, MO17, MO13, NPTS16, NST14, NFPD13, NFG+13, NNK+16, NHK+13, NNY15, Oht16, ON14, OGL10, OCL11, OLY17, OT12, OCW+15, PMC+17, PSS14, PAK15, PH17, PP19, PL14, PM13, PD12, PHT17, PVZ13, PS10,
PVAM16, RD18, RS12, Ras17, RO14a, RO14b, RFN15, RR14, RdA12, RVdMB16, RC18, RLG14, REL+14, RSR15, RSB+13, SHMO11, SF18, SLT+15, SKA19, SWM10, SSWX14, SS19, SSNT19, SOM+13, SCK18].

**dynamics**

[SJ17, SR18, SYN+12, SM16b, SK13, SKMS13, SFLG+17, SLLL13, SJ16, SZZ+18, SV11, SPZP19, SBrG14, SAvG15, Tac19, Tac17, TNY16, TFYO19, TJR19, TTC+18, US11, UGK18, Vor10, VM11, WKLC12, WBN+13, WAM17, WC11, WHL+10, WH11, WWKS11, WLC12, WLF19, WES13, WG14, Won18, Wu10, WBVE16, XCLZ19, YPvD13, YO19, YHX19, YJXZ13, Yon16, Yu12a, YFH+19, ZY+16, ZX11, ZDKM12, ZBP11, ZP13, dCLFGL13, dSVdM16].

**Dynamics-Based** [AIM+18, Vor10]. **DynamO** [BSL11].

**dysprosium** [BP18].

**E-field** [XMA+19]. **E-I** [GM17]. **EA** [MLCD11]. **EADock** [GZM11].

**EADock** [GZM11].

**E-coupling** [dVAG16]. **Early** [Tsi18, CBP+15]. **Eart** [Ano11, JHMB+09, JHMB+11, WD10]. **Easy** [SJL18, QS19, TKT11, VVV+15b, Yes12]. **Easy-to-use** [QS19]. **Ebola** [OLY17]. **Echo** [OC19]. **Economic** [PN13]. **Ecoupling** [dVAG16].

**E-coupling** [dVAG16]. **Edge** [DWZ+17, DJX+11b, KHE+19, PDG+16]. **edge-modified** [DJX+11b].

**E-diff** [DWZ+17, DJX+11b, KHE+19, PDG+16].

**E-diff** [DWZ+17, DJX+11b, KHE+19, PDG+16].

**E-diff** [DWZ+17, DJX+11b, KHE+19, PDG+16].

**E-diff** [DWZ+17, DJX+11b, KHE+19, PDG+16].

**Editor** [GKR13, GPGSM12, JW12, dSdS12b, vLBBR12, Ihl12, BCJC+14, Cor17, KR14, Man13, SFLG+17, VVB13].

**Editor** [GKR13, GPGSM12, JW12, dSdS12b, vLBBR12, Ihl12, BCJC+14, Cor17, KR14, Man13, SFLG+17, VVB13].


**Editorials** [BEFS13].

**Effect** [ABD11, CIG17, CS17, DSHLM18, GEG11, HYL+11, JZ12, KMT+19, OBW12, RRF11, SJSS19, TJR19, VS14, WZ19, dALdS+15, AB10, CSKH16, CR19, CD11, CXS10, DKT13, DJX+11b, DLW12, FCOGM12, FHK+12, GFS18, GA19, HLBlcG15, JWO15, JYS+12, KTT16, KCL+14, KLN16, LVdG10, MTvG12, ONTL16, RWR+13, SLT14, SBC+11, SY16a, Tsi19, UT15, VLGK+17, WDLG12, ZZZM13, ZLL+10, BLG10, CC11, IYK11].

**Effective** [GKV+13, IM17, YZ16, AASP18, CVG14, DR11, DMN14, DMN15, GA12, HKNH18, KS13a, KS15, LCM+14, PHC13, PRY1+17, PS13, RLD12, SSB+16, UCFR16, WXS+12, YZZ16, YZ15b, ZKH+10]. **Effects** [CS14, GBG+19, HTY19, JAH+17, JLLW19, LGOM+15, LCH+15, Mor15, NNT+19, SEM12, Tac17, WWTL19, YCK16, dCRN18, AS15a, ATIP18, AS18, AK10, ASK18, BBI+11, DMD+18, EPH+13, FAA15, FD16, GNC+18, GMG+10, HS16b, HDM+19, HLBlcG15, INT18, IN19, JMX+16, KIOY19, KG11, KYCL11, KHE+19, KKA+18, LGVA14, LHT15, LWD13, LKZM18, MUN+19, MKGA10, MBC11, MRK11, MLX+13, MCUJ15, MSG+16, MKK+19, NASH15, ORZ11, OSHG17, OCW+15, PLFS18, PDMT10, PP19, PC14, RMGB11, RRK16, SSWX14, SMP17a, SFLG+17, TM16, TNY15, TY10, UT14, VP19, VKAM12, WXY14, YNH+17, YJ11, ZPP+16, Zha11, ALW+10, THP+15]. **Efficacy** [LC17a]. **efficiencies** [RO14a]. **Efficiency** [AC11b, BB11b, BB11c, FE14, GBSE11, XFG+16, AC12, FSSW19, GSHM10,
LY10, LWL$^+$11, LZL$^+$15a, MKGA10, RO14a, XFG$^+$15, vLBBR12]. **Efficient** [AB16a, BC13, BAS14, Cas13, DSV$^+$19, DSHA15, DSAS19, DBF14, EP10, GCWS15, GRN19, GWW19, GPK12, Han11, HNS16, Het19, HHL$^+$14, HHWL17, JMS13, KNH$^+$18, LZ11, Les19, LGKS17, MKS$^+$12, NYN17, PSS14, RAN12, RJS17, SS16b, SS19a, TJB12, UCRL18, WHAS$^+$16, WM12, ZL14, ZKE$^+$17, AM10, BW11a, Boz18, CBP14, CHG$^+$16, CY$^+$10, CY13, CZZL19, CMS13, DS15, DGL$^+$13, GREA11, GWWX12, HHL$^+$17, ISK14, JZ17, Kid19, KB11a, KKH18, KV15b, LFB14, LPK16, LLZA12, LZL$^+$15a, LSW$^+$17, LAS$^+$14, MP19a, NTPT2416, NF18, OK16, PW12, PBE17, Ran13, RR14, Rod13, RSL16, SOJ13, SA13, SSMW09, SCW13, SWB$^+$12, Sun15, TO10, WJG$^+$13, WLQ19, ZWP11, Zha12a, vLBBR12, WHAS$^+$10].

**Efficiently** [WES13, ASMS10, DDK14].

EFP [CBG17].

egg [Pla11, ZP13].

egg-box [Pla11].

EGRAD [vW11].

Ehrenfest [Dil15, FED17].

eigensolver [KZZ$^+$16, KCC$^+$18].

eigensolvers [ZVY$^+$15].

eigenvalue [Coh18, HLXH17, HLXH18].

eight [HDK$^+$12].
either [TCP14].
electric [ECZWD17, LBTV11, QB10, QB11, SH11a, XTY$^+$14].

Ekectric [GH16b, LL13b, BLFZ13, BLBG$^+$13, BS10a, CXS10, GH16a, KMT$^+$19, KZK$^+$12, MRB14, PdSC18, SH15, SLX$^+$15, YN11, YJ11, YCK16, ZSL17, ZIX19].

electrical [LLL11].

electro [TMJ15].
electro/nucleophilicity [TMJ15].
electrochemical [SKGP19, SIG$^+$11, SGH$^+$16, YJ11].
electrochemistry [DSK17].

Electrode [IN19, MKO$^+$13].
electrodynamics [TAC19].
electrolyte [KS18].
electrolytes [HAL14].
electrolytic [SV11].
electromagnetic [SEM12].

Electron [BK11, Bar14, BLG11, BWKW10a, BWKW10b, CEBO15, HS16a, HRML$^+$13, HGCCGR$^+$16, KGR$^+$16, KKGW19, LLX$^+$19, PI17, VSP19, VV19, WWU12, ACD$^+$13a, ACD$^+$13b, ABGD12, BH12, BT18, CDB10, CA10, CWHH11, CC18c, CJPTC18, CTP13, CXD$^+$19, DAAGR15, ED15, EP12, ESM$^+$12, EP15, FRS14, FWS$^+$18, FED17, FCY15, GND$^+$12, HSH15, HPT17, HEMCZE$^+$14, HAP$^+$12, HBL12, IYK11, Jan16, JSQB11, JCF19, KPL13, KTK17, KKA$^+$18, KYG$^+$15, LW16, uLhY11, LRV18, LHO17, LYL16, LLJ12, LP11c, MRC$^+$18, MKGA10, MRB14, MT19b, Mat14, MBFP15, MKH$^+$13, MCK17a, NYH$^+$17, NLL19, NS17, PAK17, PGDO16, PSC11, PI17, PN13, PTB$^+$15, PHT17, PC16, Ras17, Rod13, REL17, RSK14, SFM$^+$18, SZ19, SB14, SHB17, SGLH13, SK11, SSA$^+$17, UCRL18, VGG$^+$11, VEET12, VL17a, VCL18].

electron [VI17, VYb16, WLW$^+$10, WMM11, XBS19, YKH$^+$10, YLL11, ZPP$^+$16, ZCWX18, ZGS$^+$10, dLC18a, dLvNC18a, GMBM18, SDP18].
electron-correlation [NYH$^+$17].
electron-deficient [YLL11].
electron-hole [PTB$^+$15].
electron-pair [WWU12].
electron-sharing [JSF19].
electron-vibrational [CJPTC18].
electron-withdrawing [CWHH11].

Electronegativity [FCY15, vS18].

Electronic [AMQ$^+$14, AM19a, AM19b, ASS10, BAD$^+$19, DSB$^+$19, DADGR15, DGSVVM19, GND$^+$12, GNI18, HLWD15, Ibr17, JLL19, KYCL11, KKL$^+$13, KKGW19, LLBO12, LS11b, LKZM18, MT19b, MP19b, MAP10,
NSN19, ND19, NIIT15, PMC+17, RLA+11, SZL19, TN12, TNI+19a, TN10, TFQ+10, TS15b, VI17, WRM+12, YW12, ZRCC11, ZLX+19, AR15, AK10, AC12, BLZ+13, CPRS18, DKE+17, DHOG13, DMD+18, EVR18, EH13, EWK+13, EBPK17b, FB10, GTT10, GRARO+14, GWX+12, GZZ12, HASR+12, HS14a, HSB+11, Hu16a, IIF+10, KKH19, KKPT11, KSM17, KG11, KKA+18, Kop15b, Kos16, KP10, LGOM+15, LX11, LBTV11, LBTV12, LZX+10, LSH+11, LLSW14, MC10, MA16, MCF10, MCF+18, Mat10, NC14, NCT18, NF1+16, OLA15, PiSc18, PHK14, PTB+15, PY1M16, PyY13, RCM+13a, RML+15, RR12, RR11, SFA17, SLP+12].

Electronically [SIT18, SB19, SRS14, SB15, SKGB13, Tac19, TFQ+11, TD10, TS15a, TNG+10, TS11, TG12a, Tu19, TEDT18, VVP12, VHR16, VAR12, VBM13, VLK+17, VGTL16, WHL+10, WGL12, WJC+13, WO15, WSGN11, WZK+13, YK13, YFH+19, ZJM13, wZbZ11, ZBB16, ZZZ+19, dCDP15, dVAG16, vSGP10].

Electrons [Sah18, EKH14, FHZA+18, WCY+11, WRG+17, XhD15, YAO13, YMP14, YZL+15, ZBB16, ZDZM13, ZBP11, KGM12].

Electrostatics [BSG18a, CZY11, FGM11, FP17a, KFY+13, LPLA13, MBA11, MBC13, NL+11, SDZ17, SWPR11, UHH+11, XYY17, YMP14].

Element [BCCO10, GPK+16, RMGB11, TG12b, TCX+13, XYX17].

Elementary [LPLB16, ZIM13]. Elements [TKN13, BV14, CWZB10, Hl13, JJJ16, LFB14, SK15a, KTN10, KYG+15, Lar11, LCA17, LCM16, Mat14, NF18, OHR18, PV10, RB13a, Ty10, VMR17, VV18, YKF+11, YWJ+16, YAO18, YMP14, YZL+15, ZDZM13, ZBP11, KGM12].

Elongation [OLA15, MKGA10, MKGA10]. Elongation-MP2 [MKGA10].

Elucidating [HNHR13, TDP+12]. Elucidation [CPLL11, TNY16].

Embedded [DSF17, GMS+10, HS15, KMT+19, ZFS18]. Embedding [CCB15, ESD18, ESM+12, HH16a, HH17, Hf14, KOK17, KSR17, NF18, NOK16, RR12, SDF+17, SS16b]. Embelin [CPR18]. emerges [MNNK10a].

Emission [CSC+18, LXF11, MCLD10, PLP+16, SGWA17, WDP+12, ZLL+10]. emitted [P111]. emitters [FWS+18, ZG19]. emitting [FWS+18, ZG19].

Emphasis [RCM+13b, PD11]. Empirical

Enantioselective [ORZ11]. enantioselectivity [OAN15b]. encapsulated [EOO+16, STS15]. encapsulating [WZH+18]. encapsulation [YDGZ15]. encoded [RSL16]. encoder [LDH+14]. end [HDL+17, SL10]. ended [RJR14, Zin15]. endo [FB14a]. Endohedral [NKD18, FL15, MCK17a, MCK17b, ZSL+11, ZYG+14]. endohedrally [NKD18, FL15, GLF16, MCK17a, MCK17b, ZSL+11, ZYG+14]. endothelial [JK14a]. Enediyne [DCHL12]. Energy [DK11, ELKE19, Jia19, Kop19a, LFN+10, LPLB16, MYKO18, NK19, OSI+19, PK19, SN16b, SSGS15, Spr18, SKGB13, VL19, VSP19, WM12, ZQH19, AMGB10, AAB+19, AC11a, Anol10a, AK10, AK16, BCSCJ+13, BPM15, BRL16, BH15, BS16a, BRLS08, BRLS12, BACSCJ+10, BG17, Bon14, Boz18, BD11, BWMSM10, BB11b, BB11c, BG12, CM13a, CK10, CDM+15, CLA16, CY09, CXY10, CZ13, CH16, CSXZ17, Che17, CF18, CS17, CHR+12b, CHR+12a, COH19, CKP10, CM+10, CP12, CWZB10, DGG+11, DWR17, DBG11, DS12b, DH14, DWC17, EV14, FMNC11, Fer17, FED17, FC0G14, FSSW17, FCCP17, FLM11, GS14, IS15, GH12, GO13, dCGCRN19, GMO16, HNYH19, HDL+17, HHNK19, He13, HDM+15, HH15, HG13, HYMZ16, HYUS11, HJK13j, HGW18, HYD10, HDH15a, HDH15b]. Energy [HDHL15c, IMK+16, IS13, IT19, JCPC11, JL13, JZ12, JZZM14, JCX10, KCB+12, KTT16, KB10, KIOY19, KNH16, KN17, KHWB17, KDR+18, Kid9, KB11a, Kop15a, Kop16, Kop17a, Kop18, KLS10, KMLS10, KC1+14, LRVM18, LMZ11a, LZ12, LYO13, LZZ14, LGL11, LP11b, LX11, LH11, LSH+11, LZY12b, LLSW14, LAW+16, MCvD13, MCC11, MK13b, MPA10, MPA12, MSC+10, MJL14a, MSBF16, MHO18, MK19, MUGNVJ+18, MLN+18, MSÅ12, MAP18, MB14, MB16, MLCD11, MIOM13, NZM18, NCT18, NFT+16, OKS17, ORS16, OK16, OOT15, OZS+13, PBLdS12, PG18, PBL19, PZCL16, PBB11, PM18b, PBE16, PJ13, RS17a, RLD17, RAR+11, RDT14, RS13, RCM+13a, RML+15, RF15, RVVK13, RLA18,
HNWF12, HH17, HZSS17, HDHL15a, HDHL15b, HDHL15c, JCGVPHT17, KT19, KPG18, KB14b, LLBO12, LLW12, LWGZ15, LGC19, LX11, LSH+11, LYSS11, MPSG11, MGCC19, MEH18, NYN17, PH10b, RRCH16, RR14, SFCCK+14, SFCCK+15, SRF+17, SZZS16, TSN17, WHL+10, WHX+10, YD17, YHX19, YLZ+10, YB11, YYT12, LZL+10, PGW+17].

**Excited-State**

[FHG+19, YKNN19, SGWA17, FD14, GA18, HH17, HZSS17, KT19, LWGZ15, MPSG11, NYN17, PH10b, WHL+10, WHX+10, YD17, YHT12, LZZ+10].

**excited-states** [LLBO12].

**exciton** [HRH+17, LSH+11, SEJ+18, WZ19, ZLL+19].

**exciton-phonon** [WZ19].

**EXcitonic** [JCGM18, NNT+19, LCK+18, ZMMM12].

**excluded** [LWZ+17, Yan14].

**exclusive** [dLC18a].

**Exhaustive** [DKV18].

**exhibited** [RWR+13].

**Existence** [BMB13, WD10, NKD18].

**existing** [KT18].

**Exothermic** [LWL+16].

**expand** [BK17c, Car14].

**expanded** [MLQ+12, TSNC+17, YSSB12].

**Expanding** [GMZ12, UCRL18].

**Expansions** [LZG+11].

**Expected** [Clo15, AF14].

**Expedited** [DJD12].

**expensive** [LDZW17].

**experiment** [GNC+18, JAH+17, SA+10].

**Experimental** [CAM19, MRC+18, NHF+10, AvKSP16, BRG12, DCOD13, EOO+16, GPIC+16, HJ13, KP10, POG10a, SB10, SGS+16, SKMS13, VZ14, CI+10].

**experiments** [CBP14, HCB11].

**explained** [FL15].

**Explicit** [WG14, BEM14, CCOH14, CBG16, EK15, ENK+17, GLB16, HDL+17, KJDB12, LH11, RD12, SYH12, SKMS13, ZHL+12].

**Explicitly** [yOT+16, SM17].

**Exploiting** [HB14, BYE+16].

**Exploration** [FHG+19, OSI+19, ZGS+10, BGL+18, CF18, IWW12, LAW+16, NJR18, OKS17, OKY18, RDR16, Sti15, SSP+19b].

**explore** [JCPC11, SE+10, MCC12].

**explorer** [SYN+12].

**Exploring** [BHB12, BPPS17, BPPS19, BC10, DSHL18, ELKE19, FD19, MTM14, PJJ13, TS17, VHS+19, ZTR+18, ZT14, dSDLB17, RDR16, NOK16].

**explosion** [GC18].

**explosive** [YP+10].

**Exponential** [BBO16, BB11b].

**expressions** [Gav12].

**extended** [GWZX12, IN19, KUDG12, LRvdSM15, SSWX14, TSN17, YB16, Pon11].

**Extending** [LMZ11a, Man13, TTh+19, VBV13a, VVB13, PPH+12].

**extensible** [GCW14, JYC+16, LAS+14].

**Extension** [AIQ19, HSN14, PFVL14, SDZ17, VVW+18, YHVM12, Cam15, LL11, RLLHL12, Ras17].

**extensions** [NYH+17].

**Extensive** [JW12, SLHW09, YB11, CF14, KM13].

**Extent** [OSA19, GFGS18].

**exterior** [HL19].

**exterior/interior** [HL19].

**external** [GKSS14, KMT+19, PdSC18, SEM12, XTN18, XMA+19, ZSL17, ZX19].

**extra** [PFAS+19].

**extract** [MDTD16].

**extracted** [HN15].

**Extracting** [WSW19].

**Extraction** [CVG14, UVsvdWK19, VVG13].

**extrapolation** [CC11, LC+13, OAN15a, SRR16].

**Extreme** [HRHI17, Cam15, DS12a, JBSQ11, CCR18].

**eXtreme-Pressure** [CCR18].
Extremely [ZM11].

F [ATP18, CXW14, CXS10, GPK+F, GTK10, HBL12, LZJ+F, Li14a, Li14b, MP19b, PMG+F, Rab12, STM+F, TFQ+F, TFQ+F, TCPPC14, WLY+F, WCY+F, YS13, ZYL12, ZLL12, BWKW10b, CCM15, Cht10, DKE+F, II10, JLLW19, KIOY19, LZL+F, MLGB16, MSPC19, SMiN+F, SYH12, TCPPC14, Yu12a, ZWY+F]

F-ATP [SYH12]. F12 [BBG+F]

Kid19, KLJ\textsuperscript{+17}, KSK11, KT10, KFT18, KGJZ19, KMLS10, KVR10, Lar11, LvDH13, LC17b, LM18a, LPS\textsuperscript{+13}, LPE\textsuperscript{+10}, LN15, LLvG10, LvG13c, LL13b, LDG\textsuperscript{+15}, LCL\textsuperscript{+18}, MRO17, MBC11, MSS\textsuperscript{+13}, MTvG12, MBE16, MLC13, MHRR11, MP17b, NB19, NTNY15, ON14, PHC13, PLZ17, PdSc18, PG15, PZCL16, PLH16, PVM10, PS10, PNG10, Rod13, SH15, ST11, SM14b, SK17, SS19, SzBM13, Sie15, SGY\textsuperscript{+18}, SS13c, SCSW13, SM15]. field [SYZ\textsuperscript{+17}, SBvG14, Tak14, TYN15, VV\textsuperscript{+18}, VHA\textsuperscript{+10}, VPR10, Vik11, VVLG17, WXL17, WS19, WTH\textsuperscript{+16}, WC14, WZK\textsuperscript{+13}, WDHZ13, XP13, XVA\textsuperscript{+16}, XMA\textsuperscript{+19}, Yan11, YWZ14, YJXZ13, YJ11, YN15, YCK16, YHYM12, ZSL17, ZL11, ZSYH12, ZX19, ZDKM12, ZP13, ZM10, ZCGM11]. field-based [HKR12]. field-dependant [PNG10]. field-dependent [DP15].

