FOUNDATIONS
ADVANCES

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Supporting information for article:

Extension of the transferable aspherical pseudoatom data bank for the comparison of molecular electrostatic potentials in structure–activity studies

Prashant Kumar, Barbara Gruza, Sławomir Antonii Bojarowski and Paulina Maria Dominiak

SUPPORTING INFORMATION

Extension of the transferable aspherical pseudoatom data bank for the comparison of molecular electrostatic potentials in structure–activity studies

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Table 1S. Atom types in the UBDB2018 databank. The *D* symbol represents dummy atom required for coordinate system definition. The first letter in the atom type code goes for a chemical element symbol. The T letter marks atom types which need further improvement in atom type definition or more entries from model molecules to confirm parametrization. The meaning of atom labelling of the Nearest and Next-Nearest Neighbour Atom Types is given in the Table 2S.

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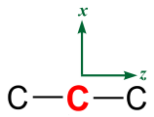
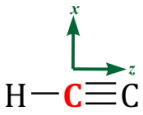
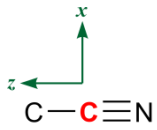
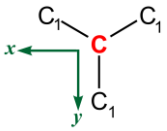
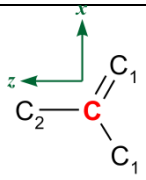
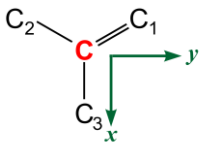
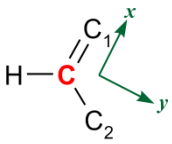
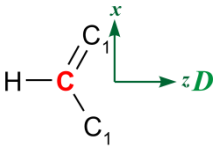
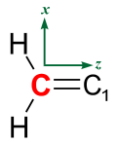
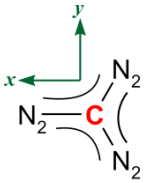
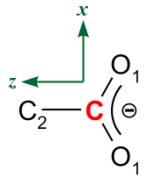
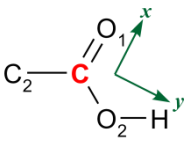
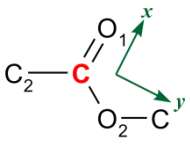
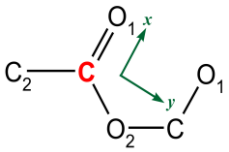
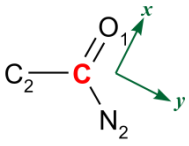
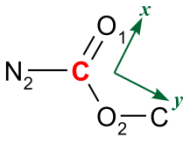
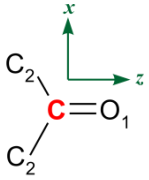
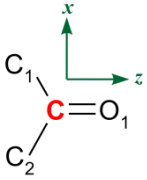
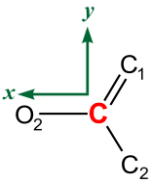
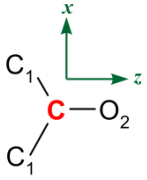
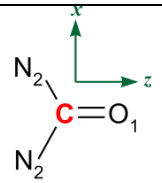
 C203	 C202	 C201	 C522	 C313-T
 C516	 C311	 C312-T	 C300-T	 C310
 C301	 C302	 C303	 C510	 C304
 C305	 C306*	 C307	 C523	 C314-T



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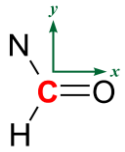

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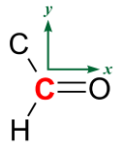

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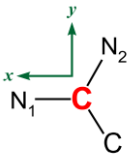

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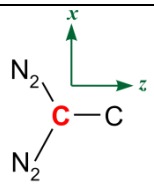

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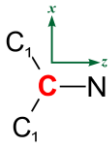

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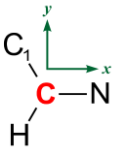

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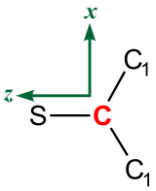

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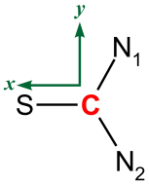

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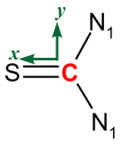

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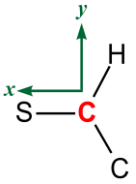

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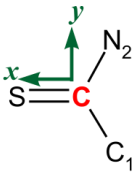

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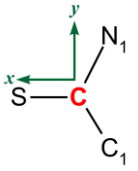

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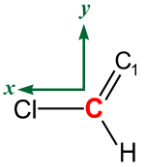

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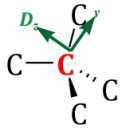

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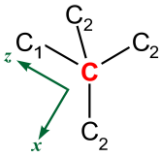

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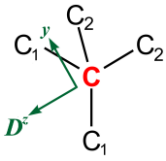

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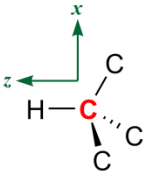

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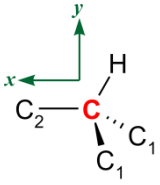

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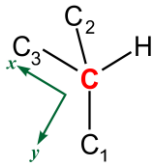

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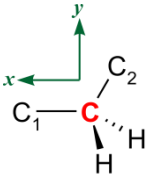

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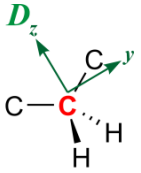

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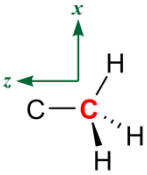

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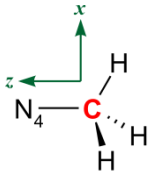

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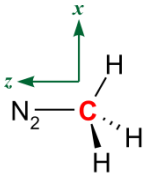

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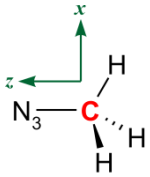

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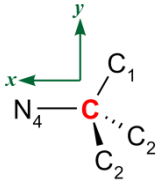

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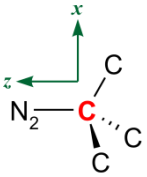

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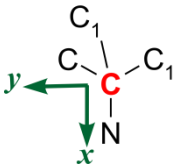

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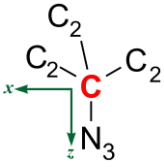

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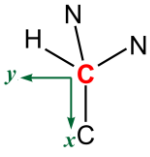

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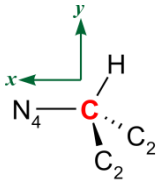

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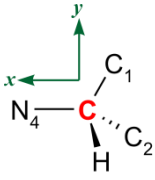

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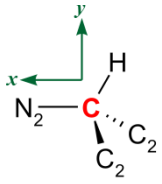

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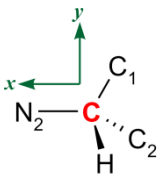
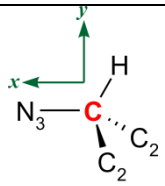
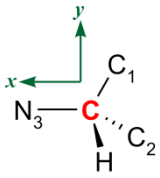
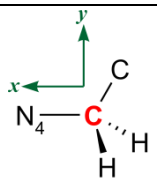
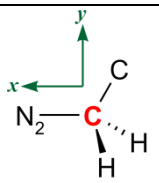
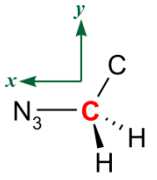
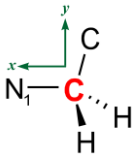
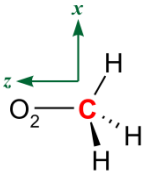
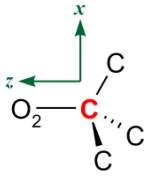
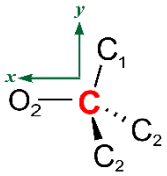
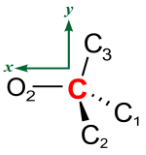
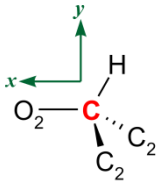
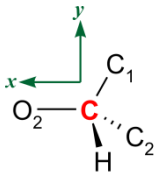
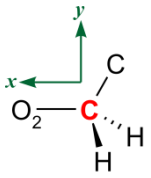
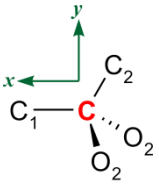
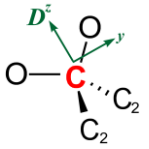
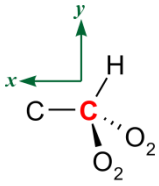
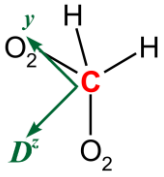
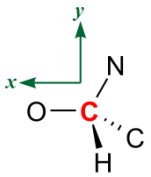
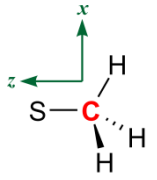
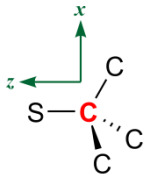
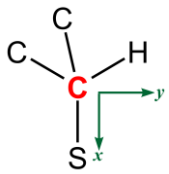
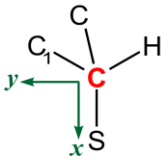
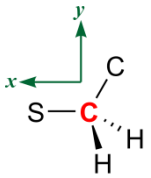
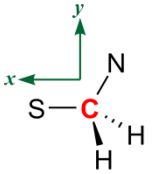
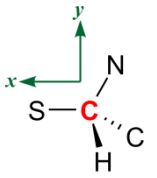
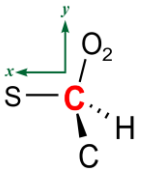
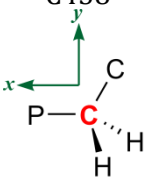
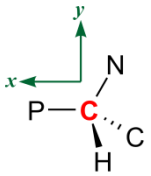
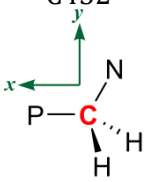
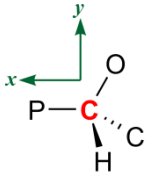
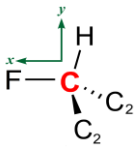
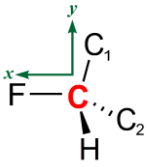
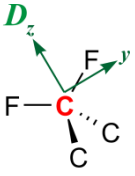
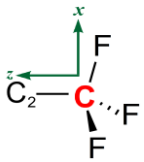
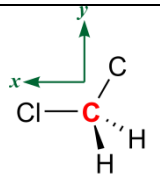
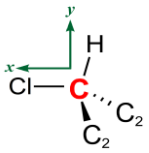
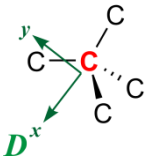
 C421	 C424*	 C425	 C412	 C418
 C423	 C476	 C427	 C428	 C464*
 C460	 C430*	 C431	 C429	 C443
 C444	 C440	 C468	 C450	 C433
 C439	 C459	 C438	 C434	 C452
 C453	 C461	 C432	 C446-T4	 C448
 C447	 C855*	 C466	 C455	 C756



