Università degli Studi di Padova

Facoltà di Medicina e Chirurgia

CORSO DI LAUREA TRIENNALE IN TECNICHE DELLA PREVENZIONE NELL'AMBIENTE E NEI LUOGHI DI LAVORO

Presidente Prof. Bruno Saia

TESI DI LAUREA

PREDIZIONE DELLA TOSSICITA' ACQUATICA DI COMPOSTI ORGANICI: UNA NUOVA STRATEGIA *IN SILICO* PER LA PREDIZIONE SU LARGA SCALA DELLA TOSSICITA' DI DATABASE DI COMPOSTI CHIMICI

RELATORE: PROF. MASSIMO RIOLFATTI
CORRELATORE: PROF. STEFANO MORO

LAUREANDO: ANGELO CIRILLO

ANNO ACCADEMICO 2006 - 2007

INDICE

alle donne della mia vita che hanno saputo

aiutarmi e sostenermi portando pazienza e dandomi

l'energia necessaria per poter arrivare alla stesura di questa tesi di laurea

a Stefano amico da sempre e a Magda per l'aiuto dato

ad un laureando "atipico"

ai miei genitori

INTRODUZIONE

Il problema di predire la tossicità dei composti rappresenta un punto cruciale nello sviluppo della chimica da quando ci sono strette leggi che regolano l'uso di sostanze, in particolare per quelle che hanno bisogno di essere introdotte nel mercato in quantità superiore ad una tonnellata l'anno. *(1)* Il primo giugno 2007 infatti, una nuova regolazione comunitaria europea sulle sostanze chimiche e la loro sicurezza è entrata in vigore ed è chiamata REACH acronimo che sta per Registration, Evaluation, Authorization and Restriction of Chemical substances *(1)*.

Il REACH è entrato in vigore sostituendo numerose direttive e regolamenti, mirando a rafforzare la protezione della salute umana e dell'ambiente dagli effetti nocivi delle sostanze chimiche e al tempo stesso cercando di migliorare la competitività e la capacità di innovazione dell'industria chimica europea. Infatti, la Commissione Europea per la Valutazione dell'Impatto Esteso, (Extended Impact Assessment of the European Commission) riporta che le malattie causate dagli agenti chimici sono presunte all'1% del totale di tutti i tipi di malattie nell'EU; quindi, se il REACH producesse un calo del 10% di queste malattie, il risultato corrisponderebbe ad uno 0,1% di riduzione del totale delle malattie nell'EU, e ciò equivarrebbe a circa 4500 morti di cancro evitate ogni anno *(1)*.

Lo scopo di questo nuovo Regolamento è di migliorare la protezione della salute umana e dell'ambiente attraverso una migliore e precoce identificazione delle proprietà intrinseche delle sostanze chimiche, fornendo informazioni di sicurezza su di esse, "coprendo tutte le sostanze, sia che esse siano state prodotte, importate, usate come intermedi o messe sul mercato, oppure usate da sole, in preparati o in codici, a meno che siano radioattivi, soggetti a supervisione doganale, o non siano intermediari non-isolati". *(1)*

Il principale parametro per determinare la tossicità di una sostanza è la dose (livello di concentrazione): infatti, quasi tutte le sostanze, in certe dosi o in determinate circostanze possono essere tossiche. Quest'ultimo concetto è ben riassunto dalla frase attribuibile a Paracelso: "*sola dosis venenum facit*" [trad: *è la dose che fa (di una sostanza) il veleno*].

Non vi è nessuna differenza tra la il concetto di tossicologia legata ai farmaci e quello legato alla realtà industriale in quanto entrambi studiano il rapporto che esiste tra dose e risposta. Il concetto di dose in farmacologia si riferisce ad un rapporto dose/beneficio nell'organismo umano mentre in tossicologia si mira a determinare gli effetti indesiderati che quella dose provoca all'organismo.

Diventa quindi fondamentale abbinare ad ogni composto un valore di dose di tossicità. La tossicologia, studiando gli effetti sull'ecosistema quando le sostanze sono presenti ad una dose superiore a quella in cui non danno nessun

effetto, contribuisce ad interpretare i livelli informativi che derivano ad esempio dall'epidemologia e dalla bioanalisi.

Al fine di stabilire se una sostanza è tossica e quindi definire il rapporto dose/effetto il metodo principale è quello sperimentale con l'utilizzo di metodiche che prevedono l'uso di cavie di laboratorio. Questo metodo risale al fisiologico francese Claude Bernard (1813 – 1878) e consente di tracciare delle curve dose-effetto.

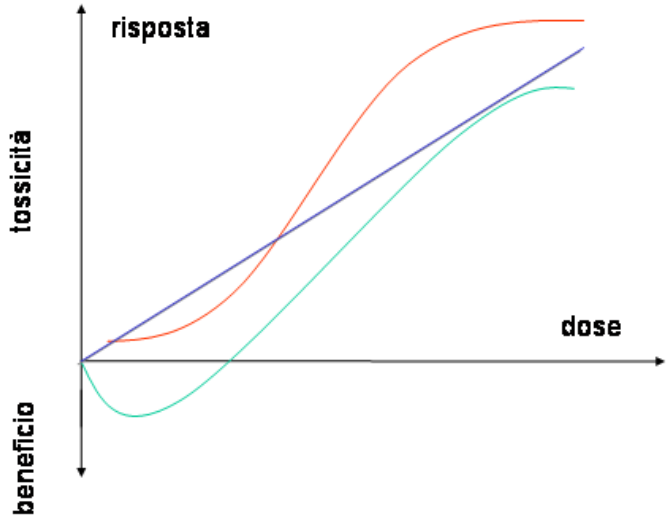


Figura 1. *Esempio di curva dose/effetto*

Da un primo esame di queste curve si può notare quali siano le risposte ai bassi livelli ed agli alti livelli di esposizione e anche com'è la pendenza nella parte iniziale della curva, che è anche la parte più significativa della curva stessa. La curva dose risposta più comune è quella rossa che ha il tipico andamento detto a sigmoide.

La distribuzione rappresentata da questa curva è significativa per tre aspetti principali:

a) non tocca l'asse delle X ovvero c'è una soglia che sta a significare che al disotto di un certo livello non c'è risposta;

b) viene raggiunta una dose massima a cui pur aumentando la dose non corrisponde un aumento di tossicità (risposta costante): ciò avviene per saturazione dei sistemi metabolici;

c) La pendenza della curva è indice della tossicità della sostanza in quanto maggiore è la pendenza e più tossica è la sostanza ovvero per piccoli incrementi di dose si hanno alti valori di tossicità.

La curva colorata in blu è lineare senza soglie ed è tipica di una rapporto dose risposta presente nelle sostanze genotossiche e cancerogene per le quali non esiste una soglia e anche una sola molecola potrebbe indurre un effetto. Infine la curva verde manifesta un andamento che a basse dosi porta ad un beneficio mentre ad alte dosi una tossicità. Questo viene detto effetto ermetico per cui alle basse dosi una data funzione viene stimolata ed alle alte dosi vieni inibita. *(2)*

Gli studi tossicologici su sistemi bersaglio sono generalmente condotti utilizzando differenti dosi di sostanza tossica capaci di coprire un largo intervallo di concentrazione. I risultati di ogni studio mostreranno generalmente, ma non sempre, effetti dannosi ad alte dosi ed effetti lievi a basse dosi. Se la sostanza è tossica sarà così identificata la dose alla quale gli effetti dannosi compaiono (livello di effetto EL). Lo studio identificherà anche la dose massima alla quale

non si osservano effetti (livello di nessun effetto osservato NOEL). Bisogna evidenziare che la natura e la severità degli effetti osservati varierà con il tipo di test, il tempo di esposizione, la specie bersaglio; questo fatto mette in discussione qualunque confronto conclusivo dell'effetto tossico tra una specie e l'altra. Come conseguenza studi di tossicità condotti in modo diverso potranno risultare in differenti valori di EL e di NOEL: la valutazione del rischio dovrebbe basarsi sullo studio più sensibile che fornisce il minimo valore di NOEL. Qualche volta il termine NOEL è sostituito da NOAEL dove la lettera A sta per *avverso*, indicando con essa il carattere dell'effetto, rispetto ad un effetto non nocivo.

I risultati di studi di tossicità possono essere usati in due modi diversi: per predire livelli sicuri di esposizione dell'uomo e per predire livelli potenzialmente tossici e la natura probabile degli effetti dannosi.

Nel primo caso i risultati degli studi di tossicità possono essere usati per predire la più elevata quantità di un sostanza tossica assorbita su base giornaliera da un essere umano senza alcun danno sostanziale. Talvolta tale quantità viene riferita all'unità di peso del soggetto e viene assunta come pari al NOEL diviso per 100: ciò al fine di una maggiore garanzia a protezione degli esposti, tenuto conto che gli esseri umani possono essere più sensibili alle sostanze tossiche degli animali utilizzati nei test di tossicità per differenze tossicocinetiche e tossicodinamiche nell'iter della sostanza stessa (adsorbimento, metabolizzazione, escrezione per la tossicocinetica; attività contro la cellula, i tessuti, gli organi per la tossicodinamica).

Nel secondo caso i risultati degli studi della tossicità possono essere usati per predire la natura di effetti nocivi che si possono registrare negli esseri umani ed a quali livelli di esposizione tali danni si possano registrare.

Per la maggior parte degli effetti tossici prodotti da un particolare composto c'è un valore di esposizione al di sotto del quale gli effetti nocivi non si osservano. A basse esposizioni il corpo può tollerare alcuni disturbi alle sue funzioni biochimiche e fisiologiche senza alcun segnale o sintomo di malattia. A volte l'organismo è capace di rimediare ad alcuni danni derivati dal contatto con alcuni composti purché questo sia limitato nel tempo. In altri casi il risanamento non può avvenire, il che si traduce in danno permanente e malattie a lungo termine.

Quando i danni sono di natura genetica al DNA ed ai cromosomi o peggio, si hanno forme di cancro per danneggiamento del DNA e si parla di effetti genotossici o carcinogenici. Questi effetti possono essere rilevati mediante test in vitro, ad esempio esponendo batteri alle sostanze tossiche da testare (test di Ames) o cellule isolate animali o umane alla sostanza stessa. Se risultano effetti genotossici in vitro, si passa ai test in vivo su animali per confermare o meno i risultati in vitro. Il danno al DNA è un evento di tutti i giorni (si pensi all'esposizione alla componente ultravioletta dello spettro solare, all'esposizione ai radicali liberi dell'ossigeno, alla divisione cellulare) cosicché il nostro organismo deve porvi rimedio con provvedimenti ed iniziative che si ripetono per milioni di volte al giorno. Questi studi hanno dimostrato che danni al DNA

possono prodursi anche a dosi molto basse, crescendo ovviamente nettamente al crescere della dose. Questi campioni vengono definiti positivi, nel senso che producono danno genotossico. Ad oggi non è possibile definire livelli di nessun effetto per i composti chimici positivi. I danni a cellule e DNA non riparati possono avere due conseguenze negative, in quanto possono provocare divisione e mutazione cellulare.

Gli effetti cancerogenici vengono osservati e misurati esponendo animali, generalmente topi o ratti di età giovane a dosi giornaliere di tossico esaminando il numero ed il tipo di tumori che si sviluppano, ma le conclusioni a tale tipo di approccio soffrono di accuratezza in quanto riferite a specie diverse da quella che si intende proteggere, l'uomo. C'è infine da osservare che l'esposizione a dosi anche piccole, se anche non produce alcun effetto nel tempo breve, di fatto lo produce certamente nel lungo, lunghissimo tempo; questo tipo di rilevazione per motivi pratici non è di reale esecuzione.

Per i composti cancerogenici, differenti approcci ci dicono se ci sia un reale rischio di cancro ai valori di esposizione che realisticamente possono essere del tipo di quelli incontrati dagli esseri umani. Tali approcci si basano usualmente su curve dose/risposta, ottenute durante test animali. Queste curve relazionano l'incidenza del cancro alle variabilità delle dosi giornaliere assunte per tutta la vita.

Di recente, per dare una giusta risposta alle svariate domande nate dal nuovo regolamento, si è cercato di sviluppare e di valutate nuove strategie

finalizzate a predire la tossicità dei composti chimici. *(3)* In particolare, nuove applicazioni in silico sono state sviluppate a supporto della valutazione dei dati di tossicità per le diverse sostanze chimiche.

Attualmente, due tipi principali di sistemi per predire la tossicità sono oggi disponibili: i programmi correlativi o "guidati dai dati" e i sistemi esperti basati su regole. *(4)*

I sistemi correlativi, come MCASE, TOPKAT, MDL QSAR, MetaDrug, vengono usati per processare grandi database di molecole non correlate, senza una previa organizzazione allo scopo di estrarre una relazione struttura-attività (SAR) mediante strumenti statistici. *(5-8)*

Il più grande svantaggio di tali sistemi è la facilità con cui una tale predizione necessita di un'attenta validazione dei risultati. Tali metodi sono migliori per una primaria identificazione di livelli di "allerta" piuttosto di una determinazione esatta del valore di tossicità all'interno dei livelli stessi. I sistemi basati su regole, come il DEREK, l'OncoLogic o l'Hazard-Expert che costruiscono associazioni e generalizzazioni da piccoli gruppi di sostanze chimiche o da gruppi di sostanze chimiche che agiscono in maniera simile in classi basate su definizioni di chimica organica e di comprensione meccanicistica e usando giudizi di esperti e il razionale basato sul meccanismo di azione all'interno delle classi *(9-11)*.

I sistemi basati su regole base tipicamente sono più limitati nella loro applicazione rispetto ad un tipo di approccio correlativo, ma possono offrire una

interpretabilità chimica e biologica maggiore per i prodotti chimici che vengono predetti. *(4)*

Diversi approcci di Relazioni Quantitative Struttura Attività (QSAR) sono stati studiati per la tossicità nell'acqua, parametro questo decisivo nel profilo di tossicità dei composti chimici *(12-16)*. In particolare, Colombo e i suoi collaboratori hanno recentemente proposto in una pubblicazione differenti modelli QSAR per l'analisi della tossicità in acqua, partendo da un grande dataset di composti industriali organici. In questo lavoro sono stati usati semplici descrittori costituzionali e descrittori chimico quantistici per classificare tutti i composti in differenti sottoinsiemi strutturali *(15)*. Per ogni sottoinsieme di molecole la successiva selezione automatica di descrittori è applicata per costruire dei modelli QSAR.

Iniziando da questo lavoro, nella presente tesi viene riportato il risultato di una applicazione QSAR per lo stesso dataset pubblico di prodotti chimici industriali (551 composti chimici), omettendo l'iniziale classificazione in sottoinsiemi strutturali, con lo scopo di sviluppare un modello generale di predizione della tossicità in acqua di composti chimici. In particolare, tre differenti classi di descrittori molecolari sono stati combinati insieme usando il metodo lineare dei minimi quadrati parziali (PLS): il vettore di autocorrelazione del potenziale elettrostatico molecolare (*auto*MEP), i descrittori Sterimol e i valori di log*D* (a pH 7.4). Si è ottenuto così un apprezzabile e robusto modello

con dei buoni coefficienti di correlazione statistica sia nello step di calibrazione del modello, sia in quello di validazione interna.

Questo modello è stato usato per predire la tossicità in acqua di una serie di 1977 composti estratti da un database pubblico MMsINC. *(17)* Lo schema di lavoro è riportato nella Figura 2.

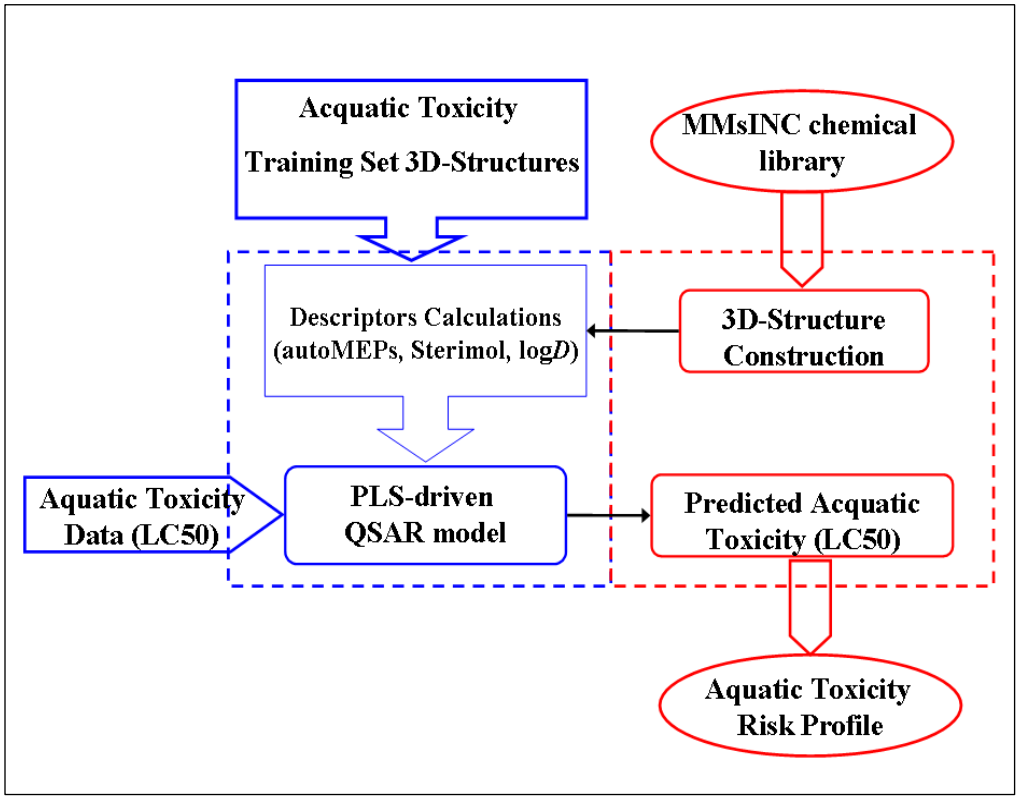


Figura 2. *Flowchart della strategia QSAR proposta.*

SCOPO DELLA TESI

Come anticipato nell'Introduzione, l'applicazione di tecniche computazionali per valutare il rischio che le sostanze chimiche hanno sulla salute pubblica e sull'ambiente - tossicologia computazionale – rappresenta un interessante ramo della ricerca finalizzata al miglioramento della vita. In particolare, i computer-based modeling methods – metodi di modellistica basati sull'uso dei computer- in grado di relazionare le strutture chimiche con l'attività biologica qualitativa (SAR) e la potenza biologica quantitativa (QSAR) sono considerati uno strumento molto utile per l'analisi della valutazione del rischio delle sostanze chimiche tossiche.

In questo lavoro viene dunque proposto un modello QSAR per predire la tossicità in acqua di nuovi composti al fine di estendere la sua applicabilità ad una larga scala di sostanze chimiche.

Scopo dunque del lavoro è creare un modello QSAR e applicarlo per la predizione di valori di tossicità in acqua per sostanze chimiche in genere.

MATERIALI E METODI

Metodologie computazionali.

Tutti i gli studi di modellistica sono stati elaboratii su un cluster linux 16 CPU (Intel Core^{TM} 2 Quad CPU 2, 40 GHz).

Tutte le analisi PLS sono state effettuate utilizzando il software di statistica "The Unscrambler". *(18)*

Costruzione delle strutture molecolari.

I modelli 3D dei composti chimici sono stati ottenuti usando il generatore di strutture 3D Corina, che è una parte integrante del software AdrianaCode (versione 2.1). *(19)* Questo software genera automaticamente le coordinate 3D degli atomi partendo dalla costituzione di una molecola come espressa da una tavola di connessione o da una stringa lineare. Un conformero a bassa energia è generato per ogni composto, iniziando da molecole espresse in notazioni di legame di valenza, combinando frammenti monocentrici con lunghezze e angoli di legame standard e usando angoli diedri adatti. Vedi Figura 3.

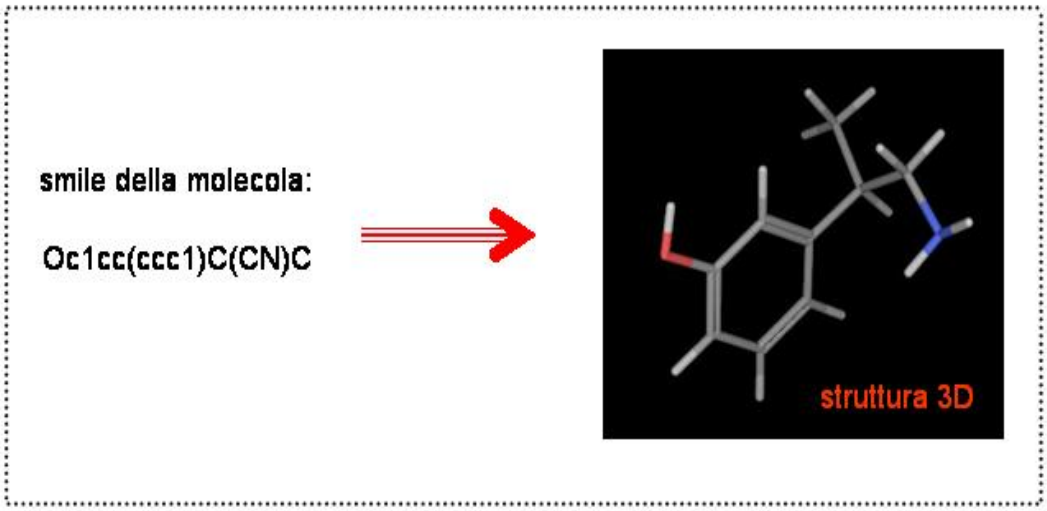


Figura 3. *esempio di molecola in notazione smile e in 3D.*

Training e Test sets.

Una raccolta di 551 prodotti chimici industriali disponibili pubblicamente sono stati selezionati per ricavare il nostro modello *auto*MEP/PLS. *(15)*

Un test esterno è stato selezionato dal database MMsINC. *(17)* MMsINC è un database free-web di composti disponibili commercialmente o pubblicamente per applicazioni chemoinformatiche e di screening virtuale. MMsINC contiene più di 4 milioni di composti chimici non ridondanti in formato 3D. MMsINC è accessibile sul sito web : http://mms.dsfarm.unipd.it/MMsINC/ .

Una ricerca per similarità è stata dedotta sui primi 153 composti del training set, identificati come molecole con "anelli alifatici e composti poliaromatici". *(15)* Sono stati selezionati tutti i composti analoghi con valori PM < 500 Da e valori di Sterimol L (valori che definiscono la dimensione delle molecole) inclusi nell'intervallo di 6.79 – 19.75 Å (corrispondenti al minimo e al

massimo valori L delle 153 molecole). Ne è derivato un set finale di 1977 molecole.

(Vedi Materiale Supplementare per le strutture molecolari.)

Calcolo dei descrittori molecolari.

I vettori autocorrelati del potenziale molecolare elettrostatico (*auto*MEP) sono stati calcolati usando AdrianaCode (versione 2.1). *(19)* I descrittori molecolari *auto*MEP sono stati introdotti qualche anno fa da Gasteiger e collaboratori. *(20-22)* Il Potenziale Elettrostatico Molecolare si deriva per ogni molecola da un modello classico di carica puntiforme ed è ottenuto muovendo una carica positiva puntuale sulla superficie di Van der Waals, ed è calcolata a vari punti j su questa superficie seguendo questa equazione :

$$V_j = \sum_{i}^{atoms} \frac{q_i}{r_{ji}}$$

Dove q_i rappresenta la carica parziale di ogni atomo i, e r_{jj} è la distanza tra i punti j e l'atomo i. Iniziando dal modello 3D di una molecola e dalle sue cariche atomiche parziali, il potenziale elettrostatico è calcolato per punti sulla superficie molecolare. Le cariche atomiche parziali vengono calcolate attraverso il metodo PEOE e la sua estensione a sistemi coniugati, come implementato nel software AdrianaCode. La superficie accessibile al solvente o superficie di Connolly, con

un solvente avente raggio di 2.0 Å è stata usata per proiettare il corrispondente MEP. Il passaggio successivo è stato l'applicazione della funzione di autocorrelazione per ottenere il vettore di autocorrelazione. La prima applicazione di questi vettori come descrittori molecolari è stata pubblicata da Moreau e Broto, che applicarono le nozioni matematiche classiche di una funzione di autocorrelazione alla topologia di strutture molecolari *(23-24*). Il vettore di autocorrelazione è presentato come un descrittore intrinseco della distribuzione di una proprietà atomica lungo il grafico molecolare. Ogni componente del vettore di autocorrelazione è calcolato come segue :

$$A(d) = \sum p_i p_j$$

Dove A è il coefficiente di autocorrelazione relativo alle coppie di atomi *i* e *j, pj* è la proprietà atomica, e d è la distanza topologica *i j*. Partendo da questo concetto è stato introdotto un nuovo descrittore 3D, basato sull'autocorrelazione di proprietà per punti distinti sulla superficie molecolare *(20-22)*. Le differenti componenti del vettore di autocorrelazione sono calcolate in questo modo :

$$A\ (d_{\text{lower}}, d_{\text{upper}}) = 1/L \sum p_i p_j \quad (d_{\text{lower}} < d_{\text{ij}} < d_{\text{upper}})$$

dove la distanza d_{ij} appartiene all'intervallo d_{lower} ,d_{upper} e L è il numero delle distanze nello stesso intervallo. L'applicazione di questo concetto rende possibile confrontare differenti proprietà molecolari, dato che questo descrittore 3D rappresenta un'espressione compressa della distribuzione della proprietà p sulla

superficie molecolare. I parametri per il calcolo del coefficiente di autocorrelazione sono i seguenti :

d_{lower} = *1 Å;*

d_{upper} = *13 Å;*

L = 12;

densità dei punti sulla superficie= 10 punti/ Å^2 *;*

fattore di riduzione dell raggio di vdW= 1000.

Tutti i parametri sono stati cambiati in vari modi per vedere se era possibile migliorare la capacità del modello, ma non ci sono stati risultati significativi. Considerando le distanze da 1 a 13 Å, con un'ampiezza di passo di 1Å sono stati calcolati 12 coefficienti di autocorrelazione. Questa trasformazione produce un'unica impronta digitale per ogni molecola in considerazione.

I descrittori 3D–Sterimol (L, B1, B2, B3, B4) sono stati calcolati usando il software Molecular Operating Enviroment (MOE, ver. 2007.09) *(25)*. Essi vennero introdotti da Verloop nel 1976 per spiegare i volumi di sostituti molecolari con differenti geometrie.*(26)*. La successiva trasposizione di questo concetto all'intera molecola permette di ottenere valori di Sterimol per la definizione sterica globale di molecole. I cinque descrittori sono dunque intrinsecamente indipendenti dai movimenti di traslazione e rotazione della molecola, e di conseguenza, possono essere usati insieme ai descrittori *auto*MEP*(27)*. Infine, è stato calcolato il descrittore log*D* a pH 7.4. usando il software ACDLabs (versione 10) *(28)*.

Dati di tossicità.

In questo lavoro la tossicità in acqua è espressa come pLC_{50}. Il valore di LC_{50} si riferisce alla concentrazione letale somministrata a pesciolini "Fathead" (*Pimephales promelas*) esposti a 96- flussi nello stadio giovane. I valori di LC_{50} sono espressi in mmo l/L. Tutti i dettagli sono stati già riportati da Colombo e i suoi collaboratori. *(15)*.

RISULTATI E DISCUSSIONE

Le relazioni struttura-attività sono essenziali per le ricerche in tossicologia. Le proprietà biologiche dei nuovi composti sono spesso derivate da proprietà di materie simili esistenti, i cui rischi sono già conosciuti. In ogni caso i tossicologi oggi si confrontano con il compito di esaminare un largo numero di diverse sostanze chimiche con strumenti diversi, per via di un incremento di controlli diversi della tossicità, usando risorse limitate e meno animali. I test sugli animali e quelli *in vitro* sono ancora considerati essenziali per sostenere le valutazioni di rischio, ma spesso sono troppo costosi e richiedono tempo per essere applicati a tutta la gamma di sostanze chimiche per le quali sono necessari alti livelli di screening tossicologico. L'applicazione di tecniche computazionali per valutare il rischio che le sostanze chimiche hanno sulla salute pubblica e sull'ambiente è chiamata tossicologia computazionale. I Computer-based modeling methods – metodi di modellistica basati sull'uso dei computer- in grado di relazionare le strutture chimiche con l'attività biologica qualitativa (SAR) e la potenza biologica quantitativa (QSAR) sono considerati uno strumento molto utile per l'analisi della valutazione del rischio delle sostanze chimiche tossiche *(3,4,29-30).* Le comunità scientifiche hanno dibattuto recentemente, a causa dell'importanza crescente nell'uso dei metodi QSAR e SAR, sulla definizione di un insieme di principi per definire la validità, la riproducibilità e la qualità di questi modelli. *(29-30)*. In più, nel 2007 l'Organizzazione per lo Sviluppo e la Cooperazione Economica

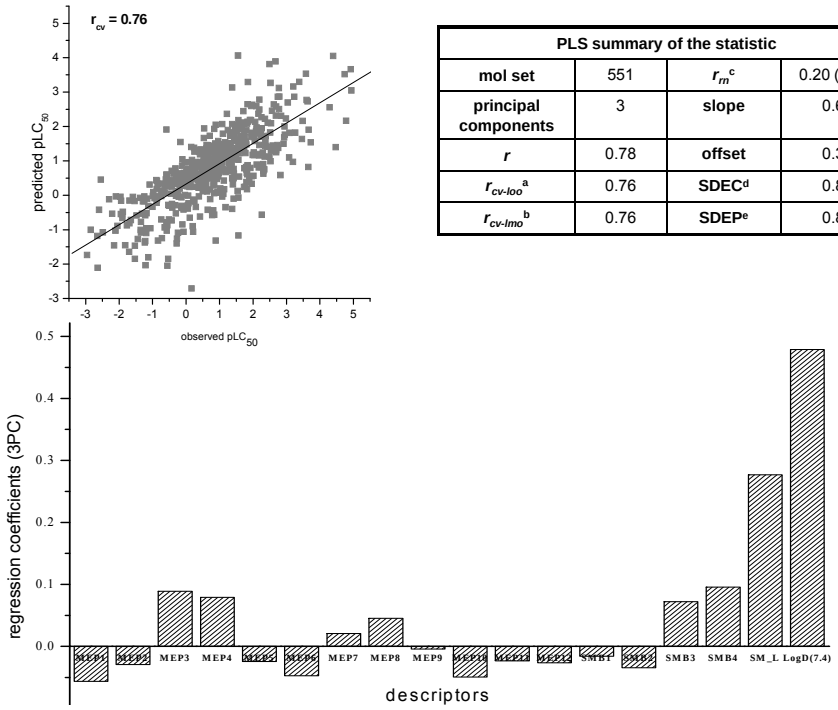
(Organisation for Economic Co-operation and Development - OECD) ha pubblicato una guida per gli scienziati sulla validità dei diversi metodi QSAR e SAR.*(30)*

In questo lavoro viene proposto un modello QSAR alternativo per predire la tossicità in acqua dei nuovi composti con lo scopo specifico di estendere la sua applicabilità ad una larga scala di sostanze chimiche. Colombo e i suoi collaboratori in una loro recente pubblicazione propongono l'uso di diversi descrittori molecolari per dividere il set iniziale in sottoinsiemi di moelcole strutturalmente più simili, proponendo poi un modello specifico QSAR per ogni sottoinsieme di composti *(15).* Partendo da questo lavoro, abbiamo selezionato lo stesso set di 551 sostanze chimiche includendo perciò tutte le differenti strutture chimiche, con lo scopo di avere un modello generale utile per valutare i nuovi composti diversi come strutture, senza fare prima una classificazione. Come anticipato, abbiamo deciso di integrare tre differenti classi di descrittori molecolari usando la PLS: i vettori autocorrelati di potenziale elettrostatico molecolare (*auto*MEP), i descrittori Sterimol e i valori log*D* (a pH 7.4). Recentemente, abbiamo riportato che i vettori *auto*MEP in combinazione con la PLS e/o le tecniche di Analisi di Risposta di Superficie (RSA) possono rappresentare un'alternativa e un utile approccio di relazione quantitativa struttura attività tridimensionale (3D–QSAR) (*27,31-36*). Infatti, le complementarietà elettrostatiche e topologiche rappresentano due concetti-chiave nei diversi processi di riconoscimento molecolare. In più, la conseguente introduzione del

vettore di autocorrelazione rende le informazioni MEP invariate rispetto la rotazione e traslazione spaziale delle molecole e questo si può considerare un valore aggiunto per classificare un largo numero di composti chimici non relazionati. Le proprietà topologiche sono state prese in considerazione usando i descrittori Sterimol implementati da Verloop. Anche i parametri Sterimol sono stati usati in diverse applicazioni 3D–QSAR *(37–38)*. Infine log*D*, o il coefficiente di partizione effettiva per sistemi dissociativi, dà la descrizione corretta degli equilibri complessi di partizione. Il log*D* riflette il reale comportamento di un componente ionizzabile in una soluzione con valore pH, tenendo in considerazione tutte le differenti specie ionizzate presenti. Questo parametro è spesso usato nella valutazione delle proprietà farmacocinetiche pH-dipendenti, come l'assorbimento, la bio-disponibilità, il metabolismo e la tossicità di farmaci *(28,39)*. Abbiamo considerato la combinazione di queste tre classi di proprietà molecolari come strategia chemocentrica per relazionare il profilo tossicologico alla chimica delle molecole.

Come si può vedere nella Figura 4 è stato ottenuto un modello statisticamente robusto, con coefficiente di correlazione di calibrazione r = 0,78 con 3 componenti principali (PCs) e un coefficiente di correlazione cross-validato LOO (leave-one-out) $r_{cv\text{-}LOO}$ =0.76. Seguendo i principi per una validazione migliore dei modelli QSAR *(29),* e' stata effettuata anche la validazione LMO (leave many out) con 10 gruppi di ≈ 50 molecole ognuno, che hanno portato ad un coefficiente di correlazione LMO $r_{cy–LMO}$ = 0,76 (con 3 PCs).

In più la randomizzazione Y della pLC_{50} ha confermato la validità del modello, dato che il coefficiente di correlazione r_{rm} = 0.20 (con 1 PC). Infine abbiamo anche verificato che tutte e tre le categorie di descrittori sono statisticamente rilevanti. In particolare abbiamo trovato che le variabili indipendenti più significative sono il log*D*, l'*auto*MEP 1, 3, 4 e gli Sterimol B3, B4, L, confermando che entrambi gli aspetti dinamici e cinetici sono rilevanti nel descrivere il comportamento chimico tossico dei composti del training set.



PLS summary of the statistic			
mol set	551	r_m[c]	0.20 (1PC)
principal components	3	**slope**	0.60
r	0.78	**offset**	0.31
$r_{cv\text{-}loo}$[a]	0.76	**SDEC**[d]	0.85
$r_{cv\text{-}lmo}$[b]	0.76	**SDEP**[e]	0.88

Figura 4. *Modello QSAR, risultati: (in alto) grafico delle pLC_{50} sperimentali vs pLC_{50} predette del training set; (in basso) variable influence plot (VIP) – grafico delle variabili più influenti del modello, che riporta il peso di ogni descrittore nel modello PLS.* [(a)]*Cross-validated r dopo la procedura di leave-one-out:* $r_{cv\text{-}LOO} = [(SD - PRESS)/SD]^{1/2}$, *SD =*

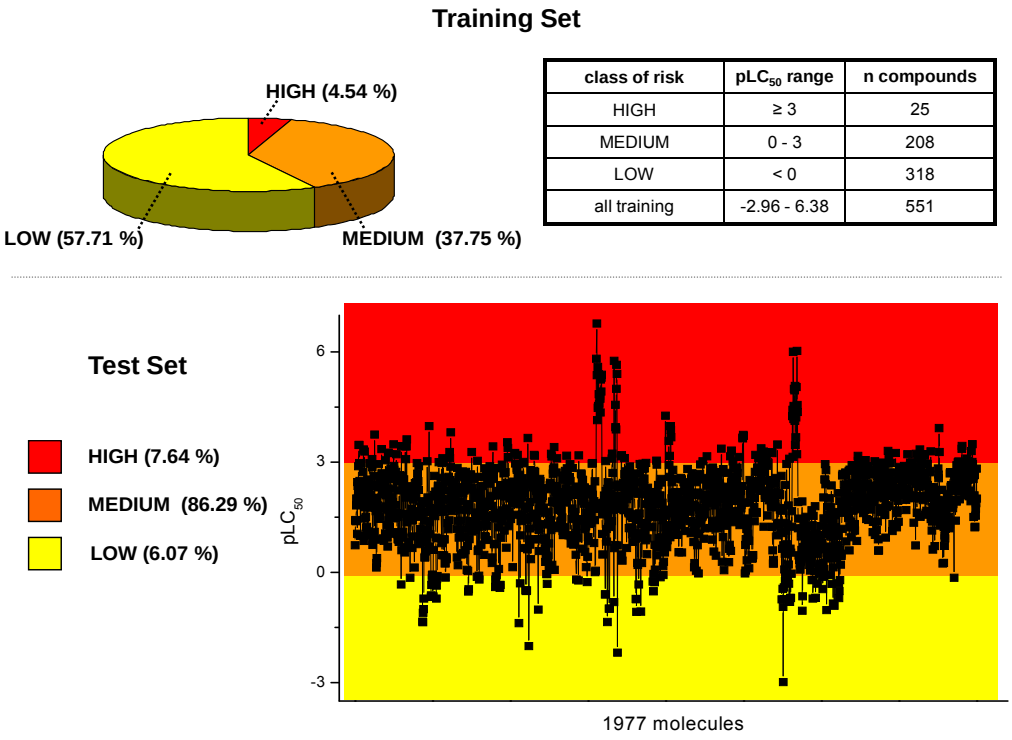
$(Y_{actual} - Y_{mean})^2$ and PRESS = $\sum(Y_{predicted} - Y_{actual})$; [(b)] $r_{cv\text{-}LMO}$ dopo leave-many-out; [(c)] r_{rn} dopo randomizzazione; [(d)] SDEC: Root mean square error di calibrazione; [(e)] SDEP: Root mean square error di predizione dopo cv-LOO.

Come anticipato, lo scopo principale di questo lavoro è quello di estendere l'applicabilità del nostro modello di predizione ad una larga scala di prodotti chimici. A questo proposito abbiamo raccolto un gran set di composti dal database pubblico disponibile MMsINC. In questa fase preliminare del progetto, abbiamo preferito selezionare una raccolta di nuovi composti con il profilo di descrizione abbastanza simile a quello presente nelle prime 153 molecole del set di preparazione, identificate come "anelli alifatici e composti poliaromatici".

Sono stati applicati per la scelta di questo primo test set una soglia di peso molecolare (PM) minore di 500 Da e valori di Sterimol inclusi nell'intervallo di 6.79 – 19.75 Å (il valore L minimo e massimo per i 153 composti). Di conseguenza abbiamo ottenuto e successivamente valutato un dataset di 1977 derivati applicando il nostro modello PLS per la predizione della tossicità in acqua di questi composti chimici presi in esame.

Come già anticipato nell'introduzione, uno degli svantaggi maggiori di un qualsiasi modello QSAR è rappresentato dalla qualità numerica della predizione del modello. Infatti, tali metodi sono migliori per una identificazione di classi di "pericolo" piuttosto che per una più fine distinzione di variazioni quantitative di attività all'interno di queste classi. Come conseguenza abbiamo raggruppato

quindi le nostre predizioni in tre classi di "allerta" (definite in ALTO, MEDIO e BASSO rischio) basandoci sull'intervallo numerico dei dati sperimentali di tossicità in acqua, come mostrato in Figura 5.



class of risk	pLC_{50} range	n compounds
HIGH	≥ 3	25
MEDIUM	0 - 3	208
LOW	< 0	318
all training	-2.96 - 6.38	551

Figura 5. *Classificazione dei composti basata sul livello di rischio tossico: training set e test set.*

Gli stessi limiti di classificazione sono stati poi applicati ai valori predetti del test set (Figura 5): 151 molecole sono state classificate come altamente tossiche, 1706 come mediamente tossiche e 120 con basso valore di tossicità.

