

**Logistic Discrimination between Drugs and Non-Drugs Including Disease-Specificity by
Assigning Probabilities Based on Molecular Properties.**

Alfonso T. García-Sosa, Mare Oja, Csaba Hetényi, Uko Maran

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Figure S1. Superposition of histograms of relative frequencies of binding free energy (DG, in kcal/mol) for drug and non-drug compounds in the training set.

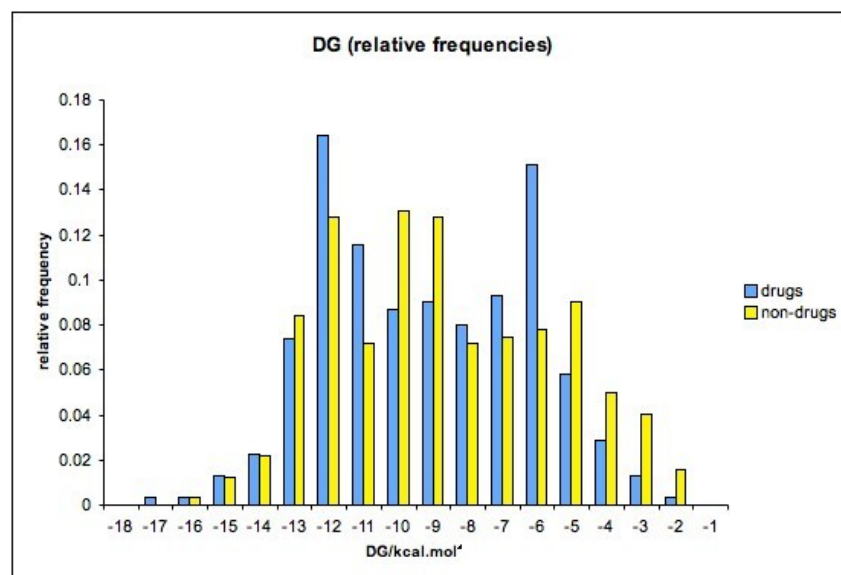


Table S1. Names, drug status, training or validation set and disease category of all compounds.

Name	Drug status	Set	Disease category
Acarbose	drug	Training	DC1
Acetazolamide	drug	Training	DC13
Adenosine	drug	Training	DC3
Alclometasone	drug	Training	DC4, DC13
Allopurinol	drug	Training	DC9
Alprazolam	drug	Training	DC10
Alprenolol	drug	Training	DC3
Amantadine	drug	Training	DC10
Amiloride	drug	Training	DC3
Aminocaproic_Acid	drug	Training	DC2
Amiodarone	drug	Training	DC3
Amitriptyline	drug	Training	DC10
Amlodipine	drug	Training	DC3
Amodiaquine	drug	Training	DC11
Amphetamine	drug	Training	DC10
Amprenavir	drug	Training	DC7
Anastrozole	drug	Training	DC8
Apomorphine	drug	Training	DC5, DC10
Aprepitant	drug	Training	DC1
Argatroban	drug	Training	DC2
Aripiprazole	drug	Training	DC10
Astemizole	drug	Training	DC12
Atenolol	drug	Training	DC3
Atovaquone	drug	Training	DC11
Atropine	drug	Training	DC1, DC10, DC13
Azelaic_Acid	drug	Training	DC4
Azelastine	drug	Training	DC12
Baclofen	drug	Training	DC9
Benztropine	drug	Training	DC10

Betamethasone	drug	Training	DC1, DC3, DC4, DC6, DC12, DC13
Bicalutamide	drug	Training	DC8
Bosentan	drug	Training	DC3
Brinzolamide	drug	Training	DC13
Bupivacaine	drug	Training	DC10
Buprenorphine	drug	Training	DC10
Bupropion	drug	Training	DC10
Buspirone	drug	Training	DC10
Cabergoline	drug	Training	DC5, DC10
Caffeine	drug	Training	DC10
Candesartan	drug	Training	DC3
Captopril	drug	Training	DC3
Carbachol	drug	Training	DC10, DC13
Celecoxib	drug	Training	DC8, DC9
Cerivastatin	drug	Training	DC3
Chlordiazepoxide	drug	Training	DC10
Chloroprocaine	drug	Training	DC10
Chlorpheniramine	drug	Training	DC12
Chlorpromazine	drug	Training	DC10
Chlorzoxazone	drug	Training	DC9
Cimetidine	drug	Training	DC1
Ciprofloxacin	drug	Training	DC7, DC13
Cisapride	drug	Training	DC1
Citalopram	drug	Training	DC10
Clarithromycin	drug	Training	DC7
Clofibrate	drug	Training	DC3
Clomifene	drug	Training	DC5
Clomipramine	drug	Training	DC10
Clonazepam	drug	Training	DC10
Clonidine	drug	Training	DC13
Clotrimazole	drug	Training	DC1, DC4, DC5
Clozapine	drug	Training	DC10
Codeine	drug	Training	DC10, DC12
Cyproheptadine	drug	Training	DC12
Daunorubicin	drug	Training	DC8
Decamethonium	drug	Training	DC14
Desipramine	drug	Training	DC10
Desogestrel	drug	Training	DC5
Dexamethasone	drug	Training	DC1, DC3, DC4, DC6, DC12, DC13
Dextromethorphan	drug	Training	DC12
Diazepam	drug	Training	DC10
Diazoxide	drug	Training	DC10, DC14
Dibucaine	drug	Training	DC14
Diclofenac	drug	Training	DC9, DC13
Dicloxacillin	drug	Training	DC7
Dienestrol	drug	Training	DC5
Diethylstilbestrol	drug	Training	DC5, DC8
Dihydroergotamine	drug	Training	DC10
Diltiazem	drug	Training	DC3
Diphenhydramine	drug	Training	DC4, DC12
Dipyridamole	drug	Training	DC2
Dobutamine	drug	Training	DC3
Dofetilide	drug	Training	DC3
Domperidone	drug	Training	DC1
Dopamine	drug	Training	DC3
Dorzolamide	drug	Training	DC13
Doxazosin	drug	Training	DC3
Doxorubicin	drug	Training	DC8
Droperidol	drug	Training	DC10
Duloxetine	drug	Training	DC10
Edrophonium	drug	Training	DC14
Enalapril	drug	Training	DC3
Epinephrine	drug	Training	DC1, DC2, DC3, DC12, DC13
Ergotamine	drug	Training	DC10
Erythromycin	drug	Training	DC4, DC7, DC13
Estradiol	drug	Training	DC5, DC8
Estrone	drug	Training	DC5
Ethacrynic_Acid	drug	Training	DC14
Ethanol	drug	Training	DC14
Ethinylestradiol	drug	Training	DC5
Ethoxzolamide	drug	Training	DC14

Etoposide	drug	Training	DC8
Felodipine	drug	Training	DC3
Fenofibrate	drug	Training	DC3
Fentanyl	drug	Training	DC10
Fexofenadine	drug	Training	DC12
Flecainide	drug	Training	DC3
Fluconazole	drug	Training	DC4, DC7
Fluorouracil	drug	Training	DC8
Fluoxetine	drug	Training	DC10
Fluoxymesterone	drug	Training	DC5
Fluphenazine	drug	Training	DC10
Flurazepam	drug	Training	DC10
Flurbiprofen	drug	Training	DC9, DC13
Fulvestrant	drug	Training	DC8
Gabapentin	drug	Training	DC10
Gatifloxacin	drug	Training	DC7, DC13
Gemcitabine	drug	Training	DC8
Gemfibrozil	drug	Training	DC3
Glyburide	drug	Training	DC1
Granisetron	drug	Training	DC1
Grepafloxacin	drug	Training	DC7
Guanabenz	drug	Training	DC14
Guanethidine	drug	Training	DC3, DC13
Haloperidol	drug	Training	DC10
Hydrocortisone	drug	Training	DC1, DC3, DC4, DC6, DC13
Hydromorphone	drug	Training	DC10
Ibuprofen	drug	Training	DC3, DC5, DC9
Iloprost	drug	Training	DC2
Imatinib	drug	Training	DC8
Imipramine	drug	Training	DC10
Indinavir	drug	Training	DC7
Indomethacin	drug	Training	DC14
Irbesartan	drug	Training	DC3
Isoniazid	drug	Training	DC7
Isoproterenol	drug	Training	DC14
Itraconazole	drug	Training	DC7
Ketamine	drug	Training	DC10
Ketoconazole	drug	Training	DC4, DC5, DC7
Ketoprofen	drug	Training	DC9
Lamivudine	drug	Training	DC7
Lamotrigine	drug	Training	DC10
Lansoprazole	drug	Training	DC1
Latanoprost	drug	Training	DC13
Levallorphan	drug	Training	DC14
Levetiracetam	drug	Training	DC10
Levocabastine	drug	Training	DC12, DC13
Levodopa	drug	Training	DC10
Levorphanol	drug	Training	DC14
Lidocaine	drug	Training	DC3, DC4, DC10, DC12, DC13
Lindane	drug	Training	DC11
Lisuride	drug	Training	DC5, DC10
Loperamide	drug	Training	DC1
Lorazepam	drug	Training	DC10
Losartan	drug	Training	DC3
Lovastatin	drug	Training	DC3
Loxapine	drug	Training	DC10
Lysinopril	drug	Training	DC3
Maprotiline	drug	Training	DC10
Marimastat	drug	Training	DC14
Mazindol	drug	Training	DC1
Mecamylamine	drug	Training	DC3
Medroxyprogesterone	drug	Training	DC5, DC8
Melatonin	drug	Training	DC10
Memantine	drug	Training	DC10
Mesoridazine	drug	Training	DC10
Methadone	drug	Training	DC10
Methazolamide	drug	Training	DC13
Methotrexate	drug	Training	DC8
Methoxamine	drug	Training	DC3
Methylphenidate	drug	Training	DC10
Methysergide	drug	Training	DC10
Metoclopramide	drug	Training	DC1

Miconazole	drug	Training	DC1, DC4, DC5, DC7, DC13
Midazolam	drug	Training	DC10
Mifepristone	drug	Training	DC5
Milrinone	drug	Training	DC3
Minoxidil	drug	Training	DC3, DC4
Misoprostol	drug	Training	DC1
Morphine	drug	Training	DC5, DC10, DC12, DC13
Nalidixic	drug	Training	DC7
Naloxone	drug	Training	DC14
Naltrexone	drug	Training	DC10
Naratriptan	drug	Training	DC10
Nefazodone	drug	Training	DC10
Nelfinavir	drug	Training	DC7
Nicardipine	drug	Training	DC3
Nicotine	drug	Training	DC10
Nifedipine	drug	Training	DC3
Nimodipine	drug	Training	DC3
Nisoldipine	drug	Training	DC3
Nitrendipine	drug	Training	DC3
Norethindrone	drug	Training	DC14
Norfloxacin	drug	Training	DC7, DC13
Norgestrel	drug	Training	DC5
Nortriptyline	drug	Training	DC10
Novobiocin	drug	Training	DC14
Ofloxacin	drug	Training	DC7
Olanzapine	drug	Training	DC10
Olopatadine	drug	Training	DC13
Omapatrilat	drug	Training	DC14
Omeprazole	drug	Training	DC1
Ondansetron	drug	Training	DC1
Orphenadrine	drug	Training	DC9, DC10
Ouabain	drug	Training	DC14
Oxandrolone	drug	Training	DC1
Oxymetazoline	drug	Training	DC12, DC13
Paclitaxel	drug	Training	DC8
Papaverine	drug	Training	DC1, DC5
Paroxetine	drug	Training	DC10
Pentostatin	drug	Training	DC8
Pergolide	drug	Training	DC10
Perhexiline	drug	Training	DC3
Perphenazine	drug	Training	DC10
Phentolamine	drug	Training	DC3, DC5
Phenylephrine	drug	Training	DC3, DC12, DC13
Phenytoin	drug	Training	DC10
Physostigmine	drug	Training	DC13, DC14
Picrotoxin	drug	Training	DC14
Pilocarpine	drug	Training	DC10, DC13
Pimozide	drug	Training	DC10
Pindolol	drug	Training	DC3
Pioglitazone	drug	Training	DC1
Piperazine	drug	Training	DC11
Pirenzepine	drug	Training	DC1
Piroxicam	drug	Training	DC9, DC13
Pramipexole	drug	Training	DC10
Pravastatin	drug	Training	DC3
Prazosin	drug	Training	DC3
Prednisolone	drug	Training	DC1, DC3, DC4, DC6, DC12, DC13
Prilocaine	drug	Training	DC10
Procainamide	drug	Training	DC3
Procaine	drug	Training	DC3, DC4, DC7
Prochlorperazine	drug	Training	DC10
Procyclidine	drug	Training	DC10
Progesterone	drug	Training	DC5, DC8
Promazine	drug	Training	DC10
Promethazine	drug	Training	DC4, DC12
Propafenone	drug	Training	DC3
Propranolol	drug	Training	DC3
Pseudoephedrine	drug	Training	DC12
Pyrimethamine	drug	Training	DC11
Quetiapine	drug	Training	DC10
Quinidine	drug	Training	DC3
Raloxifene	drug	Training	DC5

Raltitrexed	drug	Training	DC8
Ramelteon	drug	Training	DC14
Ranitidine	drug	Training	DC1
Reboxetine	drug	Training	DC10
Reserpine	drug	Training	DC3
Risperidone	drug	Training	DC10
Ritonavir	drug	Training	DC7
Rizatriptan	drug	Training	DC10
Ropinirole	drug	Training	DC10
Rosiglitazone	drug	Training	DC1
Salmeterol	drug	Training	DC12
Saquinavir	drug	Training	DC7
Scopolamine	drug	Training	DC1, DC10, DC13
Sertraline	drug	Training	DC10
Sildenafil	drug	Training	DC5
Sotalol	drug	Training	DC3
Sparfloxacin	drug	Training	DC7
Spiroglactone	drug	Training	DC3
Stavudine	drug	Training	DC7
Sulfamethoxazole	drug	Training	DC7
Sulfanilamide	drug	Training	DC4, DC7
Sulpiride	drug	Training	DC10
Sumatriptan	drug	Training	DC10
Tacrine	drug	Training	DC10
Tacrolimus	drug	Training	DC4, DC8
Tamoxifen	drug	Training	DC8
Telithromycin	drug	Training	DC7
Terazosin	drug	Training	DC5
Terbutaline	drug	Training	DC12
Terfenadine	drug	Training	DC12
Testolactone	drug	Training	DC14
Testosterone	drug	Training	DC5
Theophylline	drug	Training	DC12
Thioridazine	drug	Training	DC10
Tiagabine	drug	Training	DC10
Ticlopidine	drug	Training	DC2
Tipranavir	drug	Training	DC7
Tolazamide	drug	Training	DC1
Tolbutamide	drug	Training	DC1
Topiramate	drug	Training	DC10
Tramadol	drug	Training	DC10
Trandolapril	drug	Training	DC3
Tranylcypromine	drug	Training	DC10
Travoprost	drug	Training	DC13
Trazodone	drug	Training	DC10
Triazolam	drug	Training	DC10
Trifluoperazine	drug	Training	DC10
Trihexyphenidyl	drug	Training	DC10
Trimethaphan	drug	Training	DC3
Trimethoprim	drug	Training	DC7
Trimetrexate	drug	Training	DC11
Tripelennamine	drug	Training	DC4, DC12
Tripolidine	drug	Training	DC12
Troglitazone	drug	Training	DC1
Tubocurarine	drug	Training	DC9
Valproic	drug	Training	DC10
Vardenafil	drug	Training	DC5
Vasopressin	drug	Training	DC6
Venlafaxine	drug	Training	DC10
Verapamil	drug	Training	DC3
Vinblastine	drug	Training	DC8
Vincristine	drug	Training	DC8
Warfarin	drug	Training	DC2
Zidovudine	drug	Training	DC7
Ziprasidone	drug	Training	DC10
Zolpidem	drug	Training	DC10
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2tct	non-drug	Training	
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4er4	non-drug	Training	
4sga	non-drug	Training	
5apr	non-drug	Training	
5er1	non-drug	Training	
5hvp	non-drug	Training	
5sga	non-drug	Training	
5std	non-drug	Training	
6apr	non-drug	Training	
6cpa	non-drug	Training	
6rnt	non-drug	Training	
7hvp	non-drug	Training	
830c	non-drug	Training	
8cpa	non-drug	Training	
8hvp	non-drug	Training	
GalNag	non-drug	Training	
OleicAcid	non-drug	Training	
om12	non-drug	Training	
om13	non-drug	Training	
om14	non-drug	Training	
om15	non-drug	Training	
om16	non-drug	Training	
om17	non-drug	Training	
om18	non-drug	Training	
om19	non-drug	Training	
om23	non-drug	Training	
om99_1	non-drug	Training	
Acamprosate	drug	Validation	DC10
Acebutolol	drug	Validation	DC3
Acetophenazine	drug	Validation	DC10
Agomelatine	drug	Validation	DC10
Albendazole	drug	Validation	DC11
Albuterol (salbutamol)	drug	Validation	DC14
Alcaftadine	drug	Validation	DC13
Alfuzosin	drug	Validation	DC5
AMOXAPINE	drug	Validation	DC10
Atomoxetine	drug	Validation	DC10
Atosiban	drug	Validation	DC5
Benperidol	drug	Validation	DC10
Brimonidine GTP	drug	Validation	DC13
Brompheniramine	drug	Validation	DC12
Capsaicin	drug	Validation	DC4
CARBAMAZEPINE	drug	Validation	DC10
Carbinoxamine	drug	Validation	DC12
Carnitine	drug	Validation	DC1
Carvedilol	drug	Validation	DC3
Cetirizine (+) isomer	drug	Validation	DC12
Chloroquine	drug	Validation	DC11
Ciclesonide	drug	Validation	DC12
Cyclopentolate	drug	Validation	DC13
Cyclosporin A	drug	Validation	DC8
Darifenacin	drug	Validation	DC5
Desvenlafaxine	drug	Validation	DC10
Dexmedetomidine	drug	Validation	DC14
Dichlorphenamide	drug	Validation	DC13
Dicyclomine	drug	Validation	DC14
Dienogest	drug	Validation	DC5
Diflunisal	drug	Validation	DC10
Diphenylpyraline	drug	Validation	DC12
DOXEPIN	drug	Validation	DC10
Ephedrine,(-)	drug	Validation	DC12
Erlotinib	drug	Validation	DC8
Escitalopram	drug	Validation	DC10
Ethopropazine	drug	Validation	DC14
FENOLDOPAM	drug	Validation	DC3
Fenoprofen	drug	Validation	DC9
Flumazenil	drug	Validation	DC14
Fluvoxamine	drug	Validation	DC10
Gallamine	drug	Validation	DC9
Gefitinib	drug	Validation	DC8
Guanfacine	drug	Validation	DC3
Homatropine	drug	Validation	DC1
Hydralazine	drug	Validation	DC14

Hydrocodone	drug	Validation	DC12
Hydroxyamphetamine	drug	Validation	DC13
Hydroxyzine	drug	Validation	DC10
ILOPERIDONE	drug	Validation	DC10
Ipratropium	drug	Validation	DC12
Ketorolac	drug	Validation	DC9
LABETALOL	drug	Validation	DC3
Lanreotide	drug	Validation	DC6
Mebendazole	drug	Validation	DC11
Meclizine	drug	Validation	DC14
Meclofenamate	drug	Validation	DC9
Mefenamic acid	drug	Validation	DC9
Meloxicam	drug	Validation	DC9
Menthol	drug	Validation	DC14
Meperidine	drug	Validation	DC14
Methacholine	drug	Validation	DC14
METHAMPHETAMINE	drug	Validation	DC10
Metoprolol	drug	Validation	DC3
Milnacipran	drug	Validation	DC10
Mirtazepine	drug	Validation	DC10
Montelukast	drug	Validation	DC12
Nabilone	drug	Validation	DC1
Nabumetone	drug	Validation	DC9
Nalbuphine	drug	Validation	DC10
Naphazoline	drug	Validation	DC13
Nebivolol	drug	Validation	DC3
NOREPINEPHRINE	drug	Validation	DC14
Octreotide	drug	Validation	DC8
Oxazepam	drug	Validation	DC10
OXPRENOLOL	drug	Validation	DC14
Oxycodone	drug	Validation	DC10
Oxymorphone	drug	Validation	DC14
Oxytocin	drug	Validation	DC14
Pancuronium	drug	Validation	DC14
Paracetamol	drug	Validation	DC10
Pemetrexed	drug	Validation	DC8
Pentagastrin	drug	Validation	DC14
Pentazocine	drug	Validation	DC10
Pentoxifylline	drug	Validation	DC3
Phenelzine	drug	Validation	DC10
PHENOXYBENZAMINE	drug	Validation	DC3
Protriptyline	drug	Validation	DC10
ROFECOXIB	drug	Validation	DC9
Succinylcholine	drug	Validation	DC14
Sulfasalazine	drug	Validation	DC1
Sulindac	drug	Validation	DC9
Suprofen	drug	Validation	DC13
Tadalafil	drug	Validation	DC5
Tamsulosin	drug	Validation	DC5
Tetrahydrozoline	drug	Validation	DC13
Thiabendazole	drug	Validation	DC14
Thiothixene	drug	Validation	DC10
TIZANIDINE	drug	Validation	DC9
Tolmetin	drug	Validation	DC9
Trimipramine	drug	Validation	DC10
TROPICAMIDE	drug	Validation	DC13
Uliprastat	drug	Validation	DC5
Vecuronium	drug	Validation	DC14
Zafirlukast	drug	Validation	DC12
Zaleplon	drug	Validation	DC10
2g94	non-drug	Validation	
2gyi	non-drug	Validation	
2gzl	non-drug	Validation	
2h15	non-drug	Validation	
2h3e	non-drug	Validation	
2h5a	non-drug	Validation	
2h6t	non-drug	Validation	
2ha2	non-drug	Validation	
2hrm	non-drug	Validation	
2hw2	non-drug	Validation	
2i2c	non-drug	Validation	
2i2e	non-drug	Validation	

2i4j	non-drug	Validation	
2i4w	non-drug	Validation	
2i4z	non-drug	Validation	
2iuz	non-drug	Validation	
2j4k	non-drug	Validation	
2j7d	non-drug	Validation	
2j7f	non-drug	Validation	
2j7g	non-drug	Validation	
2jh5	non-drug	Validation	
2nsj	non-drug	Validation	
2o1c	non-drug	Validation	
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2oxy	non-drug	Validation	
2oyk	non-drug	Validation	
2p2a	non-drug	Validation	
2p3b	non-drug	Validation	
2p4y	non-drug	Validation	
2pq9	non-drug	Validation	
2pu1	non-drug	Validation	
2q8z	non-drug	Validation	
2qbq	non-drug	Validation	
2qnn	non-drug	Validation	
2qnp	non-drug	Validation	
2qpu	non-drug	Validation	
2qv4	non-drug	Validation	
2r2b	non-drug	Validation	
2r6w	non-drug	Validation	
2rke	non-drug	Validation	
2uxz	non-drug	Validation	
2v8w	non-drug	Validation	
2zb0	non-drug	Validation	
2zcg	non-drug	Validation	
3b2t	non-drug	Validation	
3b5j	non-drug	Validation	
3b68	non-drug	Validation	
3baj	non-drug	Validation	
3bc3	non-drug	Validation	
3bft	non-drug	Validation	
3bfu	non-drug	Validation	
3bgz	non-drug	Validation	
3bkk	non-drug	Validation	
3bkl	non-drug	Validation	
3bva	non-drug	Validation	
3c1k	non-drug	Validation	
3c56	non-drug	Validation	
3cct	non-drug	Validation	
3ccw	non-drug	Validation	
3ccz	non-drug	Validation	
3cd0	non-drug	Validation	
3cd5	non-drug	Validation	
3cd7	non-drug	Validation	
3cda	non-drug	Validation	
3cdb	non-drug	Validation	
3cj5	non-drug	Validation	
3cke	non-drug	Validation	
3cm2	non-drug	Validation	
3cow	non-drug	Validation	
3coy	non-drug	Validation	
3coz	non-drug	Validation	
3cpj	non-drug	Validation	
3d0e	non-drug	Validation	
3d1x	non-drug	Validation	
3d4z	non-drug	Validation	
3d50	non-drug	Validation	
3d52	non-drug	Validation	
3d7k	non-drug	Validation	
3d83	non-drug	Validation	
3d94	non-drug	Validation	
3dd8	non-drug	Validation	

3ddf	non-drug	Validation	
3ddg	non-drug	Validation	
3djk	non-drug	Validation	
3e5a	non-drug	Validation	
3e5u	non-drug	Validation	
3e64	non-drug	Validation	
3e8r	non-drug	Validation	
3e93	non-drug	Validation	
3ebl	non-drug	Validation	
3eeb	non-drug	Validation	
3eko	non-drug	Validation	
3ekr	non-drug	Validation	
3eqr	non-drug	Validation	
3f15	non-drug	Validation	
3f16	non-drug	Validation	
3f17	non-drug	Validation	
3f18	non-drug	Validation	
3f19	non-drug	Validation	
3f1a	non-drug	Validation	
3f80	non-drug	Validation	
3f8c	non-drug	Validation	
3f8f	non-drug	Validation	
Acetyldigitoxin	drug	Further tests	DC3
Arbutamine	drug	Further tests	DC3
Atorvastatin	drug	Further tests	DC3
Benazepril	drug	Further tests	DC3
Bendroflumethiazide	drug	Further tests	DC3
Bepidil	drug	Further tests	DC3
Betaxolol	drug	Further tests	DC3
Bethanidine	drug	Further tests	DC3
Bisoprolol	drug	Further tests	DC3
Bretylum	drug	Further tests	DC3
Bumetanide	drug	Further tests	DC3
Carteolol	drug	Further tests	DC3
Chlorothiazide	drug	Further tests	DC3
Colestipol	drug	Further tests	DC3
Cyclothiazide	drug	Further tests	DC3
Deserpine	drug	Further tests	DC3
Deslanoside	drug	Further tests	DC3
Dextrothyroxine	drug	Further tests	DC3
Digoxin	drug	Further tests	DC3
Disopyramide	drug	Further tests	DC3
Encainide	drug	Further tests	DC3
Eplerenone	drug	Further tests	DC3
Eprosartan	drug	Further tests	DC3
Ergoloid	drug	Further tests	DC3
Esmolol	drug	Further tests	DC3
Ezetimibe	drug	Further tests	DC3
Flumethasone	drug	Further tests	DC3
Fluocinolone	drug	Further tests	DC3
Fluocinonide	drug	Further tests	DC3
Fluorometholone	drug	Further tests	DC3
Fluvastatin	drug	Further tests	DC3
Fosinopril	drug	Further tests	DC3
Furosemide	drug	Further tests	DC3
Heparin	drug	Further tests	DC3
Hydrochlorothiazide	drug	Further tests	DC3
Hydrocortamate	drug	Further tests	DC3
Hydroflumethiazide	drug	Further tests	DC3
Ibutilide	drug	Further tests	DC3
Indapamide	drug	Further tests	DC3
Isosorbide	drug	Further tests	DC3
Isradipine	drug	Further tests	DC3
Lercarnidipine	drug	Further tests	DC3
Levosimendan	drug	Further tests	DC3
Metaraminol	drug	Further tests	DC3
Methyclothiazide	drug	Further tests	DC3
Methyldopa	drug	Further tests	DC3
Metolazone	drug	Further tests	DC3
Mexiletine	drug	Further tests	DC3
Midodrine	drug	Further tests	DC3
Moexipril	drug	Further tests	DC3

Nadolol	drug	Further tests	DC3
Nicergoline	drug	Further tests	DC3
Nitroglycerin	drug	Further tests	DC3
Olmesartan_medoximil	drug	Further tests	DC3
Pentosan_polysulfate	drug	Further tests	DC3
Perindopril	drug	Further tests	DC3
Quinapril	drug	Further tests	DC3
Ramipril	drug	Further tests	DC3
Ranolazine	drug	Further tests	DC3
Remikren	drug	Further tests	DC3
Rescinnamine	drug	Further tests	DC3
Rosuvastatin	drug	Further tests	DC3
Simvastatin	drug	Further tests	DC3
Telmisartan	drug	Further tests	DC3
Tocainide	drug	Further tests	DC3
Tolazoline	drug	Further tests	DC3
Torsemide	drug	Further tests	DC3
Triamterene	drug	Further tests	DC3
Trichlormethiazide	drug	Further tests	DC3
Valsartan	drug	Further tests	DC3
Butoconazole	drug	Further tests	DC5
Carboprost	drug	Further tests	DC5
Chlorotrianisene	drug	Further tests	DC5
Ciclopirox	drug	Further tests	DC5
Dinoprost	drug	Further tests	DC5
Dinoprostone	drug	Further tests	DC5
Dutasteride	drug	Further tests	DC5
Dydrogesterone	drug	Further tests	DC5
Econazole	drug	Further tests	DC5
Etonogestrel	drug	Further tests	DC5
Finasteride	drug	Further tests	DC5
Flavoxate	drug	Further tests	DC5
Furazolidone	drug	Further tests	DC5
Norgestimate	drug	Further tests	DC5
Oxybutynin	drug	Further tests	DC5
Ritodrine	drug	Further tests	DC5
Solifenacin	drug	Further tests	DC5
Terconazole	drug	Further tests	DC5
Tioconazole	drug	Further tests	DC5
Tolterodine	drug	Further tests	DC5
Trospium	drug	Further tests	DC5
Abacavir	drug	Further tests	DC7
Adefovir	drug	Further tests	DC7
Aminosalicilic_acid	drug	Further tests	DC7
Amoxicillin	drug	Further tests	DC7
Ampicillin	drug	Further tests	DC7
Atazanavir	drug	Further tests	DC7
Azlocillin	drug	Further tests	DC7
Carbenicillin	drug	Further tests	DC7
Cefaclor	drug	Further tests	DC7
Cefadroxil	drug	Further tests	DC7
Cefprozil	drug	Further tests	DC7
Ceftazidime	drug	Further tests	DC7
Cefuroxime	drug	Further tests	DC7
Cephalexin	drug	Further tests	DC7
Cinoxacin	drug	Further tests	DC7
Clomocycline	drug	Further tests	DC7
Dapsone	drug	Further tests	DC7
Delavirdine	drug	Further tests	DC7
Demeclocycline	drug	Further tests	DC7
Didanosine	drug	Further tests	DC7
Doxycycline	drug	Further tests	DC7
Efavirenz	drug	Further tests	DC7
Emtricitabine	drug	Further tests	DC7
Enoxacin	drug	Further tests	DC7
Ertapenem	drug	Further tests	DC7
Ethambutol	drug	Further tests	DC7
Famciclovir	drug	Further tests	DC7
Flucloxacillin	drug	Further tests	DC7
Gemifloxacin	drug	Further tests	DC7
Hetacillin	drug	Further tests	DC7
Idoxuridine	drug	Further tests	DC7

Levofloxacin	drug	Further tests	DC7
Linezolid	drug	Further tests	DC7
Lomefloxacin	drug	Further tests	DC7
Loracarbef	drug	Further tests	DC7
Meropenem	drug	Further tests	DC7
Mezlocillin	drug	Further tests	DC7
Minocycline	drug	Further tests	DC7
Moxifloxacin	drug	Further tests	DC7
Netilmicin	drug	Further tests	DC7
Nevirapine	drug	Further tests	DC7
Nitrofurantoin	drug	Further tests	DC7
Oseltamivir	drug	Further tests	DC7
Oxacillin	drug	Further tests	DC7
Pefloxacin	drug	Further tests	DC7
Penciclovir	drug	Further tests	DC7
PenicillinG	drug	Further tests	DC7
PenicillinV	drug	Further tests	DC7
Piperacillin	drug	Further tests	DC7
Pyrazinamide	drug	Further tests	DC7
Rimantadine	drug	Further tests	DC7
Spectinomycin	drug	Further tests	DC7
Sulfadiazine	drug	Further tests	DC7
Sulfamethizole	drug	Further tests	DC7
Sulfapyridine	drug	Further tests	DC7
Tetracycline	drug	Further tests	DC7
Tinidazole	drug	Further tests	DC7
Trovafoxacin	drug	Further tests	DC7
Voriconazole	drug	Further tests	DC7
Zalcitabine	drug	Further tests	DC7
Adinazolam	drug	Further tests	DC10
Alfentanil	drug	Further tests	DC10
Almotriptan	drug	Further tests	DC10
Ambenonium	drug	Further tests	DC10
Anileridine	drug	Further tests	DC10
Bethanecol	drug	Further tests	DC10
Biperiden	drug	Further tests	DC10
Butorphanol	drug	Further tests	DC10
Chlorprothixene	drug	Further tests	DC10
Clobazam	drug	Further tests	DC10
Clorazepate	drug	Further tests	DC10
Cocaine	drug	Further tests	DC10
Dezocine	drug	Further tests	DC10
Disulfiram	drug	Further tests	DC10
Donepezil	drug	Further tests	DC10
Dyclonine	drug	Further tests	DC10
Eletriptan	drug	Further tests	DC10
Entacapone	drug	Further tests	DC10
Estazolam	drug	Further tests	DC10
Eszopiclone	drug	Further tests	DC10
Ethchlorvynol	drug	Further tests	DC10
Ethosuximide	drug	Further tests	DC10
Ethotoin	drug	Further tests	DC10
Etomidate	drug	Further tests	DC10
Felbamate	drug	Further tests	DC10
Frovatriptan	drug	Further tests	DC10
Galantamine	drug	Further tests	DC10
Halazepam	drug	Further tests	DC10
Isocarboxacid	drug	Further tests	DC10
Mephénytoin	drug	Further tests	DC10
Mepivacaine	drug	Further tests	DC10
Meprobamate	drug	Further tests	DC10
Metharbital	drug	Further tests	DC10
Methohexital	drug	Further tests	DC10
Methoxyflurane	drug	Further tests	DC10
Methypylon	drug	Further tests	DC10
Metixene	drug	Further tests	DC10
Minaprine	drug	Further tests	DC10
Mirtazapine	drug	Further tests	DC10
Moclobemide	drug	Further tests	DC10
Modafinil	drug	Further tests	DC10
Oxcarbazepine	drug	Further tests	DC10
Paramethadione	drug	Further tests	DC10

Pemoline	drug	Further tests	DC10
Pentobarbital	drug	Further tests	DC10
Phenacemide	drug	Further tests	DC10
Phensuximide	drug	Further tests	DC10
Pregabalin	drug	Further tests	DC10
Primidone	drug	Further tests	DC10
Progabide	drug	Further tests	DC10
Proparacaine	drug	Further tests	DC10
Propiomazine	drug	Further tests	DC10
Propofol	drug	Further tests	DC10
Propoxyphene	drug	Further tests	DC10
Pyridostigmine	drug	Further tests	DC10
Remifentanil	drug	Further tests	DC10
Remoxipride	drug	Further tests	DC10
Riluzole	drug	Further tests	DC10
Rivastigmine	drug	Further tests	DC10
Ropivacaine	drug	Further tests	DC10
Secobarbital	drug	Further tests	DC10
Sevoflurane	drug	Further tests	DC10
Sufentanil	drug	Further tests	DC10
Talbutal	drug	Further tests	DC10
Temazepam	drug	Further tests	DC10
Thiopental	drug	Further tests	DC10
Tolcapone	drug	Further tests	DC10
Triflupromazine	drug	Further tests	DC10
Trimethadione	drug	Further tests	DC10
Vigabatrin	drug	Further tests	DC10
Zolmitriptan	drug	Further tests	DC10
Zonisamide	drug	Further tests	DC10
Zopiclone	drug	Further tests	DC10

Table S2. Discarded cross-terms due to strong (Pearson)correlation or anti-correlation.

MW ~ NoC ; MW ~ Wiener ind. ; MW ~ MSA ; MW ~ PSA ; MW ~ apolarSA ; MW ~ donor Count ; MW ~ acceptor count
MW ~ rotatable bond count ; MW ~ atom count ; MW ~ hydrogen count ; MW ~ NHA ; MW ~ molpol ; MW ~ Harary ind. ; MW ~ bond
count; MW ~ hyper Wiener ind. ; MW ~ Platt ind. ; MW ~ Randic ind. ; MW ~ Szeged ind. ; MW ~ Wiener polarity ; MW ~ ΔG/NHA ; MW
~ ΔG/MW; MW ~ ΔG/MSA

NoC ~ Wiener ind. ; NoC ~ MSA ; NoC ~ apolarSA ; NoC ~ rotatable bond count ; NoC ~ atom count ; NoC ~ hydrogen count; NoC ~ NHA
; NoC ~ molpol ; NoC ~ Harary ind. ; NoC ~ bond count ; NoC ~ hyper Wiener ind. ; NoC ~ Platt ind. ; NoC ~ Randic ind. ; NoC ~ Szeged
ind. ; NoC ~ Wiener polarity ; NoC ~ ΔG/apolarSA ; NoC ~ ΔG/NoC

Wiener ind. ~ MSA ; Wiener ind. ~ apolarSA ; Wiener ind. ~ donor count ; Wiener ind. ~ acceptor count ; Wiener ind. ~ rotatable bond count
; Wiener ind. ~ atom count ; Wiener ind. ~ hydrogen count ; Wiener ind. ~ NHA ; Wiener ind. ~ molecular polarizability ; Wiener ind. ~
Harary ind. ; Wiener ind. ~ bond count ; Wiener ind. ~ hyper Wiener ind. ; Wiener ind. ~ Platt ind. ; Wiener ind. ~ Randic ind. ; Wiener ind.
~ Szeged ind. ; Wiener ind. ~ Wiener polarity

MSA ~ PSA ; MSA ~ apolar SA ; MSA ~ donor count ; MSA ~ acceptor count ; MSA ~ rotatable bond count ; MSA ~ atom count ; MSA ~
hydrogen count ; MSA ~ NHA ; MSA ~ molpol ; MSA ~ Harary ind. ; MSA ~ Platt ind. ; MSA ~ Randic ind. ; MSA ~ Szeged ind. ; MSA ~
Wiener polarity ; MSA ~ ΔG/NHA ; MSA ~ ΔG/MSA ; MSA ~ ΔG/apolarSA

PSA ~ donor count ; PSA ~ acceptor count ; PSA ~ NHA ; PSA ~ Harary ind. ; PSA ~ Szeged ind.

apolarSA ~ acceptor count ; apolarSA ~ rotatable bond count ; apolarSA ~ atom count ; apolarSA ~ hydrogen count ; apolarSA ~ NHA ;
apolarSA ~ molpol ; apolar SA ~ Harary ind. ; apolarSA ~ bond count ; apolarSA ~ hyper Wiener ind. ; apolarSA ~ Platt ind. ; apolarSA ~
Randic ind. ; apolarSA ~ Szeged ind. ; apolar SA ~ Wiener polarity ; apolarSA ~ ΔG/apolarSA

donor count ~ acceptor count ; donor count ~ rotatable bond count ; donor count ~ atom count ; donor count ~ hydrogen count ; donor count
~ NHA ; donor count ~ molpol ; donor count ~ Harary ind. ; donor count ~ bond count ; donor count ~ Platt ind. ; donor count ~ Randic ind.
; donor count ~ Szeged ind. ; donor count ~ Wiener polarity

acceptor count ~ rotatable bond count ; acceptor count ~ atom count ; acceptor count ~ hydrogen count ; acceptor count ~ NHA ; acceptor
count ~ molpol ; acceptor count ~ Harary ind. ; acceptor count ~ bond count ; acceptor count ~ hyper Wiener ind. ; acceptor count ~ Platt ind.
acceptor count ~ Randic ind. ; acceptor count ~ Szeged ind. ; acceptor count ~ Wiener polarity ; acceptor count ~ ΔG/MW

rotatable bond count ~ atom count ; rotatable bond count ~ hydrogen count ; rotatable bond count ~ NHA ; rotatable bond count ~ molpol ;
rotatable bond count ~ Harary ind. ; rotatable bond count ~ bond count ; rotatable bond count ~ hyper Wiener ind. ; rotatable bond count ~
Platt ind. ; rotatable bond count ~ Randic ind. ; rotatable bond count ~ Szeged ind. ; rotatable bond count ~ Wiener polarity

atom count ~ hydrogen count ; atom count ~ NHA ; atom count ~ molpol ; atom count ~ Harary ind. ; atom count ~ bond count ; atom count
~ hyper Wiener ind. ; atom count ~ Platt ind. ; atom count ~ Randic ind. ; atom count ~ Szeged ind. ; atom count ~ Wiener polarity ; atom
count ~ ΔG/apolarSA

hydrogen count ~ NHA ; hydrogen count ~ molpol ; hydrogen count ~ Harary ind. ; hydrogen count ~ bond count ; hydrogen count ~ hyper
Wiener ind. ; hydrogen count ~ Platt ind. ; hydrogen count ~ Randic ind. ; hydrogen count ~ Szeged ind. ; hydrogen count ~ Wiener polarity
hydrogen count ~ ΔG/apolar SA

NHA ~ molpol ; NHA ~ Harary ind. ; NHA ~ bond count ; NHA ~ hyper Wiener ind. ; NHA ~ Platt ind. ; NHA ~ Randic ind. ; NHA ~
Szeged ind. ; NHA ~ Wiener polarity ; NHA ~ ΔG/NHA ; NHA ~ ΔG/MS

Balaban ind. ~ Harary ind. ; Balaban ind. ~ bond count ; Balaban ind. ~ hyper Wiener ind. ; Balaban ind. ~ Platt ind. ; Balaban ind. ~ Randic
ind. ; Balaban ind. ~ Szeged ind. ; Balaban ind. ~ Wiener polarity ; Balaban ind. ~ ring count

molpol ~ Harary ind. ; molpol ~ bond count ; molpol ~ hyper Wiener ind. ; molpol ~ Platt ind. ; molpol ~ Randic ind. ; molpol ~ Szeged ind.
; molpol ~ Wiener polarity ; molpol ~ ΔG/apolarSA aromatic ring count ~ aromatic atom count

Harary ind. ~ bond count ; Harary ind. ~ hyper Wiener ind. ; Harary ind. ~ Platt ind. ; Harary ind. ~ Randic ind. ; Harary ind. ~ Szeged ind. ;
Harary ind. ~ Wiener polarity

bond count ~ hyper Wiener ind.; bond count ~ Platt ind. ; bond count ~ Randic ind. ; bond count ~ Szeged ind. ; bond count ~ Wiener
polarity ; bond count ~ ΔG/apolarSA ; bond count ~ ΔG/NoC

hyper Wiener ind. ~ Platt ind. ; hyper Wiener ind. ~ Randic ind. ; hyper Wiener ind. ~ Szeged ind. ; hyper Wiener ind. ~ Wiener polarity

Platt ind. ~ Randic ind. ; Platt ind. ~ Szeged ind. ; Platt ind. ~ Wiener polarity ; Platt ind. ~ ΔG/apolar SA ; Platt ind. ~ ΔG/NoC

Randic ind. ~ Szeged ind. ; Randic ind. ~ Wiener polarity ; Randic ind. ~ ΔG/apolarSA Szeged ind. ~ Wiener polarity

ΔG/NHA ~ ΔG/MW ; ΔG/NHA ~ ΔG/apolarSA ; ΔG/NHA ~ ΔG/NoC ΔG/MW ~ ΔG/MSA ; ΔG/MW ~ ΔG/apolarSA ; ΔG/MW
~ ΔG/NoC ΔG/MSA ~ ΔG/apolarSA ; ΔG/MSA ~ ΔG/NoC

ΔG/apolarSA ~ ΔG/NoC

Table S3. Full results of molecular properties for all compounds studied. Training and Validation data sets.