C437



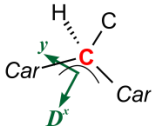
C837*



C407-5M-T3

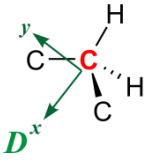
C465-6M

C457-3M

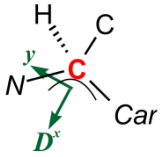


C472-5M

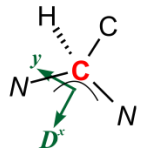
C458-3M



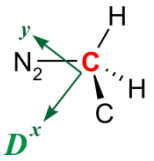
C406-5M



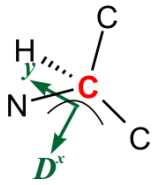
C469-5M



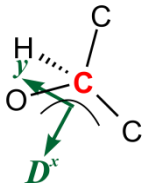
C471-5M-T



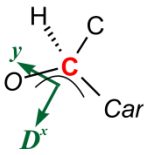
C419-5M



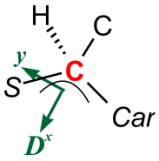
C475-4M-T



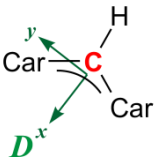
C473-4M



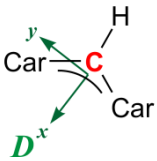
C711-5M



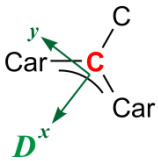
C712-5M



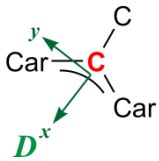
C330-6M



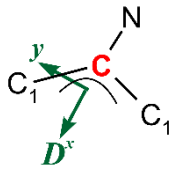
C331-5M



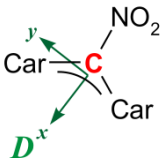
C332-6M



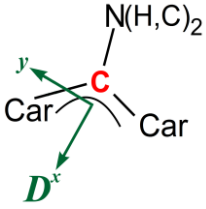
C333-5M



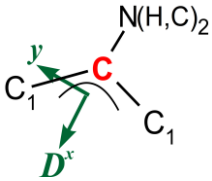
C706-6M-T



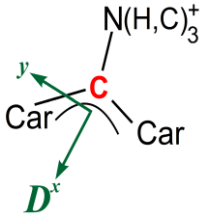
C334-6M



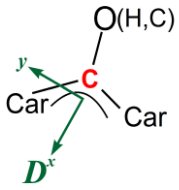
C338-6M



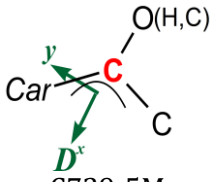
C550-5M-T



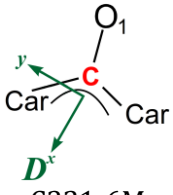
C340-6M



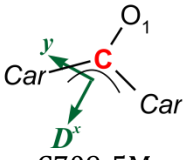
C341-6M



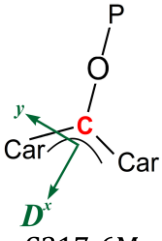
C729-5M



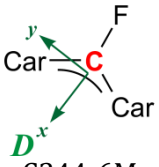
C321-6M



C709-5M



C317-6M



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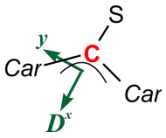

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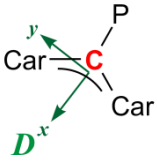

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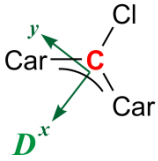

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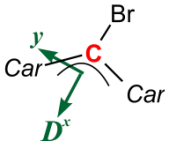

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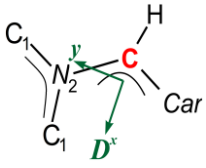

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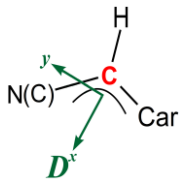

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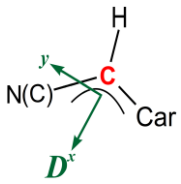

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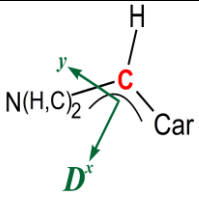

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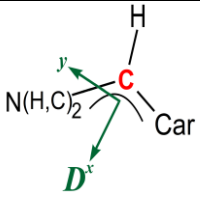

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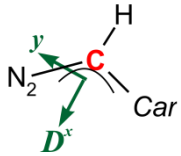

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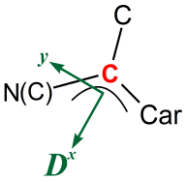

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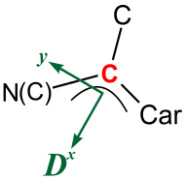

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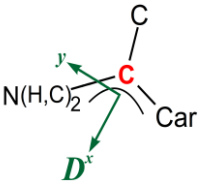

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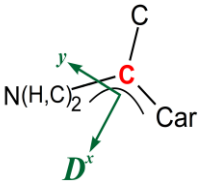

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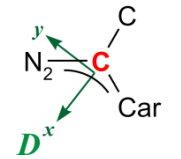

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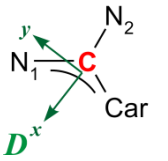

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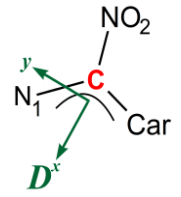

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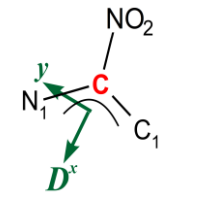

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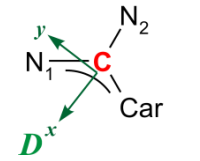

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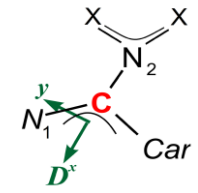

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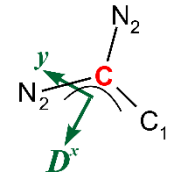

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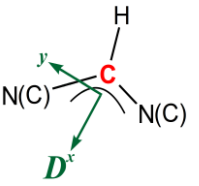

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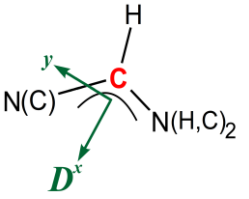

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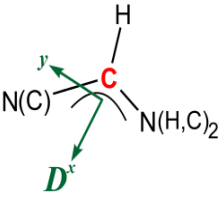

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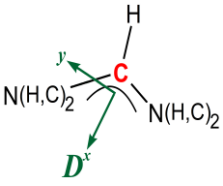

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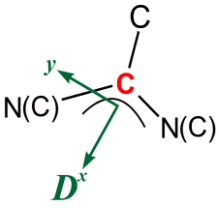

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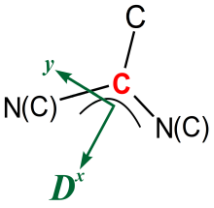

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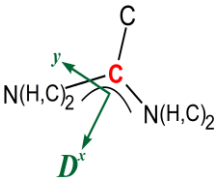
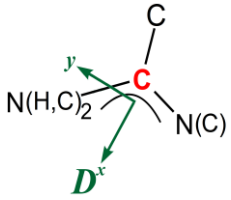


C366-5M-T4



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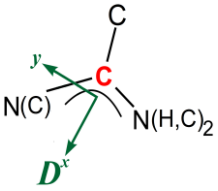

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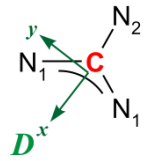

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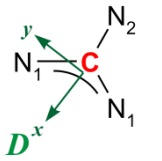

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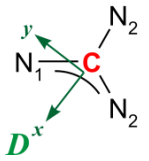

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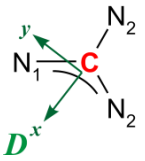

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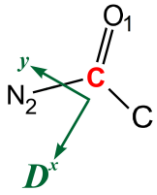
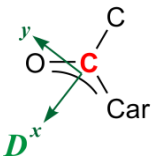


C518-4M



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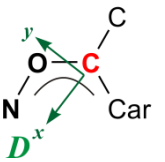

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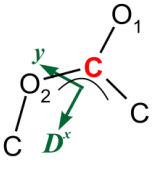

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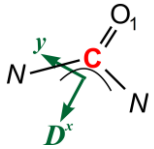
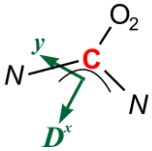


C378-6M



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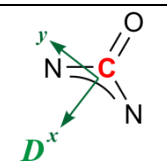
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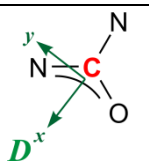
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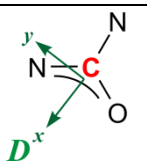
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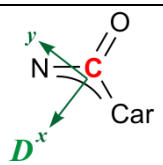
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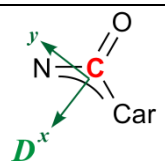
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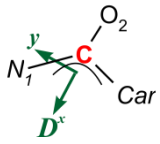
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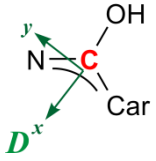
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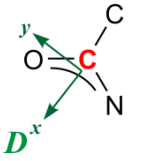
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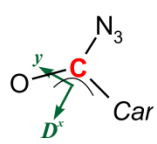
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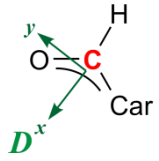
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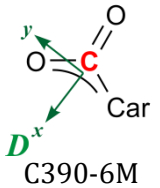
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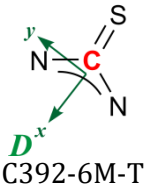
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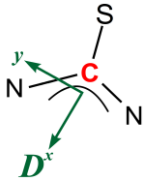
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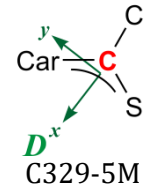
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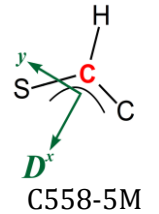
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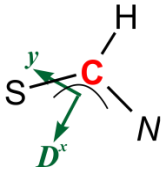
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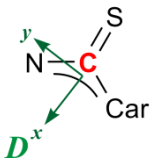
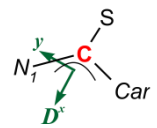
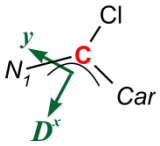
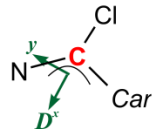
C567-5M

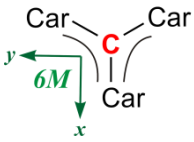

C393-6M-T2

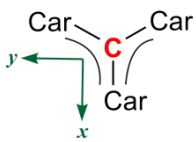

C394-6M

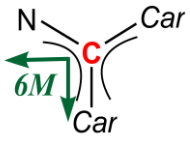

C555-5M-T

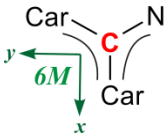

C563-6M

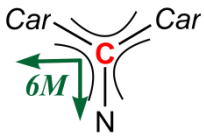

C573-5M


C501-11M


C507-12M


C702-12M


C503-11M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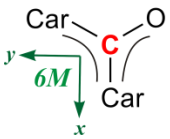
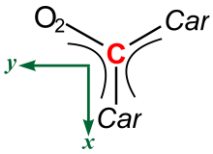

C504-11M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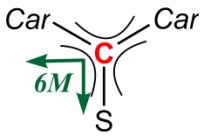
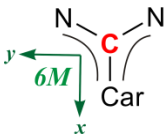
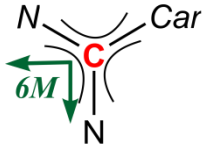
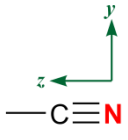
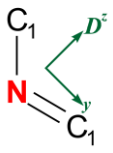
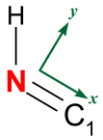
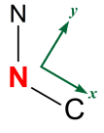
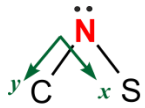

