Electronic supplementary materials *Mendeleev Commun.*, 2023, **33**, 806–808

Why pay more? QTAIM descriptors of non-covalent interactions in S22 from promolecular electron density

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Table S1. Atomic coordinates obtained for the **S22** set at the B3LYP-D3/aug-cc-pVTZ level.

2-pyridoxine_2-aminopyridine

O1 -1.41227664236 -1.888083177134 0.5159562151439999

N2 -1.4588197008605999 0.3776605997012 0.2638111052498

C3 -4.140696415921 0.33090774249780003 -0.21805338691179998

C4 -3.4437658426164 1.5642221278111998 -0.225533446756

C5 -2.1049569583242 1.5432887989122 0.017948383273

C6 -2.076859728172 -0.8669759833053999 0.29330487317279996

C7 -3.4928112557502 -0.8409037398002 0.0352895907058

H8 -5.201511075560799 0.32638859821579996 -0.4352077605052

H9 -3.9512961362924 2.4889055711262 -0.43741685416599996

H10 -1.4894013834866 2.43344322606 0.0224010731306

H11 -4.001620159433999 -1.7925750614826 0.0432633966572

H12 -0.4365295568928 0.3863943875096 0.42755659559979997

N13 1.4706849324862 0.38543052318219995 0.4005086605942

C14 2.0984130126082 -0.7752632101156 0.1265335474582

C15 3.455785541884 -0.7996686530404 -0.2678819176522

C16 4.1558412723474 0.3791675138364 -0.3354988340926

C17 3.5120689996808 1.582182899188 -0.0278246601178

C18 2.1765591452199997 1.5214496673153999 0.3190486229012

H19 3.9187789460655997 -1.7449688856538 -0.5140553952922

H20 5.1917382216552 0.3773288303002 -0.648174907388

H21 4.0384678518564 2.5203569134559998 -0.069941217879

H22 1.6338255806797999 2.4342549458456 0.5436503424312

N23 1.3930990903665998 -1.9230039611306 0.2513670565402

H24 1.8079084806184 -2.7776473357426 -0.0695250601434

H25 0.3823133566414 -1.9087814495687998 0.4120081230038

adenine_thymine_stack

N1 0.9695573199252 2.5407713760732 -0.4395550482904

C2 -0.3469945551996 2.8899902123995997 -0.6794542291751999

H3 -0.6130837168477999 3.6075050674752 -1.437908242971

N4 -1.1872858749858 2.260159901226 0.0944317264888

C5 -0.3921726838508 1.4549057532856 0.8929945203324

C6 -0.6991131444638 0.5011058315122 1.8756547339426

N7 -1.9745192478292 0.24280335776739997 2.247124107565

H8 -2.1515310161892 -0.627847410212 2.7193654138004

H9 -2.7059836422554002 0.6122044578188 1.6645345893055998

N10 0.3092952904458 -0.16272304579660002 2.4615050117357997

C11 1.5615722748366 0.11101574084319998 2.0789737969802

H12 2.336369362041 -0.4529092178066 2.583978425644

N13 1.9764827702191998 0.9659337969178 1.1426739953936

C14 0.9558622738202001 1.6150009970382 0.5776107864392

H15 1.7892211874359998 2.9250344276312 -0.8763673301818

N16 0.6609647646439999 -0.531989707669 -2.0045315063162

C17 1.2744379579718 -1.3944118589434 -1.1279757033856

H18 2.3540563515612 -1.407212257465 -1.1836864667109999

C19 0.5874784535254 -2.159320709835 -0.2602308479992

C20 1.2390375993084 -3.0814537383892002 0.721382753407

H21 0.9253396847248 -2.8268388448908 1.7334882091341999

H22 0.9573264831293999 -4.120507934331 0.5475978400182

H23 2.3230372381635997 -2.9975754115977997 0.6579467664352

C24 -0.872228184766 -2.0651618814722 -0.271795738224

O25 -1.625612622411 -2.6849139383785996 0.45666182898319996

N26 -1.3999790442153999 -1.1784234858538 -1.2236310686638

H27 -2.4061728237824003 -1.101554767303 -1.255066974813

C28 -0.708062393201 -0.38204042147280004 -2.1105197990284

O29 -1.2299003276254001 0.3761357886984 -2.9025358054594

H30 1.1953022323009999 0.0197108225548 -2.6527968770252

adenine_thymine_wc

N1 0.9213861597776 -0.3697986412346 -0.36136751792719995

C2 1.6592145893033998 -0.2362673709186 0.7589547874134

C3 3.037745486565 0.0004745209978 0.6017598469458

C4 3.5063466588327996 0.0858441034882 -0.7078791699178

N5 2.7866334259914 -0.032378275185 -1.8282290402446

C6 1.5052581140162 -0.26005768971959997 -1.5659047349981998

N7 4.0682097840322 0.162196792162 1.5105164433812

C8 5.1294857192944 0.3460325165432 0.7712587939278

N9 4.8542040395712 0.3116412882644 -0.579684251266

N10 1.0637787449901999 -0.3323275112706 1.9566509665327998

H11 0.8363127487495999 -0.37787702373759996 -2.4108563260805997

H12 6.1294113829286 0.5113223763888 1.1377172086679999

H13 5.5038995986072 0.4311704610722 -1.3371276370977998

H14 0.047992059176599995 -0.347547855224 2.0209842522798

H15 1.6147502715542 -0.15383964292679997 2.7768217355656

N16 -3.8430389208286 0.17436731831320001 -1.5181135049234

C17 -4.538202673241 0.26178193278899997 -0.33708858606500003

C18 -3.9545065020148 0.071814779669 0.8619695965383999

C19 -2.5207730658998 -0.210316293758 0.878731119032

N20 -1.8961448163817998 -0.2536389956178 -0.3542964507214

C21 -2.4845253948040003 -0.100017057343 -1.586454281394

C22 -4.6880830972437995 0.1584781172988 2.1630946575492

O23 -1.8717414584262 -0.3881659022284 1.9080186683495999

O24 -1.8884694679503997 -0.19153660045579998 -2.6428203205704

H25 -4.306211838741599 0.283106114036 -2.4045726681312

H26 -0.8636861770813999 -0.4111589372742 -0.35543967002619997

H27 -5.5886841091059996 0.49946310332999994 -0.434493743223

H28 -4.788490070286199 -0.8224811583292 2.6295473113908

H29 -4.1358320028561995 0.7817054262683999 2.8657780524697998

H30 -5.681921174702199 0.5797247017852 2.0279871716852003

ammonia_dimer

N1 -3.5941717635263997 0.1227746972494 -5.83209278e-05

H2 -4.1282808159282 0.4154407919524 -0.8118303630528

H3 -4.1280520037879995 0.4153008238424 0.8119176777528

H4 -2.7364753854486 0.6640364005375999 -0.0001283420254

N5 3.5941238991953997 -0.12278735523499999 9.6734104e-06

H6 4.1281712597928 -0.415331050604 -0.8118477889502

H7 2.7365159365119998 -0.6641888572956 3.7804619199999996e-05

H8 4.128168873191 -0.41524545573899996 0.8118996538819999

benzene_ammonia

C1 -0.7361448962738 0.5505962215244 -1.2025957403198

C2 -1.4237378027212 0.4236708321516 0.00031549711599999995

C3 -0.7363650457374 0.551832026162 1.2031968729243998

C4 0.6322662431332 0.8034859194294 1.2040647016653998

C5 1.3200146544154 0.9286762334181999 0.0002627960798

C6 0.6325161854308 0.802072490233 -1.2035308648814

H7 -1.2671348506278 0.4517462653796 -2.1382954835372