Train:

	Name	ID	DG	DrugOrNonDrug	logP	formula
1	Acarbose	DR001	-9.86	1	-6.82	C25H43NO18
2	Acetazolamide	DR002	-11.25	1	-0.44	C4H6N4O3S2
3	Adenosine	DR003	-7.53	1	-2.73	C10H13N5O4
4	Alclometasone	DR004	-12.76	1	1.18	C22H29ClO5
5	Allopurinol	DR005	-6.08	1	-0.80	C5H4N4O
6	Alprazolam	DR006	-5.90	1	2.44	C17H13ClN4
7	Alprenolol	DR007	-13.58	1	2.84	C15H23NO2
8	Amantadine	DR008	-6.82	1	2.31	C10H17N
9	Amiloride	DR009	-7.64	1	0.43	C6H8ClN7O
10	AminocaproicAcid	DR010	-6.76	1	0.05	C6H13NO2
11	Amiodarone	DR011	-8.73	1	7.91	C25H29I2NO3
12	Amitriptyline	DR012	-13.33	1	4.93	C20H23N
13	Amlodipine	DR013	-9.39	1	1.70	C20H25ClN2O5
14	Amodiaquine	DR014	-10.55	1	3.99	C20H22ClN3O
15	Amphetamine	DR015	-8.70	1	1.76	C9H13N
16	Amprenavir	DR016	-11.87	1	2.12	C25H35N3O6S
17	Anastrozole	DR017	-6.95	1	0.86	C17H19N5
18	Apomorphine	DR018	-11.53	1	3.12	C17H17NO2
19	Aprepitant	DR019	-6.82	1	3.91	C23H21F7N4O3
20	Argatroban	DR020	-10.11	1	0.70	C23H36N6O5S
21	Aripiprazole	DR021	-7.67	1	3.41	C23H27Cl2N3O2
22	Astemizole	DR022	-12.28	1	4.46	C28H31FN4O
23	Atenolol	DR023	-10.67	1	0.46	C14H22N2O3
24	Atovaquone	DR024	-9.85	1	6.27	C22H19ClO3
25	Atropine	DR025	-13.77	1	1.83	C17H23NO3
26	AzelaicAcid	DR026	-5.53	1	1.71	C9H16O4
27	Azelastine	DR027	-8.08	1	3.94	C22H24ClN3O
28	Baclofen	DR028	-8.76	1	1.33	C10H12ClN2O2
29	Benztropine	DR029	-12.31	1	4.28	C21H25NO
30	Betamethasone	DR030	-13.36	1	1.14	C22H29FO5
31	Bicalutamide	DR031	-9.67	1	2.53	C18H14F4N2O4S
32	Bosentan	DR032	-11.35	1	3.56	C27H29N5O6S
33	Brinzolamide	DR033	-13.49	1	-1.77	C12H21N3O5S3
34	Bupivacaine	DR034	-6.17	1	3.57	C18H28N2O
35	Buprenorphine	DR035	-6.58	1	3.83	C29H41NO4
36	Bupropion	DR036	-9.23	1	3.60	C13H18ClNO
37	Buspirone	DR037	-10.00	1	1.17	C21H31N5O2
38	Cabergoline	DR038	-7.94	1	2.28	C26H37N5O2
39	Caffeine	DR039	-6.30	1	-2.04	C8H10N4O2
40	Candesartan	DR040	-13.53	1	2.78	C24H20N6O3
41	Captopril	DR041	-12.69	1	0.64	C9H15N3O3S
42	Carbachol	DR042	-12.31	1	-2.06	C6H15N2O2
43	Celecoxib	DR043	-6.76	1	3.62	C17H14F3N3O2S
44	Cerivastatin	DR044	-12.12	1	3.42	C26H34FN5O5
45	Chlordiazepoxide	DR045	-6.82	1	2.86	C16H14ClN3O
46	Chlorprocaine	DR046	-6.17	1	2.80	C13H19ClN2O2
47	Chlorpheniramine	DR047	-12.76	1	3.24	C16H19ClN2
48	Chlorpromazine	DR048	-12.08	1	3.88	C17H19ClN2S
49	Chlorzoxazone	DR049	-7.48	1	1.61	C7H4ClN2O2
50	Cimetidine	DR050	-5.90	1	-0.50	C10H16N6S
51	Ciprofloxacin	DR051	-4.39	1	0.40	C17H18FN3O3
52	Cisapride	DR052	-10.71	1	3.61	C23H29ClFN3O4
53	Citalopram	DR053	-12.45	1	3.54	C20H21FN2O
54	Clarithromycin	DR054	-5.47	1	1.66	C38H69NO13
55	Clofibrate	DR055	-5.57	1	3.32	C12H15ClO3
56	Clomifene	DR056	-12.34	1	7.25	C26H28ClNO
57	Clomipramine	DR057	-11.69	1	3.61	C19H23ClN2
58	Clonazepam	DR058	-12.37	1	2.67	C15H10ClN3O3
59	Clonidine	DR059	-11.96	1	1.88	C9H9Cl2N3
60	Clotrimazole	DR060	-6.47	1	5.23	C22H17ClN2
61	Clozapine	DR061	-9.80	1	2.12	C18H19ClN4
62	Codeine	DR062	-8.60	1	1.08	C18H21NO3
63	Cyproheptadine	DR063	-9.44	1	4.68	C21H21N
64	Daunorubicin	DR064	-7.26	1	0.14	C27H29NO10
65	Decamethonium	DR065	-7.94	1	1.08	C16H38N2
66	Desipramine	DR066	-12.97	1	2.75	C18H22N2
67	Desogestrel	DR067	-7.44	1	4.01	C22H30O
68	Dexamethasone	DR068	-9.85	1	1.14	C22H29FO5
69	Dextromethorphan	DR069	-8.35	1	3.04	C17H23NO
70	Diazepam	DR070	-11.30	1	2.92	C16H13ClN2O
71	Diazoxide	DR071	-6.97	1	1.40	C8H7ClN2O2S
72	Dibucaine	DR072	-6.17	1	4.22	C20H29N3O2

73	Diclofenac	DR073	-8.40	1	3.75	C14H11Cl2N02
74	Dicloxacillin	DR074	-11.87	1	3.66	C19H17Cl2N3O5S
75	Dienestrol	DR075	-14.35	1	5.91	C18H18O2
76	Diethylstilbestrol	DR076	-15.01	1	5.48	C18H20O2
77	Dihydroergotamine	DR077	-12.58	1	1.71	C33H37N5O5
78	Diltiazem	DR078	-6.25	1	2.84	C22H26N2O4S
79	Diphenhydramine	DR079	-10.76	1	3.16	C17H21N0
80	Dipyridamole	DR080	-13.05	1	-2.82	C24H40N8O4
81	Dobutamine	DR081	-7.69	1	3.59	C18H23N03
82	Dofetilide	DR082	-10.32	1	1.82	C19H27N3O5S2
83	Domperidone	DR083	-11.47	1	1.81	C22H24ClN5O2
84	Dopamine	DR084	-10.67	1	0.92	C8H11N02
85	Dorzolamide	DR085	-12.68	1	-0.43	C10H16N2O4S3
86	Doxazosin	DR086	-12.63	1	1.38	C23H25N5O5
87	Doxorubicin	DR087	-7.05	1	-0.47	C27H29N011
88	Droperidol	DR088	-9.44	1	2.60	C22H22FN3O2
89	Duloxetine	DR089	-11.93	1	4.05	C18H19N0S
90	Edrophonium	DR090	-9.96	1	0.37	C10H16N0
91	Enalapril	DR091	-9.82	1	2.13	C20H28N2O5
92	Epinastine	DR092	-10.47	1	1.94	C16H15N3
93	Epinephrine	DR093	-8.77	1	0.55	C9H13N03
94	Ergotamine	DR094	-6.62	1	1.71	C33H35N5O5
95	Erythromycin	DR095	-6.21	1	1.14	C37H67N013
96	Estradiol	DR096	-13.33	1	4.23	C18H24O2
97	Estrone	DR097	-12.99	1	3.63	C18H22O2
98	EthacrynicAcid	DR098	-6.74	1	3.30	C13H12Cl2O4
99	Ethanol	DR099	-6.62	1	-0.08	C2H6O
100	Ethinylestradiol	DR100	-13.01	1	4.25	C20H24O2
101	Ethoxzolamide	DR101	-12.69	1	0.90	C9H10N2O3S2
102	Etoposide	DR102	-7.17	1	1.04	C29H32O13
103	Felodipine	DR103	-5.56	1	3.62	C18H19Cl2N04
104	Fenofibrate	DR104	-7.23	1	5.33	C20H21ClO4
105	Fentanyl	DR105	-12.75	1	3.93	C22H28N2O
106	Fexofenadine	DR106	-6.13	1	5.64	C32H39N04
107	Flecainide	DR107	-7.29	1	4.62	C17H20F6N2O3
108	Fluconazole	DR108	-13.44	1	-1.95	C13H12F2N6O
109	Fluorouracil	DR109	-6.28	1	-0.81	C4H3FN2O2
110	Fluoxetine	DR110	-12.34	1	4.65	C17H18F3N0
111	Fluoxymesterone	DR111	-10.04	1	1.96	C20H29F03
112	Fluphenazine	DR112	-7.91	1	3.12	C22H26F3N3O5S
113	Flurazepam	DR113	-10.71	1	3.78	C21H23ClFN3O
114	Flurbiprofen	DR114	-6.84	1	3.76	C15H13F02
115	Fulvestrant	DR115	-12.59	1	8.93	C32H47F5O3S
116	Gabapentin	DR116	-2.41	1	1.39	C9H17N02
117	Gatifloxacin	DR117	-5.30	1	0.77	C19H22FN3O4
118	Gemcitabine	DR118	-6.35	1	-0.77	C9H11F2N3O4
119	Gemfibrozil	DR119	-7.21	1	3.35	C15H22O3
120	Glyburide	DR120	-7.77	1	4.68	C23H28ClN3O5S
121	Granisetron	DR121	-12.99	1	1.75	C18H24N4O
122	Grepafloxacin	DR122	-6.17	1	1.09	C19H22FN3O3
123	Guanabenz	DR123	-11.46	1	3.56	C8H8Cl2N4
124	Guanethidine	DR124	-5.70	1	1.15	C10H22N4
125	Haloperidol	DR125	-12.78	1	3.98	C21H23ClFN02
126	Hydrocortisone	DR126	-11.63	1	0.52	C21H30O5
127	Hydromorphone	DR127	-5.46	1	0.87	C17H19N03
128	Ibuprofen	DR128	-4.75	1	3.64	C13H18O2
129	Iloprost	DR129	-8.96	1	3.19	C22H32O4
130	Imatinib	DR130	-6.47	1	2.88	C29H31N7O
131	Imipramine	DR131	-12.12	1	2.99	C19H24N2
132	Indinavir	DR132	-13.53	1	2.91	C36H47N5O4
133	Indomethacin	DR133	-5.35	1	3.62	C19H16ClN04
134	Irbesartan	DR134	-4.77	1	3.77	C25H28N6O
135	Isoniazid	DR135	-5.40	1	-0.82	C6H7N3O
136	Isoproterenol	DR136	-10.12	1	1.43	C11H17N03
137	Itraconazole	DR137	-8.61	1	1.52	C35H38Cl2N8O4
138	Ketamine	DR138	-9.82	1	2.88	C13H16ClN0
139	Ketoconazole	DR139	-10.91	1	1.80	C26H28Cl2N4O4
140	Ketoprofen	DR140	-6.41	1	3.22	C16H14O3
141	Lamivudine	DR141	-4.50	1	-0.79	C8H11N3O3S
142	Lamotrigine	DR142	-5.67	1	3.15	C9H7Cl2N5
143	Lansoprazole	DR143	-12.87	1	1.49	C16H14F3N3O2S
144	Latanoprost	DR144	-7.75	1	4.40	C26H40O5
145	Levallorphan	DR145	-12.30	1	3.91	C19H25N0
146	Levetiracetam	DR146	-3.27	1	-0.63	C8H14N2O2
147	Levocabastine	DR147	-9.96	1	5.03	C26H29FN2O2
148	Levodopa	DR148	-6.93	1	-1.76	C9H11N04
149	Levorphanol	DR149	-12.68	1	3.29	C17H23N0
150	Lidocaine	DR150	-6.17	1	2.10	C14H22N2O
151	Lindane	DR151	-4.09	1	3.83	C6H6Cl6

152	Lisuride	DR152	-12.31	1	1.93	C20H26N4O
153	Loperamide	DR153	-11.57	1	5.46	C29H33ClN2O2
154	Lorazepam	DR154	-13.64	1	3.47	C15H10Cl2N2O2
155	Losartan	DR155	-11.76	1	2.35	C22H23ClN6O
156	Lovastatin	DR156	-10.50	1	4.54	C24H36O5
157	Loxapine	DR157	-11.34	1	2.55	C18H18ClN3O
158	Lysinopril	DR158	-13.05	1	1.24	C21H31N3O5
159	Maprotiline	DR159	-6.82	1	5.06	C20H23N
160	Marimastat	DR160	-9.27	1	0.35	C15H29N3O5
161	Mazindol	DR161	-12.74	1	2.73	C16H13ClN2O
162	Mecamylamine	DR162	-8.18	1	2.66	C11H21N
163	Medroxyprogesterone	DR163	-12.92	1	3.50	C22H32O3
164	Melatonin	DR164	-13.77	1	1.26	C13H16N2O2
165	Memantine	DR165	-8.55	1	3.52	C12H21N
166	Mesoridazine	DR166	-7.84	1	2.87	C21H26N2O5
167	Methadone	DR167	-12.37	1	4.59	C21H27NO
168	Methazolamide	DR168	-11.12	1	-0.71	C5H8N4O3S2
169	Methotrexate	DR169	-15.64	1	-0.61	C20H22N8O5
170	Methoxamine	DR170	-7.12	1	0.83	C11H17NO3
171	Methylphenidate	DR171	-11.63	1	2.08	C14H19NO2
172	Methysergide	DR172	-12.54	1	0.88	C21H27N3O2
173	Metoclopramide	DR173	-9.44	1	2.18	C14H22ClN3O2
174	Miconazole	DR174	-6.35	1	5.02	C18H14Cl4N2O
175	Midazolam	DR175	-11.24	1	3.22	C18H13ClFN3
176	Mifepristone	DR176	-13.23	1	3.79	C29H35NO2
177	Milrinone	DR177	-9.31	1	1.15	C12H9N3O
178	Minoxidil	DR178	-9.94	1	0.22	C9H15N5O
179	Misoprostol	DR179	-5.92	1	3.57	C22H38O5
180	Morphine	DR180	-12.75	1	0.76	C17H19NO3
181	NalidixicAcid	DR181	-11.71	1	0.80	C12H12N2O3
182	Naloxone	DR182	-12.97	1	0.57	C19H21NO4
183	Naltrexone	DR183	-13.01	1	0.70	C20H23NO4
184	Naratriptan	DR184	-12.34	1	1.39	C17H25N3O2S
185	Nefazodone	DR185	-11.27	1	1.88	C25H32ClN5O2
186	Nelfinavir	DR186	-11.87	1	6.00	C32H45N3O4S
187	Nicardipine	DR187	-9.85	1	3.40	C26H29N3O6
188	Nicotine	DR188	-10.02	1	1.13	C10H14N2
189	Nifedipine	DR189	-8.63	1	1.84	C17H18N2O6
190	Nimodipine	DR190	-6.92	1	2.53	C21H26N2O7
191	Nisoldipine	DR191	-7.77	1	2.92	C20H24N2O6
192	Nitrendipine	DR192	-6.93	1	2.26	C18H20N2O6
193	Norethindrone	DR193	-12.82	1	3.21	C20H26O2
194	Norfloxacin	DR194	-4.15	1	0.21	C16H18FN3O3
195	Norgestrel	DR195	-10.71	1	3.78	C21H28O2
196	Nortriptyline	DR196	-12.28	1	4.69	C19H21N
197	Novobiocin	DR197	-13.23	1	4.12	C31H36N2O11
198	Ofloxacin	DR198	-3.33	1	0.26	C18H20FN3O4
199	Olanzapine	DR199	-10.35	1	0.70	C17H20N4S
200	Olopatadine	DR200	-10.22	1	3.42	C21H23NO3
201	Omapatrilat	DR201	-11.22	1	2.59	C19H24N2O4S2
202	Omeprazole	DR202	-7.51	1	0.20	C17H19N3O3S
203	Ondansetron	DR203	-12.28	1	0.19	C18H21N3O
204	Orphenadrine	DR204	-7.12	1	3.59	C18H23NO
205	Ouabain	DR205	-10.35	1	-1.24	C29H44O12
206	Oxandrolone	DR206	-9.83	1	4.15	C19H30O3
207	Oxymetazoline	DR207	-12.08	1	3.04	C16H24N2O
208	Paclitaxel	DR208	-5.81	1	2.96	C47H51NO14
209	Papaverine	DR209	-3.44	1	3.00	C20H21NO4
210	Paroxetine	DR210	-14.18	1	3.59	C19H20FN3O3
211	Pentostatin	DR211	-17.06	1	-2.89	C11H16N4O4
212	Pergolide	DR212	-12.37	1	3.65	C19H26N2S
213	Perhexiline	DR213	-7.80	1	6.20	C19H35N
214	Perphenazine	DR214	-7.94	1	2.82	C21H26ClN3O5
215	Phentolamine	DR215	-12.59	1	1.67	C17H19N3O
216	Phenylephrine	DR216	-9.03	1	0.52	C9H13NO2
217	Phenytoin	DR217	-6.51	1	2.22	C15H12N2O2
218	Physostigmine	DR218	-11.32	1	0.89	C15H21N3O2
219	Picrotoxin	DR219	-7.43	1	-0.99	C15H18O7
220	Pilocarpine	DR220	-7.36	1	0.25	C11H16N2O2
221	Pimozide	DR221	-11.22	1	5.36	C28H29F2N3O
222	Pindolol	DR222	-11.71	1	1.53	C14H20N2O2
223	Pioglitazone	DR223	-8.27	1	2.34	C19H20N2O3S
224	Piperazine	DR224	-5.46	1	-0.77	C4H10N2
225	Pirenzepine	DR225	-11.69	1	0.58	C19H21N5O2
226	Piroxicam	DR226	-6.51	1	1.89	C15H13N3O4S
227	Pramipexole	DR227	-12.30	1	0.76	C10H17N3S
228	Pravastatin	DR228	-6.92	1	2.24	C23H36O7
229	Prazosin	DR229	-14.01	1	0.59	C19H21N5O4
230	Prednisolone	DR230	-11.87	1	1.02	C21H28O5

231	Prilocaine	DR231	-6.17	1	2.10	C13H20N2O
232	Procainamide	DR232	-8.18	1	1.65	C13H21N3O
233	Procaine	DR233	-6.17	1	2.18	C13H20N2O2
234	Prochlorperazine	DR234	-8.08	1	3.53	C20H24ClN3S
235	Procyclidine	DR235	-7.87	1	4.16	C19H29NO
236	Progesterone	DR236	-15.01	1	3.52	C21H30O2
237	Promazine	DR237	-6.28	1	3.26	C17H20N2S
238	Promethazine	DR238	-12.12	1	3.36	C17H20N2S
239	Propafenone	DR239	-8.18	1	3.20	C21H27NO3
240	Propranolol	DR240	-13.70	1	3.03	C16H21NO2
241	Pseudoephedrine	DR241	-8.08	1	1.39	C10H15NO
242	Pyrimethamine	DR242	-12.04	1	3.35	C12H13ClN4
243	Quetiapine	DR243	-6.95	1	1.74	C21H25N3O2S
244	Quinidine	DR244	-8.73	1	2.83	C20H24N2O2
245	Raloxifene	DR245	-13.84	1	5.19	C28H27NO4S
246	Raltitrexed	DR246	-8.42	1	-0.49	C21H22N4O6S
247	Ramelteon	DR247	-14.81	1	2.45	C16H21NO2
248	Ranitidine	DR248	-9.27	1	0.47	C13H22N4O3S
249	Reboxetine	DR249	-12.22	1	3.07	C19H23NO3
250	Reserpine	DR250	-8.20	1	2.92	C33H42N2O9
251	Risperidone	DR251	-13.36	1	2.46	C23H27FN4O2
252	Ritonavir	DR252	-14.76	1	3.94	C37H48N6O5S2
253	Rizatriptan	DR253	-11.41	1	-0.39	C15H19N5
254	Ropinirole	DR254	-10.17	1	2.25	C16H24N2O
255	Rosiglitazone	DR255	-10.05	1	1.52	C18H19N3O3S
256	Salmeterol	DR256	-10.47	1	4.18	C25H37NO4
257	Saquinavir	DR257	-14.05	1	3.83	C38H50N6O5
258	Scopolamine	DR258	-13.74	1	0.79	C17H21NO4
259	Sertraline	DR259	-13.40	1	5.14	C17H17ClN2
260	Sildenafil	DR260	-12.28	1	0.12	C22H30N6O4S
261	Sotalol	DR261	-6.21	1	0.89	C12H20N2O3S
262	Sparfloxacin	DR262	-6.62	1	-0.34	C19H24F2N4O3
263	Spiroinolactone	DR263	-11.25	1	3.41	C24H32O4S
264	Stavudine	DR264	-4.50	1	-1.35	C10H12N2O4
265	Sulfamethoxazole	DR265	-11.08	1	1.36	C10H11N3O3S
266	Sulfanilamide	DR266	-8.28	1	0.54	C6H8N2O2S
267	Sulpiride	DR267	-6.82	1	1.16	C15H23N3O4S
268	Sumatriptan	DR268	-11.53	1	0.66	C14H21N3O2S
269	Tacrine	DR269	-10.91	1	2.56	C13H14N2
270	Tacrolimus	DR270	-12.82	1	3.27	C44H69NO12
271	Tamoxifen	DR271	-12.68	1	7.10	C26H29NO
272	Telithromycin	DR272	-6.44	1	1.72	C43H65N5O10
273	Terazosin	DR273	-11.13	1	0.27	C19H25N5O4
274	Terbutaline	DR274	-5.63	1	1.42	C12H19NO3
275	Terfenadine	DR275	-10.26	1	7.10	C32H41NO2
276	Testolactone	DR276	-6.82	1	3.68	C19H24O3
277	Testosterone	DR277	-12.22	1	3.60	C19H28O2
278	Theophylline	DR278	-7.87	1	-2.01	C7H8N4O2
279	Thioridazine	DR279	-8.58	1	4.90	C21H26N2S2
280	Tiagabine	DR280	-9.49	1	2.64	C20H25N2O2S2
281	Ticlopidine	DR281	-9.20	1	2.93	C14H14ClNS
282	Tipranavir	DR282	-15.14	1	6.62	C31H33F3N2O5S
283	Tolazamide	DR283	-5.46	1	2.48	C14H21N3O3S
284	Tolbutamide	DR284	-5.46	1	2.18	C12H18N2O3S
285	Topiramate	DR285	-3.63	1	-0.18	C12H21N2O8S
286	Tramadol	DR286	-7.87	1	2.43	C16H25NO2
287	Trandolapril	DR287	-11.65	1	3.47	C24H34N2O5
288	Tranylcypromine	DR288	-9.44	1	1.36	C9H11N
289	Travoprost	DR289	-6.62	1	4.57	C26H35F3O6
290	Trazodone	DR290	-10.80	1	0.97	C19H22ClN5O
291	Triazolam	DR291	-12.69	1	3.06	C17H12Cl2N4
292	Trifluoperazine	DR292	-8.13	1	3.83	C21H24F3N3S
293	Trihexyphenidyl	DR293	-13.64	1	4.52	C20H31NO
294	Trimethaphan	DR294	-6.82	1	4.69	C22H25N2O5S
295	Trimethoprim	DR295	-16.21	1	1.32	C14H18N4O3
296	Trimetrexate	DR296	-14.51	1	2.04	C19H23N5O3
297	Tripelennamine	DR297	-11.59	1	1.84	C16H21N3
298	Triprolidine	DR298	-12.42	1	4.01	C19H22N2
299	Troglitazone	DR299	-9.01	1	3.60	C24H27NO5S
300	Tubocurarine	DR300	-9.11	1	3.42	C37H41N2O6
301	ValproicAcid	DR301	-4.49	1	2.74	C8H16O2
302	Vardenafil	DR302	-11.39	1	1.33	C23H32N6O4S
303	Vasopressin	DR303	-12.71	1	-4.29	C46H65N15O12S2
304	Venlafaxine	DR304	-11.08	1	2.83	C17H27NO2
305	Verapamil	DR305	-9.87	1	4.70	C27H38N2O4
306	Vinblastine	DR306	-10.14	1	2.79	C46H58N4O9
307	Vincristine	DR307	-8.63	1	2.59	C46H56N4O10
308	Warfarin	DR308	-6.21	1	2.96	C19H16O4
309	Zidovudine	DR309	-4.83	1	-0.76	C10H14N5O4

310	Ziprasidone	DR310	-10.67	1	2.68	C21H21ClN4OS	
311	Zolpidem	DR311	-10.98	1	1.21	C19H23N3O	
312		1a30	ND001	-5.86	0	-1.23	C15H25N3O8
313		1a4k	ND002	-10.91	0	0.06	C21H23N3O7
314		1a4r	ND003	-9.08	0	-5.28	C10H16N6O10P2
315		1a7x	ND004	-13.23	0	3.82	C51H76N2O14
316		1a94	ND005	-10.71	0	0.90	C40H67N11O9
317		1abo	ND006	-6.09	0	-0.29	C48H76N10O12S
318		1af6	ND007	-2.49	0	-4.13	C12H22O11
319		1afk	ND008	-9.03	0	-7.06	C10H16N5O13P3
320		1afl	ND009	-8.57	0	-7.06	C10H16N5O13P3
321		1aj7	ND010	-5.28	0	1.27	C11H14N07P
322		1apv	ND011	-12.28	0	2.05	C24H44F2N4O6
323		1apw	ND012	-10.91	0	2.62	C24H44F2N4O5
324		1awi	ND013	-5.52	0	-0.88	C50H72N10O11
325		1ax0	ND014	-4.27	0	-2.13	C8H15N06
326		1b05	ND015	-9.71	0	-1.26	C15H31N5O4S
327		1b1h	ND016	-9.59	0	0.29	C22H37N5O4
328		1b32	ND017	-9.69	0	-0.65	C17H35N5O4S
329		1b3f	ND018	-9.39	0	-2.61	C18H33N7O4
330		1b3g	ND019	-9.13	0	-0.29	C18H37N5O4
331		1b3l	ND020	-8.02	0	-2.04	C14H29N5O4
332		1b40	ND021	-9.92	0	-0.18	C21H35N5O4
333		1b46	ND022	-7.20	0	-1.29	C17H33N5O4
334		1b51	ND023	-10.05	0	-2.64	C15H31N5O5
335		1b52	ND024	-9.70	0	-2.18	C16H33N5O5
336		1b58	ND025	-8.98	0	-0.47	C21H35N5O5
337		1b5i	ND026	-9.60	0	-3.12	C16H32N6O5
338		1b5j	ND027	-10.14	0	-2.76	C17H34N6O5
339		1b6h	ND028	-10.67	0	-0.58	C17H35N5O4
340		1b7h	ND029	-10.91	0	-0.02	C18H37N5O4
341		1b9j	ND030	-8.12	0	-0.08	C18H37N5O4
342		1bai	ND031	-10.50	0	0.90	C40H67N11O9
343		1bb0	ND032	-11.40	0	0.94	C23H38N6O5S
344		1bcj	ND033	-5.05	0	-2.13	C8H15N06
345		1bjr	ND034	-10.47	0	-3.82	C34H59N11O11
346		1bma	ND035	-6.25	0	4.30	C27H36F3N4O3
347		1bn1	ND036	-12.74	0	0.31	C12H14N2O4S3
348		1bn3	ND037	-13.49	0	-0.14	C13H12N2O5S3
349		1bn4	ND038	-12.70	0	-0.21	C12H14N2O5S3
350		1bnn	ND039	-13.64	0	-0.28	C13H14N2O5S3
351		1bnq	ND040	-12.95	0	-2.13	C11H19N3O5S3
352		1bnt	ND041	-13.36	0	-1.04	C13H14N2O6S3
353		1bnu	ND042	-13.23	0	-2.26	C11H12N2O5S4
354		1bnw	ND043	-12.39	0	-1.06	C9H10N2O4S4
355		1btn	ND044	-6.00	0	-7.29	C6H15O15P3
356		1bxo	ND045	-13.64	0	2.32	C30H47N4O9P
357		1bxr	ND046	-4.64	0	-6.71	C10H17N6O12P3
358		1byk	ND047	-6.82	0	-5.54	C12H23O14P
359		1bzh	ND048	-9.23	0	-3.04	C39H51FN8O19S
360		1c3x	ND049	-5.02	0	-0.19	C5H4IN5O
361		1c4u	ND050	-14.14	0	-0.01	C23H29BrN6O5S
362		1c4v	ND051	-14.73	0	1.13	C30H36N6O3
363		1c5c	ND052	-9.49	0	0.45	C12H11N07S2
364		1c70	ND053	-14.05	0	4.21	C39H48N4O5
365		1ca8	ND054	-12.95	0	0.94	C23H38N6O5S
366		1cgl	ND055	-9.37	0	2.78	C33H47N5O7
367		1cil	ND056	-12.87	0	-0.43	C10H16N2O4S3
368		1cka	ND057	-7.81	0	0.46	C46H79N11O8
369		1ct8	ND058	-8.90	0	1.85	C20H19Cl2F3N3O8P
370		1ctt	ND059	-6.17	0	-1.88	C9H14N2O5
371		1d3d	ND060	-12.40	0	6.92	C32H35BrN2O2S
372		1d4k	ND061	-12.58	0	5.27	C41H54N4O6
373		1d6v	ND062	-8.42	0	3.39	C23H27N04
374		1dar	ND063	-6.76	0	-5.75	C10H15N5O11P2
375		1db1	ND064	-12.63	0	4.98	C27H44O3
376		1det	ND065	-5.87	0	-4.52	C10H14N5O8P
377		1dfo	ND066	-9.14	0	-1.03	C20H21N7O7
378		1dif	ND067	-14.54	0	4.01	C44H56F2N8O6
379		1dl7	ND068	-8.86	0	-0.82	C11H18N2O6P
380		1dmp	ND069	-13.03	0	4.78	C33H36N4O3
381		1dud	ND070	-6.58	0	-4.77	C9H14N2O11P2
382		1e2l	ND071	-5.85	0	-1.06	C12H16N2O4
383		1e2n	ND072	-6.15	0	-2.57	C12H16N4O5
384		1e4w	ND073	-10.36	0	-3.14	C41H51N9O14
385		1e4x	ND074	-10.35	0	-4.26	C36H52N10O12
386		1e66	ND075	-13.49	0	4.43	C18H19ClN2
387		1e6q	ND076	-4.30	0	-2.49	C6H11N4O4
388		1elb	ND077	-9.76	0	4.09	C23H35F3N4O3

389	1ele	ND078	-9.35	0	2.95	C17H19F6N3O3
390	1ent	ND079	-9.49	0	2.49	C32H51N6O7P
391	1epo	ND080	-10.86	0	3.10	C32H49F2N5O7
392	1epq	ND081	-11.17	0	2.63	C27H44N3O6S2
393	1evh	ND082	-4.39	0	0.76	C31H41N5O7
394	1f1j	ND083	-12.00	0	-2.97	C20H32N4O11
395	1f3f	ND084	-6.37	0	-5.04	C10H15N2O13P3
396	1f4e	ND085	-4.04	0	0.82	C12H15N04S
397	1f4x	ND086	-7.62	0	-1.89	C12H23N07
398	1f90	ND087	-10.81	0	-0.79	C48H83N11O15
399	1f9e	ND088	-11.87	0	-0.66	C26H34N4O12
400	1fch	ND089	-12.82	0	-1.90	C29H47N7O9
401	1fcz	ND090	-12.58	0	6.76	C24H26O3
402	1fjs	ND091	-13.58	0	1.32	C25H24F2N6O5
403	1fkn_om99-2	ND092	-12.00	0	-1.52	C41H64N8O14
404	1fkx	ND093	-6.88	0	-2.98	C10H12N4O4
405	1fkx	ND094	-3.03	0	-2.29	C10H13N4O5
406	1fl3	ND095	-9.27	0	3.64	C19H19N03
407	1fmb	ND096	-13.64	0	4.96	C32H42N2O5S
408	1fwu	ND097	-5.05	0	-6.24	C20H35N018S
409	1g98	ND098	-7.77	0	-4.30	C5H11O9P
410	1ga8	ND099	-2.45	0	-3.71	C12H22O10
411	1gar	ND100	-13.64	0	-1.52	C27H38N7O12PS
412	1gux	ND101	-9.49	0	-2.26	C51H73N11O18S
413	1gvu	ND102	-12.28	0	1.39	C39H60N8O8
414	1gvw	ND103	-9.49	0	2.49	C32H51N6O7P
415	1gvx	ND104	-9.85	0	-0.86	C43H62N10O12
416	1gww	ND105	-3.51	0	-4.31	C12H22O11
417	1h6h	ND106	-7.23	0	-3.58	C17H32O16P2
418	1hdt	ND107	-10.59	0	0.72	C27H36N6O6
419	1hef	ND108	-12.28	0	2.73	C36H53N5O7
420	1heg	ND109	-10.56	0	0.99	C29H47N5O7
421	1hgt	ND110	-9.31	0	-1.10	C59H82N10O22
422	1hhh	ND111	-11.59	0	0.35	C58H78N10O15
423	1hhi	ND112	-11.21	0	2.84	C49H75N9O11
424	1hkk	ND113	-10.90	0	4.33	C56H79N9O12
425	1hi5	ND114	-5.51	0	-5.40	C10H15N5O10P2
426	1hmr	ND115	-8.94	0	7.02	C18H36O2
427	1hmt	ND116	-7.89	0	7.02	C18H36O2
428	1hn4	ND117	-7.23	0	6.57	C22H44F3O6P
429	1hp5	ND118	-8.94	0	-1.36	C8H13N04S
430	1hpo	ND119	-12.58	0	5.32	C28H28N2O5S
431	1hps	ND120	-12.58	0	5.07	C38H46N4O5
432	1hpx	ND121	-12.69	0	3.02	C33H41N5O6S2
433	1hvi	ND122	-13.74	0	3.04	C44H58N8O6
434	1hvj	ND123	-14.26	0	4.07	C44H58N8O5
435	1hvk	ND124	-13.80	0	3.04	C44H58N8O6
436	1hvr	ND125	-12.97	0	8.27	C41H38N2O3
437	1hxb	ND126	-13.53	0	3.83	C38H50N6O5
438	1ibc	ND127	-13.98	0	-1.39	C28H35N7O9
439	1if8	ND128	-13.15	0	2.46	C19H21N3O3S
440	1iht	ND129	-11.53	0	-1.14	C71H101N15O17
441	1iiq	ND130	-10.21	0	2.24	C38H50N6O7
442	1ikt	ND131	-4.64	0	5.44	C21H36O4
443	1is0	ND132	-9.55	0	-2.22	C28H39N4O14P
444	1ivp	ND133	-10.26	0	5.19	C45H59N7O7
445	1j8v	ND134	-4.93	0	-3.66	C24H35N017S
446	1jd6	ND135	-10.08	0	2.03	C47H66N8O11
447	1jet	ND136	-9.88	0	-1.51	C15H31N5O4
448	1jeu	ND137	-9.30	0	-2.04	C17H33N5O6
449	1jev	ND138	-9.39	0	-0.30	C23H36N6O4
450	1jfh	ND139	-2.79	0	-2.35	C14H26O9S2
451	1jlr	ND140	-4.55	0	-6.98	C10H16N5O14P3
452	1jn2	ND141	-5.57	0	2.06	C22H23N3O6S2
453	1jn4	ND142	-6.75	0	-6.70	C19H25N7O14P2
454	1joc	ND143	-6.30	0	-5.85	C6H14O12P2
455	1joj	ND144	-5.75	0	2.90	C50H58N8O10S
456	1jp5	ND145	-12.58	0	1.60	C37H56N8O8
457	1jq9	ND146	-11.52	0	0.80	C33H48N6O8
458	1jyq	ND147	-11.87	0	-1.86	C31H37N5O15P2
459	1k9r	ND148	-4.50	0	1.56	C32H45N5O8
460	1kdk	ND149	-12.34	0	4.50	C19H30O2
461	1kdz	ND150	-11.22	0	4.27	C29H39N3O6
462	1kel	ND151	-9.94	0	0.04	C13H19N2O7P
463	1ksn	ND152	-12.82	0	5.39	C25H26N4O4
464	1l8s	ND153	-3.81	0	4.14	C26H57N06P
465	1lbf	ND154	-10.71	0	-3.00	C12H18N09P
466	1lkk	ND155	-9.35	0	-1.50	C27H39N4O14P
467	1lrt	ND156	-7.69	0	-6.66	C20H27N7O13P2S

468		1lzq	ND157	-11.44	0	4.00	C38H49N507
469		1m0b	ND158	-12.03	0	4.01	C38H49N507
470		1m48	ND159	-6.94	0	3.65	C26H30N403
471	1m4h_om00-3	ND160	-12.95	0	0.64	C44H69N7015	
472		1m5w	ND161	-5.82	0	-3.36	C5H1107P
473		1m6p	ND162	-6.95	0	-3.78	C6H1309P
474		1m83	ND163	-4.63	0	-6.63	C10H16N5013P3
475		1mcb	ND164	-6.60	0	-1.97	C27H35N707
476		1mcj	ND165	-5.15	0	-1.14	C22H28N604
477		1mf4	ND166	-10.90	0	-1.31	C26H42N807
478		1mf1	ND167	-5.31	0	0.22	C25H43N508
479		1mj7	ND168	-11.38	0	1.02	C23H29N207P
480		1moq	ND169	-4.71	0	-3.85	C6H14N08P
481		1mpa	ND170	-10.97	0	-6.45	C63H83N15023S
482		1mq6	ND171	-15.22	0	3.32	C23H20C13N504S
483		1msn	ND172	-12.40	0	4.38	C32H37N305S
484		1mtr	ND173	-11.46	0	4.58	C33H48N406
485		1n5r	ND174	-7.72	0	5.58	C27H34N4
486		1n8u	ND175	-8.23	0	5.45	C12H25Br0
487		1nf8	ND176	-10.67	0	0.46	C10H1006
488		1nh0	ND177	-13.29	0	1.03	C37H43N5011
489		1nje	ND178	-5.18	0	-2.95	C9H14N307P
490		1nm6	ND179	-13.70	0	2.15	C27H33C1N602
491		1nq7	ND180	-9.27	0	6.16	C23H3202
492		1nw4	ND181	-12.37	0	-2.73	C11H14N404
493		1nw5	ND182	-7.11	0	-3.67	C15H23N605S
494		1nw1	ND183	-3.26	0	-1.78	C19H27N505S2
495		1o23	ND184	-6.41	0	-6.91	C15H24N2017P2
496		1o70	ND185	-6.13	0	-5.38	C9H14N2012P2
497		1oai	ND186	-6.82	0	-5.64	C41H58N10015
498		1oar	ND187	-10.09	0	1.89	C14H807S
499		1odj	ND188	-5.59	0	-3.08	C10H13N505
500		1ody	ND189	-11.05	0	4.97	C45H58N607
501		1osv	ND190	-4.75	0	5.78	C26H4404
502		1ow4	ND191	-7.75	0	2.87	C16H13N03S
503		1p19	ND192	-5.61	0	-4.77	C10H13N408P
504		1p6d	ND193	-4.01	0	2.16	C21H43N07P
505		1p6e	ND194	-3.98	0	3.09	C18H37N06PS2
506		1pme	ND195	-12.82	0	3.10	C21H16FN30S
507		1pro	ND196	-15.42	0	4.34	C34H37N306
508		1ps3	ND197	-3.12	0	-3.04	C8H12N206
509		1pvn	ND198	-13.40	0	-4.78	C9H14N309P
510		1px4	ND199	-4.40	0	-0.65	C9H1805S
511		1q84	ND200	-15.07	0	4.96	C42H58N8
512		1qan	ND201	-6.11	0	-4.36	C14H20N605S
513		1qbr	ND202	-14.42	0	4.82	C41H38N605S2
514		1qbu	ND203	-13.96	0	4.31	C34H36N404S
515		1qf2	ND204	-8.08	0	2.71	C22H24N204S
516		1qi0	ND205	-3.20	0	-4.31	C12H22011
517		1qin	ND206	-10.91	0	-2.86	C17H21IN408S
518		1qk3	ND207	-7.02	0	-4.52	C10H14N508P
519		1qkb	ND208	-10.02	0	-0.86	C17H35N504
520		1qsc	ND209	-5.02	0	-1.85	C36H53N7013
521		1r4w	ND210	-5.52	0	-4.23	C10H17N306S
522		1rdn	ND211	-2.51	0	-2.13	C8H15N06
523		1re8	ND212	-12.99	0	4.54	C27H26N206
524		1r1e	ND213	-7.91	0	-5.03	C10H16N5013P3S
525		1ro7	ND214	-4.34	0	-6.13	C20H30FN4016P
526		1ryh	ND215	-10.31	0	-7.06	C10H17N6013P3
527		1s63	ND216	-12.34	0	1.41	C22H20C1N50
528		1sl3	ND217	-16.17	0	1.34	C21H17C12F2N903
529		1sqa	ND218	-12.56	0	2.82	C23H21N70
530		1str	ND219	-6.50	0	-6.78	C29H45N11010S
531		1swr	ND220	-9.44	0	0.46	C10H16N203S
532		1syi	ND221	-7.43	0	-4.28	C10H13N304
533		1szd	ND222	-6.19	0	-6.48	C15H23N5014P2
534		1ta6	ND223	-12.46	0	2.92	C24H35C1N404
535		1tkb	ND224	-8.32	0	-1.26	C13H20N307P2S
536		1tmb	ND225	-9.20	0	-0.27	C36H47N908
537		1tsy	ND226	-6.76	0	-3.55	C9H13N208P
538		1tys	ND227	-7.48	0	-3.32	C10H15N208P
539		1u1b	ND228	-10.63	0	-9.36	C20H29N7020P4
540		1ua4	ND229	-5.76	0	-4.17	C10H14N507P
541		1uio	ND230	-5.93	0	-3.33	C10H12N405
542		1urg	ND231	-7.94	0	-4.31	C12H22011
543		1uxb	ND232	-2.94	0	-5.28	C17H29N014
544		1v16	ND233	-5.28	0	-2.30	C12H19N407P2S
545		1v48	ND234	-10.63	0	-1.48	C10H14F2N504P
546		1vac	ND235	-11.40	0	-0.84	C45H74N10013

