

Design of Novel Phosphoinositol 3-kinase Inhibitors for Non-Hodgkin's Lymphoma: Molecular Docking, Molecular Dynamics, and Density Functional Theory Studies on Gold Nanoparticles

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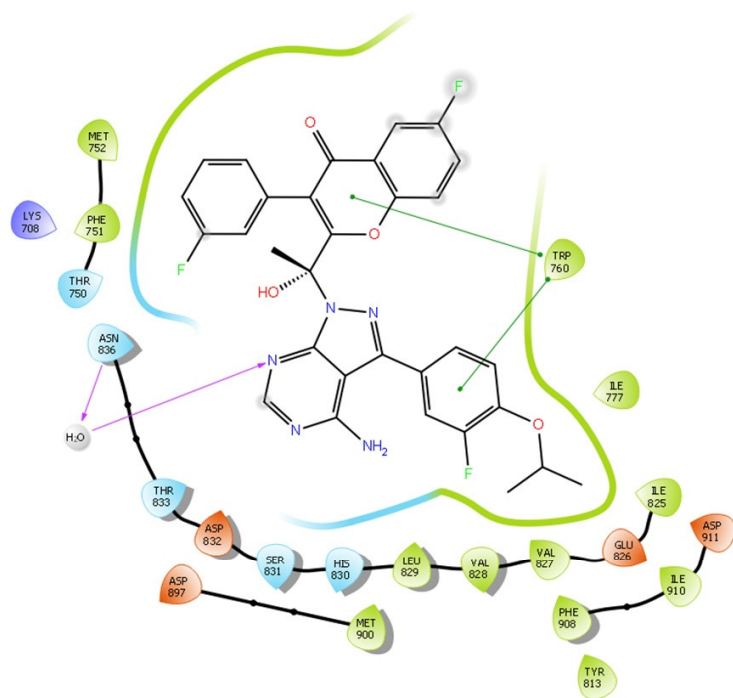
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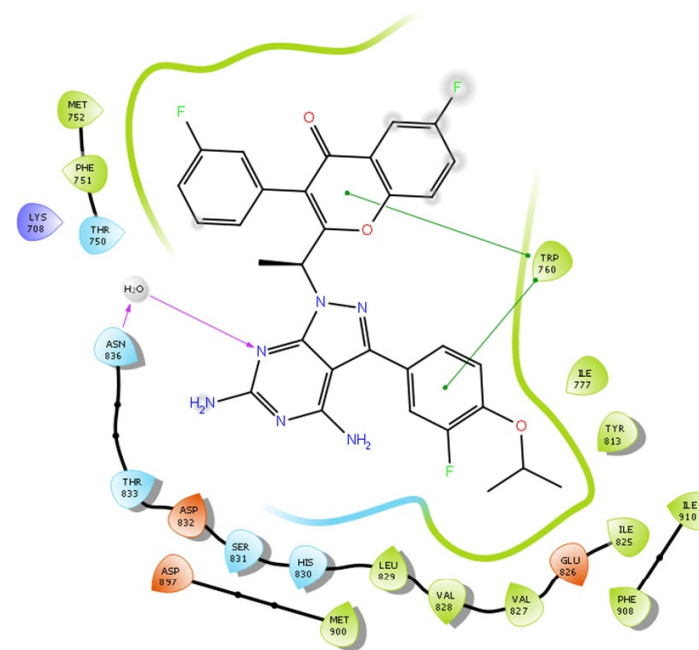
⁹Department of Pharmacology and Toxicology, College of Pharmacy, Taibah University, Al-Madinah Al-Munawwarah 30078, Saudi Arabia

*Corresponding author: Abdulrahim A. Alzain,

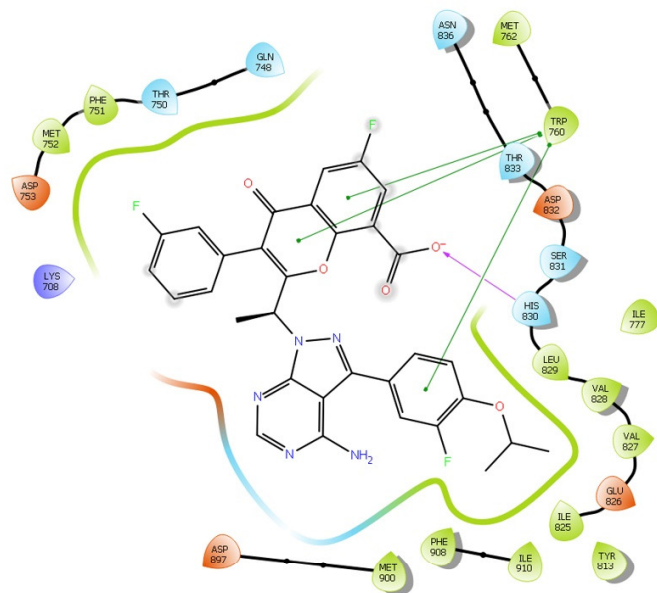
E-mail: abdulrahim.altoam@uofg.edu.sd; abdulrahim.altoam@gmail.com (A.A.A)