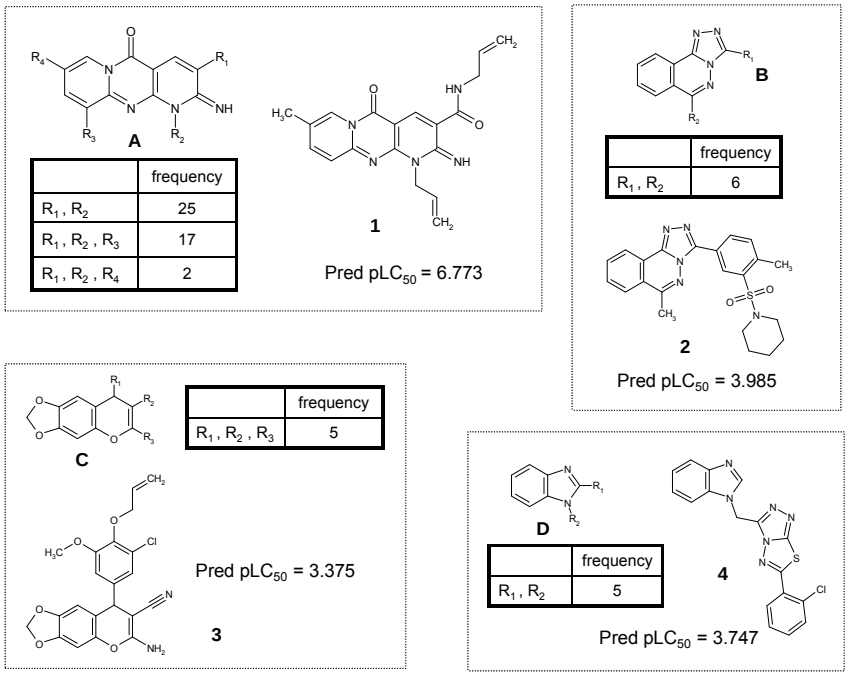


Figura 6. *Scaffolds del test set altamente tossici più rappresentativi. Per ogni scaffold viene riportata la frequenza e un esempio di molecola con il suo valore di* pLC_{50} *predetto.*

Prima di tutto abbiamo focalizzato la nostra attenzione su quei composti che presentano un "alto rischio" di tossicità in acqua del test set sopramenzionato. Quattro tra le classi chimiche più rappresentate, classificate come potenzialmente "ad alto rischio tossico", sono raggruppate nella Figura 6, insieme con un esempio di composto chimico. E' interessante osservare che lo scaffold A è

rappresentato 44 volte in questo database e, in particolare, compare nelle prime 50 molecole più tossiche. In più, lo scaffold A risulta completamente assente nelle rimanenti due classi del test set, differentemente dagli altri scaffolds riportati, per i quali alcuni composti sono presenti anche nella categoria a "medio rischio" di tossicità predetta. Dato che tutti questi scaffolds non sono rappresentati nel training set, sarebbe molto interessante validare sperimentalmente i valori di pLC_{50}, per verificare la capacità del modello nella predizione della tossicità, non solo di composti chimici analoghi a quelli del training set, ma anche per composti chimici in generale. Sottolineiamo il fatto che la validazione più apprezzabile per il modello QSAR sarebbe, infine, quella di valutare sperimentalmente la tossicità in acqua sia di composti chimici predetti come altamente tossici, che di quelli predetti a bassa tossicità. Stiamo collaborando con diversi istituti per validare sperimentalmente il nostro modello di predizione.

CONCLUSIONI E PROSPETTIVE

L'applicazione dei metodi QSAR, come quello presentato in questo lavoro è particolarmente utile per l'identificazione nei grandi database chimici di quelle molecole che potrebbero presentare un alto livello di rischio di tossicità in acqua, o semplicemente per verificare in breve tempo se il composto interessato presenta tossicità, aiutando così il miglioramento della produzione di composti chimici in concordanza con le leggi internazionali per ridurre l'inquinamento ambientale.

In questo contesto abbiamo riportato il risultato di un nuovo modello statistico QSAR robusto, basato sulle combinazioni di differenti famiglie di descrittori molecolari: i vettori *auto*MEP, i parametri Sterimol e i valori log*D*. Questo modello è stato usato nella predizione della tossicità in fase acquosa per una larga gamma di composti chimici estratti dal database MMsINC. Tre classi di allerta di rischio di tossicità sono state introdotte con lo scopo di raggruppare efficacemente i composti chimici in base alla loro tossicità.

Infine, stiamo lavorando per incorporare il nostro modello QSAR nel database MMsINC, attraverso un'interfaccia grafica basata sul web, per predire facilmente e rapidamente il profilo di rischio di tossicità in acqua di qualsiasi composto chimico specifico definito. Questo nuovo strumento sarà incluso nella prossima versione del MMsINC con il nome di MMsINC/AqToxPred.

BIBLIOGRAFIA

1 http://ecb.jrc.it/reach/reach-legislation/: REACH in brief.

2 Trevisan, A. (2008) Materiale delle lezioni di Tossicologia Industriale, corso di laurea in triennale in tecniche della prevenzione nell'ambiente e nei luoghi di lavoro.

3 Benfenati, E. (2007) Predicting toxicity through computers: a changing word. *Chem. Cent. J. 32*, 1-7.

4 Muster, W., Breidenbach, A., Fischer, H., Kirchner, S., Muller, L., Pahler, A. (2008) Computational toxicology in drug development. *Drug. Disc. Today. 13*, 303-310.

5 MCASE software. http://www.multicase.com/products/prod09.htm

6 TOPKAT software. http://www.accelrys.com/products/topkat/

7 MDL QSAR software. http://www.mdl.com/products/predictive/qsar/index.jsp

8 MetaDrug software: http://www.genego.com/metadrug.php

9 DEREK software: http://www.lhasalimited.org/index.php?cat=2&sub_cat=2#

10 OncoLogic software: http://www.epa.gov/oppt/newchems/tools/oncologic.htm

11 HazardExpert software: http://www.compudrug.com/

12 Lo Piparo, E., Fratev, F., Lemke, F., Mazzatorta, P., Smiesko, M.,

Fritz, J. I., Benfenati, E. (2006) QSAR models for daphnia magna toxicity prediction of benzoxazinone allelochemicals and their transformation products. *J. Agric. Food Chem. 54*, 1111 -1115.

13 Mazzatorta, P., Smiesko, M., Lo Piparo, E., Benfenati, E. (2005) QSAR Model for predicting pesticide aquatic toxicity. *J. Chem. Inf. Mode., 45*, 1767 -1774.

14 Castillo-Garit, J. A., Marrero-Ponce, Y., Escobar, J., Torrens, F., Rotondo, R. (2008) A novel approach to predict aquatic toxicity from molecular structure. *Chemosphere. 73*, 415–427.

15 Colombo, A., Benfenati, E., Karelson, M., Maran, U. (2008) The proposal of architecture for chemical splitting to optimize QSAR models for aquatic toxicity. *Chemosphere. 72*, 772–780.

16 Zhu, H., Tropsha, A., Fourches, D., Varnek, A., Papa, E., Gramatica, P., Oberg, T., Dao, P., Cherkasov, A., Tetko, IV. (2008) Combinatorial QSAR modeling of chemical toxicants tested against Tetrahymena pyriformis. *J. Chem. Inf. Model. 48*, 766-784.

17 Fanton, M., Floris, M., Frau, G., Masciocchi, J., Sturlese, M., Palla, P., Cedrati, F., Rodriguez-Tom, P., Moro, S. (2008) MMsINC: A new public large-scale chemoinformatics database system. *Biotechno - International Conference on Biocomputation, Bioinformatics, and Biomedical Technologies*., pp. 64-69.

18 The Unscrumbler software, version 9.6. (2003) CAMO Process AS:

Oslo, Norway.

19 AdrianaCode software, version 2.0. (2003) Molecular Networks GmbH: Erlangen, Germany.

20 Gasteiger, J., Li, X., Rudolph, C., Sadovski, J., Zupan, J. (1994) Representation of Molecular Electrostatic Potential by Topological Feature Maps. *J. Am. Chem. Soc. 116*, 4608-4620.

21 Wagener, M., Sadovski, J., Gasteiger, J. (1995) Autocorrelation of molecular surface properties for modeling corticosteroid binding globulin and cytosolic Ah receptor activity by neural networks. *J. Am. Chem. Soc. 117*, 7769-7778.

22 Bauknecht, H., Zell, A., Bayer, H., Levi, P., Wagener, M., Sadowski, J., Gasteiger, J. (1996) Locating biologically active compounds in medium-sized heterogeneous datasets by topological autocorrelation vectors: dopamine and benzodiazepine Agonists. *J. Chem. Inf. Comput. Sci. 36*, 1205-1213.

23 Moreau, G., Broto, P. (1980) The autocorrelation of a topological structure: a new molecular descriptor. *Nouv. J. Chim. 4*, 359-360.

24 Moreau, G., Broto, P. (1980) Autocorrelation of molecular structures, application to SAR studies. *Nouv. J. Chim. 4*, 757-764.

25 Molecular Operating Environment (MOE) software, version 2006.08. (2006) Chemical Computing Group: Montreal, Canada.

26 Verloop, A. (1987) The sterimol approach to drug design. Marcel

Dekker, New York.

27 Bacilieri, M., Varano, F., Deflorian, F., Marini, M., Catarzi, D., Colotta, V., Filacchioni, G., Galli, A., Costagli,C., Kaseda, C., Moro S. (2007) Tandem 3D-QSARs approach as a valuable tool to predict binding affinity data: design of new Gly/NMDA receptor antagonists as a key study. *J. Chem. Inf. Model. 47*, 1913-1922.

28 ACDLabs software. http://www.acdlabs.com/

29 Gramatica, P. (2007) Principles of QSAR models validation: internal and external. *QSAR Comb. Sci. 26*, 694 – 701.

30 http://www.oecd.org/dataoecd/55/35/38130292.pdf

31 Moro, S., Bacilieri, M., Ferrari, C., Spalluto, G. (2005) Autocorrelation of molecular electrostatic potential surface properties combined with Partial Least Squares analysis as alternative attractive aool to generate Ligand-Based 3D-QSARs. *Curr. Drug Discov. Technol, 2*, 13-21.

32 Moro, S., Bacilieri, M., Cacciari, B., Spalluto, G. (2005) Autocorrelation of molecular electrostatic potential surface properties combined with Partial Least Squares analysis as new strategy for the prediction of the activity of human A_3 adenosine receptor antagonists. *J. Med. Chem, 48*, 5698-5704.

33 Moro, S., Bacilieri, M., Cacciari, B., Bolcato, C., Cusan, C., Pastorin, G., Klotz, K. N., Spalluto, G. (2006) The application of a 3D-QSAR (autoMEP/PLS) approach as an efficient pharmacodynamic-driven

filtering method for small-sized virtual library: application to a lead optimization of a human A_3 adenosine receptor antagonist. *Bioorg. Med. Chem. 14*, 4923-4932.

34 Bacilieri, M., Kaseda, C., Spalluto, G., Moro, S. (2007) Response Surface Analysis as alternative 3D-QSAR tool: human A_3 adenosine receptor antagonists as a key study. *Lett. Drug Des. Discov. 4*, 122-127.

35 Michielan, L., Bacilieri, M., Schiesaro, A., Bolcato, C., Pastorin, G., Spalluto, G., Cacciari, B., Klotz. K.N., Kaseda, C., Moro, S. (2008) Linear and non linear 3D-QSAR approaches in tandem with ligand-based homology modeling as computational strategy to depict the pyrazolo-triazolo-pyrimidine antagonists binding site of the human adenosine A2A receptor. *J. Chem. Inf. Mod. 48*, 350-363.

36 Michielan, L., Bacilieri, M., Kaseda, C., Moro, S. (2008) Prediction of the aqueous solvation free energy of organic compounds by using autocorrelation of molecular electrostatic potential surface properties combined with response surface analysis. *Biorg. Med. Chem. 16*, 5733-5742.

37 Bacilieri, M., Varano, F., Deflorian, F., Marini, M., Catarzi, D., Colotta, V., Filacchini, G., Galli, A., Costagli, C., Kaseda, C., Moro, S. (2007) Tandem 3D-QSAR approach as a valuable tool to predict binding affinity data: design of new Gly/NMDA receptor antagonists as a key study. *J. Chem. Inf. Model. 47*, 1913-1922.

38 Leonard, J.T., Roy, K. (2006) Comparative QSAR modeling of CCR5 receptor binding affinity of substituted 1-(3,3-diphenylpropyl)-piperidinyl amides and ureas. *Bioorg. Med. Chem. Lett. 16*, 4467-4474.

39 Pliska, V., Testa, B., van de Waterbeemd, H. (1995) Lipophilicity in drug action and toxicology. In Methods and Principles in Medicinal Chemistry Vol4 (Mannhold, R., Kubinyi, H., Timmerman, H. Eds) pp 22-24, VHC.

MATERIALE SUPPLEMENTARE

Tabella 1. **Training Set – 551 composti**

ID	Smiles	pLC_{50}	classe in articolo Colombo
M1	Clc1ccc(Oc2ccccc2[N+](=O)[O-])cc1	2.1	A
M2	OC(C#C)(c1ccccc1)c1ccccc1	1.3	A
M3	ClCCOC(=O)NC1CCCCC1	0.8	A
M4	O=C1NC(=O)NC(=O)C1(CC)c1ccccc1	-0.3	A
M5	O=C1NC(=O)NC(=O)C1(C(CCC)C)CC	0.7	A
M6	O=C1NC(=O)NC(=O)C1(CCC(C)C)CC	0.4	A
M7	O=C1N(C)C(=O)N(c2ncn(c12)C)C	0.1	A
M8	O=C1c2c(cccc2)C(=O)C=C1C	3.2	A
M9	N1CCN=C1Cc1ccccc1	-0.3	A
M10	O1C2CC(=O)N3C4C5(C6N(CC(C(C24)C6)=CC1)CC5)c1c3cccc1	2.5	A
M11	O(C(=O)NC)c1c2c(ccc1)cccc2	1.4	A
M12	n1cc(ccc1)C1N(CCC1)C	1.5	A
M13	O1c2c(cccc2)C(O)=C(CC=2C(Oc3c(cccc3)C=2O)=O)C1=O	1.8	A
M14	O(c1ccc(cc1)C=O)c1ccccc1	1.6	A
M15	Clc1c(Cc2c(O)c(Cl)cc(Cl)c2Cl)c(O)c(Cl)cc1Cl	4.3	A
M16	S=C1NC(=O)C(C(CCC)C)(CC)C(=O)N1	1	A
M17	O=C1NC(=O)NC1(C)C	-2.1	A
M18	OC1(CCCCC1)C#C	-0.3	A
M19	O=C(\C=C\C=1C(CCCC=1C)(C)C)C	1.6	A
M20	Clc1cc(cc(Cl)c1O)C(C)(C)c1cc(Cl)c(O)c(Cl)c1	2.4	A
M21	NC1(CCC(CC1)C(N)(C)C)C	0.4	A
M22	C1Cc2c3c1cccc3ccc2	2	A
M23	[nH]1cc(c2c1cccc2)C	1.2	A
M24	O1c2c(CC1C(C)=C)c1OC3C(c4cc(OC)c(OC)cc4OC3)C(=O)c1cc2	4.9	A
M25	O(C(=O)c1ccccc1C(Oc1ccccc1)=O)c1ccccc1	3.6	A
M26	Oc1ccccc1C(=O)Nc1ccccc1	1.7	A
M27	Oc1c2c(ccc1)cccc2	1.5	A
M28	Oc1ccccc1-c1ccccc1	1.4	A
M29	c12c(cccc1)cccc2	1.3	A
M30	n1c2c(cccc2)ccc1	0.2	A
M31	N(CC)(CC)C1CCCCC1	0.9	A
M32	O1c2cc(ccc2OC1)\C=C/C=C\C(=O)N1CCCCC	1.6	A

	1		
M33	Clc1cc(Cc2cc(Cl)ccc2O)c(O)cc1	2.9	A
M34	O\N=C/1\CCCCC\1	-0.3	A
M35	n1ccccc1C#N	-0.8	A
M36	n1ccccc1CC	-0.6	A
M37	O1C(OCC1CO)(C)C	-2.1	A
M38	N12CN3CN(C1)CN(C2)C3	-2.6	A
M39	O(c1ccccc1)c1ccccc1	1.6	A
M40	OCCN1CCNCC1	-1.7	A
M41	n1cc(ccc1C)CC	0.2	A
M42	n1ccc(cc1)C	-0.6	A
M43	OC1CCCCC1	-0.9	A
M44	O=C1CCCCC1	-0.9	A
M45	n1cc(ccc1)C	-0.2	A
M46	N1CCN(CC1)C	-1.4	A
M47	n1ccccc1C	-1	A
M48	N1CCNCC1C	-1.4	A
M49	[nH]1cccc1	-0.5	A
M50	O1CCCC1	-1.5	A
M51	o1cccc1	0.1	A
M52	C1CCCCC1	1.3	A
M53	n1ccccc1	-0.1	A
M54	O1COCOC1	-1.8	A
M55	Clc1ccc(cc1)C(O)(C(Cl)(Cl)Cl)c1ccc(Cl)cc1	2.8	A
M56	P(Oc1ccccc1)(Oc1ccccc1)(Oc1ccccc1)=O	2.6	A
M57	O(C(=O)c1ccccc1O)c1ccccc1	2.3	A
M58	O=C(c1ccccc1)c1ccccc1	1.1	A
M59	N(c1ccccc1)c1ccccc1	1.7	A
M60	O1CCOCC1	-2.1	A
M61	O=C1CC(CC(=O)C1)(C)C	-1.9	A
M62	S1(=O)(=O)NC(=O)c2c1cccc2	-2	A
M63	o1c2c(c3c1cccc3)cccc2	2	A
M64	O(C(=O)c1ccc(N)cc1O)c1ccccc1	1.7	A
M65	N1CCN(CC1)CCN	-1.2	A
M66	o1c2c(cccc2)cc1	0.9	A
M67	N12CCN(CC1)CC2	-1.2	A
M68	C12CC3CC(C1)CC(C2)C3	2.7	A
M69	O=C1NC(=O)NC(=O)C1(C(CCC)C)CC=C	1	A
M70	BrC=1C(=O)N(C(CC)C)C(=O)NC=1C	0.2	A
M71	Fc1ccc(Oc2ccc(F)cc2)cc1	2.2	A
M72	OC1CC2CCC1(C)C2(C)C	0.4	A
M73	O=C1CC2CCC1(C)C2(C)C	0.9	A

M74	O1C(C2CCC1(CC2)C)(C)C	0.2	A
M75	OC(=O)C1(C2CCC=3C(CC\C(\C=3)=C(/C)\C)C2(CCC1)C)C	2.3	A
M76	O1CCc2c1cccc2	0.2	A
M77	OC1C2CC(C1)CC2	-0.3	A
M78	C12CC(CC1)C=C2	1	A
M79	OC(=O)c1nc(ccc1)C(O)=O	-0.3	A
M80	O=Cc1cccnc1	0.8	A
M81	OC(=O)C1(C2CC=C3C(CCC(=C3)C(C)C)C2(CCC1)C)C	2.1	A
M82	O1c2c(cccc2)C(=O)C=C1c1ccccc1	1.8	A
M83	OC(CCC1C2(C(CCC1=C)C(CCC2)(C)C)C)(C=C)C	3.4	A
M84	O=CN(c1ccccc1)c1ccccc1	0.9	A
M85	O(c1ccc([N+](=O)[O-])cc1)c1ccccc1	1.9	A
M86	S(=O)(Cc1ccccc1)Cc1ccccc1	0.5	A
M87	O1CCN(CC1)CCO	-1.3	A
M88	o1c(ccc1C)C	0.1	A
M89	o1cc(nc1)C	-1.2	A
M90	[nH]1ccnc1C	-0.5	A
M91	O=C1C2CC3CC1CC(C2)C3	0.4	A
M92	O1C(CCC1=O)CCCCCC	1	A
M93	NC12CC3CC(C1)CC(C2)C3	0.8	A
M94	Oc1nc(cc(C)c1C#N)C	-0	A
M95	P(=O)(c1ccccc1)(c1ccccc1)c1ccccc1	0.7	A
M96	ClC1CCCCC1Cl	0.9	A
M97	O(c1ccc(O)cc1)c1ccccc1	1.6	A
M98	Brc1ccsc1	1.4	A
M99	S(Sc1ccccc1)c1ccccc1	3.3	A
M100	n1ccc(cc1)-c1ccccc1	1	A
M101	Brc1ccc(nc1)N	-0	A
M102	O=C(C)c1ccncc1	-0.1	A
M103	n1(c2c(c3c1cccc3)cccc2)C=C	4.8	A
M104	O(Cc1ccccc1)c1cc(N)ccc1	1.3	A
M105	O1c2c(CC1(C)C)cccc2OC(=O)NC	2.4	A
M106	Oc1ccc(N=Nc2ccccc2)cc1	2.2	A
M107	OC(=O)C1(C2CCc3c(ccc(c3)C(C)C)C2(CCC1)C)C	2.2	A
M108	O(c1ccc(O)cc1)c1ccc(O)cc1	1.6	A
M109	Brc1nc(Br)[nH]c1Br	1.6	A
M110	Clc1c(Cl)c(Cl)nc(Cl)c1Cl	2.7	A
M111	OC1CC(CCC1C(C)C)C	0.9	A
M112	S(=O)(=O)(n1ccnc1)c1ccc(cc1)C	0.7	A

M113	OC1CCCCC1c1ccccc1	0.6	A
M114	O1CCCC1COC(=O)C(C)=C	0.7	A
M115	N1CCN(CC1)Cc1ccccc1	0.6	A
M116	OCCCc1cccnc1	-0	A
M117	Clc1ccc(cc1)C(=O)c1ccccc1N	2	A
M118	O(C(=O)C=C)C1CCCCC1	2	A
M119	n1c(cccc1-c1ccccc1)-c1ccccc1	3	A
M120	Clc1ccc(O)nc1	-0.9	A
M121	n1ccc(cc1)CCc1ccncc1	0.1	A
M122	S=C1N(CC)C(=O)CC(=O)N1CC	-1.4	A
M123	Clc1cc2nc(sc2cc1)S	1.8	A
M124	Clc1nc(nc(c1)C)N	-0	A
M125	n1ccccc1N(C)C	-0	A
M126	OC(=O)C1(C2CC=C3C(CCC(C3)(C=C)C)C2(CCC1)C)C	2.5	A
M127	Brc1ncccc1O	-0.4	A
M128	Clc1ncccc1O	-0.7	A
M129	NCCCN1CCN(CC1)CCCN	-1.2	A
M130	ClCCN1CCCC1	0.1	A
M131	BrC1C2CCC(C)(C1=O)C2(C)C	0.5	A
M132	o1cc(cc1Cc1ccccc1)COC(=O)C1C(C)(C)C1\C=C(\C)/C	4.7	A
M133	Brc1ccc(cc1)C(=O)c1cccnc1	1.1	A
M134	O=C(c1ccccc1)c1ccncc1	0.3	A
M135	O1C(CCC1(C)C)(C)C	-0.1	A
M136	Oc1cccnc1[N+](=O)[O-]	-0.1	A
M137	Clc1nc(O)ccc1	-0.2	A
M138	n1c(C)c(nnc1N)C	-0.9	A
M139	Clc1nc(ccc1)C	-0.3	A
M140	o1c(C)c(nc1C)C	-0.6	A
M141	BrCC1OCCCC1	-0.1	A
M142	Clc1ccc(cc1)C(C(C)C)C(OC(C#N)c1cc(Oc2ccccc2)ccc1)=O	4.9	A
M143	Cl\C(\Cl)=C\C1C(C)(C)C1C(OCc1cc(Oc2ccccc2)ccc1)=O	4.4	A
M144	O(c1cc(ccc1)C=O)c1ccc(cc1)C(C)(C)C	2.8	A
M145	FC(F)Oc1ccc(cc1)C(C(C)C)C(OC(C#N)c1cc(Oc2ccccc2)ccc1)=O	6.4	A
M146	Clc1cc(Oc2cc(ccc2)C=O)ccc1Cl	3	A
M147	Oc1c2c(cccc2)c([N+](=O)[O-])cc1[N+](=O)[O-]	1.8	A
M148	S(CCC)CCSCCC	1.4	B1
M149	S(CCCCSCCC)CCC	1.8	B1

M150	N(N)(C)C	0.9	B1
M151	O(CC)CC	-1.5	B1
M152	OCC	-2.5	B1
M153	OC	-3	B1
M154	OC(C)C	-2.2	B1
M155	ClC(Cl)Cl	0.2	B1
M156	S(=O)(C)C	-2.6	B1
M157	ClC(Cl)(Cl)C(Cl)(Cl)Cl	2.2	B1
M158	OCCC	-1.9	B1
M159	OCCCC	-1.4	B1
M160	OCCCCC	-0.7	B1
M161	ClC(Cl)(Cl)C	0.4	B1
M162	ClCCl	-0.6	B1
M163	IC(I)I	2.1	B1
M164	OC(C)(C)C	-1.9	B1
M165	FC(F)(F)CO	-0.1	B1
M166	ClC(Cl)(Cl)C(Cl)Cl	1.4	B1
M167	OC(CC)(CC)C	0.8	B1
M168	P(OCCOCCCC)(OCCOCCCC)(OCCOCCCC)=O	1.6	B1
M169	OCC(C)C	-1.3	B1
M170	ClC(CCl)C	-0.1	B1
M171	NC(CN)C	-1.1	B1
M172	OC(CC)C	-1.7	B1
M173	OC(CN)C	-1.5	B1
M174	ClC(Cl)CCl	0.2	B1
M175	ClC(Cl)C(Cl)Cl	0.9	B1
M176	BrC(CO)CBr	0.5	B1
M177	ClC(CCl)CCl	0.3	B1
M178	OCCN(C(C)C)C(C)C	-0.1	B1
M179	OCCN(CC)CC	-1.2	B1
M180	N(CCC)(CCC)CCC	0.4	B1
M181	OCCN(CCO)CCO	-1.9	B1
M182	OCC(CCCC)CC	0.7	B1
M183	BrCCC	0.3	B1
M184	ClCCCl	-0.1	B1
M185	ClCCO	0.2	B1
M186	NCCC	-0.7	B1
M187	NCCN	-0.6	B1
M188	OC(CC(O)C)(C)C	-2	B1
M189	NC(CC(C)(C)C)(C)C	0.7	B1
M190	S(C(C)(C)C)C(C)(C)C	0.7	B1
M191	O(C(C)C)C(C)C	-0.9	B1

M192	BrCCCBr	1.9	B1
M193	BrCCCC	0.6	B1
M194	NCCCC	-0.6	B1
M195	NCCCN	-1.2	B1
M196	O(CCN)C	-0.8	B1
M197	N(CC)CC	-1.1	B1
M198	S(SC(C)(C)C)C(C)(C)C	2.1	B1
M199	C(CCC)CC	1.5	B1
M200	ClCCCCCl	0.4	B1
M201	NCCCCC	-0.3	B1
M202	OCCNCC	-1.2	B1
M203	BrCCCCCC	1.7	B1
M204	NCCCCCC	0.3	B1
M205	OCCCCCC	0	B1
M206	OCCNCCO	-2.7	B1
M207	O(CCO)CCO	-2.8	B1
M208	S(CCC)CCC	0.7	B1
M209	NCCCCCCC	0.7	B1
M210	OCCCCCCC	0.5	B1
M211	BrCCCCCCCC	2.4	B1
M212	NCCCCCCCC	1.4	B1
M213	OCCCCCCCC	0.9	B1
M214	O(CCOCC)CCO	-2.3	B1
M215	NCCCCCCCCC	1.8	B1
M216	O(CCOCCO)CCO	-2.6	B1
M217	OCCCCCCCCCC	1.8	B1
M218	ClC(Cl)(Cl)CO	-0.3	B1
M219	NCCCCCCCCCCCC	3.3	B1
M220	P(OCCCC)(OCCCC)(OCCCC)=O	1.4	B1
M221	ClCC(O)C	-0.4	B1
M222	OCCN	-1.5	B1
M223	ClCCCCl	-0.1	B1
M224	O(CCCC)CCCC	0.6	B1
M225	OCCCCCCCCC	1.4	B1
M226	N(CCCCCC)CCCCCC	2.4	B1
M227	S(CCCC)CCCC	1.6	B1
M228	NC(C(C)C)C	-0.5	B1
M229	OC(C(C)C)C(C)C	-0.2	B1
M230	ClCCCCCCl	0.8	B1
M231	BrCCCCCCC	2.1	B1
M232	S(SCCC)CCC	1.8	B1
M233	NC(CCCCCC)C	1.4	B1

M234	O(CCCCC)CCCCC	1.7	B1
M235	FC(F)(F)C(O)C(F)(F)F	-0.2	B1
M236	O(C(C)(C)C)C	-0.9	B1
M237	NCCCCCCCCCC	2.2	B1
M238	NCCCCCCCCCCCCC	3.5	B1
M239	S(SC(C)C)C(C)C	1.3	B1
M240	S(CCSCC)CC	0.4	B1
M241	ClCCCN(C)C	0.1	B1
M242	NCC(C)(C)C	-0.7	B1
M243	ClC(Cl)(Cl)C(O)(C)C	0.1	B1
M244	O(C(OCC)CN(CC(OCC)OCC)C)CC	-0.4	B1
M245	NCCCCCCCCCCC	2.9	B1
M246	FC(F)(C(O)(C)C)C(F)F	-0.6	B1
M247	NC(CC)C	-0.6	B1
M248	S(CCCCSCC)CC	1.5	B1
M249	S(CCCCCCSC)C	1.3	B1
M250	O(CC)C(=O)N	-1.8	B2
M251	Cl\C(\Cl)=C\Cl	0.5	B2
M252	O(C(=O)C)C	-0.6	B2
M253	Cl\C(\C(\Cl)=C(\Cl)/Cl)=C(/Cl)\Cl	3.5	B2
M254	O(C(=O)CC(OCC)=O)CC	1	B2
M255	O(C(=O)CCCCC(OCCCC)=O)CCCC	1.9	B2
M256	O(C(=O)C)CCC	0.2	B2
M257	O(C(=O)CCCCCCCCC(OCC)=O)CC	2	B2
M258	O(C(=O)C)CCOCC	0.5	B2
M259	OC(=O)CCCCCCCC	0.2	B2
M260	O(C(=O)CCCCC)CC	1.2	B2
M261	O(C(=O)C)CCCC	0.8	B2
M262	ClC(Cl)=C(Cl)Cl	1.1	B2
M263	OC(=O)CC	-1.7	B2
M264	O(C(=O)CCC(OCCCC)=O)CCCC	1.7	B2
M265	O(C(=O)CCCCC(OCC)=O)CC	1.1	B2
M266	O(C(=O)C)CC	-0.4	B2
M267	OC(=O)CCCCC	-0.4	B2
M268	O(C(=O)C)CCCCCC	1.5	B2
M269	O(C(C)(C)C)C(=O)C	-0.4	B2
M270	ClC(Cl)C(=O)N	-0.3	B2
M271	O=CN(CCCC)CCCC	0.3	B2
M272	C(=C\C=C(\C)/C)(/C)\C	1.5	B2
M273	O(CC)C(=O)N(C(OCC)=O)C(OCC)=O	1.2	B2
M274	ClC(C(OCC)=O)C(OCC)=O	2.3	B2
M275	S(\C(=N\OC(=O)NC)\C)C	1.9	B2

M276	S(\C(=N/OC(=O)NC)\C(=O)N(C)C)C	1.4	B2
M277	O=CCCCCC	0.9	B3
M278	O=C(C)C	-2.2	B3
M279	O=CC	0.2	B3
M280	O=C(C(C)(C)C)C	0.1	B3
M281	O=C(CC)C	-1.7	B3
M282	O(C(=O)C(C)=C)CC=C	2.1	B3
M283	O=CC(CC)C	0.9	B3
M284	O=C(CC)CC	-1.3	B3
M285	O\N=C(\CC)/C	-1	B3
M286	O=C(CCCN(CC)CC)C	-0.3	B3
M287	O(CCCC)C(=O)\C=C\C(OCCCC)=O	2.7	B3
M288	O(C(=O)C=C)CC(C)C	1.8	B3
M289	OCC=C	2.3	B3
M290	O\N=C\C	-0.1	B3
M291	O=C(CCC)C	-1.2	B3
M292	O=C(CC(C)C)C	-0.7	B3
M293	O=C(CCC(C)C)C	-0.1	B3
M294	O=C(CCCCC)C	-0.1	B3
M295	O=CCCCC	0.8	B3
M296	O=C(CC\C=C(\C)/C)C	0.2	B3
M297	O=C(CCCCCC)C	0.6	B3
M298	O=C(CCCCCCCCC)C	2.1	B3
M299	S(C(\C=N\OC(=O)NC)(C)C)C	2.3	B3
M300	O=CC(CCC)C	0.7	B3
M301	O=C(CC(=O)C)C	-0.2	B3
M302	O=CCCC	0.6	B3
M303	O=C(CCCC)CCCC	0.7	B3
M304	C(C(C)=C)(C)=C	1.1	B3
M305	O=C(C(C)C)C	-1	B3
M306	O=CCC(C)C	1.4	B3
M307	O=C(CCCC)C	-0.6	B3
M308	O=C(CCCCCCCCCCC)C	2.7	B3
M309	O=C(CCCCCCCC)C	1.4	B3
M310	ClC(C=C)CCl	1.1	B3
M311	O(C(=O)C=C)CCO	1.4	B3
M312	O=C(CCCCCCC)C	1	B3
M313	O(C(=O)C(C)=C)CCO	-0.2	B3
M314	OC(CC=C)C=C	0.4	B3
M315	OCC\C=C\CC	-0.6	B3
M316	OCC\C=C\CC	-0.4	B3
M317	O(C(=O)C=C)CC(O)C	1.6	B3

M318	C(CCCC=C)CCC=C	2.7	B3
M319	ClCC(CCl)=C	2.8	B3
M320	O(C(=O)C(C)=C)CCOCC	0.8	B3
M321	O(C(=O)C=C)CCCCCC	2.2	B3
M322	O=CC(C(CC)C)C	0.9	B3
M323	O(C(C)C)C(=O)C(C)=C	0.5	B3
M324	OC(CCC)C=C	0.5	B3
M325	O=C(CCCCCCCCCC)C	2.2	B3
M326	OC(CC\C=C(\CC\C=C(\C)/C)/C)(C=C)C	2.2	B3
M327	O=C(C(CN(C)C)C)C	1.2	B3
M328	OC(CC)(C#C)C	-1.1	B4
M329	N#CCC	-1.4	B4
M330	OCC#C	1.6	B4
M331	N#CCC=C	-0.4	B4
M332	OCC#CCO	0.2	B4
M333	N#CCCCCC#N	-1.3	B4
M334	OC(C#C)(C)C	-1.6	B4
M335	N#CCCCCCCC#N	-0.6	B4
M336	OCC#CC	0.8	B4
M337	OC(CCCCC)C#C	2.5	B4
M338	OCCC#C	0.3	B4
M339	OC(C(C)C)(C#C)C	-0.3	B4
M340	OC(CC#C)C	0.4	B4
M341	N#CCCCCCCCC	1.5	B4
M342	N#CCCCCCCCCCCC	2.6	B4
M343	OCC#CCCCCCCC	2.2	B4
M344	N(CC#C)(CC#C)CC#C	-0.3	B4
M345	OC(CCCC)C#C	1.8	B4
M346	OC(CCC(C)C)(C#C)C	0.5	B4
M347	OC(C#C)C	0.8	B4
M348	Oc1ccc([N+](=O)[O-])cc1[N+](=O)[O-]	1.1	C1
M349	Clc1c(O)c(Cl)cc(Cl)c1Cl	2.3	C1
M350	Clc1ccc(O)cc1C	1.3	C1
M351	NC(Cc1ccccc1)C	1.1	C1
M352	Nc1ccccc1	-0.2	C1
M353	c1ccccc1	0.5	C1
M354	Oc1ccc(cc1)C(CC)(C)C	1.8	C1
M355	Clc1cccc(Cl)c1C(Cl)Cl	2.4	C1
M356	Clc1c(O)c(Cl)c(Cl)c(Cl)c1Cl	3.1	C1
M357	Clc1cc(Cl)cc(Cl)c1O	1.3	C1
M358	FC(F)(F)c1cc(O)ccc1[N+](=O)[O-]	1.4	C1
M359	Oc1ccccc1[N+](=O)[O-]	-0.1	C1

M360	Oc1c(cc([N+](=O)[O-])cc1[N+](=O)[O-])C(CC)C	2.5	C1
M361	N(CC)(CC)c1ccccc1	1	C1
M362	OCCN(CC)c1cc(ccc1)C	0.5	C1
M363	c1cccc(C)c1C	0.8	C1
M364	Oc1ccccc1C	0.9	C1
M365	Clc1ccccc1Cl	1.2	C1
M366	Clc1ccccc1N	1.4	C1
M367	Fc1ccccc1C	0.8	C1
M368	Clc1ccccc1O	1	C1
M369	c1c(C)c(ccc1C)C	1.2	C1
M370	Clc1cc(ccc1Cl)C	1.7	C1
M371	Clc1cc(N)ccc1Cl	1.4	C1
M372	O=[N+]([O-])c1cc([N+](=O)[O-])ccc1N	1.1	C1
M373	Oc1ccc(cc1)C(C)(C)C	1.5	C1
M374	c1ccccc1C(C)C	1.3	C1
M375	O=[N+]([O-])c1ccccc1	0	C1
M376	O=[N+]([O-])c1cc(ccc1)C	0.7	C1
M377	N(C)(C)c1ccc(cc1)C	0.4	C1
M378	O=[N+]([O-])c1ccc(N)cc1	0	C1
M379	Oc1ccc([N+](=O)[O-])cc1	0.4	C1
M380	O=[N+]([O-])c1ccc([N+](=O)[O-])cc1	2.4	C1
M381	c1ccccc1CC	0.9	C1
M382	NCc1ccccc1	0	C1
M383	N(C)c1ccccc1	0	C1
M384	N(CC)c1cc(ccc1)C	0.4	C1
M385	OC(CCc1ccccc1)(C)C	0.4	C1
M386	N(Cc1ccccc1)(C)C	0.6	C1
M387	Nc1ccc(cc1)CCCC	1.2	C1
M388	Oc1ccc(cc1)CCCCCCCCC	3.2	C1
M389	Oc1ccc(cc1C)C	0.9	C1
M390	Brc1ccc(N)cc1	0.6	C1
M391	c1cc(ccc1C)C	1.1	C1
M392	Oc1ccc(cc1)C	0.8	C1
M393	Clc1ccc(N)cc1	0.6	C1
M394	Clc1ccc(O)cc1	1.3	C1
M395	Nc1ccc(cc1)C	-0.1	C1
M396	c1ccccc1C	0.4	C1
M397	Clc1ccccc1	0.8	C1
M398	Oc1ccccc1	0.5	C1
M399	Brc1cc(Br)cc(Br)c1O	1.7	C1
M400	Oc1ccc(N)cc1[N+](=O)[O-]	0.6	C1
M401	OCCN(CCO)c1ccccc1	-0.6	C1