547	1vwf	ND236	-7.55	0	-4.93	C36H54N12010S2
548	1w1d	ND237	-8.90	0	-8.95	C6H16O18P4
549	1w1g	ND238	-10.47	0	-9.81	C9H22O20P4
550	1w4o	ND239	-7.12	0	-4.58	C9H13N209P
551	1w4p	ND240	-6.47	0	-3.55	C9H13N208P
552	1w4q	ND241	-7.17	0	-3.40	C9H12FN208P
553	1w6y	ND242	-7.31	0	3.08	C18H18O2
554	1wc1	ND243	-5.46	0	-6.68	C10H16N5012P4
555	1wht	ND244	-5.05	0	1.03	C11H12O4
556	1ws1	ND245	-13.03	0	1.49	C19H33N3O6
557	1x39	ND246	-12.58	0	-1.95	C15H19N3O4
558	1x8r	ND247	-8.36	0	-4.99	C10H16O13P2
559	1x8t	ND248	-10.63	0	-4.99	C10H16O13P2
560	1x9d	ND249	-5.40	0	-3.28	C13H24O10S
561	1xd0	ND250	-9.72	0	-8.45	C31H55N023
562	1xh2	ND251	-7.23	0	-8.78	C31H53N023
563	1xk5	ND252	-8.18	0	-7.98	C23H34N10018P3
564	1xq0	ND253	-8.65	0	0.99	C16H13BrN6O3S
565	1xqk	ND254	-3.65	0	-2.60	C11H14N307P
566	1y0l	ND255	-12.28	0	2.02	C14H19N3O2
567	1y3n	ND256	-7.57	0	-2.75	C12H16O12
568	1y6r	ND257	-13.80	0	-0.61	C12H17N5O2S
569	1yc1	ND258	-8.41	0	0.75	C19H16N2O6
570	1yej	ND259	-10.17	0	1.31	C16H23N208P
571	1z1r	ND260	-12.58	0	1.20	C29H40N4O7S
572	1z71	ND261	-12.52	0	4.56	C22H22C12F2N4O3
573	1zap	ND262	-13.33	0	5.49	C42H70N6O5
574	1zsf	ND263	-13.53	0	2.98	C38H49N5O8
575	1zsr	ND264	-13.40	0	2.98	C38H49N5O8
576	2a4m	ND265	-6.17	0	-1.61	C11H12N2O2
577	2a0e	ND266	-10.39	0	0.83	C40H69N11O8
578	2ayr	ND267	-12.68	0	6.46	C30H31N05S
579	2b7f	ND268	-9.96	0	-1.07	C49H80N12013S
580	2bak	ND269	-10.14	0	2.18	C32H37N7O4
581	2bmz	ND270	-5.05	0	-3.54	C12H22O10
582	2bok	ND271	-8.94	0	-0.20	C22H32N5O2
583	2bvd	ND272	-8.18	0	-3.31	C12H23N08
584	2cgr	ND273	-9.92	0	3.05	C23H20N4O2
585	2dqt	ND274	-10.53	0	2.47	C28H36C12F3N6O8P
586	2er6	ND275	-9.85	0	-0.86	C43H62N10O12
587	2er9	ND276	-10.09	0	0.62	C45H67N11O9
588	2gst	ND277	-8.28	0	-1.53	C24H27N3O7S
589	2h65	ND278	-11.17	0	-1.63	C23H37N5O10
590	2hrp	ND279	-11.32	0	-1.04	C52H83N15O12S
591	2i3h	ND280	-10.09	0	1.34	C24H33N5O5
592	2izl	ND281	-8.18	0	0.56	C10H17N3O2S
593	2msb	ND282	-3.93	0	-9.92	C32H56O27
594	2qwb	ND283	-3.74	0	-3.74	C11H19N09
595	2rkm	ND284	-5.32	0	-1.21	C12H26N4O3
596	2std	ND285	-13.44	0	4.64	C15H18C13N0
597	2tct	ND286	-12.28	0	-0.31	C22H23C1N2O8
598	2toh	ND287	-5.67	0	-2.57	C9H13N5O3
599	2vaa	ND288	-11.50	0	-1.32	C44H66N12O12
600	2vab	ND289	-11.71	0	-0.84	C46H64N10O12
601	3er3	ND290	-9.67	0	4.93	C42H67N7O8
602	3er5	ND291	-12.28	0	-1.65	C62H93N17O12
603	3gst	ND292	-9.17	0	-1.53	C24H27N3O7S
604	456c	ND293	-13.33	0	2.63	C19H20C1N06S
605	4er2	ND294	-12.69	0	2.76	C34H63N5O9
606	4er4	ND295	-9.27	0	-0.94	C54H80N16O8
607	4sga	ND296	-4.45	0	0.61	C24H32N4O6
608	5apr	ND297	-10.60	0	2.33	C35H55N7O7S2
609	5er1	ND298	-8.20	0	3.22	C28H48N4O5
610	5hvp	ND299	-10.50	0	1.43	C31H57N5O9
611	5sga	ND300	-3.89	0	0.20	C24H32N4O7
612	5std	ND301	-14.32	0	5.34	C23H19F2N3
613	6apr	ND302	-10.60	0	2.76	C34H63N5O9
614	6cpa	ND303	-15.72	0	1.74	C22H27N2O8P
615	6rnt	ND304	-3.23	0	-4.17	C10H14N5O7P
616	7hvp	ND305	-11.59	0	0.17	C42H68N8O11
617	830c	ND306	-12.66	0	2.44	C19H20C1N06S
618	8cpa	ND307	-12.48	0	1.28	C21H25N2O8P
619	8hvp	ND308	-12.28	0	-1.46	C40H73N9O12
620	Gal_Nag	ND309	-3.81	0	-4.10	C14H25N011
621	OleicAcid	ND310	-6.71	0	6.50	C18H34O2
622	om12	ND311	-6.34	0	1.88	C29H47N5O7
623	om13	ND312	-7.50	0	2.54	C31H51N5O7
624	om14	ND313	-8.11	0	3.54	C31H52N4O8S
625	om15	ND314	-9.83	0	2.23	C34H56N6O8

626	om16	ND315	-11.23	0	2.89	C36H60N6O8
627	om17	ND316	-9.96	0	5.11	C36H61N5O7S
628	om18	ND317	-10.95	0	3.89	C36H61N5O9S
629	om19	ND318	-7.14	0	5.12	C32H54N4O6S
630	om23	ND319	-11.05	0	4.25	C37H63N5O9S
631	om99_1	ND320	-10.16	0	-0.70	C36H57N7O11
	exactmass	NumberofCarbons	wienerindex	MSA	PSA	apolarsurfacearea
1	645.25	25	7413	738.94	309.14	429.80
2	221.99	4	257	229.89	125.64	104.25
3	267.10	10	657	303.12	113.52	189.60
4	408.17	22	1682	488.72	94.83	393.89
5	136.04	5	105	154.04	74.69	79.35
6	308.08	17	926	362.76	43.07	319.69
7	249.17	15	711	368.66	29.46	339.20
8	151.14	10	124	213.77	26.00	187.77
9	229.05	6	368	222.40	47.89	174.51
10	131.09	6	114	199.65	37.30	162.35
11	645.02	25	2897	626.90	53.03	573.87
12	277.18	20	882	398.42	13.59	384.83
13	408.15	20	1836	506.60	61.83	444.77
14	355.15	20	1580	465.17	46.71	418.46
15	135.10	9	126	211.90	26.00	185.90
16	505.22	25	3813	659.78	111.87	547.91
17	293.16	17	1015	413.11	78.29	334.82
18	267.13	17	680	340.94	54.05	286.89
19	534.15	23	4275	600.47	93.59	506.88
20	508.25	23	3704	644.02	122.84	521.18
21	447.15	23	3204	557.51	53.48	504.03
22	458.25	28	4090	610.86	40.64	570.22
23	266.16	14	890	379.84	46.53	333.31
24	366.10	22	1705	424.46	54.37	370.09
25	289.17	17	959	387.02	60.12	326.90
26	188.10	9	344	267.95	74.60	193.35
27	381.16	22	1795	492.39	48.48	443.91
28	213.06	10	318	261.77	37.30	224.47
29	307.19	21	1161	424.04	22.82	401.22
30	392.20	22	1670	483.29	94.83	388.46
31	430.06	18	2378	475.24	103.61	371.63
32	551.18	27	4854	698.27	142.00	556.27
33	383.06	12	1142	457.98	136.10	321.88
34	288.22	18	958	435.34	30.66	404.68
35	467.30	29	2624	641.76	72.51	569.25
36	239.11	13	454	337.12	17.07	320.05
37	385.25	21	2514	520.61	90.34	430.27
38	451.29	26	3064	613.35	80.35	533.00
39	194.08	8	258	251.58	61.82	189.76
40	440.16	24	3326	538.79	118.81	419.98
41	217.08	9	297	276.49	106.76	169.73
42	147.11	6	139	232.70	26.30	206.40
43	381.08	17	1654	435.24	59.29	375.95
44	459.24	26	3124	623.17	99.88	523.29
45	299.08	16	828	326.50	48.19	278.31
46	270.11	13	700	366.12	39.89	326.23
47	274.12	16	718	376.49	26.48	350.01
48	318.10	17	896	404.24	52.48	351.76
49	168.99	7	143	176.79	26.30	150.49
50	252.12	10	664	332.92	90.13	242.79
51	331.13	17	1234	385.48	71.20	314.28
52	465.18	23	3560	589.85	58.35	531.50
53	324.16	20	1298	440.51	46.61	393.90
54	747.48	38	9201	1058.99	193.26	865.73
55	242.07	12	468	324.13	35.53	288.60
56	405.19	26	2488	553.27	22.82	530.45
57	314.15	19	995	430.36	27.18	403.18
58	315.04	15	959	349.06	75.25	273.81
59	229.02	9	301	253.28	12.36	240.92
60	344.11	22	1225	434.74	17.82	416.92
61	326.13	18	1082	407.04	39.54	367.50
62	299.15	18	824	369.57	52.28	317.29
63	287.17	21	928	379.27	13.59	365.68
64	527.18	27	4100	619.58	159.82	459.76
65	258.30	16	883	480.88	0.00	480.88
66	266.18	18	759	385.47	13.59	371.88
67	310.23	22	1004	420.50	20.23	400.27
68	392.20	22	1670	482.97	94.83	388.14
69	257.18	17	602	363.78	22.82	340.96
70	284.07	16	726	337.84	32.67	305.17
71	229.99	8	268	242.08	54.88	187.20
72	343.23	20	1654	503.41	52.78	450.63

73	295.02	14	706	335.35	37.30	298.05
74	469.03	19	2402	510.26	136.36	373.90
75	266.13	18	814	357.65	40.46	317.19
76	268.15	18	814	378.30	40.46	337.84
77	583.28	33	6191	720.79	137.23	583.56
78	414.16	22	2077	536.94	94.73	442.21
79	255.16	17	736	378.70	22.82	355.88
80	504.32	24	3652	662.74	172.20	490.54
81	301.17	18	1346	421.96	60.69	361.27
82	441.14	19	3074	571.96	107.86	464.10
83	425.16	22	2853	527.36	85.87	441.49
84	153.08	8	160	211.32	40.46	170.86
85	324.03	10	634	369.94	113.28	256.66
86	451.19	23	3556	556.82	106.95	449.87
87	543.17	27	4392	629.58	180.05	449.53
88	379.17	22	2452	471.68	66.80	404.88
89	297.12	18	931	393.03	37.47	355.56
90	166.12	10	190	262.46	20.23	242.23
91	376.20	20	1982	507.31	94.26	413.05
92	249.13	16	587	312.61	25.95	286.66
93	183.09	9	256	250.21	60.69	189.52
94	581.26	33	6191	704.18	137.23	566.95
95	733.46	37	8842	1028.19	204.26	823.93
96	272.18	18	724	370.28	40.46	329.82
97	270.16	18	724	360.64	37.30	323.34
98	302.01	13	744	339.20	63.60	275.60
99	46.04	2	4	88.05	20.23	67.82
100	296.18	20	941	394.99	40.46	354.53
101	258.01	9	442	285.83	89.41	196.42
102	588.18	29	5464	684.21	160.83	523.38
103	383.07	18	1300	447.12	52.60	394.52
104	360.11	20	1716	469.56	52.60	416.96
105	336.22	22	1680	480.40	33.90	446.50
106	501.29	32	5214	697.62	91.35	606.27
107	414.14	17	2232	480.75	35.53	445.22
108	306.10	13	1000	358.03	81.65	276.38
109	130.02	4	84	145.10	64.07	81.03
110	309.13	17	1148	400.00	9.23	390.77
111	336.21	20	1083	443.91	57.53	386.38
112	437.17	22	2618	539.87	86.30	453.57
113	387.15	21	1747	490.90	46.26	444.64
114	244.09	15	626	311.98	37.30	274.68
115	606.32	32	7474	791.81	76.74	715.07
116	171.13	9	193	252.16	37.30	214.86
117	375.16	19	1627	452.62	80.43	372.19
118	263.07	9	560	291.42	84.58	206.84
119	250.16	15	705	378.44	46.53	331.91
120	493.14	23	3998	603.68	85.89	517.79
121	312.20	18	1195	416.93	48.48	368.45
122	359.16	19	1499	436.04	71.20	364.84
123	230.01	8	331	246.42	24.72	221.70
124	198.18	10	352	303.10	25.95	277.15
125	375.14	21	2035	475.96	50.89	425.07
126	362.21	21	1425	467.79	94.83	372.96
127	285.14	17	712	349.76	60.12	289.64
128	206.13	13	404	307.51	37.30	270.21
129	360.23	22	2018	484.47	77.76	406.71
130	493.26	29	5324	650.27	82.92	567.35
131	280.19	19	882	411.57	27.18	384.39
132	613.36	36	7788	830.56	114.67	715.89
133	357.08	19	1424	430.64	68.53	362.11
134	428.23	25	3125	562.48	87.13	475.35
135	137.06	6	121	173.45	41.99	131.46
136	211.12	11	400	299.02	60.69	238.33
137	704.24	35	12096	866.67	125.40	741.27
138	237.09	13	388	311.59	17.07	294.52
139	530.15	26	4692	643.15	89.76	553.39
140	254.09	16	724	327.29	54.37	272.92
141	229.05	8	369	263.53	89.65	173.88
142	255.01	9	417	272.23	38.67	233.56
143	369.08	16	1631	422.14	87.08	335.06
144	432.29	26	3531	614.83	86.99	527.84
145	283.19	19	794	384.30	33.82	350.48
146	170.11	8	190	235.50	47.73	187.77
147	420.22	26	2806	552.92	74.68	478.24
148	197.07	9	321	244.14	77.76	166.38
149	257.18	17	578	357.30	33.82	323.48
150	234.17	14	556	363.03	30.66	332.37
151	287.86	6	174	247.18	32.30	214.88

152	338.21	20	1442	452.73	60.04	392.69
153	476.22	29	3458	639.89	64.48	575.41
154	320.01	15	819	339.80	49.66	290.14
155	422.16	22	2665	537.65	90.86	446.79
156	404.26	24	2246	540.51	72.83	467.68
157	327.11	18	1075	402.53	48.77	353.76
158	405.23	21	2362	540.51	105.26	435.25
159	277.18	20	810	394.42	12.00	382.42
160	331.21	15	1180	475.72	103.70	372.02
161	284.07	16	702	334.61	46.18	288.43
162	167.17	11	161	276.03	12.00	264.03
163	344.24	22	1276	472.47	54.37	418.10
164	232.12	13	561	321.89	42.09	279.80
165	179.17	12	192	275.02	26.00	249.02
166	386.15	21	1604	498.73	88.76	409.97
167	309.21	21	1044	467.23	30.66	436.57
168	236.00	5	304	248.90	112.85	136.05
169	454.17	20	3832	530.43	149.50	380.93
170	211.12	11	358	303.93	38.69	265.24
171	233.14	14	498	327.19	26.30	300.89
172	353.21	21	1586	471.12	55.82	415.30
173	299.14	14	902	409.57	39.89	369.68
174	413.99	18	1547	452.95	27.05	425.90
175	325.08	18	1035	376.64	30.18	346.46
176	429.27	29	2590	569.39	50.89	518.50
177	211.07	12	425	268.60	67.89	200.71
178	209.13	9	358	278.03	75.49	202.54
179	382.27	22	2331	564.29	83.83	480.46
180	285.14	17	712	340.19	63.28	276.91
181	232.08	12	470	295.91	71.14	224.77
182	327.15	19	1047	392.25	80.35	311.90
183	341.16	20	1189	417.38	80.35	337.03
184	335.17	17	1266	453.70	71.90	381.80
185	469.22	25	4032	626.62	76.23	550.39
186	567.31	32	5398	769.97	113.49	656.48
187	479.21	26	3884	614.55	112.01	502.54
188	162.12	10	191	237.23	26.48	210.75
189	346.12	17	1280	425.46	98.42	327.04
190	418.17	21	2290	537.42	107.65	429.77
191	388.16	20	1814	498.62	98.42	400.20
192	360.13	18	1491	449.29	98.42	350.87
193	298.19	20	941	388.99	37.30	351.69
194	319.13	16	1116	397.91	71.84	326.07
195	312.21	21	1053	413.65	37.30	376.35
196	263.17	19	759	371.98	12.00	359.98
197	612.23	31	7671	746.45	158.05	588.40
198	361.14	18	1484	441.95	94.66	347.29
199	312.14	17	958	399.37	67.78	331.59
200	337.17	21	1448	450.09	60.12	389.97
201	408.12	19	1905	483.01	149.13	333.88
202	345.11	17	1419	445.31	96.31	349.00
203	295.17	18	997	392.50	48.48	344.02
204	269.18	18	825	405.50	22.82	382.68
205	584.28	29	5312	705.09	206.60	498.49
206	306.22	19	907	431.12	46.53	384.59
207	260.19	16	681	393.68	32.59	361.09
208	853.33	47	14767	1043.16	209.26	833.90
209	339.15	20	1534	461.30	49.81	411.49
210	329.14	19	1445	415.54	27.69	387.85
211	268.12	11	670	316.91	100.10	216.81
212	314.18	19	945	430.45	54.68	375.77
213	277.28	19	802	435.53	12.00	423.53
214	403.15	21	2000	509.92	86.30	423.62
215	281.15	17	911	379.49	46.18	333.31
216	167.09	9	206	238.74	40.46	198.28
217	252.09	15	617	311.01	46.17	264.84
218	275.16	15	760	384.48	53.48	331.00
219	310.11	15	787	357.19	105.59	251.60
220	208.12	11	367	288.32	44.12	244.20
221	461.23	28	3961	595.80	49.73	546.07
222	248.15	14	687	353.97	45.25	308.72
223	356.12	19	1917	444.65	93.59	351.06
224	86.08	4	27	139.65	24.10	115.55
225	351.17	19	1540	442.70	77.45	365.25
226	331.06	15	1116	368.63	106.30	262.33
227	211.11	10	318	270.58	37.66	232.92
228	424.25	23	2600	555.40	124.29	431.11
229	383.16	19	2195	479.31	101.63	377.68
230	360.19	21	1425	447.61	94.83	352.78

231	220.16	13	488	334.04	17.07	316.97
232	235.17	13	618	351.92	30.66	321.26
233	236.15	13	618	347.20	39.89	307.31
234	373.14	20	1544	475.15	66.07	409.08
235	287.22	19	903	428.92	33.82	395.10
236	314.22	21	1052	433.53	34.14	399.39
237	284.13	17	789	385.57	52.48	333.09
238	284.13	17	744	386.56	52.48	334.08
239	341.20	21	1786	485.01	46.53	438.48
240	259.16	16	792	371.30	29.46	341.84
241	165.12	10	202	250.76	20.23	230.53
242	248.08	12	498	310.79	25.78	285.01
243	383.17	21	1956	492.38	94.30	398.08
244	324.18	20	1258	417.90	55.94	361.96
245	473.17	28	3843	592.12	108.59	483.53
246	458.13	21	3432	544.33	177.60	366.73
247	259.16	16	735	361.20	26.30	334.90
248	314.14	13	1227	431.16	86.17	344.99
249	313.17	19	1166	431.24	27.69	403.55
250	610.29	33	6944	785.27	112.34	672.93
251	410.21	23	2793	529.61	74.51	455.10
252	720.31	37	10769	902.15	169.58	732.57
253	269.16	15	871	376.41	60.09	316.32
254	260.19	16	759	390.54	30.66	359.88
255	357.11	18	1883	438.43	107.18	331.25
256	415.27	25	3802	606.83	69.92	536.91
257	670.38	38	9512	886.39	114.99	771.40
258	303.15	17	1081	379.60	72.65	306.95
259	305.07	17	770	374.69	12.00	362.69
260	474.20	22	3086	617.70	140.85	476.85
261	272.12	12	706	372.39	62.75	309.64
262	394.18	19	1781	474.76	81.55	393.21
263	416.20	24	1905	524.92	85.74	439.18
264	224.08	10	433	247.80	78.87	168.93
265	253.05	10	535	302.72	68.55	234.17
266	172.03	6	152	203.49	42.52	160.97
267	341.14	15	1251	440.91	82.41	358.50
268	295.14	14	859	406.53	71.90	334.63
269	198.12	13	326	264.66	12.89	251.77
270	803.48	44	12629	1076.29	188.71	887.58
271	371.22	26	2141	537.32	22.82	514.50
272	811.47	43	14388	1110.24	192.55	917.69
273	387.19	19	2195	494.84	97.72	397.12
274	225.14	12	468	329.78	60.69	269.09
275	471.31	32	4424	685.48	54.05	631.43
276	300.17	19	928	378.08	43.37	334.71
277	288.21	19	802	394.82	37.30	357.52
278	180.06	7	211	223.75	72.68	151.07
279	370.15	21	1444	484.90	77.78	407.12
280	375.13	20	1596	475.79	107.37	368.42
281	263.05	14	533	318.03	41.83	276.20
282	602.21	31	6752	736.37	101.94	634.43
283	311.13	14	1014	405.93	85.21	320.72
284	270.10	12	685	360.52	59.59	300.93
285	339.10	12	948	419.68	97.90	321.78
286	263.19	16	670	396.52	43.05	353.47
287	430.25	24	2772	551.78	94.26	457.52
288	133.09	9	119	191.46	26.00	165.46
289	500.24	26	4909	633.39	96.22	537.17
290	371.15	19	2003	471.04	66.48	404.56
291	342.04	17	1035	381.69	43.07	338.62
292	407.16	21	2075	505.14	66.07	439.07
293	301.24	20	1039	452.26	33.82	418.44
294	365.17	22	1584	464.35	37.14	427.21
295	290.14	14	946	388.82	53.47	335.35
296	369.18	19	1952	491.01	53.47	437.54
297	255.17	16	742	379.38	40.07	339.31
298	278.18	19	953	391.55	26.48	365.07
299	441.16	24	3093	560.07	110.16	449.91
300	609.30	37	6292	802.84	90.97	711.87
301	144.12	8	131	234.15	37.30	196.85
302	488.22	23	3398	642.54	141.67	500.87
303	1083.44	46	29219	1292.76	284.55	1008.21
304	277.20	17	792	421.02	43.05	377.97
305	454.28	27	3698	676.02	74.30	601.72
306	810.42	46	11658	1050.83	185.15	865.68
307	824.40	46	12104	1046.43	191.87	854.56
308	308.10	19	1092	374.96	63.60	311.36
309	268.10	10	701	308.01	115.08	192.93

310	412.11	21	2344	483.28	81.91	401.37
311	309.18	19	1137	406.26	56.61	349.65
312	375.16	15	1828	474.32	146.04	328.28
313	429.15	21	2710	499.07	118.05	381.02
314	442.04	10	2115	463.30	225.94	237.36
315	940.53	51	20679	1250.74	215.01	1035.73
316	845.51	40	17999	1130.93	169.15	961.78
317	1016.54	48	28494	1302.64	318.00	984.64
318	342.12	12	1110	397.83	189.53	208.30
319	507.00	10	2671	514.78	282.54	232.24
320	507.00	10	2671	516.68	282.54	234.14
321	303.05	11	981	366.51	139.46	227.05
322	522.32	24	4130	729.23	108.74	620.49
323	506.33	24	3910	712.49	88.51	623.98
324	988.54	50	28655	1232.91	313.24	919.67
325	221.09	8	354	271.13	107.22	163.91
326	377.21	15	1766	507.85	110.24	397.61
327	435.28	22	3020	605.16	71.44	533.72
328	405.24	17	2126	559.79	96.74	463.05
329	411.26	18	2493	557.78	100.12	457.66
330	387.28	18	2080	559.88	71.44	488.44
331	331.22	14	1506	459.74	71.44	388.30
332	421.27	21	2719	581.76	71.44	510.32
333	371.25	17	1880	512.28	85.03	427.25
334	361.23	15	1766	496.81	91.67	405.14
335	375.25	16	1910	519.71	91.67	428.04
336	437.26	21	2972	594.49	91.67	502.82
337	388.24	16	2102	523.81	88.51	435.30
338	402.26	17	2321	548.73	88.51	460.22
339	373.27	17	1933	535.97	71.44	464.53
340	387.28	18	2126	559.19	71.44	487.75
341	387.28	18	2102	560.61	71.44	489.17
342	845.51	40	17999	1132.53	169.15	963.38
343	510.26	23	4380	654.06	175.24	478.82
344	221.09	8	354	271.34	107.22	164.12
345	797.44	34	18551	1046.45	187.77	858.68
346	521.27	27	4606	695.25	63.24	632.01
347	346.01	12	1017	393.22	113.28	279.94
348	371.99	13	1131	390.33	136.10	254.23
349	362.01	12	1180	407.52	122.51	285.01
350	374.01	13	1131	412.52	136.10	276.42
351	369.05	11	983	433.59	136.10	297.49
352	390.00	13	1270	422.47	156.33	266.14
353	379.96	11	988	389.12	175.34	213.78
354	337.95	9	750	350.12	141.52	208.60
355	419.96	6	1221	416.97	290.40	126.57
356	638.31	30	6630	843.54	150.92	692.62
357	506.01	10	2891	519.30	273.31	245.99
358	422.08	12	1858	464.39	245.87	218.52
359	986.30	39	21906	1141.37	357.59	783.78
360	276.95	5	178	202.36	74.43	127.93
361	580.11	23	4541	620.55	127.30	493.25
362	528.28	30	5234	670.11	84.78	585.33
363	345.00	12	946	369.52	142.57	226.95
364	652.36	39	9364	872.46	114.92	757.54
365	510.26	23	4380	652.63	175.24	477.39
366	625.35	33	8646	844.16	120.56	723.60
367	324.03	10	634	369.94	113.28	256.66
368	913.61	46	23409	1242.44	190.92	1051.52
369	587.02	20	4768	626.71	156.53	470.18
370	230.09	9	414	259.21	90.23	168.98
371	590.16	32	5319	703.70	84.88	618.82
372	698.40	41	10868	940.60	100.90	839.70
373	381.19	23	2494	502.50	74.60	427.90
374	443.02	10	2115	458.62	246.17	212.45
375	416.33	27	2677	602.03	60.69	541.34
376	363.06	10	1230	388.84	189.83	199.01
377	471.15	20	4127	535.82	168.44	367.38
378	830.43	44	16308	1087.57	161.70	925.87
379	305.09	11	949	400.42	111.39	289.03
380	536.28	33	4837	699.69	84.71	614.98
381	388.01	9	1460	392.86	211.78	181.08
382	252.11	12	567	297.38	89.87	207.51
383	296.11	12	862	362.80	130.47	232.33
384	893.36	41	20065	1061.76	276.01	785.75
385	816.38	36	15546	1005.87	239.04	766.83
386	298.12	18	842	363.67	12.89	350.78
387	203.08	6	262	233.07	125.77	107.30
388	472.27	23	3502	633.60	51.21	582.39

389	427.13	17	2580	493.86	51.21	442.65
390	662.36	32	8198	908.22	153.30	754.92
391	653.36	32	7856	860.13	131.56	728.57
392	570.27	27	4935	756.28	159.24	597.04
393	595.30	31	6784	754.14	177.01	577.13
394	504.21	20	4004	621.05	200.41	420.64
395	463.98	10	2316	464.66	247.89	216.77
396	269.07	12	578	330.41	93.41	237.00
397	293.15	12	825	388.03	105.45	282.58
398	1053.61	48	31808	1389.21	279.12	1110.09
399	594.22	26	6811	718.25	206.48	511.77
400	637.34	29	8360	835.15	163.11	672.04
401	362.19	24	2034	492.16	54.37	437.79
402	526.18	25	4668	589.60	125.26	464.34
403	892.45	41	22054	1146.10	251.62	894.48
404	252.09	10	568	286.21	113.52	172.69
405	269.09	10	657	305.53	133.69	171.84
406	309.14	19	1550	398.81	54.37	344.44
407	566.28	32	5491	771.24	96.89	674.35
408	609.16	20	4915	684.87	297.04	387.83
409	246.01	5	402	267.93	174.56	93.37
410	326.12	12	1011	383.51	169.30	214.21
411	715.20	27	11002	850.18	275.02	575.16
412	1159.49	51	38940	1422.87	361.86	1061.01
413	768.45	39	13772	1030.33	171.56	858.77
414	662.36	32	8198	906.83	153.30	753.53
415	910.45	43	21075	1153.71	241.33	912.38
416	342.12	12	1134	392.77	189.53	203.24
417	554.12	17	4060	651.35	275.66	375.69
418	540.27	27	5568	691.54	121.10	570.44
419	667.39	36	9108	913.56	114.81	798.75
420	577.35	29	6554	795.87	114.81	681.06
421	1282.56	59	54834	1583.30	411.25	1172.05
422	1154.56	58	43261	1467.00	295.87	1171.13
423	965.56	49	26200	1300.15	194.09	1106.06
424	1069.58	56	35320	1416.93	227.91	1189.02
425	427.03	10	1925	446.69	226.20	220.49
426	284.27	18	1313	481.38	37.30	444.08
427	284.27	18	1313	481.33	37.30	444.03
428	492.28	22	4478	708.32	84.03	624.29
429	219.06	8	274	247.22	107.58	139.64
430	504.17	28	4114	599.57	112.84	486.73
431	638.35	38	8805	863.52	109.35	754.17
432	667.25	33	8500	838.81	174.82	663.99
433	794.45	44	15471	1064.65	161.70	902.95
434	778.45	44	15056	1058.12	141.47	916.65
435	794.45	44	15471	1067.06	161.70	905.36
436	606.29	41	7167	781.31	84.71	696.60
437	670.38	38	9512	887.72	114.99	772.73
438	613.25	28	7250	732.09	200.19	531.90
439	371.13	19	1975	465.45	64.52	400.93
440	1435.75	71	99224	1828.59	337.28	1491.31
441	702.37	38	11058	932.83	114.81	818.02
442	352.26	21	2046	566.52	36.92	529.60
443	686.22	28	8934	824.03	256.75	567.28
444	809.45	45	16391	1074.13	156.38	917.75
445	641.16	24	6676	717.67	319.57	398.10
446	918.49	47	21682	1192.22	221.27	970.95
447	345.24	15	1624	485.23	71.44	413.79
448	403.24	17	2321	542.09	108.74	433.35
449	460.28	23	3413	620.10	87.23	532.87
450	402.10	14	1442	471.47	199.67	271.80
451	522.99	10	3140	530.65	302.51	228.14
452	489.10	22	3391	563.23	141.29	421.94
453	637.09	19	6929	664.96	294.07	370.89
454	340.00	6	752	347.85	234.06	113.79
455	962.40	50	23457	1200.45	234.86	965.59
456	740.42	37	12668	975.88	155.51	820.37
457	656.35	33	9232	865.58	146.04	719.54
458	781.18	31	12110	907.70	267.95	639.75
459	627.33	32	7965	812.28	183.65	628.63
460	290.22	19	802	411.10	37.30	373.80
461	525.28	29	5081	712.84	108.74	604.10
462	346.09	13	1382	432.86	164.05	268.81
463	446.20	25	3644	573.12	92.68	480.44
464	510.39	26	5847	808.34	95.03	713.31
465	351.07	12	1364	407.08	174.56	232.52
466	674.22	27	8549	817.60	256.75	560.85
467	667.09	20	7670	686.58	310.39	376.19

468	687.36	38	10680	921.22	114.81	806.41
469	687.36	38	10680	919.94	114.81	805.13
470	446.23	26	3876	581.58	80.81	500.77
471	935.49	44	24304	1214.98	271.85	943.13
472	214.02	5	272	249.01	134.10	114.91
473	260.03	6	443	284.15	166.72	117.43
474	507.00	10	2891	516.63	282.54	234.09
475	569.26	27	5757	709.30	164.92	544.38
476	440.22	22	2940	562.12	110.55	451.57
477	578.32	26	6188	754.26	149.66	604.60
478	541.31	25	4972	724.08	156.47	567.61
479	476.17	23	3786	608.18	127.78	480.40
480	259.05	6	443	288.48	146.49	141.99
481	1449.55	63	83163	1698.87	425.87	1273.00
482	567.03	23	4317	617.02	119.68	497.34
483	575.25	32	5842	743.96	130.56	613.40
484	596.36	33	6693	827.27	89.90	737.37
485	414.28	27	2458	593.62	4.93	588.69
486	264.11	12	455	356.32	20.23	336.09
487	226.05	10	445	231.14	104.06	127.08
488	733.30	37	12278	903.44	189.41	714.03
489	307.06	9	859	345.40	140.92	204.48
490	508.24	27	4074	645.03	46.61	598.42
491	340.24	23	1638	509.53	37.30	472.23
492	266.10	11	657	310.59	122.23	188.36
493	399.15	15	1993	475.24	196.22	279.02
494	469.15	19	3634	546.86	157.57	389.29
495	566.06	15	4467	579.88	311.16	268.72
496	404.00	9	1584	402.51	232.01	170.50
497	930.41	41	25091	1144.95	271.85	873.10
498	320.00	14	906	324.13	137.35	186.78
499	283.09	10	753	316.48	133.49	182.99
500	794.44	45	16909	1060.87	122.65	938.22
501	420.32	26	2239	602.82	77.76	525.06
502	299.06	16	874	353.25	62.75	290.50
503	348.05	10	1191	370.78	188.18	182.60
504	452.28	21	3015	676.20	108.94	567.26
505	458.18	18	2456	640.77	151.76	489.01
506	377.10	21	1871	456.57	77.85	378.72
507	583.27	34	6059	763.26	126.64	636.62
508	232.07	8	374	256.12	128.65	127.47
509	339.05	9	1077	354.88	186.35	168.53
510	238.09	9	354	300.91	115.45	185.46
511	674.48	42	12010	925.25	57.19	868.06
512	384.12	14	1845	439.26	155.89	283.37
513	758.23	41	11625	867.20	218.23	648.97
514	596.25	34	6244	723.89	151.47	572.42
515	412.15	22	2446	510.92	123.83	387.09
516	342.12	12	1134	394.53	189.53	205.00
517	568.01	17	3102	539.65	174.58	365.07
518	363.06	10	1330	386.55	189.83	196.72
519	373.27	17	1910	535.22	71.44	463.78
520	791.37	36	14380	996.79	248.14	748.65
521	307.08	10	969	361.10	147.54	213.56
522	221.09	8	354	271.58	107.22	164.36
523	474.18	27	4266	581.64	100.90	480.74
524	538.97	10	3140	537.83	317.53	220.30
525	632.14	20	6178	691.79	294.67	397.12
526	522.01	10	3140	533.28	293.28	240.00
527	405.14	22	2578	495.55	75.51	420.04
528	551.08	21	4925	589.20	117.52	471.68
529	411.18	23	2812	505.09	66.70	438.39
530	739.31	29	10991	889.51	254.93	634.58
531	244.09	10	500	294.82	79.67	215.15
532	239.09	10	492	270.41	86.71	183.70
533	559.07	15	4570	590.12	285.12	305.00
534	478.23	24	3593	622.24	74.03	548.21
535	424.05	13	1952	493.56	176.03	317.53
536	733.35	36	10920	908.66	156.47	752.19
537	308.04	9	859	320.74	155.44	165.30
538	322.06	10	969	348.31	155.44	192.87
539	811.04	20	11110	829.01	406.75	422.26
540	347.06	10	1191	374.39	169.86	204.53
541	268.08	10	657	300.68	133.49	167.19
542	342.12	12	1134	391.88	189.53	202.35
543	471.16	17	2655	547.44	243.90	303.54
544	425.04	12	1952	486.89	188.92	297.97
545	337.08	10	1176	383.93	130.91	253.02
546	962.54	45	23914	1274.23	231.39	1042.84

547	878.35	36	18335	1058.60	317.75	740.85
548	499.93	6	1794	489.45	346.74	142.71
549	573.97	9	2976	585.49	376.20	209.29
550	324.04	9	896	330.52	175.67	154.85
551	308.04	9	815	321.87	155.44	166.43
552	326.03	9	896	326.73	155.44	171.29
553	266.13	18	724	346.10	37.30	308.80
554	521.97	10	2891	528.45	265.47	262.98
555	208.07	11	390	261.48	74.60	186.88
556	399.24	19	2125	546.40	134.36	412.04
557	305.14	15	1090	379.79	98.74	281.05
558	406.01	10	1394	425.53	247.97	177.56
559	406.01	10	1394	425.95	247.97	177.98
560	372.11	13	1284	432.26	194.60	237.66
561	809.32	31	14124	934.20	388.29	545.91
562	807.30	31	14124	915.92	388.29	527.63
563	831.13	23	14269	903.96	408.30	495.66
564	448.00	16	1959	457.68	119.84	337.84
565	331.06	11	1099	370.73	148.02	222.71
566	261.15	14	760	360.26	55.12	305.14
567	352.06	12	1264	362.88	203.44	159.44
568	295.11	12	774	352.85	107.33	245.52
569	368.10	19	1709	436.12	124.90	311.22
570	402.12	16	2538	506.19	156.53	349.66
571	588.26	29	5552	757.32	136.78	620.54
572	498.10	22	3578	576.57	67.39	509.18
573	738.54	42	11602	1063.20	142.87	920.33
574	703.36	38	11058	929.61	135.04	794.57
575	703.36	38	11058	927.38	135.04	792.34
576	204.09	11	369	260.13	53.09	207.04
577	831.53	40	17524	1142.78	139.72	1003.06
578	517.19	30	4922	663.45	94.80	568.65
579	1076.57	49	34036	1385.10	305.10	1080.00
580	583.29	32	7479	756.96	110.61	646.35
581	326.12	12	1014	387.83	158.30	229.53
582	398.26	22	2223	533.17	74.82	458.35
583	309.14	12	916	377.49	139.84	237.65
584	384.16	23	2306	483.76	73.45	410.31
585	742.17	28	8541	875.35	180.55	694.80
586	910.45	43	21075	1151.35	241.33	910.02
587	905.51	45	21228	1199.88	219.90	979.98
588	501.16	24	3916	591.82	154.27	437.55
589	543.25	23	5206	693.56	177.02	516.54
590	1141.61	52	39201	1480.50	279.43	1201.07
591	471.25	24	3634	614.03	117.89	496.14
592	243.10	10	500	296.13	74.96	221.17
593	872.30	32	15704	998.84	425.21	573.63
594	309.11	11	858	369.37	164.75	204.62
595	274.20	12	844	394.72	54.37	340.35
596	333.05	15	828	405.68	17.07	388.61
597	478.11	22	2546	517.48	165.95	351.53
598	239.10	9	504	286.84	96.92	189.92
599	954.49	44	25674	1227.15	238.17	988.98
600	948.47	46	26875	1204.80	238.34	966.46
601	797.51	42	14473	1103.67	163.72	939.95
602	1267.72	62	56122	1600.28	297.92	1302.36
603	501.16	24	3916	591.16	154.27	436.89
604	425.07	19	2162	498.77	110.31	388.46
605	685.46	34	10287	975.89	163.11	812.78
606	1080.63	54	35721	1375.38	223.32	1152.06
607	472.23	24	3808	603.24	132.76	470.48
608	749.36	35	10530	970.24	173.25	796.99
609	520.36	28	4754	756.44	80.67	675.77
610	643.42	31	8558	901.52	163.11	738.41
611	488.23	24	4156	617.63	152.99	464.64
612	375.15	23	1985	468.34	25.78	442.56
613	685.46	34	10287	975.14	163.11	812.03
614	478.15	22	3812	596.14	137.01	459.13
615	347.06	10	1099	375.47	169.86	205.61
616	860.50	42	18280	1160.04	199.84	960.20
617	425.07	19	2227	498.47	110.31	388.16
618	464.13	21	3615	571.89	137.01	434.88
619	871.54	40	18524	1182.29	214.32	967.97
620	383.14	14	1601	450.74	186.37	264.37
621	282.26	18	1313	461.63	37.30	424.33
622	577.35	29	6776	801.39	114.81	686.58
623	605.38	31	7512	849.71	114.81	734.90
624	640.35	31	7915	886.99	140.26	746.73
625	676.42	34	10317	943.25	131.88	811.37

626	704.45	36	11301	989.62	131.88	857.74
627	707.43	36	10832	1001.51	140.11	861.40
628	739.42	36	11772	1026.33	157.33	869.00
629	622.38	32	7552	886.24	123.04	763.20
630	753.43	37	12386	1051.04	157.33	893.71
631	763.41	36	14291	1000.23	197.25	802.98

