

Supplementary table 1: List of drugs and their binding energies to ACE and ACE2.

Ligand	Human ACE	Human ACE2
	Binding energy (kcal/mol)	Binding energy (kcal/mol)
(S)-NICARDIPINE	-8.6	-6.0
(S)-NITRENDIPINE	-7.5	-6.5
17-BETA ESTRADIOL	-8.2	-5.7
4-AMINOPYRIDINE	-3.9	-4.0
4-PHENYLAMINO-3-QUINOLINECARBONITRILE	-8.2	-6.5
ABACAVIR	-8.2	-6.3
ABARELIX	-6.0	-4.4
ABEMACICLIB	-9.1	-6.7
ABIRATERONE ACETATE	-9.8	-7.0
ACALABRUTINIB	-9.6	-7.2
ACAMPROSATE	-5.7	-4.5
ACARBOSE	-8.2	-6.0
ACEBUTOLOL	-7.3	-5.6
ACETAMINOPHEN	-5.5	-5.6
ACETAZOLAMIDE	-6.2	-5.1
ACETOHEXAMIDE	-8.6	-6.3
ACETOHYDROXAMIC ACID	-3.9	-3.5
ACETOPHENAZINE	-8.0	-6.2
ACETYLCHOLINE	-4.3	-3.5
ACETYLCYSTEINE	-4.7	-3.9
ACETYLDIGITOXIN	-10.0	-7.1
ACRISORCIN	-5.9	-5.8
ACYCLOVIR	-6.7	-5.2
ADAPALENE	-9.2	-7.3
ADEFOVIR DIPIVOXIL	-7.6	-4.8
ADENOSINE	-7.0	-5.5
ALATROFLOXACIN	-10.6	-6.4
ALBENDAZOLE	-6.9	-5.2
ALBUTEROL	-6.6	-5.2
ALCAFTADINE	-9.0	-5.8
ALCLOMETASONE DIPROPIONATE	-8.6	-6.5
ALFENTANIL	-7.4	-4.9
ALFUZOSIN	-7.7	-5.6
ALISKIREN	-7.5	-5.9
ALITRETINOIN	-7.4	-5.6
ALLOPURINOL	-5.6	-5.1
ALMOTRIPTAN	-7.0	-6.0

ALOSETRON	-8.3	-6.4
ALPELISIB	-8.7	-6.6
ALPHA-TOCOPHEROL	-7.4	-5.8
ALPHA-TOCOPHEROL ACETATE	-7.8	-5.6
ALPRAZOLAM	-8.6	-5.9
ALPROSTADIL	-6.2	-5.3
ALTRETAMINE	-5.1	-4.1
ALVIMOPAN	-8.3	-6.4
AMANTADINE	-5.5	-4.6
AMBENONIUM	-7.6	-5.5
AMBRISENTAN	-7.8	-5.2
AMCINONIDE	-10.7	-7.4
AMDINOCILLIN	-7.1	-5.8
AMIFAMPRIDINE	-4.1	-4.2
AMIFOSTINE	-4.8	-3.8
AMIKACIN	-7.2	-5.4
AMILORIDE	-6.4	-5.9
AMINOCAPROIC ACID	-4.9	-4.4
AMINOGLUTETHIMIDE	-7.4	-5.7
AMINOLEVULINIC ACID	-4.7	-5.3
AMINOMETHYLBENZOIC ACID	-6.4	-3.9
AMINOPTERIN	-9.0	-5.1
AMINOSALICYLIC ACID	-6.1	-5.4
AMIODARONE	-7.4	-5.8
AMITRIPTYLINE	-7.7	-6.7
AMLEXANOX	-8.7	-4.4
AMLODIPINE	-6.7	-4.2
AMODIAQUINE	-7.5	-6.9
AMOXAPINE	-8.8	-5.5
AMOXICILLIN	-8.2	-6.2
AMPHETAMINE	-5.3	-5.2
AMPHOTERICIN B	-7.1	-6.0
AMPICILLIN	-8.1	-5.8
AMPRENAVIR	-7.5	-5.1
ANAGRELIDE	-7.2	-5.7
ANASTROZOLE	-8.0	-6.0
ANGIOTENSIN II	-9.5	-6.1
ANIDULAFUNGIN	-6.6	-5.7
ANILERIDINE	-8.3	-6.0
ANISINDIONE	-7.5	-5.5
ANTAZOLINE	-7.4	-5.1

APALUTAMIDE	-10.1	-6.8
APOMORPHINE	-8.1	-5.8
APRACLONIDINE	-6.5	-5.5
APREPITANT	-8.3	-6.3
ARBUTAMINE	-7.6	-5.9
ARFORMOTEROL	-7.4	-6.3
ARGATROBAN	-9.4	-6.0
ARIPIRAZOLE	-8.8	-6.5
ARTEMETHER	-8.4	-5.4
ASCORBIC ACID	-5.9	-4.8
ASENAPINE	-8.3	-6.0
ASPIRIN	-6.1	-4.6
ATAZANAVIR	-8.5	-6.4
ATENOLOL	-6.0	-5.3
ATOVAQUONE	-8.9	-6.8
ATROPINE	-6.9	-5.2
AVATROMBOPAG	-6.9	-7.4
AXITINIB	-9.3	-7.0
AZACITIDINE	-6.6	-5.1
AZATADINE	-8.0	-6.0
AZATHIOPRINE	-6.5	-5.1
AZELAIC ACID	-5.2	-4.1
AZELASTINE	-9.0	-6.6
AZILSARTAN KAMEDOXOMIL	-9.6	-6.4
AZITHROMYCIN	-6.6	-5.5
AZLOCILLIN	-9.4	-6.7
AZTREONAM	-7.7	-6.2
BACAMPICILLIN	-7.7	-5.6
BACITRACIN	-5.3	-4.0
BACLOFEN	-6.0	-6.3
BALOXAVIR	-9.0	-6.4
BALOXAVIR MARBOXIL	-8.6	-6.4
BALSALAZIDE	-8.2	-6.6
BARICITINIB	-8.4	-5.6
BECLOMETHASONE DIPROPIONATE	-7.8	-6.6
BENAZEPRIL	-7.5	-5.9
BENDROFLUMETHIAZIDE	-8.4	-6.1
BENZHYDROCODONE	-9.0	-7.0
BENZNIDAZOLE	-7.9	-6.3
BENZONATATE	-5.9	-4.8
BENZOYL PEROXIDE	-6.9	-6.5

BENZPHETAMINE	-6.1	-5.7
BENZQUINAMIDE	-7.5	-5.7
BENZTHIAZIDE	-8.4	-6.3
BENZTROPINE	-7.8	-5.3
BENZYL ALCOHOL	-5.0	-4.8
BENZYL BENZOATE	-6.3	-6.2
BEPOTASTINE	-8.4	-6.0
BEPRIDIL	-7.1	-4.7
BESIFLOXACIN	-8.6	-5.6
BETAINE	-4.0	-3.2
BETAMETHASONE	-9.3	-6.4
BETAMETHASONE ACETATE	-9.2	-6.5
BETAMETHASONE BENZOATE	-10.8	-6.5
BETAMETHASONE DIPROPIONATE	-8.8	-5.5
BETAMETHASONE PHOSPHATE	-8.6	-6.6
BETAMETHASONE VALERATE	-9.7	-5.7
BETAXOLOL	-6.6	-5.2
BETAZOLE	-4.4	-4.6
BETHANECHOL	-4.5	-3.8
BETRIXABAN	-8.5	-6.5
BEXAROTENE	-9.2	-6.4
BICALUTAMIDE	-8.9	-7.0
BICTEGRAVIR	-9.7	-7.8
BIMATOPROST	-7.6	-6.2
BINIMETINIB	-7.6	-5.5
BIOTIN	-6.4	-5.5
BIPERIDEN	-8.0	-6.1
BISOPROLOL	-6.1	-5.1
BISPHOSPHONATE	-5.8	-5.5
BITOLTEROL	-8.1	-5.7
BLEOMYCIN	-4.1	-4.7
BMS-354825	-8.6	-6.5
BOCEPREVIR	-8.1	-5.4
BOSENTAN	-8.4	-5.2
BREXANOLONE	-8.5	-6.0
BRIGATINIB	-8.8	-6.4
BRIMONIDINE	-7.2	-5.2
BRINZOLAMIDE	-7.2	-4.9
BROMFENAC	-7.8	-5.7
BROMODIPHENHYDRAMINE	-6.8	-4.7
BROMPHENIRAMINE	-7.0	-6.2