H8 -2.4850152620218 0.21101321852619997 0.0002662992514

H9 -1.2674468604476 0.45385241236319995 2.1390071248012

H10 1.1588611353315998 0.9043408592172 2.1430607653125997

H11 2.3821650278768 1.1348302248436 0.0002845453778

H12 1.1593701959079998 0.9018235922916 -2.1425420048667996

N13 0.1921030188524 -3.0571699433628 -0.0008902289304

H14 0.745147856781 -3.2910527709916 -0.8167953732355999

H15 0.7452443897966 -3.2917164526722 0.8147374080909999

H16 0.0627015962596 -2.0515301782132 -0.0005463201402

benzene_dimer1

C1 -0.0059753576813999995 0.0030314975906 1.1389086203954

C2 -0.000948687445 -1.2013991320448 1.8328815325948

C3 0.0057757404018 -1.2091453853043999 3.223785092184

C4 0.009082713224999999 -0.0066182796306 3.9262834434421996

C5 0.0056106732844 1.2003188587009999 3.2314662986380003

C6 -0.0008577796128 1.2029767763788 1.8403973173808

H7 -0.0091487866398 0.0047616198498 0.0602327175532

H8 -0.0037438373722 -2.1242001709719998 1.273324849009

H9 0.0079269417706 -2.1530332417896 3.7526261312268

H10 0.014506543634999999 -0.0099853778854 5.007253325709

H11 0.008100528686 2.1401527942093996 3.7669099535834003

H12 -0.0032517264312 2.1304159086684002 1.2887135462876

C13 -1.3950039743208 0.0017252273442 -2.5423286258099997

C14 -0.6975109038434 1.2054394478038 -2.5479273131674

C15 0.6932404265351999 1.2057241836864 -2.5329131218666

C16 1.3907027304874 0.0019510390337999998 -2.5136340572738

C17 0.6930860012276 -1.2019126536086 -2.5076790941895997

C18 -0.6977226446368 -1.2019138654308 -2.5198948440636

H19 -2.4763560250918 0.0018570302068 -2.5578809032102

H20 -1.2372337940259999 2.1422408114862 -2.5675012950659997

H21 1.2325799998929998 2.1431825878404003 -2.5371075560088

H22 2.4721644485215997 0.0023943595787999997 -2.5023645447414

H23 1.2326010718406 -2.1391274709167996 -2.4935571374114

H24 -1.2376243182824 -2.1388365647954 -2.51261649176

benzene_dimer2

C1 -1.1350080769497999 -1.4506457325742 0.0001601245762

C2 -1.5331693956082 -0.8785422758571999 1.2026087475642

C3 -1.5334914228054 -0.8791084667064 -1.2024496337218

C4 -2.3319653990778 0.25886564297619996 1.2029071415826

C5 -2.7370558906168 0.8245058698026 -0.0001486360784

C6 -2.332294252697 0.2582873021542 -1.2030418919777999

H7 -1.2150792658574001 -1.3146011112645999 -2.1387668506221997

H8 -2.6401252862074 0.7067261396158 -2.1380664650168

H9 -3.3765004392828 1.6972314943521998 -0.0002847835088

H10 -2.6391647715893995 0.7080193232408 2.1377525448572

H11 -1.214355040693 -1.3135621986296 2.1389890744714

H12 -0.49703179640359996 -2.3228710438927997 0.0003645573938

C13 1.1409248914478 1.4541113006433999 0.0001597964846

C14 1.536991376991 0.8815470604414 -1.2027234684963999

C15 1.5366454890676 0.8808893479112 1.2028434388942

C16 2.3308545444218 -0.2592888546812 -1.2032796313846001

C17 2.7314964895825997 -0.8276630741022 -0.00014274101319999998

C18 2.330535126082 -0.2599228916982 1.2031800555839998

H19 0.5061852609946 2.328756419807 0.0003979856944

H20 1.2175990093453999 1.3167154234956 2.1388326488633997

H21 2.6353016464616 -0.7118419396396 2.1375439050586

H22 3.3640799232078002 -1.7047595666978 -0.0003682775292

H23 2.6362598485629998 -0.7105556036038 -2.1377483907942

H24 1.218367415748 1.3177074349072 -2.1387192720484

benzene_hcn

C1 -0.7054905307748 -1.0110575205732 1.2041436024034

C2 -1.4030445522046 -0.9807386975286 -0.0002124340192

C3 -0.705568738287 -1.0118962814568 -1.2045428634216

C4 0.6848771176448 -1.0649903396428 -1.2045554261548

C5 1.3823949272871998 -1.0922367330237999 -0.0001119268618

C6 0.6849683588604001 -1.0641800486432 1.2043269791487998

H7 -1.2438663721002001 -0.9873157910797999 2.1414397229268

H8 -2.4832784244684003 -0.9247779336958 -0.000264113738

H9 -1.243937313971 -0.9887427408251999 -2.1418082332951998

H10 1.2239297801902 -1.0830981913088 -2.1416716148946002

H11 2.4633237240188 -1.1341921713504002 -9.36489846e-05

H12 1.2241515595282 -1.0816770096254 2.1413271292981997

N13 0.0003858727642 3.6062096454187995 0.0012211516434000001

C14 0.060661231641800005 2.4613041985093997 0.0006486370931999999

H15 0.1260825114688 1.3958782431824 0.00015303885599999998

benzene_methane

C1 1.2772380398566 -0.14139239797 -0.559528499459

C2 0.6583029204505999 -1.3055849900507999 -1.0061815925516

C3 -0.7108330897203999 -1.3119773680312 -1.2558937444777998

C4 -1.4652846294189998 -0.1609330944466 -1.0569376647042

C5 -0.8471358609094 0.9988466603224 -0.6002547161472

C6 0.523312769668 1.0112548412116 -0.3631920088558

H7 2.3384805044837997 -0.1309751880374 -0.3491399620474

H8 1.2404861660567998 -2.2026316691906 -1.1735863149754

H9 -1.185342747193 -2.208206437612 -1.6277970721592

H10 -2.5266126042423998 -0.1693618734866 -1.2704408550516

H11 -1.4346970623114 1.888439235897 -0.42029367947679996

H12 0.9967480065276 1.9137900430163999 -0.0032660089993999998

C13 0.2276143994798 0.36113153539799997 3.5013903060348

H14 0.8260284529576 1.250270672506 3.6958278236244

H15 -0.7886505221751999 0.5342856662268001 3.8516204265083998

H16 0.2135752540798 0.1581455065016 2.4325875631672003

H17 0.656770986685 -0.4851011422546 4.0334092932332

benzene_water

C1 0.9858076704141999 -0.6584674425126 -1.2056991693478

C2 0.4576686997692 0.6281697496254 -1.2055472946877999

C3 0.19759377994879998 1.2744777840586001 -0.0001255691222

C4 0.457440866612 0.6282640283342 1.2054036752358

C5 0.9853847391745999 -0.658443433616 1.2057412232823999

C6 1.2450042890214 -1.3031631501546 9.13999696e-05

H7 1.1938358851046 -1.1588955426152 -2.1417142085928003

H8 0.24353087972319998 1.1282379755772 -2.1390302711344003

H9 -0.2191618655496 2.2722882570230003 -0.0002711941664

H10 0.2434536141514 1.1283737790406 2.1388605631083997

H11 1.193100658288 -1.1585965770824 2.1420011987822

H12 1.6699289655568 -2.2977030896306 5.86437276e-05

O13 -3.1068461655156 0.1266469983584 7.83345154e-05

H14 -3.1481609414916 -0.8344738429577999 0.000127029659

H15 -2.1647048358696 0.3350081096032 2.5638771e-05

ethene_dimer

C1 -0.46801830695679997 -0.4680752202658 -1.9288526542872