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3	4	8		2	32	13 19
4	3	6		2	57	29 28
5	2	4		0	14	4 10
6	0	4		1	35	13 22
7	2	3		8	41	23 18
8	1	1		0	28	17 11
9	4	9		1	23	8 15
10	2	3		5	22	13 9
11	0	3		11	60	29 31
12	0	1		3	44	23 21
13	2	8		10	53	25 28
14	2	5		6	47	22 25
15	1	1		2	23	13 10
16	3	9		11	70	35 35
17	0	4		6	41	19 22
18	2	3		0	37	17 20
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20	5	11		8	71	36 35
21	1	7		7	57	27 30
22	1	5		8	65	31 34
23	3	5		8	41	22 19
24	1	4		2	45	19 26
25	1	4		5	44	23 21
26	2	4		8	29	16 13
27	0	4		3	51	24 27
28	2	4		4	26	12 14
29	0	2		4	48	25 23
30	3	6		2	57	29 28
31	2	10		7	43	14 29
32	2	10		10	68	29 39
33	2	9		7	44	21 23
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35	2	5		5	75	41 34
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37	0	7		6	59	31 28
38	2	6		8	70	37 33
39	0	3		0	24	10 14
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45	1	5		1	35	14 21
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625	7	14	20	104	56	48

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414	69.19	1	1
415	92.18	1	2
416	28.97	2	0
417	47.16	1	0
418	55.92	0	2
419	72.40	0	2
420	61.07	0	1
421	125.27	1	2
422	118.18	2	3
423	101.71	0	2
424	112.98	1	3
425	34.68	3	0
426	34.73	0	0
427	34.73	0	0
428	47.39	0	0
429	20.46	2	0
430	53.79	3	2
431	71.28	1	3
432	71.79	2	2
433	86.72	2	2
434	86.09	2	2
435	86.72	2	2
436	73.63	1	6
437	75.01	3	2
438	59.53	2	1
439	41.65	0	3
440	146.97	3	2
441	75.69	0	3
442	40.64	0	1
443	63.67	1	1
444	88.90	3	2
445	56.37	3	1
446	95.47	2	2
447	36.49	0	0
448	41.05	0	0
449	51.17	0	2
450	37.29	2	0
451	39.89	3	0
452	50.37	0	3
453	53.76	5	0
454	25.23	1	0
455	101.87	1	5
456	78.58	1	2
457	69.00	0	2
458	72.42	0	3
459	64.22	3	1
460	33.64	4	0
461	56.59	0	2
462	32.08	0	1
463	49.35	0	3
464	56.82	0	0
465	30.99	0	1
466	62.55	0	1
467	57.84	5	0

468	74.55	0	3
469	74.55	0	3
470	49.02	1	2
471	93.99	0	1
472	17.17	0	0
473	20.21	1	0
474	39.73	3	0
475	56.77	2	1
476	45.31	2	1
477	58.55	0	1
478	54.73	1	0
479	48.33	0	2
480	20.99	1	0
481	140.12	2	2
482	53.81	2	2
483	62.73	1	3
484	65.28	1	2
485	54.43	0	4
486	26.07	0	0
487	20.80	1	0
488	74.11	0	3
489	25.90	2	0
490	55.12	2	2
491	41.67	0	1
492	25.12	2	1
493	38.87	1	2
494	46.61	2	0
495	45.03	3	0
496	31.23	2	0
497	90.82	0	2
498	29.90	1	2
499	24.75	3	0
500	89.49	0	4
501	47.76	4	0
502	33.66	0	3
503	28.63	3	0
504	47.46	0	0
505	48.03	0	0
506	43.66	2	2
507	63.84	1	4
508	19.53	2	0
509	27.20	2	0
510	22.95	1	0
511	80.76	5	3
512	36.82	3	0
513	81.68	3	4
514	65.30	3	3
515	44.04	1	2
516	28.97	2	0
517	46.99	0	1
518	29.77	3	0
519	40.16	0	0
520	77.38	1	1
521	28.29	0	0
522	19.52	1	0
523	50.81	1	3
524	42.63	3	0
525	51.84	3	0
526	40.60	3	0
527	43.43	2	2
528	48.84	1	3
529	46.96	1	3
530	70.44	2	0
531	24.13	2	0
532	22.61	2	0
533	45.98	4	0
534	50.29	2	1
535	38.80	2	0
536	75.07	2	2
537	25.45	2	0
538	27.24	2	0
539	65.62	5	0
540	29.66	3	0
541	23.59	3	0
542	28.97	2	0
543	40.47	2	0
544	38.06	2	0
545	27.20	2	0
546	98.33	0	1

547	85.60	4	0
548	35.41	1	0
549	42.25	1	0
550	26.17	2	0
551	25.45	2	0
552	25.36	2	0
553	31.83	2	2
554	41.34	3	0
555	21.14	0	1
556	40.57	1	0
557	30.71	2	1
558	32.00	1	0
559	32.00	1	0
560	33.13	2	0
561	71.46	5	0
562	71.20	5	0
563	68.80	6	0
564	39.84	0	3
565	28.97	2	0
566	29.31	1	1
567	28.63	2	0
568	31.18	2	1
569	39.12	2	2
570	37.51	0	1
571	61.76	1	2
572	46.64	0	3
573	83.02	3	1
574	75.18	0	3
575	75.18	0	3
576	23.34	0	2
577	87.88	0	1
578	60.45	1	4
579	108.61	3	0
580	64.34	4	2
581	28.32	2	0
582	44.11	3	1
583	28.29	2	0
584	42.43	0	3
585	65.80	0	2
586	92.18	1	2
587	93.96	3	1
588	52.21	1	2
589	51.95	0	0
590	117.83	2	2
591	50.58	1	2
592	24.63	2	0
593	74.85	5	0
594	26.65	1	0
595	29.60	0	0
596	33.23	1	1
597	45.70	3	1
598	22.08	2	0
599	96.27	0	2
600	96.18	2	2
601	85.79	2	1
602	131.35	5	1
603	52.21	1	2
604	41.92	1	2
605	72.22	0	0
606	113.75	5	1
607	48.22	2	1
608	78.63	2	1
609	58.03	0	1
610	66.72	0	0
611	48.89	2	1
612	41.25	1	3
613	72.22	0	0
614	47.26	0	2
615	29.66	3	0
616	89.02	1	1
617	41.92	1	2
618	45.43	0	2
619	88.94	0	0
620	33.33	2	0
621	34.49	0	0
622	60.71	0	1
623	64.38	0	1
624	67.49	0	1
625	71.27	0	1

626		74.94	0		1
627		76.62	0		1
628		78.05	0		1
629		67.90	0		1
630		79.88	0		1
631		77.52	0		1
	aromaticatomCount	balabanindex	hararyindex	bondCount	hyperwienerindex
1	0	1.35	207.69	90	43344
2	5	2.18	33.71	19	677
3	0	1.65	63.95	34	1939
4	0	1.70	121.28	60	5609
5	0	1.66	24.25	15	198
6	17	1.59	81.47	38	2770
7	6	2.22	51.82	41	2544
8	0	1.79	30.00	30	226
9	0	2.36	42.23	23	1001
10	0	2.75	16.84	21	297
11	15	1.54	122.50	62	13598
12	12	1.48	72.71	46	2780
13	6	2.21	110.94	54	6378
14	12	1.37	90.31	49	6284
15	6	2.13	22.08	23	287
16	12	1.63	145.86	72	17351
17	6	1.90	76.55	42	3289
18	12	1.45	72.72	40	1840
19	12	1.49	163.69	61	19663
20	6	1.70	149.10	73	16457
21	12	0.96	111.13	60	18350
22	18	1.01	136.94	69	22647
23	6	1.98	55.10	41	3650
24	12	1.18	99.26	48	6917
25	6	1.33	70.84	46	3348
26	0	2.92	29.18	28	1216
27	12	1.45	105.02	54	6803
28	6	2.36	37.17	26	867
29	12	1.36	82.79	51	3953
30	0	1.71	122.14	60	5555
31	12	1.96	112.07	44	10485
32	12	1.46	176.15	71	22463
33	5	2.16	82.56	45	3870
34	6	1.82	69.41	50	3290
35	6	1.42	168.69	81	8888
36	6	2.46	46.01	34	1327
37	0	1.08	102.74	62	13028
38	9	1.47	140.43	73	12891
39	0	2.23	41.35	25	565
40	23	1.17	138.05	57	15608
41	0	2.57	38.19	29	748
42	0	3.21	20.83	24	348
43	12	1.68	98.35	42	6270
44	6	2.18	136.63	68	13340
45	12	1.58	74.53	37	2425
46	6	2.25	52.57	37	2488
47	6	1.72	59.85	39	2256
48	12	1.47	72.37	42	2875
49	6	1.97	27.80	16	302
50	0	1.85	46.16	33	2534
51	10	1.42	90.59	45	4135
52	12	1.31	122.85	63	19542
53	12	1.59	87.89	47	4554
54	0	2.13	283.13	123	43636
55	6	2.39	45.52	31	1426
56	18	1.37	109.28	59	11485
57	12	1.73	78.04	47	3194
58	12	1.79	79.29	34	2952
59	6	1.86	38.72	24	778
60	18	1.55	99.75	45	3580
61	12	1.48	85.69	45	3453
62	6	1.50	87.32	47	2211
63	12	1.59	81.17	46	2773
64	12	1.48	182.48	71	17274
65	0	3.13	47.55	55	4022
66	12	1.57	68.05	44	2282
67	0	1.62	89.65	56	3020
68	0	1.71	122.14	60	5555
69	6	1.51	67.37	45	1642
70	12	1.63	69.49	35	2077
71	6	2.13	40.81	22	616
72	6	1.72	86.97	55	6833

73	12	1.74	60.58	31	2195
74	11	1.33	123.44	50	9877
75	12	1.96	65.45	39	2641
76	12	1.96	65.45	41	2641
77	15	0.92	215.64	87	31219
78	12	1.66	117.17	57	7726
79	12	1.68	59.11	41	2371
80	0	1.47	160.75	79	14864
81	12	1.38	69.25	46	6115
82	12	1.50	101.32	57	18090
83	12	0.94	117.31	58	14454
84	6	2.07	25.98	22	377
85	5	2.00	64.14	36	1777
86	12	1.09	136.32	62	18380
87	12	1.45	189.16	72	18705
88	12	1.12	103.63	53	12374
89	15	1.39	70.64	42	3076
90	6	2.50	30.52	28	431
91	6	1.84	97.96	56	8193
92	12	1.51	67.20	37	1515
93	6	2.18	33.52	26	667
94	15	0.92	215.64	85	31219
95	0	2.13	274.06	120	42047
96	6	1.36	71.70	47	2154
97	6	1.36	71.70	45	2154
98	6	2.42	59.22	31	2511
99	0	1.63	2.50	8	5
100	6	1.58	82.70	49	2981
101	6	1.69	47.66	27	1292
102	12	1.19	209.85	80	24949
103	6	2.21	95.91	45	4047
104	12	1.63	87.55	47	7600
105	12	1.29	88.20	55	7214
106	18	1.20	155.06	79	31140
107	6	1.78	102.57	49	9610
108	6	1.71	77.46	36	3189
109	0	2.09	19.53	12	160
110	12	1.66	72.94	41	4312
111	0	1.63	97.91	56	3226
112	12	1.22	118.60	59	11825
113	12	1.71	105.13	52	6417
114	12	1.77	55.99	32	2003
115	6	1.02	174.82	91	52053
116	0	2.48	30.18	29	442
117	10	1.63	109.35	52	5551
118	0	2.02	58.59	30	1571
119	6	2.21	52.77	40	2523
120	12	1.22	127.07	63	23152
121	6	1.32	83.26	50	4319
122	10	1.36	102.91	51	5136
123	6	2.26	36.75	22	948
124	0	2.08	35.73	36	1078
125	12	1.32	91.64	51	9946
126	0	1.45	107.41	59	4757
127	6	1.59	82.19	44	1815
128	6	2.14	40.95	33	1240
129	0	1.72	89.61	59	9623
130	12	0.90	152.51	72	32339
131	12	1.48	72.71	47	2780
132	12	1.20	208.96	96	43374
133	15	1.56	94.14	43	5036
134	17	1.17	131.12	64	14751
135	0	2.24	22.38	17	263
136	6	2.15	40.95	32	1200
137	18	0.70	227.52	93	94912
138	6	1.92	49.49	33	952
139	12	0.98	150.63	68	26511
140	12	1.70	60.35	34	2349
141	0	1.76	43.03	27	1026
142	6	1.76	48.33	24	1122
143	6	1.33	89.64	41	6763
144	6	1.51	111.18	72	20290
145	6	1.38	77.55	49	2282
146	0	2.52	30.30	26	425
147	12	1.20	127.18	63	12918
148	6	2.33	37.31	25	893
149	6	1.56	68.11	45	1484
150	6	2.26	49.40	39	1742
151	0	2.76	31.60	18	357

152	9	1.31	95.40	54	5260
153	18	1.36	145.60	70	15775
154	12	1.59	74.96	33	2365
155	12	1.19	117.47	56	12270
156	0	1.52	113.79	67	9114
157	12	1.49	85.83	44	3398
158	6	1.99	108.76	61	9905
159	12	1.36	76.68	47	2364
160	0	5.22	78.54	51	3997
161	12	1.42	71.90	36	1978
162	0	2.16	33.45	34	310
163	0	1.49	101.63	60	4135
164	9	1.79	50.37	34	1816
165	0	1.63	39.25	36	372
166	12	1.26	99.62	55	5828
167	12	2.33	84.20	51	3102
168	0	2.51	38.21	22	797
169	6	1.29	129.38	57	21228
170	6	2.44	42.38	32	931
171	6	2.00	51.95	37	1371
172	9	1.29	101.57	56	5865
173	6	2.42	62.27	42	3275
174	12	1.40	89.96	41	5856
175	12	1.55	87.31	39	3138
176	6	1.46	141.92	71	9882
177	0	1.73	47.81	26	1162
178	0	1.80	43.44	31	955
179	0	2.22	91.61	65	11736
180	6	1.59	82.19	44	1815
181	0	2.15	53.85	30	1238
182	6	1.40	99.43	49	2987
183	6	1.36	105.42	53	3548
184	9	1.47	80.30	50	4862
185	12	1.09	126.91	68	23502
186	12	1.36	178.95	88	26175
187	12	1.62	147.45	66	18656
188	0	1.74	31.02	27	441
189	6	2.25	96.41	44	3902
190	6	2.26	121.31	57	8643
191	6	2.23	111.98	53	6233
192	6	2.34	100.29	47	4924
193	0	1.58	82.70	51	2981
194	6	1.68	84.25	43	3722
195	0	1.54	88.38	54	3378
196	12	1.57	68.05	43	2282
197	16	1.31	204.92	83	46787
198	6	1.38	104.30	49	5100
199	11	1.54	80.43	45	2983
200	12	1.53	92.90	50	5160
201	6	1.54	102.28	53	7796
202	6	1.41	85.72	45	5599
203	6	1.48	79.86	46	3296
204	12	1.94	64.49	44	2662
205	0	1.16	204.54	90	25934
206	0	1.64	84.07	55	2752
207	6	1.82	62.29	44	2085
208	18	1.23	374.19	119	80544
209	12	1.42	91.57	48	5931
210	12	1.18	85.32	47	5764
211	0	1.61	63.41	37	2023
212	9	1.58	80.93	51	2902
213	0	1.46	65.92	57	2515
214	12	1.30	101.28	56	8675
215	12	1.42	71.18	42	2926
216	6	2.29	29.47	25	511
217	12	1.76	64.90	33	1665
218	6	1.59	69.40	43	2359
219	0	1.59	89.48	44	2011
220	0	1.76	42.91	32	997
221	18	1.03	138.86	67	20947
222	9	1.60	53.82	39	2409
223	6	1.12	84.67	47	9618
224	0	2.00	10.00	16	42
225	6	1.31	101.74	50	5421
226	6	1.67	84.52	38	3726
227	0	1.79	38.28	32	897
228	0	1.96	116.00	67	11488
229	11	1.27	107.94	52	9815
230	0	1.45	107.41	57	4757

231	6	2.28	44.47	36	1544
232	6	2.01	47.59	38	2197
233	6	2.01	47.59	37	2197
234	12	1.21	92.16	52	5998
235	6	1.43	71.63	52	2888
236	0	1.54	88.56	56	3379
237	12	1.51	67.21	42	2482
238	12	1.60	68.67	42	2176
239	12	1.57	84.21	53	8059
240	10	1.54	58.38	41	2849
241	6	2.33	29.66	27	489
242	6	2.01	52.60	31	1403
243	12	1.35	102.48	55	8420
244	6	1.38	90.20	51	4299
245	21	1.08	140.72	65	19937
246	11	1.36	124.69	56	18021
247	6	1.47	61.23	42	2468
248	5	1.92	62.51	43	5567
249	12	1.59	80.95	48	3929
250	12	1.17	213.77	91	37489
251	9	0.96	118.32	61	13856
252	12	1.31	234.83	101	66714
253	9	1.36	64.87	41	3086
254	6	1.62	58.98	44	2570
255	6	1.13	85.07	46	9223
256	12	1.27	100.67	68	25807
257	12	1.16	238.43	103	54001
258	6	1.34	76.86	46	3869
259	12	1.54	68.23	39	2383
260	6	1.46	140.91	66	13191
261	6	2.26	52.80	38	2571
262	6	1.59	116.19	55	6183
263	0	1.37	125.98	65	6609
264	0	1.71	47.74	29	1222
265	11	1.85	51.45	29	1646
266	6	2.18	26.63	19	340
267	6	1.90	79.24	47	4644
268	9	1.87	64.59	42	2986
269	6	1.66	45.77	31	791
270	0	1.71	311.87	129	68684
271	18	1.50	105.84	59	9074
272	0	1.34	317.64	127	91348
273	6	1.27	107.94	56	9815
274	6	2.38	45.53	35	1416
275	18	1.12	143.62	79	25125
276	0	1.60	82.95	49	2882
277	0	1.35	78.11	52	2370
278	0	1.87	36.83	22	444
279	12	1.30	94.03	54	5138
280	10	1.35	89.45	52	6331
281	11	1.27	52.19	33	1638
282	12	1.35	190.23	78	39510
283	6	1.70	68.56	43	3768
284	6	2.33	53.14	36	2397
285	0	1.84	80.86	45	2928
286	6	1.87	62.11	45	1982
287	0	1.58	123.15	67	12017
288	6	1.48	23.05	22	258
289	6	1.65	133.28	71	30548
290	12	0.98	93.07	51	9626
291	17	1.55	87.31	38	3138
292	12	1.35	109.06	55	8473
293	6	1.63	76.32	55	3474
294	12	1.33	101.07	55	5724
295	6	1.85	70.18	40	3232
296	12	1.50	101.84	52	8230
297	6	1.65	58.78	41	2398
298	6	1.35	69.87	45	3219
299	12	1.08	122.89	61	15902
300	24	1.14	234.20	92	28021
301	0	3.50	20.95	25	300
302	6	1.40	146.28	69	15106
303	12	1.59	433.95	143	212193
304	6	2.03	66.20	48	2486
305	12	1.78	129.58	72	19459
306	15	1.09	371.16	125	55265
307	15	1.09	381.04	124	57408
308	12	1.71	84.08	41	3477
309	0	1.78	61.24	34	2197

310	12	1.00	106.52	53	11279
311	6	1.66	82.87	48	3784
312	0	4.88	89.78	50	7512
313	6	1.29	128.29	57	12000
314	0	1.50	108.54	46	8949
315	6	1.34	382.23	147	132966
316	6	3.24	298.23	127	129339
317	0	1.01	396.77	152	237349
318	0	2.18	83.55	46	3625
319	0	1.67	126.50	49	11193
320	0	1.67	126.63	49	11229
321	6	2.22	60.65	34	3962
322	0	5.82	151.13	79	19551
323	0	5.63	143.01	78	18551
324	0	0.73	405.55	152	243690
325	0	2.48	42.85	30	923
326	0	4.47	82.38	55	7779
327	6	2.60	114.67	68	14030
328	0	4.72	92.39	61	9424
329	0	2.58	104.90	62	11079
330	0	4.84	93.75	63	9073
331	0	4.02	70.97	51	6803
332	6	2.71	110.34	65	12230
333	0	2.57	90.29	59	8162
334	0	4.47	82.38	55	7779
335	0	4.68	88.30	58	8341
336	6	2.65	115.84	66	13626
337	0	4.78	93.09	58	9234
338	0	4.84	97.79	61	10346
339	0	4.62	87.48	60	8505
340	0	4.72	92.39	63	9424
341	0	4.78	93.09	63	9234
342	6	3.24	298.23	127	129339
343	6	1.41	140.73	75	24154
344	0	2.48	42.85	30	923
345	0	4.84	251.38	114	165389
346	12	1.98	155.23	74	22779
347	11	1.71	69.05	36	3824
348	11	1.66	84.51	37	3866
349	11	1.62	73.38	37	4688
350	11	1.66	84.51	39	3866
351	5	2.01	78.19	42	3130
352	11	1.62	90.18	40	4479
353	10	1.75	79.45	36	3222
354	10	1.64	60.09	30	2556
355	0	3.16	88.41	39	3934
356	6	2.39	208.13	92	32669
357	0	1.52	124.17	50	13562
358	0	1.99	102.33	51	7293
359	6	2.61	379.16	120	143259
360	0	1.89	32.00	17	382
361	6	1.17	151.61	68	24745
362	12	1.21	174.65	79	27362
363	10	2.07	79.48	34	2885
364	21	1.00	229.73	101	55155
365	6	1.41	140.73	75	24154
366	12	1.43	196.01	94	54242
367	5	2.00	64.14	36	1777
368	0	1.12	340.59	148	192061
369	12	1.92	154.98	57	25012
370	0	1.79	48.41	31	1101
371	21	0.99	163.04	78	30042
372	18	1.22	249.12	109	65102
373	12	1.27	101.45	57	12847
374	0	1.50	108.54	45	8949
375	0	1.56	117.41	76	12495
376	0	1.66	90.04	40	4050
377	6	1.42	135.54	57	23110
378	12	1.49	317.63	119	105496
379	6	2.29	61.66	38	3694
380	24	1.37	188.38	80	20870
381	0	1.78	83.97	39	5907
382	0	1.73	58.96	36	1622
383	0	2.04	73.08	38	2648
384	12	1.79	336.29	117	137820
385	6	2.24	292.55	111	102067
386	6	1.29	76.06	43	2609
387	5	2.19	40.97	26	581
388	6	2.70	128.52	68	16793

389	6	2.46	107.11	48	12379
390	6	2.13	211.05	98	45505
391	6	1.79	217.05	97	41566
392	6	2.09	160.04	83	24570
393	6	1.11	200.69	88	37314
394	0	5.51	139.59	66	19183
395	0	1.69	103.94	44	10823
396	6	1.94	57.72	34	1678
397	0	2.68	64.53	43	2720
398	0	3.40	404.43	157	265204
399	6	2.93	179.96	76	38432
400	6	2.86	197.51	92	50355
401	12	1.44	101.33	55	9110
402	6	1.44	168.54	65	22172
403	6	2.96	314.72	127	179715
404	0	1.71	58.87	32	1626
405	0	1.65	63.95	34	1939
406	12	1.52	73.02	43	7440
407	16	1.63	177.81	84	27559
408	0	1.86	187.26	77	21759
409	0	4.04	40.11	25	1192
410	0	1.90	76.97	45	3294
411	6	1.85	209.42	87	76889
412	12	2.45	464.00	155	323430
413	6	1.69	270.64	117	90120
414	6	2.13	211.05	98	45505
415	12	1.76	340.27	129	145958
416	0	2.11	82.64	46	3781
417	0	2.78	142.09	67	20112
418	12	1.96	162.87	76	29982
419	12	2.22	225.07	102	51126
420	6	2.75	173.43	88	37653
421	12	1.88	546.24	175	515774
422	18	1.24	483.11	165	390252
423	12	2.26	367.38	145	205867
424	18	1.48	431.43	159	299373
425	0	1.54	102.71	44	8008
426	0	2.92	52.40	55	7128
427	0	2.92	52.40	55	7128
428	0	3.67	107.06	75	30801
429	0	2.09	40.39	28	645
430	12	1.12	157.86	68	20019
431	18	1.42	218.55	96	50442
432	12	1.27	212.74	90	49938
433	12	1.46	295.47	119	101480
434	12	1.45	285.06	118	99478
435	12	1.46	295.47	119	101480
436	32	1.07	231.02	90	34476
437	12	1.16	238.43	103	54001
438	6	1.64	199.15	81	38910
439	15	1.36	92.48	49	9271
440	12	0.98	597.59	208	1375648
441	18	1.69	242.04	103	66511
442	6	1.99	80.91	61	11018
443	6	2.19	216.27	87	52242
444	10	1.20	303.18	122	110487
445	6	1.44	201.48	81	35971
446	12	1.46	357.01	135	152540
447	0	4.28	76.95	54	7220
448	0	4.84	97.79	60	10346
449	9	1.97	129.76	70	15742
450	0	1.96	92.94	52	5157
451	0	1.49	130.27	50	14968
452	17	1.48	135.83	58	16321
453	0	1.03	190.27	71	41698
454	0	2.96	67.27	34	2218
455	27	1.16	385.73	132	160052
456	9	1.58	256.82	111	83319
457	12	2.09	212.70	96	56002
458	18	1.69	258.46	92	73300
459	6	1.31	208.96	93	46804
460	0	1.35	78.11	54	2370
461	12	2.03	158.34	78	26195
462	6	2.29	74.61	42	5646
463	18	1.35	130.71	61	18875
464	0	3.36	112.96	90	47046
465	6	2.30	75.81	41	5583
466	6	3.07	207.15	85	49985
467	0	0.97	194.20	74	48975

468	18	1.68	232.96	101	64600
469	18	1.68	232.96	101	64600
470	12	1.27	126.76	65	21398
471	6	3.15	339.36	135	197354
472	0	3.81	32.11	23	743
473	0	2.54	46.69	29	1267
474	0	1.52	124.17	49	13562
475	6	1.64	182.62	78	28067
476	6	1.58	128.82	62	12382
477	6	2.94	174.97	83	32640
478	0	3.00	161.12	81	25491
479	12	1.75	125.24	63	19904
480	0	2.54	46.69	30	1267
481	12	1.42	626.17	188	970412
482	11	1.22	152.60	59	21826
483	18	1.32	186.16	81	29782
484	12	1.68	195.28	93	34890
485	20	1.40	130.77	68	9329
486	0	2.78	31.52	38	1820
487	0	2.53	46.26	26	1270
488	18	1.65	255.25	98	75968
489	0	1.86	64.88	35	3004
490	12	1.25	153.22	72	18772
491	6	2.51	87.58	57	6745
492	5	1.65	63.95	35	1939
493	9	1.49	100.99	52	8634
494	0	1.47	111.59	59	22065
495	0	1.47	152.16	62	23741
496	0	1.78	90.22	40	6353
497	12	2.07	332.79	125	209084
498	12	1.90	82.22	32	2671
499	0	1.59	69.09	35	2276
500	20	1.32	290.41	119	125247
501	0	1.46	128.38	77	8730
502	16	1.49	73.19	36	2732
503	0	1.58	82.50	38	4283
504	0	4.57	104.77	72	15090
505	0	4.54	95.69	64	11584
506	12	1.41	103.20	46	7424
507	24	1.26	206.01	84	28198
508	0	2.01	50.48	29	885
509	0	1.81	75.78	37	3839
510	0	2.47	42.79	33	917
511	17	0.74	239.88	115	88065
512	0	1.50	94.82	48	8062
513	24	1.05	282.74	98	65748
514	18	1.06	205.41	84	30637
515	12	1.37	110.11	55	10995
516	0	2.11	82.64	46	3781
517	6	2.51	114.76	52	14988
518	0	1.53	88.01	40	4873
519	0	4.68	88.30	60	8341
520	6	2.26	278.49	110	95098
521	0	4.07	59.25	36	3756
522	0	2.48	42.85	30	923
523	18	1.16	143.76	64	22962
524	0	1.49	130.27	50	14968
525	0	1.77	196.60	74	32501
526	0	1.49	130.27	51	14968
527	12	1.15	109.87	52	12556
528	17	1.27	156.00	57	27066
529	16	1.21	124.04	55	12564
530	0	2.20	244.88	97	66890
531	0	1.47	45.38	33	1663
532	0	2.04	52.91	31	1363
533	0	1.14	151.91	62	24994
534	6	1.38	130.54	70	18142
535	0	1.74	91.81	47	9004
536	12	1.58	269.87	103	58939
537	0	1.86	64.88	34	3004
538	0	1.82	70.13	37	3438
539	0	1.20	252.76	84	69656
540	0	1.58	82.50	39	4283
541	0	1.65	63.95	33	1939
542	0	2.11	82.64	46	3781
543	0	2.40	136.05	62	10195
544	0	1.74	91.81	46	9004
545	0	1.61	73.80	37	4628
546	6	3.52	364.39	142	174327

547	0	1.32	305.10	117	136840
548	0	3.42	111.96	44	6027
549	0	3.26	139.18	55	12013
550	0	1.98	71.98	35	2888
551	0	1.97	65.93	34	2663
552	0	1.98	71.98	34	2888
553	10	1.36	71.70	41	2154
554	0	1.52	124.17	49	13562
555	6	2.19	40.82	27	1109
556	0	2.82	103.42	61	8671
557	6	1.57	76.32	43	3967
558	0	2.97	93.25	41	4715
559	0	2.97	93.25	41	4715
560	0	2.03	87.70	49	4446
561	0	1.10	282.68	114	100180
562	0	1.10	282.68	112	100180
563	0	0.94	270.45	93	106238
564	17	1.51	100.57	42	8194
565	0	1.74	74.12	37	3896
566	6	1.64	59.74	39	2640
567	0	2.07	88.03	41	4264
568	5	1.55	68.30	39	2420
569	12	1.53	107.14	46	6109
570	6	2.00	89.39	50	14215
571	12	1.69	187.19	83	26337
572	18	1.37	132.20	57	18164
573	6	1.51	265.71	126	68267
574	18	1.69	242.04	102	66511
575	18	1.69	242.04	102	66511
576	9	1.76	42.96	28	1018
577	6	3.10	288.15	128	126789
578	22	1.00	157.06	72	27199
579	0	1.70	413.02	157	298931
580	12	0.88	193.47	85	45888
581	0	1.90	77.03	45	3329
582	6	1.38	117.01	64	9185
583	0	1.91	71.24	45	3017
584	18	1.47	110.48	51	9404
585	12	2.41	232.41	85	44752
586	12	1.76	340.27	129	145958
587	6	1.45	345.85	135	151365
588	12	1.60	145.48	64	18510
589	0	5.42	156.47	74	27993
590	9	1.44	453.08	166	340338
591	9	1.62	140.59	69	17307
592	0	1.47	45.38	34	1663
593	0	1.26	316.97	119	102877
594	0	2.87	71.88	40	2576
595	0	4.03	54.45	44	3169
596	6	1.93	65.70	39	2768
597	6	1.78	155.36	59	8926
598	0	1.98	52.71	31	1456
599	12	2.26	353.24	135	202813
600	12	1.34	356.19	135	228630
601	6	1.74	286.90	126	90521
602	6	1.06	546.60	189	544843
603	12	1.60	145.48	64	18510
604	12	1.47	107.46	50	9455
605	0	5.54	215.48	110	68107
606	6	1.05	445.52	163	298673
607	6	1.54	138.07	68	19189
608	6	1.76	248.04	108	60477
609	6	2.80	152.11	85	24548
610	0	5.47	197.23	101	53716
611	6	1.50	143.65	69	21572
612	18	1.39	110.13	50	7642
613	0	5.54	215.48	110	68107
614	12	1.72	126.93	61	20682
615	0	1.71	84.45	39	3542
616	6	2.22	312.99	130	128880
617	12	1.41	106.24	50	10067
618	12	1.70	119.74	58	19847
619	0	6.36	309.82	133	132987
620	0	2.15	98.26	52	5805
621	0	2.92	52.40	53	7128
622	6	2.66	171.65	88	40971
623	6	2.77	185.56	94	45328
624	6	2.88	192.82	96	47923
625	6	2.87	215.84	104	68630

626	6	2.96	230.55	110	75321		
627	6	2.84	223.05	110	72358		
628	6	2.96	238.54	112	78287		
629	6	2.75	184.77	97	45766		
630	6	3.04	244.47	115	82795		
631	6	2.93	254.50	111	102934		
	plattindex	randicindex	ringCount	szegedindex	wienerpolarity	DG_NHA	DG_MW
1	330	38.76	4	11511	86	-0.22	-0.02
2	60	8.48	1	294	14	-0.87	-0.05
3	116	14.60	3	955	32	-0.40	-0.03
4	234	24.85	4	3216	66	-0.46	-0.03
5	44	6.63	2	185	12	-0.61	-0.04
6	126	16.02	4	1613	40	-0.27	-0.02
7	142	17.93	1	873	21	-0.75	-0.05
8	126	11.94	3	352	15	-0.62	-0.05
9	66	10.56	1	518	21	-0.51	-0.03
10	74	9.42	0	114	6	-0.75	-0.05
11	220	26.26	3	3952	50	-0.28	-0.01
12	162	19.43	3	1385	35	-0.63	-0.05
13	186	23.24	2	2608	47	-0.34	-0.02
14	166	21.03	3	2562	39	-0.42	-0.03
15	78	10.12	1	189	9	-0.87	-0.06
16	258	30.68	3	4538	50	-0.34	-0.02
17	146	18.13	2	1395	33	-0.32	-0.02
18	142	16.68	4	1669	40	-0.58	-0.04
19	216	25.64	4	6189	59	-0.18	-0.01
20	268	30.91	3	5056	57	-0.29	-0.02
21	218	25.06	4	4951	46	-0.26	-0.02
22	244	28.93	5	6085	51	-0.36	-0.03
23	142	17.93	1	1142	21	-0.56	-0.04
24	170	20.21	4	3141	47	-0.38	-0.03
25	172	19.23	3	1373	32	-0.66	-0.05
26	100	12.46	0	344	10	-0.43	-0.03
27	194	22.57	4	3090	47	-0.30	-0.02
28	86	11.60	1	438	17	-0.63	-0.04
29	188	21.17	4	1805	35	-0.54	-0.04
30	234	24.85	4	3180	70	-0.48	-0.03
31	148	19.23	2	3158	47	-0.33	-0.02
32	238	30.46	4	7212	64	-0.29	-0.02
33	166	18.93	2	1578	38	-0.59	-0.04
34	186	21.04	2	1354	31	-0.29	-0.02
35	326	32.49	7	5957	86	-0.19	-0.01
36	120	14.74	1	589	20	-0.58	-0.04
37	238	25.50	4	3770	42	-0.36	-0.03
38	270	30.48	4	4867	57	-0.24	-0.02
39	86	10.58	2	423	25	-0.45	-0.03
40	186	24.34	5	5035	54	-0.41	-0.03
41	106	12.57	1	320	19	-0.91	-0.06
42	86	10.58	0	139	7	-1.23	-0.08
43	140	17.99	3	2432	41	-0.26	-0.02
44	238	29.41	2	4176	52	-0.37	-0.03
45	120	15.97	3	1383	37	-0.32	-0.02
46	128	16.09	1	877	24	-0.34	-0.02
47	134	16.79	2	1042	25	-0.67	-0.05
48	146	17.76	3	1636	33	-0.58	-0.04
49	50	6.95	2	241	13	-0.68	-0.04
50	110	14.49	1	693	18	-0.35	-0.02
51	164	18.68	4	2237	43	-0.18	-0.01
52	222	26.81	3	5082	49	-0.33	-0.02
53	166	19.92	3	1925	39	-0.52	-0.04
54	472	51.63	3	15073	104	-0.11	-0.01
55	106	13.53	1	612	21	-0.35	-0.02
56	200	25.37	3	3550	43	-0.43	-0.03
57	168	19.77	3	1562	37	-0.53	-0.04
58	110	14.65	3	1578	39	-0.56	-0.04
59	80	10.34	2	437	17	-0.85	-0.05
60	146	19.36	4	1882	44	-0.26	-0.02
61	158	18.79	4	1973	41	-0.43	-0.03
62	180	19.00	5	2007	51	-0.39	-0.03
63	162	19.22	4	1679	40	-0.43	-0.03
64	254	29.92	5	8110	81	-0.19	-0.01
65	216	23.25	0	883	15	-0.44	-0.03
66	156	18.56	3	1230	34	-0.65	-0.05
67	222	22.96	4	1999	50	-0.32	-0.02
68	234	24.85	4	3180	70	-0.35	-0.03
69	176	18.19	4	1240	38	-0.44	-0.03
70	116	14.95	3	1237	36	-0.57	-0.04
71	74	9.39	2	532	22	-0.50	-0.03
72	196	23.44	2	2348	36	-0.25	-0.02

73	98	13.71	2	1054	27	-0.44	-0.03
74	176	21.07	4	3243	53	-0.40	-0.03
75	124	17.25	2	1198	30	-0.72	-0.05
76	136	17.93	2	1198	30	-0.75	-0.06
77	328	35.48	8	10230	88	-0.29	-0.02
78	198	24.25	3	3093	50	-0.22	-0.02
79	140	17.67	2	1024	24	-0.57	-0.04
80	292	33.15	4	6054	60	-0.36	-0.03
81	156	20.12	2	1804	28	-0.35	-0.03
82	200	24.43	2	4082	35	-0.36	-0.02
83	210	24.04	5	4322	49	-0.38	-0.03
84	70	9.94	1	248	13	-0.97	-0.07
85	134	15.11	2	918	33	-0.67	-0.04
86	216	25.90	5	6448	59	-0.38	-0.03
87	256	30.48	5	8622	83	-0.18	-0.01
88	186	22.32	4	3654	43	-0.34	-0.02
89	142	17.96	3	1388	29	-0.57	-0.04
90	98	12.21	1	281	16	-0.83	-0.06
91	202	23.97	2	2247	38	-0.36	-0.03
92	128	15.44	4	1107	36	-0.55	-0.04
93	84	11.72	1	372	17	-0.67	-0.05
94	316	34.76	8	10230	88	-0.15	-0.01
95	460	50.49	3	14528	101	-0.12	-0.01
96	184	19.24	4	1536	39	-0.67	-0.05
97	176	18.33	4	1536	39	-0.65	-0.05
98	100	13.82	1	1012	29	-0.35	-0.02
99	26	3.81	0	4	0	-2.21	-0.14
100	188	20.30	4	1925	46	-0.59	-0.04
101	90	11.61	2	645	22	-0.79	-0.05
102	294	32.92	7	9870	83	-0.17	-0.01
103	154	19.34	2	1930	45	-0.22	-0.01
104	160	20.33	2	2436	37	-0.29	-0.02
105	198	23.25	3	2538	36	-0.51	-0.04
106	282	33.71	4	7602	64	-0.17	-0.01
107	178	20.77	2	2970	36	-0.26	-0.02
108	118	15.56	3	1307	30	-0.61	-0.04
109	36	5.46	1	144	10	-0.70	-0.05
110	140	17.69	2	1634	30	-0.56	-0.04
111	226	22.81	4	2204	58	-0.42	-0.03
112	214	24.64	4	4387	49	-0.26	-0.02
113	182	22.06	3	2632	48	-0.40	-0.03
114	104	14.05	2	1002	27	-0.38	-0.03
115	358	37.64	4	9987	70	-0.31	-0.02
116	110	12.42	1	274	15	-0.20	-0.01
117	190	21.62	4	2883	51	-0.20	-0.01
118	104	12.99	2	796	31	-0.35	-0.02
119	142	17.30	1	873	24	-0.40	-0.03
120	224	26.79	3	5456	49	-0.24	-0.02
121	188	20.56	4	1982	39	-0.56	-0.04
122	188	21.14	4	2693	49	-0.24	-0.02
123	64	10.09	1	444	17	-0.82	-0.05
124	134	15.35	1	512	16	-0.41	-0.03
125	182	21.69	3	3058	39	-0.49	-0.03
126	234	24.27	4	2759	59	-0.45	-0.03
127	172	17.63	5	1790	49	-0.26	-0.02
128	116	14.37	1	572	19	-0.32	-0.02
129	220	25.15	2	2352	34	-0.34	-0.02
130	246	30.50	5	8302	56	-0.17	-0.01
131	168	19.77	3	1385	35	-0.58	-0.04
132	348	40.54	5	10287	68	-0.30	-0.02
133	142	18.52	3	2137	42	-0.21	-0.01
134	230	26.67	5	4516	51	-0.15	-0.01
135	50	7.77	1	184	11	-0.54	-0.04
136	108	14.22	1	544	19	-0.67	-0.05
137	330	38.79	7	18445	81	-0.18	-0.01
138	120	13.98	2	640	28	-0.61	-0.04
139	242	28.44	5	6879	56	-0.30	-0.02
140	110	14.96	2	1092	28	-0.34	-0.03
141	92	11.63	2	548	20	-0.30	-0.02
142	72	10.66	2	710	25	-0.35	-0.02
143	138	17.46	3	2248	36	-0.51	-0.03
144	266	30.80	2	3865	39	-0.25	-0.02
145	188	20.14	4	1866	42	-0.59	-0.04
146	96	11.13	1	209	15	-0.27	-0.02
147	232	26.51	4	4762	59	-0.32	-0.02
148	78	11.43	1	451	18	-0.50	-0.04
149	176	18.29	4	1436	39	-0.67	-0.05
150	138	16.79	1	702	23	-0.36	-0.03
151	72	7.50	1	282	21	-0.34	-0.01