BRZ	-7.4	-4.9
BUCLIZINE	-8.9	-6.1
BUDESONIDE	-9.7	-6.2
BUMETANIDE	-7.5	-5.2
BUPIVACAINE	-7.0	-5.9
BUPRENORPHINE	-7.6	-5.9
BUPROPION	-6.5	-5.2
BUSPIRONE	-8.7	-7.2
BUSULFAN	-5.7	-4.5
BUTABARBITAL	-6.5	-4.8
BUTALBITAL	-6.6	-4.7
BUTENAFINE	-7.4	-6.1
BUTOCONAZOLE	-6.6	-4.8
BUTORPHANOL	-7.6	-6.2
CABAZITAXEL	-5.9	-5.9
CAFFEINE	-6.0	-4.9
CALCIFEDIOL	-8.6	-6.2
CALCIPOTRIENE	-8.7	-6.7
CANDESARTAN CILEXETIL	-8.9	-6.7
CANDICIDIN	-6.0	-6.3
CANNABIDIOL	-7.4	-5.3
CAPECITABINE	-7.4	-6.1
CAPREOMYCIN	-8.8	-6.4
CAPSAICIN	-7.3	-5.8
CAPTOPRIL	-5.6	-4.2
CARBACHOL	-4.7	-3.7
CARBAMAZEPINE	-7.9	-7.7
CARBENICILLIN	-8.3	-6.1
CARBENICILLIN INDANYL	-9.4	-7.1
CARBIDOPA	-6.9	-5.7
CARBINOXAMINE	-6.7	-5.9
CARGLUMIC ACID	-5.9	-5.2
CARISOPRODOL	-6.1	-5.4
CARMUSTINE	-5.0	-4.3
CARPHENAZINE	-7.8	-5.6
CARPROFEN	-8.1	-6.0
CARTEOLOL	-7.6	-5.3
CARVEDILOL	-8.4	-6.1
CEFACLOR	-7.8	-5.8
CEFADROXIL	-8.0	-6.4
CEFAMANDOLE NAFATE	-8.3	-6.3

CEFAZOLIN	-8.2	-6.4
CEFDINIR	-7.8	-6.1
CEFDITOREN PIVOXIL	-8.4	-6.4
CEFIXIME	-7.3	-6.4
CEFMENOXIME	-7.7	-6.7
CEFMETAZOLE	-7.4	-6.0
CEFONICID	-7.4	-7.1
CEFOPERAZONE	-9.8	-6.5
CEFORANIDE	-7.8	-6.9
CEFOTAXIME	-7.4	-5.9
CEFOTETAN	-8.0	-6.4
CEFOTIAM	-7.7	-5.8
CEFOXITIN	-7.1	-5.5
CEFPIRAMIDE	-9.8	-6.8
CEFPODOXIME PROXETIL	-8.0	-5.8
CEFPROZIL	-8.3	-6.0
CEFTAROLINE	-8.6	-7.1
CEFTAZIDIME	-7.9	-6.4
CEFTIBUTEN	-7.4	-6.2
CEFTIZOXIME	-7.6	-6.0
CEFTRIAZONE	-8.4	-7.0
CEFUROXIME	-7.5	-6.2
CEFUROXIME AXETIL	-8.0	-5.9
CELECOXIB	-8.3	-6.5
CEPHALEXIN	-8.0	-5.9
CEPHALOGLYCIN	-8.1	-6.0
CEPHALOTHIN	-7.3	-5.8
CEPHAPIRIN	-7.8	-6.0
CEPHRADINE	-8.0	-5.9
CERIVASTATIN	-7.3	-5.6
CERULETIDE	-6.2	-6.2
CETIRIZINE	-7.4	-5.1
CETRORELIX	-9.1	-6.2
CEVIMELINE	-5.8	-4.4
CHENODIOL	-8.4	-6.0
CHLOPHEDIANOL	-7.0	-4.8
CHLORAMBUCIL	-6.3	-4.5
CHLORAMPHENICOL	-7.0	-5.4
CHLORAMPHENICOL PALMITATE	-7.4	-4.8
CHLORDIAZEPOXIDE	-7.5	-5.4
CHLORHEXIDINE	-9.5	-6.9

CHLORMEZANONE	-6.8	-5.1
CHLOROPROCAINE	-6.5	-5.1
CHLOROQUINE	-6.7	-4.9
CHLOROTHIAZIDE	-7.0	-5.3
CHLOROTRIANISENE	-7.7	-5.7
CHLOROXINE	-6.4	-5.4
CHLORPHENESIN CARBAMATE	-6.2	-5.1
CHLORPHENIRAMINE	-7.0	-5.7
CHLORPHENTERMINE	-5.5	-4.8
CHLORPROMAZINE	-7.0	-5.0
CHLORPROPAMIDE	-6.6	-6.0
CHLORTETRACYCLINE	-8.3	-6.5
CHLORTHALIDONE	-8.0	-6.6
CHLORZOXAZONE	-6.6	-5.5
CICLESONIDE	-10.4	-7.0
CICLOPIROX	-6.8	-6.8
CIDOFOVIR	-6.4	-5.6
CILASTATIN	-6.4	-5.5
CILOSTAZOL	-9.0	-6.5
CIMETIDINE	-6.4	-4.9
CINACALCET	-7.0	-5.3
CINOXACIN	-6.8	-5.4
CIPROFLOXACIN	-8.1	-5.8
CISATRACURIUM	-7.4	-4.1
CITALOPRAM	-7.8	-5.5
CLADRIBINE	-7.2	-6.4
CLARITHROMYCIN	-8.3	-4.8
CLAVULANATE	-6.5	-5.1
CLEMASTINE	-7.4	-5.0
CLIDINIUM	-7.7	-6.3
CLINDAMYCIN	-6.8	-5.7
CLINDAMYCIN PALMITATE	-7.1	-5.0
CLINDAMYCIN PHOSPHATE	-5.6	-5.2
CLIOQUINOL	-6.5	-5.8
CLOBAZAM	-7.9	-5.7
CLOBETASOL PROPIONATE	-9.8	-6.5
CLOCORTOLONE PIVALATE	-8.5	-7.3
CLOFAZIMINE	-9.3	-6.4
CLOFIBRATE	-6.1	-4.6
CLOMIPRAMINE	-7.8	-5.1
CLONAZEPAM	-8.0	-5.9

CLONIDINE	-6.4	-5.0
CLOPIDOGREL	-7.5	-5.4
CLORAZEPATE	-8.1	-6.1
CLOTTRIMAZOLE	-7.4	-5.2
CLOXACILLIN	-8.4	-6.7
CLOZAPINE	-8.3	-6.1
COCAINE	-7.2	-5.8
CODEINE	-7.7	-5.9
COLCHICINE	-8.0	-5.2
COLFOSCERIL PALMITATE	-6.2	-4.3
COLISTIMETHATE	-5.6	-3.6
COLISTIN	-5.5	-4.8
CONIVAPTAN	-10.2	-7.8
COPANLISIB	-9.0	-6.8
CORTISONE ACETATE	-8.7	-6.6
CRIZOTINIB	-9.1	-7.3
CROMOLYN	-8.7	-7.1
CROTAMITON	-6.2	-4.5
CYCLACILLIN	-7.3	-5.9
CYCLIZINE	-7.7	-5.5
CYCLOBENZAPRINE	-8.2	-5.5
CYCLOPENTOLATE	-6.8	-4.8
CYCLOPHOSPHAMIDE	-5.2	-4.1
CYCLOSPORINE	-5.1	-4.5
CYCLOTHIAZIDE	-9.1	-6.0
CYCRIMINE	-7.6	-6.8
CYPROHEPTADINE	-9.4	-6.0
CYSTEAMINE	-2.6	-2.2
CYTARABINE	-6.4	-4.9
DABIGATRAN ETEXILATE	-8.9	-5.7
DACARBAZINE	-5.8	-5.4
DACOMITINIB	-9.9	-6.7
DACTINOMYCIN	-7.7	-4.2
DALFAMPRIDINE	-3.9	-4.0
DALFOPRISTIN	-9.0	-6.8
DANAZOL	-9.1	-7.1
DANTROLENE	-8.4	-6.4
DAPIPRAZOLE	-8.2	-6.8
DAPSONE	-7.4	-5.4
DAPTOMYCIN	-4.3	-3.5
DARIFENACIN	-9.5	-6.7