C2 0.4680640598596 0.46812959880259997 -1.9289646446506

H3 -0.8726548996426 -0.872705743257 -1.0092632987405998

H4 0.8727962489124 0.8729014181456 -1.0094838345055999

H5 -0.8719201702552 -0.8720297581413999 -2.8487085842588

H6 0.871854345555 0.8719694263296 -2.8489210235697997

C7 -0.4680708121964 0.4680589638562 1.9289013494308

C8 0.46802628699119997 -0.4681250213956 1.9289206592089998

H9 -0.8726802367809999 0.872828804066 1.009361927309

H10 0.872698043688 -0.8728741495002 1.0093956942848

H11 -0.8719845979202 0.8719361938256001 2.8487892418743996

H12 0.8718900387459999 -0.8720145124655999 2.8488251731964

ethene_ethine

C1 5.344718e-07 -0.6629599690406 -2.1584861612241997

C2 -3.9476828e-06 0.6629371560908 -2.1583543160271996

H3 0.9202395113863999 -1.2332139522412 -2.1569481895147997

H4 -0.9202069033148 -1.2332641079216 -2.156818482205

H5 -0.9202149098082 1.2332281342652 -2.1565982586562

H6 0.9202449989829999 1.2331711415792 -2.156754821851

C7 -1.12874094e-05 3.2777409200000004e-05 2.9429098263985995

C8 -3.0009797799999996e-05 2.91736934e-05 1.7450469502874

H9 -6.2760748e-06 -2.09978624e-05 0.6807367180724

H10 -1.1721337e-05 6.0644027999999994e-05 4.0062139128042

formamide_dimer

C1 -2.0138200546858 0.0381970379208 -1.6139989999999999e-06

O2 -1.4284776785648 1.1156635104566002 -8.5832996e-06

N3 -1.4236807729926 -1.164255056488 7.355602e-06

H4 -1.9915278497565998 -1.9923049982127998 2.063802e-06

H5 -0.4004824767678 -1.2470119556069998 3.4608372e-06

H6 -3.1142600302336 -0.0038509963221999995 -3.2279979999999998e-06

C7 2.013791023871 -0.038208743382400004 -1.719835e-06

O8 1.4284298301092 -1.1156653149604 -3.8735976e-06

N9 1.4236909332486 1.1642639414202 5.3023836e-06

H10 1.9915995113122 1.9922697707001997 7.7048608e-06

H11 0.40050090810719996 1.2470922745474 7.778945999999999e-07

H12 3.1142366510612 0.0038105299276 -7.646651e-06

formic_acid_dimer

C1 -1.8947821302556 -0.1927066227276 -3.1962471999999997e-06

O2 -1.4808174806214 1.0505038043036 1.58013148e-05

O3 -1.1965127791772 -1.1907264234246 -1.75370252e-05

H4 -2.9881166418975997 -0.2525838636158 -3.2174144e-06

H5 -0.4811320012056 1.112800847745 5.926815999999999e-06

C6 1.8947846703195999 0.1927047758894 -1.5399138e-06

O7 1.4808060185825997 -1.0504989146804 1.9156316e-05

O8 1.196533538908598 1.1907387109842 -1.3875099599999999e-05

H9 2.9881202403216 0.2525643739164 -7.3926446e-06

H10 0.48111655973319994 -1.1127966883902 5.8791898e-06

indole_benzene_stack

C1 0.5800506872488 0.9683220497594 -1.4841515157098

C2 -0.8006310356638 1.1366141276661998 -1.4981555870594

C3 -1.5912575371261999 0.35338204884859997 -2.3333088442191996

C4 -0.9937275687989999 -0.5999761663788 -3.1526800646064

C5 0.3875247106978 -0.7669922907614 -3.1406728328196

C6 1.1752998156907999 0.0205368566594 -2.3066863011402003

H7 1.1991290345135999 1.5605868358405999 -0.8194123270895999

H8 -1.2547125670916 1.8738520028956 -0.8505494952534001

H9 -2.665466324664 0.48025033969939995 -2.3414296087484

H10 -1.6017216588657999 -1.2134643937104 -3.8074371192146

H11 0.8380216138482 -1.507578388395 -3.7879047784902

H12 2.251728767335 -0.10055967322319999 -2.2937857129692

H13 -3.1422528902144 0.2332848118944 1.9684765625764

C14 -2.1022825831484 0.0149355339856 1.7782247952852

C15 -1.1309656497626 0.9144160918666 2.173066398466

H16 -1.4370719692334 1.8340046218923998 2.6453769479044

C17 0.2181539999052 0.6043581577884 1.9575017821368

C18 1.4701068509624 1.2695549018956 2.1925648610868

H19 1.6209370683964 2.2290034444512 2.6550654081836

C20 2.45821916907 0.4577262375106 1.7108474545062

N21 1.8954504369693999 -0.6888253031657999 1.1897418787428

C22 0.5266778887896 -0.6292261516594 1.3185209486129998

C23 -0.45313498716179995 -1.5191765428746 0.8871304333296

H24 -0.1997131881832 -2.4260121312411997 0.35756168711799996

C25 -1.7717423561605998 -1.1855563507 1.1297785931866

H26 -2.5649712219844 -1.84562558403 0.8061683116821999

H27 2.3955807145679997 -1.423987157629 0.7264669613848

H28 3.5248911104578 0.5992835755947999 1.6940045070860001

indole_benzene_t-shape

C1 3.0147736557618 1.679621897407 0.1003950294498

C2 3.0467106001185997 1.0796297709594 -1.1519022648694

C3 3.2040829693484 -0.2980109767488 -1.256571856897

C4 3.296423064261 -1.0819387314698 -0.1098141847352

C5 3.1898940924673997 -0.48400730602739994 1.1425181201328

C6 3.0641231145564 0.8970367887655999 1.2482011712374

H7 2.9808682358902 2.7561713380454 0.1821357759656

H8 2.9787208128666003 1.6997098347969999 -2.0398414492848

H9 3.2459663545261996 -0.7439291129065999 -2.2395391272022

H10 3.4314920364045998 -2.1501872958742 -0.1944791058458

H11 3.2016514295828 -1.0890310928787998 2.0351981382076

H12 3.0181513376166 1.3697334120566 2.220000907288

H13 0.650469273114 -0.3013089640956 -0.013052013028

N14 -0.279888805472 -0.6764454069475999 0.008932378478800001

C15 -0.5893583707672 -2.0167989570761997 0.1250627181072

C16 -1.9460001765482 -2.175392435615 0.1561589065718

C17 -2.5182857717293996 -0.8640635141722 0.0547241813006

C18 -1.4435941021497998 0.05379429562099999 -0.0293563875032

C19 -1.6533082155268 1.4255254362627998 -0.1205883371614

C20 -2.9636700605196 1.8874327461206 -0.1378099869568

C21 -4.0423748248389995 0.9872322706004 -0.065047096649

C22 -3.8255946132563996 -0.3753738753344 0.0333902896006

H23 0.198751567579 -2.7479174053691997 0.1849622004308

H24 -2.4862285765094 -3.1029552531460003 0.24980509710139998

H25 -0.8094863655346 2.109773745189 -0.1674914179832

H26 -3.1244482745638003 2.9530845766388 -0.2230387228984

H27 -5.058209496695 1.3501103857555998 -0.09137315604940001

H28 -4.6559182932708 -1.0641162718696 0.09842017731599999

methane_dimer

C1 -0.0046207680092 -0.1052047464698 1.9511971633676

H2 -1.0719834004248 0.0952895061016 1.855049935863

H3 0.5340245952738 0.4175304867298 1.1623907394725999

H4 0.1755000016442 -1.1750925676355999 1.8556753049116

H5 0.34618610574639996 0.2444043442312 2.9200839857738

C6 0.0042603964292 0.105045219867 -1.950824054425

H7 0.3191201680372 -0.3060680756322 -2.9080292230394003