C564-11M


C505-11M-T

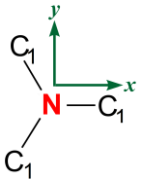

C701-12M

Nitrogen				
				
N101	N205	N204	N206	N203-T

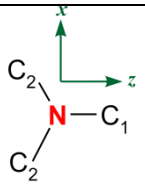
N202



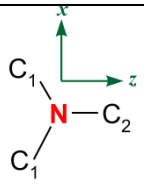
N208



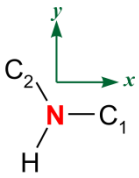
N333-T*



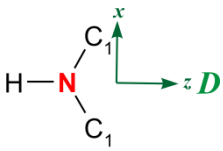
N313



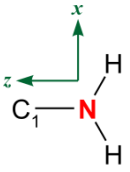
N314



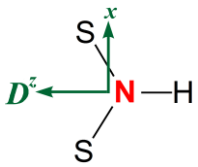
N315



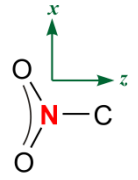
N311



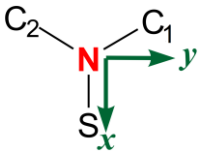
N310



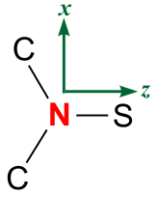
N334-T2



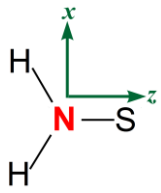
N312



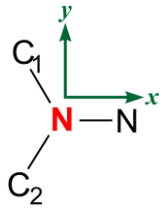
N319-T4



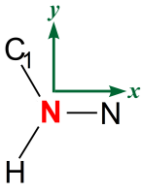
N399



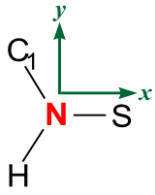
N332



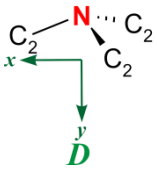
N336



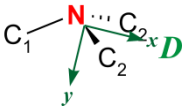
N317



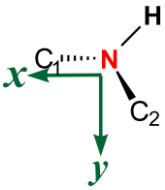
N309



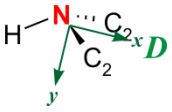
N301



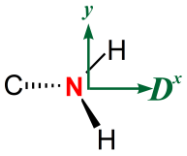
N306



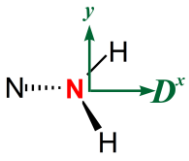
N305



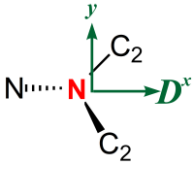
N303



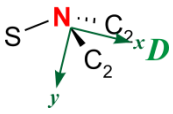
N302



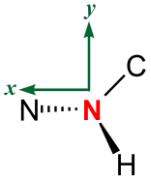
N308



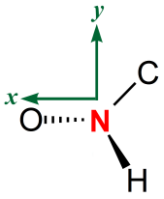
N836*



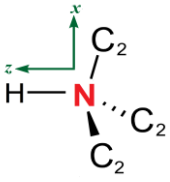
N304



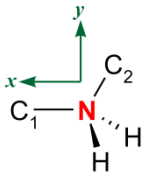
N307



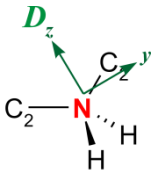
N330-T



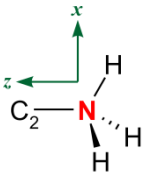
N404



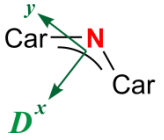
N403



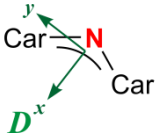
N402



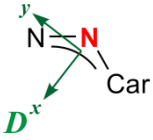
N401



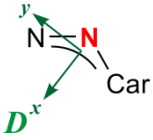
N211-5M



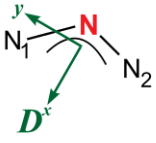
N210-6M



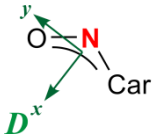
N213-5M

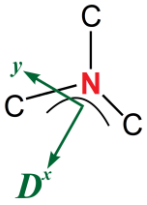


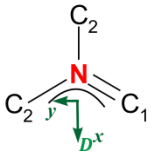
N215-6M

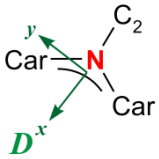


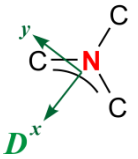
N207-5M

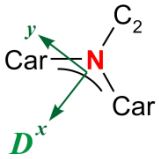

N212-5M

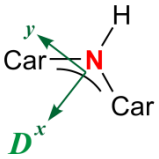

N331-5M-T

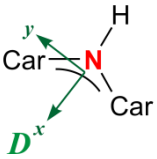

N324-5M

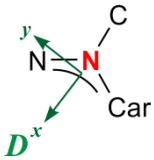

N323-5M

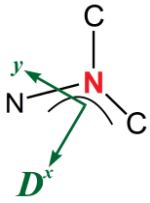

N325-6M-T


N322-6M-T


N321-5M


N320-6M


N326-6M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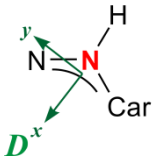
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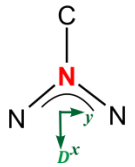
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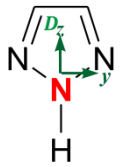
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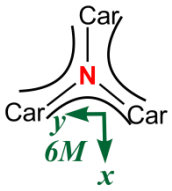
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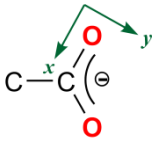
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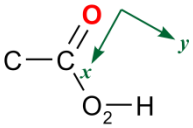
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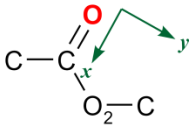
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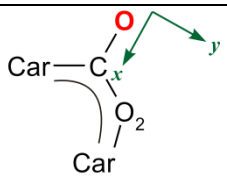
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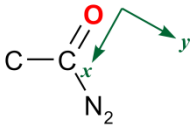
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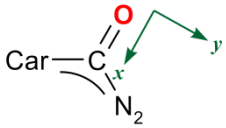
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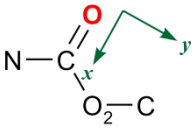
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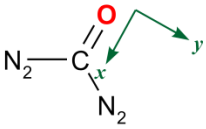
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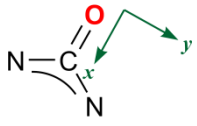
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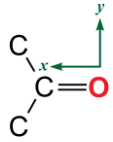
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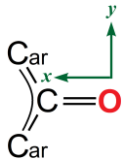
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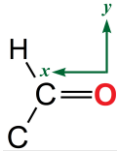
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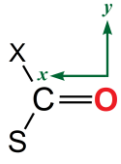
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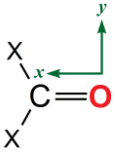
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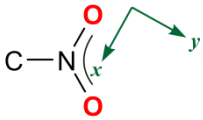
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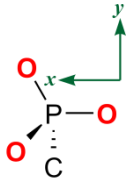
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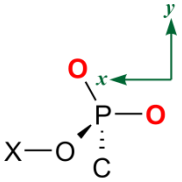
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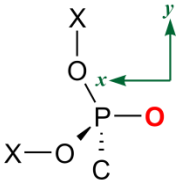
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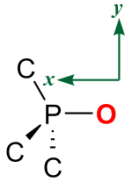
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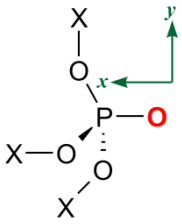
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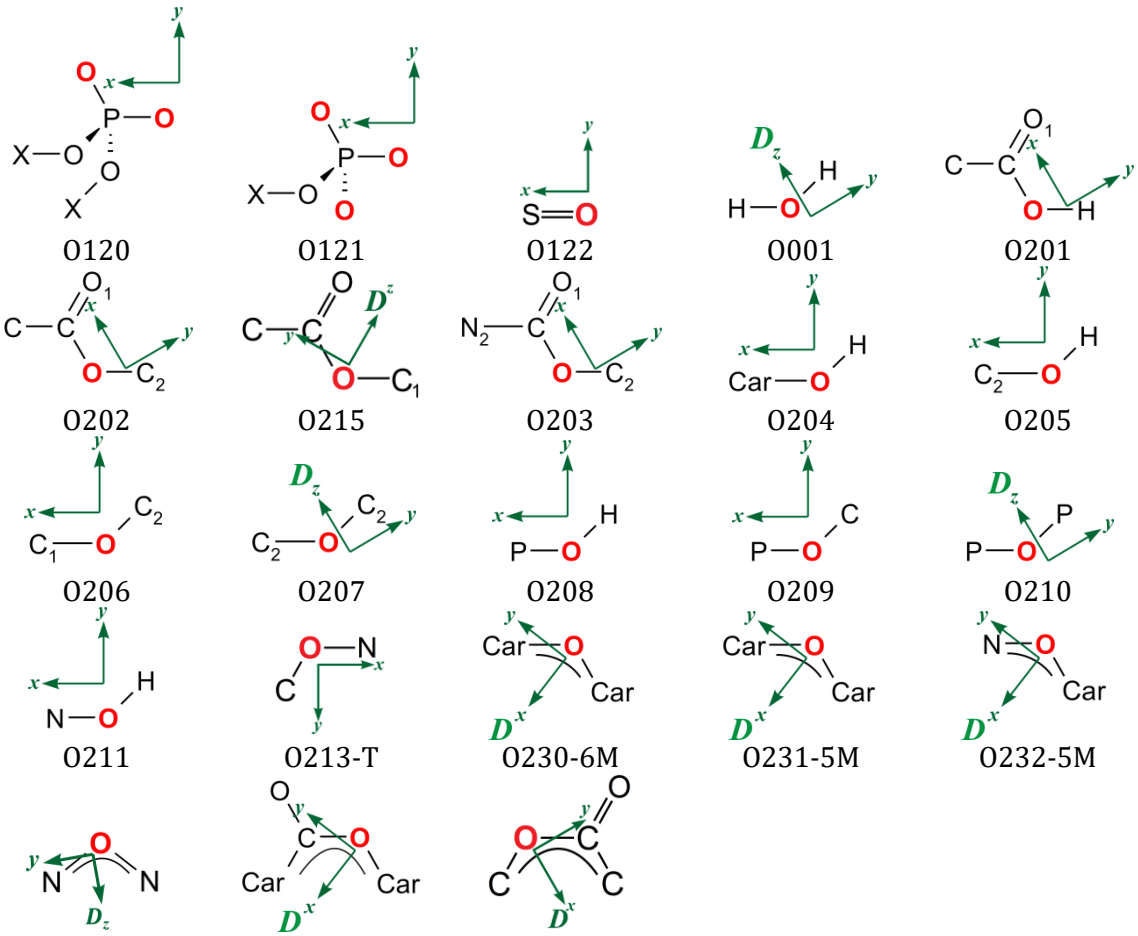
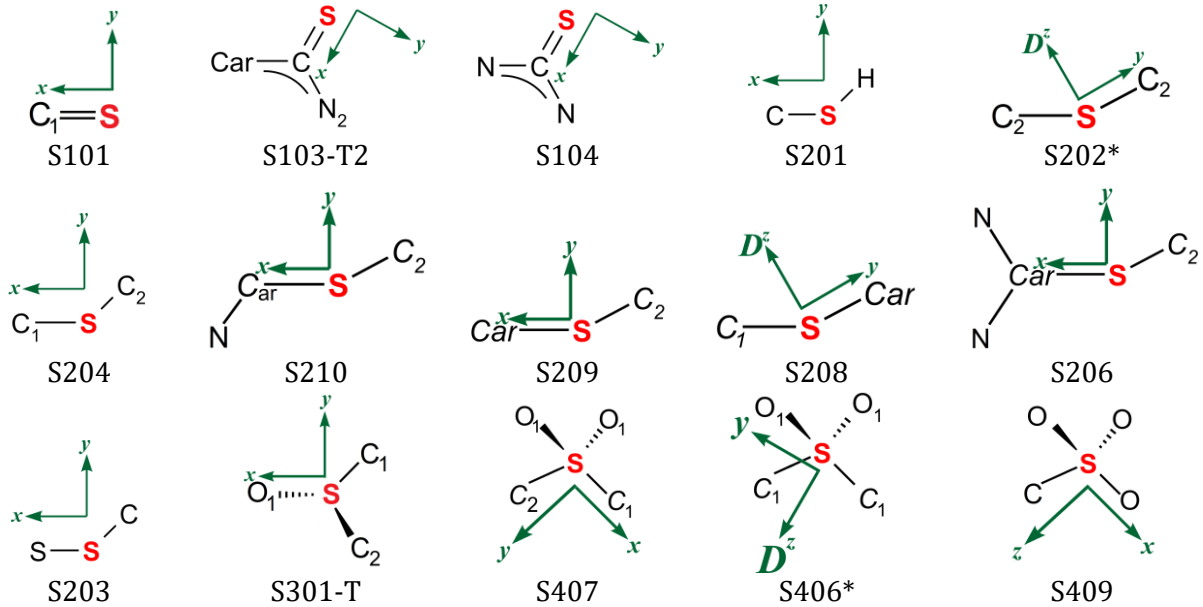
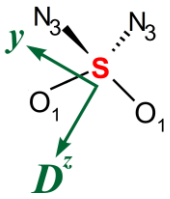