DARUNAVIR	-8.8	-5.4
DASATINIB	-8.9	-6.6
DAUNORUBICIN	-9.8	-6.2
DECITABINE	-6.5	-5.9
DEFERASIROX	-9.4	-7.1
DEFERIPRONE	-5.4	-4.6
DEFEROXAMINE	-7.1	-6.3
DEFLAZACORT	-9.3	-6.9
DEGARELIX	-4.8	-5.2
DELAFLXACIN	-8.6	-6.5
DELAVIRDINE	-8.6	-6.6
DEMECARIUM	-8.0	-5.3
DEMECLOCYCLINE	-8.3	-6.3
DESERPIDINE	-9.0	-6.6
DESFLURANE	-4.9	-4.7
DESIPRAMINE	-7.4	-5.5
DESLANOSIDE	-7.5	-7.9
DESLORATADINE	-8.3	-6.0
DESOGESTREL	-7.9	-5.7
DESONIDE	-9.9	-6.6
DESOXIMETASONE	-9.6	-6.4
DESOXYCORTICOSTERONE ACETATE	-8.3	-6.7
DESOXYCORTICOSTERONE PIVALATE	-8.6	-6.8
DESVENLAFAXINE	-6.9	-5.2
DEXAMETHASONE	-9.3	-6.6
DEXBROMPHENIRAMINE	-6.9	-4.8
DEXCHLORPHENIRAMINE	-6.9	-6.0
DEXMEDETOMIDINE	-6.5	-4.9
DEXMETHYLPHENIDATE	-6.8	-5.3
DEXPANTHENOL	-5.3	-4.3
DEXRAZOXANE	-7.0	-6.2
DEXTROTHYROXINE	-6.3	-5.2
DEZOCINE	-8.8	-5.6
DIAZEPAM	-7.9	-5.8
DIAZOXIDE	-6.7	-5.1
DIBUCAINE	-7.5	-5.6
DICHLORPHENAMIDE	-7.0	-4.7
DICLOFENAC	-6.9	-6.0
DICLOXACILLIN	-8.1	-6.1
DICUMAROL	-8.5	-6.4
DICYCLOMINE	-6.5	-5.1

DIDANOSINE	-7.2	-5.7
DIENESTROL	-7.3	-5.5
DIENOGEST	-8.5	-6.7
DIETHYLCARBAMAZINE	-5.2	-3.9
DIETHYLPROPION	-6.2	-4.3
DIETHYLSTILBESTROL	-6.9	-5.5
DIFENOXIN	-9.0	-6.6
DIFLORASONE DIACETATE	-8.4	-6.5
DIFLUNISAL	-7.7	-6.3
DIFLUPREDNATE	-8.9	-6.4
DIGITOXIN	-11.2	-8.0
DIGOXIN	-7.7	-7.4
DIHYDROCODEINE	-7.3	-5.8
DIHYDROERGOTAMINE	-12.7	-7.4
DILTIAZEM	-7.1	-4.9
DIMENHYDRINATE	-6.2	-4.7
DIMERCAPROL	-3.1	-2.7
DINOPROST	-7.0	-5.0
DINOPROSTONE	-6.7	-4.5
DIPHEMANIL	-8.0	-6.1
DIPHENHYDRAMINE	-6.8	-4.5
DIPHENIDOL	-7.2	-5.1
DIPHENOXYLATE	-8.4	-6.5
DIPHENYLPYRALINE	-7.5	-7.0
DIPIVEFRIN	-7.4	-5.5
DIPYRIDAMOLE	-7.0	-4.6
DISOPYRAMIDE	-7.2	-5.1
DISULFIRAM	-4.6	-3.5
DOCETAXEL	-9.4	-6.5
DOCOSANOL	-5.5	-3.8
DOFETILIDE	-7.6	-5.9
DOLASETRON	-8.6	-6.2
DONEPEZIL	-9.1	-6.9
DOPAMINE	-5.9	-5.3
DORAVIRINE	-8.5	-6.5
DORIPENEM	-7.8	-6.5
DORZOLAMIDE	-7.1	-5.6
DOXACURIUM	-7.1	-5.0
DOXAPRAM	-8.0	-5.3
DOXAZOSIN	-9.6	-6.7
DOXEPIN	-8.1	-5.3

DOXERCALCIFEROL	-9.5	-6.7
DOXORUBICIN	-9.3	-6.0
DOXYCYCLINE	-8.4	-6.5
DOXYLAMINE	-6.5	-4.7
DROMOSTANOLONE PROPIONATE	-8.7	-6.6
DRONABINOL	-8.2	-5.8
DRONEDARONE	-8.0	-5.4
DROPERIDOL	-9.6	-6.8
DROSPIRENONE	-10.6	-6.9
DULOXETINE	-6.8	-6.6
DUTASTERIDE	-10.2	-7.1
DUVELISIB	-9.3	-6.7
DYCLONINE	-6.9	-5.4
DYDROGESTERONE	-8.6	-6.4
DYPHYLLINE	-6.6	-5.4
ECHOTHIOPHATE	-4.6	-3.8
ECONAZOLE	-7.9	-6.0
EDARAVONE	-6.4	-5.9
EDROPHONIUM	-5.9	-4.1
EFAVIRENZ	-7.2	-5.2
EFLORNITHINE	-4.9	-4.5
ELAGOLIX	-8.7	-5.9
ELETRIPTAN	-8.0	-6.8
EMEDASTINE	-7.0	-5.3
EMTRICITABINE	-6.4	-4.9
ENALAPRIL	-7.7	-6.0
ENALAPRILAT	-7.7	-6.5
ENASIDENIB	-9.1	-7.2
ENCORAFENIB	-8.4	-7.1
ENFLURANE	-4.9	-4.7
ENOXACIN	-8.0	-5.6
ENTACAPONE	-7.2	-5.9
ENTECAVIR	-7.3	-6.0
EPINASTINE	-8.8	-5.9
EPINEPHRINE	-6.0	-5.2
EPIRUBICIN	-8.4	-5.7
EPOPROSTENOL	-7.5	-5.3
EPROSARTAN	-7.5	-5.7
EPTIFIBATIDE	-7.4	-6.6
EQUILIN	-8.5	-7.0
ERAVACYCLINE	-8.7	-6.7

ERDAFITINIB	-8.1	-5.7
ERGOALCIFEROL	-9.6	-6.4
ERIBULIN	-10.3	-7.8
ERLOTINIB	-7.9	-6.4
ERTAPENEM	-9.1	-6.6
ERTUGLIFLOZIN	-8.2	-6.7
ERYTHROMYCIN	-8.4	-5.2
ERYTHROMYCIN ESTOLATE	-8.5	-5.1
ERYTHROMYCIN ETHYLSUCCINATE	-8.9	-5.1
ESCITALOPRAM	-7.5	-5.5
ESKETAMINE	-6.3	-5.9
ESMOLOL	-6.5	-5.1
ESTAZOLAM	-8.0	-5.8
ESTRADIOL	-8.2	-6.3
ESTRADIOL CYPIONATE	-9.6	-7.3
ESTRADIOL VALERATE	-8.6	-6.0
ESTRAMUSTINE PHOSPHATE	-7.9	-6.2
ESTRONE	-8.5	-6.1
ESTROPIPATE	-9.1	-6.5
ESZOPICLONE	-8.3	-5.9
ETELCALCETIDE	-8.0	-5.7
ETHAMBUTOL	-4.8	-3.8
ETHCHLORVYNOL	-5.0	-4.7
ETHINAMATE	-6.4	-5.4
ETHINYL ESTRADIOL	-8.6	-6.5
ETHIONAMIDE	-5.4	-5.2
ETHOPROPAZINE	-7.0	-4.8
ETHOSUXIMIDE	-5.7	-4.8
ETHOTOIN	-6.5	-5.8
ETHOXZOLAMIDE	-6.4	-5.4
ETHYLESTRENOL	-7.8	-6.2
ETHYNODIOL DIACETATE	-8.2	-6.4
ETIDOCAINE	-6.4	-4.8
ETIDRONATE	-5.4	-4.2
ETODOLAC	-7.1	-5.4
ETOMIDATE	-6.9	-5.7
ETONOGESTREL	-8.5	-5.7
ETOPOSIDE	-9.6	-6.4
ETOPOSIDE PHOSPHATE	-8.8	-6.1
ETRETINATE	-7.7	-5.9
EXEMESTANE	-8.5	-5.9