H8 -1.0627163843893999 -0.0701945416368 -1.8110002306437998

H9 0.5582948697512 -0.3814772839922 -1.1497445810456

H10 0.2019344159414 1.175767658437 -1.9247990402347999

phenol_dimer

C1 -2.0535097030064 0.179901593881 0.3732662360632

O2 -0.731502341924 0.5129523566248 0.364536358895

H3 -0.30529032920259996 0.3650119117938 1.2182574151014

C4 -2.7228285793924 -0.21953868933579998 1.5282369035364

C5 -4.0669388735934 -0.572780119183 1.4591083420916

C6 -4.7518142502359995 -0.5175779242966 0.25139135648579997

C7 -4.0804927080154 -0.095100895766 -0.8934605638666

C8 -2.7386378318923996 0.2513263784736 -0.8415407561006

H9 -2.1857121229654 -0.2471203711648 2.4696522458486

H10 -4.575992618279599 -0.9067014465283999 2.3496850442958

H11 -5.791769174039399 -0.8079905588876 0.1983317796686

H12 -4.6171524873942 -0.0193100639572 -1.8288128739549998

H13 -2.2177968355454 0.5865647925045999 -1.7282392145043999

O14 1.7920631962521998 0.07209982247600001 1.726514601009

C15 2.573988486227 -0.10446178304159999 0.6004569264088

H16 2.2951033817527997 0.5550955003892 2.3891251948299996

C17 2.0073393988978 -0.7854572383831999 -0.47193087866379996

C18 2.7586081378602 -1.0061256952682 -1.6183725827394

C19 4.0746718814776 -0.5587793869591999 -1.7068674335164

C20 4.6242772981208 0.136177117398 -0.6369549631461999

C21 3.8822296000354 0.357789102223 0.521168161882

H22 0.9858706957522 -1.1228989356786 -0.39739978630399997

H23 2.31008925134 -1.5401439297983999 -2.4432031256392

H24 4.650566632429199 -0.7299553688628 -2.6050367309836

H25 5.6352410427062 0.5196212576142 -0.6970106382386

H26 4.328718652619799 0.895570049976 1.3490846761616

pyrazine_dimer

C1 -1.2673121100523999 -1.2463983131872 -0.6952413354921999

C2 -1.2673749978036 -1.2466117261893999 0.6953845527674

N3 -0.27767147247859997 -1.7957421879072 1.3977904509877999

C4 0.7112325094926 -2.3415015719366 0.6960146579769999

C5 0.7111749029578001 -2.3414835798166 -0.6960911721132

N6 -0.2776726207992 -1.7954943570378 -1.3977551176392

H7 -2.0781582194724 -0.7913061432117999 -1.2505581442492

H8 -2.078354661672 -0.7918700427116 1.2508137434809998

H9 1.5247603443986 -2.7936651327888 1.2505975311166

H10 1.5244780004096 -2.7939222719343997 -1.2507736898468

C11 -0.3258871737068 2.141309168929 1.1303265537848

C12 0.8847686394879999 1.4564702474965998 1.1297451648859997

N13 1.4979304421366 1.109483868128 3.49840898e-05

C14 0.8848291088865999 1.4563702959782001 -1.1297332054179998

C15 -0.3257740773572 2.1413110528097996 -1.1304071743578

N16 -0.9393033743485999 2.4874954281376 -7.43921244e-05

H17 -0.8140241157854 2.4020274710852 2.0607933153592

H18 1.3592425508516 1.1676856933853998 2.0584045333375998

H19 1.3592390053455998 1.1673238453932 -2.0583416191274

H20 -0.8137287169258 2.4021702279738 -2.060930642861

uracil_dimer_hb

O1 -1.442338643767 0.9853377374069999 -0.0018746677761999999

C2 -0.6140209316704 1.895637380388 -0.0014126936361999998

N3 0.7377672351506 1.6748630557522 -0.0025692588605999997

C4 1.6451218697202 2.6971037584325996 -0.0018342860504

C5 1.2795120797788 3.9921511130582 0.00015928317999999998

C6 -0.127714073953 4.3406940542296 0.002431026461

N7 -0.97927378441 3.2146814869326 0.0004666467994

O8 -0.6021714960678 5.4571024543296 0.0063758093546

H9 2.0062168017376 4.7866336803872 0.001045421549

H10 1.039570246986 0.6888734850048 -0.002513419787

H11 -1.9714030549795998 3.4044509754471997 0.0021140899754

H12 2.6815888093896 2.3949248859186 -0.0027272825922

O13 1.4420327089336 -0.9849595218774 -0.0017298470855999998

C14 0.6138263468926 -1.8953673980437997 -0.001261935546

N15 -0.7380031224274 -1.6748989923659998 -0.0023939679856

C16 -1.6450668720427999 -2.6974666700766 -0.0017175806932

C17 -1.2793153147793999 -3.9924957150742 0.0001601245762

C18 0.12803428077100001 -4.3406733844588 0.0024224537450000003

N19 0.9792654657004 -3.2143649420402003 0.0005921365445999999

O20 0.602888503217 -5.456895343861199 0.0059940165682

H21 -2.0060644455238 -4.786960586624 0.0009379345073999999

H22 -1.0403637576878 -0.689161459469 -0.0024426578374

H23 1.9714311226867998 -3.4039224727976 0.0023235182522

H24 -2.6815199789469997 -2.3952875858906 -0.0025448636626

uracil_dimer_stack

N1 1.9838059229016 -1.1699005709836 0.010375436463399999

C2 1.9910728978352 -0.7679705064504 -1.29622323492

H3 2.2338374508332 -1.5359429444077999 -2.0151120794066

C4 1.7020890280769998 0.4949022543722 -1.656966219903

H5 1.710666638992 0.8022795213244 -2.6870132959828

C6 1.3249571374056 1.4659745901783998 -0.6471714815638

O7 0.955379931542 2.6090324580358 -0.8521101529094

N8 1.4005613750546 0.969564098721 0.6648424845562

H9 1.1620362206234 1.6083822199784001 1.4107331724704

C10 1.6879650657065999 -0.32270010777979996 1.0667643362158001

O11 1.6717128948384 -0.690883173058 2.2205875086098

H12 2.1467586010674 -2.13135367913 0.2595979381356

N13 -1.9836073428147998 1.1699958657179999 0.011268612926400001

C14 -1.9900256770741998 0.7681933388566 -1.2953554379298

H15 -2.2316149318757996 1.5362915523164 -2.014482185869

C16 -1.7011769228454 -0.49473494882339997 -1.6560339740806

H17 -1.7090658906592 -0.8018541558567999 -2.686196448443

C18 -1.325172556 -1.4660976562791999 -0.6461203078282

O19 -0.9557331962346 -2.6092117812624003 -0.8509392363234

N20 -1.4016871208358 -0.9697896405287999 0.6659125394341999

H21 -1.16360543512 -1.6086644105052 1.4118936589186

C22 -1.6889720687876 0.3225160854348 1.0677789118626

O23 -1.6735254474662 0.6905539119702 2.2216604739778

H24 -2.1466565698716 2.1314176834509997 0.2604870769552

water_dimer

O1 -1.621091996425 -0.10192514812799999 -3.280916e-07

H2 -2.0127420568159997 0.7759016869528 1.3705762000000001e-06

H3 -0.663081087759 0.0461216248404 -3.17508e-07

O4 1.4239041874968 0.1016665854882 -1.0901108000000002e-06

H5 1.74974795786 -0.3845417653722 -0.765355203638

H6 1.7497443012262 -0.384540712304 0.7653555687721999

Table S2. Local properties at the intermolecular (3,-1) critical points of electron density calculated at the B3LYP/aug-cc-pVTZ level for **S22** set.