152	198	22.38	4	2587	45	-0.49	-0.04
153	248	29.73	4	5135	60	-0.34	-0.02
154	106	14.30	3	1367	38	-0.65	-0.04
155	190	23.86	4	3815	46	-0.39	-0.03
156	258	27.91	3	3450	47	-0.36	-0.03
157	154	18.36	4	1959	41	-0.49	-0.03
158	220	26.26	2	2649	40	-0.45	-0.03
159	174	19.43	4	1782	40	-0.32	-0.02
160	184	22.33	0	1180	34	-0.40	-0.03
161	124	15.09	4	1190	37	-0.64	-0.04
162	138	13.90	2	238	21	-0.68	-0.05
163	242	24.40	4	2540	57	-0.52	-0.04
164	116	14.59	2	770	22	-0.81	-0.06
165	150	14.44	3	504	21	-0.66	-0.05
166	200	22.88	4	2900	44	-0.30	-0.02
167	180	21.87	2	1404	39	-0.54	-0.04
168	72	9.67	1	347	17	-0.79	-0.05
169	186	24.90	3	5654	51	-0.47	-0.03
170	108	14.05	1	508	22	-0.47	-0.03
171	134	15.71	2	750	24	-0.68	-0.05
172	206	23.28	4	2849	48	-0.48	-0.04
173	146	18.21	1	1136	29	-0.47	-0.03
174	136	17.65	3	2128	35	-0.25	-0.02
175	130	16.43	4	1786	43	-0.49	-0.03
176	270	29.21	5	4848	65	-0.41	-0.03
177	82	11.43	2	717	24	-0.58	-0.04
178	108	13.36	2	620	22	-0.66	-0.05
179	246	27.72	1	2401	34	-0.22	-0.02
180	168	17.85	5	1790	49	-0.61	-0.04
181	100	12.98	2	860	29	-0.69	-0.05
182	186	20.04	5	2485	58	-0.54	-0.04
183	210	21.19	6	2761	59	-0.52	-0.04
184	186	20.82	3	1881	34	-0.54	-0.04
185	244	28.57	4	5553	48	-0.34	-0.02
186	324	37.14	4	7517	63	-0.30	-0.02
187	226	28.29	3	5288	57	-0.28	-0.02
188	98	11.36	2	291	14	-0.83	-0.06
189	148	19.00	2	1898	45	-0.35	-0.02
190	198	24.45	2	3193	49	-0.23	-0.02
191	184	22.75	2	2558	48	-0.28	-0.02
192	160	20.25	2	2202	45	-0.27	-0.02
193	204	20.81	4	1925	46	-0.58	-0.04
194	152	18.18	3	2048	41	-0.18	-0.01
195	216	22.06	4	2112	49	-0.47	-0.03
196	150	18.22	3	1230	34	-0.61	-0.05
197	286	35.58	4	12299	80	-0.30	-0.02
198	178	20.33	4	3098	51	-0.13	-0.01
199	160	18.66	4	1662	38	-0.47	-0.03
200	172	21.34	3	2207	41	-0.41	-0.03
201	192	22.52	3	2675	46	-0.42	-0.03
202	152	19.11	3	2061	39	-0.31	-0.02
203	170	18.96	4	1610	38	-0.56	-0.04
204	152	18.89	2	1144	27	-0.36	-0.03
205	352	37.31	6	9773	94	-0.25	-0.02
206	226	22.19	4	1880	48	-0.45	-0.03
207	160	18.60	2	980	29	-0.64	-0.05
208	430	50.15	7	24136	129	-0.09	-0.01
209	160	20.48	3	2610	42	-0.14	-0.01
210	168	19.60	4	2286	35	-0.59	-0.04
211	132	15.70	3	909	32	-0.90	-0.06
212	194	20.87	4	1879	39	-0.56	-0.04
213	234	23.15	3	1261	27	-0.39	-0.03
214	202	23.43	4	3418	43	-0.29	-0.02
215	142	17.98	3	1342	28	-0.60	-0.04
216	82	11.18	1	297	14	-0.75	-0.05
217	108	14.24	3	951	32	-0.34	-0.03
218	158	17.89	3	1145	36	-0.57	-0.04
219	178	17.58	5	1343	54	-0.34	-0.02
220	118	13.43	2	424	19	-0.49	-0.04
221	240	28.05	5	5913	54	-0.33	-0.02
222	136	16.77	2	887	22	-0.65	-0.05
223	162	20.02	3	2743	33	-0.33	-0.02
224	60	6.81	1	54	3	-0.91	-0.06
225	176	20.94	4	2515	47	-0.45	-0.03
226	124	16.40	3	1902	42	-0.28	-0.02
227	118	13.44	2	479	17	-0.88	-0.06
228	250	28.64	2	3530	46	-0.23	-0.02
229	178	21.91	4	3779	47	-0.50	-0.04
230	222	23.60	4	2759	59	-0.46	-0.03

231	126	15.61	1	614	20	-0.39	-0.03
232	132	16.52	1	774	21	-0.48	-0.03
233	128	16.09	1	774	21	-0.36	-0.03
234	188	21.62	4	2736	40	-0.32	-0.02
235	200	21.60	3	1264	30	-0.37	-0.03
236	228	22.59	4	2117	48	-0.65	-0.05
237	146	17.76	3	1448	31	-0.31	-0.02
238	146	17.76	3	1403	33	-0.61	-0.04
239	184	22.91	2	2272	32	-0.33	-0.02
240	142	17.69	2	1160	25	-0.72	-0.05
241	92	11.89	1	283	15	-0.67	-0.05
242	100	13.53	2	832	26	-0.71	-0.05
243	194	23.13	4	3233	45	-0.26	-0.02
244	186	21.28	4	2296	42	-0.36	-0.03
245	224	27.52	5	5768	54	-0.41	-0.03
246	188	24.24	3	4644	48	-0.26	-0.02
247	158	17.35	3	1005	27	-0.78	-0.06
248	148	18.67	1	1312	22	-0.44	-0.03
249	168	20.37	3	1748	33	-0.53	-0.04
250	338	37.55	6	12370	84	-0.19	-0.01
251	228	25.00	5	4686	51	-0.45	-0.03
252	354	43.23	4	11931	69	-0.30	-0.02
253	142	17.32	3	1209	25	-0.57	-0.04
254	162	18.54	2	989	25	-0.54	-0.04
255	156	19.68	3	2607	33	-0.40	-0.03
256	242	29.33	2	4437	37	-0.35	-0.03
257	376	43.48	5	12982	77	-0.29	-0.02
258	174	18.94	4	1572	35	-0.62	-0.05
259	138	16.47	3	1442	34	-0.67	-0.04
260	240	27.46	4	4838	59	-0.37	-0.03
261	134	16.51	1	946	21	-0.35	-0.02
262	206	22.80	4	3170	55	-0.24	-0.02
263	262	26.19	5	3654	61	-0.39	-0.03
264	100	12.47	2	643	23	-0.28	-0.02
265	94	12.63	2	731	22	-0.65	-0.04
266	60	8.53	1	236	13	-0.75	-0.05
267	170	19.95	2	1606	34	-0.30	-0.02
268	150	17.82	2	1162	27	-0.58	-0.04
269	110	12.94	3	750	25	-0.73	-0.06
270	490	54.14	4	23036	105	-0.22	-0.02
271	200	25.33	3	3104	41	-0.45	-0.03
272	478	53.04	5	22149	109	-0.11	-0.01
273	202	23.28	4	3779	47	-0.40	-0.03
274	120	15.47	1	619	19	-0.35	-0.03
275	286	33.47	4	6506	58	-0.29	-0.02
276	194	19.89	4	2094	45	-0.31	-0.02
277	212	21.00	4	1683	44	-0.58	-0.04
278	74	9.37	2	352	22	-0.61	-0.04
279	196	22.44	4	2640	42	-0.34	-0.02
280	186	21.98	3	1980	35	-0.38	-0.03
281	116	13.84	3	878	23	-0.54	-0.03
282	276	33.13	4	10007	71	-0.36	-0.03
283	156	18.23	2	1323	31	-0.26	-0.02
284	126	15.61	1	853	23	-0.30	-0.02
285	174	18.44	3	1348	35	-0.16	-0.01
286	166	19.04	2	1038	30	-0.41	-0.03
287	250	28.22	3	3391	48	-0.38	-0.03
288	78	9.37	2	182	10	-0.94	-0.07
289	256	30.55	2	5491	47	-0.19	-0.01
290	182	21.32	4	2999	39	-0.42	-0.03
291	126	16.02	4	1786	43	-0.55	-0.04
292	200	22.83	4	3582	46	-0.29	-0.02
293	212	22.85	3	1552	33	-0.62	-0.05
294	204	22.62	5	2338	41	-0.26	-0.02
295	130	17.37	2	1466	33	-0.77	-0.06
296	172	22.31	3	3180	47	-0.54	-0.04
297	140	17.66	2	1030	23	-0.61	-0.05
298	158	19.04	3	1356	27	-0.59	-0.04
299	218	25.59	4	4911	53	-0.29	-0.02
300	330	38.26	7	17576	90	-0.20	-0.01
301	92	10.98	0	131	10	-0.45	-0.03
302	252	28.71	4	5313	61	-0.33	-0.02
303	500	61.82	4	44246	113	-0.17	-0.01
304	178	20.29	2	1170	30	-0.55	-0.04
305	256	30.77	2	4706	55	-0.30	-0.02
306	474	51.25	9	20687	140	-0.17	-0.01
307	468	50.95	9	21439	142	-0.14	-0.01
308	136	17.69	3	1828	38	-0.27	-0.02
309	116	14.22	2	989	29	-0.25	-0.02

310	190	21.91	5	3723	44	-0.38	-0.03
311	170	20.23	3	1649	36	-0.48	-0.04
312	174	22.27	0	1828	33	-0.23	-0.02
313	208	23.92	4	4194	54	-0.35	-0.03
314	156	19.95	3	2720	44	-0.32	-0.02
315	552	61.75	5	35462	118	-0.20	-0.01
316	454	55.08	1	18512	85	-0.18	-0.01
317	582	63.30	6	29316	118	-0.09	-0.01
318	166	20.11	2	1511	43	-0.11	-0.01
319	164	21.41	3	3325	47	-0.29	-0.02
320	164	21.41	3	3325	47	-0.28	-0.02
321	114	15.10	1	1233	24	-0.26	-0.02
322	292	34.13	0	4130	59	-0.34	-0.02
323	290	33.57	0	3910	54	-0.31	-0.02
324	602	61.63	10	30025	123	-0.08	-0.01
325	106	13.27	1	518	23	-0.28	-0.02
326	196	24.25	0	1766	32	-0.39	-0.03
327	242	29.62	1	3272	40	-0.31	-0.02
328	220	26.65	0	2126	34	-0.36	-0.02
329	220	27.03	1	2546	36	-0.32	-0.02
330	230	27.44	0	2080	36	-0.34	-0.02
331	182	22.44	0	1506	27	-0.35	-0.02
332	230	28.37	1	2962	39	-0.33	-0.02
333	218	25.40	1	1927	35	-0.28	-0.02
334	196	24.25	0	1766	32	-0.40	-0.03
335	208	25.50	0	1910	34	-0.37	-0.03
336	232	28.91	1	3296	41	-0.29	-0.02
337	206	25.55	0	2102	34	-0.36	-0.02
338	218	26.80	0	2321	35	-0.36	-0.03
339	218	26.19	0	1933	33	-0.41	-0.03
340	230	27.44	0	2126	34	-0.40	-0.03
341	230	27.44	0	2102	34	-0.30	-0.02
342	454	55.08	1	18512	85	-0.18	-0.01
343	268	31.00	3	5802	51	-0.33	-0.02
344	106	13.27	1	518	23	-0.34	-0.02
345	408	49.58	0	18551	78	-0.19	-0.01
346	264	31.76	2	5470	53	-0.17	-0.01
347	122	15.53	2	1306	29	-0.61	-0.04
348	124	15.76	3	1786	40	-0.59	-0.04
349	124	16.01	2	1526	31	-0.58	-0.04
350	136	16.44	3	1786	40	-0.59	-0.04
351	154	17.68	2	1381	37	-0.59	-0.04
352	138	17.00	3	2015	43	-0.56	-0.03
353	126	15.22	3	1419	36	-0.60	-0.03
354	100	12.98	2	856	24	-0.65	-0.04
355	132	17.67	1	1641	36	-0.25	-0.01
356	336	39.29	2	10121	69	-0.31	-0.02
357	168	21.85	3	3549	48	-0.15	-0.01
358	182	22.37	2	2722	46	-0.25	-0.02
359	416	52.54	2	36929	107	-0.14	-0.01
360	52	7.43	2	295	16	-0.42	-0.02
361	248	28.64	4	6263	61	-0.39	-0.02
362	284	33.27	5	7442	66	-0.38	-0.03
363	112	14.86	2	1568	37	-0.43	-0.03
364	366	42.45	6	12381	74	-0.29	-0.02
365	268	31.00	3	5802	51	-0.37	-0.03
366	336	40.23	3	9780	60	-0.21	-0.01
367	134	15.11	2	918	33	-0.68	-0.04
368	570	61.66	5	24034	100	-0.12	-0.01
369	192	24.94	2	6136	56	-0.24	-0.02
370	110	13.40	2	590	25	-0.39	-0.03
371	282	32.39	6	7718	56	-0.33	-0.02
372	396	46.14	5	15902	80	-0.25	-0.02
373	202	24.43	3	3817	41	-0.30	-0.02
374	152	19.57	3	2720	44	-0.24	-0.02
375	294	31.81	3	3718	49	-0.42	-0.03
376	136	17.30	3	1663	39	-0.24	-0.02
377	188	24.92	3	6061	54	-0.27	-0.02
378	416	51.22	4	18360	97	-0.24	-0.02
379	132	16.58	1	1201	24	-0.44	-0.03
380	274	34.29	5	6986	68	-0.33	-0.02
381	134	17.04	2	1846	33	-0.27	-0.02
382	136	15.01	3	833	30	-0.33	-0.02
383	134	16.33	2	1328	37	-0.29	-0.02
384	400	51.19	3	21457	90	-0.16	-0.01
385	388	48.36	2	16152	85	-0.18	-0.01
386	158	17.72	4	1960	39	-0.64	-0.05
387	90	11.38	2	424	24	-0.31	-0.02
388	246	29.28	1	3988	46	-0.30	-0.02

389	168	20.84	1	3042	43	-0.32	-0.02
390	354	42.06	2	8672	62	-0.21	-0.01
391	360	41.14	3	9017	74	-0.24	-0.02
392	306	35.49	2	5565	53	-0.29	-0.02
393	332	36.58	5	7468	69	-0.10	-0.01
394	230	29.27	0	4004	47	-0.34	-0.02
395	148	19.27	2	2838	39	-0.23	-0.01
396	122	14.48	2	777	28	-0.22	-0.02
397	156	18.62	1	1096	32	-0.38	-0.03
398	576	67.67	1	31951	108	-0.15	-0.01
399	260	33.55	1	7162	57	-0.28	-0.02
400	324	40.26	1	8852	63	-0.28	-0.02
401	194	23.46	3	3264	46	-0.47	-0.03
402	214	28.01	4	6885	63	-0.36	-0.03
403	452	55.37	1	22594	91	-0.19	-0.01
404	110	13.69	3	819	29	-0.38	-0.03
405	118	14.55	3	955	32	-0.16	-0.01
406	140	18.94	2	2126	27	-0.40	-0.03
407	302	35.86	3	6738	64	-0.34	-0.02
408	282	33.10	3	7180	72	-0.13	-0.01
409	80	11.74	0	402	18	-0.52	-0.03
410	164	19.55	2	1554	38	-0.11	-0.01
411	296	38.12	2	13093	67	-0.28	-0.02
412	540	67.86	2	40788	118	-0.12	-0.01
413	426	50.04	3	14450	79	-0.22	-0.02
414	354	42.06	2	8672	62	-0.21	-0.01
415	454	56.04	3	22316	90	-0.15	-0.01
416	166	20.11	2	1744	42	-0.15	-0.01
417	240	29.30	1	4734	52	-0.21	-0.01
418	258	33.33	2	6216	53	-0.27	-0.02
419	364	43.99	2	9918	72	-0.26	-0.02
420	316	38.07	1	6896	60	-0.26	-0.02
421	620	76.02	3	56847	135	-0.10	-0.01
422	590	70.81	5	45743	129	-0.14	-0.01
423	520	62.61	2	27388	103	-0.16	-0.01
424	570	68.26	4	37887	117	-0.14	-0.01
425	148	19.14	3	2463	42	-0.20	-0.01
426	212	23.48	0	1313	17	-0.45	-0.03
427	212	23.48	0	1313	17	-0.39	-0.03
428	286	31.89	0	4478	33	-0.23	-0.01
429	102	11.95	2	438	22	-0.64	-0.04
430	246	28.47	5	6601	65	-0.35	-0.02
431	336	41.15	4	10267	68	-0.27	-0.02
432	316	38.42	4	10044	70	-0.28	-0.02
433	416	51.22	4	17451	88	-0.24	-0.02
434	414	50.66	4	17000	84	-0.25	-0.02
435	416	51.22	4	17451	88	-0.24	-0.02
436	310	38.11	7	11249	82	-0.28	-0.02
437	376	43.48	5	12982	77	-0.28	-0.02
438	282	35.04	3	7888	61	-0.32	-0.02
439	168	20.99	3	2677	38	-0.51	-0.04
440	750	89.04	5	101627	150	-0.11	-0.01
441	358	44.62	3	12354	70	-0.20	-0.01
442	224	25.98	1	2508	30	-0.19	-0.01
443	306	37.94	2	9870	69	-0.20	-0.01
444	440	51.78	5	18920	91	-0.17	-0.01
445	290	34.95	4	10200	80	-0.11	-0.01
446	490	57.64	4	23247	101	-0.15	-0.01
447	194	23.69	0	1624	30	-0.41	-0.03
448	214	26.42	0	2321	35	-0.33	-0.02
449	248	30.28	2	3814	46	-0.28	-0.02
450	190	22.40	2	2196	46	-0.11	-0.01
451	168	21.83	3	3877	50	-0.14	-0.01
452	190	25.27	3	4740	54	-0.17	-0.01
453	248	30.23	5	8717	70	-0.16	-0.01
454	116	15.40	1	1036	31	-0.32	-0.02
455	458	56.64	6	26835	106	-0.08	-0.01
456	404	47.43	3	13450	79	-0.24	-0.02
457	336	41.83	2	10144	67	-0.25	-0.02
458	304	40.55	3	14812	76	-0.22	-0.02
459	346	39.16	4	8712	70	-0.10	-0.01
460	224	21.72	4	1683	44	-0.59	-0.04
461	274	33.82	2	5897	52	-0.30	-0.02
462	144	18.55	1	1688	27	-0.43	-0.03
463	202	26.55	3	5096	51	-0.39	-0.03
464	346	38.24	0	5847	34	-0.11	-0.01
465	134	18.55	1	1586	31	-0.47	-0.03
466	294	37.44	1	9461	64	-0.20	-0.01
467	258	31.64	5	9215	71	-0.18	-0.01

468	352	43.69	3	11949	67	-0.23	-0.02
469	352	43.69	3	11949	67	-0.24	-0.02
470	224	28.01	3	5286	46	-0.21	-0.02
471	484	58.75	1	24871	95	-0.20	-0.01
472	76	10.60	0	272	14	-0.45	-0.03
473	100	13.03	1	618	23	-0.43	-0.03
474	164	21.41	3	3549	48	-0.15	-0.01
475	274	33.57	3	6253	57	-0.16	-0.01
476	218	26.52	3	3319	44	-0.16	-0.01
477	288	36.48	1	6530	58	-0.27	-0.02
478	298	34.88	1	5043	57	-0.14	-0.01
479	216	27.48	2	4326	42	-0.34	-0.02
480	104	13.41	1	618	23	-0.29	-0.02
481	650	81.85	4	93843	162	-0.11	-0.01
482	196	25.21	4	5627	56	-0.42	-0.03
483	282	34.67	4	7125	68	-0.30	-0.02
484	336	39.67	3	9702	64	-0.27	-0.02
485	240	28.78	4	4220	55	-0.25	-0.02
486	146	16.31	0	455	11	-0.59	-0.03
487	80	11.92	1	607	23	-0.67	-0.05
488	332	42.89	3	13628	74	-0.25	-0.02
489	120	15.25	2	1153	27	-0.26	-0.02
490	254	30.56	4	7863	55	-0.38	-0.03
491	200	24.72	1	2044	35	-0.37	-0.03
492	122	15.00	3	955	32	-0.65	-0.05
493	182	22.33	3	2531	43	-0.26	-0.02
494	208	25.43	2	4672	42	-0.11	-0.01
495	218	26.95	3	5705	61	-0.18	-0.01
496	136	17.60	2	1995	37	-0.25	-0.02
497	430	54.91	2	26225	95	-0.10	-0.01
498	102	13.95	3	1833	44	-0.46	-0.03
499	120	15.03	3	1094	34	-0.28	-0.02
500	422	50.99	4	19673	92	-0.19	-0.01
501	312	31.60	4	4040	62	-0.16	-0.01
502	116	15.61	3	1512	33	-0.37	-0.03
503	130	16.39	3	1609	36	-0.24	-0.02
504	272	30.77	0	3015	33	-0.13	-0.01
505	238	27.48	0	2456	31	-0.14	-0.01
506	148	19.75	4	2907	42	-0.47	-0.03
507	286	35.98	5	8747	74	-0.36	-0.03
508	104	12.59	2	585	30	-0.20	-0.01
509	128	16.14	2	1263	33	-0.61	-0.04
510	120	14.41	1	518	23	-0.29	-0.02
511	438	47.22	8	17913	86	-0.30	-0.02
512	166	20.67	3	2353	41	-0.24	-0.02
513	330	41.87	7	16115	88	-0.27	-0.02
514	296	35.49	6	8619	71	-0.32	-0.02
515	190	23.73	3	2985	43	-0.28	-0.02
516	166	20.11	2	1744	42	-0.14	-0.01
517	170	23.29	1	3426	42	-0.35	-0.02
518	136	17.30	3	1803	38	-0.29	-0.02
519	218	26.19	0	1910	34	-0.39	-0.03
520	392	47.69	2	15111	84	-0.09	-0.01
521	120	16.35	0	969	24	-0.28	-0.02
522	106	13.27	1	518	23	-0.17	-0.01
523	216	27.59	4	5971	58	-0.37	-0.03
524	168	21.83	3	3877	50	-0.25	-0.01
525	260	32.21	3	8063	77	-0.10	-0.01
526	172	22.28	3	3877	50	-0.32	-0.02
527	178	22.09	4	3855	43	-0.43	-0.03
528	188	24.52	4	6624	59	-0.44	-0.03
529	174	23.96	4	4682	49	-0.41	-0.03
530	342	42.12	2	11185	74	-0.13	-0.01
531	124	13.91	2	592	18	-0.59	-0.04
532	110	13.27	2	706	26	-0.44	-0.03
533	216	26.67	4	5502	59	-0.17	-0.01
534	260	29.46	3	4386	49	-0.38	-0.03
535	158	20.48	2	2379	35	-0.32	-0.02
536	360	44.36	4	17272	81	-0.17	-0.01
537	118	14.77	2	1153	27	-0.34	-0.02
538	130	15.98	2	1309	30	-0.36	-0.02
539	292	35.98	5	13484	82	-0.21	-0.01
540	132	16.87	3	1609	36	-0.25	-0.02
541	114	14.12	3	955	32	-0.31	-0.02
542	166	20.11	2	1744	42	-0.35	-0.02
543	222	27.15	2	3793	59	-0.09	-0.01
544	154	20.05	2	2379	35	-0.20	-0.01
545	128	16.01	2	1485	34	-0.48	-0.03
546	510	61.65	1	24499	101	-0.17	-0.01

547	426	49.82	4	18795	91	-0.13	-0.01
548	148	19.94	1	2366	41	-0.32	-0.02
549	188	24.70	1	3778	49	-0.32	-0.02
550	120	15.33	2	1207	32	-0.34	-0.02
551	118	14.77	2	1109	28	-0.32	-0.02
552	118	14.77	2	1207	32	-0.34	-0.02
553	152	16.90	4	1536	39	-0.37	-0.03
554	164	21.41	3	3549	48	-0.18	-0.01
555	88	12.14	1	498	17	-0.34	-0.02
556	226	26.22	1	2176	40	-0.47	-0.03
557	148	18.59	3	1615	36	-0.57	-0.04
558	138	18.46	1	1806	42	-0.33	-0.02
559	138	18.46	1	1806	42	-0.43	-0.03
560	178	21.25	2	1965	44	-0.23	-0.01
561	424	48.83	5	22004	109	-0.18	-0.01
562	412	48.10	5	22004	109	-0.13	-0.01
563	326	39.51	6	17511	95	-0.15	-0.01
564	134	18.32	3	2814	38	-0.32	-0.02
565	120	16.28	2	1412	30	-0.17	-0.01
566	136	16.72	2	1020	27	-0.65	-0.05
567	140	18.19	2	1908	42	-0.32	-0.02
568	136	16.62	3	1102	33	-0.69	-0.05
569	150	19.77	4	2539	46	-0.31	-0.02
570	174	21.92	1	2916	32	-0.38	-0.03
571	298	35.45	3	8440	64	-0.31	-0.02
572	190	24.79	3	4854	53	-0.38	-0.03
573	482	52.66	4	14888	84	-0.25	-0.02
574	354	44.25	3	12354	70	-0.27	-0.02
575	354	44.25	3	12354	70	-0.26	-0.02
576	92	12.26	2	518	20	-0.41	-0.03
577	460	55.49	1	18028	82	-0.18	-0.01
578	252	30.35	5	7938	59	-0.34	-0.02
579	578	66.95	3	34471	113	-0.13	-0.01
580	300	35.51	6	11554	68	-0.24	-0.02
581	164	19.44	2	1564	39	-0.23	-0.02
582	242	26.59	4	3121	49	-0.31	-0.02
583	166	19.43	2	1418	36	-0.39	-0.03
584	162	22.46	3	3134	40	-0.34	-0.03
585	298	36.68	2	10437	75	-0.22	-0.01
586	454	56.04	3	22316	90	-0.15	-0.01
587	488	57.59	4	22161	91	-0.16	-0.01
588	218	27.83	3	5452	56	-0.24	-0.02
589	262	32.48	0	5206	54	-0.29	-0.02
590	602	71.04	4	40570	121	-0.14	-0.01
591	248	29.42	3	4112	53	-0.30	-0.02
592	126	14.39	2	592	18	-0.51	-0.03
593	438	51.00	5	23128	115	-0.07	0.00
594	140	17.81	1	1164	35	-0.18	-0.01
595	158	19.38	0	844	22	-0.28	-0.02
596	144	16.49	2	1020	32	-0.67	-0.04
597	208	25.23	4	5312	79	-0.37	-0.03
598	104	13.51	2	892	27	-0.33	-0.02
599	470	58.97	2	27210	96	-0.17	-0.01
600	484	57.86	4	28490	103	-0.17	-0.01
601	464	53.73	3	15554	78	-0.17	-0.01
602	688	80.38	6	57799	133	-0.13	-0.01
603	218	27.83	3	5452	56	-0.26	-0.02
604	174	21.40	3	3236	47	-0.48	-0.03
605	408	47.43	0	10287	68	-0.26	-0.02
606	594	69.02	6	37151	113	-0.12	-0.01
607	248	28.84	3	4213	51	-0.13	-0.01
608	396	45.99	3	15370	73	-0.21	-0.01
609	310	36.59	1	5060	54	-0.22	-0.02
610	372	43.68	0	8558	64	-0.23	-0.02
611	250	29.38	3	4658	53	-0.11	-0.01
612	166	21.40	4	3175	46	-0.51	-0.04
613	408	47.43	0	10287	68	-0.22	-0.02
614	206	26.70	2	4352	46	-0.48	-0.03
615	132	16.87	3	1481	37	-0.14	-0.01
616	474	55.79	2	18919	92	-0.19	-0.01
617	174	21.40	3	3301	45	-0.45	-0.03
618	194	25.45	2	4137	42	-0.39	-0.03
619	486	57.65	0	18524	93	-0.20	-0.01
620	188	22.61	2	2391	46	-0.15	-0.01
621	200	22.80	0	1313	17	-0.34	-0.02
622	316	38.07	1	7118	55	-0.15	-0.01
623	340	40.57	1	7872	59	-0.17	-0.01
624	352	41.22	1	8284	60	-0.18	-0.01
625	376	44.89	1	10722	67	-0.20	-0.01

626	400	47.39	1	11724	71	-0.22	-0.02
627	402	47.24	1	11246	70	-0.20	-0.01
628	412	48.04	1	12204	72	-0.21	-0.01
629	354	41.68	1	7912	59	-0.17	-0.01
630	424	49.29	1	12827	73	-0.21	-0.01
631	396	48.32	1	14750	78	-0.19	-0.01
DG_PSA DG_MSA DG_apolarSA DG_Wiener DG_P DG_NoC predOutcome(Eq.2)							
1	-0.03	-0.01	-0.02	0.00	-65153160.07	-0.39	1.563373e-02
2	-0.09	-0.05	-0.11	-0.04	-30.97	-2.81	4.965568e-01
3	-0.07	-0.02	-0.04	-0.01	-4045.89	-0.75	4.965568e-01
4	-0.13	-0.03	-0.03	-0.01	-0.84	-0.58	6.763213e-01
5	-0.08	-0.04	-0.08	-0.06	-38.35	-1.22	8.157188e-01
6	-0.14	-0.02	-0.02	-0.01	-0.02	-0.35	8.157188e-01
7	-0.46	-0.04	-0.04	-0.02	-0.02	-0.91	8.656406e-01
8	-0.26	-0.03	-0.04	-0.06	-0.03	-0.68	9.317344e-01
9	-0.16	-0.03	-0.04	-0.02	-2.84	-1.27	4.039296e-01
10	-0.18	-0.03	-0.04	-0.06	-6.03	-1.13	8.656406e-01
11	-0.16	-0.01	-0.02	0.00	-1.07371E-07	-0.35	8.656406e-01
12	-0.98	-0.03	-0.03	-0.02	0	-0.67	9.317344e-01
13	-0.15	-0.02	-0.02	-0.01	-0.19	-0.47	4.965568e-01
14	-0.23	-0.02	-0.03	-0.01	0	-0.53	7.525505e-01
15	-0.33	-0.04	-0.05	-0.07	-0.15	-0.97	9.317344e-01
16	-0.11	-0.02	-0.02	0.00	-0.09	-0.47	4.039296e-01
17	-0.09	-0.02	-0.02	-0.01	-0.96	-0.41	8.157188e-01
18	-0.21	-0.03	-0.04	-0.02	-0.01	-0.68	8.656406e-01
19	-0.07	-0.01	-0.01	0.00	0	-0.30	1.801764e-01
20	-0.08	-0.02	-0.02	0.00	-2.02	-0.44	2.423556e-01
21	-0.14	-0.01	-0.02	0.00	0	-0.33	5.894209e-01
22	-0.3	-0.02	-0.02	0.00	0	-0.44	7.525505e-01
23	-0.23	-0.03	-0.03	-0.01	-3.7	-0.76	7.525505e-01
24	-0.18	-0.02	-0.03	-0.01	-5.2905E-06	-0.45	8.157188e-01
25	-0.23	-0.04	-0.04	-0.01	-0.2	-0.81	8.157188e-01
26	-0.07	-0.02	-0.03	-0.02	-0.11	-0.61	8.157188e-01
27	-0.17	-0.02	-0.02	0.00	0	-0.37	8.157188e-01
28	-0.23	-0.03	-0.04	-0.03	-0.41	-0.88	8.157188e-01
29	-0.54	-0.03	-0.03	-0.01	0	-0.59	9.036362e-01
30	-0.14	-0.03	-0.03	-0.01	-0.97	-0.61	6.763213e-01
31	-0.09	-0.02	-0.03	0.00	-0.03	-0.54	3.176781e-01
32	-0.08	-0.02	-0.02	0.00	0	-0.42	3.176781e-01
33	-0.1	-0.03	-0.04	-0.01	-794.09	-1.12	4.039296e-01
34	-0.2	-0.01	-0.02	-0.01	0	-0.34	8.656406e-01
35	-0.09	-0.01	-0.01	0.00	0	-0.23	7.525505e-01
36	-0.54	-0.03	-0.03	-0.02	0	-0.71	8.656406e-01
37	-0.11	-0.02	-0.02	0.00	-0.68	-0.48	5.894209e-01
38	-0.1	-0.01	-0.01	0.00	-0.04	-0.31	6.763213e-01
39	-0.1	-0.03	-0.03	-0.02	-690.99	-0.79	8.656406e-01
40	-0.11	-0.03	-0.03	0.00	-0.02	-0.56	5.894209e-01
41	-0.12	-0.05	-0.07	-0.04	-2.91	-1.41	7.525505e-01
42	-0.47	-0.05	-0.06	-0.09	-1413.07	-2.05	8.157188e-01
43	-0.11	-0.02	-0.02	0.00	0	-0.40	5.894209e-01
44	-0.12	-0.02	-0.02	0.00	0	-0.47	5.894209e-01
45	-0.14	-0.02	-0.02	-0.01	-0.01	-0.43	7.525505e-01
46	-0.15	-0.02	-0.02	-0.01	-0.01	-0.47	7.525505e-01
47	-0.48	-0.03	-0.04	-0.02	-0.01	-0.80	8.656406e-01
48	-0.23	-0.03	-0.03	-0.01	0	-0.71	8.157188e-01
49	-0.28	-0.04	-0.05	-0.05	-0.18	-1.07	8.157188e-01
50	-0.07	-0.02	-0.02	-0.01	-18.67	-0.59	6.763213e-01
51	-0.06	-0.01	-0.01	0.00	-1.75	-0.26	5.894209e-01
52	-0.18	-0.02	-0.02	0.00	0	-0.47	4.039296e-01
53	-0.27	-0.03	-0.03	-0.01	0	-0.62	8.157188e-01
54	-0.03	-0.01	-0.01	0.00	-0.12	-0.14	9.399165e-02
55	-0.16	-0.02	-0.02	-0.01	0	-0.46	8.157188e-01
56	-0.54	-0.02	-0.02	0.00	-6.93894E-07	-0.47	8.656406e-01
57	-0.43	-0.03	-0.03	-0.01	0	-0.62	8.656406e-01
58	-0.16	-0.04	-0.05	-0.01	-0.03	-0.82	5.894209e-01
59	-0.97	-0.05	-0.05	-0.04	-0.16	-1.33	7.525505e-01
60	-0.36	-0.01	-0.02	-0.01	-3.81118E-05	-0.29	9.036362e-01
61	-0.25	-0.02	-0.03	-0.01	-0.07	-0.54	7.525505e-01
62	-0.16	-0.02	-0.03	-0.01	-0.71	-0.48	8.157188e-01
63	-0.69	-0.02	-0.03	-0.01	0	-0.45	9.317344e-01
64	-0.05	-0.01	-0.02	0.00	-5.26	-0.27	2.423556e-01
65	-0.00	-0.02	-0.02	-0.01	-0.66	-0.50	9.036362e-01
66	-0.95	-0.03	-0.03	-0.02	-0.02	-0.72	9.036362e-01
67	-0.37	-0.02	-0.02	-0.01	0	-0.34	9.317344e-01
68	-0.1	-0.02	-0.03	-0.01	-0.71	-0.45	6.763213e-01
69	-0.37	-0.02	-0.02	-0.01	-0.01	-0.49	9.036362e-01
70	-0.35	-0.03	-0.04	-0.02	-0.01	-0.71	8.157188e-01
71	-0.13	-0.03	-0.04	-0.03	-0.28	-0.87	7.525505e-01
72	-0.12	-0.01	-0.01	0.00	0	-0.31	7.525505e-01

73	-0.23	-0.03	-0.03	-0.01	0	-0.60	7.525505e-01
74	-0.09	-0.02	-0.03	0.00	0	-0.62	3.176781e-01
75	-0.35	-0.04	-0.05	-0.02	-1.76597E-05	-0.80	9.036362e-01
76	-0.37	-0.04	-0.04	-0.02	-4.96868E-05	-0.83	9.036362e-01
77	-0.09	-0.02	-0.02	0.00	-0.25	-0.38	4.039296e-01
78	-0.07	-0.01	-0.01	0.00	-0.01	-0.28	5.894209e-01
79	-0.47	-0.03	-0.03	-0.01	-0.01	-0.63	9.036362e-01
80	-0.08	-0.02	-0.03	0.00	-8623.79	-0.54	1.801764e-01
81	-0.13	-0.02	-0.02	-0.01	0	-0.43	8.157188e-01
82	-0.1	-0.02	-0.02	0.00	-0.16	-0.54	4.965568e-01
83	-0.13	-0.02	-0.03	0.00	-0.18	-0.52	6.763213e-01
84	-0.26	-0.05	-0.06	-0.07	-1.28	-1.33	8.656406e-01
85	-0.11	-0.03	-0.05	-0.02	-34.12	-1.27	5.894209e-01
86	-0.12	-0.02	-0.03	0.00	-0.53	-0.55	3.176781e-01
87	-0.04	-0.01	-0.02	0.00	-20.8	-0.26	1.801764e-01
88	-0.14	-0.02	-0.02	0.00	-0.02	-0.43	7.525505e-01
89	-0.32	-0.03	-0.03	-0.01	0	-0.66	8.656406e-01
90	-0.49	-0.04	-0.04	-0.05	-4.25	-1.00	9.036362e-01
91	-0.1	-0.02	-0.02	0.00	-0.07	-0.49	5.894209e-01
92	-0.4	-0.03	-0.04	-0.02	-0.12	-0.65	8.656406e-01
93	-0.14	-0.04	-0.05	-0.03	-2.47	-0.97	8.157188e-01
94	-0.05	-0.01	-0.01	0.00	-0.13	-0.20	4.039296e-01
95	-0.03	-0.01	-0.01	0.00	-0.45	-0.17	9.399165e-02
96	-0.33	-0.04	-0.04	-0.02	0	-0.74	9.036362e-01
97	-0.35	-0.04	-0.04	-0.02	0	-0.72	9.036362e-01
98	-0.11	-0.02	-0.02	-0.01	0	-0.52	6.763213e-01
99	-0.33	-0.08	-0.10	-1.66	-7.96	-3.31	9.317344e-01
100	-0.32	-0.03	-0.04	-0.01	0	-0.65	9.036362e-01
101	-0.14	-0.04	-0.06	-0.03	-1.6	-1.41	6.763213e-01
102	-0.04	-0.01	-0.01	0.00	-0.65	-0.25	1.311877e-01
103	-0.11	-0.01	-0.01	0.00	0	-0.31	5.894209e-01
104	-0.14	-0.02	-0.02	0.00	-3.38227E-05	-0.36	7.525505e-01
105	-0.38	-0.03	-0.03	-0.01	0	-0.58	8.656406e-01
106	-0.07	-0.01	-0.01	0.00	-1.40464E-05	-0.19	7.525505e-01
107	-0.21	-0.02	-0.02	0.00	0	-0.43	2.423556e-01
108	-0.16	-0.04	-0.05	-0.01	-1198	-1.03	5.894209e-01
109	-0.1	-0.04	-0.08	-0.07	-40.53	-1.57	8.157188e-01
110	-1.34	-0.03	-0.03	-0.01	0	-0.73	7.525505e-01
111	-0.17	-0.02	-0.03	-0.01	-0.11	-0.50	8.157188e-01
112	-0.09	-0.01	-0.02	0.00	-0.01	-0.36	4.965568e-01
113	-0.23	-0.02	-0.02	-0.01	0	-0.51	6.763213e-01
114	-0.18	-0.02	-0.02	-0.01	0	-0.46	8.656406e-01
115	-0.16	-0.02	-0.02	0.00	-1.47914E-08	-0.39	4.965568e-01
116	-0.06	-0.01	-0.01	-0.01	-0.1	-0.27	8.656406e-01
117	-0.07	-0.01	-0.01	0.00	-0.9	-0.28	4.965568e-01
118	-0.08	-0.02	-0.03	-0.01	-37.41	-0.71	4.965568e-01
119	-0.15	-0.02	-0.02	-0.01	0	-0.48	8.656406e-01
120	-0.09	-0.01	-0.02	0.00	0	-0.34	4.039296e-01
121	-0.27	-0.03	-0.04	-0.01	-0.23	-0.72	8.157188e-01
122	-0.09	-0.01	-0.02	0.00	-0.5	-0.32	5.894209e-01
123	-0.46	-0.05	-0.05	-0.03	0	-1.43	6.763213e-01
124	-0.22	-0.02	-0.02	-0.02	-0.4	-0.57	8.157188e-01
125	-0.25	-0.03	-0.03	-0.01	0	-0.61	7.525505e-01
126	-0.12	-0.02	-0.03	-0.01	-3.51	-0.55	7.525505e-01
127	-0.09	-0.02	-0.02	-0.01	-0.74	-0.32	8.157188e-01
128	-0.13	-0.02	-0.02	-0.01	0	-0.37	9.036362e-01
129	-0.12	-0.02	-0.02	0.00	-0.01	-0.41	8.157188e-01
130	-0.08	-0.01	-0.01	0.00	-0.01	-0.22	4.965568e-01
131	-0.45	-0.03	-0.03	-0.01	-0.01	-0.64	9.036362e-01
132	-0.12	-0.02	-0.02	0.00	-0.02	-0.38	4.039296e-01
133	-0.08	-0.01	-0.01	0.00	0	-0.28	7.525505e-01
134	-0.05	-0.01	-0.01	0.00	0	-0.19	6.763213e-01
135	-0.13	-0.03	-0.04	-0.04	-35.68	-0.90	8.157188e-01
136	-0.17	-0.03	-0.04	-0.03	-0.38	-0.92	8.157188e-01
137	-0.07	-0.01	-0.01	0.00	-0.26	-0.25	2.423556e-01
138	-0.58	-0.03	-0.03	-0.03	-0.01	-0.76	8.656406e-01
139	-0.12	-0.02	-0.02	0.00	-0.17	-0.42	4.039296e-01
140	-0.12	-0.02	-0.02	-0.01	0	-0.40	8.656406e-01
141	-0.05	-0.02	-0.03	-0.01	-27.77	-0.56	6.763213e-01
142	-0.15	-0.02	-0.02	-0.01	0	-0.63	5.894209e-01
143	-0.15	-0.03	-0.04	-0.01	-0.42	-0.80	5.894209e-01
144	-0.09	-0.01	-0.01	0.00	0	-0.30	7.525505e-01
145	-0.36	-0.03	-0.04	-0.02	0	-0.65	9.036362e-01
146	-0.07	-0.01	-0.02	-0.02	-13.95	-0.41	8.157188e-01
147	-0.13	-0.02	-0.02	0.00	-9.29464E-05	-0.38	7.525505e-01
148	-0.09	-0.03	-0.04	-0.02	-398.83	-0.77	7.525505e-01
149	-0.37	-0.04	-0.04	-0.02	-0.01	-0.75	9.036362e-01
150	-0.2	-0.02	-0.02	-0.01	-0.05	-0.44	8.656406e-01
151	-0.13	-0.02	-0.02	-0.02	0	-0.68	6.763213e-01