EZETIMIBE	-8.2	-6.0
EZOGABINE	-7.5	-6.0
FAMCICLOVIR	-7.1	-5.0
FAMOTIDINE	-6.5	-5.8
FELBAMATE	-6.7	-6.3
FELODIPINE	-6.9	-4.8
FENOFIBRATE	-8.1	-6.2
FENOFIBRIC ACID	-7.9	-6.8
FENOLDOPAM	-7.9	-5.7
FENOPROFEN	-7.3	-5.9
FENTANYL	-8.0	-5.8
FESOTERODINE	-7.2	-5.4
FEXOFENADINE	-9.2	-6.2
FINASTERIDE	-8.5	-6.1
FINGOLIMOD	-6.7	-4.6
FLAVOXATE	-8.9	-6.7
FLECAINIDE	-8.1	-6.1
FLOXURIDINE	-6.7	-5.1
FLUCONAZOLE	-7.6	-6.3
FLUCYTOSINE	-5.1	-4.6
FLUDARABINE PHOSPHATE	-7.2	-5.7
FLUDROCORTISONE ACETATE	-8.7	-7.0
FLUMAZENIL	-7.9	-5.6
FLUNISOLIDE	-9.6	-6.3
FLUOCINONIDE	-9.6	-7.5
FLUOROMETHOLONE	-8.9	-6.6
FLUOROURACIL	-5.1	-4.5
FLUOXETINE	-7.5	-6.7
FLUOXYMESTERONE	-8.9	-6.7
FLUPHENAZINE	-8.0	-5.9
FLUPREDNISOLONE	-9.0	-6.4
FLURAZEPAM	-7.9	-5.4
FLURBIPROFEN	-7.8	-5.6
FLUTAMIDE	-7.1	-5.7
FLUTICASONE FUROATE	-10.0	-6.3
FLUTICASONE PROPIONATE	-8.9	-6.4
FLUVASTATIN	-7.9	-5.8
FLUVOXAMINE	-6.7	-4.9
FOLIC_ACID	-8.9	-6.9
FOMEPIZOLE	-4.0	-3.8
FONDAPARINUX	-5.8	-4.4

FORMOTEROL	-7.5	-5.7
FOSAPREPITANT	-9.3	-7.0
FOSCARNET	-4.5	-3.6
FOSFOMYCIN	-4.7	-3.5
FOSINOPRIL	-7.2	-6.2
FOSNETUPITANT	-9.9	-6.2
FOSPHENYTOIN	-8.7	-6.6
FOSTAMATINIB	-9.1	-7.1
FROVATRIPTAN	-7.5	-5.7
FULVESTRANT	-8.8	-5.5
FURAZOLIDONE	-6.7	-5.7
FUROSEMIDE	-7.6	-5.6
GABAPENTIN	-5.5	-5.8
GABAPENTIN ENACARBIL	-7.2	-5.9
GALANTAMINE	-7.7	-5.0
GALANTHAMINE	-7.8	-5.7
GALLAMINE	-5.6	-4.6
GANCICLOVIR	-6.9	-5.2
GANIRELIX	-6.2	-6.4
GATIFLOXACIN	-8.1	-5.5
GEFITINIB	-8.4	-6.2
GEMCITABINE	-6.9	-6.0
GEMFIBROZIL	-6.8	-5.3
GEMIFLOXACIN	-8.3	-6.3
GENTAMICIN	-7.3	-5.9
GENTIAN VIOLET	-6.9	-6.1
GILTERITINIB	-8.8	-6.9
GLASDEGIB	-8.6	-6.8
GLECAPREVIR	-11.5	-6.7
GLIMEPIRIDE	-10.1	-7.5
GLIPIZIDE	-10.1	-7.1
GLUCONOLACTONE	-5.6	-5.1
GLUTAMINE	-5.0	-5.3
GLUTATHIONE DISULFIDE	-6.9	-6.2
GLUTETHIMIDE	-7.2	-5.1
GLYCINE	-3.4	-5.8
GLYCOPYRROLATE	-7.7	-6.0
GLYCOPYRRONIUM	-7.7	-5.6
GOSERELIN	-6.6	-5.5
GRAMICIDIN	-5.3	-5.2
GRANISETRON	-8.0	-6.5

GREPAFLOXACIN	-7.8	-6.0
GRISEOFULVIN	-7.3	-5.4
GUAIFENESIN	-5.8	-4.6
GUANABENZ	-6.6	-5.3
GUANADREL	-6.8	-6.0
GUANETHIDINE	-6.3	-5.4
GUANFACINE	-6.9	-5.7
GUANIDINE	-3.2	-2.7
GW572016	-10.1	-7.3
HALAZEPAM	-8.1	-5.8
HALCINONIDE	-10.4	-7.0
HALOFANTRINE	-8.0	-4.7
HALOPERIDOL	-8.9	-6.8
HALOPROGIN	-5.6	-4.1
HALOTHANE	-4.1	-4.0
HETACILLIN	-8.3	-5.4
HEXACHLOROPHENE	-7.8	-5.1
HEXOCYLIUM	-7.9	-5.5
HEXYLCAINE	-7.0	-5.3
HISTAMINE	-4.3	-4.1
HISTRELIN	-7.5	-5.4
HOMATROPINE METHYLBROMIDE	-7.4	-5.9
HYDRALAZINE	-6.9	-5.9
HYDROCHLOROTHIAZIDE	-7.6	-5.7
HYDROCODONE	-7.9	-5.7
HYDROCORTAMATE	-8.3	-6.4
HYDROCORTISONE	-9.0	-5.6
HYDROCORTISONE ACETATE	-8.9	-6.6
HYDROCORTISONE BUTYRATE	-9.0	-6.1
HYDROCORTISONE CYPIONATE	-9.7	-7.5
HYDROCORTISONE PROBUTATE	-8.4	-5.5
HYDROCORTISONE VALERATE	-8.9	-6.4
HYDROFLUMETHIAZIDE	-7.9	-5.8
HYDROMORPHONE	-7.7	-5.7
HYDROXYAMPHETAMINE	-5.8	-5.3
HYDROXYCHLOROQUINE	-6.4	-4.9
HYDROXYPROGESTERONE CAPROATE	-9.3	-5.5
HYDROXYSTILBAMIDINE	-7.8	-5.6
HYDROXYUREA	-3.9	-3.8
HYDROXYZINE	-6.7	-5.6
IBANDRONATE	-6.0	-4.6