Fields [Coo19, AS15b, BHI19, BVY\textsuperscript{+12}, BAS14, CCLP12, CPN\textsuperscript{+17}, GCWS15, GMMH\textsuperscript{+16}, HDPM14, HJ10, JYC\textsuperscript{+16}, KT18, KWL\textsuperscript{+16}, LZZ\textsuperscript{+11}, LZGS11, LGL11, LTP11, LBDP12, MSK\textsuperscript{+10}, MSK\textsuperscript{+12}, MS15, ST11, SGY\textsuperscript{+18}, SEM12, TTC\textsuperscript{+18}, VV\textsuperscript{+15b}, VHA\textsuperscript{+10}, WKC\textsuperscript{+10b}, WLC12, WG12, YPKB12, ZRL\textsuperscript{+15}]. fifth [KM13, LOB18]. fifth-rung [KM13]. fifth [SY16b]. filter [MH10]. finding [Ber17, MLC13, ZQH19, GFG11, JZ17, Zim15]. fine [Hua16]. fine-structure [Hua16]. fingerprints [BHF\textsuperscript{+18}, SS13b, Yap11]. Finite [ISO\textsuperscript{+13}, ZQH19, BBG\textsuperscript{+18a}, BCCO10, BVC13, DJX\textsuperscript{+11b}, EPD\textsuperscript{+11}, Hsu14, LLH17, MLC13, MKK\textsuperscript{+19}, NPP13, SK15a, TD11, TCX\textsuperscript{+13}, WL10, XXY17]. finite-difference [LLH17, WL10]. Finite-field [ISO\textsuperscript{+13}]. finite-size [DJX\textsuperscript{+11b}, Hsu14]. Finite-Temperature [ZQH19, MKK\textsuperscript{+19}]. FIPSDock [LZL\textsuperscript{+13}]. firefly [FD14, PE11]. First [BE12, BE14, BF19a, CCJC10, DBM\textsuperscript{+15}, EB12, EBK13, EBPK17a, HFSO12, JCG\textsuperscript{+11}, LLLM11, LLB\textsuperscript{+12}, LCWW10, RRK16, THI\textsuperscript{+19}, TKN13, UGK18, YPvD13, YR13, wZbZ11, BPE16, BCCO10, BEL\textsuperscript{+11}, EMD17, EB18, GD10, GA14, Ibr17, KLZ\textsuperscript{+18}, LL10c, Lu11, MCF10, NNS15, OC19, PLZ17, RZG\textsuperscript{+13}, SBGP18, SFA17, SK12, TKC\textsuperscript{+11}, T211, WXS\textsuperscript{+12}, WYL\textsuperscript{+15}, WD10, WZK\textsuperscript{+13}, YHCS11, Zha12b, Zha12a, ZWMW10, Z12, vADC\textsuperscript{+14}, HYL\textsuperscript{+11}, NG10, SPZP18a].

First- [TKN13]. first-order [BCCO10, SK12]. First-principle [CCJC10, DBM\textsuperscript{+15}, LLB\textsuperscript{+12}]. First-Principles [HFSO12, BE12, BE14, EB12, EBK13, EBPK17a, JCG\textsuperscript{+11}, LLLM11, wZbZ11, BPE16, EMD17, EB18, GD10, KLZ\textsuperscript{+18}, PLZ17, RZG\textsuperscript{+13}, WYL\textsuperscript{+15}, WD10, ZWMW10, Z12, vADC\textsuperscript{+14}, HYL\textsuperscript{+11}, SPZP18a]. First-to-Third-Row [BF19a]. Fission [NNT\textsuperscript{+19}]. fit [BHNS14, BCG10, GDV17, KGM12, WKC\textsuperscript{+10b}]. fitted [KGJZ19]. Fitting [SN16b, BS19, Boz18, DGPM14, FN12, Gra15, Hili3, LBGS16, MKH\textsuperscript{+13}, MKM\textsuperscript{+17}, SY11, VYM15, WOH16, WOH18, ZDZM13]. five [HCD\textsuperscript{+10}, KJDB12]. five-membered [HCD\textsuperscript{+10}]. fix [WCW15]. Fixed [Jia19, AS15b, FSD\textsuperscript{+18}]. Fixed-charge [Jia19]. flake [Lin18]. flakes [SDF12]. flanks [RSG18]. flash [AGM\textsuperscript{+13}]. Flavins [Ale19]. flavonoids [PC11, ZDW18]. flavor [PFAS\textsuperscript{+19}]. Fleksy [WdVN12]. Flexibility [OXBW16, BCG10, FTW12, FMG12, GTZ\textsuperscript{+18}, KL14, LZ11, NPG17].
Flexible [GLB16, MKM+17, NG10, SC17, WdVN12, AFPI13, CPZ19, CZNA11, DVVP14, FRLN10, GBW+14, HDM+15, JC16, LS11a, LHS12, MLN+18, PL14, PS13, PJ13, RHJ11].


HLS12, HH10, HH11, HDK+12, HLW+17, HDL+17, HHNK19, HDM+15, HG13, HYUS11, HKR+14, HGW18, HHWL17, IMK+16, JMLL13, JCX10, KHWB17, Kid19, KB11a, KB11b, KBY13, LRV18, LMZ11a, LGL11, LP11b, LAW+16, MSC+10, MS13, MHO18, Mau14, MLN+18, MS˚AK12, MAP18, MBE16, MIO13, NZM18, OSR16, OK16, PGCT+12, PLBoS12, PBBP11, PPJ14, RLDJ17, RDDS10, RAR+11, RO14b, RZ16, RR14, RR19.


Frenkel [SEJ+18]. Frenkel-exciton [SEJ+18]. Frequencies [DT19, LBH+11, LLH17, SST+18, TKN19, WX12]. frequency [BMPML+13, CK10, KKA+18, LCW12, LS11b, yOTn16]. frequency-independent [yOTn16]. FRET [RO14a]. Friedel [CYY+17]. Frontier [GMBM18, Kop15a, LL13a, LHG11, LCB10, LIRL+16, LL19b, MLG18, MB16, yOTn16, ON14, Pll17, PRYI+17, RGZ+13, RvL11, SS16a, SFG+17, SK18, TCB16, TO10, UM13, UCFR16, WO15, WDHZ13, YVEI+17, ZLT13, ZCWX18, vSGP10]. function-based [WDHZ13]. function-guided [YVEI+17]. Functional [BBH19, CKH19, FAS+18, FPV13, LLX+19, MP19b, NN19, YKN19, AMK11, ALK+15, Ali18, ASW19, Ano15-59, AG12, ASS10, BY11, BLBLG+13, BS19, BK17b, BZB+13, BG13, CHG+16, CRZ+18, CR14, CWWH11, CSKH15, CSKH16, CKH17, CSXZ17, CC11, CNK97, CPL111, CB11d, DAP+18, FD16, GAI14, GHL17, GZL+12, GNCGA10, GSS13, GEG11, GAJ+17, GWJP11, Han11, HDP+17, HNF07, HNF12, HPT17, HG10, HZSS17, IN18, IKN13, IM17, JCP14, JHL+14, JW16, JYS+12, KD10, KKPT11, KOP+14, KGHK12, KB13, KZ+16.
KLN12, LCW12, LBGS16, LGW12, LBTV11, LBTV12, LHKS12, LH14b, LH17, LPM17, MMH19, MSY19, MAK+14, MWJ+11, MAP18, MFR+17, Mor15, MMJ10, NS18, NF17, NN18, NO16, NK+16, Oht16, ORZ11, OM12, PAK17, PPH+14, Pic14, PD11, QZ10b, RJPB12, RS13, Rez19, RB12.

functional [RSLML12, RHPWS13, RHT+15, RNS19, RR19, Rui11, SPS+12, SH15, SFG+17, SHL+18, SCW11, SBT17, SEF+16, SE14, SH14, ST13, SHL+13, SPH11, SH19a, SMM15a, SMM15b, SMM+18, SKTT11, SZZS16, STS15, TLDG+12, TG12a, TS10b, UvSvdWK19, VV14, Vi11, VL17a, VI17, VLGK+17, VED10, VHS+19, WKC10a, WHL+10, WCDW11, WDLG12, WYT17, WXY+10, WL14, WTH+16, WGN+16, WZC+19, XY+14, YJ11, YLZ+10, YS13, ZXS+10, ZWLX12, ZLZ14, ZYG+14, ZWY+10b, ZWY+10a, ZLHH14, ZGZ19, ZGS+10, dSdS12a, dSdS12b, CKH19].

functional [LJC+19, KAG+12].

functionalization [WWTL19].

functionalized [KYKR15, LdSRR16, LTR18, MSY19].

functionals [Ben17, CCB15, CGR16, CXD+19, DH17, DOM+11, DWC17, ELF19, FPR14, GWJR18, HG10, HBI+17, KB10, KSH13, KSSH13, Kar17, KM13, LBH+11, LAM19, LH14a, LK16a, PW12, RSG14, Rui11, SGPJS+17, Sea10, SMD+16, SH18a, SPR+13, SZX13a, SZX13b, VCL18, WYT17, Yu12b, ZTH15, ZWX19, dSdLBn17].

functions [BP18, BLZ+13, CD13, COHI19, CC11, CVG14, Fer13b, Fer13a, FFA14, Fra15, Fra16, GSHM10, GZ14, KK17a, KS18, LRER13, MY17b, Mit13, MLCD11, PHT17, Pro16, RHRC16, RVM19, SFM14, SYDS11, SM18, Sun15, TNYN16, UCRL18, WZ17, TKN13].

fundamental [CD16, VCL18, XLY10].

furan [LGC19].

furanosides [KRTB10].

Further [RTS+13, FVB10, PZA15].

fusion [CZY11].

Fuzzy [FPV13, SK12, SK17].

fuzzy-border [SK12, SK17].

FXeOXeF [ARLP13].

G [Ano15-59, BZH14, LWD13, PHK14, ILKR11].

g-tensors [PHK14].

G2R3 [Gil11].

G_membed [WHAS+16, WHAS+10].

Ga [UT15, Mit13].

Gabedit [All11].

GAFF [MPB11].

galactosidase [AKMT11].

GALAMOST [ZL+13].

GalaxyDock2 [SKKS13].

GalaxyDock3 [YBS19].

GalaxyTongDock [PBLS19].

gallium [GKB+19, YR13].

gallium-supertetrahedral [GKB+19].

gamepad [HH16b].

GAMESS [LRBB12, WSGN11].

GAMESS-UK [WSGN11].

GAMPMS [LMA15].

gap [NP+18, QZ10b, RS17a, TPH+15, VLGK+17, WZH+18].

gaps [TSN16, VCL18].

GARLEEK [PFAS+19].

Garriga [Ihl12].

Garriga-Sust [Ihl12].

Gas [ATM18, ABB+12, BGS+19, PLZ17, ARLP13, CC18c, DHE+12, FYX+10, GC13, JKS+16, KD10, LPK16, LJW11a, LPLB16, MP13, MFM+12, NIIT15, PMG+15, PSC11, RWR+13, Sea10, SYZ+17, STS15, YHG+11, ZSZ+14, ZYL+15, ZLHH14, ABB+13].

Gas-Phase [ATM18, ABB+12, FYX+10, LPLB16, PSC11, RWR+13, YHG+11, ZYL+15, ABB+13].

gaseous [HC11, YHW17].

gases [LZ14, DHE+12, SMD18].

gateway [RK15].

Gating [SBFB17].

GaudiMM [PSG+17].

Gauss [MY17a].

Gauss-type [MY17a].

GAUSSIAN
Gaussian-based [CGA19, JLCA17].

gaussian09 [RS13].

Gay [SLX15].

GB [OBW12, VM11].

GBMV2 [LC17b].

GBSA [DSX11, GR10a, IMSR18, RDDS10, STM15].

GC [GWX12, YZWC11].

GC-/AT-rich [YZWC11].

GC-related [GWX12].

GDP [SS13c].

Ge [Cas14, MCK17b, PMG16, Sak18, UT15, YW12, LYL16, WKC11].

GeauxDock [DFF15].

GeC [HSY11, Kop18].

GeH [Kop19b].

gelatinases [XDL10].

Gelessus [Spr10].

gene [CQFC10].

general [AA18, BSL11, EWK13, FNSF11, HSN14, Ish12, NLP16, PH17, RJR14, Sun15, VHA10, YHVM12].

general-contraction [HSN14].

Generalization [Sah18].

Generalized [GH16b, KCPMG12, MSPC19, AB16b, BSPP13, DSF17, FCE15, GH16a, HWLW11, LL10a, MA16, NMH19, PS13, SZTSM10, SSBW14, VMPS17, WWKS11, WHM10, WBVE16].

generally [KKK19].

generate [MPA12, MdOdQ18].

generated [HWLW11].

Generation [ADF10, AIM18, MPA10, RvL11, STF19, CAD16, GMSiG15, GKJ19, HXY15, KLJ17, KSH17, LTT16, RB13a, RGVC19, TDP12, WLF19, WHJH13, ZCGM11].

Generator [MYT18, Gar12, GPM17].

generators [CLK11, GPM17, MPA10, RvL11, STF19].

GenLocDip [GH16b].

GeO [DLSD13].

Geometric [MK11, AM19a, AM19b, CDB10, CDBM11, EH13, FXC13, HHT13a, HHT13b, LFFH16, REH13, TCB13].

geometric-quantum [CDBM11].

Geometrical [DPAB16, HRJ14, JRSHP14, NSN19, LCM14, SPR13, Tak10, Tsu19, UT14, HRJ15].

Geometrically [RIJ11].

Geometries [VL19, ZLX19, Alg17, HCP15, SRA17, STT18, Tak10, LXZ10].

Geometry [MP13, BW11b, CGA19, EPD10, ELP19, FB10, Kow11, LIRL16, MCLD10, OZS13, Pon10, RSG818, RS13, REH13, SLG15, SMM17, Tak18, VB13b, WAB17, WX12].

geometry-dependent [EPD10].

Germanium [GSMM15, ALH10, Kop18].

germylene [Kop19b].

GeSbTe [NIIT15].

GFP [UD12].

GGA [BG13, EH13].

ghost [CMF17].

ghost-hunter [CMF17].

GIANT [JCG11].

GIAO [PTK11].

GIAO-CCSD [OPR16].

gibberellin [HYZ13].

gibberellin-binding [HYZ13].

Gini [WF16].

GIPAW [SPZP18b, SPZP19].

GIST [RNSF16].

give [AA18, JT18].

glass [GF818].

glasses [You10].

Global [LVDH13, OKIS17, PRSG13, Tak10, VL19, BK17b, CPN17, CZZL19, DS15, DAA15, FDH19, GPE13, KLI11, LLI11, MP13, MB14, MO15, MCA1Y1, SKKS13, SC15, TSZQ12, Vor10, WDHZ13, XHD15, XCLZ19, ZL11, DH11].

Glu [EJ13].

glucopyranose [HH10].

glucosamine [ZBP11, ZP13].

Glucose [APY16, WFL19].

GLYCAM06 [SA10].

GLYCAM06/TIP3P [SA10].

Glycan [JSD11].

glycine [DB12, DP15, FCD10, MC10, SPZP18a, SPZP18b].

glycoconjugate
[LABSG17], glycol [MSY19, TFYO19], glycoproteins [JSD+11, PFVL14],
glycosaminoglycan [CHKR10, SZdB19, SA10], glycosidic [HH11],
glycosyltransferase [RN17], GmbH [Spr10], GMCT [UU12],
GneimoSim [LWK+14], gold
[Ano15-58, BH14, CCJC10, FHT+15, FDH19, GAMAC+14, Li14a, Li14b,
LHKS12, LH14b, MFR+11, MG14, MBFG15, SRR16, SKTT11, YLL11],
gold-thiolates [FHT+15], Goldberg [WTH+16], Good [SB10], GPCR
[LLHM16, MFR+17], GPGPU [UM13], GPR119 [HK18], GPU
[AKK+16, AGB13, BK17c, CVT+11, DZT11, HAP+12, Kan15, KGHC15,
KPF+15, KPF+19, MFR+11, MLN+18, MEH18, PZCL16, REV+17, SVB10, SOM+13,
TSH18, YLL14, YSG12, ZLL+13], GPU Accelerated
[GKHC15], GPU enabled [BK17c], GPUs
[GBL+11, HLW+17, HLEM18, KPF+15, KPF+19, MLN+18, MEH18, PZCL16,
REB19, SVB10, SOM+13], GPU-based
[KGHC15], GPU enabled [BK17c], GPUs
[GBL+11, HLW+17, HLEM18, KPF+15, KPF+19, MLN+18, MEH18, PZCL16,
REB19, SVB10, SOM+13], GPU-based
[KGHC15], GPU enabled [BK17c], GPUs
[GBL+11, HLW+17, HLEM18, KPF+15, KPF+19, MLN+18, MEH18, PZCL16,
REB19, SVB10, SOM+13], GPU-based
[KGHC15], GPU enabled [BK17c], GPUs
[GBL+11, HLW+17, HLEM18, KPF+15, KPF+19, MLN+18, MEH18, PZCL16,
REB19, SVB10, SOM+13], GPU-based
[KGHC15], GPU enabled [BK17c], GPUs
[GBL+11, HLW+17, HLEM18, KPF+15, KPF+19, MLN+18, MEH18, PZCL16,
REB19, SVB10, SOM+13], GPU-based
[KGHC15], GPU enabled [BK17c], GPUs
[GBL+11, HLW+17, HLEM18, KPF+15, KPF+19, MLN+18, MEH18, PZCL16,
REB19, SVB10, SOM+13], GPU-based
[KGHC15], GPU enabled [BK17c], GPUs
[GBL+11, HLW+17, HLEM18, KPF+15, KPF+19, MLN+18, MEH18, PZCL16,
REB19, SVB10, SOM+13], GPU-based
[KGHC15], GPU enabled [BK17c], GPUs
[GBL+11, HLW+17, HLEM18, KPF+15, KPF+19, MLN+18, MEH18, PZCL16,
REB19, SVB10, SOM+13], GPU-based
[KGHC15], GPU enabled [BK17c], GPUs
[GBL+11, HLW+17, HLEM18, KPF+15, KPF+19, MLN+18, MEH18, PZCL16,
REB19, SVB10, SOM+13], GPU-based
[KGHC15], GPU enabled [BK17c], GPUs
[GBL+11, HLW+17, HLEM18, KPF+15, KPF+19, MLN+18, MEH18, PZCL16,
REB19, SVB10, SOM+13], GPU-based
[KGHC15], GPU enabled [BK17c], GPUs
[GBL+11, HLW+17, HLEM18, KPF+15, KPF+19, MLN+18, MEH18, PZCL16,
REB19, SVB10, SOM+13], GPU-based
[KGHC15], GPU enabled [BK17c], GPUs
[GBL+11, HLW+17, HLEM18, KPF+15, KPF+19, MLN+18, MEH18, PZCL16,
REB19, SVB10, SOM+13], GPU-based
[KGHC15], GPU enabled [BK17c], GPUs
[GBL+11, HLW+17, HLEM18, KPF+15, KPF+19, MLN+18, MEH18, PZCL16,
REB19, SVB10, SOM+13], GPU-based
[KGHC15], GPU enabled [BK17c], GPUs
[GBL+11, HLW+17, HLEM18, KPF+15, KPF+19, MLN+18, MEH18, PZCL16,
REB19, SVB10, SOM+13], GPU-based
[KGHC15], GPU enabled [BK17c], GPUs
[GBL+11, HLW+17, HLEM18, KPF+15, KPF+19, MLN+18, MEH18, PZCL16,
REB19, SVB10, SOM+13], GPU-based
[KGHC15], GPU enabled [BK17c], GPUs
LRvdSM15, PHH+12, TKT11, KWG15, DDK14]. **GROMOS** [HH11, HLH+12, KAG+12, LGL11, LvG13c, MRO17, MSvG12, PLH16, PFVL14, SVB10]. **GromPy** [PHH+12]. **Ground** [GMBM18, Kop19a, BBI+11, CCM15, FAA15, GCCM15, HH16a, HWB19, Kop15a, LLBO12, LYC+13, LX11, LS11b]. **Ground-State** [Kop19a, HH16a, Kop15a, LLBO12]. **group** [Alg17, CAP17, Dry14, EHSPT16, FC16, GZZM16, GPK+16, Gil11, GWZ15, HB14, JJJ16, LZL+15b, LTR18, SSSM15, TG12b, Tsi14, VDVR14, VRKT19, WS12, WZH+18, XhD15, LdSRR16]. **group-IV** [WZH+18]. **groups** [Kan15, KV15b, LPS12, TN10, WGL+11, WZC+19]. **growing** [JZ17, Zim15]. **Grown** [SJSS19]. **growth** [BHF+18, DWZ+17, FCL+10, KHE+19, LL10c, LZLMP16, MZZ11, OME16, RS14, VMV19, WC11, XYW+14]. **GRRM17** [MHT+18]. **Grubbs** [RS17b]. **GSK3** [LJL+11]. **GTKDynamo** [BTA+13]. **GTP** [SS13c]. **guanidine** [HRJ+14, HGHP14, HRJ+15, JRSHP14]. **guanidinium** [CCCLCGRO14]. **guanine** [BZH14, CBG17, KK19, LZH+11, PDMT10]. **guanine-cytosine** [LZH+11]. **guanines** [WGL12]. **guanylthiourea** [MAPB10]. **guest** [CC18b, OAN15b, YDGZ15]. **GUI** [WCJ+14, HBJ+17, JCL+17, KLJ+17, QLKI19]. **guide** [BS15, GKV+13]. **guiding** [HS17a]. **GULP** [SN16a]. **gWEA** [YLGX14]. **H** [BSF18, BS16b, CXS10, CG12, CSNCS+18, DM15, DT19, GPK+16, HZ11, HSY+11, HVS16, JLS+10, JLH+14, LLL+11, LdSRR16, LAHS16, LWD13, MLQ+12, MCAY15, NMLD13, OKY18, OPR16, PMG+16, RMPAM15, Sak18, SNDK16, STS+10, TNY18, Tsk11, TSJ+10, TFQ+11, UT14, UT15, VIT+15, VV14, WKC10a, WKL12, WHL+10, WWKS16, WLF19, WCL+11, XFX+16, XCLZ19, YKH15, YZ15b, YZZ+17, ZYLL12, AS15a, Be17, BS10b, CK10, CKL+11, Chu10, DT19, DHE+12, EVR18, GTK10, GS11, HZ11, HRL11, JLL19, KTT+19, LJM+11b, LWD13, MSPC19, Niz13, OKIS17, PLFS18, PTK11, PJe14, Pon10, STS+10, TS15a, TKCN19, UT15, UvSvdWK19, WGL12, WWTL19, WvRSM14, XhD15, XCLZ19, YHX19, YZ15b, YZZ+17, YZL18]. **H-** [Pon10]. **H-atom** [BS10b]. **H-bonding** [WGL12]. **H-C-C-H** [YZZ+17, YZZ+17]. **H-cluster** [GS11]. **H-F** [JLLW19]. **H-FORMS** [RMPAM15]. **H-indol-** [YZZL18]. **HÔ** [BS10b]. **H/D** [Chu10, KTT16, UT15]. **H4** [BEEL14]. **hafnia** [EBPK17a]. **hafnia-based** [EBPK17a]. **hafnium** [MTS+19]. **hairpin** [LJW+11b]. **Half** [SWMW10, QS19, TS15a, WDZN16, YLT+19]. **half-lives** [QS19]. **half-sandwich** [TS15a, YLT+19]. **half-saturated** [WDZN16]. **halide** [Li14a, Li14b, NC13, ZWY+10b]. **halides** [FWB14, PGS+15, RVM19, VVP12]. **halobenzene** [CvM19, EPH+15, HvM19]. **halocyclopentadiene** [CvM19]. **halofullerenes** [TFQ+10]. **Halogen** [CvM19, FPRS14, GSMZ19, HvM17, HvM19, VVMY18, WFZ+18, ASW19].