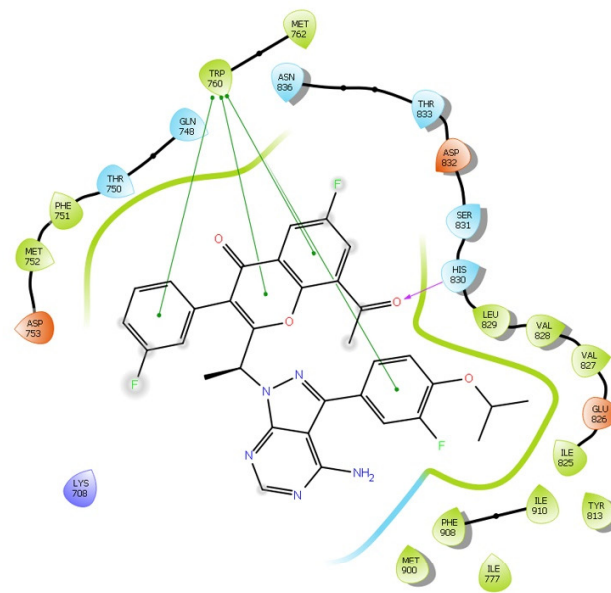
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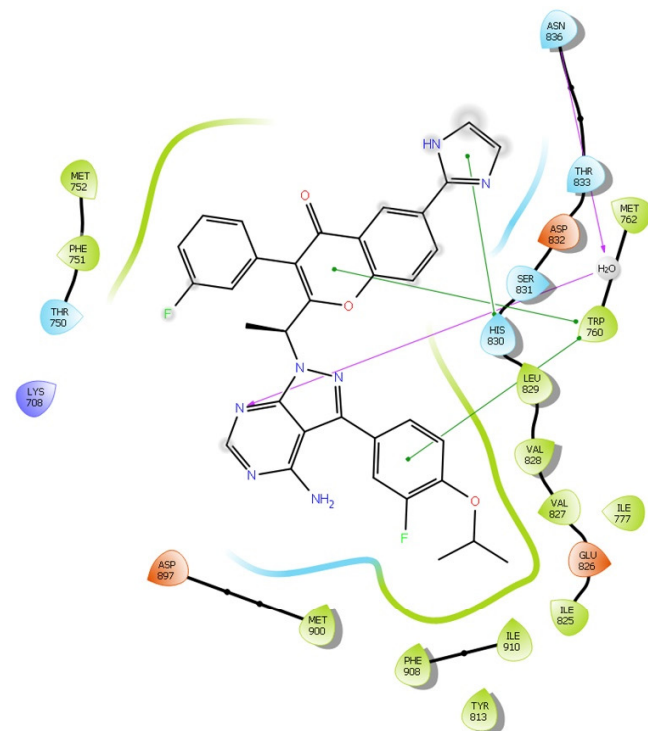
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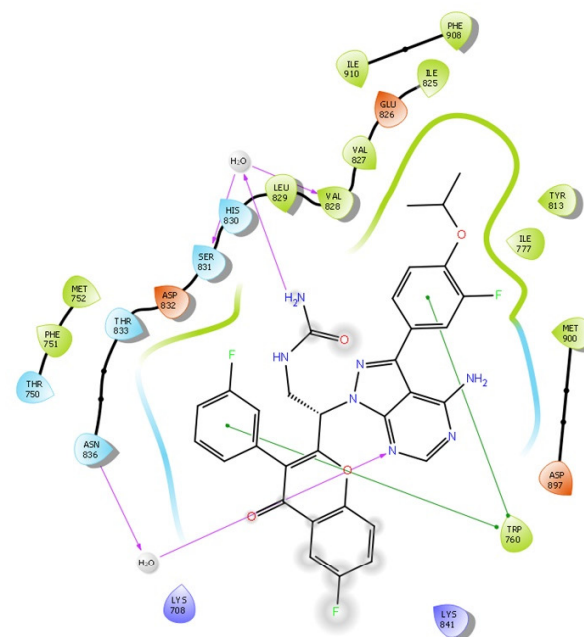
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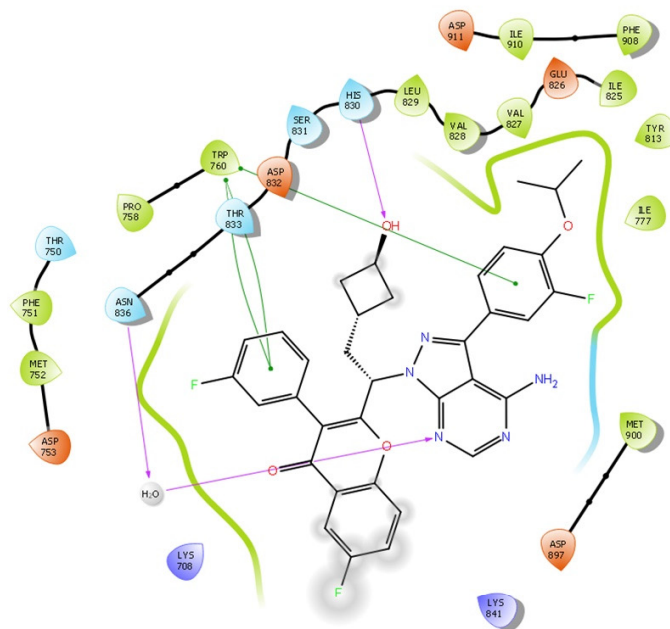
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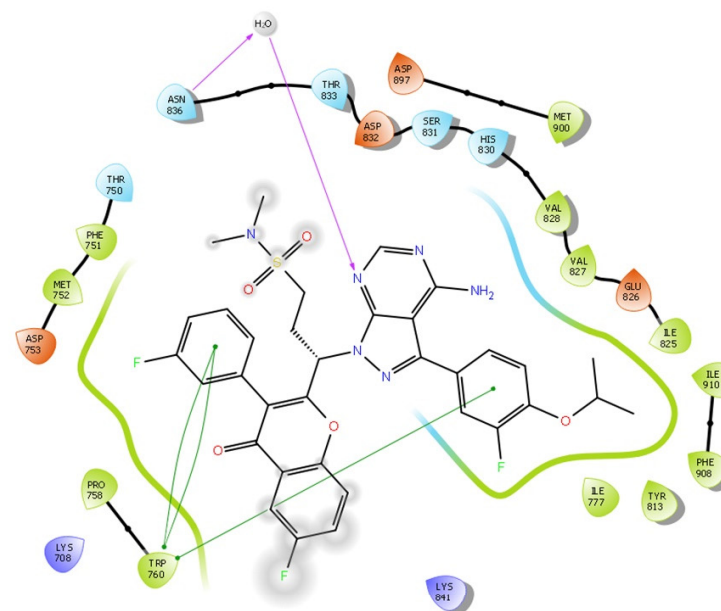
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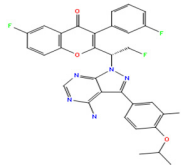
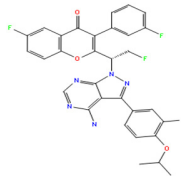
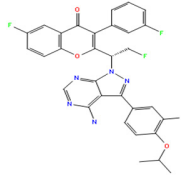
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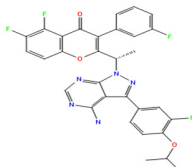
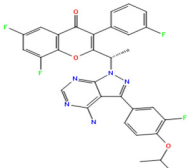
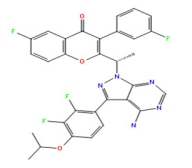
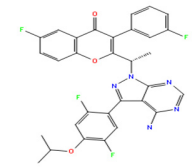