IBUPROFEN	-6.6	-6.2
IBUTILIDE	-6.9	-5.1
ICATIBANT	-7.3	-4.9
IDARUBICIN	-10.5	-6.5
IDOXURIDINE	-7.0	-5.4
IFOSFAMIDE	-5.2	-4.4
IMATINIB	-9.0	-7.9
IMIPENEM	-7.3	-4.8
IMIPRAMINE	-7.3	-5.4
IMIQUIMOD	-7.2	-7.2
IMN	-8.6	-5.8
INDACATEROL	-8.8	-6.8
INDAPAMIDE	-8.6	-6.9
INDECAINIDE	-7.3	-4.9
INDINAVIR	-9.6	-7.1
INDOMETHACIN	-8.3	-5.6
INGENOL MEBUTATE	-8.6	-6.1
IPRATROPIUM	-7.2	-5.4
IRBESARTAN	-9.0	-6.1
IRINOTECAN	-10.5	-8.1
ISOCARBOXAZID	-7.3	-5.8
ISOETHARINE	-6.6	-4.9
ISOFLURANE	-4.8	-4.7
ISOFLUROPHATE	-4.9	-3.7
ISONIAZID	-6.0	-5.2
ISOPROPAMIDE	-6.6	-5.2
ISOPROTERENOL	-6.4	-5.1
ISOSORBIDE	-5.0	-4.2
ISOSORBIDE DINITRATE	-6.6	-4.8
ISOSORBIDE MONONITRATE	-5.9	-4.7
ISOTRETINOIN	-7.7	-6.2
ISRADIPINE	-7.1	-5.1
ITRACONAZOLE	-7.5	-7.5
IVACAFTOR	-8.2	-7.0
IVOSIDENIB	-8.6	-5.7
IXABEPILONE	-8.9	-6.1
JFD00715	-7.5	-5.7
KANAMYCIN	-7.3	-5.8
KETAMINE	-6.7	-4.7
KETOCONAZOLE	-8.8	-6.9
KETOPROFEN	-7.9	-7.1



KETOROLAC	-7.6	-5.9
KETOTIFEN	-8.8	-5.7
LABETALOL	-7.8	-6.3
LACOSAMIDE	-6.5	-5.2
LACTIC ACID	-4.0	-3.5
LAMIVUDINE	-6.4	-5.3
LAMOTRIGINE	-7.2	-7.0
LANREOTIDE	-5.9	-4.4
LANSOPRAZOLE	-8.5	-5.9
LAPATINIB	-10.2	-7.3
LAROTRECTINIB	-9.8	-6.5
LATANOPROSTENE BUNOD	-7.3	-5.1
LEFLUNOMIDE	-7.6	-6.4
LENALIDOMIDE	-7.5	-5.7
LETERMOVIR	-9.0	-6.9
LETROZOLE	-8.3	-5.7
LEUCOVORIN	-8.4	-6.7
LEVALBUTEROL	-6.7	-5.9
LEVALLORPHAN	-7.8	-5.4
LEVAMISOLE	-6.1	-5.8
LEVETIRACETAM	-5.4	-4.3
LEVOBETAXOLOL	-6.7	-5.1
LEVOBUNOLOL	-7.3	-5.3
LEVOBUPIVACAINE	-7.1	-5.7
LEVOCABASTINE	-8.4	-7.9
LEVOCARNITINE	-4.6	-4.2
LEVOCETIRIZINE	-8.0	-5.9
LEVODOPA	-6.6	-6.1
LEVOFLOXACIN	-8.3	-6.0
LEVOMEFOLATE	-8.9	-6.9
LEVOMEPRMAZINE	-7.3	-4.9
LEVOMETHADYL ACETATE	-6.6	-4.7
LEVONORDEFIN	-6.2	-5.8
LEVONORGESTREL	-8.5	-6.2
LEVOPROPOXYPHENE	-6.8	-4.8
LEVORPHANOL	-7.9	-5.4
LEVOTHYROXINE	-6.5	-4.6
L-GLUTAMINE	-5.1	-4.7
L-HISTAMINE	-4.3	-7.3
LIDOCAINE	-6.2	-6.5
LIFITEGRAST	-10.4	-5.2

LINAGLIPTIN	-9.8	-6.6
LINCOMYCIN	-6.7	-5.3
LINEZOLID	-8.0	-4.8
LIOTHYRONINE	-7.4	-5.3
LISDEXAMFETAMINE	-6.4	-4.6
LISINOPRIL	-7.2	-4.8
LOFEXIDINE	-6.5	-5.9
LOMEFLOXACIN	-8.2	-6.1
LOMUSTINE	-6.3	-5.3
LOPERAMIDE	-8.4	-6.3
LOPINAVIR	-8.7	-5.9
LORACARBEF	-8.2	-6.0
LORATADINE	-8.0	-6.3
LORAZEPAM	-7.8	-5.9
LORLATINIB	-8.9	-6.2
LOSARTAN	-8.3	-6.4
LOTEPREDNOL ETABONATE	-9.0	-5.8
LOVASTATIN	-8.2	-6.2
LOXAPINE	-8.5	-5.9
LUBIPROSTONE	-7.4	-5.7
LUMEFANTRINE	-7.6	-4.7
LURASIDONE	-10.2	-7.9
LUSUTROMBOPAG	-8.4	-6.5
MACIMORELIN	-9.0	-6.4
MAFENIDE	-6.6	-4.9
MAPROTILINE	-7.7	-6.1
MARAVIROC	-9.1	-6.3
MASOPROCOL	-7.3	-6.0
MAYTANSINE	-8.7	-5.4
MAZINDOL	-8.6	-5.9
MEBENDAZOLE	-8.1	-6.6
MEBUTAMATE	-5.5	-5.5
MECAMYLAMINE	-5.8	-4.5
MECHLORETHAMINE	-3.6	-3.1
MECLIZINE	-9.4	-6.6
MECLOCYCLINE	-8.6	-6.4
MECLOFENAMATE	-7.8	-6.3
MEDROXYPROGESTERONE ACETATE	-8.4	-6.1
MEDRYSONE	-8.7	-6.6
MEFENAMIC ACID	-7.9	-5.5
MEFLOQUINE	-8.5	-6.1

MEGESTROL ACETATE	-8.6	-6.2
MELOXICAM	-8.7	-6.1
MELPHALAN	-6.2	-4.8
MEMANTINE	-6.3	-5.2
MENADIOL	-6.5	-5.6
MENADIONE	-6.8	-5.4
MENAQUINONE	-9.2	-4.9
MENTHOL	-5.8	-5.3
MEPENZOLATE	-7.8	-5.8
MEPERIDINE	-6.8	-4.9
MEPHENTERMINE	-5.6	-5.0
MEPHENYTOIN	-6.9	-4.9
MEPIVACAINE	-7.1	-5.3
MEPREDNISONE	-8.7	-6.5
MEPROBAMATE	-5.6	-5.2
MEQUINOL	-5.1	-4.7
MERCAPTOPYRINE	-5.1	-4.9
MEROPENEM	-8.0	-5.9
MESALAMINE	-5.7	-5.3
MESNA	-4.2	-3.4
MESORIDAZINE	-8.3	-5.7
MESTRANOL	-8.3	-6.6
METAPROTERENOL	-5.8	-6.0
METARAMINOL	-6.0	-6.0
METAXALONE	-6.9	-5.5
METFORMIN	-4.7	-4.2
METHACHOLINE	-4.8	-3.8
METHACYCLINE	-8.3	-6.7
METHADONE	-6.6	-5.8
METHAMPHETAMINE	-5.3	-5.3
METHARBITAL	-6.1	-4.7
METHAZOLAMIDE	-6.4	-4.9
METHDILAZINE	-8.0	-5.4
METHICILLIN	-7.2	-5.5
METHIMAZOLE	-3.8	-3.6
METHIXENE	-8.5	-5.8
METHOCARBAMOL	-6.2	-5.7
METHOHEXITAL	-7.1	-4.7
METHOTREXATE	-8.6	-6.5
METHOXAMINE	-5.8	-5.6
METHOXSALEN	-7.1	-5.1