hydrogen-bridged [ZLY+16]. hydrogen-contaminated [YR13].
Hydrogen-Disordered [MYT18]. hydrogen-storage [BEM14].
hydrogen-transfer [ZW17]. hydrogenase [GS11]. hydrogenated
[MBRC16, wZbZ11]. Hydrogenation [GBG+19, JAB16]. hydrolase
[BHNS14, LD18]. hydrolysates [LWZ+19]. hydrolyses [YZGS14a].
Hydrolysis [JAHS+19, LHT15, MFM+12, XZ11, YZGS14a]. hydperoxyl
[AAMD+11]. hydrophilic [PAK15]. hydrophobic
[ARRC15, GMMH+16, JGS+17, MBC11, PAK15, SY16b, TM16].
hydrophobic/hydrophilic [PAK15]. hydrophobicity
[CH14, SV15].hydroquinone [PNE18]. hydrosilylation
[DK19, SSD19]. hydrostatic
[FCW+14]. hydroxamate [GWZ15, GPdC+16]. hydroxamate-containing
[GPdC+16]. hydroxy [FFA14]. hydroxyapatite
[XYW+14]. hydroxybutyrate [SJD14]. hydroxycoumarin
[LZHH11]. Hydroxyl
[BHP19, DPNM11, GKR13, KS13b, Ray13, RKG11, SY16b, TM16].
hypothesized [LLB+12]. hypoxanthine
[FF11].HZSM [cCVG+14]. HZSM-5 [cCVG+14].
I50V [DLZ15]. I50V-induced [DLZ15]. IBISCO [KVQC+11]. ICD
[WAB17]. Ice [MYT18, AASP18, LPA11, TD11]. ICI [GSM19]. ICN
[KIOY19]. icosaheiral [FCW+14, GKSS14]. ID [LLHM16]. Identification
[HRB+17, KYT+17, RLL+10, DL16, JSD+11, MPNS13, RLDJ17, WSH10,
YZWC11, ZYvIZ14]. identifier [hlh12]. identifiers [GPGSM11, GPGSM12].
identify [LLHM16, LHL+10]. Identifying
[AC12, HAG10, RNS19, XTY+14, LHO17, LLJ12, She12]. identity
[Höf14, KN17, YN15]. IE [MLCD11]. IEF [GMMH+16]. IEF/PCM
[GMMH+16]. Ilhenfeldt [GPGSM12]. II
[AMK11, ALH+10, BSQ+18b, ČMD13, CK17, FPB12, FB14b, GEP+14,
HRJ+14, HRJ+15, JAB16, KPL15, LGW12, LWXC16, MLG18, MMB+17,
PHC13, SB10, TLA10, WGN+16, XP13, XWSW13, ZCK+16, vSGP10,
AKMYB18, BKWK10b, BB11c, CB11c, FXC+13, Fer13a, FVB10,
Ano17-28, Ano17y, Ano17-29, Ano17-30, Ano17-32, Ano17-33, Ano17-34, Ano17b, Ano17c, Ano17d, Ano17e, Ano17f, Ano17g, Ano17h, Ano17i, Ano17j, Ano17k, Ano17l, Ano17m, Ano17o, Ano17p, Ano17q, Ano17r, Ano17s, Ano18a, Ano18b, Ano18t, Ano18u, Ano18v, Ano18w, Ano18x, Ano18y, Ano18z, Ano18-27, Ano18-28, Ano18-30, Ano18-31, Ano18-32, Ano18-29, Ano18-33, Ano18-34, Ano18-35, Ano18-36, Ano18-37, Ano18-38, Ano18c, Ano18d, Ano18e, Ano18f, Ano18g, Ano18h]. Image [Ano18i, Ano18j, Ano18k, Ano18l, Ano18m, Ano18o, Ano18p, Ano18q, Ano18r, Ano18s, Ano19a, Ano19l, Ano19t, Ano19u, Ano19v, Ano19x, Ano19y, Ano19z, Ano19w, Ano19-27, Ano19-28, Ano19-29, Ano19-30, Ano19-31, Ano19-32, Ano19b, Ano19c, Ano19d, Ano19e, Ano19f, Ano19g, Ano19h, Ano19i, Ano19j, Ano19k, Ano19m, Ano19n, Ano19o, Ano19p, Ano19q, Ano19r, Ano19s, Cor17, LCM16, SFLG+17, YHH+13]. images [LLJ12, MBFP15]. imaging [SCF+19]. imatinib [AS10]. imidazo [QQY+18, YLZ+10, FDCJG18]. Imidazo-Pyridine [FDCJG18]. Imidazole [FD16, LWGZ15, NS10, YKH+10]. imidazolinone [CSC+18]. Imidazolium [MG15]. imidogen [Kop15a]. Imine [DK19, AS11, GG10, HDB15]. imines [ZX19]. imines-external [ZX19]. imino [GRCL12, YMY+19]. immediate [HTS17]. immersive [SFM+18]. Impact [ABM+15, DPNM11, MCS11, MKK+19, VCL18, vADC+14, JMLL13, NW17]. impacts [SSNT19]. Implementing [Nav18, SCOJ13]. Implications [CV12, VVY17, CBBG16, LP11b, LTP11, RB12]. Implicit [BEM14, CAD16, Has14, ALRM18, CBG16, EK15, FBEM11, KJDB12, KB11a, KB11b, LC17b, ML14, SSBW14, SLX+15, SCMA+17, TCC+13, WWKS11, YL13]. implicit-solvent [WWKS11]. Implicitly [Jia19]. Importance [APA+14, CPK12, ENKK+17, NMF+14, OOK11, ESM+12, Ham11, KTNN10, PBDW11, SDZ17, TNSS17, TKNN10]. important [AST+16, BZH14, MG11]. importing [FN12]. impregnated [GLZ17]. improve [CIKT13, DLL+10, DPSL16, Gon12, LLL+10, Min18, VLB+10]. Improved [BS16a, KPF+19, LRR13, CCM15, DPB+12, DSF17, GCCM15, KSR+16, MP11, OHPR18, PBLs19, RTP+13, RDRC16, SSBW14, VVV+18, XMA+19, YS10]. improvement [GSHM10, NLP+16]. Improvements [JCX10, ZFOS19, AB16b, LRBB12, BB11c]. improves [BBOB16]. Improving [AIM+18, DWL11, FSSW19, GS16, LN15, PLH16, RVM19, SB14, SACdG14, SA11, WZ17, ZWX16, ZYS+10, GS15, GFPXD17, GZ14, FZY+12, TO10].
impurities [SBC+11]. IMSPeptider [dCLFGL13]. in-depth [DPD+18].
In/Si [LGKS17]. inactive [CV12]. include [PZA15]. includes [HBKL10].
Including [KL14, SFLG+17, BL12, FAA15, FD16, LH14a, SPH11, TG12a, WC14, YB11].
inclusion [CGR16, LZ11]. Incorporating [LHO17, Yan14, CSKH16, GCCM15, ZBP11].
Incorporation [LHO17, Yan14, CSKH16, GCCM15, ZBP11]. Incremental [SPZP18a].
Incremental [ER18, RR19, DCS15, LTA+11, SR18]. increments [MS15].
In/Si [LGKS17]. inactive [CV12]. include [PZA15]. includes [HBKL10].
Including [KL14, SFLG+17, BL12, FAA15, FD16, LH14a, SPH11, TG12a, WC14, YB11].
inclusion [CGR16, LZ11]. Incorporating [LHO17, Yan14, CSKH16, GCCM15, ZBP11].
Incorporation [LHO17, Yan14, CSKH16, GCCM15, ZBP11]. Incremental [SPZP18a].
Incremental [ER18, RR19, DCS15, LTA+11, SR18]. increments [MS15].
In/Si [LGKS17]. inactive [CV12]. include [PZA15]. includes [HBKL10].
Including [KL14, SFLG+17, BL12, FAA15, FD16, LH14a, SPH11, TG12a, WC14, YB11].
inclusion [CGR16, LZ11]. Incorporating [LHO17, Yan14, CSKH16, GCCM15, ZBP11].
Incorporation [LHO17, Yan14, CSKH16, GCCM15, ZBP11]. Incremental [SPZP18a].
Incremental [ER18, RR19, DCS15, LTA+11, SR18]. increments [MS15].
Ano17-52, Ano17-53, Ano17-54, Ano17-55, Ano17-56, Ano17-57, Ano17-58, 
Ano17-59, Ano17-60, Ano17-61, Ano18-39, Ano18-40, Ano18-65, Ano18-66, 
Ano18-67, Ano18-68, Ano18-69, Ano18-41, Ano18-42, Ano18-43, Ano18-44, 
Ano18-45, Ano18-46, Ano18-47, Ano18-48, Ano18-49, Ano18-50, Ano18-51, 
Ano18-52, Ano18-53, Ano18-54, Ano18-55, Ano18-56, Ano18-57, Ano18-58, 
Ano18-59, Ano18-60, Ano18-61, Ano18-62, Ano18-63, Ano18-64, Ano19-33, 
Ano19-56, Ano19-57, Ano19-58, BMPML+13, CRZ+18]. information 
inspection \[KOY^{+12}\]. inspired \[CYY^{+17}, DSM^{+11}\]. instability \[MMH19\]. instantaneous \[RO14a\]. Instanton \[MK17, MK19, MRK11\]. Insubria \[GCC14\]. Insulator \[LLL^{+12}\]. Insulin \[MV17\]. INT \[YJXZ13\]. INT-DBD \[YJXZ13\]. Integral \[Coo19, VSP19, DL19, KSNT19, MEH18, RFN15, SS13b, Sun15, VKAM12, WXY14, YS18\]. integrals \[CHC^{+13}, PS17, PC16, RLA18, SZTSM10, WDKT19\]. integrase \[XLY12\]. Integrated \[HSW^{+19}, vRWGS17, CKKK16, MCC12, US11\]. Integrating \[APK14, LZZ14\]. Integration \[FPV13, AYY017, BB11b, BB11c, DH17, LP11a, MOS12, NSK18, dlR11, Pol13, Pop18, SJC11, SJ16, dRBO13, MYKO18\]. integrative \[ˇRez16\]. integrator \[JS17b\]. intelligence \[Aou16\]. intelligent \[CDS16\]. intensity \[dSH19\]. Inter \[CROB16, SSB11, IIHY15, SSB13\]. Inter- \[CROB16, SSB11, SSB13\]. inter-residue \[IIHY15\]. Interacting \[CM16, VSP19, ATP18, EV14, HGCCGR^{+16}, MP17a, PNE18, WL14, JCHT18\]. Interaction \[BHB19, CK10, CCCLCGRO14, CCCLRO14, Den12, NNS15, SBW12, YZWCl11, ALW^{+10}, AG12, BLFZ13, BLF14, BCNH^{+11}, BSD18, BHB^{+17}, BRLS08, BRLS12, BG17, CLFRO18, Cas13, CZH12, CYG^{+15}, CTP13, CAP17, EK17, EV14, FF11, FCCP17, FA18, GA14, GP11a, HPT17, HBL12, HLH^{+12}, HSZ^{+11}, HLXH17, HLXH18, HQSZ19, HL19, JZZM14, Kan15, KTNN10, LL10a, LMZ11a, LPS^{+13}, Li14a, Li14b, LHHW14, LZL^{+15b}, LPLB16, LCVW10, Min18, MSÁK12, MCP18, MVBD18, NGAS17, NN18, OHPR17, OHPR18, OAN15b, PRJ^{+17}, RZG^{+13}, RS13, SM16a, SS13a, SBGP18, SBV10, SHL^{+18}, SPL^{+18}, SHF11, SH19b, TYN15, Tan19, TSH^{+19}, WSH10, WYL^{+15}, YK13, YWJ^{+16}, YAO18, YCK16, YHCS11, ZRCC11, ZY14, ZW18, ZZZ^{+19}, dLvNC18b, vS18, KCB^{+12}\]. interaction-activation \[LSL^{+19}\]. interaction-based \[ZW18\]. interaction-induced \[BLFZ13\]. Interactions \[BGS^{+19}, Hes19, Sch18, WCT^{+11}, ZCK^{+16}, Abr11, ARRC15, AKK^{+16}, AO10, BSF18, BSG18a, CSS17, CIH18, CIK13, cCVG^{+14}, CKP10, CROB16, CB11a, CB11c, dRCFGRB18, DDP^{+18}, DHP^{+11}, DBG11, DLH12, EP10, ER18, GWF11, GZZM16, GZ14, HSJ18, HLvdV13, HTY19, ICS^{+12}, ICS^{+13}, IHY15, Jab18a, KSSH13, KCK^{+15}, KPH^{+19}, KGJJ19, LZLC13, LZSM19, MLGB16, MH17, MKH^{+13}, MR17, MJM^{+15}, MVKS10, MG14, MFR^{+17}, MPBJ11, OHNK11, PPJ14, PLV^{+11}, RTS^{+13}, RVM19, RMRBH^{+19}, SSIS15, SDF12, SB19, SWW^{+19}, SB11, SB13, TSSS17, TG12a, TY10, TSR^{+16}, TNG^{+10}, VVJ15, VM19, WS10, WGD^{+16}, WDS^{+19}, WZ19, WM17, XTY^{+14}, XLY12, YKO^{+11}, YZ15a, YW13, YZL^{+15}, YDGZ15, YZLI18, ZLL^{+12}, Zha11, dLC17, dLvNC18b\]. Interactive \[BRP^{+12}, BGR13\]. interactivity \[CQFC10\]. interatomic \[DPAB16, FCCP17, RLA18, YKO^{+11}, dLC17\]. intercalation \[LAM19\]. interconnections \[GLF16\]. interconversion \[HH10\]. interconversions \[TCGNT18\]. Interdependence \[WAB17\]. interest \[BCNH^{+11}, OZLSBH12\]. Interface \[SJJ18, All11, BDTFP11, CSSB11, GRP^{+12}, GCW14, HL14, JJW^{+14}, KG13, LJ112, LZdlL^{+10}, LBB^{+15}, MSSP17, NS18, OYK^{+11}, PHH^{+12}, PVZ13, RR14, RSR^{+12}, SN16a, SYDS11, SISK10, STH^{+10},
ion-pairing [KTK17]. ion/water [SV11]. Ionic
[FDCJG18, JXSW15, AFP113, APY+16, CG15, CFC15, EK15, GC11, IN19,
IM17, LEdOLd1V17, MG15, NF1+16, PS14, SCM+15, WWKS11]. ionicity
[SLY+19]. Ionisation [CTP13]. Ionization
[SHL+18, ACD+13a, ACD+13b, BG17, CG15, CBG17, GWF11, HNyH19,
LGOM+15, LK13, yOTu16, SSB+16, SGHL13, Tac17, VL17a, VCL18].
Ionicity [SLY+19]. Ionisation [CTP13]. Ionization
[SHL+18, ACD+13a, ACD+13b, BG17, CG15, CBG17, GWF11, HNyH19,
LGOM+15, LK13, yOTu16, SSB+16, SGHL13, Tac17, VL17a, VCL18].
implosions [LGVA14]. Ionized [GMBM18]. Ions
[WFZ+18, AS14, BDTP11, CCCLRO14, CC12a, EKH14, PRJ+17, PZA15,
SNS16, SGH+16, VHS+19, WKC10a, XP13]. IP [BK17b]. IP-tuned
[BK17b]. IPRO [PGL+15]. IQA [CSM16]. IR
[DCOD13, CWT+12, LWL+11, LXZ+10, WJX+10]. irGPU.proton.Net
[Kan15]. iridium [CWT+12, HDPM14, KB13]. Iridium-catalyzed [KB13].
Iridium-containing [HDPM14]. Iron
[HS14a, AKMYB18, BH19, BG13, CTR13, DK19, GBGR16, HSb+19, HS16b,
KPL13, KPL15, MC10, NH19, SBC+11, TS10b, VBMA13, EH13].
iron-containing [AKMYB18]. iron-porphyrin-carbonyl [BH19].
iron-sulfur [CTR13, HSb+19, HS16b]. irradiation [WJX+10]. Irregular
[Sch10]. isocloso [LK16b]. isoconversional [DCˇS15]. isocyanide [TLY+12].
Isoelectronic [ZLX+19]. isoindolin [YZL18]. isoindolin- [YZL18].
Isolated [FL15, DSB+19]. Isomeric [FL15]. isomerism
[dCGCRN19, RS17b]. Isomerization [BW11b, DBGO+17, EF16, BLG10,
BMFG16, LL19a, MSBF16, OKIS17, SJD11, Su10, WCL+11, ZWZ11].
Isomers [CSM16, ZWZ11, DSHL18, Kar17, OKIS17, WCL+11].
isoselectivity [OSA19]. Isoster [EdOdS18]. Isothiirane [MM19]. isotope
[KK16, MRK11, NASH15, ORZ11, UT14, UT15, VKAM12, WXY14].
isotope-substituted [UT14]. isotopomers [UT14]. isotropic
[KJS+16, Tak14]. isotropy [Tru18]. Issue
[Ano12a, Ano12b, Ano12c, Ano12d, Ano12e, Ano12f, Ano12g, Ano12h,
Ano12i, Ano12j, Ano12k, Ano12l, Ano12m, Ano12n, Ano12o, Ano12p,
Ano12q, Ano12r, Ano12s, Ano12t, Ano13a, Ano13b, Ano13c, Ano13e, Ano13f,
Ano13g, Ano13h, Ano13i, Ano13j, Ano13k, Ano13m, Ano13n, Ano13o, Ano13p,
Ano13q, Ano13r, Ano13s, Ano13t, Ano13u, Ano13v, Ano13w, Ano13x,
Ano13y, Ano13z, Ano13+27, Ano13+28, Ano13+29, Ano13+30,
Ano13+31, Ano13+32, Ano13+33, Ano13+34, Ano13+35, Ano13+36,
Ano13+37, Ano13+38, Ano13+39, Ano13+40, Ano13+41, Ano13+42,
Ano13+43, Ano13+44, Ano13+45, Ano13+46, Ano13+47, Ano13+48,
Ano13+49]. Issue
[Ano13+50, Ano14a, Ano14b, Ano14c, Ano14d, Ano14e, Ano14f, Ano14h,
Ano14i, Ano14j, Ano14k, Ano14l, Ano14m, Ano14n, Ano14o, Ano14p,
Ano14q, Ano14r, Ano14s, Ano14t, Ano14u, Ano14v, Ano14w, Ano14x,
Ano14y, Ano14z, Ano14-29, Ano14-30, Ano14-31, Ano14-32, Ano14-33,
Ano14-34, Ano14-35, Ano14-36, Ano14-37, Ano14-38, Ano14-39, Ano14-40,
Ano14-41,


KSM17, KKNN11, LCK+18, MSC+10, MCLD10, OSR16, PVL+13, PTK11, PML+12, PB14, VAMS14, WWD14, ZMMM12. Levels [Kop19a, AC12, BCSCJ+13, BY11, BACSCJ+10, HYD10, Hua16, KIOY19, KHWB17, Kop15a, Kop17a, Kop17b, Kop18, MK13b, dSAdSL13], leveraged [EPH+15]. Lewis [EHSPT16, KASH14, Liac+14]. LH1 [KPG18].