2-pyridoxine_2-aminopyridine

B3LYP		rho	lapl	g	v	h
O1	H25	0.037345	0.099815	0.029358	-0.03376	-0.0044
H12	N13	0.035911	0.069316	0.022732	-0.02814	-0.0054

adenine_thymine_stack

B3LYP						
H21	N10	0.005844	0.02	0.003911	-0.00282	0.001089
O25	N7	0.004058	0.014533	0.002792	-0.00195	0.000841
C19	N10	0.005485	0.019199	0.003699	-0.0026	0.001101
C17	N13	0.005517	0.018156	0.003449	-0.00236	0.00109
N26	C5	0.004317	0.014707	0.002771	-0.00186	0.000906
N16	C14	0.005018	0.018149	0.003497	-0.00246	0.00104
O29	N4	0.004039	0.014468	0.002769	-0.00192	0.000849

adenine_thymine_wc

B3LYP						
O23	H14	0.027207	0.084273	0.021499	-0.02193	-0.00043
H26	N1	0.046751	0.072862	0.029385	-0.04055	-0.01117
O24	H11	0.005371	0.018314	0.003651	-0.00272	0.000928

ammonia_dimer

B3LYP						
H7	H4	4.65E-06	1.50E-05	2.54E-06	-1.32E-06	1.22E-06

benzene_ammonia

B3LYP						
H16	C2	0.004847	0.016901	0.003232	-0.00224	0.000993

benzene_dimer1

B3LYP						
C17	H7	0.005241	0.018691	0.003627	-0.00258	0.001046

benzene_dimer2

B3LYP						
C2	C15	0.004434	0.013093	0.00243	-0.00159	0.000844
C3	C14	0.004426	0.013072	0.002425	-0.00158	0.000843

benzene_hcn

B3LYP						
C5	H15	0.006134	0.022864	0.004407	-0.0031	0.001309

benzene_methane

B3LYP						
H16	C6	0.004644	0.013526	0.002631	-0.00188	0.00075

benzene_water

B3LYP						
H15	C3	0.008551	0.02466	0.005233	-0.0043	0.000932

ethene_dimer

B3LYP						
H10	H3	0.003237	0.012044	0.002291	-0.00157	0.00072
H3	H9	0.003237	0.012042	0.002291	-0.00157	0.00072
H10	H4	0.003235	0.012036	0.002289	-0.00157	0.00072
H9	H4	0.003236	0.012039	0.00229	-0.00157	0.00072

ethene_ethine

B3LYP						
H9	(3,-1)	0.005637	0.015211	0.002934	-0.00206	0.000869

formamide_dimer

B3LYP						
H5	O8	0.034323	0.094307	0.026642	-0.02971	-0.00307
O2	H11	0.034318	0.094295	0.026638	-0.0297	-0.00306

formic_acid_dimer

B3LYP						
O3	H10	0.049053	0.094829	0.035889	-0.04807	-0.01218
H5	O8	0.049048	0.094831	0.035886	-0.04806	-0.01218

indole_benzene_stack

B3LYP						
C22	C1	0.007022	0.022396	0.00447	-0.00334	0.001129
C15	H8	0.00404	0.013412	0.002493	-0.00163	0.00086
C18	H7	0.004855	0.016898	0.003239	-0.00225	0.000985

indole_benzene_t-shape

B3LYP						
C4	H13	0.006532	0.022071	0.004384	-0.00325	0.001133

methane_dimer

B3LYP						
H9	H3	0.004899	0.015445	0.003073	-0.00228	0.000789

phenol_dimer

B3LYP						
H22	O2	0.009711	0.036469	0.00731	-0.0055	0.001808
O14	H3	0.014539	0.059002	0.012144	-0.00954	0.002606

pyrazine_dimer

B3LYP						
C2	C12	0.00472	0.014839	0.002788	-0.00187	0.000922
C1	C14	0.004722	0.014845	0.002789	-0.00187	0.000922
N13	(3,-1)	0.003401	0.011692	0.002148	-0.00137	0.000775

uracil_dimer_hb

B3LYP						
H22	O1	0.044512	0.106832	0.034811	-0.04291	-0.0081
O13	H10	0.044571	0.106899	0.034859	-0.04299	-0.00813

uracil_dimer_stack

B3LYP						
O19	N1	0.004774	0.018204	0.003486	-0.00242	0.001064
N20	C10	0.006221	0.023649	0.004634	-0.00336	0.001278
C22	N8	0.006219	0.023645	0.004633	-0.00335	0.001278
C16	C4	0.005136	0.014064	0.002679	-0.00184	0.000837
N13	O7	0.004777	0.018219	0.003489	-0.00242	0.001065

water_dimer						
B3LYP						
H3	O4	0.018314	0.06129	0.014145	-0.01297	0.001178

Table S3. Local properties at the intermolecular (3,-1) critical points of electron density calculated at the MP2/aug-cc-pVTZ level for **S22** set.

2-pyridoxine_2-aminopyridine						
MP2						
H12	N13	0.033556	0.080226	0.0245	-0.02894	-0.00444
O1	H25	0.034661	0.11088	0.030864	-0.03401	-0.00314
adenine_thymine_stack						
MP2						
N10	H21	0.005784	0.02136	0.004208	-0.00308	0.001132
N7	O25	0.004042	0.015353	0.002987	-0.00214	0.000851
N10	C19	0.005791	0.020121	0.003984	-0.00294	0.001046
N13	C17	0.005814	0.019024	0.003723	-0.00269	0.001033
C5	N26	0.004555	0.015508	0.003002	-0.00213	0.000875
C14	N16	0.004937	0.018897	0.003692	-0.00266	0.001032
N4	O29	0.004208	0.015131	0.00297	-0.00216	0.000813
adenine_thymine_wc						
MP2						
O23	H14	0.025078	0.091647	0.022552	-0.02219	0.000359
H26	N1	0.044009	0.087747	0.03168	-0.04142	-0.00974
O24	H11	0.004983	0.019169	0.003817	-0.00284	0.000975
ammonia_dimer						
MP2						
H4	H7	3.17E-06	1.07E-05	1.79E-06	-8.97E-07	8.93E-07
benzene_ammonia						
MP2						
C2	H16	0.004798	0.017568	0.003424	-0.00246	0.000968

benzene_dimer1

MP2

C17	H7	0.005215	0.019461	0.003851	-0.00284	0.001014

benzene_dimer2

MP2

C15	C2	0.004726	0.013802	0.002639	-0.00183	0.000812
C14	C3	0.004719	0.013781	0.002634	-0.00182	0.000811

benzene_hcn

MP2

C5	H15	0.006094	0.023645	0.00469	-0.00347	0.001221

benzene_methane

MP2

C6	H16	0.004597	0.014319	0.002802	-0.00202	0.000778

benzene_water

MP2

C3	H15	0.008152	0.02573	0.005461	-0.00449	0.000971

ethene_dimer

MP2

H3	H10	0.003103	0.012335	0.002382	-0.00168	0.000702
H3	H9	0.003102	0.012335	0.002381	-0.00168	0.000702
H10	H4	0.0031	0.012328	0.00238	-0.00168	0.000702
H9	H4	0.003101	0.012331	0.002381	-0.00168	0.000702