METHOXYFLURANE	-4.4	-4.0
METHSCOPOLAMINE	-7.6	-5.9
METHSUXIMIDE	-6.8	-6.4
METHYCLOTHIAZIDE	-6.9	-5.9
METHYL AMINOLEVULINATE	-4.7	-4.2
METHYL SALICYLATE	-5.3	-4.8
METHYLDOPA	-6.8	-4.8
METHYLDOPATE	-6.3	-5.9
METHYLERGONOVINE	-8.2	-6.4
METHYLNALTREXONE	-7.9	-6.0
METHYLPHENIDATE	-6.9	-6.3
METHYLPREDNISOLONE	-8.8	-6.1
METHYLPREDNISOLONE ACETATE	-8.3	-6.9
METHYLPREDNISOLONE SUCCINATE	-8.3	-6.8
METHYLTESTOSTERONE	-8.8	-6.4
METHYSERGIDE	-7.7	-6.1
METIPRANOLOL	-6.7	-5.2
METOCLOPRAMIDE	-6.3	-4.9
METOCURINE	-10.2	-6.7
METOLAZONE	-8.7	-6.6
METOPROLOL	-6.2	-5.1
METRONIDAZOLE	-5.6	-4.7
METYRAPONE	-6.6	-6.0
METYROSINE	-6.5	-5.8
MEXILETINE	-5.8	-4.9
MEZLOCILLIN	-9.0	-7.1
MICONAZOLE	-7.2	-5.5
MIDAZOLAM	-8.6	-6.0
MIDODRINE	-6.3	-4.9
NABILONE	-7.8	-5.4
NABUMETONE	-6.9	-5.9
NADOLOL	-7.3	-6.0
NAFARELIN	-9.7	-6.1
NAFCILLIN	-8.4	-5.9
NAFTIFINE	-8.2	-5.9
NALBUPHINE	-7.8	-6.1
NALDEMEDINE	-10.2	-7.2
NALIDIXIC_ACID	-6.6	-5.1
NALMEFENE	-8.1	-5.6
NALOXONE	-7.4	-5.4
NALTREXONE	-7.9	-5.5

NANDROLONE	-8.5	-5.8
NANDROLONE DECANOATE	-8.4	-6.2
NANDROLONE PHENPROPIONATE	-9.1	-7.2
NAPHAZOLINE	-6.9	-5.4
NAPROXEN	-7.4	-6.8
NARATRIPTAN	-7.8	-6.3
NATAMYCIN	-7.4	-6.2
NATEGLINIDE	-7.9	-6.1
NEBIVOLOL	-9.4	-6.9
NEDOCROMIL	-7.5	-5.5
NEFAZODONE	-8.7	-6.1
NELARABINE	-6.7	-5.8
NELFINAVIR	-9.0	-6.2
NEOMYCIN	-7.0	-5.3
NERATINIB	-9.0	-6.6
NETARSUDIL	-9.9	-7.3
NEVIRAPINE	-7.8	-5.4
NIACIN	-5.2	-4.7
NICARDIPINE	-8.1	-5.8
NICLOSAMIDE	-7.9	-6.2
NICOTINE	-5.4	-5.1
NIFEDIPINE	-7.2	-4.9
NILOTINIB	-9.8	-7.7
NILUTAMIDE	-7.7	-5.9
NIMODIPINE	-7.5	-4.8
NIRAPARIB	-8.6	-6.6
NITAZOXANIDE	-7.5	-6.1
NITISINONE uff	-7.8	-5.9
NITROFURANTOIN	-7.2	-5.8
NITROFURAZONE	-6.5	-5.5
NITROGLYCERIN	-5.7	-4.6
NIZATIDINE	-5.7	-4.7
NORELGESTROMIN	-8.7	-6.3
NOREPINEPHRINE	-5.9	-5.6
NORETHINDRONE	-8.5	-6.4
NORETHINDRONE ACETATE	-8.5	-6.3
NORETHYNODREL	-8.5	-6.7
NORFLOXACIN	-8.0	-5.7
NORGESTIMATE	-8.4	-6.0
NORGESTREL	-8.3	-6.2
NORTRIPTYLINE	-7.7	-5.9

NOVOBIOCIN	-9.3	-7.2
NYSTATIN	-6.8	-4.5
OCTINOXATE	-5.9	-4.7
OFLOXACIN	-7.6	-6.2
OLANZAPINE	-7.8	-6.1
OLOPATADINE	-8.0	-6.2
OLSALAZINE	-8.1	-6.5
OMADACYCLINE	-8.0	-6.3
OMEPRAZOLE	-7.5	-6.0
ONDANSETRON	-8.4	-6.1
ORLISTAT	-6.2	-4.5
ORPHENADRINE	-6.7	-4.6
OSELTAMIVIR	-7.0	-4.7
OXACILLIN	-8.5	-6.6
OXAMNIQUINE	-7.3	-6.3
OXANDROLONE	-8.5	-6.4
OXAPROZIN	-8.0	-6.6
OXAZEPAM	-7.8	-5.7
OXCARBAZEPINE	-8.1	-6.4
OXICONAZOLE	-7.3	-6.2
OXPRENOLOL	-6.1	-4.9
OXTRIPHYLLINE	-6.0	-5.0
OXYBUTYNIN	-6.9	-4.6
OXYCODONE	-7.9	-5.7
OXYMETHOLONE	-8.3	-6.9
OXYMORPHONE	-7.7	-5.8
OXYPHENBUTAZONE	-7.5	-5.5
OXYPHENCYCLIMINE	-7.9	-5.6
OXYPHENONIUM	-6.9	-5.1
OXYTETRACYCLINE	-8.2	-6.3
OZENOXACIN	-8.4	-6.5
PACLITAXEL	-10.3	-6.9
PALIPERIDONE	-10.0	-7.5
PALIPERIDONE PALMITATE	-8.7	-6.4
PALONOSETRON	-8.3	-5.9
PAMIDRONATE	-5.4	-4.2
PANCURONIUM	-8.2	-7.0
PANTOPRAZOLE	-7.9	-5.8
PANTOTHENIC ACID	-5.6	-4.3
PARAMETHADIONE	-5.5	-4.3
PARAMETHASONE ACETATE	-9.1	-5.7

PARGYLINE	-5.2	-5.2
PARICALCITOL	-8.8	-7.0
PAROMOMYCIN	-7.1	-6.1
PAROXETINE	-7.8	-6.7
PEMETREXED	-9.4	-6.6
PEMIROLAST	-7.7	-5.8
PEMOLINE	-6.3	-6.2
PENBUTOLOL	-6.8	-5.7
PENCICLOVIR	-6.6	-5.3
PENICILLAMINE	-4.3	-3.5
PENICILLIN G	-8.0	-5.8
PENICILLIN V	-7.7	-6.0
PENTAMIDINE	-6.6	-5.8
PENTAZOCINE	-8.7	-6.0
PENTOBARBITAL	-6.5	-4.9
PENTOLINIUM	-5.7	-4.6
PENTOSAN POLYSULFATE	-7.0	-5.4
PENTOSTATIN	-6.6	-5.5
PENTOXIFYLLINE	-6.6	-5.1
PERGOLIDE	-7.6	-5.7
PERPHENAZINE	-7.5	-5.5
PHENACEMIDE	-6.6	-5.7
PHENAZOPYRIDINE	-6.9	-5.6
PHENDIMETRAZINE	-5.8	-5.6
PHENELZINE	-5.9	-5.4
PHENINDIONE	-7.6	-6.8
PHENIRAMINE	-6.9	-6.1
PHENMETRAZINE	-6.2	-5.4
PHENOXYBENZAMINE	-6.0	-4.2
PHENPROCOUMON	-7.9	-6.0
PHTERMINE	-5.5	-5.3
PHTOLAMINE	-7.8	-6.4
PHENYL BUTAZONE	-7.6	-5.2
PHENYL BUTYRATE	-5.9	-5.8
PHENYLEPHRINE	-5.7	-5.6
PHENYLPROPANOLAMINE	-5.3	-5.1
PHENYTOIN	-8.1	-5.9
PHYTONADIONE	-8.6	-5.3
PIBRENTASVIR	-7.5	-6.6
PILOCARPINE	-5.9	-5.3
PIMOZIDE	-10.1	-6.9