Li [AM19a, AM19b, DDM+15, JW12, RLA+11, YCGA10, YHCS11, BWKW10a, GNI18, RLA+11, TN12, YZLZ19, YCGA10, SBW12]. Li-based [GNI18]. Li/Na [YZLZ19]. Li/Na-ion [YZLZ19]. Libcint [Sun15].


library-based [MZZ11]. LICHEM [KWL+16]. LiCl [LCL+18]. LiCN [LLL+11]. LIE [CZY11, VLb+10]. life [RHT+15]. lifetimes [CH10]. Ligand [DPOS16, KKH19, KC13a, LI19, MNNK10a, VKC10, ABD11, AG12, BKL13a, BPB11, BCG10, BBG+18b, BS10c, CMD13, CIK13, CHR+12b, CHR+12a, DFF+15, FTW12, FBEM11, FRLN10, GHIK12, GDV17, GJK+19, GS11, GZ14, HKR12, HG13, ITY+19, KLJ+17, KL14, KYB13, KTO11, KTO13, LZ11, LL+10, LL10b, LWL+11, LBS10, MC10, MGWR12, MG14, MFR+17, NST14, NHR18, NFG+13, NMF+14, OBW12, OHNK11, OGL10, OSR16, OCLM14, OOT15, PGCT+12, PK17, PPJ14, PLV+11, RL17, RZG+13, RCR+16, RO14b, RVP+11, SPL+18, SKKS13, STM+15, TLY+12, TNSS17, VVG13, Vor10, WdVN12, WNP+16, WZ17, WWW19, YZZ16, YBS19, dRBO13, AIM+18, YZZ16, SHL+11]. ligand-based [RVP+11].

ligand-binding [GDV17, MGWR12, OSR16, RO14b, WW19].

ligand-field [BBG+18b]. ligand-induced [KL14]. ligand-receptor [FRLN10, VKC10]. ligand-sized [OGL10].

ligands [CS17, GPdC+16, HRC13, KSO+19, LBC+19, LL10b, LW+11, LBS10, MC10, MGWR12, MG14, MFR+17, NST14, NHR18, NFG+13, NMF+14, OBW12, OHNK11, OGL10, OSR16, OCLM14, OOT15, PGCT+12, PKK17, PPJ14, PLV+11, RLD17, RZG+13, RCR+16, RO14b, RVP+11, SPL+18, SKKS13, STM+15, TLY+12, TNSS17, VVG13, Vor10, WdVN12, WNP+16, WZ17, WWW19, YZZ16, YBS19, dRBO13, AIM+18, YZZ16, SHL+11]. ligated [EH13, WC14]. ligating [BAD+19].

LigDockCSA [SHL+11]. light [FWS+18, GNI18, HXM+16, KDR+18, PE11, REL17, XBSS19, ZG9+19].

light-driven [HXM+16, REL17]. light-emitting [FWS+18, ZG9+19].

light-harvesting [KDR+18]. lighter [WD10]. Lightweight [RLG14]. like [AASP18, Che17, EPH+15, GRN19, KIOY+12, KD18, KB14b, MP17b, OAN15b, SDF+17, SM15, UCFR16, VHA+10, VVY18, WFZ+18, WKC11, WGN+16, ZSL+11, VVY18, YZL+19]. Limit [SN16b, Fra15, Fra16, LW16, LYC+13, OAN15a, SLT14, WTH+16].

Limitations [LvG13a, VL19, HH18]. limiting [SLT+15]. limits [GC18, II18, NSK18, PDSC18]. line [dLvNC18b]. Linear [BG12, NNT+19, KKW18, YN15, ZLY+16, ARLP13, CPV+12, DSAS19, EP12, FYB+17, FCE15, GZZ12, JZM14, JMS13, KHL19, Kid19, LP11b, MA17, MSAK12, NYH+17, PH17, RS17a, RLA+11, RR11, SS16a, Tak14, VBDS+11, WL10, YDX16, ZZZ+19]. linear-combination-based [Tak14].

Linear-scaling [BG12, YN15, NYH+17, RR11]. Linearity [IKN13].
lysine-malonylation [TYX’18]. lysoyzme [ZP13].

M [AM19b, LDJ’10, LLL’11, MCK’17a, Rab12, TLdG’12, WWKS’16, YW12, YHCS’11, JJAB’16, CCCLCGR’14, MCK’17a, TLdG’12, YHCS’11, JJAB’16].


machine-learned [FP’17a]. machines [GTZ’18, RJBH’18, RLL’10, ZWL’13], macrocycles [CMM’18, GAMSBF’16].

macrocyclic [ZRC’12]. macrolide [PG’15]. macromolecular [Kne’11b, LCA’17, LAT’10, LAT’11, PG’14, UU’12, RTP’13]. macromolecules [DG’14, DZA’11, FXC’13, OHP’17, RZ’16, ZKE’17]. macrotcyclc [ZYY’10b]. Magnetic [BHP’19, LKZM’18, MP’19b, Avd’18, BCSC’13, BP’18, BACSC’10, CPRS’18, CPN’17, CJPT’18, FNS’11, GTT’10, GBG’19, HAI’16, Ibr’17, JCG’11, KNP’12, LLLL’11, LL’12, PLSF’18, SH’18a, SIT’18, SACd’14, SB’13, SB’15, Vik’11, wZb’11, ZLZ’14, ZB’18].

Magnetically [ATM’18, ATIP’18]. magnetizabilities [ZP’16]. Magnetochemical [SvL’18]. magnetoresponsive [TDKT’10, TS’11].

magnets [BP’18]. main [ACD’13a, AC’13b, JJJ’16, XhD’15].


malonylation [TYX’18]. maltose [HYSF’19, SWM’10]. man [HDH’12].


Many [CGP’11, BDdS’13, CKK’16, HRJ’14, HRJ’15, JRSHP’14, KNH’16, LYG’13, RHPWS’13, VMP’17, WCWV’15]. Many-body [CGP’11, HRJ’14, HRJ’15, JRSHP’14, LYG’13, RHPWS’13, VMP’17].

many-core [KNH’16]. map [MKM’17]. mapper [BJP’15].

mapping [EMD’17, KZP’18b, MMM’16, NSF’16, TD’10]. Maps [ZFOS’19, GJMPAM’14, YSRSS’10]. Marburg [OLY’17]. Marcus [WBKS’19].

Marjana [CD’19]. marker [JAH’17]. Markov [BFH’13, LTT’16, WW’19].


Material [JW’12, DGL’13, HLWD’15, JBSQ’11, LL’13b, MC’16, NGAS’17, SHL’19, SMN’19, SLHW’09]. materials [BSL’16, CD’11, DLT’17, ECZW’17, EMD’17, GNI’18, KLZ’18, KB’19, Man’13, NDD’10, SB’18, SYZ’17, VBV’13a, VVB’13, VVVY’17, VVMY’18, YZLZ’19].

MATLAB [DK’14, SKA’19]. matrices [Car’14, LHO’17, Mat’14, Yon’16]. matrix
matrix-based [VGV+11]. matrix-free [ZVY+15]. matter

[BGL+18, HRB+17]. Maxima [LüC14]. Maximal [DN19]. maximum


[LLSW14]. MCSCF [ZZZ+19]. MD

[HCD+10, RSR+12, BM12, FB14b, GMASBF16, LWZ+19, LJL+11, MTVG12, OYK+11, RAR+11, SISK10, SMP17a, WTD+19, WWW19]. MD-FEP


[KKR+13]. mean [HDL+14, Kid19, KERY+16, KT10, KS12, KLS10, KML50, MIOM13, MP17b, RAR+11, SISK10, SMP17a, WTD+19, WWW19]. mean-field [Kid19].

[MIOM13]. mean-force [MP17b, RI10, VBDS+11, Vor12]. mean-field [Kid19].

[Me]. mean [HDL+14, Kid19, KERY+16, KT10, KS12, KLS10, KML50, MIOM13, MP17b, RAR+11, SISK10, SMP17a, WTD+19, WWW19]. mean-field [Kid19].

[MP17b, RI10, VBDS+11, Vor12]. mean-field [Kid19].

[MP17b, RI10, VBDS+11, Vor12]. mean-field [Kid19].

[MIOM13]. mean-force [MP17b, RI10, VBDS+11, Vor12]. mean-field [Kid19].

[MIOM13]. mean-force [MP17b, RI10, VBDS+11, Vor12]. mean-field [Kid19].

[MP17b, RI10, VBDS+11, Vor12]. mean-field [Kid19].

[MP17b, RI10, VBDS+11, Vor12]. mean-field [Kid19].
[FBKD19, LI19, VSP19, WNP+16, ZQH19, AIGP15, AOW11, BBG+11, BMR11, BAMR13, BF15, BS19, BCCO10, BMBJ11, BRP+12, BMFG16, BD11, BB11b, BK17c, CIKT13, CZY11, CL16, CH16, DK11, DC15, EFS16, EVR18, EDP+11, FGM1, Fer17, FRN15, FHZA+18, GLB16, GKH+19, GBVA11, GKY+13, GA12, dCGCRN19, GWZX12, HLS12, HH10, HTS15, HNTS15, HNS16, HYS19, HSN14, HNWF07, HNWF12, HAI+16, HBL12, HYUS11, HGW18, HHWL17, HLXH17, HLXH18, HL19, ITIN15, ISK14, ISO+13, ISM18, IO13a, IO13b, JZ17, JY+14, JMS14, JS17b, KV12, KS13a, KS15, Kan15, KSSH13, KG15, KNN11, KTO13, KB19, KB11c, KTN10, KLS10, KZP+18b, KB14b, KW15, LLHM16, LFB14, LBG16, LPC16, LCH10, LL11, LLZA12, LWZ19, LN15, LLSW14, LL19a, MK13a, MTM14, MHT+18, MC12, MKGA10, MPA12, MN15, Mat10, MDT10], method [MRK11, MA17, MJG+15, MFR+17, MS15, MNNK10b, MH10, NF18, NR11, NFDP13, NF17, NO16, OLA15, OK16, OOT15, PSS14, Pet11, PSC11, PKIC11, PPJ14, PLV+11, PM18b, Pon10, QLQ11, QB10, QB11, RHRCH16, RKGN10, RSL15, RGVC+19, Rod13, RKB+14, RFHG10, SSO19, SF18, SS13a, SCM+15, SBB10, SSWX14, SBN13a, SBN13b, SB15, STM17, SG13, SSAS10, Tak14, TKNN10, Tak10, Tak18, TSZQ12, TSNC+17, US11, UIW+10, VLB+10, VDR14, Vor10, WXS+12, WLG19, WHM10, WTH+16, YO19, YJ+16, Yon16, YAO18, YN15, YHH+13, ZDZ13, ZMM12, Zha12b, Zha12a, ZLM+15, ZGZC19, ZW17, ZFS18, ZH12, ZA15, ZZZ+19, Zim15, CKH19, JCHT18], method-based [GKJ+19]. Methodological [VKNT16], methodologies [Rob13]. Methodology [CPK19, AKI16, FF11, GAI13, GMASBF16, HPT17, OHPR17, OHPR18, RJWW12, HCD+10]. Methods [SGP18, ANO12u, Ano15-59, ASMS10, BG13, CLFRO18, CSGOA17, CXS10, CNK97, DKE+17, DCOD13, DBM+15, EHK+13, EMS+12, EV14, Fer13b, Fer13a, FB10, FSSW17, FSSW19, GA14, GFPSD17, GD10, GSS13, GM16, HCB11, HSB+11, Hsf14, HWL11, JY+13, KSM17, KB13, KHW17, LeolDLv17, LLZC13, LLSW14, MS13, MY17b, MHO18, MR17, MVK510, MOS12, NXY+17, NASH15, NC13, NC14, NTNY15, OSHG17, PN13, PVAM16, RZG+13, RRH12, Rez19, SRF+17, SS16, SACdG14, STM+15, SWW+19, SWA17, TG12b, TS15b, Tsi17, WBT10, WX12, YLCX10, YAS13, YJ17, ZGS+10, dSdLBN17], methoxy [PNE18], methoxybenzyl [YTLZ18], methyl [AARP17, BIL10, CPLL11, GZL+12, GMG+10, LL11, LSL+16, MG15, MSBF16, VKE15, YTT12], methyl-methyl [LK11], methylacetamide [HLH+12, KSK11], methacrylene [WCVW11], methylated [LRVM18], Methylation [SCW11, KYCL11, QZM11, dALdS+15], methylbenzyl [NG14], methylcobalamin [KKL+13], methylformamides [JSW10], methylysine [GHK12], methyltransferase [CPLL11, GH10, PBLdS12], Methylurea [HV17, HvM16], MetRex [Sti15], metric [CSX10, LLH16, PKIV11, SOJ14, ZT14], metrics [Hug14, PBBP11, RCM+13b], Metropolis [MO15, Pon10], Mezey [HJ13], MF [YKH15], Mg [HDM+19, LDJ+10, LLX+19, BMFG16, DOM+11,
[LLLW19]. MNX [AM19b]. MO [BRP +12, UIW +10, ZY14]. mo analyzer [DJD12]. mobilities [SFDE16]. Mode
[AIM +18, BHR15, GVP +10, YI18, SRA17, SBB10, YHCS11, YXZZ17]. Mode-tracking [BHR15]. Model [Ale19, BLS10, HM16, Jia19, MT20, Pog10, AASP18, AOW11, AS10, ALRM18, ATP18, AS15b, APA +14, AB16b, Bac12, BK17a, BH19, BEEL14, BS10b, BBG +18b, Cam15, Can10, Cam11, CGP12, CGA19, CBTZ16, CFC15, CAD16, CG12, CMS13, CJZS10, DLL +10, DSF17, FCE15, FNSF +11, GRN19, GR515, GM17, Gil11, GKR13, HLS12, HAL14, HLH +12, HOK17, HZSS17, Hug12, HRH +17, ISO +13, IN13, III18, JSXH16, Jor17, KFY +13, KCC +17, KMS +19, KR12, KOY +12, KD18, KCPMG12, KB14b, KDS17, LSL +19, LTT16, LY10, LRvdSM15, LFN +10, LPS +13, LHHW14, LZL +15a, LDG +15, LCK +18, LHMM11, ML10, MT19a, MPJ +19, MBC11, MBC13, MM +17, MHO18, NJX10, NTNY15, OPB17, PB14, PCLL11, Pla11, Pon11, Ray13, RTS +13, Ric16, RMRBH +19, REL +14, RKG11, SM14b, SDF +17, SHF11, SSBW14, SK12]. model [SK17, SLX +15, SDZ17, SZBM13, SB11, TYN15, TCC +13, Tia12, TLA10, TTh19, UIW +10, VV15, VH +19, WWKS11, WXL +12, WC13, WWW19, WNM17, WRHF10, WKC11, WCAH10, XZ11, XTY +14, XP13, YS18, YOM14, YB13, YG12, ZST14, ZKH +10, ZM10, dSDdAR10, dSH19, CCR18, FAS +18, MJBM12]. model-tuned [HZSS17]. modeled [MPA12]. modeler [BHI19, KLJ +17]. Modeling
[ASW19, CB11a, DLSA14, FD13, FTW12, GMG +10, GBS +17, HPL13, JW16, KDR +18, Mat14, NS10, NDLW13, PLP +16, SZdB19, SK11, Tia12, VY15, AKMT11, Ati16, BEM14, BPC13, Bow16, BS10c, CMD13, CLA16, CNZ11, DAG19, DWR17, DSY +11, DLmH12, EBPK17a, FZX +13, GH10, GP12, GMZ12, GWJR18, GR10b, GWZK12, HLvdV13, HBJ +17, JC16, JCL +17, KSD +12, LABS17, LLH14, LZGS11, LT13, LN15, MBA11, MJLV14b, MA17, MA14, MBP11, NSO +14, NW17, PHC13, PSS14, PSG +17, PMS16, QLK19, RJS17, SN16a, SKGP19, TTR +12, VKNT15, VAA14, VCM15, WXL17, WPM +15, WLO +17, XDL +10, XY12, YMY +19, YJ11, ZX11, DHE +12]. modelling [DBM +15]. Models [Hes19, NNT +19, ND19, BEM14, BLKP12, BPB11, CD11, Cor17, CBG16, CK17, DDP16, DSM +11, DI11, DGC14, DLC18b, EK15, EPD +10, GMPB12, GMH +16, GMG +10, GKR13, GCC +13, GDC14, GAIJ +17, HS16b, HGY15, JCP14, JGS +17, KJDB12, KKO +16, KB11b, KSR +16, KSW16, LTT16, LKL10, LZ12, LLSW14, LM18b, MPSA17, MSK12, MCJ15, MKB +13, NNS15, OLI13, PHC13, PGY15, PL18, Ray13, RTP +13, RKG11, SPHF +18, SCMA +17, SFLG +17, SAgG15, TH13, TTB +11, TLY +12, VCK10, VMP17, VZ14, WS10, WXY14, WSWD19, XTn18, YJ11, YL13, ZsA10, ZDW18, dSDdLB18]. modern [ABI16a, AB16b, DH17, Fom11, LM14, SF18, SDM +16]. modes [CBP +15, EB18, GMPB12, KKH18, LLTC12, MS17, dSH19, dSAAdSL13]. modification [Ano12u, MS +15]. modified [BD12, CH16, DPSL16, DJX +11b, GSD10, MRO17, Mit13, SMM15a, SMM15b, SM +18, XY17, XVA +16, ZZ12]. modify [ZX19]. Modifying
modular

Modulating

modulators

moieties

MOLCAS

Moldyn

molecular

molecular
PH15, PVJ10, RJBH18, RD18, RMPAM15, RLLHL12, RNSF+16, RNP13, RNVP13, RS10, RS17, RJH11, RO14b, RR14, Rda12, RC18, RLG14, RSR15, REH13, SHMO11, SSO19, SF18, Slt+15, Sax12, SWM10, SK15b, SA13, SZTSM10, Sch12, SFR+11, SHFJ18, SHF11, SMRM+17, SS19, SSNT19, SOM+13, SJ17, SR18, SYN+12, SK13, SWB+12, SLLL13, SJ16, SMD13, SKY+11, SPZP18a, SPZP19, SBvG14, SAvG15, TNYN16, TKNN10, TZ12, TJR19, TTC+18, US11, UGK18, VYM15, Vik11, Vor10, Vor12, VM11, WKL12, WBN+13, WM17, WLM+10, WH11, WCY+11, WLC12, WOH16, WXL17, WOH18, WES13, WBF17, WCDM11, WO15, WCUW15, WL14, WG14, Won18, WDKT19, XDL+10, XFG+15, YK0+11, YP+D3, YNH+17, Yo19, YLGX14, YLCX10, Yap11]. molecular [YPKB12, Yes12, Yes15, ZSTI14, ZYL16, ZX11, ZDKM12, ZSS+13, ZS19, ZLY16, ZP13, ZWX16, ZLL+13, ZA15, ZBMZH15, dSdLBNB17, dCLFGL13, dLvNC18a, AIM+18, IPAA11, KSD12, ZKH10]. molecular-mechanical [ZSTI14]. molecular-orbital [US11].

MoleculaRnetworks [MCC12]. Molecule [KR12, vRWGS17, BT18, DHO13, DGL+13, ETLS17, FAA15, GAI14, GCWS15, GBVA11, HLvdV13, HHWL17, ISO+13, IIHY15, KB11b, KKA+18, LIRL+16, MCUJ15, NLL19, PCLL11, RLL+10, SG10b, VGV+11, WF16, XYW+14, XMSZ16].
molecule-transcription [XMSZ16].

Molecules
[ATM18, Cam19, ELKE19, PiSC18, AIPG15, Ali18, AFW+18, ARAG17, AGR11a, BLDG+13, BS10a, BTMS12, BSC19, BPC19, Ben17, BS16b, BL12, CPZ19, CHG+16, CC18c, CQFC10, CYG+15, CCOH14, CXS10, CZNA11, FDI19, FE14, GWF11, GKJ+19, GP12, GPBS11, GPS12, GAJ+17, HRB+17, HSB+11, Hug12, Ih12, Kan15, KLI+17, KGFZ19, KGY+15, LPS12, LHSH12, LvG13b, LH14b, LJJ+11, LG14, MA16, MS13, Mat10, MSS+13, MH17, MBE16, MPBJ11, NII+15, OGL10, OT12, PZBA13, Pyy13, RSG18, RSG14, RK15, SFCCK+14, SFCC+15, Sch13, SG10b, SLG+17, SY16b, SM17, TZCK18, TSR+16, UNT16, VVV+15a, VHA+10, VVY18, VDVR14, WC13, WSZW15, WFS19, WWD14, WX12, You10, YKH15, YHW17, ZPP+16, Zha12b, ZIX+13, ZBB16, ZCGM11, MSPC19, SMB18].

molUP [FRC18]. Molybdaticarboranes [LK16b]. molybdocene [PM13, SDL14].