O120
O121
O122
O001
O201
O202
O215
O203
O204
O205
O206
O207
O208
O209
O210
O211
O213-T
O230-6M
O231-5M
O232-5M
O216-5M
O233-6M
O214-5M

Sulphur


S101
S103-T2
S104
S201
S202*
S204
S210
S209
S208
S206
S203
S301-T
S407
S406*
S409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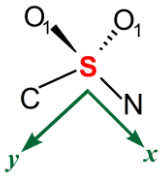
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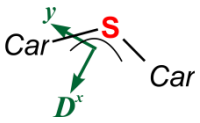
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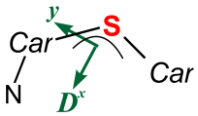
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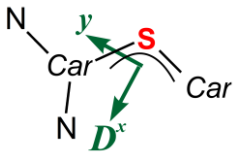
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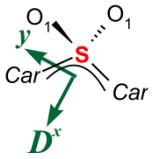
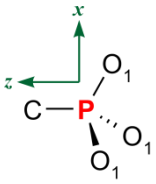

S408

Phosphorus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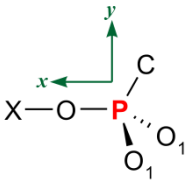
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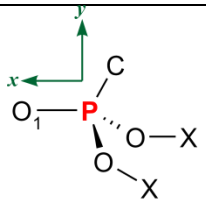
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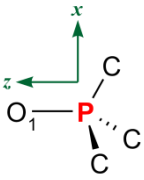
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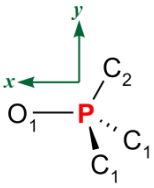
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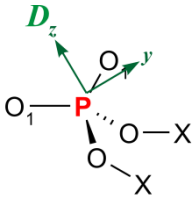
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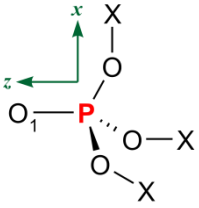
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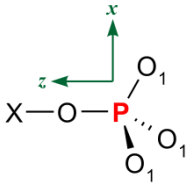
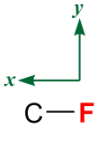
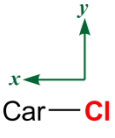
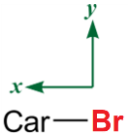
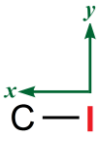
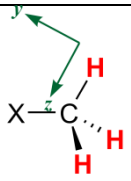

P409

Fluorine		Chlorine		Bromine	Iodine
					
F001	F002	Cl01-T	Cl02-T	Br02	I001

Hydrogen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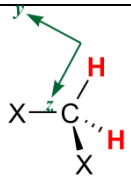
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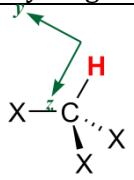
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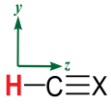
H104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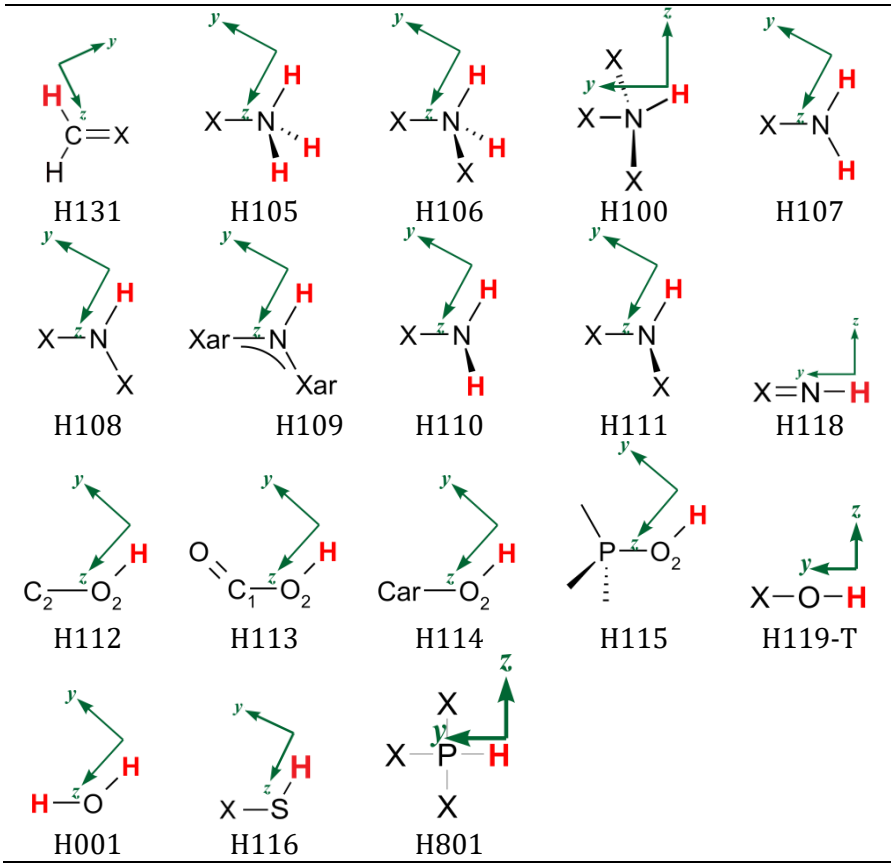


Table 2S. Labelling of the Nearest and Next-Nearest Neighbour Atom Types used in Table 1S.[a]

C	any carbon
C_1	Csp^2 aromatic and nonaromatic
C_2	Csp^3
C_3	Csp^1
Car	Csp^2 in planar ring
N	any nitrogen
N_1	$Nsp^2(2)$
N_2	$Nsp^2(3)$
N_3	$Nsp^3(3)$
N_4	$Nsp^3(4)$
O_1	$Osp^2(1)$
O_2	$Osp^3(2)$
X	any non-hydrogen atom; in the case of CPO_3 and CPO_4 groups carbon or hydrogen atoms

* - there can be two C_1 atoms, two C_2 atoms or two C_3 atoms

** - there can be two N_1 atoms, two N_2 atom, two N_3 atoms or two N_4 atoms

nM - indicates number of neighbours

T - simplified atom definition

[a] numbers in parentheses represent number of bonds to the atoms

Table 3S. Cambridge Structural Databank REFCODES for model molecules used to build the UBDB2018.

ABABIP	ABABOW	ABACAJ	ABAFUG	ABAHUI	ABALAS	ABALIA
ABATOO	ABEBUE	ABEFAO	ABEHEV	ABEKAV	ABEKEY	ABEKEZ
ABELAV	ABELEZ	ABEROP	ABIMUT	ABIPIL	ABIVUD	ABIZAM
ABUBEE	ABUGOT	ABUQAP	ABUQOD	ABURAQ	ABUTAS	ACACOX
ACAJEV	ACAMOX	ACANAC11	ACAYUY	ACAZOV	ACECAN	ACENAZ
ACERIK01	ACETSC10	ACEZIR99	ACGLUA11	ACICUK	ACIDAR	ACIDOH
ACIHEB	ACIMDC99	ACINDN	ACIRAG	ACIROU	ACIXAN	ACOREP
ACRLAC02	ACSALA01	ACUPUL	ACUZAZ99	ACXMPR	ACYHXA01	ADAGOC
ADAHET	ADAJUK01	ADAKUM	ADALAT	ADAVUW	ADAZOV	ADEKUQ
ADENCH99	ADEPAB	ADHELA10	ADIHUR	ADIMIK	ADINAD	ADITAI
ADOJAG	ADOJEI	ADONAK	ADOPIU	ADOTUJ	ADPOSD	ADULUG
ADUNAO	ADUQAS	ADUWIF	ADUXAY	ADUZAB	AEPHOS02	AFALIC
AFALUO	AFAMID	AFAYOV	AFCYDP	AFEJEC	AFEPIL	AFETEL
AFEVOW	AFEWIS	AFEZIV	AFIFOK	AFIFUR	AFIGEC	AFINAG01
AFIPIQ	AFIPOW	AFIZAS01	AFOBIH	AFOCEF	AFUGEP	AFUNEW
AFUVOM	AFUVUS	AFUYIJ	AGAGUK	AGASUY	AGEKII	AGESIO
AGIBAV	AGOCII99	AGODAD	AGONAN	AGOXOL	AGUPID	AHATAG
AHATEK	AHEBUL	AHECEW	AHECIB	AHEJAZ08	AHETOX	AHETUD
AHICIF	AHICUR	AHIKEI	AHOJIQ	AHOWOL	AHUBEM	AHUFEP
AHUZEI	AIPEPN20	AJACAP	AJACEV	AJACIX	AJAFIC	AJANAC
AJEVAN	AJEVOB	AJIDAA	AJIVIZ	AJIXIC	AJOGUC	AJOPOE01
AJUDAL	AKALAZ	AKAXAL99	AKENIO	AKEQOX	AKETUG	AKIFEF
AKILAH	AKIWOG	AKOCAE	AKOCEJ	AKOCOU	AKOPAT	AKOWAY
AKUMEA	AKUROO	AKUVEI	AKUVIM	ALAGUR	ALASAI	ALAYIW
ALAZAO	ALECIE	ALEVES	ALOVUS01	ALPHAGLY	ALUGOF	AMADAU
AMAPTZ	AMDPIM	AMEFEF	AMEGIK	AMELOU	AMELUA	AMIHXF
AMIMZA10	AMITEW	AMUMIG	ANISAT	ANTZOL10	ANUDOD	APAPYR
APEJEM	APEKEM	APEKIQ	APELAJ	APELEN	APEMOZ	APIFAH
APIPAS	APITEA	APOXOS01	APOYIO	APURAE99	AQANAI	AQARIU
AQECAA	AQEDUW	AQERAQ	AQEWOI	AQIGOW	AQINET	ARABUQ
ARACYP	ARADEC	ARBIMC10	ARCLAM01	ARFCYT99	ARGIND11	ARIQAV
AROJAU	AROMAV	AROMID	AROQEF	AROWIP	ARUBIY	ARUWEQ
ASABAZ	ASAXOJ	ASIJIW	ASIJIX	ASIYOR	ASOCOA	ASOTIM
ASOTUX	ASTROM99	ASULOP98	ASULOP99	ASUQOW	ATADUW	ATAXUO
ATAXUP	ATDZSA04	ATESIB	ATIXIM	ATIXUY	ATONOO	ATOVAG
ATOXEM	ATUBEX	ATUGAZ	ATUTAK99	ATZTHD10	AVAGIN	AVAKAK
AVEPAU	AVOTUA	AVOVIQ	AVUGUV	AVULIM	AVUSAN	AVUXAS
AWATUO	AWEBEL	AWELOE	AWENIB02	AWETED	AWIQEE	AWOLOP
AWOSOU	AWUBIF	AWUREQ	AWUYUM	AXADUZ	AXAFOV	AXAJUF
AXALAM	AXALAN	AXALOB	AXAMAN	AXANOD	AXAXED	AXEMIA
AXFSUR	AXIMEZ	AYECAJ	AYEFUF	AYIKID	AYOHEB	AYOHIF