152	-0.2	-0.03	-0.03	-0.01	-0.14	-0.62	8.157188e-01
153	-0.18	-0.02	-0.02	0.00	-4.01162E-05	-0.40	7.525505e-01
154	-0.27	-0.04	-0.05	-0.02	0	-0.91	6.763213e-01
155	-0.13	-0.02	-0.03	0.00	-0.05	-0.53	6.763213e-01
156	-0.14	-0.02	-0.02	0.00	0	-0.44	7.525505e-01
157	-0.23	-0.03	-0.03	-0.01	-0.03	-0.63	8.157188e-01
158	-0.12	-0.02	-0.03	-0.01	-0.75	-0.62	4.965568e-01
159	-0.57	-0.02	-0.02	-0.01	-5.94044E-05	-0.34	9.317344e-01
160	-0.09	-0.02	-0.02	-0.01	-4.14	-0.62	4.965568e-01
161	-0.28	-0.04	-0.04	-0.02	-0.02	-0.80	8.157188e-01
162	-0.68	-0.03	-0.03	-0.05	-0.02	-0.74	9.317344e-01
163	-0.24	-0.03	-0.03	-0.01	0	-0.59	8.656406e-01
164	-0.33	-0.04	-0.05	-0.02	-0.76	-1.06	8.656406e-01
165	-0.33	-0.03	-0.03	-0.04	0	-0.71	9.317344e-01
166	-0.09	-0.02	-0.02	0.00	-0.01	-0.37	8.157188e-01
167	-0.4	-0.03	-0.03	-0.01	0	-0.59	9.036362e-01
168	-0.1	-0.04	-0.08	-0.04	-57.05	-2.22	4.965568e-01
169	-0.1	-0.03	-0.04	0.00	-63.73	-0.78	1.311877e-01
170	-0.18	-0.02	-0.03	-0.02	-1.05	-0.65	8.157188e-01
171	-0.44	-0.04	-0.04	-0.02	-0.1	-0.83	8.656406e-01
172	-0.22	-0.03	-0.03	-0.01	-1.65	-0.60	8.157188e-01
173	-0.24	-0.02	-0.03	-0.01	-0.06	-0.67	6.763213e-01
174	-0.23	-0.01	-0.01	0.00	-6.06748E-05	-0.35	6.763213e-01
175	-0.37	-0.03	-0.03	-0.01	-0.01	-0.62	8.157188e-01
176	-0.26	-0.02	-0.03	-0.01	0	-0.46	8.656406e-01
177	-0.14	-0.03	-0.05	-0.02	-0.66	-0.78	8.157188e-01
178	-0.13	-0.04	-0.05	-0.03	-5.99	-1.10	7.525505e-01
179	-0.07	-0.01	-0.01	0.00	0	-0.27	7.525505e-01
180	-0.2	-0.04	-0.05	-0.02	-2.22	-0.75	8.157188e-01
181	-0.16	-0.04	-0.05	-0.02	-1.86	-0.98	7.525505e-01
182	-0.16	-0.03	-0.04	-0.01	-3.49	-0.68	7.525505e-01
183	-0.16	-0.03	-0.04	-0.01	-2.6	-0.65	7.525505e-01
184	-0.17	-0.03	-0.03	-0.01	-0.5	-0.73	8.157188e-01
185	-0.15	-0.02	-0.02	0.00	-0.15	-0.45	6.763213e-01
186	-0.1	-0.02	-0.02	0.00	-1.18663E-05	-0.37	4.965568e-01
187	-0.09	-0.02	-0.02	0.00	0	-0.38	4.039296e-01
188	-0.38	-0.04	-0.05	-0.05	-0.74	-1.00	9.036362e-01
189	-0.09	-0.02	-0.03	-0.01	-0.12	-0.51	4.965568e-01
190	-0.06	-0.01	-0.02	0.00	-0.02	-0.33	4.039296e-01
191	-0.08	-0.02	-0.02	0.00	-0.01	-0.39	4.965568e-01
192	-0.07	-0.02	-0.02	0.00	-0.04	-0.39	4.965568e-01
193	-0.34	-0.03	-0.04	-0.01	-0.01	-0.64	9.036362e-01
194	-0.06	-0.01	-0.01	0.00	-2.56	-0.26	5.894209e-01
195	-0.29	-0.03	-0.03	-0.01	0	-0.51	9.036362e-01
196	-1.02	-0.03	-0.03	-0.02	0	-0.65	9.317344e-01
197	-0.08	-0.02	-0.02	0.00	0	-0.43	1.311877e-01
198	-0.04	-0.01	-0.01	0.00	-1.83	-0.19	4.965568e-01
199	-0.15	-0.03	-0.03	-0.01	-2.06	-0.61	7.525505e-01
200	-0.17	-0.02	-0.03	-0.01	0	-0.49	8.157188e-01
201	-0.08	-0.02	-0.03	-0.01	-0.03	-0.59	4.965568e-01
202	-0.08	-0.02	-0.02	-0.01	-4.74	-0.44	7.525505e-01
203	-0.25	-0.03	-0.04	-0.01	-7.93	-0.68	8.656406e-01
204	-0.31	-0.02	-0.02	-0.01	0	-0.40	9.036362e-01
205	-0.05	-0.01	-0.02	0.00	-179.81	-0.36	1.801764e-01
206	-0.21	-0.02	-0.03	-0.01	0	-0.52	8.656406e-01
207	-0.37	-0.03	-0.03	-0.02	-0.01	-0.75	8.656406e-01
208	-0.03	-0.01	-0.01	0.00	-0.01	-0.12	6.653425e-02
209	-0.07	-0.01	-0.01	0.00	0	-0.17	7.525505e-01
210	-0.51	-0.03	-0.04	-0.01	0	-0.75	7.525505e-01
211	-0.17	-0.05	-0.08	-0.03	-13245.2	-1.55	5.894209e-01
212	-0.23	-0.03	-0.03	-0.01	0	-0.65	9.036362e-01
213	-0.65	-0.02	-0.02	-0.01	-4.92424E-06	-0.41	9.317344e-01
214	-0.09	-0.02	-0.02	0.00	-0.01	-0.38	6.763213e-01
215	-0.27	-0.03	-0.04	-0.01	-0.27	-0.74	8.157188e-01
216	-0.22	-0.04	-0.05	-0.04	-2.73	-1.00	8.656406e-01
217	-0.14	-0.02	-0.02	-0.01	-0.04	-0.43	8.157188e-01
218	-0.21	-0.03	-0.03	-0.01	-1.46	-0.75	7.525505e-01
219	-0.07	-0.02	-0.03	-0.01	-72.57	-0.50	5.894209e-01
220	-0.17	-0.03	-0.03	-0.02	-4.14	-0.67	8.656406e-01
221	-0.23	-0.02	-0.02	0.00	-4.89573E-05	-0.40	7.525505e-01
222	-0.26	-0.03	-0.04	-0.02	-0.35	-0.84	8.656406e-01
223	-0.09	-0.02	-0.02	0.00	-0.04	-0.44	6.763213e-01
224	-0.23	-0.04	-0.05	-0.20	-32.13	-1.36	9.036362e-01
225	-0.15	-0.03	-0.03	-0.01	-3.07	-0.62	5.894209e-01
226	-0.06	-0.02	-0.02	-0.01	-0.08	-0.43	5.894209e-01
227	-0.33	-0.05	-0.05	-0.04	-2.14	-1.23	8.157188e-01
228	-0.06	-0.01	-0.02	0.00	-0.04	-0.30	5.894209e-01
229	-0.14	-0.03	-0.04	-0.01	-3.6	-0.74	4.965568e-01
230	-0.13	-0.03	-0.03	-0.01	-1.13	-0.57	7.525505e-01

231	-0.36	-0.02	-0.02	-0.01	-0.05	-0.47	8.656406e-01
232	-0.27	-0.02	-0.03	-0.01	-0.18	-0.63	8.157188e-01
233	-0.15	-0.02	-0.02	-0.01	-0.04	-0.47	8.157188e-01
234	-0.12	-0.02	-0.02	-0.01	0	-0.40	7.525505e-01
235	-0.23	-0.02	-0.02	-0.01	0	-0.41	9.036362e-01
236	-0.44	-0.03	-0.04	-0.01	0	-0.71	9.036362e-01
237	-0.12	-0.02	-0.02	-0.01	0	-0.37	8.656406e-01
238	-0.23	-0.03	-0.04	-0.02	-0.01	-0.71	8.656406e-01
239	-0.18	-0.02	-0.02	0.00	-0.01	-0.39	8.157188e-01
240	-0.47	-0.04	-0.04	-0.02	-0.01	-0.86	8.656406e-01
241	-0.4	-0.03	-0.04	-0.04	-0.33	-0.81	9.036362e-01
242	-0.47	-0.04	-0.04	-0.02	-0.01	-1.00	7.525505e-01
243	-0.07	-0.01	-0.02	0.00	-0.13	-0.33	6.763213e-01
244	-0.16	-0.02	-0.02	-0.01	-0.01	-0.44	8.157188e-01
245	-0.13	-0.02	-0.03	0.00	-8.93842E-05	-0.49	6.763213e-01
246	-0.05	-0.02	-0.02	0.00	-26.03	-0.40	2.423556e-01
247	-0.56	-0.04	-0.04	-0.02	-0.05	-0.93	8.656406e-01
248	-0.11	-0.02	-0.03	-0.01	-3.14	-0.71	5.894209e-01
249	-0.44	-0.03	-0.03	-0.01	-0.01	-0.64	8.157188e-01
250	-0.07	-0.01	-0.01	0.00	-0.01	-0.25	2.423556e-01
251	-0.18	-0.03	-0.03	0.00	-0.05	-0.58	7.525505e-01
252	-0.09	-0.02	-0.02	0.00	0	-0.40	1.311877e-01
253	-0.19	-0.03	-0.04	-0.01	-28.02	-0.76	8.656406e-01
254	-0.33	-0.03	-0.03	-0.01	-0.06	-0.64	8.656406e-01
255	-0.09	-0.02	-0.03	-0.01	-0.3	-0.56	5.894209e-01
256	-0.15	-0.02	-0.02	0.00	0	-0.42	7.525505e-01
257	-0.12	-0.02	-0.02	0.00	0	-0.37	2.423556e-01
258	-0.19	-0.04	-0.04	-0.01	-2.23	-0.81	7.525505e-01
259	-1.12	-0.04	-0.04	-0.02	-9.70807E-05	-0.79	8.656406e-01
260	-0.09	-0.02	-0.03	0.00	-9.31	-0.56	4.039296e-01
261	-0.1	-0.02	-0.02	-0.01	-0.8	-0.52	7.525505e-01
262	-0.08	-0.01	-0.02	0.00	-14.49	-0.35	4.039296e-01
263	-0.13	-0.02	-0.03	-0.01	0	-0.47	7.525505e-01
264	-0.06	-0.02	-0.03	-0.01	-100.81	-0.45	6.763213e-01
265	-0.16	-0.04	-0.05	-0.02	-0.48	-1.11	7.525505e-01
266	-0.19	-0.04	-0.05	-0.05	-2.39	-1.38	8.157188e-01
267	-0.08	-0.02	-0.02	-0.01	-0.47	-0.45	5.894209e-01
268	-0.16	-0.03	-0.03	-0.01	-2.52	-0.82	8.157188e-01
269	-0.85	-0.04	-0.04	-0.03	-0.03	-0.84	9.036362e-01
270	-0.07	-0.01	-0.01	0.00	-0.01	-0.29	1.311877e-01
271	-0.56	-0.02	-0.02	-0.01	-1.00688E-06	-0.49	9.036362e-01
272	-0.03	-0.01	-0.01	0.00	-0.12	-0.15	9.399165e-02
273	-0.11	-0.02	-0.03	-0.01	-5.98	-0.59	4.039296e-01
274	-0.09	-0.02	-0.02	-0.01	-0.21	-0.47	8.157188e-01
275	-0.19	-0.01	-0.02	0.00	-8.1514E-07	-0.32	8.656406e-01
276	-0.16	-0.02	-0.02	-0.01	0	-0.36	8.656406e-01
277	-0.33	-0.03	-0.03	-0.02	0	-0.64	9.036362e-01
278	-0.11	-0.04	-0.05	-0.04	-805.36	-1.12	8.656406e-01
279	-0.11	-0.02	-0.02	-0.01	0	-0.41	8.157188e-01
280	-0.09	-0.02	-0.03	-0.01	-0.02	-0.47	7.525505e-01
281	-0.22	-0.03	-0.03	-0.02	-0.01	-0.66	8.656406e-01
282	-0.15	-0.02	-0.02	0.00	-3.6312E-06	-0.49	3.176781e-01
283	-0.06	-0.01	-0.02	-0.01	-0.02	-0.39	6.763213e-01
284	-0.09	-0.02	-0.02	-0.01	-0.04	-0.45	7.525505e-01
285	-0.04	-0.01	-0.01	0.00	-5.49	-0.30	4.039296e-01
286	-0.18	-0.02	-0.02	-0.01	-0.03	-0.49	8.656406e-01
287	-0.12	-0.02	-0.03	0.00	0	-0.49	5.894209e-01
288	-0.36	-0.05	-0.06	-0.08	-0.41	-1.05	9.317344e-01
289	-0.07	-0.01	-0.01	0.00	0	-0.25	4.039296e-01
290	-0.16	-0.02	-0.03	-0.01	-1.16	-0.57	6.763213e-01
291	-0.29	-0.03	-0.04	-0.01	-0.01	-0.75	7.525505e-01
292	-0.12	-0.02	-0.02	0.00	0	-0.39	5.894209e-01
293	-0.4	-0.03	-0.03	-0.01	0	-0.68	9.036362e-01
294	-0.18	-0.01	-0.02	0.00	0	-0.31	9.036362e-01
295	-0.3	-0.04	-0.05	-0.02	-0.78	-1.16	5.894209e-01
296	-0.27	-0.03	-0.03	-0.01	-0.13	-0.76	4.965568e-01
297	-0.29	-0.03	-0.03	-0.02	-0.17	-0.72	8.656406e-01
298	-0.47	-0.03	-0.03	-0.01	0	-0.65	9.036362e-01
299	-0.08	-0.02	-0.02	0.00	0	-0.38	5.894209e-01
300	-0.1	-0.01	-0.01	0.00	0	-0.25	6.763213e-01
301	-0.12	-0.02	-0.02	-0.03	-0.01	-0.56	9.036362e-01
302	-0.08	-0.02	-0.02	0.00	-0.53	-0.50	4.965568e-01
303	-0.04	-0.01	-0.01	0.00	-247860	-0.28	3.720849e-04
304	-0.26	-0.03	-0.03	-0.01	-0.02	-0.65	8.656406e-01
305	-0.13	-0.01	-0.02	0.00	0	-0.37	6.763213e-01
306	-0.05	-0.01	-0.01	0.00	-0.02	-0.22	1.801764e-01
307	-0.04	-0.01	-0.01	0.00	-0.02	-0.19	1.311877e-01
308	-0.1	-0.02	-0.02	-0.01	-0.01	-0.33	8.157188e-01
309	-0.04	-0.02	-0.03	-0.01	-27.77	-0.48	4.965568e-01

310	-0.13	-0.02	-0.03	0.00	-0.02	-0.51	5.894209e-01
311	-0.19	-0.03	-0.03	-0.01	-0.68	-0.58	8.157188e-01
312	-0.04	-0.01	-0.02	0.00	-99.52	-0.39	2.423556e-01
313	-0.09	-0.02	-0.03	0.00	-9.5	-0.52	3.176781e-01
314	-0.04	-0.02	-0.04	0.00	-1730158.33	-0.91	9.399165e-02
315	-0.06	-0.01	-0.01	0.00	0	-0.26	4.668456e-02
316	-0.06	-0.01	-0.01	0.00	-1.35	-0.27	1.079400e-02
317	-0.02	0.00	-0.01	0.00	-11.87	-0.13	3.526394e-03
318	-0.01	-0.01	-0.01	0.00	-33589.18	-0.21	2.423556e-01
319	-0.03	-0.02	-0.04	0.00	-103678272	-0.90	3.255029e-02
320	-0.03	-0.02	-0.04	0.00	-98396765.36	-0.86	3.255029e-02
321	-0.04	-0.01	-0.02	-0.01	-0.28	-0.48	4.965568e-01
322	-0.11	-0.02	-0.02	0.00	-0.11	-0.51	1.801764e-01
323	-0.12	-0.02	-0.02	0.00	-0.03	-0.45	2.423556e-01
324	-0.02	0.00	-0.01	0.00	-41.87	-0.11	7.441179e-03
325	-0.04	-0.02	-0.03	-0.01	-576.01	-0.53	5.894209e-01
326	-0.09	-0.02	-0.02	-0.01	-176.69	-0.65	3.176781e-01
327	-0.13	-0.02	-0.02	0.00	-4.92	-0.44	4.039296e-01
328	-0.1	-0.02	-0.02	0.00	-43.28	-0.57	3.176781e-01
329	-0.09	-0.02	-0.02	0.00	-3825.3	-0.52	3.176781e-01
330	-0.13	-0.02	-0.02	0.00	-17.8	-0.51	4.039296e-01
331	-0.11	-0.02	-0.02	-0.01	-879.38	-0.57	4.039296e-01
332	-0.14	-0.02	-0.02	0.00	-15.01	-0.47	4.039296e-01
333	-0.08	-0.01	-0.02	0.00	-140.39	-0.42	4.039296e-01
334	-0.11	-0.02	-0.02	-0.01	-4386.98	-0.67	3.176781e-01
335	-0.11	-0.02	-0.02	-0.01	-1468.15	-0.61	3.176781e-01
336	-0.1	-0.02	-0.02	0.00	-26.5	-0.43	3.176781e-01
337	-0.11	-0.02	-0.02	0.00	-12655.26	-0.60	2.423556e-01
338	-0.11	-0.02	-0.02	0.00	-5834.96	-0.60	2.423556e-01
339	-0.15	-0.02	-0.02	-0.01	-40.57	-0.63	4.039296e-01
340	-0.15	-0.02	-0.02	-0.01	-11.42	-0.61	4.039296e-01
341	-0.11	-0.01	-0.02	0.00	-9.76	-0.45	4.039296e-01
342	-0.06	-0.01	-0.01	0.00	-1.32	-0.26	1.079400e-02
343	-0.07	-0.02	-0.02	0.00	-1.31	-0.50	4.039296e-01
344	-0.05	-0.02	-0.03	-0.01	-681.23	-0.63	5.894209e-01
345	-0.06	-0.01	-0.01	0.00	-69174.6	-0.31	5.124412e-03
346	-0.1	-0.01	-0.01	0.00	0	-0.23	3.176781e-01
347	-0.11	-0.03	-0.05	-0.01	-6.24	-1.06	5.894209e-01
348	-0.1	-0.03	-0.05	-0.01	-18.62	-1.04	4.965568e-01
349	-0.1	-0.03	-0.04	-0.01	-20.6	-1.06	4.965568e-01
350	-0.1	-0.03	-0.05	-0.01	-25.99	-1.05	4.965568e-01
351	-0.1	-0.03	-0.04	-0.01	-1746.91	-1.18	4.039296e-01
352	-0.09	-0.03	-0.05	-0.01	-146.49	-1.03	4.039296e-01
353	-0.08	-0.03	-0.06	-0.01	-2407.46	-1.20	4.039296e-01
354	-0.09	-0.04	-0.06	-0.02	-142.26	-1.38	4.965568e-01
355	-0.02	-0.01	-0.05	0.00	-116990676	-1.00	6.653425e-02
356	-0.09	-0.02	-0.02	0.00	-0.07	-0.45	1.311877e-01
357	-0.02	-0.01	-0.02	0.00	-23796768.22	-0.46	3.255029e-02
358	-0.03	-0.01	-0.03	0.00	-2364745.32	-0.57	9.399165e-02
359	-0.03	-0.01	-0.01	0.00	-10120.49	-0.24	3.720849e-04
360	-0.07	-0.02	-0.04	-0.03	-7.78	-1.00	8.157188e-01
361	-0.11	-0.02	-0.03	0.00	-14.47	-0.61	2.423556e-01
362	-0.17	-0.02	-0.03	0.00	-1.09	-0.49	4.039296e-01
363	-0.07	-0.03	-0.04	-0.01	-3.37	-0.79	4.965568e-01
364	-0.12	-0.02	-0.02	0.00	0	-0.36	4.965568e-01
365	-0.07	-0.02	-0.03	0.00	-1.49	-0.56	4.039296e-01
366	-0.08	-0.01	-0.01	0.00	-0.02	-0.28	1.801764e-01
367	-0.11	-0.03	-0.05	-0.02	-34.64	-1.29	5.894209e-01
368	-0.04	-0.01	-0.01	0.00	-2.71	-0.17	1.563373e-02
369	-0.06	-0.01	-0.02	0.00	-0.13	-0.45	4.668456e-02
370	-0.07	-0.02	-0.04	-0.01	-468.04	-0.69	5.894209e-01
371	-0.15	-0.02	-0.02	0.00	-1.49081E-06	-0.39	7.525505e-01
372	-0.12	-0.01	-0.01	0.00	-6.75586E-05	-0.31	3.176781e-01
373	-0.11	-0.02	-0.02	0.00	0	-0.37	7.525505e-01
374	-0.03	-0.01	-0.03	0.00	-3801427.36	-0.68	9.399165e-02
375	-0.21	-0.02	-0.02	0.00	0	-0.47	8.656406e-01
376	-0.03	-0.02	-0.03	0.00	-194373.97	-0.59	2.423556e-01
377	-0.05	-0.02	-0.02	0.00	-97.94	-0.46	9.399165e-02
378	-0.09	-0.01	-0.02	0.00	0	-0.33	4.668456e-02
379	-0.08	-0.02	-0.03	-0.01	-58.54	-0.81	4.965568e-01
380	-0.15	-0.02	-0.02	0.00	0	-0.39	5.894209e-01
381	-0.03	-0.02	-0.04	0.00	-387459.13	-0.73	1.311877e-01
382	-0.07	-0.02	-0.03	-0.01	-67.17	-0.49	6.763213e-01
383	-0.05	-0.02	-0.03	-0.01	-2284.94	-0.51	4.965568e-01
384	-0.04	-0.01	-0.01	0.00	-14300.78	-0.25	3.526394e-03
385	-0.04	-0.01	-0.01	0.00	-188339.04	-0.29	5.124412e-03
386	-1.05	-0.04	-0.04	-0.02	0	-0.75	8.656406e-01
387	-0.03	-0.02	-0.04	-0.02	-1328.83	-0.72	6.763213e-01
388	-0.19	-0.02	-0.02	0.00	0	-0.42	3.176781e-01

389	-0.18	-0.02	-0.02	0.00	-0.01	-0.55	1.801764e-01
390	-0.06	-0.01	-0.01	0.00	-0.03	-0.30	1.801764e-01
391	-0.08	-0.01	-0.01	0.00	-0.01	-0.34	9.399165e-02
392	-0.07	-0.01	-0.02	0.00	-0.03	-0.41	3.176781e-01
393	-0.02	-0.01	-0.01	0.00	-0.76	-0.14	1.801764e-01
394	-0.06	-0.02	-0.03	0.00	-11199.05	-0.60	6.653425e-02
395	-0.03	-0.01	-0.03	0.00	-698456.61	-0.64	6.653425e-02
396	-0.04	-0.01	-0.02	-0.01	-0.61	-0.34	7.525505e-01
397	-0.07	-0.02	-0.03	-0.01	-591.5	-0.64	4.965568e-01
398	-0.04	-0.01	-0.01	0.00	-66.65	-0.23	1.146400e-03
399	-0.06	-0.02	-0.02	0.00	-54.26	-0.46	4.668456e-02
400	-0.08	-0.02	-0.02	0.00	-1018.33	-0.44	4.668456e-02
401	-0.23	-0.03	-0.03	-0.01	-2.18615E-06	-0.52	8.656406e-01
402	-0.11	-0.02	-0.03	0.00	-0.65	-0.54	1.801764e-01
403	-0.05	-0.01	-0.01	0.00	-397.36	-0.29	5.124412e-03
404	-0.06	-0.02	-0.04	-0.01	-6570.35	-0.69	5.894209e-01
405	-0.02	-0.01	-0.02	0.00	-590.8	-0.30	4.965568e-01
406	-0.17	-0.02	-0.03	-0.01	0	-0.49	8.157188e-01
407	-0.14	-0.02	-0.02	0.00	0	-0.43	5.894209e-01
408	-0.02	-0.01	-0.01	0.00	-8775894.19	-0.25	1.563373e-02
409	-0.04	-0.03	-0.08	-0.02	-155031.88	-1.55	4.039296e-01
410	-0.01	-0.01	-0.01	0.00	-12565.1	-0.20	3.176781e-01
411	-0.05	-0.02	-0.02	0.00	-451.66	-0.51	1.079400e-02
412	-0.03	-0.01	-0.01	0.00	-1726.9	-0.19	2.556716e-04
413	-0.07	-0.01	-0.01	0.00	-0.5	-0.31	6.653425e-02
414	-0.06	-0.01	-0.01	0.00	-0.03	-0.30	1.801764e-01
415	-0.04	-0.01	-0.01	0.00	-71.36	-0.23	5.124412e-03
416	-0.02	-0.01	-0.02	0.00	-71665	-0.29	2.423556e-01
417	-0.03	-0.01	-0.02	0.00	-27487.69	-0.43	4.668456e-02
418	-0.09	-0.02	-0.02	0.00	-2.02	-0.39	1.801764e-01
419	-0.11	-0.01	-0.02	0.00	-0.02	-0.34	1.801764e-01
420	-0.09	-0.01	-0.02	0.00	-1.08	-0.36	1.801764e-01
421	-0.02	-0.01	-0.01	0.00	-117.21	-0.16	1.207037e-04
422	-0.04	-0.01	-0.01	0.00	-5.18	-0.20	1.667707e-03
423	-0.06	-0.01	-0.01	0.00	-0.02	-0.23	1.079400e-02
424	-0.05	-0.01	-0.01	0.00	0	-0.19	7.441179e-03
425	-0.02	-0.01	-0.02	0.00	-1384049.42	-0.55	9.399165e-02
426	-0.24	-0.02	-0.02	-0.01	-8.53763E-07	-0.50	9.036362e-01
427	-0.21	-0.02	-0.02	-0.01	-7.53489E-07	-0.44	9.036362e-01
428	-0.09	-0.01	-0.01	0.00	-1.94598E-06	-0.33	4.039296e-01
429	-0.08	-0.04	-0.06	-0.03	-204.8	-1.12	6.763213e-01
430	-0.11	-0.02	-0.03	0.00	-6.02117E-05	-0.45	5.894209e-01
431	-0.12	-0.01	-0.02	0.00	0	-0.33	4.965568e-01
432	-0.07	-0.02	-0.02	0.00	-0.01	-0.38	1.311877e-01
433	-0.08	-0.01	-0.02	0.00	-0.01	-0.31	9.399165e-02
434	-0.1	-0.01	-0.02	0.00	0	-0.32	1.311877e-01
435	-0.09	-0.01	-0.02	0.00	-0.01	-0.31	9.399165e-02
436	-0.15	-0.02	-0.02	0.00	-6.9653E-08	-0.32	7.525505e-01
437	-0.12	-0.02	-0.02	0.00	0	-0.36	2.423556e-01
438	-0.07	-0.02	-0.03	0.00	-343.17	-0.50	4.668456e-02
439	-0.2	-0.03	-0.03	-0.01	-0.05	-0.69	7.525505e-01
440	-0.03	-0.01	-0.01	0.00	#VALUE!	-0.16	1.207037e-04
441	-0.09	-0.01	-0.01	0.00	-0.06	-0.27	1.311877e-01
442	-0.13	-0.01	-0.01	0.00	-1.68468E-05	-0.22	8.157188e-01
443	-0.04	-0.01	-0.02	0.00	-1584.91	-0.34	2.259390e-02
444	-0.07	-0.01	-0.01	0.00	-6.62441E-05	-0.23	1.311877e-01
445	-0.02	-0.01	-0.01	0.00	-22534.45	-0.21	1.563373e-02
446	-0.05	-0.01	-0.01	0.00	-0.09	-0.21	1.563373e-02
447	-0.14	-0.02	-0.02	-0.01	-319.71	-0.66	4.039296e-01
448	-0.09	-0.02	-0.02	0.00	-1019.72	-0.55	2.423556e-01
449	-0.11	-0.02	-0.02	0.00	-18.74	-0.41	4.039296e-01
450	-0.01	-0.01	-0.01	0.00	-624.6	-0.20	2.423556e-01
451	-0.02	-0.01	-0.02	0.00	-43452162.66	-0.46	3.255029e-02
452	-0.04	-0.01	-0.01	0.00	-0.05	-0.25	4.965568e-01
453	-0.02	-0.01	-0.02	0.00	-33830138.27	-0.36	1.079400e-02
454	-0.03	-0.02	-0.06	-0.01	-4460058.44	-1.05	1.801764e-01
455	-0.02	0.00	-0.01	0.00	-0.01	-0.12	2.259390e-02
456	-0.08	-0.01	-0.02	0.00	-0.32	-0.34	6.653425e-02
457	-0.08	-0.01	-0.02	0.00	-1.83	-0.35	9.399165e-02
458	-0.04	-0.01	-0.02	0.00	-859.91	-0.38	1.079400e-02
459	-0.02	-0.01	-0.01	0.00	-0.12	-0.14	1.311877e-01
460	-0.33	-0.03	-0.03	-0.02	0	-0.65	9.036362e-01
461	-0.1	-0.02	-0.02	0.00	0	-0.39	4.039296e-01
462	-0.06	-0.02	-0.04	-0.01	-9.07	-0.76	4.039296e-01
463	-0.14	-0.02	-0.03	0.00	-5.22262E-05	-0.51	5.894209e-01
464	-0.04	0.00	-0.01	0.00	0	-0.15	5.894209e-01
465	-0.06	-0.03	-0.05	-0.01	-10710	-0.89	3.176781e-01
466	-0.04	-0.01	-0.02	0.00	-295.67	-0.35	2.259390e-02
467	-0.02	-0.01	-0.02	0.00	-35150081.78	-0.38	1.079400e-02

468	-0.1	-0.01	-0.01	0.00	0	-0.30	1.801764e-01
469	-0.1	-0.01	-0.01	0.00	0	-0.32	1.801764e-01
470	-0.09	-0.01	-0.01	0.00	0	-0.27	5.894209e-01
471	-0.05	-0.01	-0.01	0.00	-2.97	-0.29	5.124412e-03
472	-0.04	-0.02	-0.05	-0.02	-13332.85	-1.16	5.894209e-01
473	-0.04	-0.02	-0.06	-0.02	-41877.89	-1.16	4.039296e-01
474	-0.02	-0.01	-0.02	0.00	-19750631.72	-0.46	3.255029e-02
475	-0.04	-0.01	-0.01	0.00	-615.95	-0.24	1.311877e-01
476	-0.05	-0.01	-0.01	0.00	-71.09	-0.23	4.039296e-01
477	-0.07	-0.01	-0.02	0.00	-222.55	-0.42	6.653425e-02
478	-0.03	-0.01	-0.01	0.00	-3.2	-0.21	1.311877e-01
479	-0.09	-0.02	-0.02	0.00	-1.09	-0.49	4.039296e-01
480	-0.03	-0.02	-0.03	-0.01	-33344.25	-0.79	4.039296e-01
481	-0.03	-0.01	-0.01	0.00	-30917660.76	-0.17	8.723639e-06
482	-0.13	-0.02	-0.03	0.00	-0.01	-0.66	1.311877e-01
483	-0.09	-0.02	-0.02	0.00	0	-0.39	4.039296e-01
484	-0.13	-0.01	-0.02	0.00	0	-0.35	3.176781e-01
485	-1.57	-0.01	-0.01	0.00	-2.03057E-05	-0.29	8.656406e-01
486	-0.41	-0.02	-0.02	-0.02	-2.92011E-05	-0.69	9.317344e-01
487	-0.1	-0.05	-0.08	-0.02	-3.7	-1.07	6.763213e-01
488	-0.07	-0.01	-0.02	0.00	-1.24	-0.36	4.668456e-02
489	-0.04	-0.01	-0.03	-0.01	-4616.68	-0.58	4.039296e-01
490	-0.29	-0.02	-0.02	0.00	-0.1	-0.51	4.039296e-01
491	-0.25	-0.02	-0.02	-0.01	-6.41327E-06	-0.40	9.036362e-01
492	-0.1	-0.04	-0.07	-0.02	-6643.08	-1.12	6.763213e-01
493	-0.04	-0.01	-0.03	0.00	-33255.97	-0.47	2.423556e-01
494	-0.02	-0.01	-0.01	0.00	-196.43	-0.17	1.801764e-01
495	-0.02	-0.01	-0.02	0.00	-52102436.09	-0.43	1.563373e-02
496	-0.03	-0.02	-0.04	0.00	-1470484.58	-0.68	9.399165e-02
497	-0.03	-0.01	-0.01	0.00	-2977037.98	-0.17	1.667707e-03
498	-0.07	-0.03	-0.05	-0.01	-0.13	-0.72	5.894209e-01
499	-0.04	-0.02	-0.03	-0.01	-6720.66	-0.56	4.965568e-01
500	-0.09	-0.01	-0.01	0.00	0	-0.25	1.311877e-01
501	-0.06	-0.01	-0.01	0.00	-7.88304E-06	-0.18	8.157188e-01
502	-0.12	-0.02	-0.03	-0.01	-0.01	-0.48	8.157188e-01
503	-0.03	-0.02	-0.03	0.00	-330341.29	-0.56	2.423556e-01
504	-0.04	-0.01	-0.01	0.00	-0.03	-0.19	4.965568e-01
505	-0.03	-0.01	-0.01	0.00	0	-0.22	4.039296e-01
506	-0.16	-0.03	-0.03	-0.01	-0.01	-0.61	8.157188e-01
507	-0.12	-0.02	-0.02	0.00	0	-0.45	4.039296e-01
508	-0.02	-0.01	-0.02	-0.01	-3421.01	-0.39	4.965568e-01
509	-0.07	-0.04	-0.08	-0.01	-807429.85	-1.49	1.801764e-01
510	-0.04	-0.01	-0.02	-0.01	-19.65	-0.49	6.763213e-01
511	-0.26	-0.02	-0.02	0.00	0	-0.36	5.894209e-01
512	-0.04	-0.01	-0.02	0.00	-139972.01	-0.44	2.423556e-01
513	-0.07	-0.02	-0.02	0.00	0	-0.35	1.311877e-01
514	-0.09	-0.02	-0.02	0.00	0	-0.41	4.039296e-01
515	-0.07	-0.02	-0.02	0.00	-0.02	-0.37	5.894209e-01
516	-0.02	-0.01	-0.02	0.00	-65335.61	-0.27	2.423556e-01
517	-0.06	-0.02	-0.03	0.00	-7903.6	-0.64	1.311877e-01
518	-0.04	-0.02	-0.04	-0.01	-232454.05	-0.70	2.423556e-01
519	-0.14	-0.02	-0.02	-0.01	-72.59	-0.59	4.039296e-01
520	-0.02	-0.01	-0.01	0.00	-355.39	-0.14	1.079400e-02
521	-0.04	-0.02	-0.03	-0.01	-93743.05	-0.55	3.176781e-01
522	-0.02	-0.01	-0.02	-0.01	-338.59	-0.31	5.894209e-01
523	-0.13	-0.02	-0.03	0.00	0	-0.48	4.965568e-01
524	-0.02	-0.01	-0.04	0.00	-847571.77	-0.79	3.255029e-02
525	-0.01	-0.01	-0.01	0.00	-5854498.91	-0.22	1.079400e-02
526	-0.04	-0.02	-0.04	0.00	-118374638.4	-1.03	3.255029e-02
527	-0.16	-0.02	-0.03	0.00	-0.48	-0.56	6.763213e-01
528	-0.14	-0.03	-0.03	0.00	-0.74	-0.77	1.311877e-01
529	-0.19	-0.02	-0.03	0.00	-0.02	-0.55	4.965568e-01
530	-0.03	-0.01	-0.01	0.00	-39166373.09	-0.22	7.441179e-03
531	-0.12	-0.03	-0.04	-0.02	-3.27	-0.94	6.763213e-01
532	-0.09	-0.03	-0.04	-0.02	-141575.73	-0.74	5.894209e-01
533	-0.02	-0.01	-0.02	0.00	-18693501.15	-0.41	2.259390e-02
534	-0.17	-0.02	-0.02	0.00	-0.01	-0.52	4.039296e-01
535	-0.05	-0.02	-0.03	0.00	-151.4	-0.64	3.176781e-01
536	-0.06	-0.01	-0.01	0.00	-17.13	-0.26	3.255029e-02
537	-0.04	-0.02	-0.04	-0.01	-23985.39	-0.75	3.176781e-01
538	-0.05	-0.02	-0.04	-0.01	-15627.94	-0.75	3.176781e-01
539	-0.03	-0.01	-0.03	0.00	-24351923149	-0.53	1.146400e-03
540	-0.03	-0.02	-0.03	0.00	-85196.64	-0.58	2.423556e-01
541	-0.04	-0.02	-0.04	-0.01	-12678.12	-0.59	5.894209e-01
542	-0.04	-0.02	-0.04	-0.01	-162113.99	-0.66	2.423556e-01
543	-0.01	-0.01	-0.01	0.00	-560205.45	-0.17	6.653425e-02
544	-0.03	-0.01	-0.02	0.00	-1053.5	-0.44	2.423556e-01
545	-0.08	-0.03	-0.04	-0.01	-321.02	-1.06	4.039296e-01
546	-0.05	-0.01	-0.01	0.00	-78.87	-0.25	3.526394e-03

547	-0.02	-0.01	-0.01	0.00	-642609.22	-0.21	3.526394e-03
548	-0.03	-0.02	-0.06	0.00	-7932133349	-1.48	2.259390e-02
549	-0.03	-0.02	-0.05	0.00	-67599997780	-1.16	1.079400e-02
550	-0.04	-0.02	-0.05	-0.01	-270694.85	-0.79	2.423556e-01
551	-0.04	-0.02	-0.04	-0.01	-22956.43	-0.72	3.176781e-01
552	-0.05	-0.02	-0.04	-0.01	-18010.23	-0.80	2.423556e-01
553	-0.2	-0.02	-0.02	-0.01	-0.01	-0.41	9.036362e-01
554	-0.02	-0.01	-0.02	0.00	-26133203.04	-0.55	4.668456e-02
555	-0.07	-0.02	-0.03	-0.01	-0.47	-0.46	8.157188e-01
556	-0.1	-0.02	-0.03	-0.01	-0.42	-0.69	4.039296e-01
557	-0.13	-0.03	-0.04	-0.01	-1121.19	-0.84	6.763213e-01
558	-0.03	-0.02	-0.05	-0.01	-816970.32	-0.84	1.311877e-01
559	-0.04	-0.02	-0.06	-0.01	-1038803.17	-1.06	1.311877e-01
560	-0.03	-0.01	-0.02	0.00	-10289.49	-0.42	2.423556e-01
561	-0.03	-0.01	-0.02	0.00	-2739468209	-0.31	2.425494e-03
562	-0.02	-0.01	-0.01	0.00	-4356505807	-0.23	2.425494e-03
563	-0.02	-0.01	-0.02	0.00	-781183935.4	-0.36	1.667707e-03
564	-0.07	-0.02	-0.03	0.00	-0.89	-0.54	4.965568e-01
565	-0.02	-0.01	-0.02	0.00	-1453.09	-0.33	3.176781e-01
566	-0.22	-0.03	-0.04	-0.02	-0.12	-0.88	8.157188e-01
567	-0.04	-0.02	-0.05	-0.01	-4256.92	-0.63	1.801764e-01
568	-0.13	-0.04	-0.06	-0.02	-56.22	-1.15	5.894209e-01
569	-0.07	-0.02	-0.03	0.00	-1.5	-0.44	5.894209e-01
570	-0.06	-0.02	-0.03	0.00	-0.5	-0.64	3.176781e-01
571	-0.09	-0.02	-0.02	0.00	-0.79	-0.43	2.423556e-01
572	-0.19	-0.02	-0.02	0.00	0	-0.57	4.039296e-01
573	-0.09	-0.01	-0.01	0.00	-4.3135E-05	-0.32	2.423556e-01
574	-0.1	-0.01	-0.02	0.00	-0.01	-0.36	1.311877e-01
575	-0.1	-0.01	-0.02	0.00	-0.01	-0.35	1.311877e-01
576	-0.12	-0.02	-0.03	-0.02	-251.35	-0.56	8.656406e-01
577	-0.07	-0.01	-0.01	0.00	-1.54	-0.26	1.563373e-02
578	-0.13	-0.02	-0.02	0.00	-4.39662E-06	-0.42	7.525505e-01
579	-0.03	-0.01	-0.01	0.00	-117.02	-0.20	1.146400e-03
580	-0.09	-0.01	-0.02	0.00	-0.07	-0.32	2.423556e-01
581	-0.03	-0.01	-0.02	0.00	-17510.21	-0.42	3.176781e-01
582	-0.12	-0.02	-0.02	0.00	-14.17	-0.41	5.894209e-01
583	-0.06	-0.02	-0.03	-0.01	-16701.42	-0.68	4.039296e-01
584	-0.14	-0.02	-0.02	0.00	-0.01	-0.43	6.763213e-01
585	-0.06	-0.01	-0.02	0.00	-0.04	-0.38	1.563373e-02
586	-0.04	-0.01	-0.01	0.00	-71.36	-0.23	5.124412e-03
587	-0.05	-0.01	-0.01	0.00	-2.42	-0.22	2.259390e-02
588	-0.05	-0.01	-0.02	0.00	-280.56	-0.35	2.423556e-01
589	-0.06	-0.02	-0.02	0.00	-476.49	-0.49	6.653425e-02
590	-0.04	-0.01	-0.01	0.00	-124.12	-0.22	7.879195e-04
591	-0.09	-0.02	-0.02	0.00	-0.46	-0.42	4.039296e-01
592	-0.11	-0.03	-0.04	-0.02	-2.25	-0.82	6.763213e-01
593	-0.01	0.00	-0.01	0.00	-32688316204	-0.12	7.879195e-04
594	-0.02	-0.01	-0.02	0.00	-20552.83	-0.34	3.176781e-01
595	-0.1	-0.01	-0.02	-0.01	-86.28	-0.44	5.894209e-01
596	-0.79	-0.03	-0.03	-0.02	0	-0.90	7.525505e-01
597	-0.07	-0.02	-0.03	0.00	-25.07	-0.56	2.423556e-01
598	-0.06	-0.02	-0.03	-0.01	-2106.6	-0.63	4.965568e-01
599	-0.05	-0.01	-0.01	0.00	-240.27	-0.26	2.425494e-03
600	-0.05	-0.01	-0.01	0.00	-81.01	-0.25	5.124412e-03
601	-0.06	-0.01	-0.01	0.00	0	-0.23	9.399165e-02
602	-0.04	-0.01	-0.01	0.00	-548.53	-0.20	3.720849e-04
603	-0.06	-0.02	-0.02	0.00	-310.72	-0.38	2.423556e-01
604	-0.12	-0.03	-0.03	-0.01	-0.03	-0.70	5.894209e-01
605	-0.08	-0.01	-0.02	0.00	-0.02	-0.37	9.399165e-02
606	-0.04	-0.01	-0.01	0.00	-80.74	-0.17	2.425494e-03
607	-0.03	-0.01	-0.01	0.00	-1.09	-0.19	3.176781e-01
608	-0.06	-0.01	-0.01	0.00	-0.05	-0.30	4.668456e-02
609	-0.1	-0.01	-0.01	0.00	0	-0.29	4.039296e-01
610	-0.06	-0.01	-0.01	0.00	-0.39	-0.34	9.399165e-02
611	-0.03	-0.01	-0.01	0.00	-2.45	-0.16	2.423556e-01
612	-0.56	-0.03	-0.03	-0.01	-6.5455E-05	-0.62	7.525505e-01
613	-0.06	-0.01	-0.01	0.00	-0.02	-0.31	9.399165e-02
614	-0.11	-0.03	-0.03	0.00	-0.29	-0.71	3.176781e-01
615	-0.02	-0.01	-0.02	0.00	-47775.2	-0.32	2.423556e-01
616	-0.06	-0.01	-0.01	0.00	-7.84	-0.28	1.563373e-02
617	-0.11	-0.03	-0.03	-0.01	-0.05	-0.67	5.894209e-01
618	-0.09	-0.02	-0.03	0.00	-0.65	-0.59	3.176781e-01
619	-0.06	-0.01	-0.01	0.00	-354.16	-0.31	7.441179e-03
620	-0.02	-0.01	-0.01	0.00	-47965.06	-0.27	1.801764e-01
621	-0.18	-0.01	-0.02	-0.01	-2.12189E-06	-0.37	9.036362e-01
622	-0.06	-0.01	-0.01	0.00	-0.08	-0.22	1.801764e-01
623	-0.07	-0.01	-0.01	0.00	-0.02	-0.24	1.801764e-01
624	-0.06	-0.01	-0.01	0.00	0	-0.26	1.801764e-01
625	-0.07	-0.01	-0.01	0.00	-0.06	-0.29	9.399165e-02