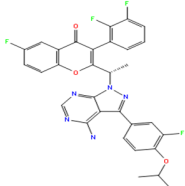
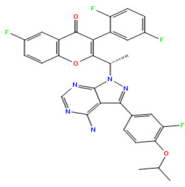
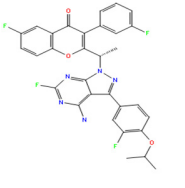
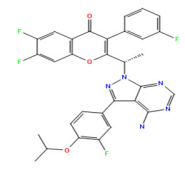
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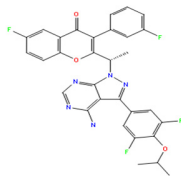
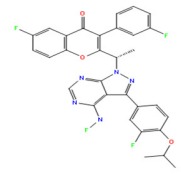
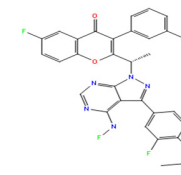
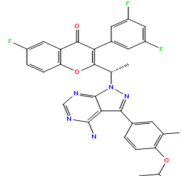
Figure S1. 2D interaction of the remaining top eight analogues in complex with PI3Kδ protein (PDB ID:4XE0) using the XP docking mode of Glide software. The hydrogen bond interactions with residues are represented by a purple dashed arrow directed towards the electron donor. The hydrophobic residues are in green color.

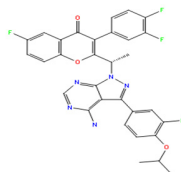
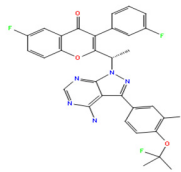
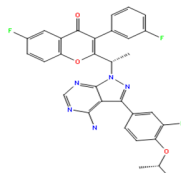
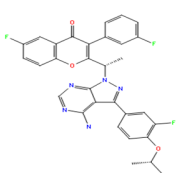
Table S1: Docking scores of the designed analogues.