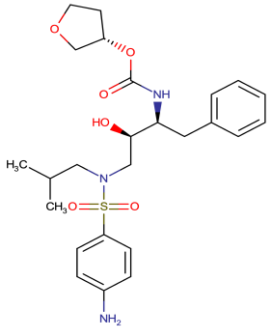
AYOHOL AYOJAZ AYOJED AYOREM AYUDUU AYUHAE AZABAF
AZACUA AZALIX AZEHOD AZESAZ AZHPXB AZIDES AZIQIJ
AZOMOS AZOPIP AZOQUC AZOROX AZUCAA AZUMOY AZURAC01
AZURUI99 BACXOV BADQIG BAFLOL BAFTAE BAGTUA BAGVAI
BAJYIV BAKFUO BAKLEG BAKLUW BALGUR BALMOR BALPIN
BAMDIC BANFIG BANKUW BANLEH BANNEL BANPAK BAQHOS01
BARCOX BARFIJ BATJUC BATSUK BATVAU BAVBOP BAWHEO
BAYGOZ BAYYAB BAZNEV BCBANN01 BCZNON BDIXNA BEBLAW
BEBWEK BEBWOU BECGOF BECRUY BECYAL BEDBAP BEDDOE
BEFSUA BEGLAC BEGVOA BEHDUO BEKBOJ98 BEKBOJ99 BEMDAZ97
BEMDAZ98 BEMDAZ99 BEMFOO BEMFUU BENTEU BEPRAP99 BERFUZ
BERHEL BERXAY BESLOC BESNUI BESPUL BESYEF BEWHUG
BEWQAV01 BEWQOK BEXGEQ BEXLIB BEXMIA BEXWEI BEYPUR
BEYVEH BEZGES BIBTAI BIBXUG BICBIZ BICSUC BIDJON
BIDMIK97 BIDMIK98 BIDMIK99 BIFPIP BIFTUH BIFVET BIFXUK
BIGUAN01 BIJSIX96 BIJSIX97 BIJSIX98 BIJSIX99 BIMSNO BIMTIB
BIPTID01 BISDIQ BIWWIO BIZDUK BIZWIS BIZYAL01 BOCDOM
BOCPUE BODCED BOGQOE BOHWUR BOLYUW BONLOG BONVIL
BOPTZO BOQJEW98 BOQJEW99 BOQVIM01 BOQYEN BORHAS BOTZOA
BOVYIV BOWYOC BOXGIE99 BOXKEE99 BOXWOA BOYHIG BOYZUL
BOZDIE BUDPEW01 BUDYAB BUDYEF BUFDEM BUFGIS BUFTED
BUGDEM BUGKIY BUGMIZ BUGXUW BUHJAP BUKKUP BUKYIP
BULXOX BUQCAT BUQLAC BUQMUX BURFIF BURKUU BURZUJ
BUSJIJ BUSPEK BUSZUM BUTFUT BUWNOW BUWSAN BUWSAO
BUXFEG BUYLAJ BZOXZT BZTZAD CAACTY CABPYR11 CABSIH10
CABZIR CADMAW CAGGUM CAINSP95 CAINSP96 CAINSP97 CAINSP98
CAKRIQ CALJIK CAMVES98 CAMVES99 CAMZOG CANCAW CANDEB01
CANELL01 CAPROA CAQYIE01 CARZAX CASBAA CASFAE CATXOK98
CATXOK99 CAVGEL CAVQUM CBOHAZ CEBNIG CECHEY CEDDIA01
CEDGUO CEDROU CEFTOW CEGBUN CEGKEG CEGVER CEHSIR
CEJSEP CELLAI CERJEP CEVYEH95 CEVYEH96 CEVYEH97 CEVYEH98
CEVYEH99 CEWCAI10 CEYCIS99 CEYNEZ CEZQII CHPYRD CHXIQL
CIBTUD CIBVEP CIDBIB CIDHON CIFTES CIJZAX CIJZUR
CINLOC CINTOK CIPMOE CIPVII CIPWOO CIQCUA CIQGEP
CIQHOB CIQHUH CIQJES CIQYEH CIRLEW CIWVAH CIWWAG
CIXWEL CIZDUK02 CIZRUY CIZYEP CMPHOA10 CMTAZP CNOXPA
COCVIZ CODPIU CODPOA CODYUP10 COHBOQ COHKOZ COHNES99
COJMUJ COJXIK COJXUW COLLEW COMXAD97 COPHEU COPREE10
CORSUY CORWAI COSFAR COSKAX COVXEQ COXZAS10 COYROZ
COZKAD COZKEH COZKIL CUCHUD CUCVAY CUDFOW CUJQED
CUMQEI CUNTAG CUQVIU CURPAI CUYKEM01 CYTIAC CYTIDI11
CYTOSC99 DABKOI DABSOR DADWEN DAFTEK99 DAJWOB DAPJAG
DAQHOS98 DAQHOS99 DAQYAV99 DASRIY DASTAS DASYEC99 DATTAU
DAXCAG01 DAYKAQ DAYWEF DAZVAB10 DEBHEX01 DECKUR DELZAW
DEMYIE DEPXUR DERFAI DERRIC DESWUT DETDOV DETFOX

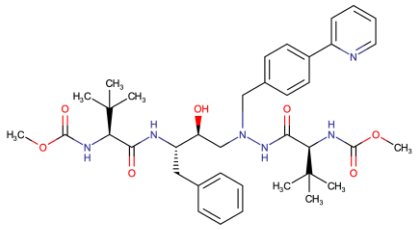
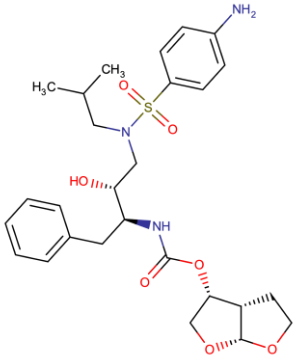
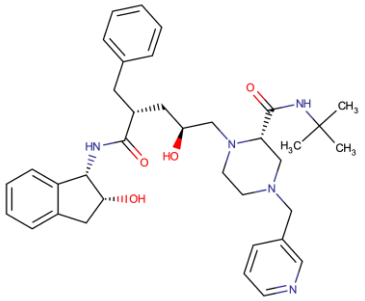
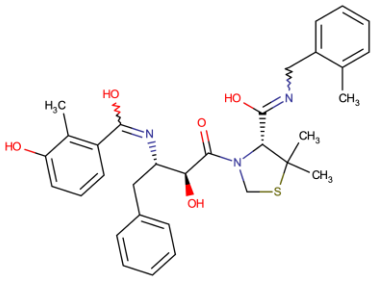
DETFOY DETFUC DEXREE DEXTAC DEXTIJ DEZTEH DHPMAD98
DHPMAD99 DIBMEH DICPUA01 DICRAI01 DIGTET DIHRAN DIJZIH
DIKWIE DINFAH01 DIPGIS12 DIUREA05 DIYHIC DNBZFX01 DNPIMZ
DOBBIH DOCYPO03 DODNUF DOGBIK99 DOLBUC DOMJUM DOMQUS
DOQSUX01 DOTTIQ DOVTAJ DOWDEY98 DOWDEY99 DOXPOV DOYNOU
DOZKOU DOZMIO DOZRIV DUBCEI DUBSID DUCXAB DUHMAW
DUHWAF DUKSOR98 DUKSOR99 DUQPAH DURYAS DUSXOF DUVGUX
DUXWIC DUZYED EKOKEU ELEYID98 ELEYID99 ELINOC EQONAZ
ERAHAG98 ERAHAG99 ESAMIU EVENIC99 EVOTUE EXOFOM95 EXOFOM96
EXOFOM97 EXOFOM98 EXOFOM99 FAGNEG99 FAGSUB FAKKAD FALBEA
FANYAV FAPKEN99 FAVWIJ FAWKUL FAXPOJ99 FAZRAZ FAZRED99
FECLUU FECMEF FECQAF FEDBOF FEFMAF FEGSEP FEHRIU
FEJJEJ FELCIK FEPNAP FESPAU99 FESPEY FESPOK FETZEJ97
FETZEJ98 FETZEJ99 FEVQED FICWAQ99 FICYOG FIKCEI98 FIKCEI99
FIMPEW FIPPEB FIQKAS99 FISKIC99 FITJEX FIWCOF FLYITU
FOJQUQ02 FOKRUS FOKWEI FONFIY99 FONMOL FORHAV FORMYB01
FOVWAO FOWREP FOWVIX FOYNUC FOYXIA99 FUBWIJ FUFYIP
FUFZAH FUGJUM01 FUGQON01 FUNNUZ FUNXAP FUPDAX FUQSAN
FUSDII FUSNOY FUTKUC FUTLEN FUWMOA FUWTOG FUXMES
FUXPIZ FUYMES GACTEM GAFNAC GAGSIR05 GAHCEY GAHTEO
GAKGEE99 GAKPEN GAKPIR GAKZIC GALHUX GAMGAD GAMKEK
GAMMOX GARVOK99 GATPAS GECLUX GEDLEH98 GEDLEH99 GEDPIP98
GEDPIP99 GEFBIE GEFTES GEFTIW GEJBIH99 GEJKUC97 GEJKUC98
GEJKUC99 GELGIN01 GELHIO10 GEPPIA GERDOW98 GERDOW99 GERFEO
GETBOX GEVREE GEXQEF GEYPOP GEZVUC GICCOK GIMKAO
GIPCAL GIQNOL GIQYEK GIQZOV GIRKOI GISLIF GLCTSM
GLPHEA98 GLPHEA99 GLUTAM02 GLYCPH98 GLYCPH99 GOCZUU GOGROL
GOJMOJ GOJPAW98 GOJPAW99 GOJPUQ99 GOPZIU98 GOPZIU99 GPHXAM
GUANPH01 GUGDAO GUNQUB97 GUNQUB99 GUPSUH GUQDUT GUQFOP
GUSSOE GUSXEZ GUVCAD GUWCOQ GUXLAO HABTEJ HAFHIF97
HAFHIF98 HAFHIF99 HAJSAN HAMROE HAMZIF HANLEP HASVII
HEGFIJ95 HEGFIJ96 HEGFIJ97 HEGFIJ98 HEGFIJ99 HEGKIO HEJCEE
HEMYON HEPDUC HEVDAO HEXZEQ HEZVEN HIDXIB HIFQES
HIFWOI HISAPH97 HISAPH98 HISAPH99 HISTAN HISTCM12 HISTPA1098
HIXGEA HIYDIC HIYJUU99 HOHCOX HOHGER HOJKUO HONLON
HOPJUR HOQZAQ HORNUZ HORTAJ HORZAQ HORZOE HORZUK
HOWYUP HOYPER HUGGEX HUSCAZ98 HUSCAZ99 HUSNEP HUXZOR
HYPRCX HYPTHO IBOCOT IFIDUW97 IFIDUW98 IFIDUW99 IFIFAE
IGAYUK99 IGIHAH IHIWIH IJICIN97 IJICIN98 IJICIN99 IJIZAC
ILIDAI ILOPUU ILOQEH INAYIH INIFUI IRISUY01 ISAXUX
ISOGAY ISOGII ISOGOO ITEJEY ITEMUR ITESIL ITICAR
ITIGAV ITINOQ ITUTEY IVOMIR IWIDEZ IWILAB IWOKEM
IWUGIQ IXAXOW IYAYIQ JABCEX JABMAD JABSEN JAFJAB98
JAFJAB99 JALQET JAPPEV JATWUW JAXSEH JAYNIG99 JEDBUQ
JEDLEK99 JEKXUT JEMSUP JETYUD JIBDIH98 JIBDIH99 JIGRAS