ethene_ethine

MP2

H9	(3,-1)	0.005612	0.016567	0.003248	-0.00235	0.000894

formamide_dimer

MP2

H5	O8	0.031794	0.104075	0.02802	-0.03002	-0.002
O2	H11	0.031789	0.104064	0.028015	-0.03001	-0.002

formic_acid_dimer

MP2

H10	O3	0.045034	0.112719	0.03784	-0.0475	-0.00966
O8	H5	0.04503	0.112712	0.037836	-0.04749	-0.00966

indole_benzene_stack

MP2

H7	C18	0.004901	0.017457	0.003428	-0.00249	0.000937
C1	C22	0.007154	0.022915	0.004643	-0.00356	0.001086
H8	C15	0.004143	0.014163	0.0027	-0.00186	0.000841

indole_benzene_t-shape

MP2

H13	C4	0.006423	0.023399	0.004709	-0.00357	0.001141

methane_dimer

MP2

H3	H9	0.004645	0.016282	0.003234	-0.0024	0.000837

phenol_dimer

MP2

O14	H3	0.013481	0.062517	0.012722	-0.00981	0.002907
O2	H22	0.009275	0.038832	0.007754	-0.0058	0.001954

pyrazine_dimer

MP2

C14	C1	0.005004	0.015611	0.003019	-0.00214	0.000884
C2	C12	0.005003	0.015605	0.003018	-0.00213	0.000883
N13	(3,-1)	0.003535	0.012354	0.002339	-0.00159	0.000749

uracil_dimer_hb

MP2

O13	H10	0.041386	0.12165	0.036696	-0.04298	-0.00628
H22	O1	0.041331	0.121571	0.036649	-0.0429	-0.00626

uracil_dimer_stack

MP2						
O19	N1	0.004738	0.018815	0.003656	-0.00261	0.001048
N20	C10	0.006552	0.024336	0.00493	-0.00375	0.001154
C22	N8	0.00592	0.023261	0.004515	-0.00321	0.0013
C16	C4	0.0056	0.015272	0.003002	-0.00219	0.000816
N13	O7	0.00474	0.01883	0.003659	-0.00261	0.001048

water_dimer

MP2						
H3	O4	0.016533	0.065258	0.014627	-0.01294	0.001688

Table S4. Local properties at the intermolecular (3,-1) critical points of electron density constructed using the promolecule model for **S22** set.

2-pyridoxine_2-aminopyridine

SIAM		rho	lapl	g	v	h
O1	H25	0.041862	0.084212	0.028562	-0.03607	-0.00751
H12	N13	0.040398	0.076972	0.026485	-0.03373	-0.00724

adenine_thymine_stack

SIAM						
H21	N10	0.010509	0.02616	0.005808	-0.00508	0.000732
C24	C6	0.009803	0.023711	0.005241	-0.00455	0.000686
C17	N13	0.009437	0.024473	0.005289	-0.00446	0.000829
C28	C5	0.008308	0.021375	0.004541	-0.00374	0.000802

adenine_thymine_wc

SIAM						
O23	H14	0.032439	0.07163	0.021439	-0.02497	-0.00353
H26	N1	0.050922	0.087814	0.034722	-0.04749	-0.01277
O24	H11	0.007268	0.020915	0.004275	-0.00332	0.000954

ammonia_dimer

SIAM						
H7	H4	2.30E-06	9.00E-06	2.00E-06	-1.10E-06	8.00E-07

benzene_ammonia

SIAM						
H16	C2	0.011029	0.024124	0.005594	-0.00516	0.000437

benzene_dimer1

SIAM						
C17	H7	0.012376	0.027216	0.006442	-0.00608	0.000362

benzene_dimer2

SIAM						
C2	C15	0.008033	0.018757	0.004051	-0.00341	0.000638
C3	C14	0.008021	0.018734	0.004045	-0.00341	0.000638

benzene_hcn

SIAM						
C5	H15	0.015345	0.03283	0.008197	-0.00819	1.09E-05

benzene_methane

SIAM						
H16	C6	0.008796	0.019136	0.004268	-0.00375	0.000516

benzene_water

SIAM						
H15	C3	0.016327	0.032392	0.00842	-0.00874	-0.00032

ethene_dimer

SIAM						
H10	H3	0.008225	0.018454	0.004038	-0.00346	0.000575
H3	H9	0.008225	0.018453	0.004038	-0.00346	0.000575
H10	H4	0.008222	0.018449	0.004037	-0.00346	0.000576
H9	H4	0.008223	0.01845	0.004037	-0.00346	0.000575

ethene_ethine

SIAM						
H9	C2	0.009986	0.02135	0.00489	-0.00444	0.000448

formamide_dimer

SIAM						
H5	O8	0.03891	0.080469	0.026273	-0.03243	-0.00616
O2	H11	0.038904	0.080462	0.026268	-0.03242	-0.00615

formic_acid_dimer

SIAM						
O3	H10	0.052214	0.092751	0.03644	-0.04969	-0.01325
H5	O8	0.05221	0.092748	0.036437	-0.04969	-0.01325

indole_benzene_stack

SIAM						
C22	C1	0.013104	0.029943	0.007082	-0.00668	0.000404

indole_benzene_t-shape

SIAM						
C4	H13	0.014339	0.030755	0.00756	-0.00743	0.000128

methane_dimer

SIAM						
H9	H3	0.009645	0.019952	0.00458	-0.00417	0.000408

phenol_dimer

SIAM						
H22	O2	0.013356	0.03558	0.008101	-0.00731	0.000794
O14	H3	0.019932	0.051722	0.012839	-0.01275	9.17E-05

pyrazine_dimer

SIAM						
C2	C12	0.008692	0.021195	0.004588	-0.00388	0.000711
C1	C14	0.008695	0.021202	0.004589	-0.00388	0.000711

uracil_dimer_hb

SIAM						
H22	O1	0.048717	0.091283	0.033915	-0.04501	-0.01109
O13	H10	0.04877	0.091329	0.033956	-0.04508	-0.01112

uracil_dimer_stack

SIAM						
C18	N1	0.008864	0.023871	0.005069	-0.00417	0.000899
N20	C10	0.011066	0.03003	0.006583	-0.00566	0.000925
C22	N8	0.011065	0.030027	0.006582	-0.00566	0.000924
C16	C4	0.00831	0.019529	0.004234	-0.00359	0.000648
N13	C6	0.008875	0.023878	0.005073	-0.00418	0.000897

water_dimer

SIAM						
H3	O4	0.022989	0.05503	0.014524	-0.01529	-0.00077

Table S5. Local properties at the intermolecular (3,-1) critical points of electron density which were observed in each model of electron density.

SIAM

2-pyridoxine_2-aminopyridine

ApprRho		rho	lapl	g	v	h
O1	H25	0.04186	0.08421	0.02856	-0.03607	-0.00751
H12	N13	0.04040	0.07697	0.02649	-0.03373	-0.00724

adenine_thymine_stack

ApprRho						
H21	N10	0.01051	0.02616	0.00581	-0.00508	0.00073
C24	C6	0.00980	0.02371	0.00524	-0.00455	0.00069
C17	N13	0.00944	0.02447	0.00529	-0.00446	0.00083
C28	C5	0.00831	0.02138	0.00454	-0.00374	0.00080

adenine_thymine_wc

ApprRho						
O23	H14	0.03244	0.07163	0.02144	-0.02497	-0.00353
H26	N1	0.05092	0.08781	0.03472	-0.04749	-0.01277
O24	H11	0.00727	0.02091	0.00428	-0.00332	0.00095

ammonia_dimer

ApprRho						
H7	H4	0.00000	0.00001	0.00000	0.00000	0.00000

M062x

2-pyridoxine_2-aminopyridine

TrueRho		rho	lapl	g	v	h
O1	H25	0.03588	0.10976	0.03082	-0.03421	-0.00338
H12	N13	0.03477	0.07426	0.02351	-0.02845	-0.00494