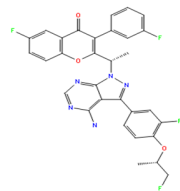
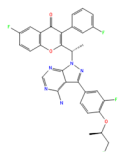
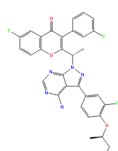
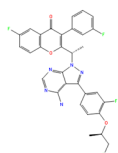
Title	Structure	docking score (kcal/mol)
Analoguue1		-7.262
Analoguue2		-7.228
Analoguue3		-7.226

Analogue4		-7.286
Analogue5		-7.684
Analogue6		-7.291
Analogue7		-7.017

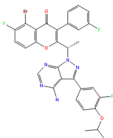
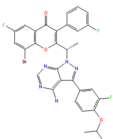
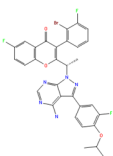
Analogue8		-7.302
Analogue9		-7.110
Analogue10		-6.884
Analogue11		-7.169

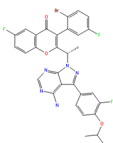
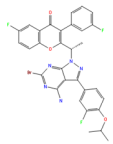
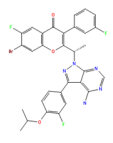
Analogue12		-7.656
Analogue13		-7.243
Analogue14		-7.081
Analogue15		-7.148

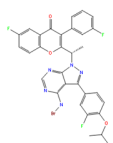
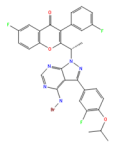
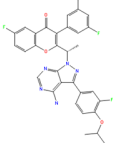
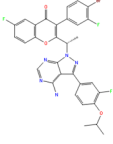
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Analogue17		-7.097
Analogue18		-6.178
Analogue19		-7.280

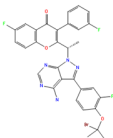
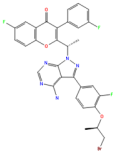
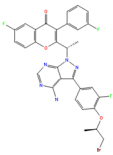
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Analogue21		-7.239
Analogue22		-7.555
Analogue23		-7.569

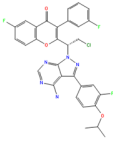
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Analogue25		-7.400
Analogue26		-7.467
Analogue27		-7.450

Analogue28		-7.480
Analogue29		-7.731
Analogue30		-7.269
Analogue31		10000.000

Analogue32		-7.487
Analogue33		10000.000
Analogue34		-7.350
Analogue35		-7.676

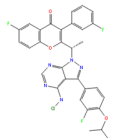
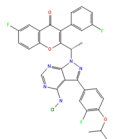
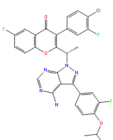
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Analogue39		-7.170

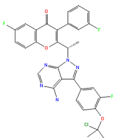
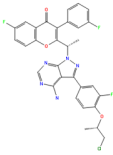
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Analogue42		-6.639
Analogue43		-6.479

Analogue44		-6.423
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Analogue46		-7.332
Analogue47		-7.329

Analogue48		-7.337
Analogue49		-7.603
Analogue50		-7.278
Analogue51		10000.000

Analogue52		-7.398
Analogue53		-5.203
Analogue54		-7.271
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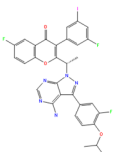
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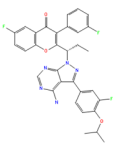
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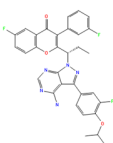
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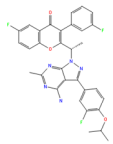
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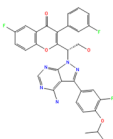
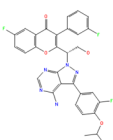
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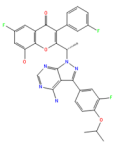
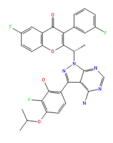
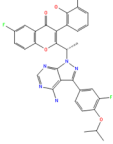
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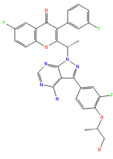
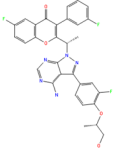
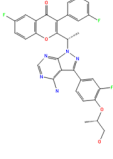
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Analogue102		-7.438
Analogue103		-7.443

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Analogue105		-7.344
Analogue106		-7.426
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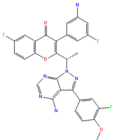
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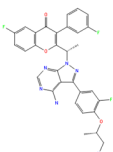
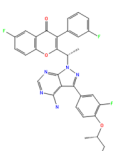
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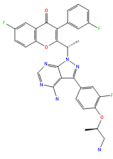
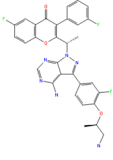
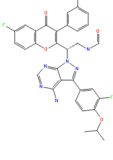
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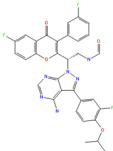
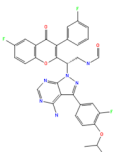
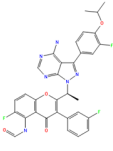
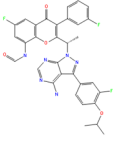
Analogue124		-7.179
Analogue125		-7.177
Analogue126		-7.177
Analogue127		-7.386

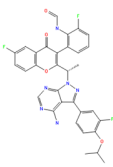
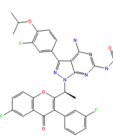
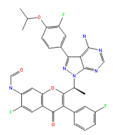
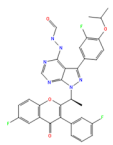
Analogue128		-7.372
Analogue129		-6.069
Analogue130		-7.324
Analogue131		-7.721