M402	Oc1ccccc1O	1.1	C1
M403	Clc1cc(Cl)ccc1Cl	1.8	C1
M404	Clc1cc(Cl)ccc1O	1.3	C1
M405	O=[N+]([O-])c1cc([N+](=O)[O-])ccc1C	0.9	C1
M406	N(C)(C)c1ccccc1	0.2	C1
M407	Clc1cc([N+](=O)[O-])ccc1	0.9	C1
M408	Clc1cc([N+](=O)[O-])ccc1N	1	C1
M409	O(CCO)c1ccccc1	-0.4	C1
M410	Oc1ccc(cc1)CC	1.1	C1
M411	Oc1c(cc(cc1C(C)(C)C)C)C(C)(C)C	2.8	C1
M412	c1c(cccc1CC)CC	1.5	C1
M413	O(C)c1cc(O)ccc1	0.2	C1
M414	O(C)c1ccc(O)cc1	0.1	C1
M415	O(C)c1ccc(OC)cc1	0.1	C1
M416	Oc1cc([N+](=O)[O-])ccc1[N+](=O)[O-]	0.7	C1
M417	Fc1ccc([N+](=O)[O-])cc1	0.7	C1
M418	Fc1ccc(N)cc1	0.8	C1
M419	Fc1cc(C(F)(F)F)c(N)cc1	0.8	C1
M420	Fc1ccc(NC)cc1	0.5	C1
M421	Oc1c(cc(cc1C)C)C	1	C1
M422	Oc1c(cc([N+](=O)[O-])cc1[N+](=O)[O-])C	2	C1
M423	c1ccccc1CCCCC	1.9	C1
M424	Clc1cc(Cl)ccc1	1.3	C1
M425	Oc1c([N+](=O)[O-])cccc1[N+](=O)[O-]	0.7	C1
M426	Brc1ccccc1Br	1.8	C1
M427	Nc1ccc(cc1)CC	0.2	C1
M428	Brc1c(O)c(Br)c(Br)c(Br)c1Br	3.7	C1
M429	Ic1cc(I)cc(I)c1O	2.6	C1
M430	Clc1cc(ccc1N)C	0.6	C1
M431	O(CC)c1cc([N+](=O)[O-])c(N)cc1	0.9	C1
M432	ClCc1ccc(cc1)CCl	3.7	C1
M433	Clc1c(Cl)c(Cl)ccc1N	1.7	C1
M434	Oc1ccc(cc1)CCC	1.1	C1
M435	Oc1c(cc(cc1C(C)(C)C)C(C)(C)C)C(C)(C)C	3.6	C1
M436	Fc1c(N)c(F)c(F)c(F)c1F	0.7	C1
M437	P(OCC)(OCC)(=O)Cc1ccccc1	-0.2	C1
M438	O(CCCC)c1ccccc1	1.4	C1
M439	Clc1c(O)c(O)c(Cl)c(Cl)c1Cl	2.3	C1
M440	Clc1cc(O)c(O)cc1	2	C1
M441	Fc1ccc(N)cc1C(F)(F)F	0.8	C1
M442	Oc1c(C)c(ccc1C)C	1.2	C1
M443	Clc1cc(OC)c(O)cc1Cl	1.6	C1

M444	Clc1cc(O)c(O)cc1Cl	2.3	C1
M445	Clc1c(N)c(Cl)c(Cl)cc1Cl	2.9	C1
M446	Clc1cc(Cl)c([N+](=O)[O-])cc1[N+](=O)[O-]	3.7	C1
M447	Clc1c(Cl)c(O)cc(Cl)c1Cl	2.8	C1
M448	O(C)c1cccc(OC)c1C	0.9	C1
M449	Clc1c([N+](=O)[O-])c(Cl)cc(Cl)c1[N+](=O)[O-]	3.1	C1
M450	BrC(Br)c1ccccc1C(Br)Br	3	C1
M451	N(Cc1ccccc1)CC	0.4	C1
M452	Nc1ccc(cc1)CCCCCCCC	3.2	C1
M453	Nc1c(cccc1C(C)C)C(C)C	1.1	C1
M454	O(C)c1c(OC)cc(cc1OC)CNCCCOC	0.3	C1
M455	Nc1ccc(cc1)CCCCCCCCCC	3.6	C1
M456	O(CCCCCC)c1ccc(N)cc1	1.8	C1
M457	Clc1cccc(NC=O)c1C	0.6	C2
M458	O(C(=O)c1cc(ccc1)C(OCCCC)=O)CCCC	2.5	C2
M459	Oc1ccccc1C(O)=O	-1.1	C2
M460	O=C(N)c1ccccc1	-0.7	C2
M461	Oc1ccccc1C(=O)N	0.1	C2
M462	O(C(=O)c1ccccc1C(OCC)=O)CC	0.8	C2
M463	O(C(=O)c1ccccc1C(OCCCC)=O)CCCC	2.5	C2
M464	O=C(N)c1ccccc1N	-0.5	C2
M465	O(C(=O)c1ccc(N)cc1)CC	0.7	C2
M466	Oc1ccc(NC(=O)C)cc1	-0.7	C2
M467	O(C(C)C)c1ccccc1OC(=O)NC	1.4	C2
M468	Oc1ccccc1C(OCC)=O	0.9	C2
M469	O=C(N(CC)CC)c1cc(ccc1)C	0.2	C2
M470	Clc1cc(NC(=O)N(C)C)ccc1Cl	1.2	C2
M471	OC(=O)c1ccccc1	-0.5	C2
M472	O(C)c1cc(O)c(cc1)C(=O)C	0.5	C2
M473	O(C(=O)C(Cc1ccccc1)C(OCC)=O)CC	1.7	C2
M474	Oc1ccccc1NC(=O)C	0.8	C2
M475	O(C(=O)c1ccc([N+](=O)[O-])cc1)C	0.9	C2
M476	O=C(N)c1ccc([N+](=O)[O-])cc1	0.1	C2
M477	Oc1cc(NC(=O)C)ccc1	-0.9	C2
M478	Clc1cc(NC(=O)CC)ccc1Cl	1.4	C2
M479	O(C(=O)c1cc(N)ccc1)CC	0.5	C2
M480	Clc1ccc(cc1)C(OC)=O	1.2	C2
M481	O(C(=O)c1ccc(cc1)C(OCCCC)=O)CCCC	2.7	C2
M482	Clc1cccc(Cl)c1C(=O)N	-0.4	C2
M483	O(C(=O)NC)c1cc(C)c(N(C)C)cc1	2	C2
M484	Oc1cc(O)ccc1C(OC)=O	0.6	C2
M485	O(C)c1ccccc1C(=O)N	0.1	C2

M486	Clc1cc(Cl)ccc1C(=O)N	0.3	C2
M487	O(C(=O)NC)c1ccc(cc1)C(C)(C)C	1.3	C2
M488	Clc1ccc(Cl)cc1C(OC)=O	1.2	C2
M489	O(C(=O)c1ccc(cc1[N+](=O)[O-])C(OC)=O)C	1.6	C2
M490	O(C(=O)c1ccc(cc1N)C(OC)=O)C	1.4	C2
M491	ClCC(=O)N(COC)c1c(cccc1CC)CC	1.7	C2
M492	Brc1cc(ccc1)C(=O)N	0.3	C2
M493	Clc1cc([N+](=O)[O-])c(cc1)C(OC)=O	0.9	C2
M494	O(CCCCCCCC)c1ccccc1NC(=O)C	2.8	C2
M495	O=C(N)c1ccc(cc1)C(C)(C)C	0.7	C2
M496	O(CCCCCC)c1ccc(cc1OC)C=O	2	C3
M497	Brc1cc(C=O)c([N+](=O)[O-])c(OC)c1O	0.6	C3
M498	O=C(CC)c1ccc(N)cc1	0	C3
M499	Oc1ccccc1C=O	1.7	C3
M500	Brc1cc(Br)cc(C=O)c1O	2.5	C3
M501	O=C(CC(=O)C)c1ccccc1	2.2	C3
M502	Oc1cc(O)ccc1C=O	1	C3
M503	O=C(C)c1ccccc1	-0.1	C3
M504	O=C(C)c1cc(N)ccc1	-0.4	C3
M505	O=Cc1ccc(N(C)C)cc1	0.5	C3
M506	O=Cc1ccccc1	1.1	C3
M507	Clc1ccc(cc1)C=O	1.8	C3
M508	O=Cc1ccc(N(CC)CC)cc1	0.9	C3
M509	O(CC)c1cc(ccc1O)C=O	0.3	C3
M510	O(C)c1cc(ccc1O)C=O	0.4	C3
M511	O=Cc1ccc(cc1)C(C)C	1.4	C3
M512	O(C)c1cccc(C=O)c1O	1.8	C3
M513	Clc1cccc(F)c1C=O	1.2	C3
M514	Fc1ccccc1C=O	2	C3
M515	FC(F)(F)c1cc(ccc1)C=O	2.3	C3
M516	O=Cc1ccccc1C	0.4	C3
M517	O=Cc1ccccc1[N+](=O)[O-]	1	C3
M518	O=Cc1ccc([N+](=O)[O-])cc1	1.2	C3
M519	N(CC=C)c1ccccc1	0.6	C3
M520	O(C)c1cc(OC)ccc1C=O	0.9	C3
M521	Clc1cc(C=O)c(O)cc1	2.3	C3
M522	Fc1c(C=O)c(F)c(F)c(F)c1F	2.3	C3
M523	O(C)c1cc(OC)cc(O)c1C=O	1.8	C3
M524	Clc1cc(Cl)ccc1C=O	2	C3
M525	BrCC(=O)c1cc(OC)ccc1OC	4.5	C3
M526	Oc1ccccc1CC=C	0.9	C3
M527	c1cc(ccc1C(C)(C)C)C=C	2.5	C3

M528	Brc1cc(C=O)c(O)cc1	2.2	C3
M529	Clc1cc(Cl)ccc1C(=O)C	1.2	C3
M530	O(Cc1ccccc1)C(=O)C(C)=C	1.6	C3
M531	Brc1cc(cc(OC)c1O)C=O	0.6	C3
M532	O(C)c1cc(OC)c(OC)cc1C=O	0.6	C3
M533	Clc1ccc(cc1[N+](=O)[O-])C(=O)C	1.6	C3
M534	O=C\C=C\c1ccc(N(C)C)cc1	1.5	C3
M535	Clc1ccc([N+](=O)[O-])cc1C=O	1.7	C3
M536	O(CC)c1ccc(cc1)C=O	0.7	C3
M537	Clc1c(Cl)c(Cl)ccc1C(=O)C	2.1	C3
M538	O(C)c1c(OC)c(OC)ccc1C(=O)C	-0	C3
M539	Oc1cc(N(CC)CC)ccc1C=O	1.6	C3
M540	ClCc1ccc(cc1)C=C	2.7	C3
M541	Oc1cc(C=O)c([N+](=O)[O-])cc1	0.6	C3
M542	OC(C#C)(C)c1ccccc1	0.1	C4
M543	FC(F)(F)c1cc(ccc1)C#N	0.6	C4
M544	FC(F)(F)c1ccccc1C#N	0.6	C4
M545	N#Cc1ccccc1C	0.4	C4
M546	O(C(=O)c1ccc(cc1)C#N)C	0.5	C4
M547	Ic1cc(cc(I)c1O)C#N	1.7	C4
M548	Brc1cc(cc(Br)c1O)C#N	1.4	C4
M549	Clc1cc(cc(Cl)c1O)C#N	0.9	C4
M550	Clc1cc(C#N)c(N)cc1	0.7	C4
M551	Clc1cccc(C)c1C#N	1	C4

Tabella 2. **Training Set –pLC_{50} sperimentali vs pLC_{50} predette**

ID	**pLC_{50} sperimentale**	**pLC_{50} predetta**
M1	2.11	1.974
M2	1.27	1.499
M3	0.77	1.363
M4	-0.32	0.75
M5	0.7	1.026
M6	0.42	0.955
M7	0.11	-0.628
M8	3.19	0.992
M9	-0.26	0.458
M10	2.54	1.349
M11	1.35	1.331

M12	1.54	0.144
M13	1.82	0.335
M14	1.63	1.645
M15	4.29	2.592
M16	1	1.308
M17	-2.11	-1.072
M18	-0.31	0.599
M19	1.58	1.578
M20	2.44	2.116
M21	0.42	-0.603
M22	1.95	1.697
M23	1.17	1.144
M24	4.94	3.096
M25	3.6	2.792
M26	1.73	1.839
M27	1.49	1.214
M28	1.44	1.614
M29	1.32	1.334
M30	0.22	0.884
M31	0.86	0.577
M32	1.56	2.025
M33	2.94	2.02
M34	-0.26	0.33
M35	-0.84	-8.38E-02
M36	-0.59	0.593
M37	-2.1	-5.71E-02
M38	-2.55	0.366
M39	1.63	1.716
M40	-1.69	-0.845
M41	0.17	0.897
M42	-0.64	7.29E-02
M43	-0.85	0.327
M44	-0.87	-0.118
M45	-0.19	0.191
M46	-1.36	-1.018
M47	-0.98	8.65E-02
M48	-1.35	-1.094
M49	-0.5	-0.305
M50	-1.48	-0.594
M51	5.00E-02	-0.38
M52	1.27	0.95
M53	-0.13	-0.364

M54	-1.82	-1.465
M55	2.79	2.869
M56	2.57	2.461
M57	2.26	1.952
M58	1.11	1.413
M59	1.65	1.431
M60	-2.05	-0.928
M61	-1.91	-0.579
M62	-1.95	-0.604
M63	1.96	1.822
M64	1.74	2.066
M65	-1.23	-1.38
M66	0.93	0.961
M67	-1.19	-1.098
M68	2.69	1.337
M69	1.04	1.244
M70	0.15	1.367
M71	2.24	1.716
M72	0.42	0.883
M73	0.95	1.081
M74	0.18	1.022
M75	2.25	2.269
M76	0.17	0.675
M77	-0.31	4.81E-02
M78	0.97	0.663
M79	-0.28	-1.374
M80	0.81	-0.417
M81	2.1	2.586
M82	1.8	1.885
M83	3.38	3.298
M84	0.88	1.181
M85	1.91	2.165
M86	0.46	1.27
M87	-1.32	-0.562
M88	0.13	0.547
M89	-1.22	-0.587
M90	-0.54	-1.77
M91	0.39	0.545
M92	0.98	1.346
M93	0.78	-0.418
M94	-3.00E-02	4.78E-03
M95	0.71	1.698

M96	0.92	0.94
M97	1.58	1.491
M98	1.42	0.775
M99	-0.11	1.036
M100	0.98	1.009
M101	-1.00E-02	0.525
M102	-0.14	-0.307
M103	4.78	2.203
M104	1.34	1.508
M105	2.42	1.424
M106	2.23	1.818
M107	2.16	2.37
M108	1.59	1.349
M109	1.58	0.553
M110	2.73	1.485
M111	0.92	1.296
M112	0.73	0.821
M113	0.6	1.354
M114	0.69	0.593
M115	0.57	0.184
M116	-4.00E-02	0.339
M117	2.04	1.716
M118	2.02	1.252
M119	3.04	2.709
M120	-0.94	-8.77E-02
M121	9.00E-02	0.568
M122	-1.35	-0.795
M123	1.8	0.395
M124	-1.00E-02	0.275
M125	-2.00E-02	0.549
M126	2.54	2.102
M127	-0.43	0.246
M128	-0.68	9.29E-02
M129	-1.19	-1.006
M130	5.00E-02	-0.291
M131	0.53	1.03
M132	4.74	3.563
M133	1.11	1.458
M134	0.25	0.926
M135	-0.12	0.855
M136	-8.00E-02	-0.407
M137	-0.22	-4.40E-02

M138	-0.88	-0.231
M139	-0.26	0.587
M140	-0.61	0.317
M141	-6.00E-02	0.576
M142	4.92	3.716
M143	4.39	4.08
M144	2.84	2.333
M145	6.38	3.984
M146	2.95	1.804
M147	1.84	0.906
M148	1.38	2.061
M149	1.84	2.635
M150	0.88	-1.284
M151	-1.54	-0.179
M152	-2.49	-1.096
M153	-2.96	-1.797
M154	-2.21	-0.545
M155	0.23	-0.126
M156	-2.64	-2.111
M157	2.19	1.48
M158	-1.89	-0.491
M159	-1.37	-8.38E-02
M160	-0.73	0.329
M161	0.4	0.603
M162	-0.59	-0.787
M163	2.13	1.211
M164	-1.94	-0.172
M165	-8.00E-02	-1.039
M166	1.43	0.645
M167	0.82	0.331
M168	1.55	3.882
M169	-1.29	-0.184
M170	-5.00E-02	0.299
M171	-1.13	-1.789
M172	-1.69	-0.161
M173	-1.53	-1.471
M174	0.21	-0.144
M175	0.92	0.481
M176	0.49	0.315
M177	0.35	0.447
M178	-0.14	-0.352
M179	-1.18	-0.53

M180	0.45	0.869
M181	-1.9	-0.679
M182	0.66	1.229
M183	0.26	0.471
M184	-0.14	-5.59E-02
M185	0.2	-0.875
M186	-0.72	-1.238
M187	-0.56	-2.005
M188	-1.96	-5.82E-02
M189	0.72	-0.103
M190	0.7	1.434
M191	-0.89	0.432
M192	1.92	0.813
M193	0.57	0.842
M194	-0.56	-0.868
M195	-1.21	-2.015
M196	-0.84	-1.31
M197	-1.07	-0.963
M198	2.11	1.939
M199	1.54	1.35
M200	0.39	0.838
M201	-0.31	-0.523
M202	-1.22	-1.33
M203	1.68	1.546
M204	0.25	-0.179
M205	2.00E-02	0.676
M206	-2.65	-1.218
M207	-2.85	-1.05
M208	0.74	1.277
M209	0.72	0.172
M210	0.53	1.064
M211	2.36	2.228
M212	1.4	0.5
M213	0.95	1.403
M214	-2.3	-0.14
M215	1.82	0.842
M216	-2.6	-0.482
M217	1.82	2.083
M218	-0.3	-1.94E-02
M219	3.26	1.861
M220	1.38	3.075
M221	-0.41	-0.356

M222	-1.53	-1.844
M223	-6.00E-02	0.435
M224	0.61	1.453
M225	1.4	1.757
M226	2.38	1.749
M227	1.61	1.919
M228	-0.51	-0.704
M229	-0.15	0.635
M230	0.75	0.942
M231	2.09	1.871
M232	1.76	1.696
M233	1.4	0.328
M234	1.7	2.114
M235	-0.16	0.268
M236	-0.88	0.173
M237	2.18	1.18
M238	3.48	2.209
M239	1.26	1.331
M240	0.4	1.317
M241	7.00E-02	-0.23
M242	-0.74	-0.709
M243	0.12	0.472
M244	-0.38	0.563
M245	2.91	1.527
M246	-0.56	0.247
M247	-0.58	-1.023
M248	1.47	1.902
M249	1.25	1.893
M250	-1.77	-0.894
M251	0.47	0.483
M252	-0.64	-0.93
M253	3.46	1.657
M254	1.02	9.71E-02
M255	1.85	3.254
M256	0.23	0.246
M257	1.98	2.618
M258	0.5	0.12
M259	0.18	0.859
M260	1.21	1.361
M261	0.81	0.635
M262	1.09	0.754
M263	-1.7	-1.644

M264	1.71	2.44
M265	1.08	2.04
M266	-0.42	-0.25
M267	-0.44	-0.286
M268	1.52	1.376
M269	-0.45	0.428
M270	-0.27	-1.188
M271	0.25	1.265
M272	1.46	1.589
M273	1.24	0.708
M274	2.31	0.652
M275	1.89	0.508
M276	1.42	0.531
M277	0.85	0.484
M278	-2.15	-1.473
M279	0.16	-2.413
M280	6.00E-02	-1.01E-02
M281	-1.65	-0.734
M282	2.11	0.899
M283	0.94	0.105
M284	-1.25	-0.185
M285	-0.99	-2.42E-02
M286	-0.33	-0.294
M287	2.69	2.592
M288	1.79	0.826
M289	2.26	-0.529
M290	-0.11	-0.838
M291	-1.16	-0.107
M292	-0.73	0.135
M293	-0.14	0.477
M294	-6.00E-02	0.651
M295	0.84	6.97E-02
M296	0.17	0.744
M297	0.55	1.053
M298	2.06	2.137
M299	2.34	0.776
M300	0.73	0.489
M301	-0.24	-0.909
M302	0.65	-0.406
M303	0.66	1.446
M304	1.08	0.975
M305	-1	-0.347

M306	1.42	-8.36E-02
M307	-0.63	0.266
M308	2.74	2.871
M309	1.44	1.811
M310	1.13	0.436
M311	1.38	-0.374
M312	0.97	1.468
M313	-0.24	0.125
M314	0.41	0.311
M315	-0.58	0.596
M316	-0.43	0.705
M317	1.56	-4.90E-02
M318	2.68	2.328
M319	2.82	0.612
M320	0.76	0.664
M321	2.16	1.807
M322	0.85	0.541
M323	0.53	0.995
M324	0.52	0.519
M325	2.19	2.495
M326	2.19	2.769
M327	1.18	-0.327
M328	-1.09	0.3
M329	-1.44	-1.253
M330	1.56	-1.123
M331	-0.43	-0.713
M332	0.21	-1.04
M333	-1.25	-0.529
M334	-1.59	-5.74E-02
M335	-0.59	0.103
M336	0.84	-0.551
M337	2.49	1.131
M338	0.29	-0.332
M339	-0.26	0.357
M340	0.38	-3.16E-02
M341	1.45	1.707
M342	2.62	2.651
M343	2.16	1.874
M344	-0.35	0.681
M345	1.8	0.754
M346	0.46	1.224
M347	0.78	-0.564

M348	1.14	0.748
M349	2.35	1.138
M350	1.29	1.009
M351	1.11	4.98E-02
M352	-0.16	0.299
M353	0.5	0.584
M354	1.8	1.483
M355	2.37	1.572
M356	3.08	1.128
M357	1.33	1.204
M358	1.36	0.881
M359	-6.00E-02	0.536
M360	2.54	1.331
M361	0.96	1.573
M362	0.53	1.654
M363	0.81	1.02
M364	0.89	0.73
M365	1.19	1.129
M366	1.35	0.714
M367	0.76	0.872
M368	0.97	0.644
M369	1.19	1.414
M370	1.74	1.476
M371	1.36	1.05
M372	1.07	1.474
M373	1.46	1.059
M374	1.28	1.3
M375	1.00E-02	0.64
M376	0.73	0.936
M377	0.42	1.184
M378	4.00E-02	0.192
M379	0.38	0.409
M380	2.37	1.557
M381	0.94	1.128
M382	2.00E-02	-0.327
M383	3.00E-02	0.733
M384	0.44	1.328
M385	0.39	1.257
M386	0.55	0.557
M387	1.17	1.438
M388	3.2	3.168
M389	0.87	0.864

M390	0.56	0.795
M391	1.08	1.145
M392	0.82	0.601
M393	0.62	0.65
M394	1.32	0.77
M395	-0.14	0.552
M396	0.41	0.855
M397	0.82	0.949
M398	0.51	0.338
M399	1.7	1.474
M400	0.63	0.119
M401	-0.61	0.447
M402	1.08	-2.68E-02
M403	1.78	1.56
M404	1.32	1.092
M405	0.87	1.49
M406	0.19	0.943
M407	0.92	1.083
M408	0.96	0.862
M409	-0.4	0.348
M410	1.07	0.914
M411	2.78	2.522
M412	1.52	1.878
M413	0.22	0.523
M414	5.00E-02	0.377
M415	7.00E-02	0.746
M416	0.74	1.162
M417	0.7	0.907
M418	0.82	0.297
M419	0.78	0.77
M420	0.51	0.767
M421	1.02	1.212
M422	2.01	0.636
M423	1.94	2.182
M424	1.26	1.25
M425	0.67	0.81
M426	1.77	1.239
M427	0.22	0.823
M428	3.72	1.573
M429	2.59	1.467
M430	0.6	0.972
M431	0.85	1.202

M432	3.65	0.86
M433	1.73	1.401
M434	1.09	1.226
M435	3.63	2.767
M436	0.69	0.816
M437	-0.17	1.525
M438	1.42	1.82
M439	2.29	1.254
M440	1.96	0.564
M441	0.77	0.911
M442	1.22	1.229
M443	1.64	1.468
M444	2.3	0.923
M445	2.93	1.713
M446	3.66	2.039
M447	2.75	1.39
M448	0.88	1.339
M449	3.09	1.89
M450	2.98	2.263
M451	0.37	0.219
M452	3.23	2.882
M453	1.1	1.782
M454	0.3	0.773
M455	3.58	3.553
M456	1.84	2.137
M457	0.56	0.869
M458	2.49	3.786
M459	-1.13	-0.319
M460	-0.74	-2.74E-02
M461	0.13	0.36
M462	0.84	1.916
M463	2.52	3.253
M464	-0.46	4.10E-02
M465	0.66	0.981
M466	-0.73	7.19E-02
M467	1.38	1.317
M468	0.92	1.338
M469	0.24	1.371
M470	1.22	2.22
M471	-0.53	-0.285
M472	0.48	0.797
M473	1.66	1.953

M474	0.84	0.373
M475	0.88	1.941
M476	0.1	0.72
M477	-0.87	0.403
M478	1.4	1.723
M479	0.52	0.936
M480	1.19	1.395
M481	2.67	3.862
M482	-0.39	0.406
M483	2.03	1.18
M484	0.56	0.837
M485	0.1	0.241
M486	0.3	0.954
M487	1.32	1.729
M488	1.17	1.536
M489	1.56	2.132
M490	1.37	1.817
M491	1.73	1.316
M492	0.33	0.553
M493	0.89	1.398
M494	2.77	3.119
M495	0.74	0.962
M496	1.95	2.593
M497	0.58	0.679
M498	1.00E-02	0.546
M499	1.73	0.259
M500	2.52	1.023
M501	2.17	0.865
M502	1.02	0.207
M503	-0.13	0.511
M504	-0.45	0.297
M505	0.51	0.649
M506	1.14	0.187
M507	1.81	0.667
M508	0.87	1.303
M509	0.28	0.782
M510	0.43	0.312
M511	1.35	0.948
M512	1.77	0.289
M513	1.23	0.759
M514	1.96	0.378
M515	2.28	0.894

M516	0.36	0.623
M517	0.96	0.554
M518	1.18	0.688
M519	0.57	1.196
M520	0.92	0.717
M521	2.31	0.721
M522	2.25	0.868
M523	1.83	0.621
M524	1.99	1.186
M525	4.47	1.78
M526	0.95	0.963
M527	2.51	1.833
M528	2.19	0.842
M529	1.21	1.346
M530	1.58	1.229
M531	0.59	0.499
M532	0.6	0.914
M533	1.56	1.044
M534	1.47	1.986
M535	1.69	1.533
M536	0.73	1.06
M537	2.05	1.583
M538	-4.00E-02	0.928
M539	1.56	1.4
M540	2.69	1.256
M541	0.6	0.338
M542	0.11	0.952
M543	0.55	1.064
M544	0.61	0.96
M545	0.42	0.518
M546	0.54	1.78
M547	1.74	0.799
M548	1.38	0.5
M549	0.89	0.515
M550	0.73	0.831
M551	1	1.023

Tabella 3. **Test Set – 1977 composti**

ID	Smiles	pLC_{50} predetta
mol1	O=C1N2C=C(C=CC2=NC=2N(CC=C)C(=N)C(=CC1=2)C(=O)NCC=C)C	6.773
mol2	O=C1N2C(=NC=3N(CCOCCO)C(=N)C(=CC1=3)C(=O)NCC=C)C(=CC=C2)C	6.032
mol3	O=C1N2C(=NC=3N(CCOC)C(=N)C(=CC1=3)C(=O)NC(C)c1ccccc1)C=CC=C2	6.004
mol4	o1cccc1CN1C=2N=C3N(C=C(C=C3)C)C(=O)C=2C=C(C(=O)NCC=C)C1=N	5.815
mol5	S(=O)(=O)(C1=CC2=C(N=C3N(C=CC=C3)C2=O)N(CC=C)C1=N)c1ccccc1	5.758
mol6	O=C1N2C(=NC=3N(C(C)C)C(=N)C(=CC1=3)C(=O)NCC=C)C=CC=C2	5.651
mol7	O=C1N2C(=NC=3N(CCOC)C(=N)C(=CC1=3)C(=O)N)C(=CC=C2)C	5.596
mol8	o1cccc1CNC(=O)C1=CC2=C(N=C3N(C=CC=C3)C2=O)N(C(C)C)C1=N	5.404
mol9	O=C1N2C(=NC=3N(CCCOC)C(=N)C(=CC1=3)C(=O)NC1CCCCC1)C=CC=C2	5.394
mol10	O=C1N2C(=NC=3N(CCCOCC)C(=N)C(=CC1=3)C(=O)NC1CCCC1)C(=CC=C2)C	5.378
mol11	O=C1N2C(=NC=3N(C(=N)C(=CC1=3)C(=O)NCC=C)C1CCCCC1)C=CC=C2	5.363
mol12	O=C1N2C(=NC=3N(CCCOCC)C(=N)C(=CC1=3)C(=O)NC1CCCC1)C=CC=C2	5.3
mol13	O=C1N2C(=NC=3N(CCCOCC)C(=N)C(=CC1=3)C(=O)NCC=C)C(=CC=C2)C	5.248
mol14	O=C1N2C(=NC=3N(CCCOC)C(=N)C(=CC1=3)C(=O)NC1CCCCC1)C(=CC=C2)C	5.075
mol15	O=C1N2C(=NC=3N(CCCOCC)C(=N)C(=CC1=3)C(=O)NCC=C)C=CC=C2	5.045
mol16	O=C1N2C(=NC=3N(CCCOC)C(=N)C(=CC1=3)C(=O)NCC=C)C=CC=C2	4.998
mol17	O=C1N2C(=NC=3N(CCCO)C(=N)C(=CC1=3)C(=O)NC1CCCCC1)C(=CC=C2)C	4.998
mol18	O=C1N2C(=NC=3N(CCCOC)C(=N)C(=CC1=3)C(=O)NCc1ccccc1)C=CC=C2	4.955
mol19	o1cccc1CNC(=O)C1=CC2=C(N=C3N(C=CC=C3)C2=O)N(CCCOCC)C1=N	4.925
mol20	O=C1N2C(=NC=3N(CCCOC)C(=N)C(=CC1=3)C(=O)NC1CCCC1)C(=CC=C2)C	4.849
mol21	O=C1N2C(=NC=3N(CCCOCC)C(=N)C(=CC1=3)C#N)C(=C	4.844

	C=C2)C	
mol22	O=C1N2C(=NC=3N(CCCOCC)C(=N)C(=CC1=3)C(=O)NC)C=CC=C2	4.801
mol23	O=C1N2C(=NC=3N(CCCOCC)C(=N)C(=CC1=3)C(=O)NC)C(=CC=C2)C	4.727
mol24	O=C1N2C(=NC=3N(CCCOCC)C(=N)C(=CC1=3)C(OCC)=O)C=CC=C2	4.594
mol25	o1cccc1CNC(=O)C1=CC2=C(N=C3N(C=CC=C3C)C2=O)N(CCCO)C1=N	4.56
mol26	O=C1N2C(=NC=3N(C(C)C)C(=N)C(=CC1=3)C(OC)=O)C=CC=C2	4.554
mol27	O=C1N2C(=NC=3N(CCCOC)C(=N)C(=CC1=3)C(=O)NCC)C=CC=C2	4.531
mol28	O1CCCC1CNC(=O)C1=CC2=C(N=C3N(C=CC=C3)C2=O)N(CCCOC)C1=N	4.528
mol29	O1CCCC1CNC(=O)C1=CC2=C(N=C3N(C=CC=C3)C2=O)N(CCCOC)C1=N	4.481
mol30	O=C1N2C(=NC=3N(C(=N)C(=CC1=3)C(OC)=O)C1CCCCC1)C(=CC=C2)C	4.423
mol31	O=C1N2C(=NC=3N(CCCn4ccnc4)C(=N)C(=CC1=3)C(=O)NCC=C)C(=CC=C2)C	4.364
mol32	O=C1N2C(=NC=3N(CCCOCC)C(=N)C(=CC1=3)C(=O)NCC)C(=CC=C2)C	4.351
mol33	s1c2N=C(SCC(=O)c3cc([N+](=O)[O-])c(OC)cc3)NC(=O)c2c(C)c1C	4.264
mol34	O=C1N2C(=NC=3N(CC=C)C(=N)C(=CC1=3)C(=O)N1CCN(CC1)C)C(=CC=C2)C	4.255
mol35	O=C1N2C(=NC=3N(CCCOCC)C(=N)C(=CC1=3)C(=O)N)C=CC=C2	4.215
mol36	O=C1N2C(=NC=3N(CCCOC)C(=N)C(=CC1=3)C(=O)NC)C=CC=C2	4.171
mol37	O=C1N2C(=NC=3N(CCOC)C(=N)C(=CC1=3)C(=O)N)C=CC=C2	4.144
mol38	O1CCCC1CNC(=O)C1=CC2=C(N=C3N(C=CC=C3C)C2=O)N(CCCOC)C1=N	4.123
mol39	S(=O)(=O)(N1CCCCC1)c1cc(ccc1C)-c1n2N=C(c3c(-c2nn1)cccc3)C	3.985
mol40	O=C1N2C(=NC=3N(CCCOC)C(=N)C(=CC1=3)C(OCC)=O)C=CC=C2	3.983
mol41	O1CCCC1CNC(=O)C1=CC2=C(N=C3N(C=CC=C3)C2=O)N(CCCO)C1=N	3.954
mol42	o1c2c(nc1-c1cc(NC(=O)c3nc[nH]n3)ccc1O)cc(cc2)C	3.928
mol43	O1CCCC1CNC(=O)C1=CC2=C(N=C3N(C=CC=C3)C2=O)N	3.891

	(CCCO)C1=N	
mol44	S(=O)(=O)(NCCC)c1cc(ccc1OC)-c1n2N=C(c3c(-c2nn1)cccc3)C	3.879
mol45	s1nc2cc(NC(=O)CSC=3NC(=O)c4c(N=3)cccc4)ccc2n1	3.809
mol46	Clc1ccccc1C=1Sc2n(N=1)c(nn2)Cn1c2c(nc1)cccc2	3.747
mol47	s1c2c(CCCC2)c(C(=O)NCCC)c1NC(=O)C1Oc2c(OC1)cccc2	3.745
mol48	s1c2c(CCCC2)c(C(=O)NCCC)c1NC(=O)C1Oc2c(OC1)cccc2	3.717
mol49	O=C1N2C(=NC=3N(CCCOCC)C(=N)C(=CC1=3)C(OC)=O)C=CC=C2	3.674
mol50	S(=O)(=O)(NC(C)C)c1cc(ccc1OC)-c1n2N=C(c3c(-c2nn1)cccc3)C	3.674
mol51	s1c2c(CCCC2)c(C(=O)NCC=C)c1NC(=O)C1Oc2c(OC1)cccc2	3.671
mol52	O(CCOC(=O)c1ccccc1)c1nc(nc(n1)NCC)NC(C)C	3.657
mol53	s1c2c(CCCC2)c(C(=O)NCC=C)c1NC(=O)C1Oc2c(OC1)cccc2	3.647
mol54	Clc1ccc(SCCNS(=O)(=O)c2cc(OC)c(OC)cc2)cc1	3.618
mol55	o1nc(nc1-c1cc(OC)c(OC)cc1OC)-c1cc(OC)c(OC)cc1	3.578
mol56	O1C2=C(C(CCCCCC)C(C#N)=C1N)C(Oc1c2cccc1)=O	3.541
mol57	Clc1cc(ccc1)C(=O)NC(=S)Nc1ccc(cc1)C(OC)=O	3.49
mol58	n12nc3nc(cc(c3c1N=C(C=C2NCCc1ccccc1)C)C)C	3.484
mol59	o1c(nnc1-c1cc(OC)c(OC)cc1)-c1cc(OC)c(OC)c(OC)c1	3.477
mol60	O=C1N2C(=NC=3N(CCCOC)C(=N)C(=CC1=3)C(=O)N1CCN(CC1)C)C(=CC=C2)C	3.47
mol61	Clc1ccccc1C=1Sc2n(N=1)c(nn2)C1Oc2c(OC1)cccc2	3.468
mol62	Clc1ccccc1C=1Sc2n(N=1)c(nn2)C1Oc2c(OC1)cccc2	3.468
mol63	S=C(Nc1cc(ccc1C)C)NC(=O)c1ccc(OCC)cc1	3.442
mol64	S(Cc1ccccc1)c1nc2n(n1)C(=O)C=1CCCCC=1N2	3.439
mol65	O1c2c(C=C(c3oc(nn3)-c3ccccc3)C1=O)cc(OC)cc2	3.431
mol66	S(CC(OC)=O)C=1n2c(nc3c2cccc3)C(C#N)=C(C=1)CCC	3.43
mol67	S(=O)(=O)(NCCO)c1cc(ccc1OC)-c1n2N=C(c3c(-c2nn1)cccc3)C	3.43
mol68	s1c(C(OCC)=O)c(nc1NC(=O)CSC=1NC(=O)C=C(N=1)C)C	3.413
mol69	O1C2=C(C(CCCCCC)C(C#N)=C1N)C(Oc1c2cccc1)=O	3.386
mol70	Clc1cc(cc(OC)c1OCC=C)C1c2c(OC(N)=C1C#N)cc1OCOc1c2	3.375
mol71	S(=O)(=O)(NCc1cc2OCOc2cc1)c1ccc(OCCC)cc1	3.367
mol72	S=C(Nc1cc(ccc1C)C)NC(=O)c1cc(OCC)ccc1	3.361
mol73	O=C1Nc2cc(ccc2C=C1CN(Cc1ccccc1)C(=O)COC)C	3.359
mol74	S=C(Nc1cc(C)c(cc1O)C)NC(=O)c1oc2c(c1)cccc2	3.346
mol75	O=C1NC(=NC(C)=C1Cc1c2c(ccc1)cccc2)N1CCN(CC1)C	3.342
mol76	s1c2c(nc1SCCNS(=O)(=O)c1cc(OC)c(OC)cc1)cccc2	3.316
mol77	S=C(Nc1cc(ccc1)C#N)NC(=O)c1ccc(cc1)C(C)(C)C	3.308

mol78	s1c2cc(ccc2nc1NC(=S)NC(=O)c1ccc(F)cc1)C	3.299
mol79	Clc1cc(ccc1C(=O)NC(=S)Nc1cc(ccc1)C(=O)C)C	3.297
mol80	s1c2CCCCc2c2-c3nc(nn3C=Nc12)-c1cc2OCOc2cc1	3.29
mol81	O1c2c(cc3OCOc3c2)C(C(C#N)=C1N)c1cc(OCC)c(OCC=C)cc1	3.288
mol82	O1c2c(ccc(OCC(=O)Nc3ccccc3CC)c2)C(=CC1=O)C	3.276
mol83	O(C(=O)c1ccc(NC(=O)c2cc(cc(c2)C)C)cc1)C	3.276
mol84	S(CCOc1ccccc1OC)c1nc2c(n1CC(=O)N)cccc2	3.275
mol85	O1c2c(cc3OCOc3c2)C(C(C#N)=C1N)c1cc(OCC)c(OCC)cc1	3.272
mol86	S(CCOc1ccccc1)c1n2-c3c(N(c2nn1)C)cccc3	3.272
mol87	O(Cc1nc([nH]n1)Nc1nc(cc(n1)C)C)c1c2c(ccc1)cccc2	3.261
mol88	Clc1cccc(NC(=S)NC(=O)Cc2ccc(OC)cc2)c1C	3.255
mol89	O1C23OC(N)=C(C2(C(C(OCCC)=O)=C1C)C(=O)c1c3cccc1)C#N	3.255
mol90	S1c2n(N=C1c1cc(F)ccc1)c(nn2)Cn1c2c([nH+]c1)cccc2	3.249
mol91	S(CC(O)=O)c1n2-c3c(N(c2nn1)CCOc1ccccc1)cccc3	3.246
mol92	O1C23OC(N)=C(C2(C(C(OCCC)=O)=C1C)C(=O)c1c3cccc1)C#N	3.238
mol93	O1C2=C(C(C(C#N)=C1N)c1ccc(OCCC)cc1)C(=O)CC(C2)(C)C	3.233
mol94	S1\C(=C/c2cc3OCOc3cc2)\C(=O)N=C1c1ccc(cc1)C	3.227
mol95	O1C2=C(C(CCCCCC)C(C#N)=C1N)C(=O)CC(C2)(C)C	3.225
mol96	S=C(Nc1cc(ccc1O)C(CC)C)NC(=O)CC(C)C	3.223
mol97	O=C1N2C(=NC=3N(CCOCCO)C(=N)C(=CC1=3)C#N)C(=CC=C2)C	3.217
mol98	Clc1cccc(NC(=O)c2cc3OCCOc3cc2)c1N1CCN(CC1)CC	3.216
mol99	S=C(N(CC)c1ccccc1)NC(=O)Cc1ccc(OC)cc1	3.216
mol100	S=C(Nc1c2c3c(CCc3ccc2)cc1)NC(=O)c1occc1	3.201
mol101	S(CCC)C=1NC(=O)C(C(OC)=O)C(C=1C#N)c1ccccc1C	3.199
mol102	Brc1ccc(cc1)Cn1c2c(nc1NCCCC)N(C)C(=O)N(C)C2=O	3.197
mol103	O=C1N(C)C(=O)N(c2nc(n(c12)Cc1ccc(cc1)C)NCCCC)C	3.195
mol104	S(CCOc1ccccc1C)c1nc2c(n1CC(O)CO)cccc2	3.188
mol105	O=C1N(c2cc(ccc2C)C)C(=O)c2c1cc(cc2)C(OCC=C)=O	3.183
mol106	o1nc(nc1Cc1ccc(OC)cc1)-c1cc(OC)c(OC)cc1	3.181
mol107	S(CCC)C=1NC(=O)C(C(OC)=O)C(C=1C#N)c1ccccc1C	3.177
mol108	S=C(Nc1cc(ccc1O)C(CC)C)NC(=O)CC(C)C	3.176
mol109	S(=O)(=O)(NC(C)(C)C)c1cc(-c2n3N=C(c4c(-c3nn2)cccc4)C)c(cc1)C	3.171
mol110	O(C)c1cc(C(NC(=O)c2ccccc2)C)c(cc1OC)CC	3.17
mol111	S(=O)(=O)(N1CCCCCC1)c1ccc(OCCCC)cc1	3.163
mol112	S(CCOc1ccccc1C)c1nc2c(n1CC(O)CO)cccc2	3.162
mol113	O1C2=C(C(C#Cc3ccccc3)C(C#N)=C1N)C(=O)CC(C2)(C)C	3.158
mol114	O1C2=C(C(CCCCCC)C(C#N)=C1N)C(=O)CC(C2)(C)C	3.154