PINACIDIL	-6.4	-4.4
PINDOLOL	-6.4	-5.1
PIOGLITAZONE	-8.6	-6.3
PIPECURONIUM	-7.3	-6.3
PIPERACILLIN	-9.2	-6.4
PIPERONYL BUTOXIDE	-6.4	-5.8
PIPOBROMAN	-5.3	-4.6
PIRBUTEROL	-6.5	-5.1
PIROXICAM	-8.7	-6.4
PITAVASTATIN	-8.5	-6.1
PLAZOMICIN	-7.3	-5.6
PLECANATIDE	-4.2	-2.0
PLICAMYCIN	-9.7	-6.3
PODOFILOX	-7.9	-5.6
POLYTHIAZIDE	-7.6	-6.1
POSACONAZOLE	-7.8	-6.2
PRALATREXATE	-10.0	-7.3
PRALIDOXIME	-5.3	-6.9
PRAMIPEXOLE	-5.9	-4.9
PRAMOXINE	-6.4	-4.4
PRASTERONE	-8.3	-5.0
PRASUGREL	-8.4	-5.9
PRAVASTATIN	-7.7	-6.0
PRAZEPAM	-8.1	-6.3
PRAZIQUANTEL	-8.6	-5.5
PRAZOSIN	-7.7	-6.4
PREDNICARBATE	-8.5	-6.0
PREDNISOLONE	-8.3	-7.2
PREDNISOLONE TEBUTATE	-8.8	-6.2
PREDNISON	-8.9	-6.3
PREGABALIN	-5.2	-6.4
PRILOCAINE	-6.6	-4.9
PRIMAQUINE	-7.0	-6.0
PRIMIDONE	-6.8	-5.1
PROBENECID	-6.8	-4.9
PROBUCOL	-8.7	-5.1
PROCAINAMIDE	-6.3	-5.1
PROCAINE	-5.9	-4.9
PROCARBAZINE	-6.6	-5.0
PROCHLORPERAZINE	-7.5	-5.2
PROCYCLIDINE	-7.6	-5.7



PROGESTERONE	-8.6	-6.3
PROGUANIL	-6.9	-6.2
PROMAZINE	-7.0	-5.1
PROMETHAZINE	-7.2	-4.7
PROPAFENONE	-6.8	-4.8
PROPANTHELINE	-8.0	-5.4
PROPARACAINE	-5.6	-6.1
PROPIOMAZINE	-7.6	-4.5
PROPOFOL	-6.2	-5.4
PROPOXYPHENE	-6.7	-5.9
PROPRANOLOL	-7.2	-4.8
PROPYLTHIOURACIL	-5.5	-5.5
PROTIRELIN	-8.1	-5.1
PROTOKYLOL	-8.0	-6.2
PROTRIPTYLINE	-7.2	-5.9
PRUCALOPRIDE	-7.2	-5.8
PSEUDOEPHEDRINE	-5.7	-5.5
PTERIDINE	-8.0	-5.2
PYRAZINAMIDE	-4.9	-4.7
PYRIDOSTIGMINE	-5.6	-4.8
PYRIDOXINE	-5.3	-5.1
PYRILAMINE	-6.5	-4.6
PYRIMETHAMINE	-6.8	-5.4
PYRVINIUM	-8.0	-7.1
QUAZEPAM	-7.2	-5.8
QUETIAPINE	-7.5	-5.8
QUINAPRIL	-7.8	-6.3
QUINESTROL	-9.1	-7.2
QUINETHAZONE	-7.2	-5.8
QUINIDINE	-8.1	-5.9
QUININE	-7.4	-6.2
RABEPRAZOLE	-7.8	-6.0
RALOXIFENE	-9.4	-6.5
RAMELTEON	-7.6	-6.0
RAMIPRIL	-8.2	-5.8
RANITIDINE	-6.1	-5.0
RANOLAZINE	-8.4	-6.3
RAPACURONIUM	-5.7	-5.6
RASAGILINE	-6.1	-4.9
REGADENOSON	-7.7	-6.4
REMIFENTANIL	-6.8	-4.8

REPAGLINIDE	-8.0	-5.6
RESCINNAMINE	-9.0	-6.5
RESERPINE	-6.3	-6.4
RETAPAMULIN	-8.3	-5.6
REVEFENACIN	-10.6	-6.9
RIBAVIRIN	-6.8	-5.4
RIBOCICLIB	-8.7	-7.3
RIBOFLAVIN	-7.8	-6.4
RIBOFLAVIN PHOSPHATE	-8.3	-6.2
RIFAMYCIN	-6.3	-6.0
RIFAPENTINE	-6.4	-6.5
RIFAXIMIN	-6.6	-5.9
RILPIVIRINE	-9.2	-6.4
RILUZOLE	-6.9	-4.8
RIMANTADINE	-6.2	-5.1
RIMEXOLONE	-8.9	-6.7
RISEDRONATE	-6.5	-5.1
RISPERIDONE	-9.7	-7.7
RITODRINE	-7.7	-4.8
RITONAVIR	-9.0	-5.8
RIVAROXABAN	-9.0	-7.1
RIVASTIGMINE	-6.7	-4.9
RIZATRIPTAN	-7.0	-5.5
ROCURONIUM	-9.0	-5.5
ROFECOXIB	-8.1	-5.8
ROFLUMILAST	-7.7	-5.7
ROMIDEPSIN	-10.1	-6.2
ROPINIROLE	-6.1	-4.8
ROPIVACAINE	-7.3	-5.3
ROSIGLITAZONE	-7.7	-5.7
ROSUVASTATIN	-7.9	-6.0
ROTIGOTINE	-7.5	-5.7
RUCAPARIB	-9.4	-6.9
RUXOLITINIB	-8.5	-6.1
SAFINAMIDE	-7.8	-6.1
SALMETEROL	-7.3	-6.0
SAPROPTERIN	-7.2	-5.4
SAQUINAVIR	-9.7	-5.3
SARALASIN	-8.9	-7.1
SARECYCLINE	-8.4	-5.9
SAXAGLIPTIN	-7.8	-5.9

SCH	-7.6	-6.1
SCOPOLAMINE	-7.1	-5.6
SECNIDAZOLE	-5.9	-4.4
SECOBARBITAL	-6.7	-4.7
SEGESTERONE ACETATE	-8.7	-6.0
SELEGILINE	-5.3	-5.4
SERTACONAZOLE	-7.6	-5.8
SERTRALINE	-7.8	-5.7
SEVOFLURANE	-5.1	-4.9
SIBUTRAMINE	-6.9	-4.6
SILDENAFIL	-8.5	-6.6
SILODOSIN	-8.2	-5.8
SIMVASTATIN	-8.5	-6.4
SIPONIMOD	-9.3	-7.1
SIROLIMUS	-7.5	-6.6
SITAGLIPTIN	-8.9	-7.1
SOLIFENACIN	-8.7	-6.2
SOLRIAMFETOL	-6.1	-5.5
SORAFENIB	-9.6	-7.7
SOTALOL	-6.3	-5.5
SPARFLOXACIN	-8.1	-6.1
SPECTINOMYCIN	-7.7	-5.4
SPIRAPRIL	-7.1	-5.7
STANOZOLOL	-8.8	-6.6
STAVUDINE	-6.8	-5.1
STIRIPENTOL	-7.0	-5.4
STREPTOMYCIN	-7.6	-5.5
STREPTOZOCIN	-6.8	-5.7
SUCCIMER	-4.5	-3.6
SUCCINYLBCHOLINE	-5.1	-4.3
SUFENTANIL	-7.4	-5.2
SULBACTAM	-6.6	-4.8
SULCONAZOLE	-7.5	-5.2
SULFACETAMIDE	-6.1	-5.8
SULFACYTINE	-7.3	-5.5
SULFADIAZINE	-7.0	-5.9
SULFADOXINE	-6.9	-5.3
SULFAMERAZINE	-7.4	-5.8
SULFAMETHAZINE	-7.7	-5.9
SULFAMETHIZOLE	-7.0	-5.7
SULFAMETHOXAZOLE	-7.4	-5.4