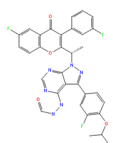
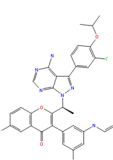
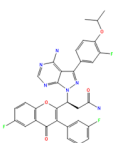
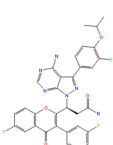
Analogue132		-7.399
Analogue133		-5.842
Analogue134		-7.288
Analogue135		-7.281

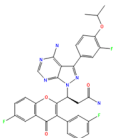
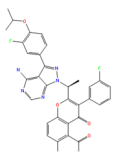
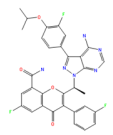
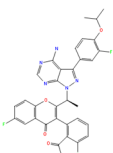
Analogue136		-6.939
Analogue137		10000.000
Analogue138		10000.000
Analogue139		10000.000

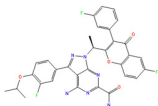
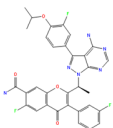
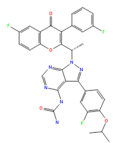
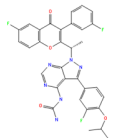
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Analogue141		-7.140
Analogue142		-6.964
Analogue143		-7.542

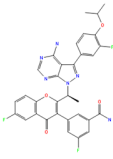
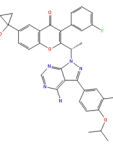
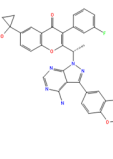
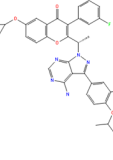
Analogue144		-7.208
Analogue145		-7.202
Analogue146		-7.202
Analogue147		-7.633

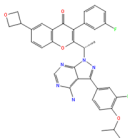
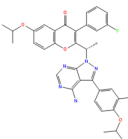
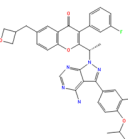
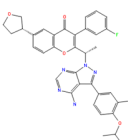
Analogue148		-8.119
Analogue149		-7.397
Analogue150		-7.703
Analogue151		-7.514

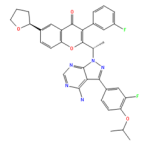
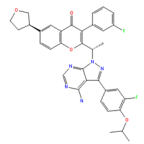
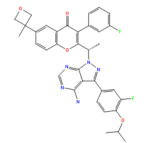
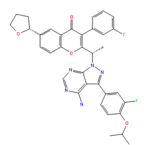
Analogue152		-7.444
Analogue153		-7.717
Analogue154		-6.188
Analogue155		-7.028

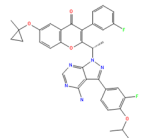
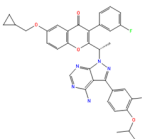
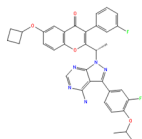
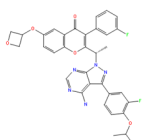
Analogue156		-7.209
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Analogue158		-7.505
Analogue159		-7.711

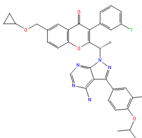
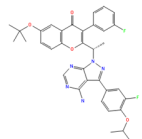
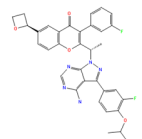
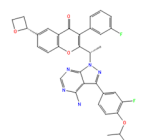
Analogue160		-7.580
Analogue161		-7.499
Analogue162		-7.922
Analogue163		-6.344

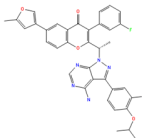
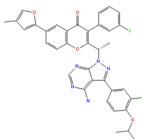
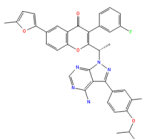
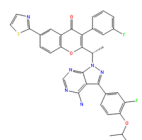
Analogue164		-4.694
Analogue165		-7.041
Analogue166		-7.636
Analogue167		-7.434

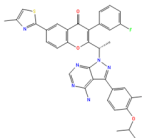
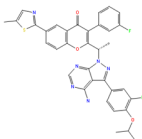
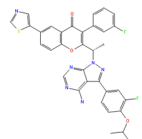
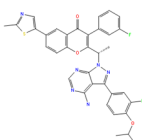
Analogue168		-7.635
Analogue169		-7.549
Analogue170		-7.296
Analogue171		-7.920

Analogue172		-7.697
Analogue173		-7.833
Analogue174		-8.461
Analogue175		-7.779

Analogue176		-7.734
Analogue177		-7.923
Analogue178		-7.497
Analogue179		-7.822

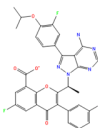
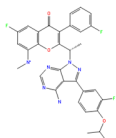
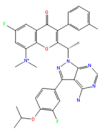
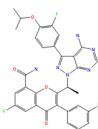
Analogue180		-7.546
Analogue181		-7.588
Analogue182		-7.785
Analogue183		-7.672