mol115	O=C1N2C(=NC=3N(CCOC)C(=N)C(=CC1=3)C(OC)=O)C=CC=C2	3.146
mol116	O1c2c(C3=C(CCC3)C1=O)c(OCC(=O)N(CC)CC)cc(c2)C	3.14
mol117	S=C(Nc1cc(cc(c1)C)C)NC(=O)c1cc(OC)c(OC)cc1	3.139
mol118	S(CC(OCCCC)=O)C=1NC(=O)CC(C=1C#N)c1ccccc1	3.134
mol119	S(CC(OCCCC)=O)C=1NC(=O)CC(C=1C#N)c1ccccc1	3.134
mol120	O1c2c(cc3OCOc3c2)C(C(C#N)=C1N)c1cc(OCC)c(OCC#C)cc1	3.119
mol121	Clc1cc(cc(OC)c1OCC=C)C1c2c(OC(N)=C1C#N)cc1OCOc1c2	3.119
mol122	S=C(NC(=O)Cc1c2c(ccc1)cccc2)N1CCc2c1cccc2	3.116
mol123	S=C(Nc1cc(ccc1O)C(C)C)NC(=O)c1ccc(F)cc1	3.113
mol124	Clc1cc(cc(OC)c1OCC=C)C1c2c(OC(N)=C1C#N)cc(O)cc2	3.112
mol125	S(CC(=O)NCC=C)c1nc(c2CCc3c(-c2n1)cccc3)C(F)(F)F	3.111
mol126	S(Cc1[nH+]c2c([nH]1)cccc2)c1[nH+]c2c(n1CC)cccc2	3.108
mol127	O1c2c(cc3OCOc3c2)C(C(C#N)=C1N)c1cc(OCC)c(OCC#C)cc1	3.107
mol128	o1c(ccc1C(OCCCC)=O)CC(=O)c1ccc(O)cc1O	3.105
mol129	Clc1cc2OCOc2cc1C1C2=C(N=C(C)C1C(OCC=C)=O)CCCC2=O	3.103
mol130	O1c2c(cc3OCOc3c2)C(C(C#N)=C1N)c1cc(OCC)c(OCC=C)cc1	3.099
mol131	S=C(Nc1cc(ccc1C)C)NC(=O)c1ccccc1F	3.099
mol132	O1C2=C(C(C(C#N)=C1N)c1ccc(OCCC)cc1)C(=O)CC(C2)(C)C	3.096
mol133	S1\C(=C/C=2C(=O)N3C(=NC=2NC(C)C)C=CC=C3)\C(=O)N(C)C1=S	3.094
mol134	S(=O)(=O)(NC)c1cc(ccc1C)-c1n2N=C(c3c(-c2nn1)cccc3)C	3.086
mol135	S(CC[NH+](CC)CC)c1nc2n(c3c(cc(cc3)C)c2nn1)CC	3.083
mol136	S=C(Nc1ccc(cc1)C(OC)=O)NC(=O)c1ccccc1	3.058
mol137	O=C1n2nc(nc2NC(=C1)C)NCc1c2c(ccc1)cccc2	3.049
mol138	Oc1cc2c(n(CCCC)c(C)c2C(OCC)=O)cc1	3.043
mol139	O1c2c(C(=CC1=O)C)c(O)cc(c2)CCCCCC	3.035
mol140	O(C)c1cc(C(NC(=O)c2ccc(OC)cc2)C)c(cc1OC)CC	3.03
mol141	s1c2CCCCc2nc1NC(=O)C(Sc1nncn1C)CC	3.028
mol142	S(CCOc1ccccc1)c1nc2c(n1CCO)cccc2	3.026
mol143	Clc1cc(C)c(OCC(Oc2cc([N+](=O)[O-])ccc2)=O)cc1	3.025
mol144	Brc1cc(ccc1OCC(=O)NC1CCCCC1)CC	3.023
mol145	S(CCOc1ccccc1OC)c1nc2c(n1CCO)cccc2	3.022
mol146	Brc1cc(S(=O)(=O)N2CCN(CC2)c2ccccc2)c(OC)cc1	3.021
mol147	Clc1ccccc1NC(=S)NC(=O)c1cc(OCC)ccc1	3.017
mol148	Clc1cc(ccc1)C(=O)NC(=S)Nc1ccccc1C(OC)=O	3.009
mol149	S=C(NC1CCCC1)NC(=O)c1ccc(OC(C)C)cc1	3.007

mol150	S1CCSC12CCC1(CC2(CCC12SCCS2)C(OC)=O)C(OC)=O	3.005
mol151	S(CC(OCCC)=O)C=1NC(=O)CC(C=1C#N)c1ccc(cc1)C	3.004
mol152	S(CCOc1ccccc1OC)c1nc(cc(n1)C)C	3
mol153	Clc1cc(NC(=S)NC(=O)c2cc(ccc2)C)ccc1OC	2.996
mol154	S=C(Nc1cc(cc(C)c1O)C)NC(=O)c1ccccc1OC	2.995
mol155	S=C(Nc1cc(ccc1C)C)NC(=O)c1ccccc1	2.993
mol156	Brc1oc(cc1)C(=O)NC(=S)Nc1cc(ccc1)C	2.992
mol157	O(CC(=O)Nc1ccccc1C(=O)N)c1ccccc1C(CC)C	2.991
mol158	O(CC)c1cc(ccc1OCC)CC(=O)Nc1ccc(cc1)C	2.988
mol159	S=C(NC(=O)c1ccccc1C)NCCC=1CCCCC=1	2.983
mol160	s1cccc1-c1nc(nc(c1)C(F)(F)F)NC(=[NH2+])Nc1ccccc1	2.983
mol161	S1CCN=C1SC(CC)C(=O)Nc1sc(C(OCC)=O)c(n1)C	2.978
mol162	O=C1C2=C(NC(=C1)CCC)NN(C2=O)c1ccccc1	2.976
mol163	s1c2CCCCc2c2c1N=C(SCC(=O)N1CCCCC1)NC2=O	2.975
mol164	O=C(NCCCc1nc2c(n1CC=C)cccc2)c1ccccc1	2.974
mol165	S(CC(OCCC)=O)C=1NC(=O)CC(C=1C#N)c1ccc(cc1)C	2.968
mol166	O1C(=CC=2OC(N)=C(C#N)C3(C=2C1=O)c1c(N(C(=O)C)C3=O)cccc1)C	2.968
mol167	FC(F)(F)C=1n2nc(cc2N=C2C=1CCc1c2cccc1)C(=O)NCCOC	2.966
mol168	Clc1ccccc1OCC(=O)NC(=S)Nc1cc(C)c(cc1)C	2.962
mol169	S=C(Nc1ccc(cc1)CC)NC(=O)c1ccccc1OC	2.962
mol170	S1CCN=C1SC(CC)C(=O)Nc1sc(C(OCC)=O)c(n1)C	2.959
mol171	O1C(=CC=2OC(N)=C(C#N)C3(C=2C1=O)c1c(N(C(=O)C)C3=O)cccc1)C	2.956
mol172	Brc1ccc(NC(=S)NC(=O)CC(C)C)cc1C	2.956
mol173	FC(F)(F)C(=O)c1c2c(n(c1)CC(=O)N1CCCC1)cccc2	2.955
mol174	Clc1cc(NC(=S)NC(=O)c2ccccc2F)c(OC)cc1	2.952
mol175	O1c2c(cc3OCOc3c2)C(C(C#N)=C1N)c1cc(OCC)c(OCC)cc1	2.952
mol176	s1c2CC(CCc2c(C#N)c1NC(=O)CN1CCCC1)C(C)(C)C	2.951
mol177	O=Cc1c2c(n(CC(=O)NC3CCCCC3)c1C)cccc2	2.95
mol178	s1c(C(=O)C)c(C)c(C(OCC)=O)c1NC(=O)CSc1ncccn1	2.95
mol179	S=C(Nc1cc(ccc1)C(=O)C)NC(=O)c1ccccc1F	2.949
mol180	O1C2C=CC13C(C2C(OCCC)=O)C(=O)N(C3)c1ccc(cc1)CC	2.948
mol181	Brc1cc(ccc1)C(=O)NC(=S)Nc1ccccc1C	2.947
mol182	O1c2c(C3=C(CCCC3)C1=O)ccc(OCC(OCC=C)=O)c2C	2.944
mol183	s1cc(nc1NC(=O)c1occc1)C1=Cc2c(OC1=O)cccc2	2.944
mol184	O(CCOC)c1nc2N(C)C(=O)N(C)C(=O)c2n1Cc1c2c(ccc1)cccc2	2.943
mol185	s1ccc(C)c1C1C2=C(OC(N)=C1C#N)c1c(OC2=O)cccc1	2.941
mol186	Clc1cc(ccc1)C(=O)NC(=S)Nc1cc(ccc1)C	2.938
mol187	S=C(Nc1ccc(OC)cc1)NC(=O)c1cc(ccc1)C	2.936
mol188	O1C(=C(C(OCC)=O)C2(c3c(NC2=O)cccc3)C(C#N)=C1N)c1ccccc1	2.935

mol189	S(=O)(=O)(N1CCCCC1)c1ccc(OCCCC)cc1	2.93
mol190	O(CC)c1ccccc1\C=C/1\C(=O)N(NC\1=O)c1cc(C)c(cc1)C	2.92
mol191	O1c2cc(ccc2OC1)CNC(=O)Cn1cc(c2c1cccc2)C(=O)C1CC1	2.919
mol192	O(CC(=O)Nc1ccccc1OCC)c1c(cccc1C)C	2.913
mol193	O(CC(=O)Nc1ccc(cc1)C#N)c1ccccc1C(C)C	2.912
mol194	s1c2c(CCCC2)c(C(OCC)=O)c1NC(=O)c1nn(cc1)CC	2.91
mol195	O1c2c(cc3OCOc3c2)C(C(C#N)=C1N)c1cc(OC)c(OCC=C)cc1	2.909
mol196	Clc1cc(cc(OC)c1OCC=C)C1c2c(OC(N)=C1C#N)cc(O)cc2	2.901
mol197	O(CC(=O)Nc1ccccc1C(=O)N)c1ccccc1C(CC)C	2.898
mol198	Clc1cc(C)c(OCC(Oc2ccc(OC)cc2)=O)cc1	2.895
mol199	Clc1ccc(cc1)-c1nc2n(n1)C(=O)C(C)=C(N2)C	2.893
mol200	O1c2c(ccc(N(CC)CC)c2)C(=CC1=O)COC(=O)C	2.892
mol201	O(c1cc(C)c(cc1)C)c1ccc(cc1)-c1nc(nc(n1)N)N	2.89
mol202	Clc1ccc(cc1)CN1CCN(CC1)c1nc2N(C)C(=O)NC(=O)c2n1CCC	2.89
mol203	S=C(Nc1cc(ccc1)C(=O)C)NC(=O)c1ccccc1OC	2.889
mol204	S(C)c1ccc(cc1)C1C2=C(OC(N)=C1C#N)CC(CC2=O)(C)C	2.883
mol205	S=C(NC(C)c1ccccc1)NC(=O)c1ccc(OC)cc1	2.883
mol206	S=C(NC(C)c1ccccc1)NC(=O)c1ccc(OC)cc1	2.883
mol207	O(CC)c1cc(ccc1OCC)C(NC(=O)Cc1ccccc1)C	2.88
mol208	O(C)c1c(OC)cc(cc1OC)C(Oc1ccccc1C(=O)C)=O	2.879
mol209	Clc1ccc(S(=O)(=O)c2cc(S(=O)(=O)N3CCCC3)c(cc2)C)cc1	2.877
mol210	Brc1ccc(OCC(=O)N(CC)c2ccccc2)cc1	2.869
mol211	S=C(Nc1ccc(cc1O)C)NC(=O)c1c2c(ccc1)cccc2	2.865
mol212	Clc1ccc(NC(=O)c2ccccc2)cc1[N+](=O)[O-]	2.865
mol213	O1CCCC1COC(=O)C1C(C2=C(N=C1C)CCCC2=O)c1ccc(N(C)C)cc1	2.862
mol214	Clc1ccc([N+](=O)[O-])cc1NC(=S)NC(=O)c1cc(ccc1)C	2.862
mol215	Clc1ccccc1OCC(=O)NCCC=1CCCCC=1	2.861
mol216	O1c2c(cc3OCOc3c2)C(C(C#N)=C1N)c1cc(OC)c(OCC)cc1	2.856
mol217	[nH+]1c2c(n(CCc3ccccc3)c1C1CC1)cccc2	2.856
mol218	FC(F)(F)c1cc(NC(=O)C(=O)NC(C)c2ccccc2)ccc1	2.854
mol219	O1CCCC1COC(=O)C1C(C2=C(N=C1C)CC(CC2=O)(C)C)c1cc(O)ccc1	2.851
mol220	Clc1c2c(sc1C(=O)N1CCCC1C(OCC)=O)cccc2	2.849
mol221	Clc1cc(NC(=S)NC(=O)c2cc(F)ccc2)ccc1OC	2.848
mol222	Clc1cc(C(=O)NC(=S)Nc2ccc(F)cc2)c(OC)cc1	2.846
mol223	S=C1NC(=O)\C(=C\c2ccc(N(CC)CC)cc2OCCC)\C(=O)N1	2.846
mol224	O1c2cc(ccc2OC1)C1N(CCCC)C(=O)C(=O)C1C(=O)c1ccc(OC)cc1	2.845
mol225	Oc1cc(ccc1)C1C2=C(N=C(C)C1C(OCC=C)=O)CC(CC2=O)(C)C	2.844

mol226	Clc1cc(ccc1)C(=O)NC(=S)Nc1ccc(F)cc1	2.843
mol227	O1c2c(cc3OCOc3c2)C(C(C#N)=C1N)c1cc(OC)c(OCC)cc1	2.842
mol228	s1c2c(CCCC2)c(C(OC)=O)c1NC(=O)CCC(OCC)=O	2.841
mol229	O(CC(=O)N(CC)c1ccccc1)c1cc(ccc1C)C	2.84
mol230	O(C)c1cc(ccc1O)C1C2=C(N=C(C)C1C(OCC=C)=O)CC(CC2=O)(C)C	2.837
mol231	S(CCC#N)c1nnc(n1CC=C)-c1ccncc1	2.836
mol232	n1cc(ccc1-c1ccc(cc1)C#N)CCCC	2.834
mol233	Clc1ccc(cc1)Cn1c2c(nc1NCCCOC)N(C)C(=O)N(C)C2=O	2.832
mol234	S=C(NCc1ccc(OC)cc1)NCc1ccc(OC)cc1	2.831
mol235	O1C(N(N=C1c1ccc(cc1)C)C(=O)C)c1ccc(cc1)C	2.827
mol236	O=C1Nc2c(C=C1CN(Cc1ccccc1)C(=O)C(C)C)cccc2	2.827
mol237	O(C)c1cc2N(C(=O)CN3C(=O)C4C(CCCC4)C3=O)C(C=C(c2cc1)C)(C)C	2.826
mol238	S=C(Nc1ccccc1C)NC(=O)COc1ccccc1C	2.821
mol239	O(C)c1ccc(OC)cc1NC(=O)c1cc(OC)cc(OC)c1	2.82
mol240	O1CCCC1COC(=O)C1C(C2=C(N=C1C)CCCC2=O)c1ccc(N(C)C)cc1	2.818
mol241	Clc1cc(NC(=O)C(=O)NC2CCCCC2)ccc1Cl	2.814
mol242	O(CC)c1ccccc1\C=C\1/C(=O)N(NC/1=O)c1cc(C)c(cc1)C	2.811
mol243	O(C)c1cc2N(C(=O)CN3C(=O)C4C(CCCC4)C3=O)C(C=C(c2cc1)C)(C)C	2.811
mol244	Clc1ccc(OC(=O)COc2ccc(cc2)CC)cc1	2.811
mol245	FC(F)(F)C(=O)c1c2c(n(c1)CC(=O)N(CC)CC)cccc2	2.809
mol246	o1c(ccc1[N+](=O)[O-])C(=O)Nc1ccc(cc1)CCCC	2.809
mol247	Clc1ccccc1OCC(=O)N(CC)c1ccccc1	2.807
mol248	Clc1ccc(NC(=O)NNC(=O)c2ccccc2C)cc1	2.801
mol249	Clc1ccc(OC(=O)COc2cc(ccc2C)C)cc1	2.801
mol250	s1c(C(=O)N(C)C)c(nc1NC(=O)c1ccccc1OCC)C	2.8
mol251	S(CC=C)c1nc(ccc1C#N)-c1ccccc1	2.798
mol252	Clc1ccc(NC(=S)NC(=O)c2cc(F)ccc2)cc1	2.798
mol253	O1CCCC1COC(=O)C1C(C2=C(N=C1C)CCCC2=O)c1ccc(N(C)C)cc1	2.797
mol254	S=C(Nc1nccc(c1)C)NC(=O)c1ccc(OCC)cc1	2.797
mol255	Brc1cc(ccc1)Cn1c2c(nc1NCCO)N(C)C(=O)N(C)C2=O	2.792
mol256	s1c2CCCCc2c2-c3nc(nn3C=Nc12)C(C)(C)C	2.79
mol257	S(CC=C)c1nc(N)c(C#N)c(-c2ccccc2)c1C#N	2.789
mol258	O1c2c(cc3OCOc3c2)C(C(C#N)=C1N)c1cc(OC)c(OCC=C)cc1	2.788
mol259	O(C)c1cc(ccc1OC)C(NC(=O)c1ccccc1)CC	2.787
mol260	Brc1cc(OC)c(OC)cc1CNCCc1cc2OCOc2cc1	2.784
mol261	O(CCOCC)c1nc2N(C)C(=O)N(C)C(=O)c2n1CCc1ccccc1	2.782
mol262	O(CC(=O)n1nc(cc1C)C)c1ccccc1-c1ccccc1	2.78

mol263	FC(F)(F)c1cc(NC(=O)C(=O)NC(C)c2ccccc2)ccc1	2.78
mol264	S=C(Nc1cc(OC)ccc1OC)NC(=O)c1ccc(OC)cc1	2.779
mol265	O1c2c(C=C(c3oc(nn3)-c3ccc(cc3)C)C1=O)cccc2	2.778
mol266	O(C(=O)C=1C=Nc2n(nc(C)c2-c2ccccc2)C=1C)CC	2.778
mol267	S(=O)(=O)(N1CCN(CC1)C)c1ccc(OCCCC)cc1	2.777
mol268	Clc1cc(C(=O)NC(=S)Nc2ccccc2C)c(OC)cc1	2.776
mol269	O(C)c1cc(ccc1OC)C1n2nc(nc2NC(C1)c1ccc(cc1)CC)N	2.776
mol270	O(CC)c1ccccc1NC(=O)c1cc([N+](=O)[O-])c(OCC)cc1	2.775
mol271	S(CCO)c1ccc(cc1)Cc1ccc(SCCO)cc1	2.773
mol272	O=C1N(C)C(=O)N(c2nc(n(c12)Cc1c2c(ccc1)cccc2)NCC=C)C	2.772
mol273	Clc1c2c(sc1C(=O)N1CCCC1C(OCC)=O)cccc2	2.771
mol274	Clc1ccc(OCC(Oc2cc([N+](=O)[O-])ccc2)=O)cc1	2.765
mol275	S(CCC)C=1NC(=O)C(C(OC)=O)C(C=1C#N)c1ccccc1C	2.762
mol276	s1c(ncc1CNC(=O)c1ccc([N+](=O)[O-])cc1)-c1ccccc1	2.762
mol277	s1c(C)c(C)c(C(OC(C)C)=O)c1NC(=O)c1occc1	2.761
mol278	Clc1cc(C(=O)NC(=S)Nc2cc(F)ccc2)c(OC)cc1	2.759
mol279	O(C)c1ccc(cc1)-c1c2CC(CCc2nc(N)c1C#N)C	2.759
mol280	FC(F)C=1n2ncc(c2N=C(C=1)c1ccc(cc1)C)C(=O)NCC=C	2.746
mol281	O=C1N(C(=O)C2C1CCCC2)c1ccc(cc1)C(OCC)=O	2.742
mol282	s1cccc1-c1c(C#N)c(nc(SCC(=O)C(C)(C)C)c1C#N)N	2.74
mol283	O=C1N(C(=O)C2C1CCCC2)c1ccc(cc1)C(OCC)=O	2.74
mol284	S(CCC)c1nc2N(C)C(=O)N(C)C(=O)c2n1Cc1ccc(F)cc1	2.739
mol285	S(CCCC)c1[nH+]c2cc(ccc2n1C)C	2.738
mol286	O(CCn1c2c(nc1C(O)C)cccc2)c1ccccc1	2.736
mol287	S(CCC)C=1NC(=O)C(C(OC)=O)C(C=1C#N)c1ccccc1C	2.735
mol288	S(CC[NH+]1CCCCC1)c1nc2n(c3c(cc(F)cc3)c2nn1)C	2.733
mol289	Brc1cc(ccc1OC)C(Oc1ccc(cc1)C(=O)C)=O	2.733
mol290	O(CCO)c1ccc(cc1OC)C1C2=C(N=C(C)C1C#N)CC(CC2=O)(C)C	2.732
mol291	O(C)c1cc(ccc1OC)C1n2nc(nc2NC(C1)c1ccc(cc1)C)N	2.732
mol292	S=C(Nc1cc(OC)ccc1OC)NC(=O)COc1ccccc1	2.731
mol293	S(C(C(=O)Nc1ccc(S(=O)(=O)N)cc1)C)C=1NC(=O)C=C(N=1)C	2.731
mol294	Brc1cc(ccc1OC)C(Oc1ccc(OC)cc1)=O	2.728
mol295	Clc1cc(NC(=O)c2ccc(cc2)CC)c(N2CCOCC2)cc1	2.727
mol296	S=C(Nc1cc(F)ccc1)NC(=O)c1ccccc1C	2.721
mol297	O1c2c(ccc(O)c2)C(C(C#N)=C1N)c1cc(OCC)c(OCC#C)cc1	2.721
mol298	S=C(Nc1ccc(OC)cc1OC)NC(=O)c1cc(OC)ccc1	2.721
mol299	n1nnn(CCC)c1NCc1ccc(N(CC)CC)cc1	2.718
mol300	O1c2c(C=C(C(=O)N3CCc4c(C3)cccc4)C1=O)cccc2CC=C	2.718
mol301	Fc1ccc(cc1)C(=O)CC(C(C#N)C#N)c1ccccc1	2.718
mol302	o1c(nnc1-c1cc2OCOc2cc1)-c1ccc(cc1)C	2.717

mol303	S=C(NC(=O)c1ccc(cc1)-c1ccccc1)N1CCCC1	2.715
mol304	O1c2c(ccc(O)c2)C(C(C#N)=C1N)c1cc(OCC)c(OCC#C)cc1	2.715
mol305	Clc1ccc([N+](=O)[O-])cc1NC(=S)NC(=O)c1ccccc1	2.713
mol306	Clc1cc2c(OC(=O)C=C2C)cc1OCCCC	2.711
mol307	S=C(NC(=O)Cc1ccc(OC)cc1)N1CCCc2c1cccc2	2.711
mol308	O1C(C)=C(C(OCC=C)=O)C2(c3c(NC2=O)cccc3)C(C(OCC)=O)=C1N	2.711
mol309	O=C(N\N=C\c1ccc(cc1)C)c1c2c([nH]c1)cccc2	2.708
mol310	O1CCCC1COC(=O)C1C(C2=C(N=C1C)CC(CC2=O)(C)C)c1cc(O)ccc1	2.708
mol311	S(c1ncc([N+](=O)[O-])cc1)c1nc2c(n1C)cccc2	2.706
mol312	S=C(Nc1ccc(cc1)C#N)NC(=O)c1ccccc1C	2.705
mol313	O(CC(=O)Nc1cc(ccc1)C#N)c1ccccc1C(C)C	2.704
mol314	Brc1oc(cc1)C(=O)Nc1cc2c(cc1)C(=O)N(C)C2=O	2.702
mol315	Clc1cc(NC(=S)NC(=O)c2ccccc2)ccc1C	2.7
mol316	S=C(Nc1ccc(F)cc1)NC(=O)c1cc(ccc1)C	2.699
mol317	S(=O)(=O)(N(CC)CC)c1ccc(OCCCC)cc1	2.699
mol318	Clc1cc(NC(=S)NC(=O)c2ccccc2F)ccc1C	2.698
mol319	O(C(=O)CCCc1c2c([nH]c1)cccc2)CC(=O)c1ccccc1	2.698
mol320	Clc1cccc(NC(=O)c2ccc(cc2)CC)c1N1CCOCC1	2.696
mol321	O(C(=O)c1ccc(NC(OC)=O)cc1)CCCC	2.696
mol322	S(CCC)C=1NC(=O)CC(C=1C#N)c1ccc(cc1)CC	2.695
mol323	Clc1cc(cc(OC)c1O)C1NC(=O)N(C)C(C)=C1C(OCCOCC)=O	2.695
mol324	o1c(ccc1CO)-c1ccc(cc1)C(OC(C)C)=O	2.689
mol325	s1c2CC(CCc2c(C#N)c1NC(=O)CN1CCCC1)C(C)(C)C	2.687
mol326	O=C1N=C(Nc2c1cccc2)Nc1nc(c2cc(C)c(cc2n1)C)C	2.686
mol327	O=C1c2c(N(CC(=O)NC=3C(=O)N(N(C)C=3C)c3ccccc3)C1=O)cccc2	2.685
mol328	Clc1ccc(cc1)C(=O)NC(=S)Nc1cc(ccc1)C(=O)C	2.685
mol329	Clc1ccccc1OCC(=O)Nc1cc(ccc1)C(=O)C	2.685
mol330	O1CCCC1COC(=O)C=1C(C2C(=NC=1C)CCCC2=O)c1ccc(N(C)C)cc1	2.685
mol331	S=C(Nc1cc(ccc1)C)NC(=O)CCc1ccccc1	2.684
mol332	Clc1cc(NC(=S)NC(=O)c2ccccc2OC)ccc1C	2.684
mol333	S=C(Nc1cc(ccc1)C(=O)C)NC(=O)c1cc(ccc1)C	2.682
mol334	s1cccc1-c1onc(n1)-c1ccc(OC)cc1	2.679
mol335	s1c2nc3CCCCc3cc2c(N)c1C(OC)=O	2.678
mol336	s1cccc1-c1nc(SCC(=O)NCC=C)nc(c1)C(F)(F)F	2.675
mol337	O1CCOc2c1cc1c(NC(=O)CC1c1cc(OC)c(OC)c(OC)c1)c2	2.671
mol338	S=C(NC(=O)c1ccc(cc1)C(C)(C)C)N1CCCCCC1	2.671
mol339	S(CCC)C=1NC(=O)CC(C=1C#N)c1ccc(cc1)CC	2.669
mol340	O=C1N(C(=O)C2C1CCCC2)c1ccc(cc1)C(OCC)=O	2.668
mol341	S=C(Nc1ccc(cc1)CC)NC(=O)c1cc(F)ccc1	2.667

mol342	Brc1cc(ccc1C)C(Oc1ccc(OC)cc1)=O	2.667
mol343	S(=O)(=O)(N1CCCCC1)c1ccc(cc1)C(OCC#C)=O	2.665
mol344	S=C(Nc1cc(OC)ccc1OC)NC(=O)c1ccccc1	2.662
mol345	O=C(NC(C)c1ccccc1)Cn1nc(nn1)-c1ccccc1	2.662
mol346	s1cc(-c2cc3c(cc2)cccc3)c(C(OC)=O)c1N	2.659
mol347	O=C1NC(=O)N(c2nc(n(c12)C)N(CCCC)CCCC)C	2.658
mol348	O1CCOc2c1cc1c(NC(=O)CC1c1ccc(OC)c(OC)c1OC)c2	2.656
mol349	Clc1ccccc1C(=O)NC(=S)N(C)C1CCCCC1	2.654
mol350	S=C(Nc1cccnc1)NC(=O)c1ccc(OCC)cc1	2.653
mol351	O(C)c1ccc([N+](=O)[O-])cc1NCc1ccc(OCC)cc1	2.652
mol352	S(=O)(=O)(NCCCO)c1c(cc(cc1C(C)C)C(C)C)C(C)C	2.645
mol353	S=C(Nc1ccc(cc1)C(=O)C)NC(=O)C1CCCCC1	2.644
mol354	O(C(=O)COc1cc2c(cc1)cccc2)c1ccccc1[N+](=O)[O-]	2.641
mol355	Clc1ccccc1C=1Sc2n(N=1)c(nn2)C(C)C	2.641
mol356	Clc1cc(-n2c(ccc2C)C)ccc1OC	2.64
mol357	O(C)c1ccc([N+](=O)[O-])cc1NCc1cc(OC)c(OC)cc1	2.639
mol358	S(=O)(=O)(N(CC(=O)NCCOC)c1ccc(cc1)C)c1ccccc1	2.639
mol359	O(C)c1ccc(cc1)CC(=O)N\N=C\c1ccc(O)cc1O	2.639
mol360	S1c2n(N=C1c1ccc(OC)cc1)c(nn2)C(C)C	2.636
mol361	S(CC(=O)N1CCCCCC1)C1=[NH+]C([O-])=C(CCCC)C(=O)N1	2.636
mol362	O(CC(=O)NC1CCCCCC1)c1ccccc1C	2.633
mol363	Brc1oc(cc1)C(Oc1ccc(Cl)cc1)=O	2.631
mol364	O(C)c1cc2N(C(=O)CN3C(=O)C4C(CCCC4)C3=O)C(C=C(c2cc1)C)(C)C	2.629
mol365	O(C(=O)c1c2c(n(c1)CC(=O)Nc1ccc(cc1)C)cccc2)C	2.628
mol366	S(CC(=O)NC1CCCCC1)C=1NC(=O)CC(C=1C#N)c1ccc(F)cc1	2.626
mol367	O(CC(=O)Nc1ccc(cc1)C(=O)N)c1ccccc1C(CC)C	2.625
mol368	S=C(Nc1ccc(cc1)C(OC)=O)NC(=O)c1ccccc1OC	2.625
mol369	S(CC(=O)Nc1cc2OCCOc2cc1)C=1NC(=O)C=C(N=1)CCC	2.624
mol370	Clc1cc(Cl)ccc1CNc1nc2n(n1)C(=O)C=1CCCC=1N2	2.622
mol371	s1c2c(nc1-n1ncc3c1CC(CC3=O)C)cccc2	2.622
mol372	s1c2c(nc1-n1ncc3c1CC(CC3=O)C)cccc2	2.622
mol373	O(CC(=O)Nc1cccc([N+](=O)[O-])c1C)c1ccc(cc1)CC	2.62
mol374	Clc1ccccc1OCC(=O)Nc1ccc(N(C(=O)C)C)cc1	2.619
mol375	O1C2=C(C(C(C(OCC)=O)=C1N)c1ccc(cc1C)C)C(=O)CC(C2)(C)C	2.618
mol376	O1CCOc2c1cc1c(NC(=O)CC1c1cc(OC)c(OC)c(OC)c1)c2	2.613
mol377	O(C)c1ccc(cc1)CNc1nc2n(n1)C(=O)C=C(N2)C	2.607
mol378	S=C(Nc1cc(ccc1)C)NC(=O)c1ccc(F)cc1	2.606
mol379	Fc1ccc(cc1)CCNCc1cc(OC)c(OC)c(OC)c1	2.604
mol380	O(C)c1ccccc1NC(=O)/C(/NC(=O)c1ccc(cc1)C)=C\c1cccnc1	2.604

mol381	Clc1ccccc1OCC(=O)NC1CCCCCC1	2.602
mol382	Brc1ccc(N2C(=O)c3c(cccc3[N+](=O)[O-])C2=O)cc1	2.602
mol383	S(=O)(=O)(N(CC(=O)N(CC)CC)c1cc([N+](=O)[O-])ccc1)c1ccccc1	2.602
mol384	s1c2c(CCCC2)c(C(=O)N)c1NC(=O)c1cc(OC)c(OC)c(OC)c1	2.599
mol385	S(=O)(=O)(N(CCO)C)c1cc(-c2n3N=C(c4c(-c3nn2)cccc4)C)c(cc1)C	2.599
mol386	Brc1oc(cc1)C(Oc1ccc(cc1)C(=O)CC)=O	2.599
mol387	S=C(NC(=O)c1ccc(cc1)C(C)(C)C)NCC1OCCC1	2.597
mol388	S=C(Nc1cc([N+](=O)[O-])ccc1F)NC(=O)c1cc(OC)ccc1	2.597
mol389	Clc1cc(NC(=O)c2cc([N+](=O)[O-])c(OC)cc2)ccc1C	2.596
mol390	O1c2cc(ccc2OC1)-c1c2CCCCCc2nc(N)c1C#N	2.594
mol391	S=C(Nc1cc([N+](=O)[O-])ccc1F)NC(=O)c1cc(ccc1)C	2.594
mol392	O1c2c(C3=C(CCC3)C1=O)ccc(OCC(OCC=C)=O)c2C	2.593
mol393	S=C(Nc1ccc(OC)cc1OC)NC(=O)c1cc(ccc1)C	2.592
mol394	O1C2=C(C(C(C#N)=C1N)c1cc(O)ccc1)C(Oc1c2cccc1)=O	2.59
mol395	OCCCc1c2c(n(c1)Cc1ccccc1)cccc2	2.589
mol396	O1C2=C(C(C(C(OCC)=O)=C1N)c1ccc(OCCCC)cc1)C(=O)CCC2	2.588
mol397	Clc1nc(nc(n1)NCC=C)NC1CCCCC1	2.583
mol398	Brc1cc(ccc1OCC(=O)NC(C)(C)C)CC	2.582
mol399	Brc1cc(ccc1OCC(=O)Nc1sccn1)CC	2.582
mol400	O(CC(=O)Nc1ccccc1C(=O)N)c1ccccc1C(C)C	2.581
mol401	OC1(c2c(-c3c1cccc3)cccc2)CC#CCN(C(C)C)CCO	2.579
mol402	Fc1ccc(cc1)C(Oc1ccc(cc1)C(=O)CC)=O	2.576
mol403	Brc1cc(Cl)c(OCC(=O)n2nc(cc2C)C)cc1	2.574
mol404	OC1(c2c(N(C)C1=O)cccc2)CC(=O)c1ccc(cc1)C(C)(C)C	2.574
mol405	O=C1N(CC(C1)c1ccccc1)C(=O)c1cc([N+](=O)[O-])ccc1	2.573
mol406	O=C1N(C2N(C)C(=O)N(C2N1C)CCCC)CCCC	2.572
mol407	S1C(C)C(=O)N(CCc2ccccc2)C1c1ccccc1	2.572
mol408	O(CCn1c2c(nc1C)cccc2)c1ccccc1	2.571
mol409	S(C(C(=O)Nc1ccc(S(=O)(=O)N)cc1)C)C=1NC(=O)C=C(N=1)C	2.571
mol410	Clc1ccccc1OCCCCCCN1CCOCC1	2.57
mol411	FC(F)(F)C(=O)c1c2c(n(c1)CC(=O)N1CCCC1)cc(cc2)C(OC)=O	2.569
mol412	s1c2c(CCC2)c(C(OCC)=O)c1NC(=O)CSC1=NC(=O)C(=NN1)C	2.566
mol413	Clc1cc(ccc1OCC=C)C1c2c(OC(N)=C1C#N)cc1OCOc1c2	2.565
mol414	O=C1n2c3c(nc2N(Cc2ccccc2)C(=C1)C)cccc3	2.563
mol415	O=C(NC(C)c1ccccc1)Cn1nc(nn1)-c1ccccc1	2.563
mol416	S=C(Nc1ncccc1)NC(=O)c1ccc(OCC)cc1	2.561
mol417	O=C(n1nc(cc1)C)c1ccc(NC(=O)CC(C)C)cc1	2.56

mol418	O(CC(=O)N(CC)c1ccccc1)c1ccccc1C	2.56
mol419	S=C(Nc1ccc(cc1O)C)NC(=O)c1cc(OC)ccc1	2.555
mol420	Clc1ccccc1OCC(Oc1ccc(Cl)cc1)=O	2.554
mol421	Clc1ccc([N+](=O)[O-])cc1NC(=O)c1oc([N+](=O)[O-])cc1	2.553
mol422	Fc1cc(ccc1)Cn1c2c(nc1NCCO)N(C)C(=O)N(C)C2=O	2.552
mol423	Clc1cc(Cl)ccc1OCCCC(=O)N1CCN(CC1)C	2.55
mol424	O(CC(Oc1ccc(OC)cc1)=O)c1ccccc1C	2.549
mol425	O1c2c(ccc(O)c2)C(C(C#N)=C1N)c1ccc(OCCCC)cc1	2.548
mol426	S1C=2N(CN(C1)c1ccccc1)C(=O)CC(c1ccc(OC)cc1OC)C=2C#N	2.548
mol427	S1C=2N(CN(C1)c1ccccc1)C(=O)CC(c1ccc(OC)cc1OC)C=2C#N	2.548
mol428	S=C(Nc1cc([N+](=O)[O-])ccc1F)NC(=O)c1cc(F)ccc1	2.547
mol429	s1cccc1-c1onc(n1)-c1cc(OC)ccc1	2.547
mol430	s1c2c(nc1NC(=O)CCCCC)cccc2	2.546
mol431	O(CC(=O)N(CC)c1ccccc1)c1ccc(cc1)CC	2.546
mol432	S=C(Nc1cc(ccc1)C(=O)C)NC(=O)COc1cc(ccc1)C	2.545
mol433	O(CC(=O)Nc1ccc(cc1)C(=O)N)c1ccccc1C(CC)C	2.544
mol434	S(=O)(=O)(CCc1nc2c(n1CCC#N)cccc2)c1ccc(cc1)C	2.544
mol435	Fc1ccccc1N1CCN(CC1)Cc1nc2N(C)C(=O)N(C)C(=O)c2n1CCC	2.543
mol436	o1cccc1CNC(=O)c1cc(OCC)c(OCC)c(OCC)c1	2.542
mol437	O(C(=O)c1cc(C)c(-n2c(ccc2C)C)cc1)C	2.54
mol438	S(CCC)c1nc2OC(Nc3c(-c2nn1)cccc3)(C)C	2.539
mol439	S=C(Nc1cc(C)c(cc1)C)NC(=O)c1cc(F)ccc1	2.539
mol440	Clc1cc(OC)c(NC(=S)NC(=O)CC)cc1OC	2.538
mol441	O1CCCC1COC(=O)C1C(C2C(N=C1C)=CC(CC2=O)(C)C)c1cc(O)ccc1	2.538
mol442	O(CC)c1ccc(cc1[N+](=O)[O-])C(=O)NC1CCCC1	2.538
mol443	Clc1ccccc1CNC(=O)C(=O)Nc1ccc(N(C)C)cc1	2.536
mol444	O=C(NC1CCCCC1)C(=O)Nc1c2c(ccc1)cccc2	2.533
mol445	O(CCC)c1nc2N(C)C(=O)N(C)C(=O)c2n1Cc1ccccc1	2.533
mol446	OC(C#CCN(C(C)C)C)(C1CCCC1)c1ccccc1	2.532
mol447	O(C)c1cc(NCC(O)CN2C=3N(c4c2cccc4)C(=O)C=C(C)C=3C#N)ccc1	2.531
mol448	OCCCc1c2c(n(c1)-c1ccccc1)cccc2	2.531
mol449	S(=O)(=O)(N)c1ccc(NC(=O)c2oc([N+](=O)[O-])cc2)cc1	2.529
mol450	Clc1ccc(OC(=O)COc2cc(ccc2)C)cc1	2.528
mol451	Clc1ccccc1NC(=S)NC(=O)c1cc(ccc1)C	2.528
mol452	O=C1N(C)C(=O)N(c2nc(n(c12)CC(=O)c1ccccc1)N1CCN(CC1)CC)C	2.526
mol453	S=C(Nc1ccc(OC)cc1)NC(=O)c1cc(F)ccc1	2.524
mol454	O(C)c1ccc(OC)cc1NC(=O)C1Nc2n(c3c(n2)cccc3)C(=O)C1	2.523