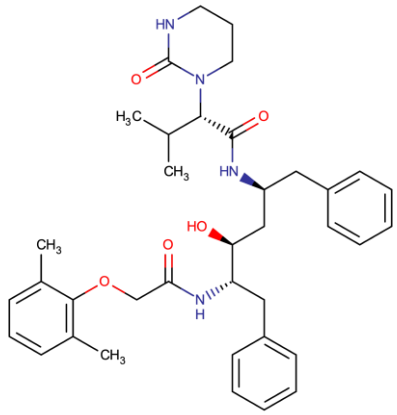
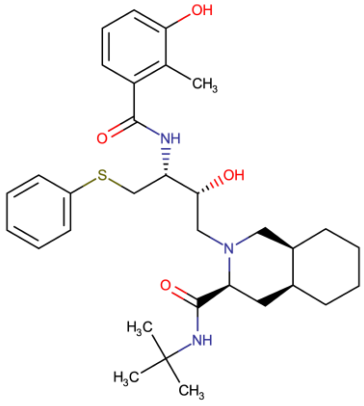
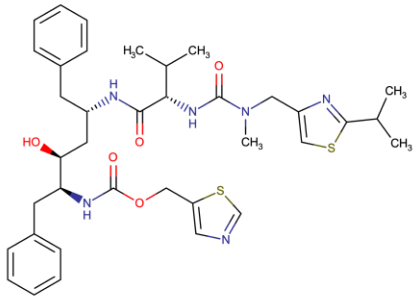
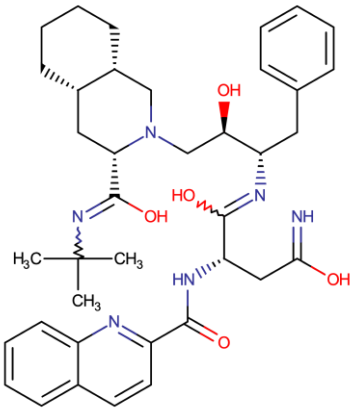
JIPJUO JIWHUT JIYREO98 JIYREO99 JIYWET96 JIYWET97 JIYWET98
JIYWET99 JODHAN JODKEU JOGFAN JOPXOB JOPYUI JOSGUV
JOWWIB JOXDEF JUDWEK JUKNIO JULXEV JULZEX JUMMEL
JUNBEB JUPLOX JURDIL JURLIR JURZED KACTUE99 KADPUA
KAKLUE KAPWAZ KASNOH KAYWIR01 KECFIJ KECGOO99 KEHZAY98
KEHZAY99 KEPHUI KEPNUO KERKOI01 KETLAX KETSAF KEZREM
KGULAM KICJEL99 KIHVAY97 KIHVAY98 KIHVAY99 KIHVEC KIKKIZ
KIMNID99 KISGAW KITREK KIWVIW KOCHOZ KOFKUL98 KOFKUL99
KOFLOG KOJGUM KOKBER98 KOMHAV01 KOTPEO KOTXAU KOVCAZ
KULREP KUMZOJ KUNBAY KUNBIG KUPGIN KUPZUS KUQBEF
KUSQEW KUSQIA KUTHOW KUVYAC KUXXUY KUYBAJ LABRUB98
LABRUB99 LABVIT98 LABVIT99 LALNIN03 LAPFIR98 LAPFIR99 LARGPH97
LARGPH98 LARGPH99 LAVHAR LAXTIO98 LAXTIO99 LAXYOY98 LAXYOY99
LCYSTN04 LESJEY LESJOI LIDYEC LIQWEN LOMTEM98 LOMTEM99
LOPXUJ LTYRGG98 LTYRGG99 LUFBOD99 MABZAR99 MADCMP99 MAJDOR
MAJGAG99 MALAMS98 MALAMS99 MAMDEK01 MAPNUN MATDUG MDPIZO
MEDMEO MEPVAE01 MERQUW MEYCIC MHPTEC98 MHPTEC99 MIETDZ20
MINOSP MIPWEN98 MIQNEF98 MIQNEF99 MIQNIJ98 MIQNIJ99 MISTAJ
MMCPUR96 MMCPUR97 MMCPUR98 MMCPUR99 MOBCIQ MOBYIL98 MOBYIL99
MOGZAK MOGZEO MOPMOT96 MOPMOT98 MOPMOT99 MOSRUH99 MOTJOU
MPHTAZ11 MPROLA10 MSMNIT MUBVOV MUGKAA01 MUHCOH98 MUHCOH99
MUJBIE MUJTAM MULFIK MUNVAS98 MUNVAS99 MURYED99 MURYIH99
MUSYIJ MUTDOW MUYYUA MUZNEC NAFHUY NAGGEH NAGLEN98
NAGLEN99 NAJQOG NALCYS02 NAMZAC NAPRLA02 NARGIX99 NEFGAG98
NEFGAG99 NEQNIG NETGIC97 NETGIC98 NETGIC99 NEZNAH NIPBEV
NITRBE01 NIYDOO01 NMACEP01 NOKNOR NOLHIF01 NOREPH01 NOWCAD99
NOZXEF NUHJIK NUHKIL NUNFIL NUPTAV NURCEJ NUTGEO99
NUVHAP NUVKEW NUVKIA NUXXEJ NUXZAJ OBIDAE OCAHAC
OCASER OCIPEV OFOYEN OGEYAA OGUGIG OHIPUR OHIWOT
OJUHOS OJUHUY OKESOM OKETUT OLINEE OQODOP OQUPEW
OSEJON OVAQAF OVAQEJ OVAZUI OVUYEL PABMUA98 PABMUA99
PABSOC PAGXOL99 PAKWON PAYWIX PEFDOT PEXTAN98 PEYSES
PHOGLY04 PINPAD01 PIPVAL PIYKIR PIZHAH POBMIC POJQEK98
POMDAW PONTIV99 POTHRE01 POVKIU PROAPH02 PUKVOI PUMYIH
PUNJOZ PURBAH PURBEL PURQOK PURREB PUSVIK PUSYOT
QACLAH QAFTUN QAKWAB99 QANJUL98 QANJUL99 QAXDEY99 QAXDIC99
QEBBUW QECCIK QECNIV QEKXUZ QEVPEM QEZLOW QIJHUM97
QIJHUM98 QIJHUM99 QINGAV QOTNAP QUBVUE97 QUBVUE98 QUBVUE99
QULVEY98 QULVEY99 QUNZAC RADGAF98 RADGAF99 RADKOX98 RADKOX99
RAFBAB RAJFIR RAJXUW97 RAJXUW98 RAJXUW99 RAMVOQ01 RAWFOM
RAXKAD96 RAXKAD97 RAXKAD98 RAXKAD99 RECZIJ REDTUR RESTOY
RIPGEE RIQKEH RISCUR RIWBUV RIWLAK99 RODFAR99 RUKCEH
RULHIR RUNGAK RUWFEU SADMEQ99 SADMUG99 SAFFEK SAHBUZ99
SAKHUI SANPEE SARZAM SASBIX98 SASBIX99 SATCEW99 SATNAC
SATNEH SAVSOX99 SAYWAQ99 SAZCOL SCCHRN06 SCGMPT99 SEDBUZ99

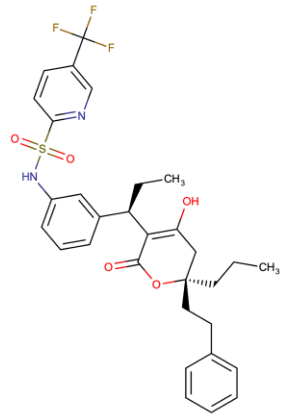
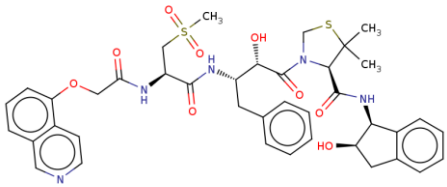
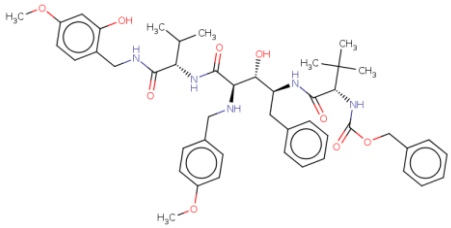
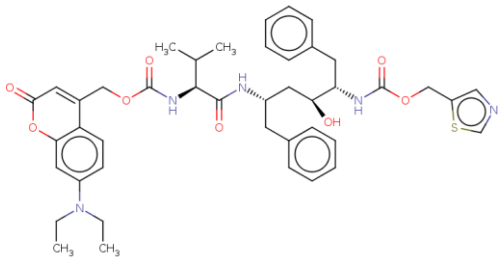
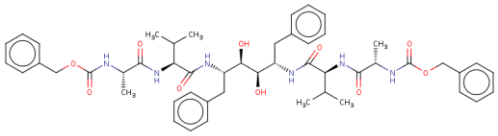
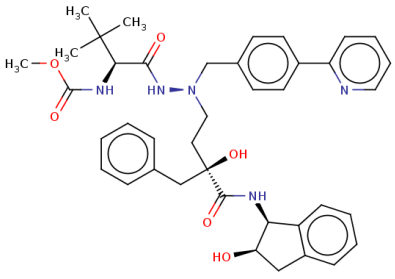
SEGGER98	SEGGER99	SEJSIJ	SEKWIO99	SERPOP01	SEWGEG	SIHPAB
SIYLOB	SIZXAA	SOFMEG	SOJDEA	SUFNUC98	SUFNUC99	SUGFIJ
SULBOS	SULSIC	SUMPAR99	SUNWUV	SURREC	TAHJIV99	TEDZUY
TEJDAN96	TEJDAN97	TEJDAN98	TEJDAN99	TEJMOK98	TEJMOK99	TEJNEB95
TEJNEB96	TEJNEB97	TEJNEB98	TEJNEB99	TEKNAY97	TEKNAY98	TEKNAY99
TEQZAR01	TERMIM99	TERNOT99	TERYAQ01	TERYAQ02	TEVHEH01	TIRPAL
TIXPIZ	TMEYPH	TODNUV97	TODNUV98	TODNUV99	TONQAO99	TOZLOJ
TPHCUR97	TPHCUR98	TPHCUR99	TPYPOP10	TUBERC01	TUDMOU99	TUGWUN
TUGXAU	TUNTUT	TURYIQ	TURZEN	TUSVEK	TUWVOY	TUYWUH
UHAWUV	UNOCAB	VAFVUU	VALTUX97	VALTUX98	VANREH	VANRIL
VARNIM	VASSAL	VEFZIP	VEGKIB97	VEGKIB98	VEGKIB99	VELTIQ
VIGNII97	VIGNII98	VIGNII99	VINXAS	VIOLME98	VIOLME99	VIRYEA
VISVIC	VOCKIH	VOJJIN98	VOJJIN99	VOMKOZ	VOMZAY	VOVSAA
VOWGAP	VOWTEG98	VOWTEG99	VUMMIZ	VUMMOF	VUMMUL	VUPJUM
VUWCEW	VUXKAA99	VUXKEE	VUXKII	VUXKOO	VUXLAB	VUXLEF
VUYMAD98	VUYMAD99	WAFROK10	WAKWUB	WALFOG	WALWOW	WAZDEG
WEBFISmol1	WEJBIW	WEKHEA02	WELWUF	WEPMAH	WETNAK	WEVKEO
WIFREI	WIPCAZ98	WIPCAZ99	WIZZEL	WOBXAM	WOCSAI99	WOGWEV
WOLRUK	WOMCAC	WOMYEC	WONJAK	WOQZOR94	WOQZOR95	WOQZOR96
WOQZOR97	WOQZOR98	WOQZOR99	WOTZEK99	WOVXOU01	WUCZOL	WUKWEF
WUKWIJ	WUQPAB	WUSJEZ	WUXBIA99	XACMEBZ	XAJNIG	XANOPT99
XATXEV98	XATXEV99	XAZWOL99	XEGLAW98	XEGLAW99	XIHSEM96	XIHSEM97
XIHSEM98	XIHSEM99	XODXOF	XOPNEV	XORNOH	XOWGOF98	XOWGOF99
XOYFIA	XUCHAE	XUHQUM	XUJWUU	XUQPIK	XURNIJ	XUSTUC
XUTCEW	XUTDEX	XUZJUX01	YAJZUF	YALLON99	YANQEK99	YAYDAD
YAYSOH	YEHYOZ	YEMFOL99	YENKEH	YEQCIG98	YEQCIG99	YIRNOC
YOPSUR	YURNAA	ZAYJOY	ZAYPAQ99	ZEHKEC	ZEJMOQ99	ZETKUE
ZIKFOO99	ZILHOR02	ZONFOX	ZOZWAM	ZUMHUM	ZUPPAD	ZURLOP
ZUSXAO	ZUTFOL	ZUTKAC	ZUTKEG	ZZZSBA97	ZZZSPS99	ZZZUEE04