626	-0.09	-0.01	-0.01	0.00	-0.01	-0.31	9.399165e-02
627	-0.07	-0.01	-0.01	0.00	-7.73142E-05	-0.28	1.311877e-01
628	-0.07	-0.01	-0.01	0.00	0	-0.30	9.399165e-02
629	-0.06	-0.01	-0.01	0.00	-5.41624E-05	-0.22	2.423556e-01
630	-0.07	-0.01	-0.01	0.00	0	-0.30	9.399165e-02
631	-0.05	-0.01	-0.01	0.00	-50.92	-0.28	2.259390e-02

Validat:

	Name	DG	DrugOrNonDrug	logP	formula
	Acamprosate	-6.80	1	-1.11	C5H11N04S
	acebutolol	-9.38	1	1.68	C18H28N2O4
	acetophenazine	-11.72	1	2.04	C23H29N3O2S
	Agomelatine	-8.96	1	2.76	C15H17N02
	Albendazole	-6.80	1	2.45	C12H15N3O2S
	albuterol_salbutamol	-8.56	1	1.44	C13H21N03
	alcaftadine	-11.57	1	0.75	C19H21N3O
	Alfuzosin	-11.55	1	0.86	C19H27N5O4
	AMOXAPINE	-11.82	1	2.31	C17H16ClN3O
	Atomoxetine	-11.85	1	3.95	C17H21NO
	Atosiban	-11.49	1	-2.86	C43H67N11O12S2
	Benperidol	-14.37	1	2.75	C22H24FN3O2
	BrimonidineGTP	-11.96	1	0.86	C11H10BrN5
	Brompheniramine	-11.17	1	3.41	C16H19BrN2
	capsaicin	-8.36	1	4.58	C18H27N03
	CARBAMAZEPINE	-6.80	1	2.30	C15H12N2O
	Carbinoxamine	-11.74	1	2.62	C16H19ClN2O
	Carnitine	-6.80	1	-2.34	C7H16N03
	carvedilol	-12.18	1	3.37	C24H26N2O4
	Cetirizineplusisomer	-11.55	1	2.81	C21H25ClN2O3
	Chloroquine	-9.47	1	4.01	C18H26ClN3
	ciclesonide	-10.10	1	4.29	C32H44O7
	Cyclopentolate	-11.95	1	2.39	C17H25N03
	CyclosporinA	-8.05	1	4.57	C62H111N11O12
	Darifenacin	-12.34	1	4.54	C28H30N2O2
	Desvenlafaxine	-10.05	1	2.51	C16H25N02
	Dexmedetomidine	-12.23	1	2.32	C13H16N2
	Dichlorphenamide	-10.09	1	1.27	C6H6Cl2N2O4S2
	Dicyclomine	-12.52	1	5.50	C19H35N02
	dienogest	-12.23	1	2.30	C20H25N02
	Diflunisal	-6.91	1	4.69	C13H8F2O3
	Diphenylpyraline	-11.55	1	3.70	C19H23N0
	DOXEPIIN	-13.66	1	3.99	C19H21N0
	Ephedrine-	-10.01	1	1.39	C10H15N0
	erlotinib	-12.04	1	2.54	C22H23N3O4
	Escitalopram	-12.18	1	3.54	C20H21FN2O
	ethopropazine	-10.47	1	4.21	C19H24N2S
	FENOLDOPAM	-11.63	1	2.01	C16H16ClN03
	Fenoprofen	-7.56	1	3.14	C15H14O3
	flumazenil	-12.23	1	0.86	C15H14FN3O3
	Fluvoxamine	-11.96	1	3.20	C15H21F3N2O2
	Gallamine	-7.83	1	3.46	C24H45N3O3
	Gefitinib	-11.89	1	3.02	C22H24ClFN4O3
	Guanfacine	-10.45	1	2.21	C9H9Cl2N3O
	Homatropine	-10.33	1	1.76	C16H21N03
	Hydralazine	-6.95	1	0.37	C8H8N4
	Hydrocodone	-10.81	1	1.19	C18H21N03
	Hydroxyamphetamine	-7.21	1	1.36	C9H13N0
	Hydroxyzine	-12.23	1	2.71	C21H27ClN2O2
	ILOPERIDONE	-13.54	1	4.04	C24H27FN2O4
	Ipratropium	-13.44	1	1.44	C20H30N03
	Ketorolac	-13.21	1	1.33	C15H13N03
	LABETALOL	-10.77	1	2.52	C19H24N2O3
	Lanreotide	-12.64	1	1.82	C54H71N11O10S2
	Mebendazole	-6.80	1	2.54	C16H13N3O3
	Meclizine	-8.97	1	5.76	C25H27ClN2
	Meclofenamate	-9.11	1	4.16	C14H11Cl2N02
	MefenamicAcid	-9.24	1	3.35	C15H15N02
	Meloxicam	-9.32	1	0.27	C14H13N3O4S2
	Menthol	-6.80	1	3.21	C10H20O
	Meperidine	-8.68	1	2.63	C15H21N02
	Methacholine	-10.38	1	-0.72	C8H18N02
	METHAMPHETAMINE	-10.75	1	2.15	C10H15N
	Metoprolol	-10.68	1	1.63	C15H25N03
	Milnacipran	-10.97	1	1.91	C15H22N2O
	mirtazepine	-11.82	1	1.57	C17H19N3
	Montelukast	-11.74	1	7.89	C35H36ClN03S
	Nabilone	-10.40	1	6.80	C24H36O3
	Nabumetone	-6.36	1	3.06	C15H16O2

Nalbuphine	-11.43	1	1.41	C21H27N04
Naphazoline	-11.21	1	2.44	C14H14N2
Nebivolol	-10.31	1	2.74	C22H25F2N04
NOREPINEPHRINE	-12.64	1	0.16	C8H11N03
octreotide	-14.54	1	0.30	C49H66N10O10S2
Oxazepam	-8.78	1	2.84	C15H11ClN2O2
OXPRENOLOL	-11.02	1	2.02	C15H23N03
oxycodone	-10.96	1	0.28	C18H21N04
Oxymorphone	-12.25	1	-0.04	C17H19N04
Oxytocin	-12.64	1	-2.67	C43H66N12O12S2
Pancuronium	-5.77	1	4.42	C35H60N2O4
paracetamol	-6.76	1	0.45	C8H9N02
Pemetrexed	-7.04	1	0.53	C20H21N5O6
Pentagastrin	-12.37	1	1.31	C37H49N7O9S
Pentazocine	-11.77	1	3.69	C19H27N0
Pentoxifylline	-5.58	1	-1.69	C13H18N4O3
Phenelzine	-6.90	1	1.08	C8H12N2
PHENOXYBENZAMINE	-12.30	1	4.72	C18H22ClN0
Protriptyline	-12.03	1	4.72	C19H21N
ROFECOXIB	-10.53	1	3.21	C17H14O4S
Succinylcholine	-7.53	1	-2.91	C14H30N2O4
Sulfasalazine	-3.54	1	1.51	C18H14N4O5S
Sulindac	-6.26	1	3.55	C20H17F03S
Suprofen	-8.10	1	2.24	C14H12O3S
tadalafil	-10.89	1	1.47	C22H19N3O4
Tamsulosin	-12.53	1	2.86	C20H28N2O5S
Tetrahydrozoline	-10.82	1	1.95	C13H16N2
Thiabendazole	-8.60	1	1.77	C10H7N3S
Thiothixene	-14.30	1	3.14	C23H29N3O2S2
2g94	-12.99	0	1.57	C30H54N6O8S
2gyi	-9.55	0	-3.04	C4H9N05
2gzl	-6.58	0	-2.92	C23H31N5O13P2S
2h15	-7.74	0	-0.42	C12H22N2O7S
2h3e	-7.77	0	-4.05	C6H11N2O7P
2h5a	-6.95	0	-3.33	C5H11O8P
2h6t	-9.85	0	2.76	C34H63N5O9
2ha2	-6.35	0	-2.91	C14H30N2O4
2hrm	-4.85	0	-4.50	C10H16N2O10P2
2hw2	-4.05	0	2.11	C43H58N4O12
2i2c	-6.41	0	-3.45	C20H24N10O6S2
2i2e	-6.00	0	-8.99	C20H27N10O16P3
2i4j	-8.41	0	5.72	C27H36N2O4
2i4w	-15.80	0	2.44	C33H49N2O12PS
2i4z	-7.78	0	5.72	C27H36N2O4
2iuz	-7.57	0	-4.63	C16H18N8O4
2j4k	-6.62	0	-4.15	C9H13N2O9P
2j7d	-9.73	0	-3.40	C10H16N2O6
2j7f	-8.66	0	-5.19	C9H12N2O6
2j7g	-9.55	0	-3.21	C10H14N2O6
2jh5	-8.78	0	-0.53	C17H22ClN3O5S2
2nsj	-6.53	0	-6.00	C9H14N3O9P
2o1c	-6.44	0	-3.48	H407P2
2o2u	-8.73	0	3.03	C16H13FN2O5
2o4j	-13.77	0	2.88	C27H42O3
2o4k	-14.26	0	4.55	C38H52N6O7
2o4r	-12.82	0	2.88	C27H42O3
2o8h	-10.37	0	-0.05	C24H29N5O4S
2oag	-11.55	0	2.40	C21H19F3N4O2S
2oi2	-8.60	0	-3.31	C6H14O10P2
2ov4	-6.47	0	-7.86	C10H17N5O16P4
2oxd	-9.31	0	3.68	C7H2Br4N2O
2oxx	-9.14	0	3.93	C7H2Br4N2S
2oxy	-8.90	0	4.03	C7H2Br4N2
2oyk	-7.23	0	-3.74	C12H23N08
2p2a	-8.36	0	-4.37	C14H14N6O4
2p3b	-11.57	0	5.54	C50H64N6O10
2p4y	-12.28	0	6.73	C28H22ClF3N2O6
2pq9	-11.06	0	-4.42	C10H14F2O14P2
2pu1	-7.99	0	-2.64	C2H5FN05P
2q8z	-7.75	0	-4.12	C9H14N3O9P
2qbq	-10.15	0	5.97	C23H28BrN05S
2qnn	-9.76	0	3.00	C34H31F6N5O6S2
2qnp	-8.74	0	5.52	C30H29I2N3O4S2
2qpu	-4.91	0	-4.09	C19H35N012
2qv4	-3.46	0	-8.78	C31H53N023
2r1y	-6.15	0	-2.39	C8H14O7
2r2b	-5.73	0	-6.59	C27H42O22

	2r6w	-12.76	0	5.70	C29H29N04S
	2rke	-5.57	0	-1.79	C2H405S
	2rkp	-6.19	0	0.35	C12H12Cl2N204
	2uwd	-11.39	0	2.47	C19H17ClN205
	2uxz	-11.57	0	5.17	C36H45BrN406
	2uy0	-9.44	0	4.63	C36H43BrN407
	2v00	-4.99	0	1.64	C12H13N30
	2v8w	-9.31	0	-5.54	C11H19N5014P3
	2vpn	-9.17	0	-0.75	C6H10N202
	2zb0	-9.03	0	6.58	C24H20N402
	2zcq	-12.04	0	1.30	C16H1907PS
	3b2t	-7.10	0	-4.41	C11H17N509P2
	3b5j	-7.75	0	-5.05	C16H16N8016P2
	3b68	-11.46	0	2.25	C19H18F3N306
	3baj	-4.22	0	-8.45	C31H55N023
	3bc3	-9.29	0	6.71	C47H55N705S
	3bft	-8.85	0	-3.84	C5H11N303S
	3bfu	-8.56	0	-3.84	C5H11N303S
	3bgz	-8.54	0	5.37	C21H15N02
	3bkk	-8.30	0	3.12	C28H30N206
	3bkl	-8.41	0	2.89	C30H31N306
	3bva	-8.90	0	-0.36	C35H67N1108
	3c1k	-12.88	0	-0.25	C26H34N605S
	3c56	-10.76	0	-4.68	C5H13N010P2
	3cct	-10.32	0	5.13	C33H35FN206
	3ccw	-6.64	0	2.36	C27H32FN305
	3ccz	-9.94	0	1.76	C28H34FN306
	3cd0	-10.33	0	2.76	C27H31F2N305
	3cd5	-10.77	0	3.79	C31H36N205
	3cd7	-10.70	0	5.50	C33H34F2N205
	3cda	-10.34	0	4.34	C33H36FN307S
	3cdb	-9.57	0	3.72	C33H35F2N307S
	3cj5	-8.64	0	2.41	C22H30BrN304
	3cke	-8.32	0	1.24	C15H26F207P2
	3cm2	-8.82	0	2.40	C28H37N503
	3cow	-9.42	0	-3.08	C16H24N608S
	3coy	-8.21	0	-3.15	C16H25N707S
	3coz	-7.60	0	-3.54	C15H23N707S
	3cpj	-6.44	0	-5.95	C10H15N5011P2
	3cs7	-14.57	0	3.68	C28H29F3N402
	3d0e	-11.46	0	1.53	C21H27N703
	3d1x	-11.81	0	3.83	C38H50N605
	3d4z	-6.67	0	-2.73	C8H12N204
	3d50	-6.51	0	1.88	C15H29N04
	3d52	-4.48	0	-0.41	C13H16ClN306
	3d7k	-6.28	0	-3.86	C20H29N4011P3S
	3d83	-11.40	0	3.71	C28H30N403
	3d94	-9.28	0	3.79	C30H31N7
	3dd8	-10.71	0	3.68	C16H21N05S2
	3ddf	-6.35	0	-0.71	C13H18N204
	3ddg	-8.18	0	-0.57	C14H20N204
	3dj k	-14.44	0	2.46	C27H38N208S
	3e5a	-11.23	0	1.37	C23H28N80S
	3e5u	-7.99	0	1.67	C8H7Cl03
	3e64	-9.70	0	3.01	C17H20N402S
	3e8r	-13.29	0	3.21	C28H25N304
	3e93	-12.08	0	4.13	C30H32N403
	3ebl	-8.60	0	1.91	C19H2405
	3eeb	-8.03	0	-11.41	C6H18024P6
	3eko	-9.14	0	1.41	C11H9N04
	3eqr	-11.87	0	2.26	C29H38N80
	3f15	-11.05	0	-2.45	C12H18N207S
	3f16	-11.22	0	-1.37	C10H14N206S
	3f17	-11.77	0	1.15	C14H14N204S
	3f18	-10.10	0	-1.53	C10H13FN205S
	3f19	-9.80	0	-0.63	C8H9FN204S
	3f1a	-9.84	0	-0.79	C8H10N204S
	3f80	-5.76	0	-2.20	C6H12N204
	3f8c	-10.47	0	2.81	C27H28N60
	3f8f	-9.04	0	0.14	C27H29N010
exactmass	NumberofCarbons	wienerindex	MSA	PSA	apolarsurfacearea
181.04	5	190	227.61	79.82	147.79
336.20	18	1568	483.07	63.60	419.47
411.20	23	2410	541.66	103.37	438.29
243.13	15	642	339.35	26.30	313.05
265.09	12	676	336.86	92.31	244.55
239.15	13	560	352.71	60.69	292.02

307.17	19	1053	398.78	48.48	350.30
389.21	19	2380	519.46	84.13	435.33
313.10	17	936	375.53	35.18	340.35
255.16	17	728	378.73	9.23	369.50
993.44	43	22869	1243.34	264.35	978.99
381.19	22	2452	491.11	66.80	424.31
291.01	11	515	272.57	30.82	241.75
318.07	16	718	381.41	26.48	354.93
305.20	18	1411	446.24	46.53	399.71
236.09	15	521	282.92	20.31	262.61
290.12	16	851	391.32	35.71	355.61
162.11	7	170	248.63	57.53	191.10
406.19	24	3062	539.27	63.71	475.56
388.16	21	2068	502.84	73.71	429.13
319.18	18	1212	455.52	26.48	429.04
540.31	32	4484	690.88	99.13	591.75
291.18	17	929	418.41	60.12	358.29
1201.84	62	37337	1731.15	303.13	1428.02
426.23	28	2965	571.10	39.89	531.21
263.19	16	672	391.69	54.05	337.64
200.13	13	353	297.45	28.68	268.77
303.91	6	398	290.41	85.04	205.37
309.27	19	1099	483.20	39.89	443.31
311.19	20	1082	396.92	61.09	335.83
250.04	13	597	279.33	57.53	221.80
281.18	19	930	401.47	22.82	378.65
279.16	19	882	388.09	22.82	365.27
165.12	10	202	250.50	20.23	230.27
393.17	22	2396	516.39	62.70	453.69
324.16	20	1298	440.50	46.61	393.89
312.17	19	988	436.11	52.48	383.63
305.08	16	851	365.08	60.69	304.39
242.09	15	650	318.55	46.53	272.02
303.10	15	956	363.94	74.78	289.16
318.16	15	1216	421.74	30.82	390.92
423.35	24	2827	681.69	68.46	613.23
446.15	22	3020	551.05	67.06	483.99
245.01	9	384	266.24	29.43	236.81
275.15	16	854	362.81	60.12	302.69
160.07	8	182	202.90	25.78	177.12
299.15	18	824	378.93	49.12	329.81
151.10	9	166	224.21	20.23	203.98
374.18	21	1831	503.48	56.64	446.84
426.20	24	3379	554.58	75.15	479.43
332.22	20	1371	467.58	46.53	421.05
255.09	15	693	312.23	59.30	252.93
328.18	19	1607	444.66	57.53	387.13
1097.48	54	33809	1380.40	270.41	1109.99
295.10	16	1138	356.93	84.08	272.85
390.19	25	2177	526.61	27.18	499.43
295.02	14	682	335.75	37.30	298.45
241.11	15	602	324.48	37.30	287.18
351.03	14	1115	364.27	131.07	233.20
156.15	10	150	257.42	20.23	237.19
247.16	15	568	359.60	39.89	319.71
160.13	8	170	268.52	26.30	242.22
149.12	10	168	241.09	12.00	229.09
267.18	15	906	406.31	38.69	367.62
246.17	15	572	367.59	30.66	336.93
265.16	17	687	356.71	40.07	316.64
585.21	35	6351	744.08	95.72	648.36
372.27	24	1826	556.09	46.53	509.56
228.12	15	566	320.42	26.30	294.12
357.19	21	1356	450.32	83.51	366.81
210.12	14	431	280.75	12.36	268.39
405.18	22	2692	500.21	58.92	441.29
169.07	8	198	220.59	60.69	159.90
1018.44	49	23347	1271.70	246.57	1025.13
286.05	15	727	320.86	49.66	271.20
265.17	15	834	383.53	38.69	344.84
315.15	18	907	393.63	69.35	324.28
301.13	17	788	364.28	80.35	283.93
1006.44	43	23044	1241.87	272.19	969.68
572.46	35	5163	829.32	52.60	776.72
151.06	8	166	201.60	37.30	164.30
427.15	20	3252	511.67	151.56	360.11
767.33	37	13349	975.17	190.04	785.13

285.21	19	870	415.13	33.82	381.31
278.14	13	834	374.93	78.89	296.04
136.10	8	133	208.02	38.00	170.02
303.14	18	1046	419.40	22.82	396.58
263.17	19	759	368.31	12.00	356.31
314.06	17	1061	370.04	68.82	301.22
290.22	14	1078	459.06	52.60	406.46
398.07	18	2428	423.24	134.17	289.07
356.09	20	1517	420.13	73.58	346.55
260.05	14	653	311.81	82.61	229.20
389.14	22	1914	458.55	95.57	362.98
408.17	20	2488	549.85	70.21	479.64
200.13	13	339	273.57	12.36	261.21
201.04	10	293	213.16	66.34	146.82
443.17	23	2491	567.55	108.59	458.96
658.37	30	8439	913.83	158.08	755.75
151.05	4	125	184.45	110.02	74.43
679.11	23	8407	774.21	262.60	511.61
338.11	12	948	424.05	88.67	335.38
254.03	6	476	283.59	138.78	144.81
230.02	5	296	248.53	146.49	102.04
685.46	34	10287	978.20	163.11	815.09
290.22	14	1078	459.05	52.60	406.45
386.03	10	1460	404.62	202.55	202.07
822.41	43	13890	1029.90	213.30	816.60
564.13	20	5399	606.67	237.18	369.49
756.08	20	10498	785.94	364.83	421.11
452.27	27	3755	640.38	81.71	558.67
728.27	33	10137	941.60	184.90	756.70
452.27	27	3755	641.07	81.71	559.36
386.15	16	1944	476.17	123.64	352.53
324.04	9	948	330.07	175.67	154.40
260.10	10	556	314.45	128.20	186.25
244.07	9	465	274.63	136.04	138.59
258.09	10	569	299.64	136.04	163.60
447.07	17	2289	501.15	141.31	359.84
339.05	9	1077	365.75	181.38	184.37
177.94	0	88	178.09	143.91	34.18
300.07	16	925	346.77	81.13	265.64
414.31	27	2717	588.17	60.69	527.48
704.39	38	10532	971.67	145.48	826.19
414.31	27	2717	587.96	60.69	527.27
483.19	24	3364	613.81	127.53	486.28
448.12	21	2828	514.95	81.89	433.06
308.01	6	693	350.32	190.44	159.88
586.96	10	4121	589.29	338.88	250.41
445.69	7	262	262.68	45.35	217.33
461.67	7	262	272.66	60.37	212.29
429.70	7	211	247.88	28.68	219.20
309.14	12	894	378.29	139.84	238.45
330.11	14	1446	374.12	118.18	255.94
908.47	50	23427	1201.50	161.34	1040.16
574.11	28	5277	658.75	95.95	562.80
457.98	10	1875	445.93	257.20	188.73
172.99	2	118	177.75	116.67	61.08
339.05	9	1051	352.71	199.52	153.19
509.09	23	2818	586.90	112.07	474.83
783.16	34	10875	867.44	146.36	721.08
812.97	30	5195	753.83	112.22	641.61
469.22	19	2939	566.81	209.76	357.05
807.30	31	13968	920.64	388.29	532.35
222.07	8	350	259.21	127.45	131.76
718.22	27	8254	821.33	369.58	451.75
487.18	29	4229	616.68	108.59	508.09
139.98	2	66	146.88	100.05	46.83
318.02	12	764	336.85	87.74	249.11
388.08	19	1761	419.97	72.83	347.14
708.25	36	8580	882.27	126.52	755.75
722.23	36	8880	878.41	133.24	745.17
215.11	12	485	286.86	44.10	242.76
538.01	11	3372	565.72	290.80	274.92
142.07	6	117	183.44	49.66	133.78
396.16	24	2809	503.20	79.84	423.36
386.06	16	1720	461.31	139.32	321.99
425.05	11	1925	461.88	205.97	255.91
638.02	16	5566	642.36	318.30	324.06
441.11	19	3128	518.36	109.42	408.94

809.32	31	14124	936.89	388.29	548.60
829.40	47	17871	1053.47	126.17	927.30
193.05	5	205	219.28	82.83	136.45
193.05	5	205	218.02	82.83	135.19
313.11	21	1205	391.35	53.09	338.26
490.21	28	4442	623.47	111.90	511.57
529.22	30	5517	663.14	127.69	535.45
769.52	35	13642	1067.14	152.08	915.06
542.23	26	5445	693.87	127.15	566.72
309.00	5	759	343.44	193.68	149.76
574.25	33	5714	734.60	119.99	614.61
497.23	27	4261	643.53	112.65	530.88
527.24	28	4816	678.41	132.88	545.53
515.22	27	4634	650.85	112.65	538.20
516.26	31	5165	673.86	99.76	574.10
576.24	33	5733	730.05	99.76	630.29
637.23	33	7122	788.64	142.28	646.36
655.22	33	7338	797.65	142.28	655.37
479.14	22	2704	562.34	87.62	474.72
418.11	15	2300	508.50	132.91	375.59
491.29	28	3949	645.90	64.80	581.10
460.14	16	2911	538.66	182.34	356.32
459.15	16	2911	542.68	162.11	380.57
445.14	15	2661	513.22	162.11	351.11
443.02	10	2115	459.30	271.27	188.03
510.22	28	4519	635.09	59.90	575.19
425.22	21	2645	551.64	99.09	452.55
670.38	38	9512	886.57	114.99	771.58
200.08	8	262	238.15	98.74	139.41
287.21	15	986	411.69	80.92	330.77
345.07	13	1344	384.12	131.61	252.51
626.08	20	4820	719.04	274.15	444.89
470.23	28	4403	611.52	69.85	541.67
489.26	30	4583	631.19	70.26	560.93
371.09	16	1364	434.73	94.27	340.46
266.13	13	754	338.80	77.76	261.04
280.14	14	846	366.62	91.35	275.27
550.23	27	4846	722.41	130.33	592.08
464.21	23	3554	588.66	124.01	464.65
186.01	8	205	212.32	57.53	154.79
344.13	17	1429	444.98	71.20	373.78
467.18	28	4261	583.74	88.52	495.22
496.25	30	4905	644.80	65.92	578.88
332.16	19	1002	398.31	83.83	314.48
659.86	6	3300	628.58	459.42	169.16
219.05	11	417	260.77	82.69	178.08
514.32	29	5130	718.04	66.42	651.62
334.08	12	1069	407.96	155.13	252.83
290.06	10	740	345.11	121.31	223.80
306.07	14	1040	368.15	91.85	276.30
292.05	10	708	340.32	125.67	214.65
248.03	8	473	277.95	91.85	186.10
230.04	8	392	270.03	91.85	178.18
176.08	6	247	235.07	83.12	151.95
452.23	27	4027	591.58	93.77	497.81
527.18	27	4100	619.58	159.82	459.76
donorCount	acceptorCount	rotatablebondCount	atomCount	hydrogenCount	NHA
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1	6	7	58	29	29
1	3	4	35	17	18
2	5	5	33	15	18
4	4	5	38	21	17
0	3	1	44	21	23
2	9	8	55	27	28
1	4	0	38	16	22
1	2	6	40	21	19
11	25	18	135	67	68
1	5	6	52	24	28
2	5	1	27	10	17
0	2	5	38	19	19
2	4	9	49	27	22
1	3	0	30	12	18
0	4	6	39	19	20
2	4	4	27	16	11
3	5	10	56	26	30
1	6	8	52	25	27

1	4	8	48	26	22
1	7	6	83	44	39
1	4	7	46	25	21
5	23	15	196	111	85
1	4	7	62	30	32
2	3	4	44	25	19
1	1	2	31	16	15
2	8	2	22	6	16
0	3	8	57	35	22
1	3	2	48	25	23
2	5	2	26	8	18
0	2	4	44	23	21
0	2	3	42	21	21
2	2	3	27	15	12
1	7	11	52	23	29
0	4	6	45	21	24
0	3	5	46	24	22
4	5	1	37	16	21
1	2	4	32	14	18
0	6	3	36	14	22
1	7	10	43	21	22
0	6	18	75	45	30
1	9	8	55	24	31
2	6	2	24	9	15
1	4	4	41	21	20
2	4	1	20	8	12
0	4	1	43	21	22
2	2	2	24	13	11
1	5	8	53	27	26
0	6	8	58	27	31
1	4	6	54	30	24
1	3	3	32	13	19
4	5	8	48	24	24
15	22	29	148	71	77
2	5	4	35	13	22
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2	3	3	33	15	18
2	8	1	36	13	23
1	1	1	31	20	11
0	3	4	39	21	18
0	3	4	29	18	11
1	1	3	26	15	11
2	4	9	44	25	19
1	3	5	40	22	18
0	3	0	39	19	20
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1	2	2	30	14	16
3	7	6	54	25	29
4	4	2	23	11	12
13	21	17	137	66	71
2	5	1	31	11	20
2	4	9	42	23	19
1	5	1	44	21	23
2	5	0	41	19	22
12	26	17	135	66	69
0	6	6	101	60	41
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6	10	9	52	21	31
8	16	23	103	49	54
1	2	2	48	27	21
0	4	5	38	18	20
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0	3	8	43	22	21
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2	7	11	56	28	28
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1	3	1	21	7	14

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5	6	3	19	9	10
6	17	12	75	31	44
2	9	2	44	22	22
5	9	6	27	11	16
5	8	2	25	11	14
8	14	22	111	63	48
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5	12	6	40	16	24
6	16	5	117	58	59
6	16	7	62	24	38
9	24	12	76	27	49
1	6	13	69	36	33
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1	6	13	69	36	33
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5	7	3	32	14	18
1	10	5	50	22	28
6	11	5	36	14	22
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7	9	4	44	23	21
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8	16	25	130	64	66
1	10	8	62	22	40
7	16	9	42	14	28
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6	12	4	36	14	22
3	7	7	59	28	31
3	17	12	84	31	53
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10	13	5	67	35	32
17	24	12	108	53	55
5	7	3	29	14	15
13	22	15	91	42	49
2	6	7	64	29	35
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3	7	2	32	12	20
3	8	4	44	17	27
5	10	15	92	45	47
5	11	14	91	43	48
2	4	3	29	13	16
8	19	8	52	19	33
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2	5	5	50	20	30
3	6	8	44	19	25
5	13	6	44	17	27
4	23	7	58	16	42
3	12	8	49	18	31
17	24	12	110	55	55
7	13	21	115	55	60
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2	2	3	39	15	24
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11	19	29	121	67	54
2	10	9	72	34	38
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5	8	12	77	35	42
4	8	12	68	32	36
5	9	13	72	34	38
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4	8	12	76	34	42
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5	11	13	81	35	46
1	7	5	60	30	30
3	9	13	52	26	26
4	8	8	73	37	36
5	13	6	55	24	31
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5	13	6	53	23	30
8	14	6	43	15	28
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4	5	1	26	12	14
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6	10	4	39	16	23
6	16	12	68	29	39
2	7	7	65	30	35
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1	6	4	45	21	24
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2	10	12	76	38	38
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12	24	12	54	18	36
3	4	1	25	9	16
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molecularpolarizability	aliphaticringCount	aromaticringCount			
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36.87	0	1			
46.90	2	2			
29.02	0	2			
28.97	1	1			
26.61	0	1			
35.24	3	1			
41.35	2	1			
33.85	2	2			
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99.60	2	1			
40.80	2	2			
25.39	2	1			
32.45	1	1			
34.81	0	1			
27.07	1	2			
32.52	1	1			
16.58	0	0			
47.94	0	4			
42.30	1	2			
38.25	1	1			
58.15	6	0			
32.84	1	1			
129.41	1	0			
49.84	2	3			
30.72	1	1			
23.99	1	1			
26.39	0	1			
36.70	2	0			
35.00	4	0			
23.94	0	2			
34.27	1	2			
34.19	1	2			
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35.71	1	2
37.89	1	2
31.76	1	2
26.96	0	2
29.87	2	1
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50.14	0	1
46.15	2	2
23.35	0	1
30.28	2	1
18.64	0	2
32.47	4	1
17.95	0	1
42.09	1	2
45.71	1	3
37.58	2	1
27.10	1	2
36.95	0	2
118.41	0	5
32.09	1	2
46.69	1	3
29.64	0	2
27.37	0	2
34.54	2	1
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28.55	1	1
17.83	0	0
19.21	0	1
30.35	0	1
28.99	1	1
31.28	3	1
67.57	2	3
43.40	2	1
27.91	0	2
38.25	5	1
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40.25	2	2
17.44	0	1
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30.19	0	1
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31.21	4	1
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41.60	1	2
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34.61	2	1
27.84	2	0
16.82	0	1
35.02	0	2
33.57	1	2
33.58	1	2
31.27	0	0
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37.72	1	2
27.01	0	2
41.52	3	3
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23.12	2	1
50.61	2	2
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20.44	0	0
17.70	1	0
72.22	0	0
31.27	0	0
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62.99	6	0
50.77	1	2

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36.18	4	0
26.17	2	0
23.33	2	0
21.15	2	0
22.87	2	0
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27.48	2	0
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29.75	1	2
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77.42	1	2
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44.80	3	0
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26.78	1	1
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56.29	0	5
32.73	1	0
11.48	0	0
27.20	2	0
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71.62	1	4
72.97	1	4
43.14	3	0
71.20	5	0
19.06	1	0
61.85	3	0
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10.65	0	0
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38.48	2	1
71.82	1	3
71.77	1	3
23.53	1	1
41.85	3	0
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37.94	0	2
71.46	5	0
92.13	1	4
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52.60	0	3
57.79	0	4
79.87	0	0
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23.42	0	0
63.35	0	4
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58.47	1	3
62.34	0	4
68.68	0	4
67.94	0	4
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43.19	3	0
41.37	3	0
34.83	3	0
51.28	4	2
45.28	3	1
75.01	3	2

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	31.13		1		1
	56.87		2		1
	53.48		3		2
	61.18		5		2
	38.22		2		1
	27.26		1		1
	29.09		1		1
	57.48		1		2
	49.70		4		1
	17.54		0		1
	40.13		1		2
	53.66		2		3
	57.87		2		4
	34.23		5		0
	45.61		1		0
	21.69		0		2
	58.30		3		2
	31.41		0		1
	27.08		0		1
	32.87		0		2
	26.12		0		1
	21.80		0		1
	22.02		0		1
	16.32		0		0
	55.22		3		3
	52.29		3		2
aromaticatomCount	balabanindex	hararyindex	bondCount	hyperwienerindex	
0	3.15	23.81	21		530
6	2.42	79.51	52		6784
12	1.24	112.32	61		10772
10	1.74	55.09	36		2083
6	1.67	54.29	34		2362
6	2.25	49.66	38		1788
6	1.53	86.57	47		3256
6	1.32	103.22	57		11517
12	1.57	80.78	41		2813
12	1.69	59.32	41		2311
6	1.88	376.32	137		160243
12	1.12	103.63	55		12374
6	1.33	52.82	29		1527
6	1.72	59.85	39		2256
6	2.02	66.80	49		6722
12	1.85	60.41	32		1332
6	1.88	63.78	40		2849
0	3.61	24.75	26		417
19	1.01	112.14	59		16535
12	1.44	98.42	54		9281
6	1.57	71.86	49		4904
0	1.26	189.67	88		19780
6	1.90	70.23	47		3078
0	4.22	539.73	196		260224
18	1.24	134.13	66		13271
6	1.85	61.83	45		1979
6	1.83	43.54	32		920
6	2.86	48.63	22		1001
0	1.75	74.21	58		3946
0	1.50	87.54	51		3595
12	1.86	56.92	27		1793
12	1.39	70.63	46		3070
12	1.48	72.71	44		2780
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12	1.44	110.02	54		10435
12	1.59	87.89	47		4554
12	1.73	78.16	48		3136
12	1.53	74.31	39		2609
12	1.69	54.80	33		2135
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6	2.62	108.53	75		13204
12	1.12	120.93	58		14698
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6	1.50	87.32	47		2211
6	1.97	25.65	24		408

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12	1.58	80.29	49	7193
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12	1.50	74.83	37	4359
18	1.28	106.69	58	9430
12	1.80	61.64	31	2046
12	1.83	56.36	34	1799
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6	1.99	57.57	40	1590
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6	1.94	25.38	26	413
6	1.94	54.58	44	3788
6	2.00	57.04	41	1601
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18	1.08	179.93	81	35269
6	1.65	105.21	65	7273
10	1.77	50.45	34	1881
6	1.29	110.71	58	4276
10	1.41	48.26	32	1205
12	1.08	108.95	57	13790
6	2.39	30.04	23	473
21	1.44	412.06	141	145934
12	1.63	69.35	33	2076
6	2.12	55.79	42	3116
6	1.49	94.40	48	2432
6	1.57	89.12	45	2008
6	1.92	388.40	137	156187
0	1.19	203.27	106	23725
6	1.97	25.65	20	408
11	1.34	117.91	54	17402
15	1.70	259.79	105	87384
6	1.52	74.49	50	2798
0	1.93	65.77	39	2839
6	2.02	21.64	22	323
12	1.64	66.57	44	3926
12	1.57	68.05	43	2282
12	1.61	76.98	38	3738
0	3.60	57.42	49	4741
6	1.28	102.69	44	12034
12	1.46	92.19	44	5806
11	1.69	55.20	31	2194
15	1.10	125.14	53	6568
12	1.56	100.07	57	12466
6	1.59	44.87	33	851
6	1.61	40.07	23	754
12	1.29	120.70	62	10546
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0	1.84	80.86	46	2928
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0	3.60	57.42	49	4741
0	1.78	83.97	41	5907
6	1.41	331.33	121	78198
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0	0.93	238.14	81	69348
12	1.32	127.96	71	19693
12	1.35	231.20	101	61625
12	1.32	127.96	71	19693
0	1.42	113.28	49	7462
0	1.87	70.66	35	3279
0	2.04	58.60	35	1542
0	2.19	54.26	30	1214
0	2.00	58.12	33	1624
5	1.37	104.48	52	10574
0	1.81	75.78	37	3839
0	3.75	18.75	12	173
11	1.39	71.72	36	3093
0	1.54	116.88	74	12917
12	1.79	248.27	105	59701
0	1.54	116.88	74	12917

12	1.24	148.74	67	14958
12	1.20	125.84	53	12970
0	4.10	52.33	31	2419
0	1.51	146.66	54	21457
6	2.19	41.13	17	585
6	2.19	41.13	17	585
6	1.87	36.83	16	444
0	1.96	71.70	45	2846
6	1.40	84.40	40	5778
24	1.35	345.51	133	181990
24	1.27	184.76	66	25670
0	3.23	110.31	42	6685
0	3.94	22.10	14	245
0	1.85	76.45	37	3640
11	1.57	124.40	61	12726
24	1.36	277.51	88	59505
24	1.34	195.71	74	23022
0	1.59	133.49	69	13023
0	1.12	283.57	112	97732
0	2.50	42.90	29	891
0	1.97	255.47	93	40542
21	1.04	146.02	68	22817
0	3.39	15.17	11	127
6	1.56	68.81	34	2358
6	1.71	104.59	46	6471
18	1.45	222.00	95	47335
18	1.46	231.29	94	48564
6	1.48	45.53	30	1538
0	1.48	136.99	54	16170
0	2.32	22.72	20	245
23	1.13	115.83	53	13870
12	1.61	86.82	45	7495
0	1.54	102.71	46	8008
0	1.33	205.31	62	25420
12	1.70	119.03	50	16043
0	1.10	282.68	114	100180
24	1.14	298.68	119	123821
0	2.30	29.58	23	504
0	2.30	29.58	23	504
21	1.46	90.92	42	3860
18	1.47	147.81	68	22649
21	1.25	167.62	73	29740
0	5.98	254.28	120	91723
6	1.49	159.00	74	31413
0	3.72	50.33	30	2926
23	1.63	198.74	80	26675
12	1.58	150.59	70	20790
12	1.72	164.41	74	23650
12	1.53	156.27	70	23303
17	1.31	163.05	77	28205
23	1.63	198.25	79	26821
23	1.50	217.15	84	36285
23	1.52	226.97	84	36655
6	1.51	115.37	62	12532
0	3.77	83.40	51	12494
12	1.34	157.90	76	17948
0	1.51	123.80	57	13760
0	1.51	123.80	58	13760
0	1.55	117.78	55	12310
0	1.50	108.54	45	8949
12	1.11	164.59	71	22935
5	1.31	126.89	61	10937
12	1.16	238.43	103	54001
0	2.19	40.97	27	581
0	2.21	60.56	49	4019
6	1.75	77.57	40	5480
6	1.82	178.04	70	22410
12	0.99	142.56	69	24695
12	0.93	163.91	74	23551
6	1.49	87.22	47	5171
6	1.61	59.40	38	2544
6	1.86	64.81	41	2863
12	1.68	163.18	78	23746
6	1.10	132.35	65	17644
6	2.30	29.69	19	510
12	1.40	86.30	46	5744
18	1.02	144.94	64	22908