mol455	Clc1cc2C3=C(CCC3)C(Oc2cc1OCC(OCC=C)=O)=O	2.522
mol456	O=C1N(C2N(C)C(=O)N(C2N1C)CCCC)CCCC	2.521
mol457	Fc1ccc(cc1)C1C(=CN(C=C1C(OC)=O)C1CCCC1)C(OC)=O	2.52
mol458	O=C1N(C)C(=O)N(c2ncn(c12)CC(=O)NC(CCCCCC)C)C	2.519
mol459	S(CCOC(=O)c1ccccc1)c1nc(nc(n1)N(C)C)N(C)C	2.516
mol460	O1C2=C(C(C(C(OCC)=O)=C1N)c1ccc(OCCCC)cc1)C(=O)CCC2	2.516
mol461	O=C1N(C)C(=O)N(c2ncn(c12)CC(=O)NC(CCCCCC)C)C	2.515
mol462	S1CCC(=O)N2C1=NC(C)=C(C(OCCOC)=O)C2c1ccc(cc1)C(OC)=O	2.515
mol463	O(CCC)c1nc2N(C)C(=O)N(C)C(=O)c2n1CCC	2.515
mol464	O(C)c1cc(NCC(O)CN2C=3N(c4c2cccc4)C(=O)C=C(C)C=3C#N)ccc1	2.514
mol465	FC(F)(F)C(=O)Nc1ccccc1C(=O)NC1CCCCC1	2.514
mol466	S1C=2N(C(C(C(OC)=O)=C(N=2)C)c2ccc(OC)cc2)C(=O)C1CC	2.512
mol467	S1C=2N(C(C(C(OC)=O)=C(N=2)C)c2ccc(OC)cc2)C(=O)C1CC	2.51
mol468	O1c2c(OCC1C(NCc1cc(OC)c(OC)cc1OC)C)cccc2	2.507
mol469	[NH+]1(CCCCC1)CCCn1c2c(c3c1cccc3)cccc2	2.507
mol470	S=C(N(Cc1ccccc1)C)NC(=O)c1ccc(cc1)C	2.502
mol471	Clc1ccc(cc1)-c1nc(on1)CCC(=O)NCC=C	2.5
mol472	O(C(=O)c1cnc2c(cc(cc2)C(OC)=O)c1Nc1ccc(cc1)C(O)=O)CC	2.499
mol473	O=C1N(N=C2c3c1cccc3-c1c2cccc1)CC(=O)c1ccccc1	2.497
mol474	Clc1cc(cc(OC)c1OC(C)C)\C=C/1\NC(=S)NC\1=O	2.496
mol475	O1c2c(OCC1C(NCc1cc(OC)c(OC)cc1OC)C)cccc2	2.493
mol476	S=C(NC(=O)c1ccc(cc1)C(C)(C)C)NCC1OCCC1	2.492
mol477	O1c2cc(OCC(OCC=C)=O)ccc2C2=C(CCCC2)C1=O	2.492
mol478	O1c2c(cc3OCOc3c2)C(C(C#N)=C1N)c1cc(OC)c(OC)c(OC)c1	2.491
mol479	O=C1N(C)C(=O)N(c2nc(n(c12)CC(C)=C)NCC=C)C	2.49
mol480	S=C(Nc1cccnc1)NC(=O)c1cc(OCC)ccc1	2.488
mol481	Fc1ccccc1CNc1cc(C(OC)=O)c(N2CCOCC2)cc1	2.488
mol482	O=C1CC(Cc2nc3c(cccc3)c(NCC)c12)(C)C	2.487
mol483	S=C(Nc1cc(ccc1)C)NC(=O)Cc1ccc(OC)cc1	2.487
mol484	O1c2c(OC1)cc(cc2OC)CN1CCN(CC1)Cc1cc2OCOc2cc1	2.487
mol485	O=C1N(C2N(C)C(=O)N(C2N1C)CCCC)CCCC	2.484
mol486	s1cccc1C(=O)NC(=S)Nc1cc(ccc1)C#N	2.484
mol487	O=C1N=C(Nc2c1cccc2)Nc1nc(c2c(n1)c(ccc2)C)C	2.484
mol488	S(CCO)c1nc2N(C)C(=O)N(C)C(=O)c2n1Cc1ccc(F)cc1	2.482
mol489	S1CCC(=O)N2C1=NC(C)=C(C(OCCOC)=O)C2c1cc(OC)c(OC)cc1	2.482

mol490	Clc1cc(ccc1OCC=C)C1c2c(OC(N)=C1C#N)cc1OCOc1c2	2.479
mol491	S(CC#CCO)c1oc(nn1)-c1ccc(cc1)C	2.478
mol492	S=C(NC(=O)c1ccccc1)N1CCc2c1cccc2	2.477
mol493	Clc1ccccc1CNc1nc2n(n1)C(=CC(=N2)C)C	2.477
mol494	S=C(Nc1ccc(F)cc1)NC(=O)c1cc(F)ccc1	2.476
mol495	Clc1cc(ccc1Cl)C1c2c(OC(N)=C1C#N)cc(N)cc2	2.475
mol496	Clc1cc(Cl)ccc1C(=O)NC(=S)Nc1ncccc1C	2.471
mol497	O1CCCC1COC(=O)C=1C(C2C(=NC=1C)CC(CC2=O)(C)C)c1cccnc1	2.47
mol498	Clc1cc(ccc1)C(=O)NC(=S)Nc1ccccc1OC	2.463
mol499	O1c2cc(OCC)ccc2C2=C(CCCC2)C1=O	2.462
mol500	n1c(nc(nc1Nc1ccccc1)-n1nccc1)Nc1ccccc1	2.462
mol501	S(CC(=O)Nc1ncccc1)c1oc(nn1)-c1ccoc1C	2.461
mol502	O=C1N(C)C(=O)N(c2nc(n(c12)CCOCC)CN1CCN(CC1)c1ccccc1)C	2.461
mol503	S(CC#C)c1nc(c2cc(ccc2n1)C)C	2.46
mol504	S=C(Nc1ccccc1F)NC(=O)COc1ccccc1C	2.459
mol505	Clc1cc(ccc1C(=O)NC(=S)NC1CCCC1)C	2.458
mol506	O1CCN(CC1)CC(OC(=O)C1c2c(Oc3c1cccc3)cccc2)C	2.456
mol507	o1c2ncnc(NCCO)c2c(c1-c1ccc(OC)cc1)-c1ccc(OC)cc1	2.455
mol508	s1cccc1C(=O)NC(=S)N1CCCc2c1cccc2	2.455
mol509	O(C(=O)COc1ccccc1C)c1ccccc1[N+](=O)[O-]	2.455
mol510	O(CCOC(=O)C1C(C2=C(N=C1C)CCCC2=O)c1ccncc1)c1ccccc1	2.454
mol511	O1C(=CC=2OC(N)=C(C#N)C(C=2C1=O)c1cc(OC)c2OCOc2c1)C	2.454
mol512	O1c2n[nH]c(c2C(C(C#N)=C1N)c1c(C)c(cc(C)c1C)C)C	2.452
mol513	Clc1cc(NC(=O)C(=O)NC2CCCC2)ccc1Cl	2.451
mol514	O(C(=O)C=1Nc2n(nnn2)C(C=1C(=O)C)c1ccc(cc1)C(C)C)C	2.451
mol515	Clc1cc(NC(=O)C(=O)NCc2ccccc2)ccc1Cl	2.451
mol516	O(c1ccc(cc1)C(OC)=O)c1nc(nc(n1)NC(C)(C)C)N(C)C	2.451
mol517	S(CCOc1ccc(cc1)C)C=1NC(=O)c2c(N=1)cccc2	2.451
mol518	O1c2c(ccc(O)c2)C(C(C#N)=C1N)c1ccc(OCCCC)cc1	2.448
mol519	S=C(Nc1cc([N+](=O)[O-])c(F)cc1)NC(=O)c1cc(ccc1)C	2.448
mol520	Clc1ccc(cc1)C(=O)NC=1Oc2c(cccc2)C(=O)C=1	2.446
mol521	s1c2c(nc1SCC(OCC#C)=O)cccc2	2.44
mol522	s1cc(nc1N)C(CCC(OC)=O)(CCC)C(OCC)=O	2.44
mol523	S1C=2N(C(C(C(OC)=O)=C(N=2)C)c2ccc(OC)cc2)C(=O)C1CC	2.439
mol524	O(C(=O)COc1cc(ccc1)C)c1ccccc1[N+](=O)[O-]	2.437
mol525	S(CC=C)c1nc2[nH]c3c(cc(cc3)C)c2nn1	2.436
mol526	S1CCC(=O)N2C1=NC(C)=C(C(OCCOC)=O)C2c1cc(OC)c(OC)cc1	2.434

mol527	S(=O)(=O)(NCc1cc2OCOc2cc1)c1c2ncccc2ccc1	2.433
mol528	S=C(N1CCCC1)c1ccc(OCC(C)C)cc1	2.433
mol529	O1CCOc2c1cc(cc2)C(NC(=O)Cc1ccccc1)C	2.432
mol530	S=C(Nc1cc(ccc1)C(=O)C)NC(=O)C1CCCCC1	2.43
mol531	O=C1CC(Cc2nc(nc(c12)C)N1CCN(CC1)C(OCC)=O)C	2.429
mol532	Clc1ccc(SCC=2N=C(NC(=O)C=2)N2CCCCC2)cc1	2.427
mol533	Brc1cc(ccc1OC)C(=O)n1nnc2c1cccc2	2.427
mol534	S(=O)(=O)(N1CCN(CC1)C(=S)NCC=C)c1ccc(cc1)C	2.426
mol535	O1c2c(cc3OCOc3c2)C(C(C#N)=C1N)c1cc(OC)c(OC)cc1	2.424
mol536	Clc1cc(ccc1)C(=O)N(CC1=Cc2cc(ccc2NC1=O)C)CCOC	2.422
mol537	Clc1ccc(cc1)\C=C/1\C(=O)N(NC\1=O)c1ccc(Cl)cc1	2.422
mol538	O=C(NC(C)c1ccc(cc1C)C)Cc1ccccc1	2.416
mol539	Brc1ccc(cc1)Cn1c2c(nc1NCCO)N(C)C(=O)N(C)C2=O	2.415
mol540	O(CCOC(=O)C)c1nc(nc(n1)NCC)NC(C)C	2.414
mol541	FC(F)(F)C(=O)c1c2c(n(CC(=O)NCC3OCCC3)c1C)cccc2	2.414
mol542	Clc1cc(Cl)ccc1C(=O)NC(=S)N1CCCCCC1	2.411
mol543	FC(F)C=1n2ncc(c2N=C(C=1)c1ccccc1)C(=O)NCC=C	2.411
mol544	S=C(Nc1ccc(cc1)C(=O)C)Nc1ccc(F)cc1	2.411
mol545	o1cccc1C(=O)NC(C)c1ccc(OC)cc1	2.411
mol546	S1C=2N(C(C(C(OC)=O)=C(N=2)C)c2ccc(OC)cc2)C(=O)C1CC	2.41
mol547	O1c2c(OCC1C(NCc1cc(OC)c(OC)cc1OC)C)cccc2	2.407
mol548	S(=O)(=O)(N1CCc2c(C1)cccc2)c1cc(C)c(F)cc1	2.406
mol549	s1cccc1C1C2C(=NC(=C)C1C(OCC1OCCC1)=O)CCCC2=O	2.405
mol550	OCCN1CCN(CC1)Cc1nc2c(n1CCC)cccc2	2.405
mol551	s1c2c(nc1-c1cc(OC)ccc1)cccc2	2.403
mol552	S1CCC(=O)N2C1=NC(C)=C(C(OCC=C)=O)C2c1ccccc1F	2.401
mol553	s1cccc1C1C2C(=NC(=C)C1C(OCC1OCCC1)=O)CCCC2=O	2.401
mol554	Clc1ccccc1OCC(=O)Nc1cccc([N+](=O)[O-])c1C	2.4
mol555	Clc1cc(NC(=O)C(=O)NCCc2ccccc2)ccc1	2.399
mol556	Fc1ccc(cc1)C1C2=C(OC(N)=C1C(OCCOC)=O)CC(CC2=O)(C)C	2.398
mol557	Clc1ccc(cc1)Cn1c2c(nc1NCCC)N(C)C(=O)NC2=O	2.397
mol558	O(C)c1ccc(OC)cc1CNc1cc([N+](=O)[O-])ccc1OC	2.395
mol559	S1CCC(=O)N2C1=NC(C)=C(C(OCCOC)=O)C2c1ccc(OCC)cc1	2.395
mol560	Ic1ccc(NC(=S)NC(=O)CCC)cc1	2.394
mol561	Brc1ccc(cc1)C1C2=C(OC(N)=C1C#N)CC(CC2=O)C	2.394
mol562	s1cccc1C1CC(=O)c2c(n(nc2)-c2nc(cc(n2)C)C)C1	2.39
mol563	O(C(C)(C)C)C(=O)N1CCCC1C(=O)Nc1cc(C)c(cc1)C	2.388
mol564	Clc1cc(NC(=O)C(=O)NCC(C)C)ccc1Cl	2.388
mol565	s1cccc1C1CC(=O)c2c(n(nc2)-c2nc(cc(n2)C)C)C1	2.387
mol566	Brc1cc(ccc1OC)C(=O)n1c2c(nc1)cccc2	2.384

mol567	Clc1cc(NC(=S)NC(=O)CCC)c(cc1)C	2.382
mol568	O=Cc1c2c(n(c1)CC(=O)N1CCc3c1cccc3)cccc2	2.381
mol569	O1c2c(cc3OCOc3c2)C(C(C#N)=C1N)c1cc(OC)c(OC)cc1	2.379
mol570	Clc1cc(OC)c(S(=O)(=O)N2CCC(CC2)C)cc1OC	2.378
mol571	Clc1ccc(cc1)C(=O)N1CCNC(=O)C1CC(=O)Nc1ccc(OCC)cc1	2.377
mol572	O=C(C)c1n2-c3c(N(c2nc1C)CCCC)cccc3	2.376
mol573	O(CC(=O)Nc1c2c(nccc2)ccc1)c1ccc(cc1)CC	2.376
mol574	Clc1cc(ccc1)C(=O)NC(=S)Nc1ccccc1F	2.375
mol575	Clc1c2c(sc1C(OCCCN(C)C)=O)cccc2	2.375
mol576	S=C(NC(=O)c1ccc(cc1)C(C)(C)C)N1CCCC1	2.373
mol577	Ic1cc(ccc1C)C(=O)NC1CCCCC1	2.373
mol578	O=C1CC(Cc2nc(ncc12)Nc1cc(ccc1)C)C	2.372
mol579	s1cc(nc1N)C(CCC(OC)=O)(CCC)C(OCC)=O	2.372
mol580	S1c2n(N=C1c1ccccc1)c(nn2)C(C)C	2.371
mol581	S(C(C)C)c1nnnn1-c1c(cc(cc1C)C)C	2.371
mol582	Clc1cc(cc(OC)c1O)C1NC(=O)N(C)C(C)=C1C(OCCOCC)=O	2.368
mol583	O=C1N(C)C(=O)N(c2nc(n(c12)CCOC)CN1CCN(CC1)c1ccccc1)C	2.367
mol584	O(C)c1ccccc1\C=C/1\C(=O)N(c2ccccc2)C(=O)NC\1=O	2.365
mol585	S=C(Nc1cc([N+](=O)[O-])ccc1)NC(=O)COc1ccccc1	2.364
mol586	O1c2cc(ccc2OC1)CN1CCN(CC1)C(=O)c1ccc([N+](=O)[O-])cc1	2.364
mol587	Clc1ccc([N+](=O)[O-])cc1\C=N\\N1C(=CC(=CC1=O)C)C	2.363
mol588	S(CCOc1ccc(cc1C(C)C)C)c1nc(N)cc(n1)N	2.362
mol589	Brc1cc(OCC)c(OCC)cc1C(NC(=O)C)C	2.356
mol590	FC(F)(F)C(=O)c1c2c(n(CC(=O)N3CCOCC3)c1C)cccc2	2.356
mol591	O=C1N=C(NC(C1)C(=O)Nc1ccc(cc1)C)Nc1ccc(cc1)CC	2.355
mol592	S(CCO)c1nc2c(n1CCC)cccc2	2.354
mol593	Brc1cc(ccc1C)C(Oc1ccccc1[N+](=O)[O-])=O	2.352
mol594	O=C1N(c2cccc([N+](=O)[O-])c2C)C(=O)c2c1cccc2	2.352
mol595	Clc1ccc(cc1)C(=O)CC1OC(=O)c2c1ccc(OC)c2OC	2.352
mol596	o1c2c(cc(cc2)COCC)cc1C(OCCN(CC)CC)=O	2.352
mol597	O(CCn1c2c(nc1CCCO)cccc2)c1ccccc1	2.351
mol598	O=C1CC(Cc2nc(ncc12)Nc1cc(ccc1)C)C	2.35
mol599	FC(F)(F)C(=O)c1c2c(n(CC(=O)NCC3OCCC3)c1C)cccc2	2.35
mol600	S1CCC(=O)N2C1=NC(C)=C(C(OCC=C)=O)C2c1ccccc1F	2.35
mol601	Clc1cc(NC(=S)NC(=O)CC(C)C)c(O)cc1	2.349
mol602	S(CCOc1cc(OC)ccc1)C=1NC(=O)c2c(N=1)cccc2	2.349
mol603	O1c2c(OCC1C(NCc1cc(OC)c(OC)cc1OC)C)cccc2	2.347
mol604	S=C(NC(=O)c1cc(ccc1)C)NCc1ccccc1	2.345
mol605	OCCCN1c2n(C=C1C(C)(C)C)c1c(n2)cccc1	2.345
mol606	Clc1ccc(cc1)\C=C\1/C(=O)N(NC/1=O)c1ccc(Cl)cc1	2.344

mol607	S(=O)(=O)(NC)c1cc(-c2n3N=C(c4c(-c3nn2)cccc4)C)c(cc1)C	2.343
mol608	Clc1cc2nnn(S(=O)(=O)c3cc(OC)c(OC)cc3)c2cc1	2.339
mol609	S1CCC(=O)N2C1=NC(C)=C(C(OCC=C)=O)C2c1ccccc1	2.338
mol610	Brc1ccc(cc1)C1C2=C(OC(N)=C1C#N)CC(CC2=O)C	2.334
mol611	O=C1CC(Cc2nc(nc(c12)C)N1CCN(CC1)C(OCC)=O)C	2.334
mol612	O=C(NCCC=1CCCCC=1)CCc1ccccc1	2.333
mol613	Clc1ccccc1OCC(=O)Nc1cc([N+](=O)[O-])ccc1F	2.332
mol614	S(CC(=O)NCC=C)c1nc(cc(n1)C(F)(F)F)-c1occc1	2.331
mol615	s1cccc1C(=O)NC(=S)Nc1ccccc1OCC	2.331
mol616	S1CCC(=O)N2C1=NC(C)=C(C(OCCOC)=O)C2c1ccc(OC)cc1	2.331
mol617	Clc1cc2c(OC(=O)C=C2C)cc1OCCC	2.33
mol618	Clc1cccc(NC(=O)c2ccc(F)cc2)c1N1CCOCC1	2.33
mol619	O1C(C)=C(C(OC(C)(C)C)=O)C2(c3c(NC2=O)cccc3)C(C#N)=C1N	2.329
mol620	O(C)c1ccc([N+](=O)[O-])cc1NC(=O)Nc1ccccc1	2.328
mol621	Clc1cc(OC)c(OC)cc1C1c2c(OC(N)=C1C#N)cc1OCOc1c2	2.326
mol622	Ic1cc(C)c(NC(=S)NC(=O)CC)cc1	2.325
mol623	Brc1cc(Cl)c(OCC(=O)Nc2sccn2)cc1	2.324
mol624	O1c2c(cc3OCOc3c2)C(C(C#N)=C1N)c1cc(OC)c(OC)c(OC)c1	2.32
mol625	O(CC)c1ccccc1CNc1ccc(O)cc1	2.319
mol626	O=C1N(N=C(c2c1cccc2)c1ccc(cc1)C(=O)N(C)C1CCCCC1)C	2.317
mol627	S1CCN2C1=NC1=C(C3(CCCCC3)Cc3c1cccc3)C2=O	2.317
mol628	ClC=1C(=Nc2n(nc(n2)NCc2ccccc2F)C=1C)C	2.316
mol629	Clc1cc(C(=O)NC(=S)Nc2ncccc2C)c(OC)cc1	2.316
mol630	OC1(c2cc(ccc2NC1=O)C)CC(=O)c1ccc(cc1)CC	2.315
mol631	O1CCOc2c1cc1c(NC(=O)CC1c1ccc(OC)c(OC)c1OC)c2	2.315
mol632	O(C)c1cc(ccc1OC)C(=O)CC1(O)c2cc(OC)ccc2NC1=O	2.315
mol633	Clc1cc(cc(OC)c1O)C1NC(=O)N(C)C(C)=C1C(OCCSCC)=O	2.314
mol634	S1CCC(=O)N2C1=NC(C)=C(C(OCC)=O)C2c1ccc(cc1)C(OC)=O	2.314
mol635	O=C1N(C)C(=O)N(c2nc(n(c12)CCC)NCCC)C	2.312
mol636	O=C(NCC=C)C1C2c3c(C(C1)c1c2cccc1)cccc3	2.312
mol637	FC(F)(F)c1cc(NC(=O)C(=O)NC2CCCCC2)ccc1	2.312
mol638	s1cc(nc1NC(=O)CN1c2c(OC1=O)cccc2)-c1ccccc1	2.311
mol639	O1c2cc(OCC(OCC)=O)ccc2C2=C(CCCC2)C1=O	2.31
mol640	s1c(C)c(C)c(C(=O)N)c1NC(=S)NC(=O)c1ccccc1	2.309
mol641	S=C(Nc1ccccc1OC)NC(=O)c1cc(ccc1)C	2.308
mol642	O(C(=O)CCc1ccccc1)c1ccccc1[N+](=O)[O-]	2.306
mol643	FC(F)(F)C(=O)c1c2c(n(CC(OCC)=O)c1C)cccc2	2.304
mol644	s1c2CC(CCc2nc1NC(=O)C)c1ccccc1	2.304
mol645	Clc1cc2OCOc2cc1C1C2C(=NC(=C)C1C(OCC=C)=O)CCCC	2.303

	2=O	
mol646	S1c2n(N=C1c1occc1)c(nn2)C(C)C	2.299
mol647	S1\C(=C\c2ccccc2)\C(=O)N(c2cc(O)ccc2)C1=S	2.299
mol648	s1cccc1CNC(=O)CSc1nnc(n1-c1ccccc1)C	2.299
mol649	OC(C#CCN(C(C)C)C)(C1CCCC1)c1ccccc1	2.297
mol650	O1CCN(CC1)c1ccc(NCc2ccccc2)cc1C(OC)=O	2.297
mol651	S=C(Nc1ccccc1O)NC(=O)c1cc(ccc1)C	2.296
mol652	Clc1cc(NC(=O)C(=O)NC2CCCCC2)ccc1	2.296
mol653	s1c(nnc1SCC(=O)Nc1sc2c(CCC2)c1C(=O)N)C	2.294
mol654	Clc1cc(OC)c(NS(=O)(=O)c2ccc(OC)cc2)cc1OC	2.294
mol655	s1cccc1C(=O)NC(=S)NCCC=1CCCCC=1	2.293
mol656	S1CCC(=O)N2C1=NC(C)=C(C(OCC=C)=O)C2c1cc(F)ccc1	2.293
mol657	s1cc(nc1NCC=C)-c1ccc(F)cc1F	2.293
mol658	O=C(NCc1ccncc1)c1ccc(cc1)-c1ccccc1	2.293
mol659	s1c(nnc1SCC)NC(=O)CSc1ncccn1	2.288
mol660	O(C)c1cc(ccc1OC)C(=O)CC1(O)c2cc(OC)ccc2NC1=O	2.284
mol661	Brc1cc(Cl)ccc1OC(=O)c1occc1	2.282
mol662	S1C=2N(C(C(C(OCC)=O)=C(N=2)C)c2ccc(F)cc2)C(=O)C1C	2.279
mol663	O(CC(O)Cn1c2c(nc1NCCO)N(C)C(=O)N(C)C2=O)c1ccccc1C	2.276
mol664	S1\C(=C/2\c3c(NC\2=O)cccc3)\C(=O)N(NC(=O)Cc2ccccc2)C1=S	2.276
mol665	S1c2c(N(CC(=O)Nc3cc4OCCOc4cc3)C1=O)cccc2	2.274
mol666	O1CCN(CC1)CC(OC(=O)C1c2c(Oc3c1cccc3)cccc2)C	2.273
mol667	O=C1Nc2n(c3c(n2)cccc3)C(C1)C(=O)Nc1ccc(cc1C)C	2.273
mol668	O=C1N(CCCCCC(OC)=O)C(=O)c2c1cccc2	2.273
mol669	o1c(ccc1C)-c1c2CCCCCc2nc(N)c1C#N	2.273
mol670	s1cccc1C1C2=C(N=C(C)C1C(OCC1OCCC1)=O)CCCC2=O	2.272
mol671	Brc1cc(ccc1OC)C(=O)NC(=S)N(CC)CC	2.271
mol672	O1CCCC1COC(=O)C1C(C2=C(N=C1C)CC(CC2=O)(C)C)c1cccnc1	2.27
mol673	s1c2CCCCc2c2c1ncnc2N1CC(OC(C1)C)C	2.268
mol674	S1C=2N(C(C(C(OCC)=O)=C(N=2)C)c2ccccc2)C(=O)C1C	2.268
mol675	O=C(Nc1c2c(ccc1)cccc2)C(=O)NCc1ccccc1	2.268
mol676	O(C)c1cc(OC)c(OC)cc1C1CC(=O)Nc2c1cc(OC)c(OC)c2	2.267
mol677	O(C)c1cc(OC)c(OC)cc1C1CC(=O)Nc2c1cc(OC)c(OC)c2	2.265
mol678	S(Cc1[nH+]c2c([nH]1)cccc2)c1[nH+]c2c([nH]1)cccc2	2.265
mol679	O1CCCC1COC(=O)C1C(C2=C(N=C1C)CC(CC2=O)(C)C)c1cccnc1	2.265
mol680	s1nnc2cc(NC(=O)NCCC)ccc12	2.264
mol681	S1C=2N(C(C(C(OCC)=O)=C(N=2)C)c2ccc(F)cc2)C(=O)C1C	2.263
mol682	Clc1cc(cc(OC)c1O)C1NC(=O)N(C)C(C)=C1C(OCCSCC)=O	2.261
mol683	O(CC(=O)Nc1c2c(nccc2)ccc1)c1ccc(cc1C)C	2.261

mol684	n1n(cc(Cc2cn(nc2C)CC=C)c1C)CC=C	2.261
mol685	S1C=2N(C(C(C(OCC)=O)=C(N=2)C)c2ccc(F)cc2)C(=O)C1C	2.259
mol686	Clc1ccc(cc1)C(=O)N1CCNC(=O)C1CC(=O)Nc1ccc(OCC)cc1	2.258
mol687	S(=O)(=O)(N1CCOCC1)c1ccc(OCCCC)cc1	2.258
mol688	S(=O)(=O)(Nc1nc(ccn1)C)c1ccc(N2C(=O)C3C(CCCC3)C2=O)cc1	2.257
mol689	O=C1N(C)C(=O)N(c2nc(n(c12)CCC)NCC=C)C	2.254
mol690	Fc1cc(ccc1)C1C2C(N=C(C)C1C(OCC=C)=O)=CCCC2=O	2.251
mol691	S=C(N(CC)CC)NC(=O)c1cc(OC)c(OC)c(OC)c1	2.25
mol692	O=C(NCC=C)C1C2c3c(C(C1)c1c2cccc1)cccc3	2.25
mol693	O1c2c(C=C(C(=O)N3CCCCC3)C1=O)cccc2CC=C	2.25
mol694	S1C=2N(C(C(C(OCC)=O)=C(N=2)C)c2ccccc2)C(=O)C1C	2.249
mol695	S1C=2N(C(C(C(OCC)=O)=C(N=2)C)c2ccccc2)C(=O)C1C	2.245
mol696	s1c2CCCCc2c2c1nc(nc2N1CC[NH+](CC1)C)C	2.244
mol697	O(CC)c1ccc2c(cccc2)c1CNc1nnnn1C	2.244
mol698	S(C)c1nc([nH]n1)NCc1ccc(cc1)C	2.244
mol699	Brc1ccc(cc1[N+](=O)[O-])C=1OC(=O)c2c(N=1)cccc2	2.243
mol700	O(CCOC(=O)C1C(C2C(N=C1C)=CCCC2=O)c1ccncc1)c1ccccc1	2.235
mol701	O(Cc1cc(ccc1)C)c1ccc(cc1OC)CNc1[nH]ncn1	2.234
mol702	S1c2c(N(c3c1cccc3)C(=O)CN1CCN(CC1)C(OCC)=O)cccc2	2.234
mol703	S1CCC(=O)N2C1=NC(C)=C(C(OCC=C)=O)C2c1ccc(cc1)C(OC)=O	2.233
mol704	O(CC)c1ccc2c(cccc2)c1CNc1nnnn1CC	2.233
mol705	S(C)c1cc(OC)c(cc1)C(=O)NCCNC(=O)c1nonc1N	2.233
mol706	O=C1N(c2c3c1cccc3ccc2)CC(=O)N(Cc1ccccc1)C	2.233
mol707	O=C(NC1CCCC1)C(=O)Nc1c2c(ccc1)cccc2	2.232
mol708	S1CCC(=O)N2C1=NC(C)=C(C(OCCOC)=O)C2c1ccc(OCCC)cc1	2.23
mol709	Ic1cc(ccc1C)C(=O)Nc1sccn1	2.23
mol710	O1CCCC1CNC(=O)C(=O)Nc1cc(OC)ccc1OC	2.229
mol711	O1c2c(ccc(O)c2)C(C(C#N)=C1N)c1ccc(OCC#C)cc1	2.229
mol712	S1CCC(=O)N2C1=NC(C)=C(C(OCC=C)=O)C2c1ccccc1	2.229
mol713	O1c2cc(ccc2OC1)\C=C/1\N=C(NC\1=O)c1ccccc1	2.228
mol714	o1nc(nc1CCC(=O)NC)-c1cc(OCC)c(OC)cc1	2.227
mol715	S=C(Nc1cccnc1)NC(=O)c1cc(OC)ccc1	2.226
mol716	Fc1cc(ccc1)C1C2=C(N=C(C)C1C(OCC=C)=O)CCCC2=O	2.225
mol717	O1CCN(CC1)c1ccc(NCc2ccccc2C)cc1	2.224
mol718	Brc1oc(cc1)C(=O)N(CC)c1ccccc1	2.224
mol719	Clc1cc(OC)c(OC)cc1C1c2c(OC(N)=C1C#N)cc1OCOc1c2	2.223
mol720	Brc1cc(cc(OC)c1O)C1NC(=O)N(C)C(C)=C1C(OCCC)=O	2.223
mol721	s1cccc1C(=O)NC(=S)N(Cc1ccccc1)C	2.221

mol722	S(=O)(=O)(NCCSCc1occc1)c1ccc(OC)cc1	2.221
mol723	Clc1ccccc1OCC(=O)Nc1ccsc1C(OC)=O	2.221
mol724	Clc1sc(S(=O)(=O)NC(C)c2ccccc2)cc1	2.217
mol725	Brc1ccc(OCC(=O)NCc2sccc2)cc1	2.216
mol726	Brc1ccc(cc1)C(=O)NCCNC(=O)c1nonc1N	2.212
mol727	Clc1ccc(NC(=O)C(=O)NC2CCCCC2)cc1	2.212
mol728	O(CC=C)c1nc(nc2c1cccc2)-c1ccncc1	2.211
mol729	n1ccn(CCn2ccnc2CCCC)c1CCCC	2.211
mol730	S1CCC(=O)N2C1=NC(C)=C(C(OCCOC)=O)C2c1ccc(OC)cc1	2.209
mol731	O(CC(O)Cn1c2c(nc1NCCO)N(C)C(=O)N(C)C2=O)c1ccccc1C	2.207
mol732	S=C(NC(=O)c1occc1)N1CCCc2c1cccc2	2.205
mol733	O(C(=O)COc1ccc(cc1)C)c1ccccc1[N+](=O)[O-]	2.205
mol734	S1C=2N(C(C(C(OCC)=O)=C(N=2)C)c2ccc(F)cc2)C(=O)C1C	2.205
mol735	S(CCOC(=O)C=1C(NC(=O)N(C)C=1C)c1cc2OCOc2cc1)CC	2.201
mol736	Clc1ccc(S(=O)(=O)NCCSCc2occc2)cc1	2.201
mol737	Clc1cc(C(=O)NC(=S)Nc2ncccc2)c(OC)cc1	2.2
mol738	O=C1N(\N=C\c2ccc([N+](=O)[O-])cc2)C(=CC(=C1)C)C	2.196
mol739	Clc1cc(Cl)cc(Cl)c1NC(=S)NC(=O)CC	2.195
mol740	S(CC(=O)NCCOC)c1nc(cc(n1)C(F)(F)F)-c1occc1	2.19
mol741	O=C(Nc1cc(ccc1C)C)C(=O)NCCCC	2.189
mol742	Clc1ccc(cc1)Cn1c2c(nc1N1CCN(CC1)CC)N(C)C(=O)NC2=O	2.189
mol743	o1c2c(cc(OCC(OCC)=O)cc2)c(C(OCCOC)=O)c1C	2.188
mol744	S1C=2N(C(C(C(OCC)=O)=C(N=2)C)c2ccccc2)C(=O)C1C	2.188
mol745	o1cccc1C(=O)Nc1cc(ccc1)CC	2.188
mol746	O(CCO)c1ccc(cc1OC)C1C2C(N=C(C)C1C#N)=CC(CC2=O)(C)C	2.188
mol747	FC(F)(F)c1cc(NC(=O)c2cccnc2NCCO)ccc1	2.187
mol748	Clc1cc(NC(=O)C(=O)NC(C)C)ccc1Cl	2.187
mol749	OCCNc1nc(c2cc(ccc2n1)C)-c1ccccc1	2.187
mol750	Clc1ccc(cc1)C(=O)NCCNC(=O)c1nonc1N	2.187
mol751	O(C(=O)C=1Nc2n(nnn2)C(C=1C(=O)C)c1ccc(cc1)CC)C	2.185
mol752	O(C)c1ccccc1-c1c2n(nc1C)C(=CC(=N2)C)C	2.185
mol753	s1c2CCCCc2c2c1ncnc2N1CCCCC1	2.184
mol754	s1c(nnc1NC(=O)CSc1oc2c(n1)cccc2)C	2.184
mol755	Brc1cc(cc(OC)c1O)C1NC(=O)N(C)C(C)=C1C(OCCC)=O	2.184
mol756	O(CCNCC(O)Cn1c2c(c3c1cccc3)cccc2)C	2.184
mol757	O(C(CCN1CCCCC1)(C#C)c1ccccc1)C	2.184
mol758	Brc1cc(cc(OC)c1O)C1NC(=O)NC(C)=C1C(OC\C=C\C)=O	2.183
mol759	S=C(Nc1cc([N+](=O)[O-])ccc1)NC(=O)c1cc(F)ccc1	2.183
mol760	Fc1ccc(cc1)Cn1c2c(nc1NCCC)N(C)C(=O)NC2=O	2.18

mol761	S(=O)(=O)(NC1CCN(CC1)Cc1ccccc1)c1cc2OC(=O)N(c2cc1)C	2.179
mol762	Brc1cc(cnc1)C(=O)c1ccc(cc1)CC	2.178
mol763	O=C(Nc1cccc([N+](=O)[O-])c1C)Nc1ccccc1	2.178
mol764	O(CCNCC(O)Cn1c2c(c3c1cccc3)cccc2)C	2.177
mol765	O=C1CC(Cc2nc(nc(c12)C)N1CCN(CC1)CC)C	2.175
mol766	O=C1NC(=O)N(c2nc(n(c12)CCc1ccccc1)N1CCN(CC1)CC)C	2.175
mol767	O1CCN(CC1)CCCCCOc1ccccc1C	2.173
mol768	Fc1ccc(cc1)CCNCc1cc(OC)c2OCOc2c1	2.172
mol769	FC(F)(F)C(Oc1nc(nc(n1)NCC=C)N1CCOCC1)C(F)(F)F	2.171
mol770	Clc1ccc(cc1)C1N2C(SC(C)C2=O)=NC(C)=C1C(OC)=O	2.171
mol771	O(C)c1ccccc1C(=O)Nc1cccc(C)c1C	2.17
mol772	O=C1N(CC(=O)NC(CC(C)C)C(OC)=O)C(=O)c2c1cccc2	2.169
mol773	S=C(NCc1ccccc1)NC(=O)Cc1ccccc1	2.168
mol774	S1CCC(=O)N2C1=NC(C)=C(C(OCC=C)=O)C2c1cc(F)ccc1	2.168
mol775	S1CCC(=O)N2C1=NC(C)=C(C(OCCOC)=O)C2c1ccc(cc1)CC	2.166
mol776	O=C1CCCc2c1n(c1c2cc(cc1)C)CCC#N	2.165
mol777	S=C(Nc1ccc(F)cc1F)NC(=O)c1ccccc1F	2.164
mol778	S1c2c(N(c3c1cccc3)CC(O)CNCCCO)cccc2	2.162
mol779	S1C2(NN=C1c1ccccc1)c1c(NC2=O)c(ccc1)C	2.162
mol780	s1cccc1CNC=1CC(CC(=O)C=1)(C)C	2.162
mol781	Brc1cc(Cl)c(OC(=O)c2occc2)cc1	2.162
mol782	S(CCOC(=O)C=1C(NC(=O)N(C)C=1C)c1cc2OCOc2cc1)CC	2.16
mol783	Clc1ccc(cc1)C(NC(=O)c1occc1)C	2.16
mol784	O(C)c1ccc(OC)cc1NC(=O)C1Nc2n(c3c(n2)cccc3)C(=O)C1	2.158
mol785	n12nc(cc1N=C(C=C2N)C(C)(C)C)C(C)(C)C	2.156
mol786	Clc1ccccc1C1N2C(SCCC2=O)=NC(C)=C1C(OCCOC)=O	2.156
mol787	Brc1ccc(nc1C)NC(=O)c1ccc(F)cc1	2.156
mol788	Brc1ccc(NC(=O)CSc2sc(nn2)C)cc1	2.155
mol789	O=C1N(N=C2c3c1cccc3-c1c2cccc1)CCN1CCCCC1	2.155
mol790	O1CCCC1C(Oc1cc2c(NC(C=C2C)(C)C)cc1)=O	2.151
mol791	O=C(NC1CCCCC1)C(=O)Nc1cc(C)c(cc1)C	2.151
mol792	S1c2n(N=C1COc1ccccc1)c(nn2)C(F)(F)F	2.15
mol793	O1c2cc(ccc2OC1)CN1CCN(CC1)Cc1cc(OC)c(OC)c(OC)c1	2.148
mol794	[NH+]1(CCCC1)Cc1cc2c3c(n(c2cc1)CC)cccc3	2.148
mol795	n1n(cc(Cc2cn(nc2C)CCC)c1C)CCC	2.147
mol796	O1C=2N=CNC(=O)C=2C(C(C#N)=C1N)c1cc(OC)c(OCCC)cc1	2.143
mol797	O(C(=O)COc1ccccc1OC)c1ccccc1[N+](=O)[O-]	2.141
mol798	Clc1ccc(NC(=O)CC2Sc3c(NC2=O)cccc3)cc1	2.141
mol799	Fc1cc(ccc1)C(=O)Nc1c2c(nccc2)ccc1	2.14
mol800	Brc1cc(Cl)ccc1OCC(=O)Nc1sccn1	2.14