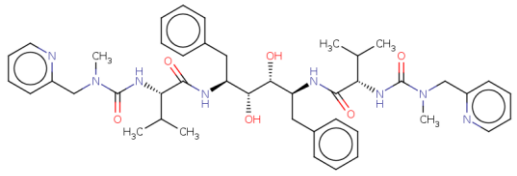
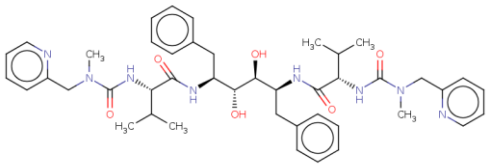
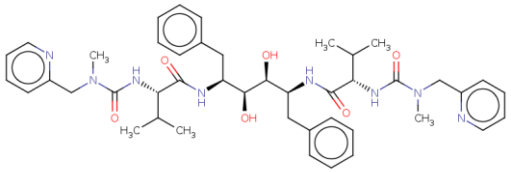
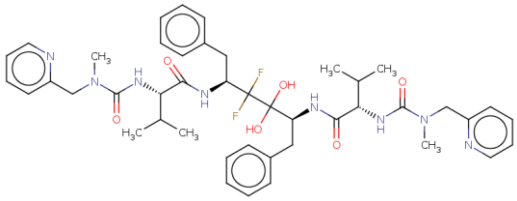
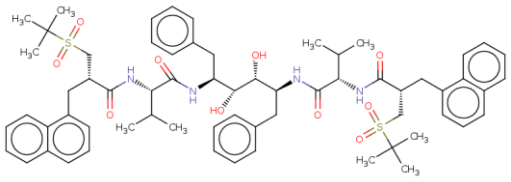
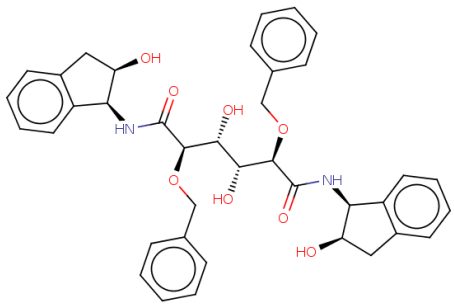
Table 4S. HIV-1 protease inhibitor compounds from the BindingDB database used in this study.

ID	Chemical Formula	Name	2D scheme
Amprenavir	$C_{25}H_{35}N_3O_6S$	Amprenavir	

Atazanavir	$C_{38}H_{52}N_6O_7$ Atazanavir	
Darunavir	$C_{27}H_{37}N_3O_7S$ Darunavir	
Indinavir	$C_{36}H_{47}N_5O_4$ Indinavir	
JE-2147	$C_{32}H_{37}N_3O_5S$ JE-2147	

Lopinavir	$C_{37}H_{48}N_4O_5$	Lopinavir	
Nelfinavir	$C_{32}H_{45}N_3O_4S$	Nelfinavir	
Ritonavir	$C_{37}H_{48}N_6O_5S_2$	Ritonavir	
Saquinavir	$C_{38}H_{50}N_6O_5$	Saquinavir	

Tipranavir	$C_{31}H_{33}F_3N_2O_5S$	Tipranavir	
Cmpd7	$C_{40}H_{45}N_5O_9S_2$	KNI-10075	
Cmpd42	$C_{46}H_{59}N_5O_9$	SDZ283-910	
Cmpd45	$C_{43}H_{51}N_5O_8S$		
Cmpd50	$C_{50}H_{64}N_6O_{10}$	TL-3, C2 symmetric inhibitor	
Cmpd65	$C_{40}H_{47}N_5O_6$		

Cmpd92	$C_{44}H_{58}N_8O_6$	
Cmpd93	$C_{44}H_{58}N_8O_6$	
Cmpd95	$C_{44}H_{58}N_8O_6$	
Cmpd97	$C_{44}H_{56}F_2N_8O_6$	
Cmpd115	$C_{64}H_{82}N_4O_{10}S_2$	
Cmpd120	$C_{38}H_{40}N_2O_8$	

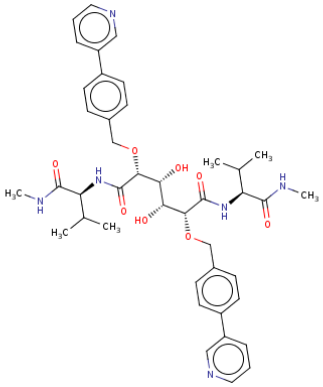
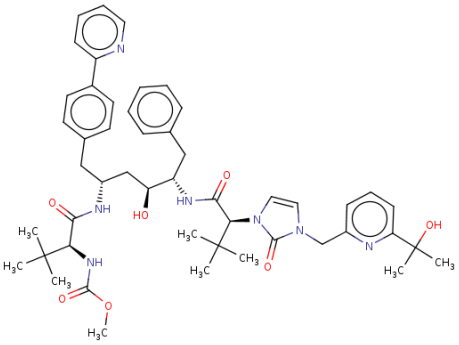
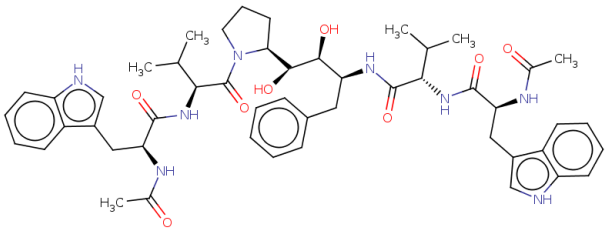
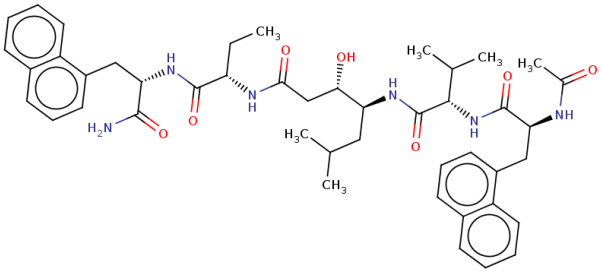
Cmpd127	$C_{42}H_{52}N_6O_8$	
Cmpd188	$C_{49}H_{63}N_7O_7$	
Cmpd213	$C_{50}H_{64}N_8O_8$	
Cmpd251	$C_{45}H_{58}N_6O_7$	

Table S5. Statistical descriptors of carbon, nitrogen, oxygen, sulfur and hydrogen pseudoatom values for atomic charge (e) computed for groups (C, N, O, S and H, respectively) and sub-groups divided basing on number of first neighbours (X_1 for one neighbour, X_3 for two, X_ 3 for three and X_4 for four, where X stands for label of element type) of pseudoatoms used to build the UBDB2018 databank. Trimmed mean - mean by dropping the top and bottom trim fraction by 10%. MAD - Median Absolute Deviation which is a robust measure of how spread out a set of data is ($MAD = median(|Y_i - median(Y_i)|)$. SE- standard error, the approximate standard deviation of a statistical sample population ($SE = \frac{\sigma}{\sqrt{n}}$).

	n	Mean	Standard deviation	Median	Trimmed mean	MAD	Min value	Max value	Range	Skew	Kurtosis	SE
Carbon												
C	12627	0.11	0.19	0.08	0.10	0.19	-0.57	0.78	1.35	0.33	0.05	0.00
C_2	177	-0.27	0.24	-0.36	-0.28	0.25	-0.57	0.25	0.82	0.30	-1.54	0.02
C_3	7289	0.00	0.11	0.00	0.00	0.12	-0.38	0.57	0.95	0.32	0.42	0.00
C_4	5161	0.27	0.16	0.26	0.27	0.17	-0.50	0.78	1.29	-0.13	0.06	0.00
Nitrogen												
N	2433	-0.01	0.09	-0.02	-0.01	0.08	-0.29	0.43	0.72	0.65	1.53	0.00
N_1	91	0.24	0.06	0.23	0.24	0.05	0.07	0.43	0.36	0.23	0.69	0.01
N_2	807	-0.03	0.06	-0.03	-0.03	0.05	-0.27	0.26	0.54	0.07	1.29	0.00
N_3	1420	0.00	0.08	-0.01	0.00	0.08	-0.29	0.33	0.62	-0.01	0.52	0.00
N_4	115	-0.12	0.07	-0.12	-0.12	0.05	-0.26	0.12	0.38	0.74	1.63	0.01
Oxygen												
O	3411	-0.20	0.08	-0.20	-0.20	0.08	-0.56	0.01	0.57	-0.70	1.74	0
O_1	1889	-0.19	0.09	-0.16	-0.18	0.08	-0.56	0.01	0.57	-1.08	1.37	0
O_2	1522	-0.22	0.05	-0.22	-0.22	0.05	-0.43	-0.01	0.42	0.21	0.78	0
Sulfur												
S	390	-0.24	0.16	-0.30	-0.25	0.12	-0.50	0.11	0.61	0.70	-0.97	0.01
S_1	56	-0.40	0.04	-0.40	-0.40	0.04	-0.50	-0.29	0.21	-0.07	0.60	0.01
S_2	229	-0.31	0.07	-0.32	-0.32	0.07	-0.44	-0.05	0.39	0.66	0.57	0.00
S_3	13	-0.05	0.04	-0.06	-0.05	0.04	-0.10	0.04	0.14	0.56	-1.03	0.01
S_4	92	0.02	0.04	0.02	0.02	0.04	-0.10	0.11	0.21	-0.06	0.08	0.00
Hydrogen												
H	9389	-0.02	0.10	-0.05	-0.03	0.07	-0.35	0.36	0.7	1.04	0.41	0

Table S5. Minimal (Vmin, e bohr^{-1}) and maximal (Vmax, e bohr^{-1}) values of potential, root mean square errors (RMSE, e bohr^{-1}) and correlation coefficients (Corr. Coef.) for molecular electrostatic potential grids computed from the UBDB, IAM and aug-PROmol models compared to the referential B3LYP/6-31G** method (REF). Molecules ordered according to the rising value of RMSE for UBDB.