adenine_thymine_stack

TrueRho						
N10	H21	0.00608	0.02008	0.00405	-0.00309	0.00097
N7	O25	0.00440	0.01476	0.00296	-0.00224	0.00073
N13	C17	0.00592	0.01831	0.00362	-0.00266	0.00096
C5	N26	0.00485	0.01459	0.00292	-0.00219	0.00073

adenine_thymine_wc

TrueRho						
O23	H14	0.02588	0.09281	0.02260	-0.02199	0.00060
H26	N1	0.04601	0.07209	0.02979	-0.04156	-0.01177
O24	H11	0.00545	0.01836	0.00375	-0.00291	0.00084

ammonia_dimer

TrueRho						
H4	H7	0.00000	0.00001	0.00000	0.00000	0.00000

mp2

2-pyridoxine_2-aminopyridine

TrueRho						
O1	H25	0.03466	0.11088	0.03086	-0.03401	-0.00314
H12	N13	0.03356	0.08023	0.02450	-0.02894	-0.00444

adenine_thymine_stack

TrueRho						
N10	H21	0.00578	0.02136	0.00421	-0.00308	0.00113
N7	O25	0.00404	0.01535	0.00299	-0.00214	0.00085
N13	C17	0.00581	0.01902	0.00372	-0.00269	0.00103
C5	N26	0.00456	0.01551	0.00300	-0.00213	0.00087

adenine_thymine_wc

TrueRho						
O23	H14	0.02508	0.09165	0.02255	-0.02219	0.00036
H26	N1	0.04401	0.08775	0.03168	-0.04142	-0.00974
O24	H11	0.00498	0.01917	0.00382	-0.00284	0.00098

ammonia_dimer

TrueRho						
H4	H7	0.00000	0.00001	0.00000	0.00000	0.00000

benzene_ammonia

ApprRho

H16	C2	0.01103	0.02412	0.00559	-0.00516	0.00044

benzene_ammonia

TrueRho

C2	H16	0.00506	0.01655	0.00332	-0.00251	0.00082

benzene_ammonia

TrueRho

C2	H16	0.00480	0.01757	0.00342	-0.00246	0.00097

benzene_dimer1

ApprRho

C17	H7	0.01238	0.02722	0.00644	-0.00608	0.00036

benzene_dimer1

TrueRho

C17	H7	0.00556	0.01856	0.00378	-0.00292	0.00086

benzene_dimer1

TrueRho

C17	H7	0.00522	0.01946	0.00385	-0.00284	0.00101

benzene_dimer2

ApprRho

C2	C15	0.00803	0.01876	0.00405	-0.00341	0.00064
C3	C14	0.00802	0.01873	0.00405	-0.00341	0.00064

benzene_dimer2

TrueRho

C15	C2	0.00476	0.01321	0.00253	-0.00177	0.00077
C14	C3	0.00475	0.01319	0.00253	-0.00176	0.00077

benzene_dimer2

TrueRho

C15	C2	0.00473	0.01380	0.00264	-0.00183	0.00081
C14	C3	0.00472	0.01378	0.00263	-0.00182	0.00081

benzene_hcn

ApprRho

C5	H15	0.01534	0.03283	0.00820	-0.00819	0.00001

benzene_hcn

TrueRho

C5	H15	0.00647	0.02274	0.00463	-0.00358	0.00105

benzene_hcn

TrueRho

C5	H15	0.00609	0.02364	0.00469	-0.00347	0.00122

benzene_methane

ApprRho

H16	C6	0.00880	0.01914	0.00427	-0.00375	0.00052

benzene_methane

TrueRho

C6	H16	0.00470	0.01368	0.00270	-0.00198	0.00072

benzene_methane

TrueRho

C6	H16	0.00460	0.01432	0.00280	-0.00202	0.00078

benzene_water

ApprRho

H15	C3	0.01633	0.03239	0.00842	-0.00874	-0.00032

benzene_water

TrueRho

C3	H15	0.00835	0.02528	0.00534	-0.00435	0.00098

benzene_water

TrueRho

C3	H15	0.00815	0.02573	0.00546	-0.00449	0.00097

ethene_dimer

ApprRho

H10	H3	0.00822	0.01845	0.00404	-0.00346	0.00058
H3	H9	0.00822	0.01845	0.00404	-0.00346	0.00058
H10	H4	0.00822	0.01845	0.00404	-0.00346	0.00058
H9	H4	0.00822	0.01845	0.00404	-0.00346	0.00058

ethene_ethine

ApprRho

H9	C2	0.00999	0.02135	0.00489	-0.00444	0.00045

formamide_dimer

ApprRho

H5	O8	0.03891	0.08047	0.02627	-0.03243	-0.00616
O2	H11	0.03890	0.08046	0.02627	-0.03242	-0.00615

formic_acid_dimer

ApprRho

O3	H10	0.05221	0.09275	0.03644	-0.04969	-0.01325
H5	O8	0.05221	0.09275	0.03644	-0.04969	-0.01325

indole_benzene_stack

ApprRho

C22	C1	0.01310	0.02994	0.00708	-0.00668	0.00040

ethene_dimer

TrueRho

H3	H10	0.00342	0.01198	0.00239	-0.00178	0.00061
H3	H9	0.00342	0.01198	0.00239	-0.00178	0.00061
H10	H4	0.00342	0.01198	0.00239	-0.00178	0.00061
H9	H4	0.00342	0.01198	0.00239	-0.00178	0.00061

ethene_ethine

TrueRho

H9	bcp	0.00560	0.01572	0.00307	-0.00221	0.00086

formamide_dimer

TrueRho

H5	O8	0.03290	0.10410	0.02804	-0.03005	-0.00201
O2	H11	0.03290	0.10409	0.02803	-0.03004	-0.00201

formic_acid_dimer

TrueRho

H10	O3	0.04793	0.09891	0.03719	-0.04966	-0.01247
O8	H5	0.04792	0.09891	0.03719	-0.04966	-0.01246

indole_benzene_stack

TrueRho

C1	C22	0.00725	0.02326	0.00471	-0.00361	0.00110

ethene_dimer

TrueRho

H3	H10	0.00310	0.01234	0.00238	-0.00168	0.00070
H3	H9	0.00310	0.01233	0.00238	-0.00168	0.00070
H10	H4	0.00310	0.01233	0.00238	-0.00168	0.00070
H9	H4	0.00310	0.01233	0.00238	-0.00168	0.00070