Moments [GH16a, Ali18, BLDK+13, CP15, CTP13, DHO13, GH16a, Lar11, NOKJ16, Tru18].

multipoles [Elk16, KGM12, SMP17b]. multiprocess [MB16].
multiprocessing [GP11b].
multiresolved [DGC14].
multisite [CK17, HS14b, MMB17].
multistart [MS16]. Multistep [DWZ17, FZY12, WDZN16].
multistate [BLKP12, FXC13, LC16, LZ14, JBB11, MBC13, SYN12, WLO17].
multithreading [TO10, ZWL13].
multivalent [AS14, FVP14].
Multiwfn [LC12].
muscarinic [SRA17].
musculus [WZQW10].
muscular [WZQW10].
mutagenic [BZH14].
mutant [FHK12, LMA15].
mutants [CSC18, RKDM14].
mutations [BH15, GMO16, KYT17, SL10, SY16a, WC11].
mutable [BMPML13].
MVPACK [BACSCJ10].
MX [Sch13].
MXenes [YZLZ19].
mycobacterium [MPNS13].
myoglobin [SHB17].
N [ATIP18, Ano15-59, BLF14, BCNH11, KBC12, KCL14, LPLB16,
NDG14, PVL13, RLZ18, ZLX19, GNI18, LZSM19, BCNH11,
BKWK10b, BMB13, BSDP16, CWT12, CCM15, DCHL12, DLW12,
GMASBF16, GZL12, HLH12, KV14, KCL14, LZL15b, MLGB16,
MSPC19, MS15, OZLSBH12, PVL13, QQY18, RHN10, RWR13,
ŠBD17, SGHL13, TSJ10, VM11, WS10, WGL11, WCL11, WYGW12,
WS12, Yu12b, YXZZ17, ZP13, HPSK12]. N-[BMB13].
-N-Bromosuccinimide-promoted [QQY18]. N-Codoped [RLZ18].
N-heterocyclic [BSDP16, CWT12, SGHL13, WS12].
N-methyl-N-phenyl-hydrazine [GZL12].
N-methylacetamide [HLH12].
N-substituted [DCHL12]. Na-ion [SMIN19, YZLZ19].
NABs [SBW12, SBW12]. NABs-Li [SBW12]. NaCl [HB15, PK19, TNY18].
NaI [OCW15]. Naïve [JL19].
Naiyang [Ano12u]. NAMI [LWZ19].
NAMI-A [LWZ19]. nano [Ano15-58, BH14, QZ10b].
nano-clusters [QZ10b].
Nanocluster [THF19]. nanobiotechnology [Fel10].
nanochannels [TM16].
nanocluster [AS15a, AAMR18, AHK19, RVKK13].
nanoclusters [AASP18, LLJ12].
nanocrystal [KC13b].
nanodisc [QLKI19].
nanoflakes [GNI18, Lin18].
nanogranular [DWZ17].
nanographene [DWZ17].
nanographenes [TSN17].
nanolayers [EBK13].
nanoparticle [CCJC10, NNS15].
nanoparticle-PMMA [NNS15].
nanoparticles [EOO16, KHL19, LZZ11].
nanopore [SM16b].
nanopores [DMN14, MJC14, SM15].
nanoporous [KB19].
nanoribbon [DJX11b, DJX11a, RRK14].
nanoribbon-based [DJX11b, DJX11a].
nanoribbons [LWZK13].
nanorings [TS15b, YDGZ15].
nanorods [LHKS12, LH14b].
nanoscale [Hei10, SWB12].
nanosheet [Bow16, MCRL17].
nanosheets [wZbZ11].
nanospheres [AAMR18].
non-equilibrium [NHN16]. non-heme [PHC13]. non-hybrid [CSKH15].
non-natural [GMZ12]. non-uniform [YWJ+16]. nonadditive [RTS+13].
Nonadiabatic [HZ11, RGVC+19, JBSQG11, KIOY19, MT19b, SRSLO15, WLF19].
Nonclassical [GC11]. Noncovalent [BGS+19, dRCFGRB18, Sch18, RLA18, SM16a, SWW+19, SBW12, TSM+16, VT14, WGD+16, WDS+19, YW13, YZLZ18, SMD18]. noncyclic [SM16a].
onempirical [BK17b, WYT17]. nonequilibrium [ASL+11, KHWB17]. Nonfitting [RZG+13].
nongeometric [KB11a]. nongeometric [KB11a]. Nonstatistical [Yu12a]. nontemplate [OL13].
Nontotally [HOM+16]. nonuniform [BD12]. norbornadiene [Ant13, WJX+10]. Nuclear
[AM19a, BCNH+11, CXS10, CSNCS+18, DHE+12, GBGR16, HRL11,}

O [AM19a, BCNH+11, CXS10, CSNCS+18, DHE+12, GBGR16, HRL11,
JM11, JLH + 14, KMS + 19, LZTV10, LLLM11, LLB + 12, LLSW14, MG11, PLFS18, PBE16, RHT + 15, SPS + 12, SBD + 17, TNY18, VV14, WHL + 10, WLF19, WRM + 12, XFX + 16, YW12, YR13, YOBP16, ZRCC12, ZXL + 19, Tsi17, BCNH + 11, BWKW10b, CK10, Chn10, CROB16, CPLL11, DT19, DHE + 12, HZ11, LZL + 15b, LCWW10, MH11, MSPC19, MS15, PBLdS12, PP19, RHNN10, RAGLL11, SZ17, SJ11, SSX + 14, TKCN19, WLF19, YZ15b, ZRCC11, ZSWL12, dCRN18. o-atom [Tsi17]. O-H [TKCN19].

[SvLK18, Aou16, BBG+11, BCSCJ+13, BCJC+14, BACSCJ+10, CCC+11, CJPTC18, DDK14, Dra19, GBW+14, HSN+18, KR14, KVQC+11, KCC+18, KGW15, KYG+15, LWK+14, LISH12, MLN+18, SKA19, SWA13, SHFJ18, SMRM+17, SJ17, SJ16, UI12, VB113b, WSGN11, ZCS+15]. packages [MSvG12, MJG+15]. packet [LWD13]. packing [MCAG+16, MP17b, NS11].

PaDEL [HLS+13, Yap11]. PaDEL-DDPredictor [HLS+13].


Parallelized [KAI19, DBDP16]. parallelizing [BMBJ11]. parameter [NB19, PFL14, SH19a, VCL18, VVL17, WDHZ13, LL11].

Parameterization [HKH18, HIJ16, ILKR11, IJH+13, MPSA17, PRRT+10, TCC+13, BAS14, CCL12, DLM12, KY13, LTP11, LCL+18, MSS+13, VLB+10, VBD11, VH1+19]. parameterizations [SH15]. parameterized [OZS+13]. Parameters [CTR13, AG11, AKMYB18, BCSCJ+13, BCJC+14, BSD18, BW15, BC13, CYG+15, DPSL16, DMAH15, FHT+15, GSD10, HLS12, HM16, HBI+17, HLH+12, KvdV14, KGK12, KGJZ19, LvDH13, LPS+13, LVG11, LHH+11, MRO17, MP11, PLS19, Pog10, RKB+14, SOY12, SZBM13, SPR+13, SPZP18b, VYM15, VLGK+17, WAM17, WOH16, WOH18, WC14, YWW+14, ZRL+15]. Parametric [LM18b].

Partitioning [VSP19, DK11, EV14, FCQGM12, FHZA+18, LZF+17, REL17, SS13a, TMJ15, VGV+11, ZW18, VV19]. partner [dVZ17].

Path [MA17, VKAM12, CY09, DL19, HXM+16, Ish10, JZ17, KSNT19, MvBD18, SRSLO15, SA13, SS13b, SMM17, TN18, TNY18, WXY14, ZT14, MYKO18, CY13]. path-based [ZT14].

Path-integral [VKAM12, WXY14]. path-search [Ish10]. PathOpt [GPE13].

Paths [SH11a, AMGB10, Ant13, CX10, Jab18a, NMLD13, RVP+11]. pathway [BHB12, HOM+16, LKL10, SJJD14, TDP+12, XLYZ10]. Pathways [JL19, CM13a, EF616, GS11, HNTS15, KGR+16, KDR+18, MTM14, NJR18, QSW+10, QB16, RCM+13a, RML+15, SJJD11, SH18b, Tsi17, WSH10, Yon16, BHH12]. pattern [CS10, LZSM19, WGL12]. Patterned [SJSS19].


PCASSO [LFB14]. PCCP [VT14]. pCCSD [Sch12]. PCM [LFN+10].


PDECO [CJL+13]. PDielec [KB16]. PDxCN [ZLL19]. peaks [LZS+17]. PEG [EOO+16]. PEG-PLA [EOO+16]. penalty [GZH10, LL19b].


peptides [BLKP12, BPC13, CR19, CCOH14, CZA11, GFG11, HSB+19, HLH+12, HWWL17, IO13b, JX10, KB10, LG13c, MZ11, MUGN18, OLY17, WNM17, XHL16, XWSW13, ZKH+10]. peptoid [MMZW14].

peptoids [WS19]. perception [AJR16, HYZ13]. Performance [Abr11, BZB+13, CSH16, CKKK16, DAP+18, DOM+11, GWR18, HSB+11, HB19, JC14, LK16a, RKB+14, SF18, SH18a, SGW17, ZWMW19, ABM+15, BLBG+13, CLF018, XSS10, CSS11, CJZS10, ESB13].
EWK$^{+13}$, GAI$^{+14}$, GRARO$^{+14}$, GSS$^{+13}$, HWLW$^{11}$, KZZ$^{+16}$, KLZ$^{+18}$, LL10a, LBB$^{12}$, LLC$^{+10}$, MHT$^{+18}$, MC$^{12}$, MG$^{11}$, OPB$^{+12}$, RRH$^{12}$, RSLS$^{13}$, SRF$^{+17}$, SPR$^{+13}$, SJ$^{16}$, TF$^{15}$, XMA$^{+19}$, YPC$^{+10}$, YMY$^{+19}$, ZHS$^{+18}$, ZST$^{+18}$, ZSLL$^{17}$, ZWL$^{13}$, SBW$^{12}$.

Pericyclic [HPT$^{16a}$, KG$^{15}$, ZZMW$^{19}$].

Period [LOB$^{18}$].

Periodic [Sce$^{07}$, Sch$^{10}$, AAC$^{+16}$, BBG$^{+18a}$, BS$^{19}$, BS$^{18}$, CMM$^{18}$, CDC$^{19}$, CEBO$^{15}$, FCD$^{10}$, Gar$^{12}$, HSH$^{15}$, HBI$^{+17}$, ITIN$^{15}$, KB$^{14a}$, LBGS$^{16}$, Man$^{13}$, MGS$^{+16}$, NN$^{18}$, NO$^{16}$, NTNY$^{15}$, RJPB$^{12}$, RLZ$^{+18}$, RNS$^{19}$, SN$^{16a}$, SSP$^{19a}$, Sie$^{15}$, SPZP$^{18b}$, TLD$^{+12}$, Tak$^{14}$, VBV$^{13a}$, VVB$^{13}$, VECT$^{12}$, VI$^{17}$, YAO$^{18}$].

Perlin [HLBLCCG$^{15}$].

Permeation [DMN$^{15}$].

Permutation [IO$^{13b}$, YO$^{19}$].

Permitrines [WD$^{10}$].

Perovskites [LLB$^{12}$, LLL$^{12}$, VVY$^{17}$, VVMY$^{18}$].

Peroxide [HW$^{19}$, KNP$^{+12}$, MK$^{13b}$, SZ$^{17}$].

Peroxo [RHPWS$^{13}$, RHT$^{+15}$, ZRCC$^{12}$].

Peroxo/superoxo [ZRCC$^{12}$].

Peroxyl [CGVBAI$^{19}$].

Peroxynitrous [BLG$^{11}$].

Persistence [XW$^{15}$].

Persistent [WZWW$^{18}$, XFTW$^{15}$].

Personal [Tsi$^{18}$].

Perspective [ABDGN$^{12}$, Dil$^{15}$, Hsu$^{14}$, JCGVPHT$^{17}$, JMX$^{+16}$, LGOM$^{15}$, MM$^{18}$, MP$^{17a}$, Niz$^{13}$, PZM$^{15}$, TNY$^{18}$, XLY$^{12}$].

Perspectives [NSK$^{18}$, DR$^{14}$, Wei$^{12a}$].

Perturbation [ELKE$^{19}$, CCM$^{15}$, CF$^{14}$, DCHL$^{12}$, FRSA$^{14}$, FSSW$^{17}$, FSSW$^{19}$, FE$^{14}$, GR$^{15}$, GCCM$^{15}$, GA$^{18}$, Hii$^{13}$, HRJ$^{+14}$, HRJ$^{+15}$, HYUS$^{11}$, JRSH$^{14}$, KKKN$^{11}$, KN$^{17}$, KSHP$^{+19}$, KM$^{13}$, LCL$^{+10}$, LLvG$^{10}$, LGL$^{11}$, LvG$^{13b}$, LvG$^{13a}$, MCC$^{11}$, MUGNY$^{+18}$, RL$^{+17}$, RAR$^{+11}$, RHPWS$^{13}$, SSSM$^{15}$, TAG$^{16}$, VDL$^{+13}$, WHAS$^{+10}$, YKH$^{15}$, ZZ$^{14}$, WHAS$^{+16}$].

Perturbation-based [KSHP$^{+19}$].

Perturbation-selection [FE$^{14}$].

Perturbations [GM$^{17}$, OS$^{16}$, Tak$^{10}$, WWCL$^{15}$].

Perturbative [SSWX$^{14}$].

Perylene [BSL$^{+16}$, SLP$^{+12}$].

Perylenebisimide [LCK$^{18}$].

Perylenediimides [QCR$^{12}$].

Pesticide [BHB$^{+17}$].

Peta [KNHN$^{16}$].

Peta-scale [KNHN$^{16}$].

Petascale [SCOJ$^{13}$, ZWL$^{13}$].

PH [LZL$^{+15b}$, dSD$^{10}$, RBC$^{+19}$, LZL$^{+15b}$, AB$^{16a}$, CS$^{14}$, CAD$^{16}$, HS$^{14b}$, MBA$^{14}$, PZ$^{15}$, PS$^{13}$, SY$^{16a}$, SOvG$^{12}$, Vor$^{12}$].

pH-dependent [SY$^{16a}$].

pH-responsive [MA$^{14}$].

Phage [MP$^{17b}$].

Phage-like [MP$^{17b}$].

PhAISTOS [BFH$^{+13}$].

Pharmacokinetics [VBDS$^{+11}$].

Pharmacophore [HRK$^{+10}$, HKRS$^{11}$, HS$^{11}$, TD$^{10}$, AKMT$^{11}$].

Phase [ATM$^{18}$, ZWM$^{10}$, ABB$^{+12}$, BE$^{12}$, BG$^{17}$, Coh$^{18}$, DSL$^{13}$, DLW$^{12}$, EMD$^{17}$, FC$^{18}$, GYX$^{+10}$, Hsu$^{14}$, KD$^{10}$, LJW$^{11a}$, LPLB$^{16}$, LGKS$^{17}$, MFM$^{+12}$, MKK$^{+19}$, NIT$^{15}$, PSC$^{11}$, RWR$^{+13}$, RSLML$^{12}$, RJS$^{17}$, SJZ$^{+15}$, SPZP$^{18a}$, VKAM$^{12}$, VED$^{10}$, YHG$^{+11}$, YSG$^{12}$, ZSZ$^{+14}$, ZWW$^{10}$, ZYR$^{+15}$, ZLH$^{114}$, dS$^{12a}$, dS$^{12b}$, ABB$^{+13}$].

Phase-change [EMD$^{17}$].

Phase-space [FC$^{18}$].

Phases [EB$^{12}$, LPAS$^{11}$].

Phen [FD$^{16}$, FHG$^{+19}$].

Phenantherline [SCSM$^{19}$, MRC$^{+18}$].

Phenol [AAMD$^{+11}$, AK$^{10}$, IYK$^{11}$, PPH$^{+14}$, TFYO$^{19}$, WH$^{+10}$, YKH$^{+10}$, AK$^{10}$].

Phenol-imidazole-base [YKH$^{+10}$].

Phenol-triethylgermanium [WHX$^{+10}$].

Phenolates [SKGB$^{13}$].

Phenols [SK$^{12}$].

Phenomena [JBSQG$^{11}$, WD$^{+12}$].

Phenoxy [IYK$^{11}$].

Phenoxy/phenol [IYK$^{11}$].
phenyl [GZL+12, ZWY+10a]. phenylacetylene [ZZL+12].
phenylacetylene-containing [ZZL+12]. phenylalanine [GWF11, PVS12].
phenylimidazo [LWL+11]. PHI [CAT+13]. philicity [Tsi19].
phosphate [MR17, SC18b, XZ11, YZGS14]. phosphatidylcholine [PVM10].
phosphatidylethanolamine [SH11a, TSW11]. phosphathione [TLM11].
phosphatidylglycerol [BH12]. phosphatidylinositol [GZ10].
phosphatidylserine [AD11a, HHK11, HHK10].
phosphatidylethanolamine [GZ10].
phosphatidylcholine [PVM10].
phosphatidylglycerol [BH12]. phosphatidylinositol [GZ10].
phosphatidylethanolamine [SH11a, TSW11].
phosphatidylethanolamine [SH11a, TSW11].
phosphatidylglycerol [BH12].
phosphatidylinositol [GZ10]. phosphatidylethanolamine [SH11a, TSW11].
phosphatidylethanolamine [SH11a, TSW11].
phosphatidylglycerol [BH12].
phosphatidylinositol [GZ10].
phosphatidylethanolamine [SH11a, TSW11].
phosphatidylethanolamine [SH11a, TSW11].
phosphatidylglycerol [BH12].
phosphatidylinositol [GZ10].
phosphatidylethanolamine [SH11a, TSW11].
phosphatidylethanolamine [SH11a, TSW11].
phosphatidylglycerol [BH12].
phosphatidylinositol [GZ10].
phosphatidylethanolamine [SH11a, TSW11].
SHL⁺18, SLX⁺15, ŠSB⁺16, SJC11, SGHL13, VCL18, YB16, ZL11.

**powdered** [KB16].  **Power** [Min18, LZL⁺15a].  **powerful** [CAT⁺13, HMO⁺18].  **powers** [WZ17].  **pp** [CD19, Spr10].  **PPI** [RMRBH⁺19].  **PPI-Detect** [RMRBH⁺19].  **PR** [TTB⁺10].  **Practical** [GR10b, SLG15, BB11b].  **pre** [RLDJ17].  **pre-computed** [RLDJ17].  **preadsorbed** [KD10].  **prebiotic** [SSNT19].  **precatalyst** [MJLV14a].  **precatalysts** [MJLV14a, MJLV14b].  **precision** [DH17, MLC13, SWW⁺19].  **predict** [ASMS10, CBH14, DLC18b, HWB19, LLvG10, LLSW14, SEF⁺16, SPZP18a, WJG⁺13].  **predictability** [BBOB16].  **predictable** [GDV17].  **predicted** [DWL11, LZW⁺11, TYX⁺18, WKLC12, YZ16, Zha12b, ZWX19].  **Predicting** [AS14, AS18, BVHI17, BPB11, cCVG⁺14, CPK19, ELKE19, GC18, GRL⁺11, JGS⁺17, Jor17, LZSM19, LDH⁺14, PGdO⁺16, RDF⁺11, SJWE10, TYX⁺18, VL19, YZ15a, DBM⁺17, Kar17, KTO13, RB13b, SMDP18, SIG⁺11, WCDM11, Yon16, Zha12b, Zha12a, ZLX⁺13, ZYS⁺10, GRL⁺12].  **Prediction** [Ano12u, AIM⁺18, CP15, CQFC10, FSD⁺18, HZSS17, KPL⁺15, LDZW17, MCAG⁺16, vOaCG10, PRP15, SRA17, SPL⁺18, WDL12, YHW17, ZYL⁺12, AGM⁺13, BLDK⁺13, Ben17, BddS13, BA11, CZAF17, DWL11, DDP16, EOA⁺11, FZY⁺12, GK10, GFPSD17, GTZ⁺18, HLS⁺13, HPL⁺18, HYMZ16, HL14, JSW10, KL14, KT10, KTO11, KB19, LXL⁺11, LMI⁺14, LZL⁺15a, LZZ14, LH11, LWL⁺10, LSH⁺11, MDT10, Mau14, MG11, MSÅK12, PML⁺12, PN13, PPJ14, PLV⁺11, RCR⁺16, RMRBH⁺19, RKB⁺14, SM11, SYH12, SSD19, TYZ⁺16, VKC10, WLF11, WH11, WXS⁺12, WXL⁺12, WWW18, XFTW15, YVEI⁺17, YLCX10, YHH⁺13, YDX16, YDGZ15, ZsA10, wZbZ11, ZvI13, ZLW10, ZHIX11, ZDW18, MSP19, SDIP18, VVL17].  **predictions** [ALK⁺15, BCP⁺10, CLA16, CS17, EOO⁺16, GAI13, KZK⁺12, PdSC18, RDDS10, RCM⁺13b, SHMO11, SA10, WZWW18].  **predictive** [LLL⁺10, WKC11].  **predictor** [CDS16].  **predictors** [GHK12].  **predissociation** [YB11].  **Preface** [GS18].  **preference** [DSHLM18, LK18].  **preferences** [FCOGM12, LGL11].  **preferential** [TKYN17].  **preorganized** [CM16].  **preorganized-interacting** [CM16].  **preparation** [JSD⁺11].  **present** [Cas14].  **presenting** [ZGZ19].  **preserving** [ZBG11].  **Press** [CD19].  **Pressure** [YAO18, AYYO17, Cam15, CCCR18, FCW⁺14, HYNS19, HRHI17, I18, LLL⁺12, MO17, NFDP13, SMM⁺18, SPZP18a, WDLG12, CCR18].  **pressures** [RHNN10].  **primary** [ALK⁺15, GAI13, VVLG17, KTN11].  **prime** [DSX⁺11].  **prime/MM** [DSX⁺11].  **primitive** [HAL14].  **principal** [PSP15].  **Principle** [WBKS19, CCJC10, DBM⁺15, LLB⁺12, MCF10, SBGP18, Tak11, YPvD13].  **Principles** [HFSO12, BE12, BE14, BPE16, EMD17, EB12, EBK13, EBPK17a, EB18, GD10, HYL⁺11, Ibr17, JCC⁺11, KLZ⁺18, LLLL11, LCWW10, NNS15, OC19, PLZ17, RZG⁺13, SFA17, SPZP18a, TZ11, UGK18, WYL⁺15, WD10, YR13, wZbZ11, Zha12b, Zha12a, ZWMW10, ZZ12, vADC⁺14, THI⁺19].
properties [SCF+19, SB11, SIT18, SLIB12, SWMW10, SZB19, SZZ+18, SIG+15, SGH+16, TN12, TFQ+10, TFQ+11, TS11, TS15b, VVW+18, VPR10, VECT12, WLC12, YW12, YCGA10, wZbZ11, ZYG+15, ZWMW10, ZB18, ZLX+13, ZBP11, ZYLX12, ZBB19, FDCJG18, SFCCK15].

property [CD13, GPS10, GBS+17, GWX+12, PH15, V˚AA14, WH11].

propionate [TN10].

propionic [CM16].

Proposal [PRYI+17].

proposed [GS11].

protease [DLZ15, NHN16, OBW12, SYH12].

protective [JAH+17].

Protegrin [RI10].

Protegrin-1 [RI10].