SULFANILAMIDE	-5.8	-5.6
SULFAPYRIDINE	-7.0	-5.9
SULFASALAZINE	-9.2	-7.2
SULFINPYRAZONE	-8.9	-6.4
SULFISOXAZOLE	-7.3	-5.7
SULFISOXAZOLE ACETYL	-7.3	-5.6
SULFOXONE	-7.7	-6.5
SUMATRIPTAN	-6.6	-5.4
SUNITINIB	-8.2	-6.3
SUPROFEN	-7.4	-6.4
TACRINE	-7.1	-5.8
TADALAFIL	-8.9	-6.9
TAFAMIDIS	-8.4	-6.2
TAFENOQUINE	-9.2	-5.7
TAFLUPROST	-7.3	-5.6
TALAZOPARIB	-8.7	-6.0
TAMOXIFEN	-7.9	-5.4
TAMSULOSIN	-7.7	-5.7
TAPENTADOL	-6.5	-4.6
TAZAROTENE	-7.5	-6.1
TAZOBACTAM	-7.4	-5.2
TECOVIRIMAT	-9.3	-6.9
TEGASEROD	-7.7	-5.5
TELAPREVIR	-9.5	-6.3
TELAVANCIN	-4.7	-4.6
TELBIVUDINE	-6.8	-5.2
TELMISARTAN	-10.4	-6.7
TELOTRISTAT	-10.3	-6.8
TELOTRISTAT ETHYL	-10.2	-6.0
TEMAZEPAM	-7.7	-6.1
TEMOZOLOMIDE	-6.5	-6.6
TEMSIROLIMUS	-7.4	-6.1
TENIPOSIDE	-8.8	-6.3
TENOFOVIR	-7.1	-5.7
TENOFOVIR DISOPROXIL	-6.5	-5.8
TERAZOSIN	-7.8	-6.0
TERBINAFINE	-7.7	-5.6
TERBUTALINE	-6.0	-4.9
TERCONAZOLE	-8.8	-6.8
TESTOLACTONE	-9.1	-6.0
TESTOSTERONE	-8.6	-6.0

TESTOSTERONE CYPIONATE	-9.5	-6.7
TESTOSTERONE ENANTHATE	-8.5	-6.3
TESTOSTERONE PROPIONATE	-8.5	-6.2
TETRABENAZINE	-7.5	-5.7
TETRACAINE	-6.1	-4.9
TETRACYCLINE	-8.2	-6.3
TETRAHYDROZOLINE	-7.0	-6.6
TEZACAFTOR	-9.0	-7.3
THALIDOMIDE	-7.8	-6.4
THEOPHYLLINE	-6.0	-4.9
THIABENDAZOLE	-6.5	-5.9
THIAMYLAL	-6.4	-4.6
THIETHYLPERAZINE	-7.3	-5.4
THIOGUANINE	-5.9	-5.5
THIORIDAZINE	-8.0	-5.5
THIOTHIXENE	-8.7	-5.9
THONZONIUM	-6.0	-5.1
TIAGABINE	-7.6	-6.2
TICARCILLIN	-7.3	-6.1
TICLOPIDINE	-6.7	-5.5
TIGECYCLINE	-8.3	-6.7
TILUDRONATE	-6.6	-5.2
TIMOLOL	-6.4	-5.1
TINIDAZOLE	-6.2	-4.7
TIOCONAZOLE	-6.9	-5.4
TIOPRONIN	-4.8	-3.6
TIOTROPIUM	-7.6	-5.9
TIROFIBAN	-7.4	-5.4
TIZANIDINE	-7.1	-5.8
TMC-114	-8.5	-5.6
TOBRAMYCIN	-7.3	-5.6
TOCAINIDE	-6.3	-5.1
TOLAZAMIDE	-8.7	-6.1
TOLAZOLINE	-5.8	-5.6
TOLBUTAMIDE	-6.9	-5.6
TOLCAPONE	-8.3	-7.3
TOLMETIN	-7.6	-5.4
TOLTERODINE	-7.3	-5.1
TOLVAPTAN	-9.4	-7.3
TOPIRAMATE	-7.5	-5.4
TOPOTECAN	-8.1	-6.1

TOREMIFENE	-7.9	-5.3
TRAMADOL	-6.6	-5.3
TRANDOLAPRIL	-8.7	-5.6
TRAVOPROST	-7.9	-6.3
TRAZODONE	-8.6	-6.7
TREPROSTINIL	-8.2	-6.0
TRETINOIN	-7.9	-6.0
TRIAMCINOLONE	-9.7	-6.6
TRIAMTERENE	-7.5	-6.5
TRIAZOLAM	-7.9	-6.1
TRICHLORMETHIAZIDE	-7.4	-5.7
TRICLABENDAZOLE	-7.3	-5.4
TRICLOFOS	-5.2	-4.3
TRICLOSAN	-6.9	-4.6
TRIDIHEXETHYL	-6.9	-6.2
TRIENTINE	-4.0	-4.1
TRIFLUOPERAZINE	-7.8	-5.9
TRIFLUPROMAZINE	-7.8	-5.1
TRIFLURIDINE	-7.4	-5.7
TRIHENXYPHENIDYL	-7.9	-5.3
TRILOSTANE	-9.2	-6.3
TRIMEPRAZINE	-7.1	-4.8
TRIMETHADIONE	-5.1	-4.3
TRIMETHAPHAN	-7.8	-5.9
TRIMETHOBENZAMIDE	-7.6	-5.3
TRIMETHOPRIM	-7.0	-5.0
TRIMIPRAMINE	-7.6	-5.5
TRIPLENNAMINE	-6.6	-5.6
TRIPROLIDINE	-7.8	-5.4
TRIPTORELIN	-6.3	-5.2
TROGLITAZONE	-10.0	-7.2
TROLEANDOMYCIN	-5.8	-5.2
TROPICAMIDE	-6.8	-5.0
TROVAFLOXACIN	-9.3	-6.4
TUBOCURARINE	-8.9	-6.8
TYLOXAPOL	-6.4	-4.5
TYROSINE	-6.4	-5.7
ULIPRISTAL ACETATE	-8.9	-6.0
UNOPROSTONE ISOPROPYL	-6.6	-5.0
URACIL MUSTARD	-5.6	-5.0
URSODIOL	-8.4	-5.9

VALACYCLOVIR	-6.7	-5.7
VALBENZAZINE	-7.8	-5.7
VALDECOXIB	-8.5	-6.2
VALGANCICLOVIR	-7.0	-5.8
VALPROIC ACID	-5.0	-4.5
VALRUBICIN	-9.9	-5.8
VALSARTAN	-7.7	-5.7
VANCOMYCIN	-7.7	-5.4
VANDETANIB	-8.7	-6.9
VARDENAFIL	-8.6	-6.7
VARENICLINE	-7.1	-5.8
VASOPRESSIN	-6.1	-3.9
VECURONIUM	-9.0	-6.9
VEMURAFENIB	-9.4	-7.6
VENLAFAXINE	-6.8	-5.4
VERAPAMIL	-7.6	-5.8
VIDARABINE	-6.9	-5.0
VIGABATRIN	-4.6	-4.5
VILAZODONE	-9.9	-7.6
VINBLASTINE	-8.2	-5.7
VINORELBINE	-8.5	-4.9
VIOMYCIN	-8.3	-5.7
VISMODEGIB	-9.3	-6.9
VITAMIN_A	-7.7	-5.9
VORINOSTAT	-7.1	-5.0
VOXILAPREVIR	-8.7	-6.5
WARFARIN	-8.2	-6.3
ZAFIRLUKAST	-9.6	-7.1
ZALCITABINE	-6.8	-5.5
ZALEPLON	-8.0	-6.7
ZANAMIVIR	-6.6	-5.1
ZIDOVUDINE	-6.9	-5.5
ZILEUTON	-7.0	-5.2
ZIPRASIDONE	-9.4	-7.4
ZOLMITRIPTAN	-7.6	-6.0
ZOLPIDEM	-7.7	-6.0
ZONISAMIDE	-6.6	-5.9

Supplementary table 2: Predicted interactions of ACE and ACE2 with RBD of SARS-CoV-2 spike protein.

<b>Feature</b>	<b>ACE-Spike protein</b>	<b>ACE2-Spike protein</b>
Z-Score	-1.2	-1.4
RMSD from the overall lowest-energy structure	$1.7 \pm 0.3$	$1.1 \pm 0.7$
Van der Waals energy	$-48.8 \pm 3.3$	$-59.6 \pm 4.7$
Electrostatic energy	$-319.7 \pm 36.8$	$-122.1 \pm 46.9$
Desolvation energy	$87.4 \pm 7.4$	$33.8 \pm 14.9$
Restraints violation energy	$39.4 \pm 25.03$	$22.5 \pm 14.15$