ethene_ethine

TrueRho

H9	bcp	0.00561	0.01657	0.00325	-0.00235	0.00089

formamide_dimer

TrueRho

H5	O8	0.03179	0.10407	0.02802	-0.03002	-0.00200
O2	H11	0.03179	0.10406	0.02802	-0.03001	-0.00200

formic_acid_dimer

TrueRho

H10	O3	0.04503	0.11272	0.03784	-0.04750	-0.00966
O8	H5	0.04503	0.11271	0.03784	-0.04749	-0.00966

indole_benzene_stack

TrueRho

C1	C22	0.00715	0.02291	0.00464	-0.00356	0.00109

indole_benzene_t-shape

ApprRho

C4	H13	0.01434	0.03075	0.00756	-0.00743	0.00013

indole_benzene_t-shape

TrueRho

H13	C4	0.00672	0.02215	0.00456	-0.00358	0.00098

indole_benzene_t-shape

TrueRho

H13	C4	0.00642	0.02340	0.00471	-0.00357	0.00114

methane_dimer

ApprRho

H9	H3	0.00964	0.01995	0.00458	-0.00417	0.00041

methane_dimer

TrueRho

H3	H9	0.00488	0.01533	0.00311	-0.00239	0.00072

methane_dimer

TrueRho

H3	H9	0.00464	0.01628	0.00323	-0.00240	0.00084

phenol_dimer

ApprRho

H22	O2	0.01336	0.03558	0.00810	-0.00731	0.00079
O14	H3	0.01993	0.05172	0.01284	-0.01275	0.00009

phenol_dimer

TrueRho

O2	H22	0.00983	0.03703	0.00755	-0.00585	0.00171
O14	H3	0.01428	0.06089	0.01254	-0.00986	0.00268

phenol_dimer

TrueRho

O2	H22	0.00927	0.03883	0.00775	-0.00580	0.00195
O14	H3	0.01348	0.06252	0.01272	-0.00981	0.00291

pyrazine_dimer

ApprRho

C2	C12	0.00869	0.02120	0.00459	-0.00388	0.00071
C1	C14	0.00869	0.02120	0.00459	-0.00388	0.00071

pyrazine_dimer

TrueRho

C2	C12	0.00507	0.01492	0.00291	-0.00209	0.00082
C14	C1	0.00508	0.01493	0.00291	-0.00209	0.00082

pyrazine_dimer

TrueRho

C2	C12	0.00500	0.01560	0.00302	-0.00213	0.00088
C14	C1	0.00500	0.01561	0.00302	-0.00214	0.00088

uracil_dimer_hb

ApprRho

H22	O1	0.04872	0.09128	0.03391	-0.04501	-0.01109
O13	H10	0.04877	0.09133	0.03396	-0.04508	-0.01112

uracil_dimer_hb

TrueRho

H22	O1	0.04323	0.11440	0.03624	-0.04388	-0.00764
O13	H10	0.04330	0.11441	0.03628	-0.04396	-0.00768

uracil_dimer_hb

TrueRho

H22	O1	0.04133	0.12157	0.03665	-0.04290	-0.00626
O13	H10	0.04139	0.12165	0.03670	-0.04298	-0.00628

uracil_dimer_stack

ApprRho

C18	N1	0.00886	0.02387	0.00507	-0.00417	0.00090
N20	C10	0.01107	0.03003	0.00658	-0.00566	0.00092
C22	N8	0.01107	0.03003	0.00658	-0.00566	0.00092
C16	C4	0.00831	0.01953	0.00423	-0.00359	0.00065
N13	C6	0.00888	0.02388	0.00507	-0.00418	0.00090

uracil_dimer_stack

TrueRho

O19	N1	0.00514	0.01834	0.00366	-0.00274	0.00092
N20	C10	0.00654	0.02381	0.00481	-0.00366	0.00114
C22	N8	0.00654	0.02380	0.00481	-0.00366	0.00114
C16	C4	0.00550	0.01443	0.00284	-0.00208	0.00077
N13	O7	0.00514	0.01835	0.00367	-0.00274	0.00092

uracil_dimer_stack

TrueRho

O19	N1	0.00474	0.01882	0.00366	-0.00261	0.00105
N20	C10	0.00655	0.02434	0.00493	-0.00375	0.00115
C22	N8	0.00592	0.02326	0.00451	-0.00321	0.00130
C16	C4	0.00560	0.01527	0.00300	-0.00219	0.00082
N13	O7	0.00474	0.01883	0.00366	-0.00261	0.00105

water_dimer

ApprRho

H3	O4	0.02299	0.05503	0.01452	-0.01529	-0.00077

water_dimer

TrueRho

H3	O4	0.01737	0.06533	0.01459	-0.01285	0.00174

water_dimer

TrueRho

H3	O4	0.01653	0.06526	0.01463	-0.01294	0.00169

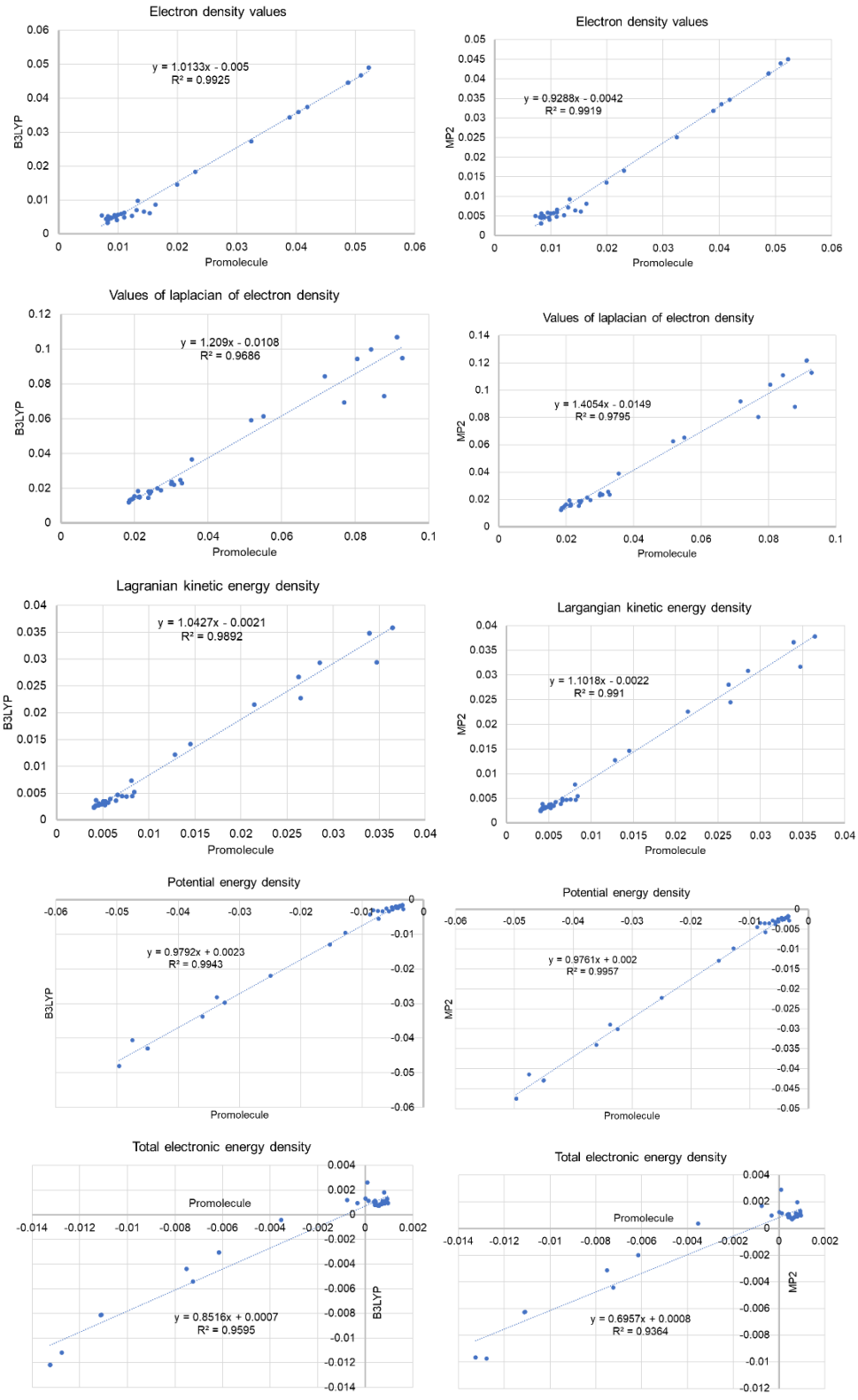

Figure S1. Scatter plots and linear trends of the QM and promolecule-based descriptors at the intermolecular (3,-1) critical points of $\rho(\mathbf{r})$ for the **S22** set.