Protein [CIKT13, CDS16, CPK19, DPOS16, GPS10, HNTS15, HS16b, JL19, LZGS11, MFEM15, MFR10, PGL+15, Ran12, RP15, Rao11, SHMO11, SKKS13, YBS19, AIGP15, AKK+16, AM10, AG12, BSZ+12, BFH+13, BPB11, BPC13, BCG10, Bow16, BDds13, BA11, CSC+18, CZA17, CFC15, CHR+12b, CHR+12a, CM13b, CCYL11, CKP10, CH14, CC12b, CBG16, CHP11, DWL11, DJ13, DVVP14, DLMH12, ESD18, FZY+12, FHW+11, FCE15, FLM11, FSC+14, GS14, GDV17, GMSdG15, GRP+12, GZ14, GRL+11, GRL+12, HAGK10, HNNR13, HMO+18, HTS15, HTS17, Has14, HZY+10, HPL+18, HKR12, HYMZ16, HJ10, HHHY10, HM13, HZ13, HQSZ19, ILKR11, IHY15, JZ12, JZZM14, JLZ+17, KYT+17, Kan15, KNE11a, KOY+12, KL14, KERY+16, KJ10, KTO11, KTO13, KDT+12, KLS10, KMLS10, LS11a, LFB14, LHL+10, LH11, LCPS13, LC16, LC17b, LZ11, LL+10, LL10b, LFM12, LPS+13].

protein [LZZ14, LLLC11, LHH11, LBS10, LMI18b, LL19b, LDH+14, MS17, MMM+16, MJC14, Mau14, MUGNVJ+18, MA17, MFEM15, MS16, MP11, MKB+13, MOS12, MNNK10a, NSK18, NST14, NS11, NFG+13, NG10, OHNK11, OCL11, CKP10, CH14, CC12b, CBG16, CHP11, DWL11, DJ13, DVVP14, DLMH12, ESD18, FZY+12, FHW+11, FCE15, FLM11, FSC+14, GS14, GDV17, GMSdG15, GRP+12, GZ14, GRL+11, GRL+12, HAGK10, HNNR13, HMO+18, HTS15, HTS17, Has14, HZY+10, HPL+18, HKR12, HYMZ16, HJ10, HHHY10, HM13, HZ13, HQSZ19, ILKR11, IHY15, JZ12, JZZM14, JLZ+17, KYT+17, Kan15, KNE11a, KOY+12, KL14, KERY+16, KJ10, KTO11, KTO13, KDT+12, KLS10, KMLS10, LS11a, LFB14, LHL+10, LH11, LCPS13, LC16, LC17b, LZ11, LL+10, LL10b, LFM12, LPS+13].
python [SH19b, HPT+16b, LRvE17, PHH+12, SHFJ18, TBJ18, Yes15].
Pytim [SHFJ18]. PYX [LWWG12].

Q [WPM+15, BS10c, GKV+13]. Q-CHEM [GKV+13]. Q-Dock [BS10c].
Q2MM [LN15]. Q5 [REL+14]. Q5/D5Cost [REL+14]. QB3 [KG15]. QC
QikProp [LP11a]. QM [BM12, Lun12, RSR+12, PLP+16, AALCM11, BH13, BZH14, CBG17, CJZS10, DSK17, FRC18, FLM11, FPB12, FB14b, GRS15, GWZ15, GCW14, HH15, HYUS11, HBR17, JHH+13, JWST10, Kid19, KTNN10, KWL+16, KWG15, LZdL+10, LFM12, LT13, LHT15, LJJ+11, MCR17, MTvG12, MJG+15, NO16, OYK+11, PMC+17, PP10, PDMT10, PL14, PLP+16, RR14, RR12, SN16a, SGDT10, SJ14, SCM+15, STM+15, SSAS10, TSC+13, UTM11, VKNT15, VKNT16, VCM15, VTKRJ15, WDP+12, vRET19, GRS15, JAHS+19, LWZ+19, RFN15, ZZY+16].
QM-only [LT13]. QM/ [GRS15, JAHS+19, LWZ+19, RFN15]. QM/EFP
[CBG17]. QM/MM [BM12, RSR+12, AALCM11, CJZS10, DSK17, FLM11, FPB12, FB14b, GWZ15, GCW14, HH15, HBR17, JHH+13, JWST10, Kid19, KTNN10, KWL+16, KWG15, LFM12, LT13, LHT15, LJJ+11, MCR17, MTvG12, MJG+15, NO16, OYK+11, PMC+17, PDMT10, PL14, RR14, RR12, SN16a, SGDT10, SJ14, SCM+15, STM+15, SSAS10, TSC+13, UTM11, VKNT15, VKNT16, VCM15, VTKRJ15, WDP+12, vRET19]. QM/MM-QMC [UTM11].
QM/MM-type [Kid19].
QM/QM' [PLP+16]. QMC [UTM11]. QMX [KKR+13]. QSAAR
[GKR13, Ray13, AKMT11, BF15, CLX+10, FCL+10, GMMH+16, GCP+13, GCC14, LLL+10, LZdL+15a, MdOdQ18, PKIC11, PPUBGD10, RK11, TTB+10, TLL+12, WMW+10, ZDW18]. QSAR/QSPR [CLX+10, GCC14].
QSARINS [GCC14]. QSARINS-chem [GCC14]. QSPR
[CD13, BRNG12, CLX+10, CD13, CD16, GCC14, KKO+16, TTR+12, XWW+11, YMY+19]. QTAIM
[BH13, BZH14, FCOGM12, FCPJM14, GMBX+16, HXM+16, JMX+16, diRL11, Rod13, RSKG14, VV15, Wei12b, WvRSM14, XFX+16, ZZZ+12, ZCWX18, dLC18a]. QTAIM-
[VV15].
QTAIM-based [FCOGM12, FCPJM14, Wei12b]. quadrupolar
[CSEMB+16], quadrupole [HBKL10, LIRL+16], quadrupoles [NLP+16].
Qualitative [YK13]. Quality [CLK11, KCK+17, KYB13, LOB18, MCF+18, MKB+13, OLB19, POB13, RB13a, RCM+13b, SC15]. QuanPol
[TSC+13]. quantification [Fer17, Ham11, PC14, SKGP19, YNH+17]. quantify
[LLHM16]. Quantifying [TMJ15, GMBX+16, MS10]. Quantitative
[DZA11, RDT14, VAA14, Wei12b, BPC13, CD13, DKL+10, NPG+18, NFG+13, REL17, RCM+13b, XFTW15, TTB+11]. Quantized [KKGW19].
Quantum [ALK+15, AC11a, APA+14, Chu10, CG12, DDM+15, FRN15, GH10, HHD16, JCHT18, KASH14, Li14a, Li14b, IWD13, MM18, Mat18, MBRC16, MS12, NNT+19, NN19, OKY18, RFN15, SCOJ13, SAGC16, SBD+17, SOY12, SR10, SHB17, TR12, UD12, VP19, VSP19, WCAH10,
WDP+12, YHX19, Aki16, ATP18, ASS+17, ARAG17, AAC+16, APY+16, ACS12, ASK18, ALH+10, Bac12, BTT10, BRP+12, BGR13, BEL+11, Cam15, CBH14, CDM10, CDB10, CDBM11, CD13, CD16, CDC19, CXW14, CHK10, CSNCS+18, CM16, CKG18, DR11, DKT13, DDP+18, DPAB16, Dra19, ECZWD17, EV14, Fer13b, Fer13a, FB10, FFA14, FC18, FLM11, GPM17, GMMH+16, GTK10, GGM+12, HZ11, HSN+18, HLvdV13, HPT+16b, HGCCGR+16, HMM10, HYUS11, HGY15, JBB+11, JSXH16, KP11, KNR+18, KVR10, KKH18, LPE+10, Lüe14, Man19b]. quantum [MP17a, MAPB10, MSvG12, ME10, MSSP17, MHRR11, MFR+11, NC13, NC14, NNK+16, NDD+10, NHK+13, NS17, OKIS17, OSR16, PML+12, PNE18, PSC11, PGW+17, PAMG16, RLLHL12, Rez19, REL+14, SLT14, SKA19, SS13b, SPZP19, Tae9, Ts18, UDK+18, VPR10, VBMA13, WKC+10b, WBT10, WLLH18, WAB17, XCLZ19, YKO+11, YLS19, YW13, YKH15, ZVY+15, dCDP15, BLG10, OSI+19, SKA19].

Quantum-chemical [KASH14, FB10, MSvG12, MFR+11].
Quantum-chemistry [DDM+15].
Quantum-classical [HLvdV13, SKA19].
Quantum-mechanical [ACS12, ECZWD17, PGW+17, Rez19].
question [YLT+19].
quasi-planar [YLT+19].
Quasi-classical [YLT+19].
quasiclassical [YLT+19].
quaternary [DSHLM18].
QuBiLS [GJMPAM+14].
quest [AOW11, EK17].
question [BZH14].
questions [AAB+19].
quick [VVV+15b].
QuickFF [VVV+15b, VV18].
quickly [vW11].
quinacridone [HSZ+11].
quinoline [HRJ+14, HGHP14, HRJ+15, JRSH14, SSD19].
quinolone [ZCK+16].
quinone [GLM+17, VSD10].
quinones [uLhY11, SDIP18].
[KERY+16, HWLW11, MP11, PBG17]. Rapid [LJW11a, LW11, LAT11, MZZ11, MRR11, MSS+13, MFR+17, NO16, PG14, RZ16, TM18, JSW10, KLOS10, JK11, WBF17]. Rapidly [OPR16, RDRC16]. RAQET [HSN+18]. rare [HNS16, LRvE17, MP13, Sea10, STS15]. rare-gas [MP13, Sea10]. RASPT2 [BH19]. Rate [AR10, AAMD+11, CSNCS+18, NMLD13, CBH14, GAI13, GKR13, HSL+11, JW10, KB19, KCL+14, MSV16, MK17, MK19, NDW15, OZLSBH12, RAGLL11, Ray13, RKG11, SSC+19, STM17, TTR+12, ZSL+10b, ZLLL12]. rates [BL12, CSAdOM17, GRL+11, GRL+12, QB16, SHB17, WAB17]. ratio [AR10, APA+14, BK15, CYY+17, CSAdOM17, CXW14, CSNCS+18, FB12, GYX+10, GZL+12, GTK10, GKR13, GJ17, HS16, He13, HLJ16, ITP+19, JZ17, JLS+10, JW16, KV12, KV13, KB15, KSK11, KK19, LGOM+15, LZY+12a, LJW+11b, LZL+16, LW13, LPMT17, MTM14, MHT+18, MPPS11, MS10, MJLV14a, MJLV14b, MTS+19, MT19b, MB16, MMJ10, NH19, NMLD13, NM19, NTNY15, OSA19, OZLSBH12, PVL+13, PG18, PNE18, PXH1+14, QLY10, RAGLL11, Ray13, RLZ+18, RSL13, RRFV+18, RN17, RKG11, RSKG14, RSK+15, SLT14, SLT+15, SJD14, SRF+17, SBH+17, STS+10, SSB+19b, SM17, SM17, TAC17, Tak14, TN18, TNY18, TSJ+10, TDP+12, TCPPC14, Tsi17, VBD11, VV14, VGT16, VMT10, Wu10, WHDL11, WCL+11, XCLZ19]. Reaction [XBSS19, YHG+11, YJ11, Yu12a, ZYLL12, ZSZ+14, ZX19, ZYR+15, Zim13]. reaction-diffusion [RSLS13]. Reactions [CC18c, ATP18, AAMD+11, ABB+12, ABB+13, APA+14, Cam15, CC18a, CSXZ17, Chu10, DSD+11, DS12a, DGSGVM19, FB14a, FC16, FFA14, GAI14, GH10, GNDA+12, GMBX+16, GSMZ19, HLS12, HYUS11, HRL11, JZ17, JC+10, KG15, KZP+18a, LLH14, LGW12, LTL3, LXF17, LJ+11, MC10, MSV16, ORZ11, OSH17, RWR+13, RB12, SSC+19, ST13, Su10, SSS+14, TM18, TN18, TKXT13, TTR+12, Tsi17, UvSvdWK19, VKAM12, VKTRJ15, VGTL16, WLHZ12, WCDM11, WSWD19, XLYZ10, YZGS14a, YND+17, Yu12b, ZSL+10b, ZSL+10a, ZW11, ZLLL12, ZMW19, ZW17, dSDLBNB17, dCRN18, dSV+16, SMB18]. reactive [DMAH15, HJL16, IHJ+13, LvDH13, MB14, NB19, RLLHL12, TDP+12]. reactivities [WS11, WS12]. Reactivity [FHG+19, QQY+18, TS14, WBKS19, BCP+10, CRZ+18, CBDS19, DI11, DI11, DI11].
HGY15, JS17a, LZH16, MAPB10, OSF12, OM12, PML+12, PRYI+17, SIT18, Sti15, YB16, ZYR+15, ZT14. read [DDK14]. reader
Reannotation [YS10]. rearrangement
[HJL16, JW15, LvDH13, YpD13]. Recasting [RHRCH16]. receive
[JT18]. Receptor
[HK18, BHF+18, CV12, ESB13, FTW12, FRLN10, HYYZ13, ILK11, LZ11, LLL+10, OME16, PPJ14, SSP+13, VKC10, WC11, YZ16]. receptor-ligand
[FTW12]. receptors [DR14, SRA17, UU12]. Recognition
[ZDT18, CXS10, EPH+15, HS12, Hsu14, ISP+10, LG14, OME16, OOK11]. recognized [CDS16]. recognizers [uLhY11]. recombination
[DS12a, SL+17, ZZL19]. Reconsideration [MS11]. Reconstruction
recursive [RJR14]. Red [Jab14, CSC+18, MTS+19]. redesign
[CGBK13, HMO+18, SL10, PGL+15]. Redesigned [XHL16].
redistribution [JCGVPHT17]. Redox [LCB10, GLM+17, INT18, KPL13, LZY+12a, MLQ+12, MKO+13, TN10, Ts17]. Redox-induced [LCB10].
redox-switchable [MLQ+12]. Reduced
[BYE+16, BBL13, SWM10, SRR16, SL+17, VI17, WRG+17]. Reduced-cost [BYE+16]. reduced-size [BBL13]. reduces [ZIJZ13].
reducing [HAGK10]. reductase [BS16a, RKDM14, STM+15, SJ16, VSD10]. Reduction
[SST+18, TN19b, AS18, BS16a, GMPB12, KPL15, LDZW17, PN13, PSC11, RLZ+18, SIG+15, YJ11, ZGS+10]. reductive
[MRC+18, dCDP15]. Reevaluating [PKK17]. Reexamination
[CLK+11].
Reference
[AIQ19, Jia19, Ail18, FHZA+18, KGM12, LvGi13b, OZL12, SHF11, SMM15a, SMM15b, SMM+18, YN15, dLC17]. reference-free
[FHZA+18]. reference-modified [SMM15a, SMM15b, SMM+18]. references [EK17]. refined [KD18]. Refinement
[Lvg13c, BC10, BS10c, CM13b, FLM11, K18, LFM12, LZZ14, LGH11, OCL11, OL13, PN13, Vor10]. reflectance [DCOD13]. Reformulating [Pro16]. Refractive [MMS16].
regime [CSAOM17]. region [MtvG12, MNNK10a]. regions
[KIOY19, MP17a, Pol13, TZ12]. Regioselective [WDZN16, BCP+10].
regression [DCS15, LLL+10, RB13a, YNH+17, YDX16]. regular [SWA13].
Regularized [YNH+17]. regularly [NPP13]. regulated [PGI19].
regulators [FCL+10]. reHiSS [CHK19]. reHiSSB [CHK19]. reHiSSB-D [CHK19]. related [BP18, FCOGM12, GWX+12, LEdOLdlV17, NDD+10, SRA17, Tzck18, TY10, WvRSM14, SMB18]. Relating [EJ13]. Relation
[KTT16, CSKH16, HSN14, SBR13]. Relations [BMPML+13]. Relationship
104


respiratory [TN19b]. Response [GPGSM12, dSdS12b, BZH14, DSAS19, DHE^+12, ESM^+12, ITIN15, KSSH13, Kid19, KZK^+12, LP11b, MRB14, RJR14, RCM^+13b, SS16a, SDF^+17, WGLG^+16]. responses [GWX^+12, MLQ^+12], responsive [MA14]. restrained [ER18, HCD^+10, KCK^+17, SR18, ZDZM13]. restraining [KOV^+12].


resulting [MvBD18]. Results [XKW18, Ber17, CBH14, CLK11, GR10a, KERY^+16, PLAG11, RAR^+11, SHL^+13, SPZP18b, WDIH13, KMLS10].


rich [BHI19, ZZWX11, ZYL^+12, ZYW11]. right [SJWE10]. Rigid [NJR18, Aou16, AGRI1a, CZNA11, DBM^+17, HDL^+14, ODB18, PG14, PKG^+19, dACP12]. rigid-body [PGK^+19]. Rigid-CLL [dACP12]. Rigidity [NPG17, OXW16, PRSG13]. rigorous [WO15]. ring [ABDG12, CPN^+17, CB11d, FNSF^+11, GWT^+17, GMBX^+16, GSMZ19, HH10, HHI1, HCD^+10, LG19, PCL11, PLH16, SP13, WCL^+11, XVN17, YHCS11, ZQ419].


Robustness [VYM15, BD11]. ROCS [HP10a]. Role

S
[AM19a, AM19b, CXS10, DT19, GTK10, LWD13, PLFS18, SPS1+12, WGN1+16, WGLG1+16, XCLZ19, YZGS1+1b, ZYG1+14, PRRT1+10, AS11, Alg17, ATP18, DT19, HOM1+16, LGW12, MH11, MSCP19, MLY1+13, RWR1+13, TKXT13, TN19b, WJX1+10, WZZW18, YZGS1+1b, Yu12b, Yu12a, YZL1+15, ZYR1+15]. S-loss [MH11]. S-nitrosothiol [TKXT13]. S. [GKR13]. S100-family [TJR19]. S371 [MV17]. SA [OBW12, VM11]. SAC [EFAC13, FE14, IN13, MN19, PH10b, SRF1+17, SCF19]. SAC-CI [EFAC13, EFS16, IN13, MN19, SRF1+17, SCF19]. SAC/SAC [IN13]. SAC/SAC-CI [IN13]. saccharide [LABSG17]. Saddie [ZH19]. Sal [LBC1+19]. salen [DSHM18]. salicylidene [PLP1+16]. Salpeter [KK17b]. salt [EK15, IPA11, OCW1+15, PZA15]. salts [Ano11, DSHM18, HJM1+09, HJM1+11, LCL1+18, ZYL1+12]. samarium [AARP17]. same [CSKH16]. same-spin [CSKH16]. sample [HRID16]. sampled [AST1+16, CDM1+15]. Sampling [AKN16, JL19, Yan16, BLKP12, BH15, BG17, CY09, CY13, CF18, CS17, DPN11, DJ13, FM10, FB14b, GFPS17, GMO16, HH10, HKD1+12, HTS15, HNS16, HS17a, HYNS19, HKN1H18, HDM1+15, HCP15, IMK1+16, ISK14, Ish10, KvdV14, KJM1+17, KTO11, KB11c, LTT16, LC16, LC17a, LL11, LMI1+14, LZZ14, LAW1+16, MZZ11, MCR17, OL13, PBDW11, SSO19, SEM12, SBN13a, ...
sandwich [TS15a, WWKS16, YLT+19]. SBN13b, STM+15, TJB12, WTD+19, YZ16, ZZ14, ZC14, ZGZC19, DAB16].

SAPT [CLFRO18, DWR17, YJ17]. SAR [WPM+15]. satellite [ACD+13a, ACD+13b], satisfy [KSH13].

saturated [WDZN16, ZWX19]. Saving [FSSW17]. Sb [ATIP18, RDT14, SLY+19]. Sand: [WS16, ZWX19].

SSAP [CLFRO18, DWR17, YJ17]. SAR [WPM+15]. Scale [XFG+16, YKNN19, AH10, CK18].

satisfied [KSH13]. saving [FSSW17]. Scents [DR14]. Schiff [GA18, SC18b, WGA18, ZLHH14].


Scope [KMS+19]. scores [LZZ14]. scoring [FM10, GSHM10, GZ14, HS11, LH017, PH11, Pro16, RZG+13, TO10, WZ17]. scoring-docking-screening [WZ17].

screened [KH17]. screened-exchange [KH17]. screening [AKMT11, CV12, GRP+12, Hei10, JBAM11, KD18, KC14, KB14b, LG11, LMA15, MNNK10b, MH10, SDF+17, WZ17, Won18, YLFX10, YZZ16].


Schemes [CSM16, Hes19, KYB13, LPLA13, MC12, WOH18, WDW12, XSL11]. Schiff [GA18, SC18b, WGA18, ZLHH14].


Scope [KMS+19]. scores [LZZ14]. scoring [FM10, GSHM10, GZ14, HS11, LH017, PH11, Pro16, RZG+13, TO10, WZ17]. scoring-docking-screening [WZ17].

screened [KH17]. screened-exchange [KH17]. screening [AKMT11, CV12, GRP+12, Hei10, JBAM11, KD18, KC14, KB14b, LG11, LMA15, MNNK10b, MH10, SDF+17, WZ17, Won18, YLFX10, YZZ16].


Schemes [CSM16, Hes19, KYB13, LPLA13, MC12, WOH18, WDW12, XSL11]. Schiff [GA18, SC18b, WGA18, ZLHH14].


Scope [KMS+19]. scores [LZZ14]. scoring [FM10, GSHM10, GZ14, HS11, LH017, PH11, Pro16, RZG+13, TO10, WZ17]. scoring-docking-screening [WZ17].

screened [KH17]. screened-exchange [KH17]. screening [AKMT11, CV12, GRP+12, Hei10, JBAM11, KD18, KC14, KB14b, LG11, LMA15, MNNK10b, MH10, SDF+17, WZ17, Won18, YLFX10, YZZ16].


Schemes [CSM16, Hes19, KYB13, LPLA13, MC12, WOH18, WDW12, XSL11]. Schiff [GA18, SC18b, WGA18, ZLHH14].


Scope [KMS+19]. scores [LZZ14]. scoring [FM10, GSHM10, GZ14, HS11, LH017, PH11, Pro16, RZG+13, TO10, WZ17]. scoring-docking-screening [WZ17].

screened [KH17]. screened-exchange [KH17]. screening [AKMT11, CV12, GRP+12, Hei10, JBAM11, KD18, KC14, KB14b, LG11, LMA15, MNNK10b, MH10, SDF+17, WZ17, Won18, YLFX10, YZZ16].


Schemes [CSM16, Hes19, KYB13, LPLA13, MC12, WOH18, WDW12, XSL11]. Schiff [GA18, SC18b, WGA18, ZLHH14].