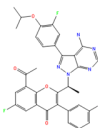
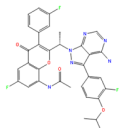
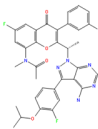
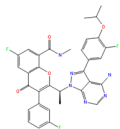
Analogue184		-7.444
Analogue185		-7.542
Analogue186		-7.791
Analogue187		-7.657

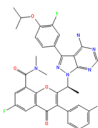
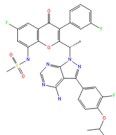
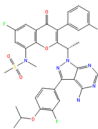
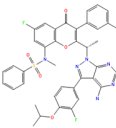
Analogue188		-7.816
Analogue189		-7.900
Analogue190		-7.797
Analogue191		-7.904

Analogue192		-7.756
Analogue193		-7.704
Analogue194		-5.903
Analogue195		-6.822

Analogue196		10000.000
Analogue197		10000.000
Analogue198		-7.683
Analogue199		-7.135

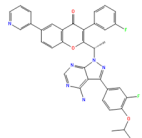
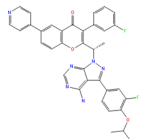
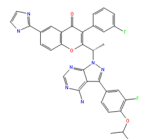
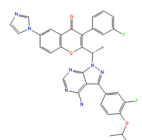
Analogue200		-7.123
Analogue201		-7.834
Analogue202		-7.923
Analogue203		-7.398

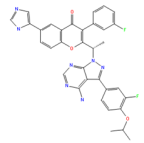
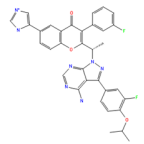
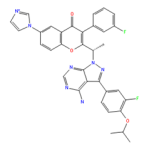
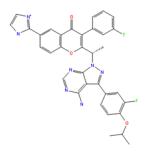
Analogue204		-6.573
Analogue205		-7.894
Analogue206		-7.908
Analogue207		-4.389

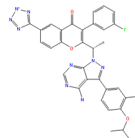
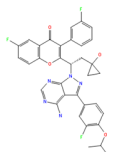
Analogue208		-3.753
Analogue209		-5.882
Analogue210		-8.298
Analogue211		-6.754

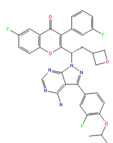
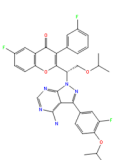
Analogue212		-4.672
Analogue213		-8.155
Analogue214		-6.735
Analogue215		-6.789

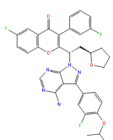
Analogue216		-7.261
Analogue217		-7.576
Analogue218		-7.567
Analogue219		-7.828

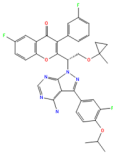
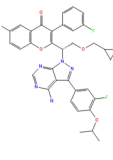
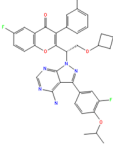
Analogue220		-7.702
Analogue221		-7.806
Analogue222		-7.725
Analogue223		-8.103

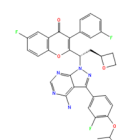
Analogue224		-7.633
Analogue225		-7.531
Analogue226		-7.820
Analogue227		-7.958

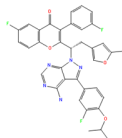
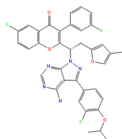
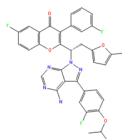
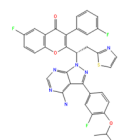
Analogue228		-7.787
Analogue229		-7.357
Analogue230		-7.257
Analogue231		-7.348

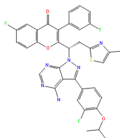
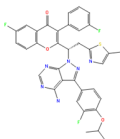
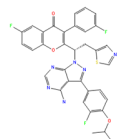
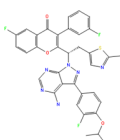
Analogue232		-7.377
Analogue233		-7.289
Analogue234		-7.391
Analogue235		-7.350

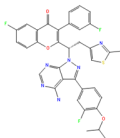
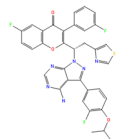
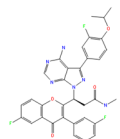
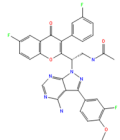
Analogue236		-7.371
Analogue237		-7.298
Analogue238		-7.395
Analogue239		-7.397

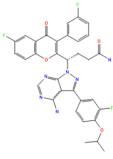
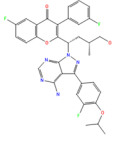
Analogue240		-7.297
Analogue241		-7.412
Analogue242		-7.383
Analogue243		-7.418

Analogue244		-7.502
Analogue245		-7.337
Analogue246		-7.237
Analogue247		-7.184

Analogue248		-7.343
Analogue249		-7.467
Analogue250		-7.462
Analogue251		-7.395

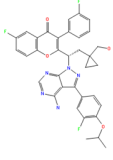
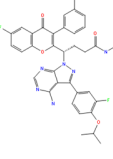
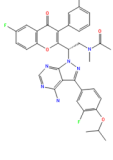
Analogue252		-7.356
Analogue253		-7.366
Analogue254		-7.370
Analogue255		-7.362