mol801	S(CC(OCCC)=O)c1nc(cc(C)c1C#N)C	2.14
mol802	O1CCN(CC1)CCCOc1ccc(cc1)C(C)(C)C	2.139
mol803	Clc1cc(Cl)ccc1NC(=S)NC(=O)C1CC1	2.138
mol804	s1c2CCCCc2c2c1ncnc2N1CC(OC(C1)C)C	2.138
mol805	O1C=2N=CNC(=O)C=2C(C(C#N)=C1N)c1cc(OC)c(OCCC)cc1	2.138
mol806	O1c2c(ccc(O)c2)C(C(C#N)=C1N)c1ccc(OCC#C)cc1	2.137
mol807	s1c2CCCCc2nc1NS(=O)(=O)c1ccc(OC)cc1	2.137
mol808	Clc1cnn(C)c1C(=O)NCCSc1nc(cc(n1)C)C(F)(F)F	2.135
mol809	[NH+]1(CCN(CC1)c1ccccc1)Cc1ccccc1	2.134
mol810	O1c2cc(OCC(OCC=C)=O)ccc2C2=C(CCC2)C1=O	2.134
mol811	O(C)c1cc(OC)c(OC)cc1CNCc1cc(OC)c(OC)cc1	2.133
mol812	S=C(Nc1ccccc1OC)NC(=O)c1cc(F)ccc1	2.132
mol813	Clc1ccc(cc1)C1N2C(SC(C)C2=O)=NC(C)=C1C(OC)=O	2.128
mol814	s1c2c(c(C(OCC)=O)c1NC(=O)CCC(O)=O)C(CCC2)C	2.126
mol815	O=C1CC(Cc2nc(nc(c12)C)N1CCN(CC1)CC)C	2.126
mol816	s1cccc1C1C2=C(N=C(C)C1C(OCC1OCCC1)=O)CCCC2=O	2.125
mol817	O1CCN(CC1)CC#CC(OC(=O)C)(CCC=C)C	2.124
mol818	S1c2n(N=C1c1ccncc1)c(nn2)-c1ccc(OC)cc1	2.123
mol819	O1CC(COC1C1C(CC(=CC1C)C)C)C	2.122
mol820	S1c2c(N(c3c1cccc3)CC(O)CNCCCO)cccc2	2.122
mol821	Brc1c2n(nc1C(=O)NCCCC)C=C(Br)C=N2	2.122
mol822	Clc1cc(N2N=C(c3c(C2=O)c(sc3)N)C(OCC)=O)ccc1C	2.121
mol823	O(CCCC)c1ccc(N2C(=O)C(N3CCCCC3)CC2=O)cc1	2.12
mol824	O=C(NC1CCCCC1)C(=O)NCCc1ccccc1	2.12
mol825	Clc1cc(ccc1OCC=C)C1c2c(OC(N)=C1C#N)cc(O)cc2	2.119
mol826	O1CCCC1CNC(=O)C(=O)Nc1cc(OC)ccc1OC	2.118
mol827	O1c2cc(ccc2OC1)CNCCc1ccccc1OC	2.118
mol828	S=C(NC(=O)c1ccc(OC)cc1)N1CCCC1	2.117
mol829	OC1(c2c(NC1=O)c(ccc2)C)CC(=O)c1ccc(cc1)CC	2.117
mol830	Brc1cc(ccc1OC)C(=O)n1nc(cc1C)C	2.114
mol831	s1c2c(c(C(OCC)=O)c1NC(=O)CCC(O)=O)C(CCC2)C	2.114
mol832	o1nc(-c2nc3c(n2CCCC)cccc3)c(n1)N	2.111
mol833	O1CCCC1COC(=O)C1C(C2C(N=C1C)=CC(CC2=O)(C)C)c1cc(O)ccc1	2.111
mol834	S(=O)(=O)(C(C)(C)C)c1ccc(cc1)CCCC	2.11
mol835	Clc1cc(ccc1OCC=C)C1c2c(OC(N)=C1C#N)cc(O)cc2	2.11
mol836	S1(=O)(=O)N(CC(=O)Nc2cc3c(cc2)cccc3)C(=O)c2c1cccc2	2.11
mol837	Clc1ccc(cc1)C1N2C(SC(C)C2=O)=NC(C)=C1C(OC)=O	2.109
mol838	O=C1N(NC(=O)c2ccc(cc2)C(C)(C)C)C(=O)c2c1cccc2	2.109
mol839	S(C(C)(C)C)CCNC(=O)CN1c2c3c(cccc3ccc2)C1=O	2.107
mol840	S1CCC(=O)N2C1=NC(C)=C(C(OCC=C)=O)C2c1ccc(cc1)C(OC)=O	2.106

mol841	Clc1ccc(cc1)C1N2C(SC(C)C2=O)=NC(C)=C1C(OC)=O	2.106
mol842	S1c2n(N=C1CCc1ccccc1)c(nn2)C(F)(F)F	2.1
mol843	OC(CCC=C)(C#CCN1CCCCC1)C	2.1
mol844	Clc1cc(NC(=O)C(=O)NC(CC)C)ccc1	2.1
mol845	Clc1cc(-n2c(ccc2C)C)c(OC)cc1	2.099
mol846	O(CC(=O)NC(C)(C)C)c1ccc(cc1)C1=NN(C)C(=O)c2c1cccc2	2.098
mol847	O1CCCC1COC(=O)C1C(C2C(=NC1=C)CC(CC2=O)(C)C)c1cccnc1	2.098
mol848	S=C(Nc1ccccc1F)NC(=O)c1ccccc1F	2.097
mol849	S1CCC(=O)N2C1=NC(C)=C(C(OCCOC)=O)C2\C=C\c1ccccc1	2.096
mol850	S1CCC(=O)N2C1=NC(C)=C(C(OCCOC)=O)C2\C=C\c1ccccc1	2.096
mol851	O=C(CCN1CCCCC1)c1cc2CCCCc2cc1	2.096
mol852	Oc1ccc(NCc2ccc(cc2)CC)cc1	2.096
mol853	S=C(Nc1ccc(F)cc1F)NC(=O)Cc1ccccc1	2.095
mol854	Clc1ccc(S(=O)(=O)NCCNC(=O)c2nonc2N)cc1	2.095
mol855	Clc1cc(ccc1)C1C(C(OCC=C)=O)=C(OC(N)=C1C#N)C	2.095
mol856	O1c2c(OCC1C(=O)NC(C)c1ccccc1)cccc2	2.094
mol857	Clc1ccccc1C1N2C(SCCC2=O)=NC(C)=C1C(OCCOC)=O	2.094
mol858	O1c2c(OCC1C(=O)NC(C)c1ccccc1)cccc2	2.094
mol859	O(C(=O)c1ccccc1C)c1ccccc1[N+](=O)[O-]	2.093
mol860	Clc1ccc(NC(=O)C(=O)NC(CC)C)cc1	2.092
mol861	O(C)c1cc(ccc1O)C1C2C(=NC(C)=C1C(OC(C)C)=O)CCCC2=O	2.09
mol862	s1nnc2cc(NC(=O)NCC=C)ccc12	2.09
mol863	o1c2c(cc(OC)cc2)c(C(=O)Cn2ccnc2)c1C	2.09
mol864	s1c2c(CCCC2)c(C#N)c1-n1cccc1C[NH2+]CCCC	2.089
mol865	Clc1ccc(cc1)C(=O)NC(=S)N(CC)CC	2.088
mol866	Clc1c2c(ccc1OCC(O)CN1CCOCC1)cccc2	2.088
mol867	S1\C(=C/c2ccccc2)\C(=O)N(CC(=O)Nc2ccccc2O)C1=S	2.086
mol868	Clc1cc(ccc1C)C(=O)Nc1ccccc1OC	2.086
mol869	Fc1ccc(cc1)C1C2=C(OC(N)=C1C(OCCOC)=O)CC(CC2=O)(C)C	2.086
mol870	S(CC(OC1CC(CCC1C(C)C)C)=O)C1=NC(=O)C(=NN1)C	2.085
mol871	S1CCC(=O)N2C1=NC(C)=C(C(OCCOC)=O)C2c1ccc(OCC)cc1	2.085
mol872	Clc1c2c(sc1C(=O)NCC=C)cccc2	2.082
mol873	S1CCC(=O)N2C1=NC(C)=C(C(OCCOC)=O)C2c1ccc(F)cc1	2.078
mol874	Clc1c(cccc1Cl)C1C(C(OCC)=O)=C(OC(N)=C1C#N)C	2.077
mol875	S=C(NC(=O)c1cc(ccc1)C)N1CCC(CC1)C	2.076
mol876	O1c2c(-c3n(nnc3C1=O)CCCC)cccc2	2.076
mol877	S=C(NC1CCCC1)NC(=O)c1ccccc1C	2.076

mol878	Clc1cc(ccc1)C1C(C(OCC=C)=O)=C(OC(N)=C1C#N)C	2.076
mol879	Clc1c2c(ccc1OCC(O)CN1CCOCC1)cccc2	2.075
mol880	S=C(Nc1ccccc1)NC(=O)c1cc(F)ccc1	2.074
mol881	Clc1ccc(OCC(O)Cn2c3c(nc2NCCO)N(C)C(=O)NC3=O)cc1	2.073
mol882	O1CCN(CC1)CC(=O)NC(CCCCC)(C)C	2.069
mol883	Clc1cc(ccc1)C1N2C(SCCC2=O)=NC(C)=C1C(OCCOC)=O	2.069
mol884	S=C(Nc1ccc(F)cc1F)NC(=O)CC(C)C	2.066
mol885	s1cc(nc1NCC=C)-c1cc([N+](=O)[O-])ccc1	2.066
mol886	O(CC(O)Cn1c2c(nc1N(C)C)N(C)C(=O)N(C)C2=O)c1ccc(cc1)C	2.065
mol887	o1cccc1C1CC(=O)c2c(nc(nc2)NC(=O)c2ccccc2)C1	2.065
mol888	Clc1ccc(cc1N(S(=O)(=O)C)CC(=O)NCC1OCCC1)C(F)(F)F	2.064
mol889	S(CC#C)c1nc(N)c(C#N)c(-c2ccc(O)cc2)c1C#N	2.06
mol890	O(Cc1ccccc1)CCN(Cc1ccccc1)CCO	2.06
mol891	FC(F)(F)c1cc(N\N=C(/C#N)\C(OCC)=O)ccc1	2.06
mol892	O(C(=O)C(C(=O)NCC=C)C1CCCCC1)CC	2.059
mol893	O1CCc2c(cccc2)C1CNC(=O)C(=O)Nc1ccccc1	2.059
mol894	O=C1CC(CC2=Nc3n(C=C12)c1c(n3)cccc1)(C)C	2.058
mol895	FC(F)(F)C1n2nc(cc2NC(C1)c1occc1)C(=O)N1CC(OC(C1)C)C	2.051
mol896	Clc1ccc(NC(=O)C(=O)NC(CC)C)cc1	2.051
mol897	Clc1ccc(N2C3=C(C=C(C(=O)NCC=C)C2=O)C(=O)CCC3)cc1	2.05
mol898	FC(F)(F)C1n2nc(cc2NC(C1)c1ccc(cc1)C)C(=O)N1CCOCC1	2.05
mol899	FC(F)(F)C1n2nc(cc2NC(C1)c1ccc(cc1)C)C(=O)N1CCOCC1	2.05
mol900	S=C(NC(=O)c1occc1)N1CCc2c1cccc2	2.049
mol901	O(CC#C)c1ccc(cc1)C1C2C(=NC=3C1C(=O)CCC=3)CCCC2=O	2.049
mol902	S(CCOc1ccccc1F)C=1NC(=O)c2c(N=1)cccc2	2.048
mol903	Clc1ccc(OCC(O)Cn2c3c(nc2NCCO)N(C)C(=O)NC3=O)cc1	2.047
mol904	Clc1cc(NC(=O)NCc2cn(nc2C)C)ccc1	2.045
mol905	O(CC(O)Cn1c2c(nc1N(C)C)N(C)C(=O)N(C)C2=O)c1ccc(cc1)C	2.045
mol906	s1c2c(nc1-c1cc(N)cc(C)c1O)cccc2	2.043
mol907	Brc1ccc(NC(=O)CN2c3c(cccc3)C(=O)C2=O)cc1	2.042
mol908	S(=O)(=O)(Nc1cc(C(O)=O)c(O)cc1)c1c2c3c(ccc2)C(=O)Nc3cc1	2.04
mol909	Clc1cc(Cl)ccc1C=1Sc2n(N=1)cnn2	2.04
mol910	Clc1ccccc1OC(=O)COc1ccccc1	2.039
mol911	OC(=O)c1c2NC(C3C(c2c([N+](=O)[O-])cc1)C=CC3)CCC	2.038
mol912	S(=O)(=O)(N1CCC(CC1)C)c1ccc(OC)cc1	2.037
mol913	s1cc(nc1C)-c1ccc(NS(=O)(=O)c2ccc([N+](=O)[O-])cc2)cc1	2.036
mol914	O=C1N(C)C(=O)N(c2nc(n(c12)CCOC)N1CCCCC1)C	2.035

mol915	Clc1cc(C)c(NC(=O)C(=O)NC(C)C)cc1	2.034
mol916	Clc1ccc(NC(=O)NNC(=O)Nc2ccccc2)cc1	2.034
mol917	S=C(NC(=O)COc1ccc(cc1)C)N1CCCC1	2.033
mol918	Clc1cc(OC)c(OC)cc1C1c2c(OC(N)=C1C#N)cc(O)cc2	2.031
mol919	S(CC(=O)c1ccccc1)c1oc(nn1)-c1ccncc1	2.031
mol920	s1cccc1\C=C/1\C(=O)N(c2cc(C)c(cc2)C)C(=O)NC\1=O	2.03
mol921	Fc1ccc(cc1)Cn1c2c(nc1NCCCO)N(C)C(=O)NC2=O	2.028
mol922	ClC=1C(=O)n2nc(nc2NC=1C)NCc1c(F)cccc1Cl	2.028
mol923	s1c2CCCc2c2c1-n1c(nnc1S)N(c1ccccc1OC)C2=O	2.027
mol924	S=C(Nc1ccc(cc1)C(C)C)NC(=O)CC	2.026
mol925	O1c2c(OCC1C(=O)NC(C)c1ccccc1)cccc2	2.026
mol926	O1c2c(OCC1C(=O)NC(C)c1ccccc1)cccc2	2.026
mol927	O1c2cc(ccc2OC1)C1N(CCCC)C(=O)C(O)=C1C(=O)c1ccc(OC)cc1	2.026
mol928	s1cccc1-c1c2c(sc1)ncnc2NCCCN1CCOCC1	2.025
mol929	S=C(N(CC)c1ccccc1)NC(=O)C1CC1	2.024
mol930	O(CC)c1c(cccc1OC)CNc1nnnn1C	2.023
mol931	FC(F)(F)C1n2nc(cc2NC(C1)c1ccc(cc1)C)C(=O)N1CCOCC1	2.023
mol932	s1cccc1C(O)(C#CCN(CC)CC)c1ccccc1	2.021
mol933	S=C1NN=C(N1CC=C)COc1cc(ccc1C)C	2.02
mol934	ClC=1C(=O)n2nc(nc2NC=1C)NCc1ccccc1F	2.019
mol935	s1c(nnc1NC(=O)CCCC)Cc1ccccc1	2.018
mol936	Ic1cc(ccc1C)C(=O)N1CCC(CC1)C	2.018
mol937	O1CCN(CC1)CC#CC(OC(=O)C)(CCC=C)C	2.017
mol938	S1CCC(=O)N2C1=NC(C)=C(C(OCCOC)=O)C2c1ccc(OCCC)cc1	2.017
mol939	Clc1nc(nc(n1)NCC=C)NC(C)(C)C	2.017
mol940	OC(CCC=C)(C#CCN1CCCCC1)C	2.016
mol941	S(=O)(=O)(N1CCCc2c1cccc2)c1ccccc1[N+](=O)[O-]	2.014
mol942	Clc1cc(NC(=O)C2n3c4c(nc3NC(=O)C2)cccc4)ccc1	2.013
mol943	S(CC(=O)C1=Cc2c(OC1=O)cccc2)c1nnnn1C	2.013
mol944	s1cccc1CNc1nc(n(n1)-c1ccccc1)N	2.011
mol945	O=C1C2(CN3CC1(CN(C2)C3(CCCC)C)C)C	2.01
mol946	Fc1ccc(cc1)C(=O)Nc1ccccc1OCC	2.009
mol947	Fc1cc(NC(=O)Nc2ccccc2)ccc1C	2.009
mol948	s1cccc1C(=O)NC(=S)Nc1ccccc1F	2.009
mol949	FC(F)(F)C1n2nc(cc2NC(C1)c1ccc(cc1)C)C(=O)N1CCOCC1	2.008
mol950	O(C(=O)c1cc(ccc1)C)c1ccccc1[N+](=O)[O-]	2.003
mol951	Brc1cc(ccc1)CNCCc1cc2OCOc2cc1	2.002
mol952	Clc1cc(NC(=O)C2n3c4c(nc3NC(=O)C2)cccc4)ccc1	2.002
mol953	FC(F)(F)c1nn(c2c1CCC2)CC(=O)NCCCC	2.002
mol954	Clc1ccc(cc1)C(=O)NCC(=O)c1ccccc1	2.001
mol955	S(C)c1ccc(cc1)CNc1ncccc1	2

mol956	S(CC(=O)Nc1ccc(F)cc1)c1nnnn1-c1ccc(O)cc1	1.999
mol957	Clc1ccc(OCc2oc(NCCN3CCOCC3)c(n2)C#N)cc1	1.998
mol958	s1c2cc(ccc2nc1N)C(=O)Nc1cc2sc(nc2cc1)N	1.998
mol959	O(C)c1ccc(cc1)C1n2nnnc2NC(C(OC)=O)=C1C(=O)C	1.995
mol960	S=C1N\C(=C/c2ccc(O)cc2)\C(=O)N1c1ccccc1	1.994
mol961	S(=O)(=O)(NCCCn1ccnc1)c1cc(ccc1C)C	1.993
mol962	Fc1ccc(cc1)C1C2=C(OC(N)=C1C#N)CC(CC2=O)C	1.991
mol963	O=C(NC1CCCCC1)NCc1cn(nc1C)CC	1.991
mol964	FC(F)(F)c1cc(N2C(=O)C(=O)C(C(=O)c3ccccc3)=C2C(OC)=O)ccc1	1.99
mol965	O(C(=O)C(C(=O)NCC=C)C1CCCCC1)CC	1.988
mol966	S(CC(=O)c1cc(ccc1C)C)c1[nH]nc(n1)-c1ccncc1	1.988
mol967	s1c(nnc1SC)NC(=O)CCc1ccccc1	1.988
mol968	S=C(Nc1cc([N+](=O)[O-])c(F)cc1)NC(=O)c1ccccc1F	1.987
mol969	s1c2c(nc1SCC#CCO)cccc2	1.986
mol970	BrC=1C=Nc2nc(nn2C=1)C(=O)NCCCC	1.984
mol971	S1\C(=C/c2ccccc2)\C(=O)N(CC(=O)Nc2ccc(O)cc2)C1=S	1.983
mol972	O=[N+]([O-])c1ccccc1CNCCc1c2c([nH]c1)cccc2	1.979
mol973	O(C)c1c2c(ccc1OC)C(=O)N(c1ccccc1C)C2=O	1.978
mol974	Clc1ccc(cc1)CNC(=O)C(=O)NCc1ccccc1	1.977
mol975	Oc1ccccc1C\C=C\c1ccccc1	1.974
mol976	Brc1oc(cc1)C(Oc1ccccc1C(=O)C)=O	1.974
mol977	O(CCCN1CCCCC1)c1ccc(cc1C)C	1.973
mol978	Clc1ccc(cc1)C(=O)NC(=S)Nc1ccccc1C#N	1.972
mol979	s1nnc2cc(NC(=O)NCCCO)ccc12	1.969
mol980	Ic1cc(C(=O)NC2CCCC2)c(Cl)cc1	1.967
mol981	O1CCc2c(cccc2)C1CNC(=O)C(=O)Nc1ccccc1	1.965
mol982	O(C(=O)C=1Nc2n(nnn2)C(C=1C(=O)C)c1ccc(cc1)C(C)C)C	1.965
mol983	Brc1cc(F)c(NC(=O)c2ccoc2C)cc1	1.964
mol984	o1cccc1CNC(=O)CCc1onc(n1)-c1ccccc1	1.963
mol985	Brc1ccc(cc1)CNc1[nH]nc(SC)n1	1.963
mol986	O1c2c(N(CCC(=O)NC3CCCCC3)C1=O)cccc2	1.961
mol987	FC(F)(F)C1n2nc(cc2NC(C1)c1occc1)C(=O)NCCOC	1.961
mol988	FC(F)(F)Oc1ccc(NC2CC(=O)N(C2=O)c2ccc(OC)cc2)cc1	1.96
mol989	Clc1cc(NC(=O)c2ccc(F)cc2)c(N2CCOCC2)cc1	1.96
mol990	Brc1c(n(nc1C)C(=O)c1sccc1)C	1.96
mol991	S1CCC(=O)N2C1=NC(C)=C(C(OCCOC)=O)C2c1ccc(cc1)CC	1.96
mol992	O1C(=Nc2c(cc(OC)c(OC)c2)C1=O)c1cc(OC)c(OC)c(OC)c1	1.958
mol993	Brc1cc(S(=O)(=O)NCCCN2CCOCC2)c(OC)cc1	1.958
mol994	Brc1ccc(nc1C)NC(=O)c1sccc1	1.957
mol995	Clc1ccccc1C(=O)N1CCN(CC1)c1ccc(F)cc1	1.953
mol996	S=C(Nc1cc(cc(c1)C)C)NC(=O)C1CC1	1.952

mol997	S=C(Nc1cc(ccc1O)C)Nc1ccccc1	1.951
mol998	O(CCCCN1CCCCC1)c1cc(ccc1)C	1.951
mol999	O(C)c1cc(OC)ccc1CNc1ccc(NC(=O)C)cc1	1.95
mol1000	S1CCC(=O)N2C1=NC(C)=C(C(OCCOC)=O)C2c1ccccc1	1.949
mol1001	S=C1NC(=O)/C(/N1)=C\c1cc(CC=C)c(O)c(OC)c1	1.948
mol1002	O(C)c1ccc(cc1C=O)-c1ccccc1	1.945
mol1003	O1C2C3C(C1(C=C2)C)C(=O)N(C3=O)c1ccc(OCCC)cc1	1.941
mol1004	S=C(Nc1ccc(NC(=O)C)cc1)NC(=O)c1ccccc1OC	1.94
mol1005	S(CC(=O)N1CCOCC1)C1=[NH+]C([O-])=C(CCCC)C(=O)N1	1.939
mol1006	O=C(Nc1ccccc1C#N)c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1	1.939
mol1007	S(CCC)c1nc(cc(COC)c1C#N)C	1.939
mol1008	S(CC#CCO)c1c2ncccc2ccc1	1.937
mol1009	S1CCC(=O)N2C1=NC(C)=C(C(OCCOC)=O)C2c1ccc(F)cc1	1.937
mol1010	S(C)c1ccc(cc1)CNc1nnnn1CCC	1.934
mol1011	O1c2cc(ccc2OC1)CNCc1ccc(cc1)C	1.93
mol1012	s1c2cc(ccc2nc1N)C(OCCOC)=O	1.929
mol1013	o1c2c(cccc2)c(C)c1C(=O)NCCC	1.929
mol1014	O(CC(=O)Nc1cccnc1)c1c(cccc1C)C	1.925
mol1015	Clc1cc(ccc1Cl)C(=O)NCc1ccncc1	1.925
mol1016	o1cccc1C1NC(=NC(=O)C1C(OCC)=O)N1CCc2c1cccc2	1.923
mol1017	O=C1Nc2n(c3c(n2)cccc3)C(C1)C(=O)Nc1ccc(cc1C)C	1.922
mol1018	O=C1N(CCOC)C(=O)C2C1C1c3c(C2c2c1cccc2)cccc3	1.922
mol1019	Clc1ccc(cc1)CN1CCN(CC1)C(CC)C	1.921
mol1020	O=C(NC(CC)C)C(=O)NCCc1ccccc1	1.921
mol1021	O=C(NC(CC)C)C(=O)NCCc1ccccc1	1.92
mol1022	Clc1ccc(cc1)C1C2=C(OC(N)=C1C(OCCOC)=O)CCCC2=O	1.92
mol1023	O=C(N1CCN(CC1)CCNC(=O)C(CC)CC)C(CC)CC	1.917
mol1024	O=C(Nc1cc(ccc1)C#N)CCC(=O)Nc1cc(ccc1)C#N	1.917
mol1025	S(=O)(=O)(NCCNC(=O)c1nonc1N)c1ccccc1	1.914
mol1026	FC(F)(F)c1cc(NC(=O)C(=O)NCC=C)ccc1	1.914
mol1027	O=C(NC1CCCC1)C(=O)Nc1cc(C)c(cc1)C	1.913
mol1028	n1nnn(CC)c1NCc1ccc(N2CCCC2)cc1	1.913
mol1029	o1cccc1C1NC(=NC(=O)C1C(OCC)=O)N1CCc2c1cccc2	1.912
mol1030	S1CCC(=O)N2C1=NC(C)=C(C(OCCOC)=O)C2c1cc(F)ccc1	1.912
mol1031	S1CCC(=O)N2C1=NC(C)=C(C(OCCOC)=O)C2c1ccc(OC(=O)C)cc1	1.911
mol1032	Fc1cc(ccc1)C1C2=C(OC(N)=C1C#N)CC(CC2=O)(C)C	1.91
mol1033	S1CCC(=O)N2C1=NC(C)=C(C(OCCOC)=O)C2c1ccc(cc1)C(OC)=O	1.903
mol1034	S=C(Nc1ccc(cc1)C#N)Nc1ccccc1	1.901
mol1035	S1c2c(N(c3c1cccc3)C(=O)NCCOC)cccc2	1.9
mol1036	FC(F)(F)c1nn(c2c1CCCC2)CC(=O)NCCC	1.9

mol1037	S(C)c1ccc(cc1)\C=N\NC(=S)N	1.9
mol1038	O1c2cc(ccc2OC1)C1N(CCCOC)C(=O)C(=O)C1C(=O)c1cccc1	1.9
mol1039	o1cccc1C(=O)NC(C)c1ccc(cc1)C	1.899
mol1040	s1nnc2cc(ccc12)C(=O)NCCOC	1.898
mol1041	S(CC(=O)N1CCOCC1)c1nnnn1-c1c(cccc1C)C	1.896
mol1042	S(=O)(=O)(N(CC(=O)NC(C)(C)C)c1ccccc1)c1ccccc1[N+](=O)[O-]	1.895
mol1043	S(=O)(=O)(N(CCC#N)CCC#N)c1cc2c(cc1)cccc2	1.895
mol1044	O(C(C)C)c1ccc(cc1)CC1CCC(=O)N(C)C1=O	1.894
mol1045	Clc1ccc(cc1)\C=C\C(=O)NC1CCS(=O)(=O)C1	1.894
mol1046	Clc1cc(NC(=O)Cn2nc([N+](=O)[O-])nc2)ccc1F	1.892
mol1047	FC(F)(F)Oc1ccc(NC2CC(=O)N(C2=O)c2ccc(OC)cc2)cc1	1.891
mol1048	Clc1cc(NC(=O)C(=O)NCC(C)C)ccc1	1.89
mol1049	s1nc2cc(NC(=O)NCCO)ccc2n1	1.889
mol1050	Clc1ccc(cc1)C(=O)C12CN3CN(C1)CN(C2)C3	1.889
mol1051	Clc1ccc(NC(=O)C(=O)NC2CCCC2)cc1	1.889
mol1052	FC(F)(F)c1nn(c2c1CCCC2)CC(=O)NC(C)(C)C	1.888
mol1053	S1c2n(N=C1c1cc3OCCOc3cc1)cnn2	1.887
mol1054	Clc1cc(NC(=O)CC(C)C)ccc1C	1.884
mol1055	O=C1NC(=O)N(c2nc(n(c12)CC(C)=C)NCCOC)C	1.884
mol1056	O=C(NC(C)c1ccc(cc1)C)c1cccnc1	1.879
mol1057	Clc1cc(ccc1)C1N2C(SCCC2=O)=NC(C)=C1C(OCCOC)=O	1.876
mol1058	S(CC#CCO)c1oc2c(n1)cccc2	1.871
mol1059	S(C)c1nc([nH]n1)NCc1ccccc1	1.87
mol1060	O=C1N(CCO)C(=O)c2c1cc(cc2)C(=O)c1cc([N+](=O)[O-])ccc1	1.869
mol1061	Clc1ccc(NC(=O)C(=O)NCC(C)C)cc1	1.868
mol1062	o1cccc1C1NC(=NC(=O)C1C(OCC)=O)N1CCc2c1cccc2	1.868
mol1063	FC(F)(F)C1n2nc(cc2NC(C1)c1occc1)C(=O)NCCOC	1.868
mol1064	Oc1ccccc1\C=N\NC(=O)c1cc(O)c(O)cc1	1.866
mol1065	S=C1NC(C(C(OCC)=O)=C(N1)C)c1ccc(OCC(=O)N)cc1	1.862
mol1066	O(C)c1ccc2c(cccc2)c1CNc1nnnn1CC	1.86
mol1067	O=C1CC(Cc2nc3c(cccc3)c(N)c12)(C)C	1.859
mol1068	O1c2c(OC1)cc(cc2OC)CNCCc1ccc(OC)cc1	1.857
mol1069	O=C(NCCC)N1CCN(CC1)c1ncccn1	1.855
mol1070	Fc1ccc(cc1)C(=O)Nc1ccc(NC(=O)C(C)C)cc1	1.855
mol1071	[NH3+]CCCc1c2c(n(Cc3ccccc3)c1C)cccc2	1.854
mol1072	o1cccc1C1NC(=NC(=O)C1C(OCC)=O)N1CCc2c1cccc2	1.853
mol1073	S=C1NN=C(N1C)c1ccc(N(C)C)cc1	1.853
mol1074	O(C)c1ccc(cc1)C1n2nnnc2NC(C(OC)=O)=C1C(=O)C	1.853
mol1075	s1ccnc1NS(=O)(=O)c1ccc(NS(=O)(=O)c2ccc(cc2)C)cc1	1.849
mol1076	FC(F)(F)C=1n2nc(cc2N=C(C=1)c1occc1)C(=O)N	1.847

mol1077	O1c2cc(ccc2OC1)CNCCc1cc(OC)c(OC)cc1	1.845
mol1078	S1CCC(=O)N2C1=NC(C)=C(C(OCCOC)=O)C2c1ccccc1	1.845
mol1079	Clc1nc(nc(n1)NCC=C)NC(C)C	1.838
mol1080	Clc1cc(NC(=O)C(=O)NC(CC)C)ccc1	1.836
mol1081	FC(F)(F)C1n2nc(cc2NC(C1)c1occc1)C(=O)NC(COC)C	1.836
mol1082	s1cccc1C(=O)NCc1cc(ccc1OC)C1=NN(C)C(=O)c2c1cccc2	1.835
mol1083	S(CC#C)c1oc2c(n1)cccc2	1.834
mol1084	S=C1NC(C(C(OCC)=O)=C(N1)C)c1ccc(OCC(=O)N)cc1	1.834
mol1085	s1c(nnc1NS(=O)(=O)c1ccc(cc1)CCCC)C	1.833
mol1086	Brc1ccc(cc1)C(=O)CC1(O)c2c(NC1=O)cccc2	1.831
mol1087	o1cccc1C1NC(=NC(=O)C1C(OCC)=O)N1CCN(CC1)CC	1.83
mol1088	Brc1ccc(cc1)CC(=O)NC(CC)(C)C	1.828
mol1089	O(C(CCN1CCCCC1)(C#C)c1ccccc1)C	1.828
mol1090	O(C(CCCN(CC)CC)(C#C)c1ccccc1)C	1.828
mol1091	o1nc(C(=O)NCCNC(=O)c2ccc(cc2)C)c(n1)N	1.826
mol1092	O(C)c1cc2C=3N(CCc2cc1OC)CN(CC=3C#N)CC(O)=O	1.826
mol1093	Ic1cc(ccc1C)C(=O)NC(C)(C)C	1.826
mol1094	O1CCN(CC1)CCCOc1c(cccc1C)C	1.823
mol1095	Clc1cccc(NC(=O)CC2OCCN(CC)C2=O)c1C	1.822
mol1096	s1ccnc1NC(=O)CSc1nc(c(nn1)-c1occc1)-c1occc1	1.819
mol1097	Clc1ccccc1-c1nc(on1)-c1cccnc1	1.819
mol1098	[NH2+](Cc1ccc(N(C)C)cc1)CCc1ccccc1	1.819
mol1099	O=C(NC1CCCC1)C(=O)NCCc1ccccc1	1.819
mol1100	O(C(C)C)c1ccc(cc1)CC1CCC(=O)N(C)C1=O	1.818
mol1101	OC(CNCCCN(C)C)Cn1c2c(c3c1cccc3)cccc2	1.818
mol1102	O(C)c1ccc2c(cccc2)c1CNc1nnnn1C	1.817
mol1103	S(=O)(=O)(NCC=C)c1cc(OC)c(OC)cc1	1.815
mol1104	O(C)c1cc(ccc1OC)CCNCc1ccncc1	1.814
mol1105	n1c(nc(nc1N)N)-c1cc(ccc1)-c1nc(nc(n1)N)N	1.814
mol1106	S=C(N(CC)CC)NC(=O)c1ccc(F)cc1	1.814
mol1107	s1cc(nc1NCC=C)-c1ccncc1	1.813
mol1108	OC(CNCCCN(C)C)Cn1c2c(c3c1cccc3)cccc2	1.813
mol1109	s1cccc1C(=O)CN1c2c(N(CC=C)C1=N)cccc2	1.808
mol1110	O1C(=N\C(=C/c2n(ccc2)C)\C1=O)c1ccccc1	1.808
mol1111	Clc1ccccc1OCCCCN1CCOCC1	1.805
mol1112	O(CC(OC)=O)c1cc2c(cc1)cccc2	1.801
mol1113	S1c2n(N=C1COc1ccc(F)cc1)cnn2	1.799
mol1114	S1CC(=O)Nc2n(nc(O)c2C1c1cc(OC)c(OC)cc1)C(C)C	1.799
mol1115	O1c2cc(ccc2OC1)CCNCc1cccc(OC)c1OC	1.798
mol1116	S=C1NN=C(N1CC)COc1cc(ccc1C)C	1.797
mol1117	Clc1ccc(cc1)CCNCc1ccncc1	1.794
mol1118	Cl\C(=C\CN1c2c(cc(cc2)C)C(=O)C1=O)\C	1.794

mol1119	S(CC(=O)Nc1ccccc1F)c1ncccc1	1.793
mol1120	Brc1ccc(NC(=O)CC)cc1Cl	1.793
mol1121	Clc1ccc(cc1)CNC(=O)C(=O)NC1CCCC1	1.792
mol1122	O(C(=O)C=1Nc2n(nnn2)C(C=1C(=O)C)c1ccc(cc1)CC)C	1.791
mol1123	O1c2cc(ccc2OC1)CCC1(NC(=O)c2c(N1)cccc2)C	1.79
mol1124	O=C(NC1CCCCC1)C(=O)NCc1ccccc1	1.788
mol1125	S(=O)(=O)(N)c1ccc(cc1)CCNC1CC(=O)N(C1=O)c1ccccc1	1.786
mol1126	Fc1ccccc1CCNCc1cc2OCOc2cc1	1.786
mol1127	O(C)c1ccc(cc1)CN1c2c(cccc2)C(=O)C1=O	1.783
mol1128	Clc1cc(cc(OC)c1OC)CNc1ccc(cc1)C(O)=O	1.781
mol1129	S=C(Nc1cccc(C(O)=O)c1C)NC(=O)c1ccc(cc1)C	1.778
mol1130	Ic1cc(ccc1C)C(=O)N1CCCCCC1	1.777
mol1131	S(C)c1ccc(cc1)CNc1nnnn1CC	1.776
mol1132	OCCCc1nc2cc([N+](=O)[O-])ccc2n1CCO	1.774
mol1133	o1nc(nc1-c1cc2OCOc2cc1)-c1cccnc1	1.772
mol1134	O=C1N(C)C(=O)N(c2nc(n(c12)CCOC)CN1CCN(CC1)Cc1cccc1)C	1.772
mol1135	S1CCC(=O)N2C1=NC(C)=C(C(OCCOC)=O)C2c1cc(F)ccc1	1.772
mol1136	Brc1ccccc1C(=O)NCCNC(=O)c1nonc1N	1.77
mol1137	o1ccc(C(=O)N2CCN(CC2)c2ccccc2OC)c1C	1.769
mol1138	O=C1Nc2cc(ccc2C=C1CN(C(=O)c1ccccc1)CCOC)C	1.768
mol1139	s1nnc2cc(ccc12)C(=O)NCC=C	1.767
mol1140	Brc1ccc(N2C(=O)C3C(C4CCC3C=C4)C2=O)cc1	1.766
mol1141	Clc1ccc(cc1)C1C2=C(OC(N)=C1C(OCCOC)=O)CCCC2=O	1.766
mol1142	O1C2=C(OC(=CC2=O)CO)C(C(C#N)=C1N)c1cc(OC)c(OCCC)cc1	1.764
mol1143	n12nc(cc1N=C(C=C2N)C)-c1ccccc1	1.764
mol1144	O1c2cc(ccc2OC1)C1C(=CN(C=C1C(OC)=O)CCOC)C(OC)=O	1.764
mol1145	O(CC)C(=O)/C(/NC(=O)C)=C/c1c2c([nH]c1)cccc2	1.763
mol1146	O1c2cc(ccc2OC1)C1N(CCCCCC)C(=O)C(=O)C1C(=O)C	1.762
mol1147	S(CCC(=O)Nc1ccccc1OC)c1nnnn1C	1.759
mol1148	O(CCCn1ccnc1)c1cc(ccc1)C	1.755
mol1149	O(Cc1ccccc1)c1ccc(cc1OC)C1NC(=O)CCC1[N+](=O)[O-]	1.753
mol1150	Brc1oc(cc1)C(Oc1ccccc1[N+](=O)[O-])=O	1.753
mol1151	[nH+]1c2n(cc1-c1cc(N)ccc1)C=CC=C2C	1.751
mol1152	O1C2=C(OC(=CC2=O)CO)C(C(C#N)=C1N)c1cc(OC)c(OCCC)cc1	1.751
mol1153	S(CC(=O)N)c1nc2N(C)C(=O)N(C)C(=O)c2n1CCCC	1.75
mol1154	O=C1CC(CC(NCCCC)=C1)(C)C	1.75
mol1155	s1c2cc([N+](=O)[O-])ccc2nc1NC(=O)CCC(O)=O	1.748
mol1156	Fc1ccccc1CNc1ccc(N2CCOCC2)cc1	1.746
mol1157	O1C2=C(C(C(C(OCCOC)=O)=C1N)c1ccncc1)C(=O)CC(C2)(	1.743