Scope [KMS+19]. scores [LZZ14]. scoring [FM10, GSHM10, GZ14, HS11, LH017, PH11, Pro16, RZG+13, TO10, WZ17]. scoring-docking-screening [WZ17].

screened [KH17]. screened-exchange [KH17]. screening [AKMT11, CV12, GRP+12, Hei10, JBAM11, KD18, KC14, KB14b, LG11, LMA15, MNNK10b, MH10, SDF+17, WZ17, Won18, YLFX10, YZZ16].


Semiempirical [FA18, SRL +15, BP18, GJK +19, GP11a, HGY15, KTN10, KB14b, LSD +10, MGWR12, Rez19, SPH11, SDL14, TKNN10, TG12a, UCFR16, WCWV15].


separation [CSKH15, DS12a, NMH19, VCL18, VL17b, YSG12]. Sequence [TYZ +16, DLY +10, DWL11, HPL +18, LXL +11, MP17b, RMRBH +19, Sti15, TXY +18, WXL +12, YZWC11, YS10, ZWP11, HYMZ16]. Sequence-based [TYZ +16, RMRBH +19, WXL +12]. sequence-reactivity [Sti15].

Sequence-specific [HYMZ16]. sequences [AnO12u, CCYL11, Fel10, HZY +10, LMZ +11b, LLLC11, LDH +14, OLA15, QLQ11, YDL +10].

[SN16b, BLL13, BLG10, BRLS08, BRLS12, CC11, HS16b, KNP+12, LS11a, LLC+10, LYC+13, LZ18, LWL+10, Mat10, OAN15a, PML+12, PGdO+16, PHK14, PD11, Pog10, PFVL14, RLD12, SPS+12, Sch13, SWM10, SG10a, SG13, VLGK+17, VVLG17, WX12, YOMT14, ZPP+16, FL15]. Sets
silicon-doped [TN12].
silicon-germanium [GSMM15].
Silver [NSN19, Tsu19, YXZZ17].
silylene [BIL10].
Similarities [PM18a].
Similarity [HS12, LMZ+11b, YDL+10, CDR10, CDB10, CDBM11, CDC19, CQFC10, GWT+17, GK15b, HRK+10, HKRS11, HS11, HSW+19, RMPAM15, TZCK18, YZZ16, ZYvIZ14].

Similarity/dissimilarity [YDL+10].
SIMONA [SWB+12].
Simple [Ano15-59, CNK97, GM17, MPSA17, AB16b, BS10b, BD12, CWZB10, KRTB10, NSP15, PHC13, PRIY+17, RHRCH16, RGVC+19, SEF+16, SS13c, YS18, dSAdSL13, KTSW11].
simplified [KOY+12].
simplify [BLZ+13].
simplifying [BL19].
SIMPRE [BCSCJ+13, BCJC+14, KR14].
SIMPRE1.2 [CSEMB+16].
simulaid [Mez10].
simulate [SLX+15].
simulated [LBC+12, MO15, LVG10, MO17, NPTS16, RHJ11, SHMO11].
simulating [HIS17, SS13c, FHT+15, PVM10, SA10].
simulation [ZSS+13, ZKH+10, ZLL+13, dCLFGL13, SGP18].
simulations [OCL11, OLY17, OCW+15, PGY15, PH17, PL19, PW17, PL14, PM13, PS13, PS10, PNG10, RD18, RdA12, RLG14, RSRR15, SSO19, SBV10, SKA19, SS13b, SHFJ18, SBT17, SIK10, SCK18, SJ17, SMP17a, SYN+12, SK13, SFLG+17, SB15, SWB+12, SMDS13, SPM+19, SV11, VSA11, VINTERJ15, VM11, WKL12, WAM17, WH11, WWSK11, WLC12, WBF17, WS19, WGI14, Won18, WCJ+14, XFG+15, XWSW13,
YKO$^{+11}$, YO$^{19}$, YSG$^{12}$, Yon$^{16}$, YHVM$^{12}$, YFH$^{+19}$, ZZY$^{+16}$, ZDKM$^{12}$]. simulator [BSL$^{11}$, KJM$^{+17}$, RLLHL$^{12}$, TCX$^{+13}$]. simultaneous [LL$^{10b}$, WZWW$^{18}$]. Single [HPL$^{+18}$, LP$^{11c}$, PM$^{18b}$, SR$^{18}$, Zim$^{15}$, AS$^{15a}$, BE$^{14}$, BP$^{18}$, BK$^{17b}$, Den$^{12}$, FTR$^{15}$, GCCM$^{15}$, KK$^{17a}$, KGJZ$^{19}$, LXL$^{+11}$, MS$^{19}$, MT$^{19b}$, MCLD$^{10}$, MEH$^{18}$, PBE$^{16}$, RHNN$^{10}$, RLDJ$^{17}$, SY$^{16b}$, SPM$^{+19}$, TSR$^{+16}$, VS$^{14}$, WLW$^{+10}$, WYL$^{+15}$, YZN$^{13}$]. single- [BE$^{14}$]. single-bond [GCCM$^{15}$]. single-configuration [MT$^{19b}$]. Single-ended [Zim$^{15}$]. single-excitation [MEH$^{18}$]. single-file [SY$^{16b}$]. single-ion [BP$^{18}$]. Single-pass [SR$^{18}$]. single-sequence-based [HPL$^{+18}$]. single-step [RLDJ$^{17}$]. single-vibronic-level [MCLD$^{10}$]. single-wall [KGJZ$^{19}$, TSR$^{+16}$]. single-walled [AS$^{15a}$, PBE$^{16}$, VS$^{14}$, WYL$^{+15}$, YZN$^{13}$]. singles [EK$^{17}$]. Singlet [NNT$^{+19}$, SZL$^{19}$, BSDP$^{16}$, HWB$^{19}$, ISO$^{+13}$, RS$^{17a}$, SSC$^{+19}$, THP$^{+15}$, TCPPC$^{14}$, ZZL$^{19}$]. singlet-triplet [RS$^{17a}$]. Singlet/ [ZZL$^{19}$]. singular [Les$^{19}$, SG$^{10a}$]. singular-value [Les$^{19}$]. SiO [DOM$^{+11}$, HEM$^{+17}$]. SiOH [LvDH$^{13}$]. SIPs [KCC$^{+18}$]. Site [CH$^{14}$, LJW$^{+11b}$, CVG$^{14}$, DAP$^{+18}$, GEP$^{+14}$, GPdC$^{+16}$, HL$^{14}$, ISP$^{+10}$, LLB$^{+12}$, LKZM$^{18}$, LLL$^{+12}$, MP$^{13}$, MNNK$^{10a}$, OHP$^{+17}$, OHPR$^{+18}$, RLDJ$^{17}$, SHF$^{11}$, SB$^{11}$, SC$^{18b}$, TYN$^{15}$, ZLX$^{+13}$]. Site-directed [CH$^{14}$]. site-identification [RLDJ$^{17}$]. sites [AIGP$^{15}$, Ano$^{12u}$, DVVP$^{14}$, DBK$^{17}$, JAHS$^{+19}$, KDT$^{+12}$, LZTV$^{10}$, LHL$^{+10}$, LL$^{10b}$, LZX$^{16}$, LG$^{14}$, MA$^{+16}$, PHC$^{13}$, PGB$^{17}$, TYZ$^{+16}$, TYX$^{+18}$, Vor$^{10}$, YZ$^{15a}$, YHI$^{+13}$, ZZL$^{+12}$]. situ [JZL$^{+17}$, LZY$^{12b}$]. six [DOM$^{+11}$, Xh$^{15}$]. Size [NNT$^{+19}$, Tak$^{18}$, AS$^{15a}$, BLBG$^{+13}$, BD$^{12}$, CC$^{12a}$, CF$^{14}$, DJX$^{+11b}$, FE$^{14}$, GZZ$^{12}$, Hsu$^{14}$, MTVG$^{12}$, SL$^{17}$, SB$^{11}$, XYX$^{17}$, Zha$^{11}$]. Size-guided [Tak$^{18}$]. size-modified [BD$^{12}$]. sized [LRV$^{+17}$, OGL$^{10}$, RK$^{15}$, WWD$^{14}$]. sizes [Lin$^{18}$]. SKATE [FM$^{10}$]. slab [BBG$^{+18a}$]. Slater [Dil$^{15}$, LRER$^{13}$, MY$^{+17b}$, SFG$^{+17}$]. Slater-function-based [SFG$^{+17}$]. Slater-type [Dil$^{15}$, MY$^{+17b}$]. slices [AKN$^{16}$]. slicing [KCC$^{+18}$]. SLIM [SSBW$^{14}$]. slit [Fom$^{13}$]. slope [Zha$^{12b}$]. Slowing [SGP$^{18}$]. SM [XMSZ$^{16}$]. SM-TF [XMSZ$^{16}$]. Small [XYW$^{+14}$, ASS$^{10}$, BTMS$^{12}$, BLKP$^{12}$, BS$^{16b}$, CQFC$^{10}$, DT$^{19}$, DGL$^{+13}$, ETL$^{17}$, GAMAC$^{+14}$, GBFD$^{12}$, KKPT$^{11}$, KGHK$^{12}$, KL$^{+17}$, KB$^{11b}$, LK$^{13}$, LHKS$^{12}$, LH$^{14b}$, Man$^{19a}$, Man$^{19b}$, MSS$^{+13}$, MBE$^{16}$, MBRC$^{16}$, MPBJ$^{11}$, NHH$^{16}$, RLL$^{+10}$, RSG$^{18}$, RS$^{13}$, SG$^{13}$, STS$^{15}$, TNY$^{18}$, VT$^{14}$, WF$^{16}$, WTH$^{+16}$, XMSZ$^{16}$, ZCGM$^{11}$]. small-molecule [ETLS$^{17}$, WF$^{16}$]. smaller [MCK$^{17b}$]. smallest [PMT$^{16}$]. SMD [ALK$^{+15}$]. smeared [ENKK$^{+17}$]. SMILES [TTB$^{+10}$]. SMILES-based [TTB$^{+10}$]. Smoluchowski [KS$^{18}$, SG$^{10a}$]. smooth [AG$^{11}$, EFS$^{16}$, JLCA$^{17}$, ZSB$^{+16}$]. smoothed [LZ$^{12}$]. SMPPS [XYX$^{17}$]. Sn [MCK$^{17b}$, PMG$^{+16}$, RDT$^{14}$, YW$^{12}$, ASS$^{10}$, PKK$^{17}$]. SnCl [dSDdAR$^{10}$]. SnO [DHE$^{+12}$]. Sodium [KLN$^{16}$, OC$^{19}$, TFYO$^{19}$]. Soft [SJC$^{11}$, WBKS$^{19}$, Ben$^{17}$, BG$^{12}$]. Soft-core [SJC$^{11}$, BG$^{12}$]. Software [AIGP$^{15}$, Aki$^{16}$, APK$^{14}$, AAC$^{+16}$, BTA$^{+13}$, BHB$^{12}$, BCSC$^{+13}$, BS$^{+12}$, Ber$^{17}$, BPJ$^{15}$, BFH$^{+13}$, BBG$^{+18b}$, CBH$^{14}$, CSEMB$^{+16}$, CZAF$^{17}$, CAT$^{+13}$,
CPK19, DMN15, DJD12, DVVP14, DBDP16, DDK14, DWC17, DSK17, ESB13, EWK+13, FN12, FSC+14, GMSdG15, Gar12, GJMPAM+14, GLW13b, GS12, GCP+13, GCC14, GBW+14, GH16b, HLS+13, HBR+17, HDH12, HPT+16b, HPSK12, HHT+13b, HH16b, HG13, HYMZ16, HKR+14, HBJ+17, HL14, HC14, IGK16, JHJ+13, JJW+14, JLCA17, JP15, JCGM18, KS13a, KS15, KK17a, Kan15, KR14, KB16, KKR+13, KDR+18, KLJ+17, KJM+17, KDT+12, Kos16, KG13, KWL+16, KK17b, KGW15, KSD+12, KYG+15, KAG+12, KSW16, KPF+15, LPS12, LJJR+12, LHSH12, Lhe15, LRvdSM15, LRvE17, LDB+17, LLZA12, LBB+15, LWZ+17, LC12, LAS+14, MHT+18, MDT16, MBR+15, MYT18, MSSP17, MB14, MB16, NKJ16, OV14].

Software
[OPB+12, OZS+13, OC14, PSS14, PGL+15, PSG+17, PW12, PPM15, PHH+12, PVZ13, PG14, RLLHL12, RNSF+16, Rast17, Řez16, RR14, RdA12, RSR+12, RCM+13b, SM14a, SFG+17, SK15b, SWA13, SMRM+17, She12, SC15, Sie15, SJ17, SvlK18, SJL18, SWB+12, SDMS13, TNYN16, TSC+13, TTR+12, TTL+12, UU12, VMRSH+17, VV+15b, VAR12, VB13b, WDdN12, WY13, WPM+15, WF16, We12d, WHH+12, WJ1G13, WG14, WCJ+14, XML+15, XYX17, YYJ+16, YYZ16, Yes12, Yes15, YHH+13, ZFS19, ZDKM12, ZLL+13, dVAG16, CCC+11, DBF14, EdOdS18, FRC18, HSW+19, MSvG12, MJG+15, SF18, SVB10, SGM+13, Yap11, ZCS+15, She12].

softerwares [All11]. solar [ACS12, DGL+13, JYS+12, LZZ+15a, MP19a, SLC+17, TZ12, VÁA14, YJN+11]. Solid [MP19b, RSK+15, ASS10, ASK18, CL16, HLS12, HBI+17, KLN12, KKH18, LOB18, OLPB19, POB13].

Solid-state [RSK+15, HBI+17, KLN12, KKH18, LOB18, OLPB19, POB13]. solids [BK11, BPC19, HAI+16, MDT13, MS15, dRL11, PON11, SNI6a]. Solubility [MSY19, KKO+16, WZW18]. solubilization [TFYO19].

solute [BRLS08, BRLS12, EOA+11, RVM19, TKT11, YKO+11, Yan11].
solute/solvent [RVM19]. solutes [GC11, PAK15]. Solution
[Cam19, PK19, AvKSP16, AK10, DR11, DBM+17, DP15, EOAO+11, GAI13, GA14, HDK+12, HAL14, HNN+17, KSI8, KTNNO10, KVR10, LVMG10, MM+17, MFM+12, PMC+17, PGW+17, SJWE10, TKNN10, UCF16, WHL+10, WC13, WLF19, XTG+11, ZLL+10, ZZ10, vADC+14]. solutions [Ber17, CFC15, EK15, Kri10, OC19, OCW+15, SM14a]. Solvate
[Jia19, RNSF+16, ZBP11, ALRM18, CBG17, CBG16, FGM11, GMHM+16, GP12, HRC13, JMLL13, JGS+17, Jor17, KSK11, LP11b, MS13, MPSA17, MBE16, NW17, OBW12, PL14, RK16a, RK16b, SM14a, SK12, SY11, SMM15a, SMM15b, SMM+18, TKYN17, TCC+13, WXL17, WWW18, YOMT14, YAS13, Yan14, ZCS+15]. solvation-free-energy [SMM15a, SMM15b]. solvational [FCL+10]. Solvatochromic [MK15].

Solvatochromism [TKYN17]. solve [PNW+16]. Solved [CD19]. Solvent
[KC13b, PK19, AKK+16, BEM14, BRLS08, BRLS12, CAD16, CBG16, EK15, FZY+12, FD16, GA19, HDL+17, Has14, HPL+18, HYUS11, JKDB12, KB11b, KCMPMG12, LHL+10, LC17b, LZZ+16, LWZ+17, MBC11, MBC13, MS11, ML14, MCU15, MCC12, MNK10a, MNK10b, PDMT10, PS13, QQY+18,
RVM19, RdA12, RRK16, SLT14, SBV10, SK17, SLX+15, SYH12, SCMA+17, SKMS13, TYN15, WWKS11, WXL+12, WBF17, YOMT14, Yan14, YJ11, BK17a]. **solvent-dependent** [HYUS11]. **Solvent-driven** [KC13b]. **solvent-induced** [AKK+16]. **Solvents** [LHT15, ISO+13, Pie14, Pog10, RK16a, RK16b]. **solvolyis** [OSS10]. **SOMA** [BMFG16]. **Solvants** [LHT15, ISO+13, Pie14, Pog10, RK16a, RK16b]. **solver** [FBY+17, FHMB15, Kan15, RR19, SHF11]. **solvers** [GRARO+14, WL10, XYX17]. **Solving** [KV13, SG10a, BYE+16, GA14, RRFV+18, SK15a]. **Song** [JW12]. **Soon** [Ano16-75, Ano16-80, Ano16-81, Ano16-82, Ano16-83, Ano16-84, Ano16-85, Ano16-86, Ano16-87, Ano16-88, Ano16-76, Ano16-77, Ano16-78, Ano16-79]. **soot** [KAR12]. **SOP** [AKK+16]. **SOP-GPU** [AKK+16]. **Sorafenib** [GMASBF16]. **sorbates** [KB19]. **Sorting** [NMF+14]. **Source** [GMBM18, TCB16, Aki16, APK14, BZH14, CD13, FBY+17, HMO+18, HLS+13, HPT17, KSD+12, MLG18, PHT17, SMRM+17, XTG+11, Yap11, Yes12]. **Source-Function** [GMBM18]. **sources** [BK13]. **Space** [vRWGS17, ACD+13a, ACD+13b, AD10, Cas13, CH16, CXS10, Coh18, DK11, DSHLM18, FC18, GA14, GK15b, HB14, HP10b, HSB+11, JCGVPHT17, LMZ11a, LLFH16, LAW+16, MBFP15, NH19, NCT18, PDG+16, SS13a, SHL+11, SCSW13, TTN19, TJB12, WDHZ13, XTn18, YD17]. **space-group** [HB14]. **spare [JYS+12]. spacings [CD13, FBvdB18, TTN19, WM17]. sweeping [yOaCG10]. sparse [LK11, LDH+14, VZ14, YHH+13]. sparsely [CBP+15]. Sparsity [HNS16, BYE+16, RR11]. sparsity-exploiting [BYE+16]. **Sparsity-weighted** [HNS16]. **Spatial** [PTB+15, HAL14, MTvG12]. **SPC** [GM17]. **SPC/E** [GM17]. **SPC/E-I** [GM17]. special [Alg17, ZZZ+19]. **species** [MAK+14, MG11, OSS10, RHT+15, SSA+17, TCPCC14, Tsi14, VRKT19, WvRSM14, ZZ10, ZLY+16]. **Specific** [DHF+11, OHNK11, CIKT13, CCM15, GCCM15, HnyH19, HYMZ16, JZZM14, KR12, LHO17, LGL11, LXFC17, MCC11, MC12, SSSM15]. **specificity** [LJW+11b, LBS10, ZX11]. **Spectra** [PAK15, TT18, AMQ+14, BG17, DCOD13, EBPK17b, FD13, FF11, GWF11, GGM+12, GZZ12, HRH+17, KASH14, Kow11, LBC+12, LX11, MAK+14, MCLD10, MKK+19, NHF+10, PMC+17, PDMT10, PDG+16, RS17a, RJS17, SGD10, SB15, SR11, TYN15, TZCK18, TG12b, Tsi14, WGL12, WWD14]. **spectral** [Ano15-58, BH14, CBDS19, HRMAL+13, KZZ+16, NSO+14, QZM11, RLG11, SFDE16]. **spectrometer** [LBB+15]. **Spectroscopic** [SS13b, GK10, KDB13, Kop15b, NC13, NC14, TCPPC14, Tsi14, VRKT19, WvRSM14, ZZ10, ZLY+16]. **spectroscopy** [DMD+18, HDM+19, HPSK12, IY18, KNR+18, LLBO12, Lin18, NC12, OC19, WHK+12, FAS+18]. **spectroscopy-oriented** [HPSK12]. **spectrum** [BLF14, KCC+18, MN19, MLCD11, RDF+11, SLLL13, TSC+13, ZDX11].
spectrum-slicing [KCC\textsuperscript{+18}]. sped [IMSR\textsuperscript{18}]. speed [TO10, VM11, YD17]. speed-up [YD17]. speeding [AO10]. sphalerite [SBC\textsuperscript{+11}]. sphere [KT12, MH10, Pop18, TH13]. spheres [HS16b]. spherical [Ano15-58, BH14, YOPB16]. spherically [Vyb15, Vyb16]. spheroidal [ZBW10b]. spider [Che17]. SPILLO [DVVP14]. Spin [ATIP18, DSM\textsuperscript{+11}, JKS\textsuperscript{+16}, KM13, MLG18, SZL19, TT18, AB10, AMQ\textsuperscript{+14}, CSEBM\textsuperscript{+16}, CSS17, CSKH16, CAP17, FAA15, FD16, GP11a, KT19, KIOY19, KSK11, KKA\textsuperscript{+18}, LXF17, MG11, MCP18, PLFS18, PS17, RRK16, SFM14, SPHF\textsuperscript{+18}, SSB\textsuperscript{+16}, SH18b, TN18, TTn19, VFRAR16, VHS\textsuperscript{+19}, YB11, ZLHH14, ZZZ\textsuperscript{+19}]. Spin-component-scaled [KM13]. spin-coupled [SH18b]. Spin-driven [DSM\textsuperscript{+11}]. spin-flip [ZLHH14]. spin-forbidden [TN18]. Spin-orbit [ATIP18, JKS\textsuperscript{+16}, AMQ\textsuperscript{+14}, FAA15, FD16, GP11a, KT19, KKA\textsuperscript{+18}, MG11, MCP18, PS17]. spin-orbital [ZZZ\textsuperscript{+19}]. spin-polarized [SFM14, VHS\textsuperscript{+19}]. spin-rotation [KIOY19]. spin-spin [PLFS18, SPHF\textsuperscript{+18}]. spin-symmetry [TTn19]. SPINE [FZY\textsuperscript{+12}]. Spinor [CC12b, Bar14]. spins [ZR10]. Spiral [SK18]. Splitting [Rob13, EHSPT16, EHT19, FZL\textsuperscript{+19}, LL19a, OT12]. SPME [NLP\textsuperscript{+16}]. SPOT [YZZ16]. SPOT-Ligand [YZZ16]. spots [HQSZ19]. Spread [BEEL14]. squaraines [AMQ\textsuperscript{+14}]. square [HDL\textsuperscript{+14}, HGW18, ISK14, Tsi19]. squared [JMS13]. squares [BCCO10]. SR [ARAG17, WMW11]. SR-ZORA [ARAG17]. SrO [BL12]. SSC [LG11]. ST [JJW\textsuperscript{+14}]. ST-analyzer [JJW\textsuperscript{+14}]. STAAR [JHH\textsuperscript{+13}]. Stabilities [BF19a, ZLX19, BLDK\textsuperscript{+13}, SIT18, TFQ\textsuperscript{+11}]. Stability [BPPS19, CSM16, EK15, GWT\textsuperscript{+17}, LdSR16, Lin18, OME16, PP10, BPPS17, CSS17, CFC15, CM16, CB11d, DLT17, DLW12, GPK\textsuperscript{+16}, GC18, Ham11, HLB15, LTR18, LIHS12, MC10, MS15, PMG\textsuperscript{+16}, PAT\textsuperscript{+10}, Rab12, SGBP18, SY16a, SPZP18a, TN12, TKCN19, VP19, XFTW15, ZRCC11, ZWMW10, ZW10]. Stabilization [KSR17, BSDP16, DBK17]. stabilize [KG11]. stabilized [AHK\textsuperscript{+19}, KASH14]. stabilizing [MvBD18]. stable [NPTS16, PBDW11, ZDZM13]. stacked [ANH\textsuperscript{+11}, HVM12, LDH\textsuperscript{+14}]. stacking [HVM12, YZZ\textsuperscript{+17}]. stages [CBP\textsuperscript{+15}]. staircase [SK18]. Stalis [LI19]. Standard [DH17, BCJC\textsuperscript{+14}, MKO\textsuperscript{+13}, PNI13, RD18, REL\textsuperscript{+14}, SRR16, VVG13, WHK\textsuperscript{+12}, WGA18]. standing [TS11]. staple [SV15]. Star [MA17]. State [CCM15, FHH\textsuperscript{+19}, GS16, Kop19a, MP19b, TT18, YKNN19, Alg17, AR10, ASS10, BS15, BBI\textsuperscript{+11}, CSAdOM17, CH10, CV12, ESM\textsuperscript{+12}, F414, GS15, GBPC19, GCCM15, GA18, GPE13, HLS12, Hei18, HNWF07, HNWF12, HH16a, HH17, HBI\textsuperscript{+17}, HWB19, HZSS17, HBR17, JZ17, KT19, KLN12, Kop15a, Kop15b, KKL\textsuperscript{+13}, KKH18, KCL\textsuperscript{+14}, LL15, LLBO12, LOB18, LZZL\textsuperscript{+10}, LFC17, MTM14, MPSG11, MCC11, MC12, MCLD10, NNY17, NMLD13, OBW12, OLBP19, OZLSBH12, POB13, PGW\textsuperscript{+17}, PHI10b, QZ10c, RAGL11, RIJ\textsuperscript{+11}, RCM\textsuperscript{+13a}, RML\textsuperscript{+15}, RR14, RGVC\textsuperscript{+19}, RSK\textsuperscript{+15}, SRF\textsuperscript{+17}, SSM15, Sie18, SGWA17, VZ14, VL17b, WHL\textsuperscript{+10}, WWW19, WHX\textsuperscript{+10}, XCLZ19, XBSS19, YWZ14, YD17, YJ19, YYT12, YL13, ZZZ\textsuperscript{+19}, Zim15].
state-of-the-art [YJ19]. state-selected [KCL+14]. State-specific [CCM15, GCCM15, LGL11, LXFC17, MCC11, MC12]. state-to-state [XCLZ19]. States [GBMB18, AST+16, ANH+11, BSL+16, BH19, DHOG13, DSV+19, EFS16, EK17, EVR18, EP15, FAA15, FD16, GO13, GA12, GTK10, HDHL15a, HDHL15b, HDHL15c, JCGVPHT17, KKH19, KT19, KKA+18, KPG18, KB14b, LLBO12, LLW12, LWW12, LGC19, LX11, LS11b, LYSS11, LCK+18, MS10, MN15, MGCC19, MH11, MEH18, PBDW11, RHRCH16, SRF+17, SSC+19, SOYC12, SMN+19, SB13, SB15, SZSS16, TN10, Tia12, TSN17, VVV+15a, XWSW13, YZGS14b, YK13, YLZ+10, YB11, ZX5+10, ZBB16, ZDT18, dLC17].