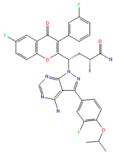
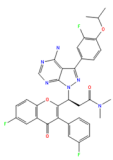
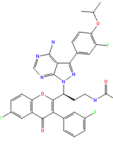
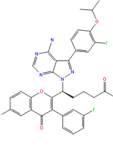
Analogue256		-7.371
Analogue257		-7.415
Analogue258		-7.346
Analogue259		-7.479

Analogue260		-7.219
Analogue261		-7.683
Analogue262		-8.425
Analogue263		-7.159

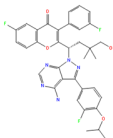
Analogue264		-7.365
Analogue265		-7.378
Analogue266		-7.265
Analogue267		-7.295

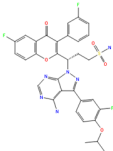
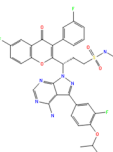
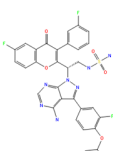
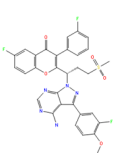
Analogue268		-8.023
Analogue269		-7.553
Analogue270		-7.309
Analogue271		-7.376

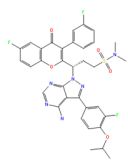
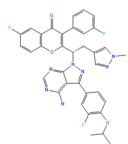
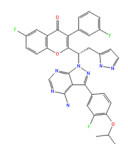
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Analogue273		-7.446
Analogue274		-7.487
Analogue275		-7.397

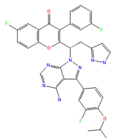
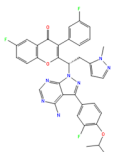
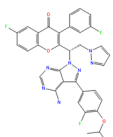
Analogue276		-7.297
Analogue277		-7.457
Analogue278		-7.117
Analogue279		-7.548

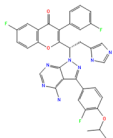
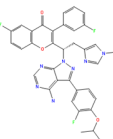
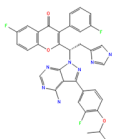
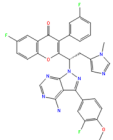
Analogue280		-7.116
Analogue281		-7.284
Analogue282		-7.873
Analogue283		-7.330

Analogue284		-7.518
Analogue285		-7.307
Analogue286		-7.637
Analogue287		-7.527

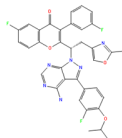
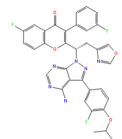
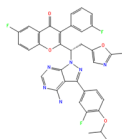
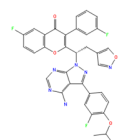
Analogue288		-7.370
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Analogue290		-7.709
Analogue291		-7.404

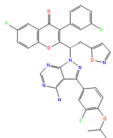
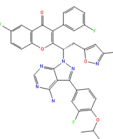
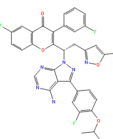
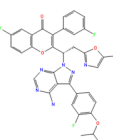
Analogue292		-7.242
Analogue293		-7.667
Analogue294		-7.639
Analogue295		-7.636

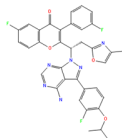
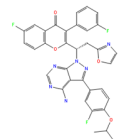
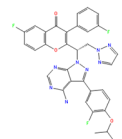
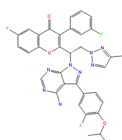
Analogue296		-7.267
Analogue297		-7.284
Analogue298		-7.404
Analogue299		-7.350

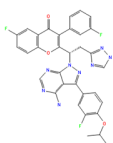
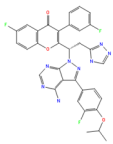
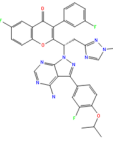
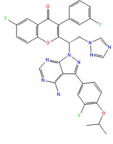
Analogue300		-7.280
Analogue301		-7.586
Analogue302		-7.585
Analogue303		-7.311

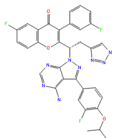
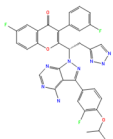
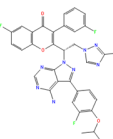
Analogue304		-7.419
Analogue305		-7.317
Analogue306		-7.682
Analogue307		-7.275

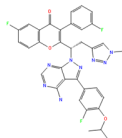
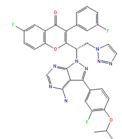
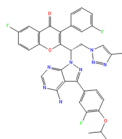
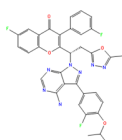
Analogue308		-7.202
Analogue309		-7.316
Analogue310		-7.306
Analogue311		-7.330

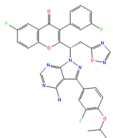
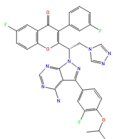
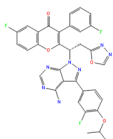
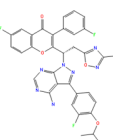
Analogue312		-7.341
Analogue313		-7.451
Analogue314		-7.525
Analogue315		-7.516