	REF		UBDB				IAM				aug-PROmol			
	Vmin	Vmax	Vmin	Vmax	Corr.Coeff	RMSE	Vmin	Vmax	Corr.Coeff.	RMSE	Vmin	Vmax	Corr.Coeff.	RMSE
Cmpd127	-0.1061	97.49	-0.0935	99.91	0.9997	0.0085	0.0000	64.73	0.9742	0.0798	-0.1066	100.14	0.9986	0.0205
Cmpd50	-0.0838	123.14	-0.0963	125.41	0.9997	0.0087	0.0000	65.58	0.9750	0.0808	-0.0970	125.72	0.9987	0.0214
Cmpd97	-0.0974	115.35	-0.1180	114.54	0.9997	0.0093	0.0000	57.39	0.9772	0.0824	-0.1188	114.67	0.9985	0.0232
Cmpd92	-0.1004	209.16	-0.0955	207.39	0.9997	0.0100	0.0000	49.72	0.9163	0.1711	-0.1235	207.58	0.9986	0.0248
Cmpd95	-0.0977	163.41	-0.1004	163.70	0.9997	0.0105	0.0000	64.84	0.9546	0.1330	-0.1227	164.02	0.9987	0.0254
Lopinavir	-0.1054	167.21	-0.1175	56.36	0.9997	0.0106	0.0000	56.58	0.9543	0.1170	-0.1369	167.09	0.9985	0.0237
Cmpd93	-0.1051	83.70	-0.1008	83.70	0.9997	0.0107	0.0000	53.33	0.9916	0.0559	-0.1257	83.84	0.9983	0.0270
Cmpd188	-0.0968	103.79	-0.0766	103.54	0.9997	0.0110	0.0000	64.74	0.9810	0.0823	-0.1048	103.85	0.9986	0.0254
Cmpd251	-0.0894	190.82	-0.0951	196.99	0.9997	0.0112	0.0000	64.83	0.9210	0.1776	-0.1149	197.34	0.9987	0.0259
Saquinavir	-0.1031	69.81	-0.1167	70.61	0.9995	0.0121	0.0000	63.55	0.9945	0.0424	-0.1292	70.85	0.9981	0.0252
Cmpd213	-0.0970	87.12	-0.1152	87.47	0.9994	0.0128	0.0000	57.98	0.9841	0.0688	-0.1209	87.50	0.9985	0.0237
Atazanavir	-0.0859	116.93	-0.0849	119.26	0.9996	0.0128	0.0000	64.30	0.9812	0.0840	-0.1143	119.05	0.9986	0.0258
Cmpd45	-0.0939	126.85	-0.1023	126.82	0.9994	0.0131	0.0000	61.56	0.9737	0.0887	-0.1066	126.92	0.9987	0.0224
Cmpd120	-0.0838	54.99	-0.1159	56.13	0.9994	0.0138	0.0000	50.92	0.9954	0.0411	-0.1155	56.27	0.9985	0.0228
Cmpd115	-0.0778	117.20	-0.0954	114.61	0.9995	0.0138	0.0000	58.07	0.9823	0.0812	-0.1023	114.74	0.9984	0.0269
Cmpd42	-0.1063	55.70	-0.0890	55.66	0.9992	0.0140	0.0000	55.93	0.9941	0.0411	-0.1155	55.59	0.9983	0.0222
JE-2147	-0.0839	158.16	-0.0971	65.13	0.9993	0.0149	0.0000	158.47	0.9977	0.0322	-0.0993	158.42	0.9987	0.0228
Cmpd65	-0.0901	153.02	-0.1156	152.24	0.9993	0.0151	0.0000	63.83	0.9614	0.1118	-0.1091	152.04	0.9985	0.0240
Indinavir	-0.1026	132.80	-0.1309	134.19	0.9993	0.0153	0.0000	62.84	0.9656	0.1098	-0.1117	134.39	0.9984	0.0265
Darunavir	-0.0829	221.02	-0.0970	218.62	0.9996	0.0154	0.0000	115.03	0.8814	0.2639	-0.1152	218.87	0.9989	0.0265
Ritonavir	-0.1003	97.97	-0.1021	98.14	0.9993	0.0157	0.0000	65.49	0.9827	0.0764	-0.1304	98.32	0.9987	0.0229
Amprenavir	-0.0836	232.94	-0.0959	220.05	0.9995	0.0161	0.0000	64.70	0.9048	0.1924	-0.1088	220.18	0.9983	0.0262
Nelfinavir	-0.0961	75.50	-0.1342	75.32	0.9991	0.0164	0.0000	50.60	0.9883	0.0581	-0.1223	75.63	0.9984	0.0238
Cmpd7	-0.1070	64.99	-0.1045	63.66	0.9986	0.0219	0.0000	63.82	0.9957	0.0417	-0.1089	63.67	0.9983	0.0263
Tipranavir	-0.0910	64.47	-0.1172	64.29	0.9961	0.0322	0.0000	56.66	0.9963	0.0342	-0.1079	64.36	0.9984	0.0236

Table S6. The statistical quantitative descriptors of electrostatic potential at the van der Waals surface (Positive Average Potential ($V_{av.}^{+}$, e bohr^{-1}), Negative Average Potential ($V_{av.}^{-}$, e bohr^{-1}) and their variance (σ^{+}, σ^{-}, e bohr^{-1}), Average Deviation (π , e^{2} bohr^{-2}), Minimal (Vmin, e bohr^{-1}) and maximal (Vmax, e bohr^{-1}) values of potential evaluated as described in the original paper by Politzer el. al. (Murray & Politzer, 1998; Forms *et al.*, 2000) using van der Waals surface thickness of 0.3 bohr.

	REF							
	$V_{av.}^{+}$	σ^{+}	$V_{av.}^{-}$	σ^{-}	Vav.	π	V_{max}	V_{min}
Cmpd127	0.0173	0.0148	-0.0218	0.0175	0.0005	0.0194	0.0982	-0.0896
Cmpd50	0.0182	0.0142	-0.0196	0.0164	0.0005	0.0177	0.0861	-0.0725
Cmpd97	0.0178	0.0122	-0.0205	0.0188	0.0005	0.0191	0.0794	-0.0840
Cmpd92	0.0165	0.0113	-0.0208	0.0192	0.0005	0.0187	0.0654	-0.0855
Cmpd95	0.0166	0.0128	-0.0189	0.0181	0.0005	0.0176	0.0834	-0.0839
Lopinavir	0.0121	0.0095	-0.0172	0.0164	0.0004	0.0145	0.0802	-0.0934
Cmpd93	0.0174	0.0130	-0.0211	0.0197	0.0006	0.0192	0.0786	-0.0895
Cmpd188	0.0151	0.0113	-0.0189	0.0162	0.0004	0.0162	0.0746	-0.0801
Cmpd251	0.0190	0.0150	-0.0214	0.0178	0.0005	0.0196	0.0853	-0.0754
Saquinavir	0.0158	0.0126	-0.0226	0.0222	0.0007	0.0191	0.0673	-0.0908
Cmpd213	0.0169	0.0145	-0.0221	0.0178	0.0005	0.0196	0.0762	-0.0817
Atazanavir	0.0152	0.0113	-0.0198	0.0178	0.0004	0.0170	0.0779	-0.0745
Cmpd45	0.0178	0.0115	-0.0209	0.0179	0.0005	0.0190	0.0656	-0.0833
Cmpd120	0.0173	0.0155	-0.0220	0.0159	0.0005	0.0197	0.0951	-0.0723
Cmpd115	0.0185	0.0130	-0.0215	0.0158	0.0004	0.0194	0.0819	-0.0700
Cmpd42	0.0158	0.0129	-0.0206	0.0174	0.0005	0.0181	0.0880	-0.0878
JE-2147	0.0117	0.0091	-0.0147	0.0112	0.0002	0.0131	0.0795	-0.0703
Cmpd65	0.0140	0.0096	-0.0189	0.0165	0.0004	0.0161	0.0666	-0.0807
Indinavir	0.0154	0.0105	-0.0222	0.0195	0.0005	0.0171	0.0685	-0.0860
Darunavir	0.0203	0.0136	-0.0236	0.0192	0.0006	0.0205	0.0839	-0.0766
Ritonavir	0.0166	0.0114	-0.0208	0.0189	0.0005	0.0180	0.0693	-0.0859
Amprenavir	0.0186	0.0148	-0.0238	0.0193	0.0006	0.0202	0.0810	-0.0730
Nelfinavir	0.0168	0.0133	-0.0221	0.0192	0.0005	0.0183	0.0822	-0.0831
Cmpd7	0.0219	0.0154	-0.0218	0.0159	0.0005	0.0219	0.1044	-0.0913
Tipranavir	0.0175	0.0132	-0.0190	0.0171	0.0005	0.0172	0.0841	-0.0799

Table S6. *Cont*.

	UBDB								aug-PROmol						
	$V_{av.}^{+}$	σ^{+}	$V_{av.}^{-}$	σ^{-}	Vav.	π	V_{max}	V_{min}	$V_{av.}^{+}$	σ^{+}	$V_{av.}^{-}$	σ^{-}	Vav.	V_{max}	V_{min}
Cmpd127	0.0214	0.0157	-0.0256	0.0189	-0.0050	0.0236	0.0963	-0.0845	0.0233	0.0175	-0.0275	0.0211	0.0020	0.1225	-0.0864
Cmpd50	0.0237	0.0166	-0.0246	0.0193	0.0031	0.0237	0.0944	-0.0858	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Cmpd97	0.0222	0.0147	-0.0260	0.0212	-0.0004	0.0240	0.0821	-0.1051	0.0208	0.0143	-0.0262	0.0230	0.0014	0.1021	-0.1089
Cmpd92	0.0200	0.0138	-0.0242	0.0190	-0.0011	0.0220	0.0806	-0.0836	0.0208	0.0141	-0.0267	0.0235	-0.0015	0.0840	-0.1003
Cmpd95	0.0211	0.0155	-0.0234	0.0190	0.0005	0.0221	0.0966	-0.0888	0.0207	0.0152	-0.0254	0.0214	0.0009	0.1011	-0.1005
Lopinavir	0.0144	0.0110	-0.0240	0.0212	-0.0008	0.0193	0.0788	-0.1116	0.0211	0.0144	-0.0295	0.0268	0.0015	0.1093	-0.1131
Cmpd93	0.0227	0.0164	-0.0253	0.0197	-0.0004	0.0239	0.0931	-0.0892	0.0207	0.0155	-0.0274	0.0243	0.0005	0.0993	-0.1042
Cmpd188	0.0227	0.0161	-0.0211	0.0154	0.0027	0.0218	0.0915	-0.0668	0.0194	0.0137	-0.0232	0.0188	0.0039	0.1078	-0.0855
Cmpd251	0.0207	0.0154	-0.0249	0.0208	0.0005	0.0227	0.0899	-0.0847	0.0260	0.0205	-0.0298	0.0230	0.0047	0.1333	-0.0942
Saquinavir	0.0216	0.0130	-0.0361	0.0267	-0.0014	0.0290	0.0947	-0.1045	0.0202	0.0143	-0.0327	0.0290	-0.0002	0.0874	-0.1131
Cmpd213	0.0211	0.0174	-0.0262	0.0234	-0.0063	0.0238	0.0861	-0.1069	0.0212	0.0158	-0.0297	0.0220	-0.0006	0.0929	-0.1010
Atazanavir	0.0192	0.0110	-0.0262	0.0188	-0.0006	0.0223	0.0721	-0.0810	0.0186	0.0122	-0.0266	0.0209	0.0019	0.0911	-0.0951
Cmpd45	0.0270	0.0155	-0.0291	0.0201	0.0028	0.0276	0.0873	-0.0892	0.0207	0.0139	-0.0252	0.0202	0.0032	0.0936	-0.0912
Cmpd120	0.0214	0.0124	-0.0338	0.0231	-0.0039	0.0279	0.0739	-0.1053	0.0222	0.0182	-0.0280	0.0210	-0.0016	0.1223	-0.0961
Cmpd115	0.0209	0.0152	-0.0231	0.0206	0.0006	0.0219	0.0840	-0.0869	0.0226	0.0160	-0.0268	0.0196	0.0038	0.1279	-0.0846
Cmpd42	0.0258	0.0181	-0.0249	0.0180	-0.0034	0.0252	0.1068	-0.0794	0.0208	0.0154	-0.0260	0.0201	0.0018	0.1038	-0.0982
JE-2147	0.0193	0.0119	-0.0261	0.0190	-0.0022	0.0001	0.0734	-0.0914	0.0265	0.0162	-0.0255	0.0196	0.0088	0.1038	-0.0812
Cmpd65	0.0195	0.0130	-0.0282	0.0214	-0.0004	0.0241	0.0705	-0.1098	0.0173	0.0110	-0.0258	0.0206	0.0000	0.0775	-0.1057
Indinavir	0.0219	0.0132	-0.0277	0.0221	0.0014	0.0241	0.0870	-0.1146	0.0200	0.0124	-0.0291	0.0240	0.0036	0.0916	-0.1017
Darunavir	0.0247	0.0166	-0.0284	0.0220	0.0025	0.0259	0.1023	-0.0881	0.0253	0.0168	-0.0290	0.0227	0.0055	0.1074	-0.0968
Ritonavir	0.0290	0.0183	-0.0274	0.0210	0.0072	0.0274	0.0971	-0.0882	0.0193	0.0130	-0.0276	0.0238	0.0025	0.0846	-0.1056
Amprenavir	0.0238	0.0179	-0.0295	0.0226	0.0016	0.0260	0.1009	-0.0874	0.0238	0.0171	-0.0294	0.0221	0.0039	0.0900	-0.0915
Nelfinavir	0.0291	0.0171	-0.0342	0.0289	0.0022	0.0339	0.1133	-0.1278	0.0220	0.0157	-0.0290	0.0251	0.0030	0.0929	-0.1050
Cmpd7	0.0270	0.0208	-0.0314	0.0242	0.0024	0.0292	0.1142	-0.0970	0.0266	0.0187	-0.0275	0.0190	0.0016	0.1533	-0.0925
Tipranavir	0.0178	0.0114	-0.0229	0.0262	0.0056	0.0457	0.1093	-0.1094	0.0229	0.0165	-0.0224	0.0205	0.0073	0.1003	-0.0918