stringent [DPOS16]. strong
[Kan15, MLZZ12, SDF12, SS19, VVY17, Vik11, ZSL17]. stronger [KSC16]. Structural [ESD18, FHG+19, GLF16, GBL+11, GTT10, GAMAC+14, GWX+12, HS17a, II10, KZK+12, KSD+12, LBTV11, MP19b, NC14, TS11, VSH19, ZWW10, AIGP15, AD10, AKK+16, ALH+10, BBOB16, BPC13, CD19, CPV+12, CDS15, CY1+10, DWL11, DH11, GWT+17, GNI18, HS17b, HVS16, KKPT11, KG11, KNE11a, KDT+12, KZ13, LL13a, MCF10, OSA19, PHC13, PGI15, PNG10, RRF11, RKB+14, RSL16, SFA17, SS13c, TYX+18, VVW+18, WC11, XMSZ16, YVEI+17, ZWW10, FAS+18, VPR10].
structurally [TZCK18]. Structure [BPPS19, BJP15, CGBK13, DXL+10, GPK+16, GWJJ12, GBGR16, HLB15, JLLW19, LAHS16, MM19, MHR11, NC12, NC13, PMG+16, Rab12, SGH+16, VDVR14, WZK+13, AFPI13, AR15, AM19a, AM19b, AC12, BPPS17, BFIH+13, BDdS13, CPRS18, CD13, CvM19, CM13b, Clo15, DKE+17, DKT13, DSB+19, DDP16, DVVP14, DGSGVM19, DLW12, EH13, EKW+13, EFOD13, FZY+12, FDH19, FSC+14, GLB16, GMDG15, GRARO+14, GP12, GK10, GRD+10, GDPC+16, GBG+19, HASR+12, HNHR13, HSB+19, HNHy19, HS14a, HHR+17, HH15, HMYM16, HZ13, HLWD15, Hua16, Ibr17, KYT+17, KKH19, KSM17, KT10, KS12, Kop19b, KKL+13, KLS10, KML10, LLBO12, LFB14, LKL10, LZJ+11, LMI+14, LYL16, LPE+10, LGL11, LWWG12, LLFH16, Mat10, MDT10, Mau14, MAPB10, MV17, NGAS17, NCT18, OCL11, OL13, OL15, PSS14, PdSC18, PML+12].
structure [PN13, RLG14, RCM+13b, RR11, SHMO11, SB10, SM11, SLP+12, SB19, SLIB12, SRS14, SYN+12, SKGB13, SPZP18a, SPZP18b, Tac19, TN12, TTB+11, TG12b, UNT16, VVP12, VHR16, VVBL17, VAA14, VBMA13, VKC10, VI17, VLHK+17, WO15, WRM+12, WSGN11, YW12, YZZ16, ZRCC11, ZHHX11, CPR18, FDCG18, OFS12, SA10]. structure-activity [DXL+10]. Structure-based [CGBK13, DXL+10, DVVP14, GLB16, VKC10, YZZ16]. structured [GEP+14].
Structures [DLT17, HDM+19, NSN19, SNS16, SZL19, ZLX+19, AHK+19, BHNS14, BPM15, Ber17, CL16, CCIO14, CBDS19, CV12, DVVP14, DH14, DLC18b, DT19, DZA11, GS12, GSS13, HSY+11, HTS17, HPL+18, HS12, Hua16, IYK11, KNE11a, KOS+12, KTO11, KTO13, KDT+12, KSW16, LABSG17, uLhY11, LZX+10, LLWS14, LL19b, Lâe14, MCS11, MMT14, MPA10, MPA12, MP13, Mau14, MN19, MH10, MCAY15, MP17b, NS18, PRP15, PNH+16, QZM11, RRCH16, Rao11, RCR+16, RV11, RJJ11, RVVK13, RSG+10, Sak18, SWA13, SFR+11, SJD11, SIT18, SPM+19, SKY+11, TN10, Tak11, TFO+10, TFO+11, Tsu19, UCFR16, WKCI11, WD10, YNH+17, ZSL+11, ZLY+16, ZP13, ÇMD13, OSI+19, PGCT+12]. studied
[Ish10, KRTB10, OLY17, RHPWS13, RI10, TS15b]. Studies [JW12, AALCM11, BLS10, BRGN12, BLG10, BIL10, DM15, DXL+10, FWS+18, GZZM16, GEP+14, JLS+10, KG15, KP11, LXFC17, LCCW10, LLJ+11, LWD13, RCM+13b, SB10, SFA17, SLHW09, SZZ+18, TNI+19a,
TDP+12, VSD10, WCAH10, YKH+10, YPC+10, YDL+10, YXZZ17, ZZL+12, ZZL+10a, ZYG+15, ZX11]. Study [BHB19, JLH+14, LLX+19, MUGNVJ+18, VL17b, AARP17, AS11, AS15a, AMMA+11, ATP18, ASMS10, ANH+11, APA+14, APY+16, ALH+10, BEM14, BE14, BHB+17, BH19, BEEL14, BSJ12, BLG11, BMD19, BRLS08, BRLS12, BL12, BEL+11, CCLP12, CCCLR14, CWHH11, CBG17, CC18c, CCJ+11, CKL+11, CXW14, CBTZ16, CL16, CSXZ17, CSC+18, cCVG+14, CBDS19, Chu10, CG12, CB11c, CPLL11, CXD+19, CB11d, DASA15, DR11, DK19, DI11, DLS13, DSX+11, EHT19, EOA+11, EvRC+18, EV14, FCL+10, FF11, FCD10, FBEM11, FL15, FPB12, FB14b, GAI14, GG10, GKB+19, GC18, GVP+10, GD10, GTK10, GWZ15, GNGCA10, GKR13, GWPJ11, HZ11, HW19, HDB15, HRL11, HBR17, HVS16, Ibr11, IIF10, INT18, IN19, IN13, IIHY15, II10, JA10, JAHS19, JCG+10, JAH+17, JJAB16, JW16, JYS+12, KD10, KKT11, KOP+14, KIOY19, KC13b, KSNT19, KB13, KT12, KG11, KMT+19, KNP+12, KS13b, KP10, LC10, LY10, uLH11, LP11a, LL13a, LA19, LL+10, LDJ+10, LZL+10, LCL+10, LZJ+11, LZH11, LWL+11, Li14a, Li14b, LGW12, LT13, LJW+11b, Lin18, LBTV11, LBTV12, LTP11, LYSS11, LHS12, LH14b, LLSW14, LHT15, Lu11, LJC+11, LPM17, MUN+19, MMS19, MSY19, MC10, MG15, MCF10, MJLV14b, MAPB10, MFM+12, MH11, MWJ+11, MS11, MPNS13, MAMF19, MN19, MHR11, MBRC16, MO17, Mor15, MIS+15, NHF+10, NH19, NGAS17, NASH15, NC12, NC13, NC14, NS18, NJX+10, NFI+16, OP16, ORZ11, OSS10, OSHG17, OSA19, OME16, OOK11, PVL+13, PGCT+12, PP10, PGC12, PGS+15, PH12, PG18, PAK17, PP19, PPH+14, QLYL10, QZ10b, RS17a, RAGLL11, RAR+11, Ray13, RS13, RS14]. study [RVCFF13, RSLML12, RKG11, RSKG14, SN16a, SSP+13, SGDT10, SJD14, SCM+15, SRF+17, SSC+19, SWM10, SBD+17, SNS16, SGS+16, SSNT19, SMN+19, SCF+19, SE14, SCMA+17, SCMM19, Su10, SKY+11, STS+10, SKTT11, SZZS16, STS15, SGHL13, SIG+15, SPZP18a, SPZP19, TM16, TYFO19, TTC+18, TLA10, TNSC+17, TSR+16, TL16, UvSvdWK19, VKNT16, VPR10, VAR12, Vik11, VLGK+17, VED10, WKC10a, WHL+10, WCCW11, WDLG12, WHZ12, WYL+15, WFL+19, WNM17, WHX+10, WD10, WMW+10, WZQW10, WS11, WHDL11, WCL+11, WYGW12, WDP+12, XDL+10, XZ11, XWW+11, XCLZ19, XBSS19, YZGS14a, YZWC11, YHG+11, YZN13, YR13, YLZ19, YJXZ13, YLZ+10, YKH15, YSR11, YCA10, YBI11, YYT12, YZ15b, ZCK+16, ZWGO16, ZTH+15, ZPP+16, ZXS+10, ZZL+10b, ZZWT12, ZYLL12, ZLL12, ZSS+14, ZDX11, ZWY+10b, ZWY+10a, ZBP11, ZZ12, ZZWX11, ZGZ19, dSDdAR10, dSdS12a, dSD12b, dSd1B17]. study [dALdS+15, vRET19, vADC+14, GMBM18]. studying [SDL14]. styrene [MG15, FXX10]. sub [LTT16, YO19]. sub-optimal [LTT16]. sub-permutation [YO19]. subdomain [LKL10]. subjected [JMX+16]. submarine [WWKS16]. Subspace [FBKD19, SBB10, SM18]. Substituent [MG+16, AS18, CWHH11, JMX+16, MLX+13, TYN15, TY10].

T [BBI+11, CSQOA17, Gil11, MSPC19, MLCD11, OPR16, SRR16, XKW18, YJ17, BBG+18b, BG13, CCR18, CSS17, CEBO15, CKL+11, CLK11, CAP17, EP12, GG10, Gar12, GP12, GA19, GBW+14, GR10b, GWZ12, HS11, HCD+10, HH18, HvM16, ITTN15, JSXH16, JS17b, KV12, KZP+18b, KGM12, KKH18, LBS16, LCP13, LPLA13, MP19a, MSC+10, MG14, MSL12, MS12, NYN17, NCV10, NLI19, NFG+13, NO16, NSK+16, NS17, ODB18, OPB+12, OC14, PAK17, PAT+10, PBBP11, PD12, QLI19, RJPB12, RVCFF13, SSO19, SCOJ13, Sch12, Sea10, SKGP19, SEJ+18, SH18b, SW+12, SG13, SMM17, TSN16, TCX+13, UT15, WCY+11, WWU12, WS11, YCK16, ZSB+11, ZS18, ZT14, HvM17].

Theoretical

[AvKSP16, AMAA+11, AWFK+19, AHK+19, BHB+17, BSDP16, CWT+12, DBM+17, DGL+13, FF1+18, GYX+10, GLZ+17, HW+19, HDHL+15c, JW+12, KCB+12, KSO+19, KMT+19, KS+13b, LCL+10, LNL+11, LYL+12, LZY+12a, Lin+18, LWG+12, LX+16, LXFC+17, LD+18, LGJ+11, MLQ+12, MSV+16, NSF+16, OSS+10, OAN+15b, PKK+17, PM+13, PE+11, RS+17b, SB+10, SMI+19, SDD+19, SKY+11, STS+10, SZZ+16, SLC+17, TPL+10, Ts+19, WMW+11, WDL+11, WS+12, XSS+19, YJ+N+11, YPC+10, YH+11, YCGA+10, YY+12, YDGZ+15, ZL+10a, ZYLL+12, ZL+11, ZSG+14, ZGY+15, ZGZ+19, ZBMZH+15, dSdLBNB+17, BL+10, BAD+19, BE+16, CZH+12, CK+11, CBTZ+16, EV+14, GG+10, HDB+15, HGP+14, LWW+12, LLD+17, LZW+11, LCL+18, MRC+18, MPSG+11, MP+19a, MKK+19, NHH+10, PH+12, PsD+18, PsD+10, Pog+10, PH0b, RZG+13, RVCF+13, RP+13, SSE+13, SCS+19, SJD+11, SLH+09].

Theoretical [SKT+11, SGH+16, Tak+11, TL+16, UCRL+18, WSH+10, WQZ+10, YK+13, YZWC+11, YN+13, YB+11, Zha+12b, dSdSL+13, HDHL+15a, HDHL+15b, KZK+12, TD+12]. Theoretically [LLX+19].

Theories [OM+12, WCWV+15].

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HG13, JLS18, KDB13, LP11a, LKI1, LDB$^{+17}$, LCA17, LBB$^{+15}$, LG11,
LP11c, MDT16, MCC12, NHK$^{+13}$, OV14, OVPK15, OC14, PNW$^{+16}$,
SDM13, SH19b, WCDM11, ZCGM11, dVAG16, JCGM18]. toolbox
[HPT$^{+16b}$. toolchain [KSH$^{+17}$. toolkit [FSC$^{+14}$, GS12, IGK16, MJBM12,
MSS$^{+13}$, MADWB11, NKJ16, PG15, PPM15, TS10a, TBJ18, ZLL$^{+13}$. Tools
[RLG14, ZFOS19, GMZ12, SLG15]. toolset [YPKB12].

topological [KFY$^{+13}$. training [DBDP16]. trajectories [AST$^{+16}$, HRID16, JZL$^{+17}$,
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trajectory [IKU$^{+11}$, JFW$^{+14}$, LWD13, LAS$^{+14}$, MKS$^{+12}$, PVZ13, RC18,
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trans-influence [Tsi19]. trans-influence/trans-effect [Tsi19].

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DWR17, DAdGR15, EFAC13, ENKK$^{+17}$, FC16, HSH15, HAP$^{+12}$, HDHL15a,
HDHL15b, HDHL15c, IYK11, JM11, JCGVHPHT17, KGR$^{+16}$, KDR$^{+18}$,
LZL$^{+10}$, LLLM11, LWGZ15, LPLB16, MEG11, MRB14, MSV16, MCF$^{+18}$,
MT19b, PGCT$^{+12}$, PG18, PAK17, PL14, PTB$^{+15}$, Ras17, RCM$^{+13a}$,
RML$^{+15}$, Ric16, REL17, RKDM14, SRF$^{+17}$, SB$^{+17}$, SMP17a, SZZ19,
SHB17, TM16, Tsi17, VKTRJ15, VMTL10, YL17b, WCT$^{+11}$, YZ19, WG14,
XBSS19, XLY12, YKH$^{+10}$, YHX19, YLZ$^{+10}$, YYT$^{+12}$, YFH$^{+19}$, ZW17,
dALdS$^{+15}$. Transferability [FP17a, ZRL$^{+15}$, HOK17]. Transferable
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Transition\textsuperscript{19, 16}, BGS\textsuperscript{+19}, OZLSBH\textsuperscript{12}, QZ\textsuperscript{10c}, YB\textsuperscript{13}, Alg\textsuperscript{17}, AR\textsuperscript{10}, BS\textsuperscript{15}, CSA\textsuperscript{15}, CMS\textsuperscript{13}, DLS\textsuperscript{13}, G1\textsuperscript{15a}, GFGS\textsuperscript{18}, GPE\textsuperscript{13}, Hsu\textsuperscript{14}, IYK\textsuperscript{11}, JZ\textsuperscript{17}, JSF\textsuperscript{19}, LYL\textsuperscript{16}, LDZW\textsuperscript{17}, LN\textsuperscript{15}, LZW\textsuperscript{+11}, LGKS\textsuperscript{17}, LLL\textsuperscript{+12}, TM\textsuperscript{14}, MS\textsuperscript{10}, MN\textsuperscript{15}, MKK\textsuperscript{+19}, NMLD\textsuperscript{13}, PHK\textsuperscript{14}, RAGL\textsuperscript{11}, RJ\textsuperscript{+11}, SJ\textsuperscript{+15},

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version [BCJC14, EVR18, KYG15, OPB12, Pyy13]. versus
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MG11, OSI12, PG15, RP15, TR12, WCT11, WvRSM14, YSBB12].
vertex [RNP13]. vertical [UD12]. vertices [LK16b, OV14, RNVP13]. Very
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VI [OSS10]. via [AKMT11, ACD13a, ACD13b, BSPP13, BH13, CS17,
DDP18, DL15, DL19, GRCL12, HGCGR16, KHW17, KKH18,
LAW18, NSO14, RO14b, RJWW12, RNSS19, SS13b, SISK10, SB15, SM17,
TM18, TZ12, WBE16, ZWP11, ZLY16]. viable [SSX14]. VIBPACK
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MK13b, Tac17, WZ19, YHX19]. vibration-rotation
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ARLP13, BZB13, CJPT18, DOM11, DHF11, DT19, EB18, HYD10,
IY18, KKA18, KCMPG12, Kow11, KKH18, LBH11, LLTC12, LBTV12,
LS1b, MCF10, MAK14, MN19, RLA11, RRR16, SS13a, SSX14,
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vibrationally [YHX19]. vibronic [MCLD10, ZTH15]. view
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JBAM11, KCI4, KLS10, KML10, LBB15, MRB14, MNNK10b, MH10,
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voltage-dependent [SFBT17]. Volume
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Ano12h, Ano12i, Ano12j, Ano12k, Ano12l, Ano12m, Ano12n, Ano12o,
Ano12p, Ano12q, Ano12r, Ano12s, Ano12t, Ano12u, Ano12v, Ano13x,
Ano13y, Ano13z, Ano13-27, Ano13-28, Ano13-29, Ano13-30,
Ano13-31, Ano13b, Ano13c, Ano13d, Ano13e, Ano13f, Ano13g, Ano13h,
Ano13i, Ano13j, Ano13k, Ano13m, Ano13n, Ano13o, Ano13p, Ano13q,
Ano13r, Ano13s, Ano13-32, Ano13-43, Ano13-51, Ano13-52, Ano13-53,
Ano13-55, Ano13-56, Ano13-57, Ano13-58, Ano13-59, Ano13-60,
Ano13-61, Ano13-62, Ano13-63, Ano13-64, Ano13-33, Ano13-34, Ano13-35,


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