	C)C	
mol1158	s1ccnc1NC(=O)CCOc1ccccc1	1.743
mol1159	o1nc(nc1CCC(=O)N(C)C)-c1ccc(cc1)C	1.742
mol1160	O(C)c1ccccc1N1C(=O)C(N2CCN(CC2)c2ccccc2)CC1=O	1.741
mol1161	O(CC)c1cc(ccc1OCC(=O)NCc1ccccc1)C(O)=O	1.739
mol1162	S1(=O)(=O)CC(Nc2ccc(OC)cc2)C(NCc2occc2)C1	1.739
mol1163	O=C1N=C(NC(C1)C(=O)Nc1ccccc1)N1CCc2c(C1)cccc2	1.738
mol1164	o1cccc1CN1CCN(CC1)C1CCCCC1C	1.738
mol1165	Clc1cc(NC(=O)CCC)ccc1C	1.734
mol1166	s1nc2c(n1)cccc2NC(=O)CCCC	1.733
mol1167	S(CC(=O)NC(Cc1ccccc1)C(OC)=O)C=1NC(=O)C=C(N=1)N	1.733
mol1168	S(CC(=O)NC(Cc1ccccc1)C(OC)=O)C=1NC(=O)C=C(N=1)N	1.733
mol1169	FC(F)(F)C(=O)c1c2c(n(c1)CC(OC)=O)cccc2	1.731
mol1170	O1CCc2c(cccc2)C1CNC(=O)C(=O)NCc1occc1	1.727
mol1171	S(=O)(=O)(N)c1ccc(N2C(=O)CCCC2=O)cc1	1.721
mol1172	O=C(Nc1ccc(NC(=O)C(C)C)cc1)Cc1ccccc1	1.717
mol1173	S(C)C1=N\C(=C/c2ccc(OC)cc2)\C(=O)N1C	1.717
mol1174	FC(F)(F)C1n2nc(cc2NC(C1)c1occc1)C(=O)NC1CC1	1.716
mol1175	O=C1N(C(=O)C2C1CCCC2)c1c2c(ccc1)cccc2	1.715
mol1176	Clc1cc(-n2nnnc2SCCCC#N)ccc1	1.713
mol1177	O(C(CCCN(CC)CC)(C#C)c1ccccc1)C	1.713
mol1178	Fc1ccc([N+](=O)[O-])cc1NC(=O)Nc1ccccc1	1.711
mol1179	O=C1N(C(=O)C2C1CCCC2)c1c2c(ccc1)cccc2	1.711
mol1180	Clc1ccc(NC(=O)NCc2occc2)cc1	1.71
mol1181	Clc1cc(C2=NNC(=S)N2c2cc3OCCOc3cc2)c(OC)cc1	1.709
mol1182	S1C=Cn2cc([nH+]c12)-c1cc(N)ccc1	1.709
mol1183	s1c(nnc1NC(=O)CCCC)CC(C)C	1.708
mol1184	S(=O)(=O)(NC1CCCC1)c1ccccc1[N+](=O)[O-]	1.708
mol1185	Clc1cccc(NC(=O)CC2OCCN(CC)C2=O)c1C	1.706
mol1186	Brc1cc(cnc1)C(=O)c1ccc(cc1)C	1.706
mol1187	[NH2+](CC1(CCCC1)c1ccccc1)CCC#N	1.703
mol1188	FC(F)(F)C1n2nc(cc2NC(C1)c1occc1)C(=O)NCCOC	1.703
mol1189	O1CCc2c(cccc2)C1CNC(=O)C(=O)NCc1occc1	1.701
mol1190	Clc1ccccc1-c1nc(on1)-c1ccncc1	1.701
mol1191	[NH2+](C(c1ccccc1)c1ccncc1)CCC	1.697
mol1192	[NH2+](C(c1ccccc1)c1ccncc1)CCC	1.697
mol1193	Clc1ccc(cc1)C(=O)n1nc(cc1)C	1.696
mol1194	Clc1ccc(-n2cnnc2)cc1C(=O)NC(CC)c1ccccc1	1.696
mol1195	o1c(ccc1C=O)-c1ccc(OC)cc1	1.691
mol1196	Brc1ccc(NC(=O)C(=O)NCC=C)cc1	1.691
mol1197	Clc1ccc(OCC(O)CN2CCOCC2)cc1	1.69
mol1198	S=C(Nc1ccc(Nc2ccccc2)cc1)NC(=O)C1CC1	1.688

mol1199	s1c2c(nc1NS(=O)(=O)c1ccc([N+](=O)[O-])cc1)cccc2	1.683
mol1200	Brc1ccc(NC(=O)CCC(OC)=O)cc1Cl	1.681
mol1201	Oc1ccc(NCc2ccc(cc2)C)cc1	1.679
mol1202	O1c2cc(ccc2OC1)CCNCc1ccc(cc1)C	1.679
mol1203	S=C(Nc1ccccc1C#N)NC(=O)Cc1ccccc1	1.678
mol1204	O1c2cc(-n3cccc3C=O)ccc2OC1	1.677
mol1205	Oc1cc(O)ccc1C(OC(CCN(CC)CC)C)=O	1.677
mol1206	s1c2CCCCc2c2c1N=C(NC2=O)NCCO	1.675
mol1207	Clc1cc(OC)c(NC(=O)C(=O)NCCN2CCNCC2)cc1OC	1.674
mol1208	s1cccc1-c1csc(N)c1C(OC)=O	1.673
mol1209	Clc1cc(NC(=O)C(=O)NC(C)C)ccc1	1.673
mol1210	Brc1ccc(NC(=O)C(=O)NCc2occc2)cc1	1.669
mol1211	O1c2cc(ccc2OC1)C1N(CCCCCC)C(=O)C(O)=C1C(=O)C	1.669
mol1212	Cl\C(=C\C[NH2+]C\C=C(\Cl)/C)\C	1.668
mol1213	S=C(Nc1ccc(F)cc1F)NC(=O)c1occc1	1.668
mol1214	[nH+]1c2n(cc1-c1ccc(N)cc1)C=CC=C2C	1.667
mol1215	S(C)c1nc([nH]n1)NCc1cc(OC)c(OC)cc1	1.665
mol1216	O=C1N=C(NC(C1)C(=O)Nc1ccc(cc1)C)N1CCc2c1cccc2	1.664
mol1217	Brc1cc(N2C(=O)C3C(C4CCC3C=C4)C2=O)ccc1C	1.659
mol1218	O(C(=O)C1=CN(C=C(C(OC)=O)C1c1ccc(cc1)C(C)C)C)C	1.659
mol1219	S=C(Nc1cccc(C)c1C)NC(=O)CC	1.658
mol1220	s1c(C)c(C)c(C(OCC)=O)c1NC(=O)CCCC(O)=O	1.655
mol1221	Clc1cc(NC(=O)C(=O)NCC=C)ccc1	1.652
mol1222	O=C(NCCc1ccccc1)C(=O)NCC=C	1.652
mol1223	s1c2CC(CCc2c2c1ncnc2N1CCOCC1)C	1.649
mol1224	O1c2c(cccc2)C(Oc2ccccc2)=C([N+](=O)[O-])C1=O	1.648
mol1225	Clc1ccccc1OC(=O)COc1ccc([N+](=O)[O-])cc1	1.648
mol1226	Clc1cc(F)c(NC(=O)c2ccoc2C)cc1	1.647
mol1227	s1cccc1C(=O)NC1CCCCCC1	1.645
mol1228	Clc1ccc(nc1)NC(=O)CSC=1NC(=O)C=C(N=1)N	1.643
mol1229	S=C(Nc1ccccc1)NCCOC=C	1.643
mol1230	O1CCN(CC1)CC#CC(O)(CCC=C)C	1.642
mol1231	[NH2+]1C(Cc2c(ccc3c2cccc3)C1C)(C)C	1.64
mol1232	[NH2+]1C(Cc2c(ccc3c2cccc3)C1C)(C)C	1.64
mol1233	o1c(ccc1C)CNCCc1cc(OC)c(OC)cc1	1.64
mol1234	O=C1CCCc2c1n(c1c2cc(cc1)C)CC(O)CNCCO	1.639
mol1235	s1nc2cc(NC(=O)NCc3occc3)ccc2n1	1.639
mol1236	Brc1ccccc1C1C2=C(OC(N)=C1C#N)CCCC2=O	1.635
mol1237	O=C1N(c2c(cc(cc2C)C)C1NC(=O)C)CC	1.635
mol1238	O=C1N(C(=O)C2C1CCCC2)c1c2c(ccc1)cccc2	1.635
mol1239	O1C2=C(C(C(C#N)=C1N)c1ccccc1)C(=O)CC(C2)C	1.634
mol1240	s1c2CCCCc2c2c1nc(nc2N1CCOCC1)C	1.634

mol1241	S(CC=C)C1=[NH+]C([O-])=C(C(CC)C)C(=O)N1	1.631
mol1242	Fc1cc(ccc1)C[NH2+]CCc1c2c([nH]c1)cccc2	1.63
mol1243	Oc1c2cc(ccc2nc(C)c1CN1CCN(CC1)CC)CC	1.629
mol1244	S=C1NN=C(N1c1ccc(OC)cc1)c1ccc(cc1)C	1.627
mol1245	o1c(ccc1CO)-c1ccc([N+](=O)[O-])cc1OC	1.627
mol1246	OCCCc1[nH]c2c(n1)cc1c(c2)cccc1	1.626
mol1247	O=C1CCCc2c1n(c1c2cc(cc1)C)CC(O)CNCCO	1.624
mol1248	S(=O)(=O)(NCCNC(=O)N1CCOCC1)c1ccccc1	1.623
mol1249	O=C1N(c2c(cc(cc2C)C)C1NC(=O)C)CC	1.62
mol1250	S(CC=C)C1=[NH+]C([O-])=C(C(CC)C)C(=O)N1	1.62
mol1251	Ic1ccccc1NC(=S)NC(=O)CC	1.619
mol1252	O=C1N(CCOC)C(=O)C2C1C1c3c(C2c2c1cccc2)cccc3	1.619
mol1253	S1c2c3c(cccc3c(S(=O)(=O)NCCCOC)cc2)C1=O	1.618
mol1254	S(=O)(=O)(N1CCN(C1)C(=O)CN1CCN(CC1)C)c1ccc(cc1)C	1.617
mol1255	S=C(Nc1ccc(F)cc1)NC(=O)C1CC1	1.614
mol1256	Clc1ccc(NC(=O)C(=O)NCC=C)cc1	1.614
mol1257	O(CC=C)CCn1nc(cc1C)C	1.612
mol1258	s1nnc2cc(NC(=O)NCCOC)ccc12	1.612
mol1259	S1C(=N)C(C#N)C(C(C#N)C1=N)c1c(C)c([N+](=O)[O-])c(cc1C)C	1.61
mol1260	Ic1cc(ccc1OC)C(=O)N1CCCC1	1.61
mol1261	O1CCOc2c1cc(NC(=O)C1n3c4c(nc3NC(=O)C1)cccc4)cc2	1.609
mol1262	O(CCCn1ccnc1)c1ccc(cc1)C	1.605
mol1263	Oc1ccccc1NC(=O)c1ccc([N+](=O)[O-])cc1	1.605
mol1264	O1C(COC12CCCCCCCCCCC2)CNCCN	1.605
mol1265	O1C2=C(C(C(C#N)=C1N)c1ccccc1)C(=O)CC(C2)C	1.604
mol1266	O(CCCC)c1ccc(NC=2NC(=O)C=C(N=2)C)cc1	1.601
mol1267	o1nc(NC(=O)c2cc3OCCOc3cc2)cc1C	1.598
mol1268	O1c2cc(ccc2OC1)CNC(=O)C(=O)NCC=C	1.594
mol1269	o1nc(cc1-c1cc(OC)c(OC)cc1)C(OC)=O	1.593
mol1270	S=C(Nc1ccccc1C#N)NC(=O)CC(C)C	1.592
mol1271	O=C1C2C(=NC(C)=C(C#N)C2c2ccccc2)CCC1	1.59
mol1272	O=C(NC(C)C)C(=O)NCCc1ccccc1	1.59
mol1273	[nH+]1c2c(n3c1NC[NH+](C3)CCC)cccc2	1.586
mol1274	BrC=1C=Nc2nc(nn2C=1)C(=O)NCCC	1.584
mol1275	Clc1ccc(cc1)-c1onc(c1)C(OC)=O	1.584
mol1276	S(=O)(=O)(NCCCn1ccnc1)c1ccc(cc1)C	1.582
mol1277	[NH3+]CC12CC3(CC(C1)CC(C3)C2)c1cc(C)c(cc1)C	1.582
mol1278	s1c2cc(OC)ccc2nc1NCc1cccnc1	1.582
mol1279	S=C1NN=C(N1C)COc1cc(ccc1C)C	1.577
mol1280	Clc1cc(N2C(=O)C3C(CCCC3)C2=O)ccc1C(O)=O	1.575
mol1281	Clc1cc(N2C(=O)C3C(CCCC3)C2=O)ccc1C(O)=O	1.575
mol1282	S=C(Nc1cc(C)c(cc1O)C)NC(=O)CC	1.571

mol1283	s1c2c(c3c1NC(NC3=O)c1ccc(cc1)CC)CCN(C2)C	1.57
mol1284	Ic1cc(ccc1C)C(=O)NCC1OCCC1	1.566
mol1285	O1c2cc(ccc2OC1)CNC(=O)C(=O)NC1CC1	1.565
mol1286	Brc1ccccc1CN1CCN(CC1)Cc1cccnc1	1.562
mol1287	Ic1cc(ccc1C)C(=O)NCC1OCCC1	1.562
mol1288	s1c2CCCCc2c2c1nc(nc2N1CC[NH2+]CC1)C	1.56
mol1289	S(CCCC)C=1NC(=O)C=C(N=1)C	1.559
mol1290	OCCCNC(c1ccccc1)c1ncccc1	1.559
mol1291	s1cccc1S(=O)(=O)N1CCCc2c1cccc2	1.556
mol1292	O(C(=O)C1C2c3c(C(c4c2cccc4)C1C(O)=O)cccc3)CCC	1.552
mol1293	O1c2c(OCC1CNCCC(OCC)=O)cccc2	1.55
mol1294	o1cccc1C1NC(=NC(=O)C1C(OCC)=O)N1CCN(CC1)CC	1.549
mol1295	O1CCN(CC1)CC#CC(O)(CCC=C)C	1.549
mol1296	OC=1c2c(cccc2)C(=O)C=1C1=CC(=O)Nc2c1cccc2	1.549
mol1297	O(C)c1cc(ccc1OC)C(=O)NCC(C)C	1.547
mol1298	S(CC#N)c1nnnn1-c1ccccc1F	1.547
mol1299	O(C(=O)C1C2c3c(C(c4c2cccc4)C1C(O)=O)cccc3)CCC	1.547
mol1300	Fc1ccccc1C1C2=C(OC(N)=C1C(OC)=O)CC(CC2=O)(C)C	1.547
mol1301	O=C1N(CCOC)C(=O)C2C1C1c3c(C2c2c1cccc2)cccc3	1.543
mol1302	Sc1nncn1NCc1ccc(cc1)C	1.541
mol1303	Oc1ccc(cc1)C(NCCCO)c1ccccc1	1.539
mol1304	O=C1NC(=O)N(C=C1)C(C(OCC)=O)C(OCC)=O	1.533
mol1305	FC(F)(F)C1n2nc(cc2NC(C1)c1occc1)C(=O)NCCOC	1.532
mol1306	S1(=O)(=O)CC(Nc2ccc(OC)cc2)C(NCc2occc2)C1	1.529
mol1307	Fc1ccc(cc1)C1C2=C(OC(N)=C1C(OCC)=O)CCCC2=O	1.528
mol1308	Brc1ccc(NC(=O)C(=O)NCC2OCCC2)cc1	1.527
mol1309	O=C1N=C(NC(C1)C(=O)Nc1ccccc1)N1CCc2c(C1)cccc2	1.526
mol1310	s1c2c(ncnc2NC(CC)CO)c2cc3c(nc12)CC(OC3)(C)C	1.526
mol1311	O=C1c2c(N(CC(=O)c3ccccc3)C1=O)cccc2	1.526
mol1312	S(=O)(Cc1oc2c(cc(OC)cc2)c1C(O)=O)c1ccccc1	1.52
mol1313	s1c2c(ncnc2NC(CC)CO)c2cc3c(nc12)CC(OC3)(C)C	1.519
mol1314	O1c2c(CC1C(=O)N1CCCCC1)cccc2	1.518
mol1315	O=C1Nc2c(cccc2)C12NCCc1c2[nH]c2c1cccc2	1.516
mol1316	[nH+]1c2c(n(CCCC)c1N)cccc2	1.513
mol1317	S(C)c1ccc(cc1)CNc1nnnn1C	1.513
mol1318	S=C(NCC=C)NNc1nc(nc(n1)N1CCCC1)N1CCCC1	1.513
mol1319	Clc1cc(ccc1Cl)CNc1nnnn1CC	1.513
mol1320	Brc1ccc(nc1C)NC(=O)CC	1.512
mol1321	O(C)c1cc(OC)ccc1CNCCCn1ccnc1	1.512
mol1322	Clc1cc(Cl)ccc1NC(=O)C1OCCC1	1.512
mol1323	Ic1cc(Cl)c(NC(=O)c2nc[nH]n2)cc1	1.511
mol1324	O1CCOc2c1cc(NC(=O)C1n3c4c(nc3NC(=O)C1)cccc4)cc2	1.511

mol1325	O(C(=O)C1C2c3c(C(c4c2cccc4)C1C(O)=O)cccc3)CCC	1.508
mol1326	O(C(=O)C1C2c3c(C(c4c2cccc4)C1C(O)=O)cccc3)CCC	1.508
mol1327	Fc1cc(ccc1)C(=O)NCc1ccccc1	1.507
mol1328	S=C(Nc1ccccc1N1CCOCC1)NC(=O)CCC	1.506
mol1329	O(CCCC)c1cc(ccc1)C1(CCCC1)C(O)=O	1.504
mol1330	Clc1cc(N2NC(=O)/C(=C\c3occc3)/C2=O)ccc1Cl	1.503
mol1331	Clc1cc(NC(=O)NC2CC2)ccc1	1.502
mol1332	Clc1cc(N2C(=O)C3C(CCCC3)C2=O)ccc1C(O)=O	1.501
mol1333	O=C1NC(=NC2=C1CCCC2)N1CCN(CC1)CC	1.5
mol1334	o1c(ccc1[N+](=O)[O-])C(=O)N(Cc1ccccc1)C	1.498
mol1335	o1cccc1C1NC(=NC(=O)C1C(OCC)=O)N1CCN(CC1)CC	1.496
mol1336	[NH+](Cc1cccnc1)(CCc1ncccc1)C	1.489
mol1337	O(C(C)(C)C)C(CC#CCN(CC)CC)C	1.486
mol1338	S(CC(=O)C)c1oc2c(n1)cccc2	1.484
mol1339	S(CCOC(=O)C)c1nc(nc(n1)N(C)C)N(C)C	1.481
mol1340	o1cccc1C1CC(=O)Nc2c1ccc1c2cccc1	1.481
mol1341	O=C(NCc1ccccc1)C(=O)NCC(C)C	1.478
mol1342	S1(=O)(=O)CC(NC(=O)C(=O)NC2CCS(=O)(=O)C2)CC1	1.478
mol1343	s1c2cc([N+](=O)[O-])ccc2nc1NC(=O)c1c(F)cccc1F	1.474
mol1344	OCCCNc1[nH]c2cc(C)c(cc2n1)C	1.471
mol1345	o1cccc1C1NC(=NC(=O)C1C(OCC)=O)N1CCN(CC1)CC	1.469
mol1346	s1c(ccc1C=O)CCCC	1.468
mol1347	S(Cc1nc(nc(n1)N)Nc1ccccc1OC)CCO	1.466
mol1348	O1c2cc(ccc2OC1)C1N(CCCOC)C(=O)C(O)=C1C(=O)c1ccccc1	1.466
mol1349	S(CC(=O)Nc1cc(F)c(F)cc1)c1nccn1C	1.466
mol1350	s1c2cc(OC)ccc2nc1NCc1ccncc1	1.466
mol1351	O1c2c(OCC1CNC(=O)C(=O)NCCCO)cccc2	1.463
mol1352	Clc1nc(nc(n1)NCCO)NCC=C	1.462
mol1353	Clc1ccc(-n2cnnc2)cc1C(=O)NCc1ccc(OC)cc1	1.46
mol1354	O1CCN(CC1)CCCNCc1c2c(ccc1)cccc2	1.459
mol1355	OC1=C(C(=O)c2ccc(cc2)C)C(N(CCC(O)=O)C1=O)c1ccc(cc1)C	1.456
mol1356	S=C(NC1CCCCC1)NC(=O)c1occc1	1.455
mol1357	s1c(nnc1SCC(=O)Nc1ccccc1)NC(=O)C	1.455
mol1358	s1c2c(nc1N1CCCCC1)CCCC2=O	1.454
mol1359	S=C(Nc1ccccc1OCC)NC(=O)CC	1.453
mol1360	O=C1N(CC(OCCC)=O)C(=O)c2c1cccc2	1.452
mol1361	O(C(=O)C(=O)c1n2c(cc1C)C=CC=C2)CC	1.452
mol1362	O1C2=C(C(C(C(OCCOC)=O)=C1N)c1ccncc1)C(=O)CC(C2)(C)C	1.452
mol1363	OCCNC(=O)C(c1ccccc1)c1ccccc1	1.451
mol1364	O1CCN(CC1)CCOc1cc2c(cc1)cccc2	1.45

mol1365	Clc1cc(NC(=O)N2CCN(CC2)C)ccc1	1.444
mol1366	Clc1ccc(cc1)CNC(=O)C(=O)NC(C)C	1.437
mol1367	O(C)c1cc2c(N(C)C(=O)C2NC(=O)C)cc1	1.434
mol1368	Clc1cc(ccc1)CNc1nnnn1CC	1.433
mol1369	O(C)c1ccc(cc1)CN(C#N)c1nc(nc(n1)N(C)C)N(C)C	1.433
mol1370	O=C(C(=O)N1CCCCCC1)c1c2c([nH]c1)cccc2	1.432
mol1371	O(C)c1cc2c(N(C)C(=O)C2NC(=O)C)cc1	1.432
mol1372	O1CCN(CC1)CCCNC1CC(=O)N(C1=O)c1ccc(cc1)C	1.43
mol1373	S=C(Nc1ccc(F)cc1)Nc1ncccc1	1.43
mol1374	Clc1ccccc1C1OCC2(SC(=O)NC2=O)CO1	1.43
mol1375	S(=O)(=O)(NC(=O)NCCCC)c1oc(cc1)C(OC(C)C)=O	1.429
mol1376	o1cccc1CNCC(O)COc1ccccc1	1.427
mol1377	O1CCCC1CNC(=O)C(=O)Nc1ccc(OC)cc1	1.421
mol1378	S(CC#N)c1nnnn1-c1ccccc1	1.42
mol1379	Brc1ccc(NC(=O)C(=O)NCC2OCCC2)cc1	1.42
mol1380	O=C1N(C)C(=O)N(c2nc([N+](=O)[O-])n(c12)Cc1ccc(cc1)C)C	1.42
mol1381	S(CC(=O)NCc1occc1)C1=[NH+]C([O-])=C(CCCC)C(=O)N1	1.419
mol1382	Brc1cc(ccc1)C(=O)NCC=C	1.419
mol1383	Clc1cc(cc(OC)c1OCC)CNc1[nH]ncn1	1.418
mol1384	OC1(c2c(NC1=O)cccc2)CC(=O)c1ccc([N+](=O)[O-])cc1	1.417
mol1385	O(C)c1cc(ccc1OC)CCNCc1cc(OC)cc(OC)c1	1.415
mol1386	S1\C(=C/c2ccccc2)\C(=O)N(CC(=O)Nc2ccc(cc2)C(O)=O)C1=S	1.415
mol1387	FC(F)(F)C(=O)c1c2c(n(CC(=O)N)c1C)cccc2	1.411
mol1388	Clc1cc(N2NC(=O)/C(=C\C=C/c3occc3)/C2=O)ccc1F	1.41
mol1389	o1nc(NC(=O)CCCOc2ccccc2)cc1C	1.409
mol1390	Oc1cc(O)ccc1C(OC(CCN(CC)CC)C)=O	1.407
mol1391	O(CCn1c2c(nc1NCCO)N(C)C(=O)NC2=O)c1ccccc1	1.406
mol1392	OCCCNc1[nH]c2c(n1)cc(cc2)C	1.405
mol1393	s1cc(nc1NCC=C)CC(OCC)=O	1.403
mol1394	O1CCCC1CNC(=O)C(=O)Nc1ccc(OC)cc1	1.403
mol1395	s1cccc1S(=O)(=O)Nc1ccccc1OCC	1.402
mol1396	O=C(Nc1c2c(ccc1)cccc2)C(=O)NC	1.4
mol1397	O(C)c1cc(NC(=O)C(=O)NC)ccc1OC	1.397
mol1398	O=C1NC(=O)N(c2nc(n(c12)CCC)NCCCO)C	1.397
mol1399	S(O)(=O)(=O)CCNCc1cc(cc(C(C)(C)C)c1O)C(C)(C)C	1.395
mol1400	Brc1ccc(S(=O)(=O)CCC(OCC)=O)cc1	1.394
mol1401	Clc1cc(N2C(=O)C3C(CC=CC3)C2=O)ccc1C(O)=O	1.394
mol1402	O=C1N(C(=O)CC1N1CCCCC1CC)c1ccc(NC(=O)C)cc1	1.393
mol1403	Fc1ccc(cc1)Cn1c2c(nc1NCCO)N(C)C(=O)NC2=O	1.389
mol1404	O(CC)c1cc2[nH]c(nc2cc1)NCCO	1.388
mol1405	O1CCN(CC1)CCCNC1CC(=O)N(C1=O)c1ccc(cc1)C	1.388

mol1406	Clc1ccc(cc1NC(=S)NC(=O)c1occc1)C(O)=O	1.387
mol1407	FC(F)(F)C(=O)Cc1nc2c(cc1)cccc2	1.384
mol1408	S=C(Nc1cc(OC)ccc1OC)NC(=O)CC	1.383
mol1409	OC(=O)c1cc2c(cc1NCCC#N)cccc2	1.381
mol1410	S=C(NC(=O)C1CC1)NCc1ccccc1	1.379
mol1411	Brc1oc(cc1)C(=O)Nc1ccccc1C#N	1.375
mol1412	O=C(Nc1nc(cc(c1)C)C)c1cc(C)c([N+](=O)[O-])cc1	1.375
mol1413	O(CCCNC(c1ccccc1)c1ccncc1)C	1.369
mol1414	s1c2c(nc1N)c(ccc2C)C	1.365
mol1415	S(=O)(=O)(N(CC(O)=O)C)c1cc2c3c(oc2cc1)cccc3	1.364
mol1416	O(C)c1cc(OC)ccc1NC(=O)C(=O)NCc1cccnc1	1.361
mol1417	O1CCN(CC1)CCCCOc1ccccc1OC	1.358
mol1418	s1c(nnc1SCC(=O)Nc1cc(F)c(F)cc1)C	1.358
mol1419	o1cccc1CNCCc1cc2OCOc2cc1	1.356
mol1420	S=C(Nc1ccccc1C(OC)=O)NC(=O)C	1.354
mol1421	Clc1ccc(Cl)cc1S(=O)(=O)NCCOC	1.352
mol1422	O=Cc1cc(C)c(N2CCCC2)cc1	1.346
mol1423	O1c2cc(ccc2OC1)CN1CCN(CC1)C(=O)CN1C(=O)C2C(CCCC2)C1=O	1.346
mol1424	S(CC(O)=O)c1nc2n(c3c(c2nn1)cccc3)CCC	1.345
mol1425	O1CCCC1CNC(CCc1ccccc1)C	1.344
mol1426	O1CCN(CC1)CCCNCc1ccc(OC)cc1OC	1.343
mol1427	Brc1c(n(nc1[N+](=O)[O-])CC(=O)NCCOC)C	1.341
mol1428	S(=O)(=O)(N1CCCCC1)c1ccc(NCCCC(O)=O)cc1	1.341
mol1429	Clc1ccccc1OCCCN1CCNCC1	1.339
mol1430	s1cccc1COc1ccc(cc1)CNCCO	1.339
mol1431	O1C2=C(C(C(C(OCC)=O)=C1N)c1ccccc1)C(=O)CCC2	1.336
mol1432	Clc1ccc(cc1)C1N(CCC(O)=O)C(=O)C(O)=C1C(=O)c1ccc(cc1)C	1.335
mol1433	O(C(=O)C(C(C(C(OC)=O)C(OC)=O)(C)C)C(OC)=O)C	1.331
mol1434	O1CCN(CC1)CCCNCc1ccc(cc1)C(C)C	1.325
mol1435	Clc1ccc(cc1)C=1O\C(=C\C(OC)=O)\C(=O)C=1	1.323
mol1436	O=C1N(CC(=O)Nc2nc(cc(n2)C)C)C(=O)C2C1CCCC2	1.32
mol1437	O=C1NC2N(CCC)C(=O)NC2N1CCC	1.318
mol1438	Fc1ccc(cc1)CC[NH2+]Cc1cccnc1	1.315
mol1439	S=C(Nc1ccc(cc1)C(=O)N)NC(=O)CC	1.314
mol1440	O=C1N(CC(=O)Nc2nc(cc(n2)C)C)C(=O)C2C1CCCC2	1.314
mol1441	O=C1N(CC(O)Cn2nc(cc2C)C)C(=O)NC1(C)C	1.313
mol1442	Fc1ccccc1Nc1nc(N2CCOCC2)c2c(n1)cccc2	1.312
mol1443	OC1=C(C(=O)c2ccccc2)C(N(CCCOC)C1=O)c1ccccc1	1.312
mol1444	n1nnn(C)c1NCc1ccccc1C	1.311
mol1445	S(CC#CCO)C=1NC(=O)c2c(N=1)cccc2	1.31
mol1446	O(C)c1c(OC)c2c(NC(=O)CC2c2ccncc2)cc1OC	1.308

mol1447	ClCC(=O)NC(Cc1ccccc1)(C)C	1.307
mol1448	O=C(N)CN1CCN(CC1)C(=O)NC1CCCCC1	1.307
mol1449	s1cc(c2CCCCc12)C(=O)N1CCOCC1	1.306
mol1450	S=C(Nc1ccc(N(C(=O)C)C)cc1)NC(=O)CCC	1.303
mol1451	s1cc(nc1N)C1=Cc2cc([N+](=O)[O-])ccc2OC1=O	1.302
mol1452	O=C1N(CC(=O)Nc2nc(cc(n2)C)C)C(=O)C2C1CCCC2	1.302
mol1453	s1cnnc1NC(=O)CSc1snc(SC)n1	1.294
mol1454	Fc1ccc(cc1)CNCCc1ccccc1	1.293
mol1455	o1c2c(NC(=O)C(C(O)=O)=C2c2ccccc2)c2c1cccc2	1.284
mol1456	S(=O)(=O)(NCCOC)c1c(cc(cc1C)C)C	1.28
mol1457	O1CCN(CC1)CCCNCc1ccccc1OCC	1.278
mol1458	O(CCCN1CCCCC1)c1ccccc1	1.277
mol1459	Brc1cc(cc(OC)c1OC)CNc1[nH]ncn1	1.275
mol1460	S(=O)(=O)(NCCCN(C)C)c1ccc(cc1)C	1.273
mol1461	Clc1cc(ccc1)CNCCCN1CCOCC1	1.265
mol1462	S(=O)(=O)(N1CCC(CC1)C(=O)NCCCOCC)C	1.265
mol1463	s1c(nnc1NC(OCCCCC)=O)C	1.264
mol1464	[NH+](CCC[NH2+]Cc1ccc(N(CC)CC)cc1)(C)C	1.264
mol1465	[NH+]=1CCNC=1Cc1cc2c(cc1)cccc2	1.263
mol1466	S(CCCC)c1nc2c(n1CC(O)=O)cccc2	1.261
mol1467	Clc1ccc(N2C3=C(C=C(C(=O)NCCO)C2=O)C(=O)CCC3)cc1	1.26
mol1468	O=C1NC2N(CCC)C(=O)NC2N1CCC	1.26
mol1469	S(C(C(O)=O)C)c1n2-c3c(Nc2nn1)cccc3	1.26
mol1470	O=C1NC2N(CCC)C(=O)NC2N1CCC	1.259
mol1471	O(CC)c1ccc(cc1)C1N(CCC(O)=O)C(=O)C(O)=C1C(=O)c1ccc(cc1)C	1.258
mol1472	Brc1ccc(cc1)C1=NNC(=S)N1c1ccc(OC)cc1	1.255
mol1473	O(C)c1cc(ccc1OC)C1C(=CN(C=C1C(OC)=O)CCOC)C(OC)=O	1.251
mol1474	O=C1N(c2c3c1cccc3ccc2)CC(=O)N1CCCC1	1.245
mol1475	Brc1cc(cnc1)C(=O)N\N=C\c1cc(O)c(O)cc1	1.244
mol1476	[NH2+](C(C)c1ccccc1)CC#C	1.243
mol1477	Oc1cc2CCC3C4CCC(=O)C4(CC(=O)C3c2cc1)C	1.243
mol1478	O=C1N(c2c3c1cccc3ccc2)CC(=O)NCCOC	1.242
mol1479	[NH+](CC1(CCCC1)c1ccccc1)(C)C	1.239
mol1480	S1(=O)(=O)N(CC(=O)N)C(C(=O)c2ccccc2)C(=O)c2c1cccc2	1.238
mol1481	O=C1N=C(NC2(CCCCC2)C1C#N)N1CCN(CC1)C(OCC)=O	1.237
mol1482	Clc1ccc(-n2cnnc2)cc1C(=O)Nc1ccc(cc1O)C	1.237
mol1483	Clc1cc(C(NC(=O)C)c2occc2)c(O)c2ncccc12	1.233
mol1484	o1nc(nc1CCC(O)=O)-c1cc(OC)c(OC)c(OC)c1	1.232
mol1485	O1c2c(N(CC(OCC)=O)C1=O)cc(cc2)C	1.232
mol1486	Clc1cc(ccc1)CNc1nnnn1C	1.231
mol1487	Fc1ccccc1CNCCCn1ccnc1	1.231

mol1488	Fc1ccccc1-n1cccc1\C=C/1\NC(=O)NC\1=O	1.227
mol1489	Brc1oc(cc1)C(=O)NC(=S)N1CCCC1	1.226
mol1490	S(CC(=O)Nc1noc(c1)C)c1ncccn1	1.226
mol1491	Clc1ccc(cc1)Cn1c2c(nc1[N+](=O)[O-])N(C)C(=O)N(C)C2=O	1.226
mol1492	OC(C(C)C)(C#CCN(CC)CC)C	1.225
mol1493	s1cc(nc1SCCCCCCC(O)=O)C	1.224
mol1494	Clc1cc2sc(nc2cc1)NC(=O)CCCC(O)=O	1.222
mol1495	O=C1N=C(NC2(CCCCC2)C1C#N)N1CCN(CC1)C(OCC)=O	1.218
mol1496	n1ccn(c1)CCCNC1CCC(CC1)CC	1.215
mol1497	n1cc(ccc1)CN1CCN(CC1)Cc1ccccc1	1.208
mol1498	O(CCCC)c1ccc(N2C(=O)C(N3CCC(CC3)C(=O)N)CC2=O)cc1	1.206
mol1499	O=C(Nc1ccc(NC(=O)C)cc1)C1CC1c1ccccc1	1.204
mol1500	N(C(C)c1ccccc1)C1CCCC1	1.203
mol1501	O(C(=O)c1nc2n(n1)C=C([N+](=O)[O-])C=N2)CCCC	1.201
mol1502	n1nnn(CCC)c1NCc1n(ccc1)C	1.2
mol1503	Fc1cc(ccc1)CNCCCn1ccnc1	1.198
mol1504	S(CC(=O)C1Oc2c(OC1)cccc2)C=1NCCN=1	1.196
mol1505	[NH2+](Cc1n(ccc1)-c1ccccc1)CCCC	1.195
mol1506	OC(C(C)C)(C#CCN(CC)CC)C	1.194
mol1507	[NH2+](Cc1n(ccc1)C)CCc1c2c([nH]c1)cccc2	1.187
mol1508	s1cccc1C=1n2ncc(c2N=CC=1)C(O)=O	1.186
mol1509	O1CCN(CC1)CCCNCc1ccc(cc1)CC	1.186
mol1510	OCCNc1[nH]c2c(n1)cc(cc2)C	1.185
mol1511	OC1=C(C(=O)c2ccc(cc2)C)C(N(CCC(O)=O)C1=O)c1ccc(cc1)C	1.18
mol1512	O(CC=C)c1nc(nc(n1)NCC)N(C)C	1.18
mol1513	Clc1ccc(-n2cnnc2)cc1C(=O)Nc1ccc(OC)cc1	1.18
mol1514	O1CCN(CC1)c1nc(nc(n1)NCCC)N1CCOCC1	1.178
mol1515	S1C2(COC(OC2)c2ccc(OC)cc2)C(=O)NC1=O	1.178
mol1516	S1C(=N)C(C#N)C(C(C#N)=C1N)c1ccc(OC)c(OC)c1OC	1.177
mol1517	Fc1ccc(cc1)C(CCN)c1ccc(OC)cc1	1.177
mol1518	O(C)c1ccccc1CNCCCn1ccnc1	1.177
mol1519	S=C1NN=C(N1c1ccc(cc1)C)c1ccccc1	1.176
mol1520	O(CC(O)CN)c1ccccc1C(C)C	1.171
mol1521	O1CCN(CC1)Cc1c(nc2c(cc(cc2)CC)c1O)C	1.164
mol1522	s1c2cc(S(=O)(=O)C)ccc2nc1NC(=O)c1cc(ccc1C(O)=O)C	1.16
mol1523	O(CC(O)Cn1ccnc1)c1ccccc1	1.159
mol1524	O(CC(O)CN)c1ccccc1C(C)C	1.157
mol1525	s1cccc1CNCCCOC(C)C	1.156
mol1526	o1c2c(cc(OCC#N)cc2)c(C(OC)=O)c1C	1.154
mol1527	S(CCOc1ccccc1)C=1NCCN=1	1.154
mol1528	o1c(C)c(cc1CC(C)C)C(=O)NCCCC(O)=O	1.153