21	1.00	159.15	74	27311		
0	1.47	101.24	52	2692		
0	3.94	165.66	54	11784		
11	1.77	48.24	26	1118		
12	1.17	164.30	80	27512		
6	2.76	73.93	40	3679		
6	2.41	59.14	33	2459		
12	1.68	68.15	36	4021		
6	2.54	59.81	32	2207		
6	2.37	45.37	25	1460		
6	2.19	41.16	25	1144		
0	3.20	26.92	23	739		
18	0.88	140.59	67	22373		
12	1.48	182.48	71	17274		
plattindex	randicindex	ringCount	szegedindex	wienerpolarity	DG_NHA	DG_MW
74	9.38	0	190	8	-0.62	-0.04
184	22.52	1	1982	31	-0.39	-0.03
220	25.56	4	4062	47	-0.40	-0.03
122	15.50	2	1028	25	-0.50	-0.04
114	14.64	2	933	23	-0.38	-0.03
132	16.70	1	744	22	-0.50	-0.04
170	19.46	4	1748	42	-0.50	-0.04
202	24.07	3	3424	43	-0.41	-0.03
142	17.15	4	1721	39	-0.54	-0.04
140	17.69	2	1028	25	-0.62	-0.05
494	58.76	3	35148	106	-0.17	-0.01
198	23.04	4	3654	43	-0.51	-0.04
96	12.31	3	890	24	-0.70	-0.04
134	16.79	2	1042	25	-0.59	-0.04
172	21.28	1	1675	26	-0.38	-0.03
102	13.84	3	928	33	-0.38	-0.03
136	17.25	2	1196	26	-0.59	-0.04
94	11.54	0	170	9	-0.62	-0.04
200	25.18	4	4077	45	-0.41	-0.03
190	23.02	3	3070	38	-0.43	-0.03
176	20.85	2	1717	31	-0.43	-0.03
350	35.77	6	7838	83	-0.26	-0.02
172	19.98	2	1128	29	-0.57	-0.04
734	83.32	1	63427	150	-0.09	-0.01
236	27.64	5	4201	54	-0.39	-0.03
166	19.14	2	996	28	-0.53	-0.04
110	13.69	2	508	21	-0.82	-0.06
72	9.77	1	580	25	-0.63	-0.03
230	23.99	2	1441	34	-0.57	-0.04
202	20.80	4	2152	47	-0.53	-0.04
82	12.09	2	984	28	-0.38	-0.03
164	19.42	3	1458	29	-0.55	-0.04
152	18.65	3	1385	35	-0.65	-0.05
92	11.89	1	283	15	-0.83	-0.06
178	23.30	3	3792	43	-0.42	-0.03
166	19.92	3	1925	39	-0.51	-0.04
170	20.26	3	1741	37	-0.48	-0.03
132	16.83	3	1449	39	-0.55	-0.04
106	14.53	2	990	24	-0.42	-0.03
130	16.07	3	1501	41	-0.56	-0.04
150	18.63	1	1531	28	-0.54	-0.04
276	31.87	1	3326	41	-0.26	-0.02
202	24.43	4	4768	48	-0.38	-0.03
74	10.83	1	508	19	-0.70	-0.04
160	17.98	3	1243	30	-0.52	-0.04
64	9.27	2	368	17	-0.58	-0.04
184	18.78	5	2007	51	-0.49	-0.04
80	10.66	1	250	11	-0.66	-0.05
196	23.35	3	2761	37	-0.47	-0.03
218	25.57	4	5026	48	-0.44	-0.03
214	23.36	3	1953	42	-0.56	-0.04
116	14.51	3	977	29	-0.70	-0.05
166	21.43	2	2114	33	-0.45	-0.03
530	65.68	5	37846	122	-0.16	-0.01
118	16.01	3	1698	32	-0.31	-0.02
204	24.47	4	3518	42	-0.32	-0.02
98	13.68	2	1046	30	-0.48	-0.03
110	14.89	2	930	27	-0.51	-0.04
126	16.28	3	1779	41	-0.41	-0.03
122	13.06	1	236	14	-0.62	-0.04
146	16.92	2	871	29	-0.48	-0.04
104	12.13	0	170	9	-0.94	-0.06

90	11.33	1	240	11	-0.98	-0.07
156	19.03	1	1158	21	-0.56	-0.04
150	17.40	2	707	29	-0.61	-0.04
152	17.33	4	1416	38	-0.59	-0.04
284	34.42	5	8915	62	-0.29	-0.02
250	27.01	3	3174	48	-0.39	-0.03
116	14.59	2	970	23	-0.37	-0.03
230	23.35	6	3158	60	-0.44	-0.03
110	13.50	3	748	21	-0.70	-0.05
206	24.00	4	4316	46	-0.36	-0.03
72	10.51	1	300	16	-1.05	-0.07
496	60.67	5	37800	112	-0.20	-0.01
106	14.30	3	1227	35	-0.44	-0.03
144	18.40	1	1014	22	-0.58	-0.04
186	19.34	5	2189	57	-0.48	-0.03
174	18.19	5	1958	55	-0.56	-0.04
492	58.91	3	35269	107	-0.18	-0.01
436	42.76	6	9407	84	-0.14	-0.01
62	9.03	1	250	11	-0.61	-0.04
180	23.49	3	4452	46	-0.23	-0.02
366	45.35	3	14503	76	-0.23	-0.02
188	20.82	3	1750	39	-0.56	-0.04
140	16.49	2	1143	32	-0.28	-0.02
72	9.78	1	196	9	-0.69	-0.05
152	18.94	2	1370	26	-0.59	-0.04
150	18.26	3	1230	34	-0.60	-0.05
128	16.20	3	1596	34	-0.48	-0.03
184	21.01	0	1078	19	-0.38	-0.03
138	19.32	3	3628	42	-0.13	-0.01
146	18.95	3	2281	40	-0.25	-0.02
100	13.62	2	924	25	-0.45	-0.03
190	21.65	6	3596	56	-0.38	-0.03
198	24.50	2	3227	40	-0.45	-0.03
122	13.64	3	628	21	-0.72	-0.05
72	9.82	3	441	17	-0.61	-0.04
224	25.86	4	4208	52	-0.48	-0.03
366	42.31	1	8563	62	-0.29	-0.02
56	8.57	0	125	12	-0.95	-0.06
270	33.46	4	10664	74	-0.15	-0.01
178	18.88	3	1348	35	-0.35	-0.02
84	12.02	0	476	17	-0.49	-0.03
86	11.22	1	429	19	-0.50	-0.03
408	47.43	0	10287	68	-0.21	-0.01
184	21.01	0	1078	19	-0.32	-0.02
144	17.83	2	1846	33	-0.20	-0.01
436	51.28	5	29430	115	-0.07	0.00
232	28.29	6	7135	67	-0.17	-0.01
278	34.60	6	12962	83	-0.12	-0.01
254	30.19	3	4834	48	-0.25	-0.02
370	42.51	4	12473	75	-0.32	-0.02
254	30.19	3	4834	48	-0.24	-0.02
172	20.41	4	2946	55	-0.27	-0.02
120	15.33	2	1263	31	-0.32	-0.02
122	15.27	2	814	32	-0.54	-0.04
102	13.24	2	699	30	-0.51	-0.04
114	14.48	2	827	30	-0.53	-0.04
190	21.82	3	2758	40	-0.31	-0.02
124	16.35	2	1263	33	-0.30	-0.02
34	5.95	0	88	6	-0.72	-0.04
124	15.30	3	1314	33	-0.42	-0.03
282	31.04	3	3798	49	-0.46	-0.03
368	45.21	3	12530	77	-0.28	-0.02
282	31.04	3	3798	49	-0.43	-0.03
242	27.71	5	6060	64	-0.31	-0.02
184	22.42	4	4407	52	-0.37	-0.03
104	14.14	0	693	19	-0.48	-0.03
180	23.67	3	4899	54	-0.18	-0.01
54	7.37	2	425	24	-0.66	-0.02
54	7.37	2	425	24	-0.65	-0.02
50	6.95	2	352	22	-0.68	-0.02
166	19.43	2	1374	36	-0.34	-0.02
130	17.37	3	1817	33	-0.35	-0.03
464	57.41	4	25695	98	-0.18	-0.01
222	27.97	5	7918	68	-0.31	-0.02
140	18.92	1	2365	45	-0.40	-0.02
42	6.76	0	118	12	-0.80	-0.05
128	16.20	2	1401	34	-0.35	-0.02

218	26.01	3	4002	48	-0.33	-0.02
306	37.40	5	14600	93	-0.18	-0.01
258	31.34	5	6844	69	-0.21	-0.01
258	29.57	3	4555	62	-0.15	-0.01
412	48.10	5	21758	109	-0.06	0.00
102	12.93	1	510	23	-0.41	-0.03
332	40.62	3	11878	96	-0.12	-0.01
236	28.77	5	6343	56	-0.36	-0.03
34	5.29	0	66	5	-0.70	-0.04
118	14.55	3	1116	34	-0.31	-0.02
150	19.92	3	2515	45	-0.42	-0.03
336	40.65	4	10087	73	-0.25	-0.02
330	40.31	4	10422	76	-0.20	-0.01
98	13.08	2	753	19	-0.31	-0.02
184	23.47	3	4187	53	-0.28	-0.02
70	8.73	1	186	11	-0.92	-0.06
170	22.91	4	4373	46	-0.30	-0.02
152	19.73	2	2284	34	-0.48	-0.03
158	19.83	3	2463	42	-0.26	-0.02
214	26.33	5	7946	76	-0.18	-0.01
166	21.86	2	4202	47	-0.37	-0.03
424	48.83	5	22004	109	-0.08	-0.01
408	51.30	5	21459	84	-0.15	-0.01
78	10.28	1	224	13	-0.74	-0.05
78	10.28	1	224	13	-0.71	-0.04
134	18.11	4	1939	40	-0.36	-0.03
228	29.77	3	5333	51	-0.23	-0.02
246	31.68	4	6650	58	-0.22	-0.02
436	51.99	0	13642	75	-0.16	-0.01
262	31.47	3	6656	55	-0.34	-0.02
98	13.76	0	759	18	-0.60	-0.03
272	34.62	4	7271	68	-0.25	-0.02
242	30.25	3	5210	53	-0.18	-0.01
256	32.06	3	5847	58	-0.26	-0.02
242	30.25	3	5714	55	-0.28	-0.02
270	32.92	4	6807	62	-0.28	-0.02
270	34.08	4	7356	67	-0.25	-0.02
288	36.23	4	9214	73	-0.23	-0.02
288	36.23	4	9506	76	-0.21	-0.01
230	25.97	3	3712	45	-0.29	-0.02
178	22.43	0	2300	29	-0.32	-0.02
276	32.15	4	5123	63	-0.25	-0.02
202	24.38	3	3569	51	-0.30	-0.02
206	24.76	3	3569	51	-0.26	-0.02
194	23.51	3	3289	49	-0.25	-0.02
152	19.62	3	2720	44	-0.23	-0.01
262	29.13	6	7065	64	-0.39	-0.03
216	25.71	4	3693	48	-0.37	-0.03
376	43.48	5	12982	77	-0.24	-0.02
94	11.79	2	424	24	-0.48	-0.03
182	21.17	1	1245	28	-0.33	-0.02
132	17.73	2	1888	35	-0.19	-0.01
238	30.38	3	5922	67	-0.16	-0.01
244	28.93	5	6741	54	-0.33	-0.02
264	30.55	7	8096	64	-0.25	-0.02
176	19.55	3	1906	39	-0.45	-0.03
132	16.58	2	954	27	-0.33	-0.02
144	17.79	2	1059	31	-0.41	-0.03
280	33.16	3	5863	59	-0.38	-0.03
230	27.14	5	5370	47	-0.34	-0.02
58	8.69	1	307	14	-0.67	-0.04
158	19.62	3	2217	37	-0.40	-0.03
216	27.32	5	6581	57	-0.38	-0.03
264	30.76	6	8012	61	-0.33	-0.02
210	20.99	5	1781	59	-0.36	-0.03
180	24.47	1	4272	51	-0.22	-0.01
78	11.72	2	602	23	-0.57	-0.04
284	33.53	5	7904	61	-0.31	-0.02
134	17.74	1	1324	33	-0.50	-0.03
108	14.72	1	950	28	-0.59	-0.04
116	15.86	2	1526	30	-0.56	-0.04
106	14.24	1	888	28	-0.53	-0.03
80	11.22	1	617	21	-0.61	-0.04
80	11.22	1	500	19	-0.66	-0.04
80	10.37	0	247	11	-0.48	-0.03
234	27.85	6	6569	55	-0.31	-0.02
254	29.92	5	8110	81	-0.24	-0.02

DG_PSA	DG_MSA	DG_apolarSA	DG_Wiener	DG_P	DG_NoC
-0.09	-0.03	-0.05	-0.04	-8.756000e+01	-1.36
-0.15	-0.02	-0.02	-0.01	-2.000000e-01	-0.52
-0.11	-0.02	-0.03	0.00	-1.100000e-01	-0.51
-0.34	-0.03	-0.03	-0.01	-2.000000e-02	-0.6
-0.07	-0.02	-0.03	-0.01	-2.000000e-02	-0.57
-0.14	-0.02	-0.03	-0.02	-3.100000e-01	-0.66
-0.24	-0.03	-0.03	-0.01	-2.060000e+00	-0.61
-0.14	-0.02	-0.03	0.00	-1.590000e+00	-0.61
-0.34	-0.03	-0.03	-0.01	-6.000000e-02	-0.7
-1.28	-0.03	-0.03	-0.02	0.000000e+00	-0.7
-0.04	-0.01	-0.01	0.00	-8.326780e+03	-0.27
-0.22	-0.03	-0.03	-0.01	-3.000000e-02	-0.65
-0.39	-0.04	-0.05	-0.02	-1.650000e+00	-1.09
-0.42	-0.03	-0.03	-0.02	0.000000e+00	-0.7
-0.18	-0.02	-0.02	-0.01	0.000000e+00	-0.46
-0.33	-0.02	-0.03	-0.01	-3.000000e-02	-0.45
-0.33	-0.03	-0.03	-0.01	-3.000000e-02	-0.73
-0.12	-0.03	-0.04	-0.04	-1.486910e+03	-0.97
-0.19	-0.02	-0.03	0.00	-1.000000e-02	-0.51
-0.16	-0.02	-0.03	-0.01	-2.000000e-02	-0.55
-0.36	-0.02	-0.02	-0.01	0.000000e+00	-0.53
-0.10	-0.01	-0.02	0.00	0.000000e+00	-0.32
-0.20	-0.03	-0.03	-0.01	-5.000000e-02	-0.7
-0.03	0.00	-0.01	0.00	0.000000e+00	-0.13
-0.31	-0.02	-0.02	0.00	0.000000e+00	-0.44
-0.19	-0.03	-0.03	-0.01	-3.000000e-02	-0.63
-0.43	-0.04	-0.05	-0.03	-6.000000e-02	-0.94
-0.12	-0.03	-0.05	-0.03	-5.400000e-01	-1.68
-0.31	-0.03	-0.03	-0.01	-3.958910e-05	-0.66
-0.20	-0.03	-0.04	-0.01	-6.000000e-02	-0.61
-0.12	-0.02	-0.03	-0.01	0.000000e+00	-0.53
-0.51	-0.03	-0.03	-0.01	0.000000e+00	-0.61
-0.60	-0.04	-0.04	-0.02	0.000000e+00	-0.72
-0.49	-0.04	-0.04	-0.05	-4.100000e-01	-1
-0.19	-0.02	-0.03	-0.01	-3.000000e-02	-0.55
-0.26	-0.03	-0.03	-0.01	0.000000e+00	-0.61
-0.20	-0.02	-0.03	-0.01	0.000000e+00	-0.55
-0.19	-0.03	-0.04	-0.01	-1.100000e-01	-0.73
-0.16	-0.02	-0.03	-0.01	-1.000000e-02	-0.5
-0.16	-0.03	-0.04	-0.01	-1.690000e+00	-0.82
-0.39	-0.03	-0.03	-0.01	-1.000000e-02	-0.8
-0.11	-0.01	-0.01	0.00	0.000000e+00	-0.33
-0.18	-0.02	-0.02	0.00	-1.000000e-02	-0.54
-0.36	-0.04	-0.04	-0.03	-6.000000e-02	-1.16
-0.17	-0.03	-0.03	-0.01	-1.800000e-01	-0.65
-0.27	-0.03	-0.04	-0.04	-2.970000e+00	-0.87
-0.22	-0.03	-0.03	-0.01	-7.000000e-01	-0.6
-0.36	-0.03	-0.04	-0.04	-3.100000e-01	-0.8
-0.22	-0.02	-0.03	-0.01	-2.000000e-02	-0.58
-0.18	-0.02	-0.03	0.00	0.000000e+00	-0.56
-0.29	-0.03	-0.03	-0.01	-4.900000e-01	-0.67
-0.22	-0.04	-0.05	-0.02	-6.200000e-01	-0.88
-0.19	-0.02	-0.03	-0.01	-3.000000e-02	-0.57
-0.05	-0.01	-0.01	0.00	-1.900000e-01	-0.23
-0.08	-0.02	-0.02	-0.01	-2.000000e-02	-0.42
-0.33	-0.02	-0.02	0.00	-1.559540e-05	-0.36
-0.24	-0.03	-0.03	-0.01	0.000000e+00	-0.65
-0.25	-0.03	-0.03	-0.02	0.000000e+00	-0.62
-0.07	-0.03	-0.04	-0.01	-5.000000e+00	-0.67
-0.34	-0.03	-0.03	-0.05	0.000000e+00	-0.68
-0.22	-0.02	-0.03	-0.02	-2.000000e-02	-0.58
-0.39	-0.04	-0.04	-0.06	-5.449000e+01	-1.3
-0.90	-0.04	-0.05	-0.06	-8.000000e-02	-1.08
-0.28	-0.03	-0.03	-0.01	-2.500000e-01	-0.71
-0.36	-0.03	-0.03	-0.02	-1.400000e-01	-0.73
-0.30	-0.03	-0.04	-0.02	-3.200000e-01	-0.7
-0.12	-0.02	-0.02	0.00	-1.512660e-07	-0.34
-0.22	-0.02	-0.02	-0.01	-1.648440e-06	-0.43
-0.24	-0.02	-0.02	-0.01	-1.000000e-02	-0.42
-0.14	-0.03	-0.03	-0.01	-4.400000e-01	-0.54
-0.91	-0.04	-0.04	-0.03	-4.000000e-02	-0.8
-0.18	-0.02	-0.02	0.00	-2.000000e-02	-0.47
-0.21	-0.06	-0.08	-0.06	-8.750000e+00	-1.58
-0.06	-0.01	-0.01	0.00	-7.290000e+00	-0.3
-0.18	-0.03	-0.03	-0.01	-1.000000e-02	-0.59
-0.28	-0.03	-0.03	-0.01	-1.100000e-01	-0.73

-0.16	-0.03	-0.03	-0.01	-5.750000e+00	-0.61
-0.15	-0.03	-0.04	-0.02	-1.343000e+01	-0.72
-0.05	-0.01	-0.01	0.00	-5.913530e+03	-0.29
-0.11	-0.01	-0.01	0.00	0.000000e+00	-0.16
-0.18	-0.03	-0.04	-0.04	-2.400000e+00	-0.84
-0.05	-0.01	-0.02	0.00	-2.080000e+00	-0.35
-0.07	-0.01	-0.02	0.00	-6.100000e-01	-0.33
-0.35	-0.03	-0.03	-0.01	0.000000e+00	-0.62
-0.07	-0.01	-0.02	-0.01	-2.734900e+02	-0.43
-0.18	-0.03	-0.04	-0.05	-5.700000e-01	-0.86
-0.54	-0.03	-0.03	-0.01	0.000000e+00	-0.68
-1.00	-0.03	-0.03	-0.02	0.000000e+00	-0.63
-0.15	-0.03	-0.03	-0.01	-1.000000e-02	-0.62
-0.14	-0.02	-0.02	-0.01	-6.118390e+03	-0.54
-0.03	-0.01	-0.01	0.00	-1.100000e-01	-0.2
-0.09	-0.01	-0.02	0.00	0.000000e+00	-0.31
-0.10	-0.03	-0.04	-0.01	-5.000000e-02	-0.58
-0.11	-0.02	-0.03	-0.01	-3.700000e-01	-0.49
-0.18	-0.02	-0.03	-0.01	-2.000000e-02	-0.63
-0.88	-0.04	-0.04	-0.03	-1.200000e-01	-0.83
-0.13	-0.04	-0.06	-0.03	-1.500000e-01	-0.86
-0.13	-0.03	-0.03	-0.01	-1.000000e-02	-0.62
-0.08	-0.01	-0.02	0.00	-3.500000e-01	-0.43
-0.09	-0.05	-0.13	-0.08	-1.046999e+04	-2.39
-0.03	-0.01	-0.01	0.00	-5.473280e+03	-0.29
-0.09	-0.02	-0.02	-0.01	-2.035000e+01	-0.64
-0.06	-0.03	-0.05	-0.02	-8.722576e+04	-1.3
-0.05	-0.03	-0.07	-0.02	-1.486467e+04	-1.39
-0.06	-0.01	-0.01	0.00	-2.000000e-02	-0.29
-0.12	-0.01	-0.02	-0.01	-5.164260e+03	-0.45
-0.02	-0.01	-0.02	0.00	-1.533590e+05	-0.48
-0.02	0.00	0.00	0.00	-3.000000e-02	-0.09
-0.03	-0.01	-0.02	0.00	-1.806554e+04	-0.32
-0.02	-0.01	-0.01	0.00	-5.862700e+09	-0.3
-0.10	-0.01	-0.02	0.00	-1.602290e-05	-0.31
-0.09	-0.02	-0.02	0.00	-6.000000e-02	-0.48
-0.10	-0.01	-0.01	0.00	-1.482550e-05	-0.29
-0.06	-0.02	-0.02	0.00	-3.231199e+05	-0.47
-0.04	-0.02	-0.04	-0.01	-9.352693e+04	-0.74
-0.08	-0.03	-0.05	-0.02	-2.443344e+04	-0.97
-0.06	-0.03	-0.06	-0.02	-1.341944e+06	-0.96
-0.07	-0.03	-0.06	-0.02	-1.548626e+04	-0.95
-0.06	-0.02	-0.02	0.00	-2.975000e+01	-0.52
-0.04	-0.02	-0.04	-0.01	-6.531087e+06	-0.73
-0.04	-0.04	-0.19	-0.07	-1.944935e+04	-0na0
-0.11	-0.03	-0.03	-0.01	-1.000000e-02	-0.55
-0.23	-0.02	-0.03	-0.01	-2.000000e-02	-0.51
-0.10	-0.01	-0.02	0.00	0.000000e+00	-0.38
-0.21	-0.02	-0.02	0.00	-2.000000e-02	-0.47
-0.08	-0.02	-0.02	0.00	-1.164000e+01	-0.43
-0.14	-0.02	-0.03	0.00	-5.000000e-02	-0.55
-0.05	-0.02	-0.05	-0.01	-1.754930e+04	-1.43
-0.02	-0.01	-0.03	0.00	-4.688778e+08	-0.65
-0.21	-0.04	-0.04	-0.04	0.000000e+00	-1.33
-0.15	-0.03	-0.04	-0.03	0.000000e+00	-1.31
-0.31	-0.04	-0.04	-0.04	0.000000e+00	-1.27
-0.05	-0.02	-0.03	-0.01	-3.973824e+04	-0.6
-0.07	-0.02	-0.03	-0.01	-1.958620e+05	-0.6
-0.07	-0.01	-0.01	0.00	-3.336720e-05	-0.23
-0.13	-0.02	-0.02	0.00	-2.286080e-06	-0.44
-0.04	-0.02	-0.06	-0.01	-2.909089e+05	-1.11
-0.07	-0.04	-0.13	-0.07	-3.485710e+03	-3.99
-0.04	-0.02	-0.05	-0.01	-1.021003e+05	-0.86
-0.09	-0.02	-0.02	0.00	-1.088020e-05	-0.44
-0.07	-0.01	-0.01	0.00	-1.000000e-02	-0.29
-0.08	-0.01	-0.01	0.00	-2.640180e-05	-0.29
-0.02	-0.01	-0.01	0.00	-6.045042e+04	-0.26
-0.01	0.00	-0.01	0.00	-2.085796e+09	-0.11
-0.05	-0.02	-0.05	-0.02	-1.509710e+03	-0.77
-0.02	-0.01	-0.01	0.00	-2.229286e+07	-0.21
-0.12	-0.02	-0.03	0.00	-2.546620e-05	-0.44
-0.06	-0.04	-0.12	-0.08	-3.434700e+02	-2.79
-0.07	-0.02	-0.02	-0.01	-2.760000e+00	-0.52
-0.16	-0.03	-0.03	-0.01	-4.000000e-02	-0.6
-0.09	-0.01	-0.02	0.00	-7.822050e-05	-0.32
-0.07	-0.01	-0.01	0.00	0.000000e+00	-0.26
-0.11	-0.02	-0.02	-0.01	-1.100000e-01	-0.42

-0.03	-0.02	-0.03	0.00	-3.227614e+06	-0.85
-0.18	-0.05	-0.07	-0.08	-5.156000e+01	-1.53
-0.11	-0.02	-0.02	0.00	-2.375160e-06	-0.38
-0.09	-0.03	-0.04	-0.01	-6.000000e-01	-0.75
-0.03	-0.02	-0.03	0.00	-1.825695e+05	-0.65
-0.02	-0.01	-0.02	0.00	-8.690144e+05	-0.48
-0.10	-0.02	-0.03	0.00	-6.000000e-02	-0.6
-0.01	0.00	-0.01	0.00	-1.190630e+09	-0.14
-0.07	-0.01	-0.01	0.00	-1.811230e-06	-0.2
-0.11	-0.04	-0.06	-0.04	-6.125569e+04	-1.77
-0.10	-0.04	-0.06	-0.04	-5.921825e+04	-1.71
-0.16	-0.02	-0.03	-0.01	-3.642480e-05	-0.41
-0.07	-0.01	-0.02	0.00	-1.000000e-02	-0.3
-0.07	-0.01	-0.02	0.00	-1.000000e-02	-0.28
-0.06	-0.01	-0.01	0.00	-2.038000e+01	-0.25
-0.10	-0.02	-0.02	0.00	-2.291000e+01	-0.5
-0.06	-0.03	-0.07	-0.01	-5.148827e+05	-2.15
-0.09	-0.01	-0.02	0.00	-7.647150e-05	-0.31
-0.06	-0.01	-0.01	0.00	-3.000000e-02	-0.25
-0.07	-0.01	-0.02	0.00	-1.700000e-01	-0.35
-0.09	-0.02	-0.02	0.00	-2.000000e-02	-0.38
-0.11	-0.02	-0.02	0.00	0.000000e+00	-0.35
-0.11	-0.01	-0.02	0.00	-3.383940e-05	-0.32
-0.07	-0.01	-0.02	0.00	0.000000e+00	-0.31
-0.07	-0.01	-0.01	0.00	0.000000e+00	-0.29
-0.10	-0.02	-0.02	0.00	-3.000000e-02	-0.39
-0.06	-0.02	-0.02	0.00	-4.800000e-01	-0.55
-0.14	-0.01	-0.02	0.00	-4.000000e-02	-0.32
-0.05	-0.02	-0.03	0.00	-1.132119e+04	-0.59
-0.05	-0.02	-0.02	0.00	-1.159527e+04	-0.51
-0.05	-0.01	-0.02	0.00	-2.633887e+04	-0.51
-0.02	-0.01	-0.03	0.00	-5.742696e+06	-0.64
-0.24	-0.02	-0.03	0.00	0.000000e+00	-0.52
-0.12	-0.02	-0.03	0.00	-3.400000e-01	-0.55
-0.10	-0.01	-0.02	0.00	0.000000e+00	-0.31
-0.07	-0.03	-0.05	-0.03	-3.579370e+03	-0.83
-0.08	-0.02	-0.02	-0.01	-9.000000e-02	-0.43
-0.03	-0.01	-0.02	0.00	-1.151000e+01	-0.34
-0.02	-0.01	-0.01	0.00	-4.547793e+04	-0.31
-0.16	-0.02	-0.02	0.00	0.000000e+00	-0.41
-0.13	-0.01	-0.02	0.00	0.000000e+00	-0.31
-0.11	-0.02	-0.03	-0.01	0.000000e+00	-0.67
-0.08	-0.02	-0.02	-0.01	-3.258000e+01	-0.49
-0.09	-0.02	-0.03	-0.01	-3.041000e+01	-0.58
-0.11	-0.02	-0.02	0.00	-5.000000e-02	-0.53
-0.09	-0.02	-0.02	0.00	-4.800000e-01	-0.49
-0.14	-0.04	-0.05	-0.04	-1.700000e-01	-1
-0.14	-0.02	-0.03	-0.01	-1.000000e-02	-0.57
-0.15	-0.02	-0.03	0.00	-1.000000e-02	-0.47
-0.18	-0.02	-0.02	0.00	0.000000e+00	-0.4
-0.10	-0.02	-0.03	-0.01	-1.100000e-01	-0.45
-0.02	-0.01	-0.05	0.00	-2.063820e+12	-1.34
-0.11	-0.04	-0.05	-0.02	-3.600000e-01	-0.83
-0.18	-0.02	-0.02	0.00	-7.000000e-02	-0.41
-0.07	-0.03	-0.04	-0.01	-3.115440e+03	-0.92
-0.09	-0.03	-0.05	-0.02	-2.631300e+02	-1.12
-0.13	-0.03	-0.04	-0.01	-8.300000e-01	-0.84
-0.08	-0.03	-0.05	-0.01	-3.422000e+02	-1.01
-0.11	-0.04	-0.05	-0.02	-4.182000e+01	-1.23
-0.11	-0.04	-0.06	-0.03	-6.068000e+01	-1.23
-0.07	-0.02	-0.04	-0.02	-9.127500e+02	-0.96
-0.11	-0.02	-0.02	0.00	-2.000000e-02	-0.39
-0.06	-0.01	-0.02	0.00	-6.550000e+00	-0.33

Table S4. Bootstrap (nonparametric) on 1,000 re-samples.

The following statistics are calculated on the multivariate logistic regressions obtained by substituting the expressions into Eq. 1.

Eq. 3:
Bootstrap Statistics :

```

      original      bias      std. error
t1*  2.9889862  0.024295128  0.30732267
t2* -0.3753449 -0.003540546  0.04142203
BOOTSTRAP CONFIDENCE INTERVAL CALCULATIONS
Based on 1000 bootstrap replicates

```

```

CALL :
boot.ci(boot.out = results, type = "bca", index = 1)

```

```

Intervals :
Level      BCa
95%      ( 2.394,  3.575 )
Calculations and Intervals on Original Scale
BOOTSTRAP CONFIDENCE INTERVAL CALCULATIONS
Based on 1000 bootstrap replicates

```

```

CALL :
boot.ci(boot.out = results, type = "bca", index = 2)

```

```

Intervals :
Level      BCa
95%      (-0.4545, -0.2933 )
Calculations and Intervals on Original Scale

```

Eq. 4:

```

Bootstrap Statistics :
      original      bias      std. error
t1*  2.71025677  0.0305438403  0.256598564
t2* -0.02634499 -0.0003006375  0.002649184
BOOTSTRAP CONFIDENCE INTERVAL CALCULATIONS
Based on 1000 bootstrap replicates

```

```

CALL :
boot.ci(boot.out = results, type = "bca", index = 1)

```

```

Intervals :
Level      BCa
95%      ( 2.146,  3.185 )
Calculations and Intervals on Original Scale
BOOTSTRAP CONFIDENCE INTERVAL CALCULATIONS
Based on 1000 bootstrap replicates

```

```

CALL :
boot.ci(boot.out = results, type = "bca", index = 2)

```

```

Intervals :
Level      BCa
95%      (-0.0314, -0.0210 )
Calculations and Intervals on Original Scale

```

Eq. 5:

```

t1*  1.69077976  0.0323524693  0.283471744
t2*  0.50598689  0.0030037653  0.078581404
t3* -0.02988067 -0.0003924046  0.003055006
BOOTSTRAP CONFIDENCE INTERVAL CALCULATIONS
Based on 1000 bootstrap replicates

```

```

CALL :
boot.ci(boot.out = results, type = "bca", index = 1)

```

```

Intervals :
Level      BCa
95%      ( 1.151,  2.263 )

```

Calculations and Intervals on Original Scale
BOOTSTRAP CONFIDENCE INTERVAL CALCULATIONS
Based on 1000 bootstrap replicates

CALL :
boot.ci(boot.out = results, type = "bca", index = 2)

Intervals :
Level BCa
95% (0.3573, 0.6660)
Calculations and Intervals on Original Scale
BOOTSTRAP CONFIDENCE INTERVAL CALCULATIONS
Based on 1000 bootstrap replicates

CALL :
boot.ci(boot.out = results, type = "bca", index = 3)

Intervals :
Level BCa
95% (-0.0355, -0.0241)
Calculations and Intervals on Original Scale

Eq. 6:

t1*	2.30067225	0.0393196650	0.356663971
t2*	0.80817618	0.0162521559	0.113261207
t3*	0.50300112	0.0080978841	0.063149842
t4*	-0.01015057	-0.0001856429	0.001251888

BOOTSTRAP CONFIDENCE INTERVAL CALCULATIONS
Based on 1000 bootstrap replicates

CALL :
boot.ci(boot.out = results, type = "bca", index = 1)

Intervals :
Level BCa
95% (1.597, 2.970)
Calculations and Intervals on Original Scale
BOOTSTRAP CONFIDENCE INTERVAL CALCULATIONS
Based on 1000 bootstrap replicates

CALL :
boot.ci(boot.out = results, type = "bca", index = 2)

Intervals :
Level BCa
95% (0.5857, 1.0154)
Calculations and Intervals on Original Scale

Eq. 7:

Bootstrap Statistics :

	original	bias	std. error
t1*	2.66961081	0.0552587630	0.327264269
t2*	0.78567358	0.0068023554	0.111674203
t3*	-0.03098791	-0.0003863474	0.003387844
t4*	-0.01114992	-0.0004487933	0.005348194

BOOTSTRAP CONFIDENCE INTERVAL CALCULATIONS
Based on 1000 bootstrap replicates

CALL :
boot.ci(boot.out = results, type = "bca", index = 1)

Intervals :
Level BCa

95% (2.015, 3.216)
 Calculations and Intervals on Original Scale
 BOOTSTRAP CONFIDENCE INTERVAL CALCULATIONS
 Based on 1000 bootstrap replicates

CALL :
 boot.ci(boot.out = results, type = "bca", index = 2)

Intervals :
 Level BCa
 95% (0.5769, 1.0019)
 Calculations and Intervals on Original Scale
 BOOTSTRAP CONFIDENCE INTERVAL CALCULATIONS
 Based on 1000 bootstrap replicates

CALL :
 boot.ci(boot.out = results, type = "bca", index = 3)

Intervals :
 Level BCa
 95% (-0.0380, -0.0248)
 Calculations and Intervals on Original Scale
 BOOTSTRAP CONFIDENCE INTERVAL CALCULATIONS
 Based on 1000 bootstrap replicates

CALL :
 boot.ci(boot.out = results, type = "bca", index = 4)

Intervals :
 Level BCa
 95% (-0.0215, 0.0002)
 Calculations and Intervals on Original Scale

Eq. 8:

Bootstrap Statistics :

	original	bias	std. error
t1*	2.0613354093	1.359692e-02	3.004708e-01
t2*	0.1533742667	6.163986e-03	6.771892e-02
t3*	-0.0001188325	-9.032671e-06	6.379956e-05
t4*	-0.0182776409	1.728144e-05	3.427764e-03

 BOOTSTRAP CONFIDENCE INTERVAL CALCULATIONS
 Based on 1000 bootstrap replicates

CALL :
 boot.ci(boot.out = results, type = "bca", index = 1)

Intervals :
 Level BCa
 95% (1.479, 2.686)
 Calculations and Intervals on Original Scale
 BOOTSTRAP CONFIDENCE INTERVAL CALCULATIONS
 Based on 1000 bootstrap replicates

CALL :
 boot.ci(boot.out = results, type = "bca", index = 2)

Intervals :
 Level BCa
 95% (0.0012, 0.2713)
 Calculations and Intervals on Original Scale
 BOOTSTRAP CONFIDENCE INTERVAL CALCULATIONS
 Based on 1000 bootstrap replicates

CALL :
boot.ci(boot.out = results, type = "bca", index = 3)

Intervals :
Level BCa
95% (-0.0002, 0.0000)
Calculations and Intervals on Original Scale
BOOTSTRAP CONFIDENCE INTERVAL CALCULATIONS
Based on 1000 bootstrap replicates

CALL :
boot.ci(boot.out = results, type = "bca", index = 4)

Intervals :
Level BCa
95% (-0.0252, -0.0114)
Calculations and Intervals on Original Scale

Eq. 9:

Bootstrap Statistics :
 original bias std. error
t1* 3.5027931 0.12981380 0.7319870
t2* -0.8239265 -0.03309284 0.2814914
t3* -0.2970891 -0.01080606 0.1293552
t4* -0.7621793 -0.01680360 0.1087372
t5* -1.8858517 0.02809676 0.6180348
BOOTSTRAP CONFIDENCE INTERVAL CALCULATIONS
Based on 1000 bootstrap replicates

CALL :
boot.ci(boot.out = results, type = "bca", index = 1)

Intervals :
Level BCa
95% (1.998, 4.812)
Calculations and Intervals on Original Scale
BOOTSTRAP CONFIDENCE INTERVAL CALCULATIONS
Based on 1000 bootstrap replicates

CALL :
boot.ci(boot.out = results, type = "bca", index = 2)

Intervals :
Level BCa
95% (-1.3350, -0.2262)
Calculations and Intervals on Original Scale
BOOTSTRAP CONFIDENCE INTERVAL CALCULATIONS
Based on 1000 bootstrap replicates

CALL :
boot.ci(boot.out = results, type = "bca", index = 3)

Intervals :
Level BCa
95% (-0.5375, -0.0252)
Calculations and Intervals on Original Scale
BOOTSTRAP CONFIDENCE INTERVAL CALCULATIONS
Based on 1000 bootstrap replicates

CALL :
boot.ci(boot.out = results, type = "bca", index = 4)

Intervals :

Level BCa
 95% (-0.9612, -0.5177)
 Calculations and Intervals on Original Scale
 BOOTSTRAP CONFIDENCE INTERVAL CALCULATIONS
 Based on 1000 bootstrap replicates

CALL :
 boot.ci(boot.out = results, type = "bca", index = 5)

Intervals :
 Level BCa
 95% (-3.194, -0.673)
 Calculations and Intervals on Original Scale

Eq. 10:

Bootstrap Statistics :

	original	bias	std. error
t1*	0.92261457	-0.0028229285	0.379320319
t2*	0.75622588	0.0125261222	0.105118444
t3*	0.15328158	0.0053450305	0.055145149
t4*	-0.02569398	-0.0002883767	0.003325823
t5*	-56.16218277	-2.1211030587	14.936559474

 BOOTSTRAP CONFIDENCE INTERVAL CALCULATIONS
 Based on 1000 bootstrap replicates

CALL :
 boot.ci(boot.out = results, type = "bca", index = 1)

Intervals :
 Level BCa
 95% (0.1640, 1.7326)
 Calculations and Intervals on Original Scale
 BOOTSTRAP CONFIDENCE INTERVAL CALCULATIONS
 Based on 1000 bootstrap replicates

CALL :
 boot.ci(boot.out = results, type = "bca", index = 2)

Intervals :
 Level BCa
 95% (0.5422, 0.9644)
 Calculations and Intervals on Original Scale
 BOOTSTRAP CONFIDENCE INTERVAL CALCULATIONS
 Based on 1000 bootstrap replicates

CALL :
 boot.ci(boot.out = results, type = "bca", index = 3)

Intervals :
 Level BCa
 95% (0.0391, 0.2521)
 Calculations and Intervals on Original Scale
 BOOTSTRAP CONFIDENCE INTERVAL CALCULATIONS
 Based on 1000 bootstrap replicates

CALL :
 boot.ci(boot.out = results, type = "bca", index = 4)

Intervals :
 Level BCa
 95% (-0.0321, -0.0190)
 Calculations and Intervals on Original Scale
 BOOTSTRAP CONFIDENCE INTERVAL CALCULATIONS

Based on 1000 bootstrap replicates

CALL :
boot.ci(boot.out = results, type = "bca", index = 5)

Intervals :
Level BCa
95% (-86.73, -28.42)
Calculations and Intervals on Original Scale

Eq. 14:

Bootstrap Statistics :
original bias std. error
t1* -4.91890873 2.18484861 0.570373032
t2* 0.42876311 -0.41711763 0.170477893
t3* 0.03134088 -0.03272111 0.009453038
t4* -0.23247168 0.22545459 0.099957275

Eq. 15:

Bootstrap Statistics :
original bias std. error
t1* 2.43616219 -3.27682854 0.670858568
t2* 1.48569099 -1.47405089 0.173606173
t3* 0.77514171 -0.77401321 0.107806197
t4* -0.20648088 0.20602827 0.029894092
t5* -0.02850488 0.02842726 0.003464385
t6* 47.78631283 -47.41006849 15.795368547

Eq. 16:

Bootstrap Statistics :
original bias std. error
t1* -3.16782641 3.13533750 1.10658068
t2* 1.97753492 -1.96314339 0.36131343
t3* -0.01644416 0.01649827 0.00467011
t4* -156.04854479 155.46315866 32.73663157
BOOTSTRAP CONFIDENCE INTERVAL CALCULATIONS
Based on 1000 bootstrap replicates

CALL :
boot.ci(boot.out = results, type = "bca", index = 1)

Intervals :
Level BCa
95% (-3.308, -3.308)
Calculations and Intervals on Original Scale

Eq. 17:

Bootstrap Statistics :
original bias std. error
t1* 5.869192563 -5.842817141 0.7007514065
t2* -1.265167959 1.253522842 0.2121949264
t3* 0.946602104 -0.947970220 0.0806648465
t4* -0.006235705 0.006229628 0.0009391184
t5* -0.167165101 0.167918758 0.0463399371

Eq. 18:

Bootstrap Statistics :
original bias std. error
t1* -0.52963403 0.23988701 0.769494546
t2* 1.49715681 -1.51694571 0.327768763
t3* -0.06613467 0.06617878 0.005635043
t4* 0.10067103 -0.10130650 0.017931663
BOOTSTRAP CONFIDENCE INTERVAL CALCULATIONS

Based on 1000 bootstrap replicates

CALL :
boot.ci(boot.out = results, type = "bca", index = 1)

Intervals :
Level BCa
95% (-3.1653, 0.5928)
Calculations and Intervals on Original Scale

Eq. 19:

Bootstrap Statistics :
original bias std. error
t1* 3.37505508 -3.41138410 0.680138167
t2* 1.45531370 -1.45376967 0.214671510
t3* -0.38260731 0.38705456 0.108991558
t4* -0.07216959 0.07270592 0.008565112
t5* 0.20072729 -0.20324224 0.058791252

Eq. 20:

Bootstrap Statistics :
original bias std. error
t1* 4.681103633 -4.691249871 0.372363626
t2* -0.608902828 0.610758740 0.124333686
t3* -0.045470302 0.045518943 0.004249099
t4* 0.007935213 -0.007924788 0.001471788
t5* -1.237256600 1.236706054 0.103285486

Eq. 21:

Bootstrap Statistics :
original bias std. error
t1* -5.656425e+00 5.713619e+00 1.130734e+00
t2* 3.981382e+00 -3.991637e+00 3.783706e-01
t3* -2.154501e-04 2.153724e-04 2.520972e-05
t4* -1.801824e+02 1.819162e+02 3.648989e+01