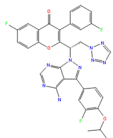
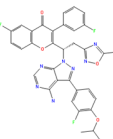
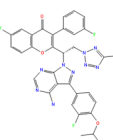
Analogue316		-7.362
Analogue317		-7.260
Analogue318		-7.191
Analogue319		-7.232

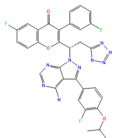
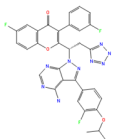
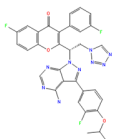
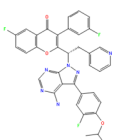
Analogue320		-7.370
Analogue321		-7.230
Analogue322		-7.646
Analogue323		-7.295

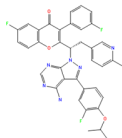
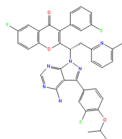
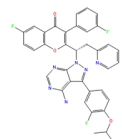
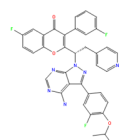
Analogue324		-7.191
Analogue325		-7.292
Analogue326		-7.349
Analogue327		-7.436

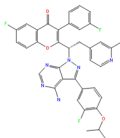
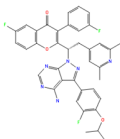
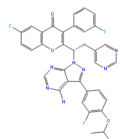
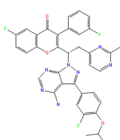
Analogue328		-7.362
Analogue329		-7.649
Analogue330		-7.272
Analogue331		-7.303

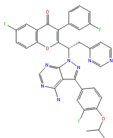
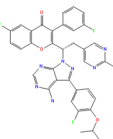
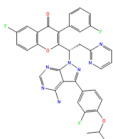
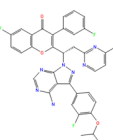
Analogue332		-7.245
Analogue333		-7.200
Analogue334		-7.322
Analogue335		-7.274

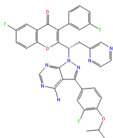
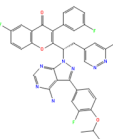
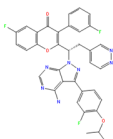
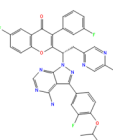
Analogue336		-7.245
Analogue337		-7.234
Analogue338		-7.254
Analogue339		-7.225

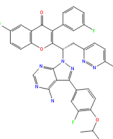
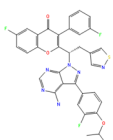
Analogue340		-7.266
Analogue341		-7.299
Analogue342		-7.258
Analogue343		-7.314

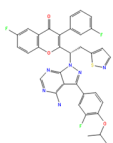
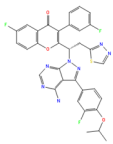
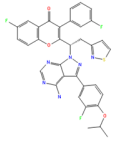
Analogue344		-7.445
Analogue345		-7.415
Analogue346		-7.344
Analogue347		-7.331

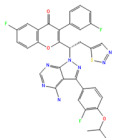
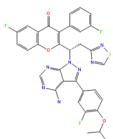
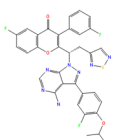
Analogue348		-7.368
Analogue349		-7.411
Analogue350		-7.423
Analogue351		-7.352

Analogue352		-7.459
Analogue353		-7.322
Analogue354		-7.404
Analogue355		-7.357

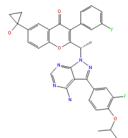
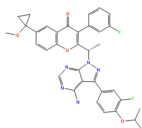
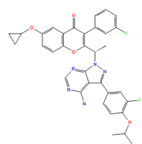
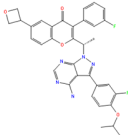
Analogue356		-7.420
Analogue357		-7.335
Analogue358		-7.488
Analogue359		-7.452

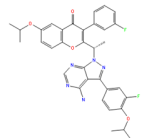
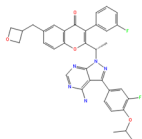
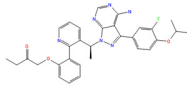
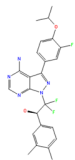
Analogue360		-7.364
Analogue361		-7.254
Analogue362		-7.426
Analogue363		-7.280

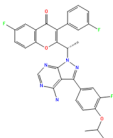
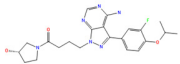
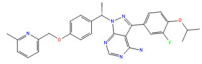
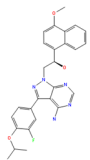
Analogue364		-7.505
Analogue365		-7.344
Analogue366		-7.342
Analogue367		-7.566

Analogue368		-7.378
Analogue369		-7.378
Analogue370		-7.353
Analogue371		-7.241

Analogue372		-7.333
Analogue373		-7.219
Analogue374		-7.693
Analogue375		-7.585

Analogue376		-7.353
Analogue377		-7.636
Analogue378		-7.434
Analogue379		-7.635

Analogue380		-7.549
Analogue381		-7.296
Analogue382		-7.920
Analogue383		-6.151

Analogue384		-5.023
Analogue385		-5.845
Analogue386		-5.601
Analogue387		-5.735

Analogue388		-4.764
Analogue389		-5.307
Analogue390		-7.092
Analogue391		-6.727