mol1529	s1cccc1C(=O)NC(=S)N1CCCCC1	1.148
mol1530	Brc1cc(N2C(=O)C3C(C4OC3(C=C4)CO)C2=O)ccc1C	1.14
mol1531	S=C1NC(=O)C=C(N)N1c1cc(ccc1)C	1.139
mol1532	s1ccc(C)c1CNn1cnnc1S	1.138
mol1533	OC=1c2c3N(CCc3ccc2)C(=O)C=1C(=O)NCCc1ccccc1	1.135
mol1534	O(CC(O)CN)c1ccc(cc1)C(C)(C)C	1.132
mol1535	O(CCC)c1ccc(cc1)C1NC(=O)CCC1[N+](=O)[O-]	1.126
mol1536	O(CCC)c1ccc(cc1)C1NC(=O)CCC1[N+](=O)[O-]	1.125
mol1537	S=C(Nc1ccc(O)cc1)NC(=O)CC	1.125
mol1538	O=C(NCc1ccccc1)C(=O)NCC=C	1.124
mol1539	O=C1c2c(N(CCN3CCCCC3)C1=O)cccc2	1.121
mol1540	O1CCC(O)(CC1(C)C)CCNCc1ccc(N(C)C)cc1	1.118
mol1541	O(C)c1c(OC)c2c(NC(=O)CC2c2ccncc2)cc1OC	1.117
mol1542	O=C1N(C)C(=O)N(c2nc(n(c12)CCOC)CN1CC(CCC1)C)C	1.113
mol1543	O1c2cc(NC(=O)Cn3c(ncc3[N+](=O)[O-])C)ccc2OC1	1.109
mol1544	O=C1NC(=O)N(c2nc(n(c12)CCOCC)CN1CCN(CC1)CC)C	1.108
mol1545	O=C1N(C)C(=O)N(c2nc(n(c12)CCCO)CN1CCN(CC1)C)C	1.102
mol1546	OC(=O)c1cc(nc2c1cccc2C)-c1ncccc1	1.098
mol1547	O=C1N=C(NC2(CCCCC2)C1C#N)N1CCN(CC1)c1ccccc1	1.098
mol1548	O1CCc2c(cccc2)C1CNC(=O)C(=O)NCCO	1.094
mol1549	FC(F)(F)C(=O)c1c2c(n(c1)CC#N)cccc2	1.093
mol1550	O(CC(O)CN)c1ccc(cc1)C(C)(C)C	1.093
mol1551	o1ccc(C(=O)NN2C(=O)c3c(cccc3)C2=O)c1C	1.093
mol1552	O1CCC(O)(CC1(C)C)CCNCc1ccc(N(C)C)cc1	1.091
mol1553	ClCC(=O)Nc1snc(SCC)n1	1.08
mol1554	O(CC)c1ccc(cc1)C1N(CCC(O)=O)C(=O)C(=O)C1C(=O)c1ccc(cc1)C	1.08
mol1555	O1CCN(CC1)Cc1nc2N(C)C(=O)N(C)C(=O)c2n1CCOCC	1.08
mol1556	O1CCc2c(cccc2)C1CNC(=O)C(=O)NCCO	1.069
mol1557	Clc1cc(N2C(=NNC2=S)c2occc2)ccc1F	1.067
mol1558	O=C1N(C)C(=O)N(c2nc([nH]c12)CNC(C)c1ccccc1)C	1.067
mol1559	OC(=O)c1cc2nnn(c2cc1)C1CCCCC1	1.066
mol1560	O1CCN(CC1)CCCNCc1ccccc1C	1.063
mol1561	S1CCNC(=O)C1CC(=O)Nc1cc(ccc1)C	1.062
mol1562	S(=O)(=O)(NCCO)c1c2c3c(ccc2)C(=O)Nc3cc1	1.062
mol1563	O=C1N(C)C(=O)N(c2nc([nH]c12)CNC(C)c1ccccc1)C	1.057
mol1564	OC=1c2c(N(CCC)C(=O)C=1C(=O)NNC(=O)CC(C)C)cccc2	1.057
mol1565	S(CC[NH2+]Cc1n(ccc1)C)c1nnnn1C	1.056
mol1566	O(CCCN1CCNCC1)c1cc(OC)ccc1	1.054
mol1567	O(CCn1c2c(nc1NCCN)N(C)C(=O)NC2=O)c1ccccc1	1.053
mol1568	O=C1NC(=O)N(c2nc(n(c12)CCO)NCC=C)C	1.052
mol1569	[NH2+]1CCn2c(ccc2)C1CCC	1.052
mol1570	[NH2+]1CCn2c(ccc2)C1CCC	1.052

mol1571	Fc1ccc(cc1)C1N(CCC(O)=O)C(=O)C(O)=C1C(=O)c1ccc(cc1)C	1.051
mol1572	o1cccc1CNCCCOC(C)C	1.05
mol1573	O1c2cc(ccc2OC1)C(=O)NCCCn1ccnc1	1.048
mol1574	O=C(NC(Cc1c2c([nH]c1)cccc2)C)C	1.046
mol1575	S=C1NC(=O)C(CCCCCC)C(=O)N1	1.043
mol1576	O=C1N=C(NC2(CCCCC2)C1C#N)N1CCN(CC1)c1ccccc1	1.043
mol1577	s1cc(nc1C)-c1ccc(N)cc1	1.038
mol1578	OC(=O)c1cc(nc2c1cccc2C)-c1cccnc1	1.037
mol1579	Fc1cc(ccc1)CNCCCN1CCOCC1	1.032
mol1580	s1cccc1C(=O)NCCCOC	1.03
mol1581	O(CCCNC(C)c1ncccc1)C	1.03
mol1582	O=C1N(C)C(=O)N(c2nc(n(c12)CCOC)CN1CC(CCC1)C)C	1.02
mol1583	O=C1N(NC(=O)C2CCCCC2)C(=O)c2c1cccc2	1.02
mol1584	O(CCC)c1ccc(cc1)C1NC(=O)CCC1[N+](=O)[O-]	1.017
mol1585	O(CCC)c1ccc(cc1)C1NC(=O)CCC1[N+](=O)[O-]	1.017
mol1586	O(C)c1c(OC)cc(cc1OC)CNCCN(C)C	1.013
mol1587	O=C1NC(=O)N(c2nc(n(c12)CCCC)N(C)C)C	1.012
mol1588	O=C1N(CCOC)C(C)=C(C1)C(OCC)=O	1.009
mol1589	S(O)(=O)(=O)c1nc2c(n1CCOc1cc(ccc1)C)cccc2	1.009
mol1590	Clc1c(NC(=O)C(=O)N)cccc1Cl	1.008
mol1591	n1ccn(c1)CCCNCc1ccccc1C	1.007
mol1592	O(C)c1cc(ccc1OC)CNCCN(C)C	1.004
mol1593	Clc1ccc(-n2cnnc2)cc1C(=O)NC1CCCCC1	1.003
mol1594	Clc1ccc(N2C(=NNC2=S)c2nc3c(cc2)cccc3)cc1C(O)=O	0.998
mol1595	O(C(C)C)c1ccc(N)cc1	0.996
mol1596	O=C1N(CC(C1)C(=O)NCCO)c1ccccc1	0.993
mol1597	O(C)c1cc(C(O)=O)c(cc1)-c1ccc(OC)cc1	0.992
mol1598	O=C(NCCc1ccncc1)NCCC	0.991
mol1599	O1CCOC1(Cc1[nH]c2c(n1)cccc2)C	0.986
mol1600	O=C1N(CC(C1)C(=O)NCCO)c1ccccc1	0.985
mol1601	Clc1ccccc1NC(=O)CC1SCCNC1=O	0.983
mol1602	Fc1ccc(cc1)C(CCN)c1ccc(OC)cc1	0.982
mol1603	O(C)c1ccc(OC)cc1CNCCCO	0.982
mol1604	O(C(C)C)c1cc(N)ccc1	0.976
mol1605	O(C)c1c(cccc1OC)CNCCN(C)C	0.974
mol1606	S1CCNC(=O)C1CC(=O)Nc1cc(ccc1)C	0.971
mol1607	Fc1cc(ccc1)C(=O)NCc1occc1	0.969
mol1608	N(CC1C2CC(C1)C=C2)(CCCN(C)C)CCCN(C)C	0.961
mol1609	O1CCN(CC1)CCCNCc1cc(ccc1)C	0.96
mol1610	O=C(Nc1ccc(cc1)C)c1ccncc1	0.959
mol1611	S1(=O)(=O)CC(CC1)C(C(=O)C)C(OCC)=O	0.959
mol1612	S(=O)(=O)(NC(CN1CCNCC1)(C)C)c1ccccc1	0.959

mol1613	Fc1ccc(OCC(=O)NC2CC2)cc1	0.956
mol1614	Fc1ccccc1C[NH2+]CC=C	0.955
mol1615	S(=O)(=O)(N1CCCCC1)c1cc(ccc1C)C(O)=O	0.954
mol1616	S(Cc1ccc(OC)cc1)C1=NC(=O)C(=NN1)C	0.952
mol1617	O=C1N(C(=O)c2c1cc([N+](=O)[O-])cc2)c1cccnc1	0.952
mol1618	S(=O)(=O)(N)c1ccc(NC(=O)C(=O)N2CCCCC2)cc1	0.95
mol1619	Clc1ccccc1NC(=O)C1N2N(C(=O)C1)C(S)=NC(=O)C2(C)C	0.949
mol1620	S(=O)(=O)(NCc1occc1)c1ccc(N)cc1	0.949
mol1621	O1C(C)(C)C(=O)CC1c1ccccc1	0.948
mol1622	Clc1ccc(cc1)C1C(=CN(C=C1C(OC)=O)CCOC)C(OC)=O	0.948
mol1623	O1CCN(CC1)CCCNC(=O)Cc1ccccc1	0.948
mol1624	Ic1cc(ccc1C)C(=O)N1CCOCC1	0.947
mol1625	O(C)c1cc2[nH]c(nc2cc1)NCCO	0.944
mol1626	o1cccc1CNC(=O)C(=O)NCc1ncccc1	0.939
mol1627	s1c(nnc1NC(=O)C)CCCCC	0.935
mol1628	o1cccc1CNC(=O)C(=O)NC1CCCC1	0.934
mol1629	Brc1cc2N(C(=O)C)C(=O)C(=O)c2cc1C	0.928
mol1630	n1ccn(c1)CCCNCc1ccc(cc1)C	0.926
mol1631	Clc1cc(NC(=O)C2n3ncnc3NC(=O)C2)c(cc1)C	0.925
mol1632	Clc1ccc(-n2cnnc2)cc1C(=O)NCc1ccccc1	0.925
mol1633	s1c(ccc1C(O)=O)-c1cc2OCCOc2cc1	0.924
mol1634	S1CC(=O)N(CC(=O)Nc2ccc(F)cc2)C1=O	0.921
mol1635	S1CCN2C3=Nc4c(C3=NN=C12)cccc4	0.918
mol1636	[NH2+](Cc1n(ccc1)-c1ccccc1)CC=C	0.918
mol1637	O(CC(O)CN)c1ccc(cc1)CC	0.915
mol1638	O(C)c1cc(ccc1OC)CNCCCO	0.914
mol1639	n1(c2c(cc(N)cc2)cc1)C	0.911
mol1640	OC1=C(C(=O)c2ccc(cc2)C)C(N(CCC(O)=O)C1=O)c1ccccc1	0.908
mol1641	S(=O)(=O)(NCCCCCCC(O)=O)c1ccccc1	0.906
mol1642	Clc1ccc(cc1)C1=NNC(=S)N1c1cc2OCCOc2cc1	0.906
mol1643	S(=O)(=O)(NCCO)c1cc2c(cc(O)cc2)cc1	0.905
mol1644	O=C1NC(CC1)C(=O)NCCCn1ccnc1	0.905
mol1645	O1C2=C(NC(=O)NC2=O)C(C(C#N)=C1N)c1cc([N+](=O)[O-])ccc1	0.902
mol1646	O1C2=C(NC(=O)NC2=O)C(C(C#N)=C1N)c1cc([N+](=O)[O-])ccc1	0.902
mol1647	S(=O)(=O)(NCCO)c1ccc(OC)cc1	0.899
mol1648	S=C(Nc1ccccc1C#N)NC(=O)CC	0.898
mol1649	O1CCN(CC1)CCCNC=1CC(CC(=O)C=1)(C)C	0.898
mol1650	Fc1ccc(cc1)C1N(CCC(O)=O)C(=O)C(O)=C1C(=O)c1ccc(cc1)C	0.891
mol1651	[NH+]=1C[NH+](CNC=1Nc1nc(c2c(n1)c(ccc2)C)C)Cc1cccnc1	0.89

mol1652	O1c2cc(NC(=O)C(=O)NC)ccc2OC1	0.89
mol1653	S1CCNC(=O)C1CC(=O)Nc1ccc(cc1)C	0.887
mol1654	Fc1ccccc1C1N(CCC(O)=O)C(=O)C(O)=C1C(=O)c1ccc(cc1)C	0.886
mol1655	O1CCN(CC1)CCCNCc1cc(OC)ccc1	0.885
mol1656	S1C=2N(N=C1c1ccccc1)C(=O)CC(=O)N=2	0.879
mol1657	S(CC(=O)Nc1cc(F)c(F)cc1)c1nncn1C	0.875
mol1658	s1ccc(C)c1CNCC(O)C	0.873
mol1659	O1CCN(CC1)CCNCc1ccccc1OC	0.871
mol1660	OCCCNC(=O)C(=O)NC1CCCCC1	0.866
mol1661	Clc1cc(NC(=O)C2n3ncnc3NC(=O)C2)c(cc1)C	0.861
mol1662	O=C1N=C(NC2(CCCCC2)C1C#N)N1CCCCC1	0.861
mol1663	Fc1ccccc1C1N(CCC(O)=O)C(=O)C(O)=C1C(=O)c1ccc(cc1)C	0.86
mol1664	S(CC#C)C=1NC(=O)C=C(C)C=1C#N	0.859
mol1665	O1C2C1CCC(OC(=O)C)C(OC(=O)C)CC2	0.859
mol1666	Clc1ccccc1NC(=O)CC1SCCNC1=O	0.856
mol1667	Fc1cc(ccc1)C1N(CCC(O)=O)C(=O)C(O)=C1C(=O)c1ccc(cc1)C	0.854
mol1668	S1(=O)(=O)CC(CC1)C(C(=O)C)C(OCC)=O	0.849
mol1669	Fc1ccc(cc1)C(=O)CNC(=O)c1occc1	0.844
mol1670	s1c2c(c3c1NC(NC3=O)c1oc(cc1)C)CCN(C2)C	0.839
mol1671	n1ccccc1CN1CCN(CC1)Cc1ncccc1	0.833
mol1672	S1CCNC(=O)C1CC(=O)Nc1ccc(cc1)C	0.832
mol1673	Clc1cc(NC(=O)C(=O)N)ccc1OC	0.828
mol1674	o1c2c(ncnc2NCCO)c2c1cccc2	0.817
mol1675	O(CC(O)CN)c1ccc(cc1)CC	0.811
mol1676	O(C)c1c(OC)cc(cc1OC)CNCCCN(C)C	0.81
mol1677	S(CC(=O)Nc1cc(O)ccc1)c1nnnn1C	0.806
mol1678	O(C)c1ccc(cc1)CNCCCn1ccnc1	0.804
mol1679	Clc1sc(cc1)C1C(=CN(C=C1C(OC)=O)CCOC)C(OC)=O	0.798
mol1680	Fc1ccc(cc1)C1C(=CN(C=C1C(OC)=O)CCOC)C(OC)=O	0.795
mol1681	o1cccc1\C=C\C(=O)NCCCN1CCOCC1	0.791
mol1682	S(=O)(=O)(N)c1oc(cc1)C(OCCC)=O	0.79
mol1683	Fc1ccc(cc1)CNCCN1CCOCC1	0.785
mol1684	Oc1n(nc(c1)-c1ccccc1)CCC#N	0.777
mol1685	S(O)(=O)(=O)c1nc2c(n1Cc1ccc(cc1)C)cccc2	0.767
mol1686	O(C)c1ccc(cc1)-c1nn(CCC#N)c(O)c1	0.766
mol1687	O(CCN1CCNCC1)c1ccc(OC)cc1	0.764
mol1688	O=C1c2c(N(CCCC#N)C1=O)cccc2	0.757
mol1689	[NH2+]1Cc2c(CC13CCCCC3)cccc2	0.757
mol1690	O=C1c2cc(ccc2N(CC#C)C1=O)C	0.757
mol1691	S(CC(=O)Nc1ccc(S(=O)(=O)N)cc1)c1nncn1C	0.752

mol1692	O=C1N(N=Cc2c1cccc2)CC(OC)=O	0.752
mol1693	O1CCOC1c1ccc(cc1)C1OCCO1	0.75
mol1694	Fc1ccccc1CNCCN1CCOCC1	0.747
mol1695	O=C1N=C(NC2(CCCCC2)C1C#N)N1CCCCC1	0.746
mol1696	O=C1N(CCOC)C(C)=C(C1)C(OC)=O	0.744
mol1697	Clc1ccccc1C1N(CCC(O)=O)C(=O)C(O)=C1C(=O)c1ccccc1	0.744
mol1698	S(C=1C(=O)NC(=O)N(C)C=1N)c1nnnn1-c1ccccc1	0.74
mol1699	[NH2+](CC#CC)CC#CC	0.739
mol1700	S(CCc1ccncc1)CCO	0.739
mol1701	Oc1nn(c2NC(=O)C=C(c12)C)C1CC(N(CC1C)C)C	0.733
mol1702	o1c(nnc1O)-c1cc(OC)c(OC)c(OC)c1	0.732
mol1703	Fc1ccccc1CNCCN(C)C	0.73
mol1704	Clc1ccc(-n2cnnc2)cc1C(=O)Nc1ccccc1	0.722
mol1705	S(=O)(=O)(NCCO)c1ccccc1[N+](=O)[O-]	0.721
mol1706	O(CC(=O)NC(C)(C)C)c1ccc(cc1OC)CNn1nnnc1N	0.716
mol1707	ClCC(=O)Nc1sc(C(=O)N(C)C)c(n1)C	0.713
mol1708	S(CC[NH3+])c1c2c([nH]c1)cccc2	0.711
mol1709	Clc1ccccc1NC(=O)C1N2N(C(=O)C1)C(S)=NC(=O)C2(C)C	0.705
mol1710	OC(=O)c1cc(nc2c1cccc2C)-c1ccncc1	0.702
mol1711	o1c(ccc1C)CNCCCN1CCOCC1	0.688
mol1712	Fc1ccccc1-c1nn(nn1)CCC#N	0.686
mol1713	Fc1ccccc1CNCCCO	0.686
mol1714	Fc1ccccc1CNCCCN(C)C	0.681
mol1715	O1CCCC1CNC(=O)C(=O)NCC(C)C	0.679
mol1716	O1CCc2c(cccc2)C1CNCC	0.677
mol1717	O1CCc2c(cccc2)C1CNCC	0.676
mol1718	ClCC(=O)NNC(=O)COc1ccc(cc1)C	0.675
mol1719	S(=O)(=O)(NCCOC)c1ccccc1	0.669
mol1720	S(CC(=O)c1ccccc1)c1ncccc1C(O)=O	0.666
mol1721	O(C)c1ccccc1CNCCN(C)C	0.665
mol1722	O=C1N(C)C(=O)N(CCCCO)C(=C1)C	0.663
mol1723	o1nc(cc1C(=O)N)-c1cc2OCOc2cc1	0.663
mol1724	o1cccc1CNC(=O)C(=O)NCCCOC	0.662
mol1725	s1c(nnc1NC(=O)C(OCC)=O)COC	0.661
mol1726	O(C)c1ccc(cc1)CNCCN(C)C	0.653
mol1727	s1c2cc(S(=O)(=O)C)ccc2nc1NC(=O)CCCC(O)=O	0.649
mol1728	ClCC(=O)Nc1ccc(OC(F)F)cc1	0.648
mol1729	Nc1ccccc1N1CCCCCC1	0.645
mol1730	OC(=O)CNC1=NC2(CCCC2)Cc2c1cccc2	0.644
mol1731	S1CCN=C1SCC(=O)Nc1ccc(S(=O)(=O)N)cc1	0.642
mol1732	s1ccc(C)c1CNCCCO	0.641
mol1733	o1cccc1CNC(=O)C(=O)NCC=C	0.632

mol1734	O1CCN(CC1)CCNCc1ccc(OC)cc1	0.632
mol1735	Fc1ccc(cc1)CNCCN(C)C	0.63
mol1736	O(C)c1c(OC)c(OC)ccc1CNCCCN(C)C	0.629
mol1737	Clc1c(cc(OC(C(O)=O)C)cc1C)C	0.627
mol1738	s1c2c(CCN(C2)C)c(C(OC)=O)c1N	0.626
mol1739	o1cccc1C(NC(=O)C)c1cc([N+](=O)[O-])c2c(nccc2)c1O	0.625
mol1740	S=C(Nc1cccc(C(O)=O)c1C)NC(=O)CC	0.625
mol1741	S1(=O)(=O)N(CC(=O)NC(C)(C)C)C(=O)c2c1cccc2	0.612
mol1742	N(CCc1ccccc1)CCC	0.609
mol1743	s1cccc1CC(=O)Nc1ccccc1C(O)=O	0.602
mol1744	O1CCN(CC1)Cc1nc2N(C)C(=O)N(C)C(=O)c2n1CCOC	0.602
mol1745	o1c(C)c(cc1C)C(=O)N1CCOCC1	0.601
mol1746	S1(=O)(=O)N(CC(=O)NC(CC)C)C(=O)c2c1cccc2	0.597
mol1747	S=C(N)C(N1C(=O)c2c(cccc2)C1=O)C	0.595
mol1748	n1ccn(c1)CCCNCc1ccc(N(C)C)cc1	0.595
mol1749	S=C(N)C(N1C(=O)c2c(cccc2)C1=O)C	0.592
mol1750	S(=O)(=O)(N)c1ccc(cc1)CNC1CC(=O)N(C1=O)c1ccc(cc1)C(O)=O	0.587
mol1751	Clc1ccc(OCC(O)CN)cc1	0.582
mol1752	o1cccc1C(NC(=O)C)c1cc([N+](=O)[O-])c2c(nccc2)c1O	0.579
mol1753	Clc1cc2C3=C(CCCC3)C(Oc2cc1OCC(O)=O)=O	0.577
mol1754	O=C(N1CCCC1)C(=O)NCc1cccnc1	0.57
mol1755	Clc1ccc(OCC(O)CN)cc1	0.565
mol1756	Clc1cc(OC)c2oc(cc2c1)C(O)=O	0.564
mol1757	O1CCN(CC1)CCCNC(=O)C(=O)NC(C)C	0.563
mol1758	O1CCN(CC1)CCCNCc1cccnc1	0.556
mol1759	s1cccc1S(=O)(=O)N1CCOCC1	0.551
mol1760	O=C(NCc1ncccc1)C(=O)NCC=C	0.542
mol1761	s1ccnc1NC(=O)CSCCO	0.541
mol1762	s1c(ccc1S(O)(=O)=O)-c1nc2c(n1C)cccc2	0.541
mol1763	O(CCCNCc1ncccc1)C	0.539
mol1764	OC(=O)CCC(=O)CCC(=O)c1ccc(cc1)C	0.537
mol1765	S1CC2NC(=O)NC2(O)C1CCCCC(OC)=O	0.529
mol1766	Clc1ncnc(NN)c1N	0.527
mol1767	ClC(=O)c1oc(cc1)C	0.517
mol1768	OC(=O)c1nn2c(N=CC=C2c2cnn(C)c2C)c1	0.509
mol1769	S1CC2NC(=O)NC2(O)C1CCCCC(OC)=O	0.508
mol1770	FC(F)(F)C=1n2nc(cc2N=C(C=1)C1(CC1)C)C(O)=O	0.507
mol1771	s1cccc1C[NH2+]C1CC1	0.499
mol1772	s1c2c(c3c1NC(NC3=O)c1ccc(F)cc1)CCN(C2)C	0.496
mol1773	[NH3+]Cc1[nH]c2c(n1)cc1c(c2)cccc1	0.49
mol1774	s1cccc1S(=O)(=O)Nc1ccc(S(=O)(=O)N)cc1	0.489
mol1775	S(CCC(N)C(O)(CC=C)CC=C)C	0.486

mol1776	O(C)c1cc(ccc1O)C1N(CCC(O)=O)C(=O)C(O)=C1C(=O)c1ccc(cc1)C	0.482
mol1777	O1c2c(cccc2)C(NCCO)=C(N)C1=O	0.478
mol1778	o1c(ccc1C)CNCCCn1ccnc1	0.471
mol1779	o1cccc1CNC(=O)C1CCC12C(C(O)=O)(C)C2(C)C	0.469
mol1780	O1c2c(OCC1C(NC(=O)CCC(O)=O)C)cccc2	0.466
mol1781	O1c2c(OCC1C(NC(=O)CCC(O)=O)C)cccc2	0.466
mol1782	Nc1ccc(cc1)CN1CCN(CC1)C	0.464
mol1783	O1CCCC1CNC(=O)C(=O)NCCCOC	0.463
mol1784	s1c2CCCc2c2c1nc(nc2O)C	0.462
mol1785	N(=C\1/N(CCC/1)C)/c1ccccc1C#N	0.461
mol1786	s1c2CCCc2c2c1ncnc2NCCC(O)=O	0.46
mol1787	OCCNC(=O)C(=O)NC1CCCCC1	0.459
mol1788	O=C(Nc1ccccc1)N1CCNCC1	0.456
mol1789	OCCCNC(C)c1ccncc1	0.453
mol1790	O(C(CC)C(O)=O)c1cccc(C)c1C	0.45
mol1791	O(C)c1ccc(cc1)C=1n2nc(cc2N=CC=1)C(O)=O	0.449
mol1792	OC(CNC1CC(CCC1)C)C	0.439
mol1793	O1CCCC1CNC(=O)C(=O)NC(C)C	0.434
mol1794	O(CC(O)CN)c1cc(OC)ccc1	0.428
mol1795	O=C(NCC=C)c1n(ncc1[N+](=O)[O-])C	0.424
mol1796	O1CCCC1CNC(=O)C(=O)NCCCOC	0.422
mol1797	O1CCN(CC1)CCNCC1CCC=CC1	0.422
mol1798	O=C1NC(=Nc2n(cnc12)COCCOC(=O)C)N	0.41
mol1799	O1CCN(CC1)CCNC(=O)C(C)C	0.407
mol1800	FC(F)(F)C(=O)NC(CC(O)=O)c1ccc(OC)cc1	0.406
mol1801	FC(F)(F)C(=O)NC(CC(O)=O)c1ccc(OC)cc1	0.405
mol1802	O(CC(O)CN)c1cc(OC)ccc1	0.401
mol1803	O1CCCC1CNC(=O)C(=O)NC(C)C	0.398
mol1804	O1c2c(OCC1C(NC(=O)CCC(O)=O)C)cccc2	0.397
mol1805	O1C(CN(CC1C)Cc1[nH]c2c(n1)N(C)C(=O)NC2=O)C	0.391
mol1806	[NH2+](CC(C)C)CC#C	0.385
mol1807	s1cccc1CNCCN(C)C	0.385
mol1808	ClC(=O)c1ccoc1C	0.383
mol1809	O1c2c(OCC1C(NC(=O)CCC(O)=O)C)cccc2	0.372
mol1810	O1CCN(CC1)CCNCc1ccncc1	0.365
mol1811	[nH+]1c2c(CCC2)c(N)c(C)c1C	0.361
mol1812	O=C(NCC#N)Cn1nc(C)c([N+](=O)[O-])c1C	0.357
mol1813	[NH2+](CCCC)CC#C	0.341
mol1814	ClC=1CSC2N(C(=O)C2NC(=O)COc2ccccc2)C=1C(O)=O	0.338
mol1815	Clc1ccc(cc1)C1N(CCC(O)=O)C(=O)C(=O)C1C(=O)c1ccc(cc1)C	0.33
mol1816	[NH2+](CC(C)C)CC#CC	0.322

mol1817	S=C1NN=C(N1CCOC)c1ccncc1	0.32
mol1818	O1CCN(CC1)CCCNC(=O)C(=O)NC1CC1	0.288
mol1819	[NH2+](CC=C)CC#CC	0.288
mol1820	S(CC(O)=O)c1nc(SCC(O)=O)nc(c1)-c1ccccc1	0.288
mol1821	O=C(N1CCCC1)C(=O)NCc1ncccc1	0.285
mol1822	Clc1cc(N2C(=O)C(N3CCC(CC3)C(O)=O)CC2=O)ccc1	0.278
mol1823	N(CCCN(CC)CC)C1CCN(CC1)C	0.268
mol1824	Clc1ccccc1NC1SC(=O)NC1=O	0.263
mol1825	Clc1ccc(-n2cnnc2)cc1C(=O)NCc1ncccc1	0.261
mol1826	Brc1oc(cc1)\C=C\1/SC(=S)N(CC(O)=O)C/1=O	0.257
mol1827	O(C(=O)CNC(=O)c1nn(cc1[N+](=O)[O-])C)CC	0.256
mol1828	O=Cc1cn(nc1)CCC	0.254
mol1829	O=C1NC(=Nc2n(cnc12)COCCO)NC(=O)C	0.253
mol1830	O1C(CN(CC1C)Cc1[nH]c2c(n1)N(C)C(=O)NC2=O)C	0.252
mol1831	FC(F)(F)C(=O)NC(CC(O)=O)c1ccccc1	0.249
mol1832	FC(F)(F)C(=O)NC(CC(O)=O)c1ccccc1	0.245
mol1833	Clc1ccc(-n2cnnc2)cc1C(=O)NC(C)C	0.241
mol1834	NCCCN1CCN(CC1)Cc1ccccc1	0.241
mol1835	ClC=1CSC2N(C(=O)C2NC(=O)COc2ccccc2)C=1C(O)=O	0.24
mol1836	ClC=1CSC2N(C(=O)C2NC(=O)COc2ccccc2)C=1C(O)=O	0.24
mol1837	Fc1ccc(cc1)CNCCCN(C)C	0.235
mol1838	o1c(C(O)=O)c(cc1C(C)(C)C)C	0.22
mol1839	O1c2cc(OC(CC)C(O)=O)ccc2OC1	0.214
mol1840	s1cccc1CNCCCN(C)C	0.213
mol1841	S(CCCS(O)(=O)=O)c1oc2c(n1)cccc2	0.205
mol1842	Clc1ccccc1NC1SC(=O)NC1=O	0.203
mol1843	O1CCN(CC1)CCNCc1cccnc1	0.203
mol1844	O1CCN(CC1)CCCNCCCC	0.199
mol1845	O=C1NC(=O)NC=C1NC(=O)\C=C/C=C\C	0.192
mol1846	O=C(Nc1cccnc1)C(=O)Nc1cccnc1	0.165
mol1847	S(=O)(=O)(N)c1oc(cc1)C(OC)=O	0.164
mol1848	n1ccccc1CNCCN(C)C	0.147
mol1849	O(CC1C2N(CCC1)CCCC2)CCCN	0.146
mol1850	S(=O)(=O)(N)c1cc2C3C(CC=C3)C(Nc2cc1)C(O)=O	0.144
mol1851	o1c(ccc1C)CNCCO	0.14
mol1852	o1c(ccc1C(O)=O)CN1CCCCC1	0.14
mol1853	S1\C(=C/c2ccc(cc2)C(O)=O)\C(=O)N(CCC(O)=O)C1=S	0.132
mol1854	O1C(CN(CC1C)Cc1[nH]c2c(n1)N(C)C(=O)NC2=O)C	0.129
mol1855	n1cc(ccc1)CNCCN(C)C	0.118
mol1856	Fc1cc(ccc1)C1N(CCC(O)=O)C(=O)C(=O)C1C(=O)c1ccc(cc1)C	0.112
mol1857	s1cc(nc1N)C1(CC(OC1)=O)C(OCC)=O	0.103
mol1858	o1nc(C(OC)=O)c(n1)N	0.0945

mol1859	OC=1c2c3N(CCCc3ccc2)C(=O)C=1C(=O)NCCN	0.0865
mol1860	OCCCCNC1CCCCC1	0.0809
mol1861	s1cccc1C(=O)NCCCC(O)=O	0.0762
mol1862	O1CCN(CC1)CCCNCC(C)C	0.0748
mol1863	S(CCC(NC(=O)c1cc([O-])c[nH+]c1)C(O)=O)C	0.0725
mol1864	O=C1N(C2=C(C=C1C(O)=O)C(=O)CCC2)c1ccccc1	0.0722
mol1865	o1cccc1CNCCCN(C)C	0.066
mol1866	O(CCCNC1CCN(CC1)CC)C	0.06
mol1867	O=C1C(C(=O)c2ccc(cc2)C)C(N(CCC(O)=O)C1=O)c1ccccc1	0.0493
mol1868	o1cccc1CNCCCO	0.0488
mol1869	S(CCc1ncccc1)CC(O)=O	0.0447
mol1870	O1CCCC1CNC(=O)C(=O)NCC(O)C	0.0425
mol1871	OC(CNCCc1ccccc1)CN	0.0419
mol1872	s1cccc1CNCCO	0.0284
mol1873	O1CCCC1CNC(=O)C(=O)NCC(O)C	0.0104
mol1874	n1ccc(cc1)CNCCN(C)C	0.00858
mol1875	n1cc(ccc1)CNCCCN(C)C	-0.0147
mol1876	S(O)(=O)(=O)c1cc(ccc1C)Cc1cc([O-])c[nH+]c1	-0.0264
mol1877	Clc1ccccc1C1N(CCC(O)=O)C(=O)C(=O)C1C(=O)c1ccccc1	-0.028
mol1878	Cl\C(=C/C[NH3+])\C	-0.0331
mol1879	S(=O)(=O)(n1nc(nc1N)C(=O)N1CCOCC1)CC	-0.0404
mol1880	O1CCCC1CNC(=O)C(=O)NCC	-0.047
mol1881	O1CCCC1CNC(=O)C(=O)NCC	-0.0482
mol1882	Sc1oc(nn1)COc1ccc(F)cc1	-0.0537
mol1883	S1C(Nc2cc(ccc2)C)C(=O)N(CC(O)=O)C1=O	-0.0578
mol1884	FC(F)Oc1ccc(cc1OC)C(O)=O	-0.0627
mol1885	O(CCNC(=O)C(=O)NC1CC1)C	-0.0706
mol1886	S1C(Nc2cc(ccc2)C)C(=O)N(CC(O)=O)C1=O	-0.0773
mol1887	S1(=O)(=O)CC(NC(Cc2ccc(O)cc2)C(O)=O)CC1	-0.0895
mol1888	S1C(Nc2ccccc2C(O)=O)C(=O)N(C)C1=O	-0.0941
mol1889	P(OC)(OC)(=O)C(O)(CC(OCC)=O)C	-0.106
mol1890	O=C1N(C2CCCCC2)C(=O)NC1CCC(O)=O	-0.11
mol1891	n1ccc(cc1)CNCCCN(C)C	-0.112
mol1892	S(CC(N)C(O)=O)C1OCCCC1	-0.12
mol1893	O1CCN(CC1)C(=O)C1CCCCC1C(O)=O	-0.132
mol1894	S(=O)(=O)(NCCO)c1ccc(cc1)\C=C\C(O)=O	-0.141
mol1895	o1nc2nc(OC)c(OC)nc2n1	-0.145
mol1896	O=[N+]([O-])c1ccc(nc1-n1ccnc1)-n1ccnc1	-0.147
mol1897	S1C(Nc2ccc(cc2)C)C(=O)N(CC(O)=O)C1=O	-0.165
mol1898	S1C(Nc2ccccc2C(O)=O)C(=O)N(C)C1=O	-0.184
mol1899	O(C)c1cc(ccc1O)C1N(CCC(O)=O)C(=O)C(=O)C1C(=O)c1ccc(cc1)C	-0.195
mol1900	P(OC)(OC)(=O)C(O)(CC(OCC)=O)C	-0.196

mol1901	S1(=O)(=O)CC(NC(Cc2ccc(O)cc2)C(O)=O)CC1	-0.197
mol1902	OCCCNC1CCN(CC1)CC	-0.208
mol1903	ClC1CC(=O)N(C1=O)c1ccc(OC(=O)C)cc1	-0.215
mol1904	Fc1cc(F)ccc1OC(C(O)=O)C	-0.215
mol1905	O(C(=O)CCCC(O)=O)CC#C	-0.217
mol1906	S=C1NC(=O)C=C(N)N1CCOC	-0.236
mol1907	O=C1NC2NC(=O)NC2N1C(C(C)C)C(O)=O	-0.25
mol1908	s1cnnc1NC(=O)CCC(C(O)=O)C	-0.25
mol1909	OC=1c2c(N(CC)C(=O)C=1[N+](=O)[O-])cccc2	-0.263
mol1910	S1\C(=C/2\c3c(N(C)C\2=O)cccc3)\C(=O)N(C(CCC(O)=O)C(O)=O)C1=S	-0.269
mol1911	S1\C(=C/2\c3c(N(C)C\2=O)cccc3)\C(=O)N(C(CCC(O)=O)C(O)=O)C1=S	-0.269
mol1912	o1cccc1C(=O)NC(CCC)C(O)=O	-0.27
mol1913	Sc1nc2N(C)C(=O)NC(=O)c2n1CCCC	-0.3
mol1914	O(C)c1cc(OC)c(OC)cc1CN	-0.301
mol1915	O1CCCC1CNC(C)C	-0.307
mol1916	O=C1N(Cc2c1c(ccc2)C(O)=O)CCOC	-0.307
mol1917	O(CCNCC)CC	-0.311
mol1918	O1CCCC1CNC(=O)C(=O)NCCO	-0.314
mol1919	o1c(ccc1C)C(=O)N1CCCCC1C(O)=O	-0.329
mol1920	O=C1NC(=NC(=N1)Nc1ccccc1)N	-0.332
mol1921	S1(=O)(=O)CC(C)C(=O)CC1C	-0.339
mol1922	S1(=O)(=O)CC(C)C(=O)CC1C	-0.339
mol1923	S1C(Nc2ccc(cc2)C)C(=O)N(CC(O)=O)C1=O	-0.344
mol1924	S1C(Nc2cc(ccc2)C(O)=O)C(=O)N(C)C1=O	-0.36
mol1925	S(=O)(=O)(N)c1c2c(cc(S(=O)(=O)N)cc2O)ccc1	-0.398
mol1926	o1nc(C)c(CCN)c1C	-0.412
mol1927	S1(=O)(=O)CC(C)C(=O)CC1C	-0.423
mol1928	NCCCN1CCN(CC1)CC	-0.448
mol1929	N(CCCN(C)C)C1CCN(CC1)C	-0.453
mol1930	O(CC(O)CNCC)CC(O)CNCC	-0.458
mol1931	O1CC(NCCC(O)=O)C(O)(CC1)C	-0.487
mol1932	O1CC(NCCC(O)=O)C(O)(CC1)C	-0.488
mol1933	O1CC(NCCC(O)=O)C(O)(CC1)C	-0.5
mol1934	O1CCN(CC1)c1nccc(c1)C(O)=O	-0.505
mol1935	O1CC(NCCC(O)=O)C(O)(CC1)C	-0.51
mol1936	S(=O)(=O)(n1nc(nc1N)C(=O)N1CCOCC1)C	-0.511
mol1937	O(CC(O)CNCC)CC(O)CNCC	-0.521
mol1938	O=C1c2c(N(C(C(O)=O)C)C1=O)cccc2	-0.6
mol1939	O=C1c2c(N(C(C(O)=O)C)C1=O)cccc2	-0.601
mol1940	S1C(Nc2ccccc2)C(=O)N(CC(O)=O)C1=O	-0.627
mol1941	O=C(NCCN)c1cccnc1	-0.652

mol1942	S1C(Nc2ccc(cc2)C(O)=O)C(=O)NC1=O	-0.654
mol1943	S1C(Nc2ccc(cc2)C(O)=O)C(=O)NC1=O	-0.662
mol1944	S1C(Nc2ccccc2)C(=O)N(CC(O)=O)C1=O	-0.67
mol1945	OCCCc1nc([nH]n1)N	-0.693
mol1946	ClC(=O)c1nnsc1	-0.693
mol1947	NC1CCN(CC1)C(C)C	-0.697
mol1948	[NH2+]1CCN=C(C=C1C)C	-0.698
mol1949	O1CCN(CC1)C(C(O)=O)C	-0.71
mol1950	S1(=O)(=O)CC(NC(CC)C(O)=O)CC1	-0.712
mol1951	S1C(Nc2cc(ccc2)C(O)=O)C(=O)N(C)C1=O	-0.712
mol1952	O=C1N(CCC1)CC1CCCNC1	-0.725
mol1953	OC(=O)c1[nH]cnc1C(=O)Nc1ccc(N)cc1	-0.73
mol1954	O=C1N(CCC1)CC1CCCNC1	-0.731
mol1955	O=C1NC2NC(=O)NC2N1C(C(O)=O)C	-0.737
mol1956	OC(=O)CCn1ncc(c1)C	-0.788
mol1957	S(O)(=O)(=O)c1cc2Cc3cc(S(O)(=O)=O)ccc3-c2cc1	-0.801
mol1958	s1cnnc1NC(=O)CCCC(O)=O	-0.806
mol1959	S=C1NCN(CN1)CCC(O)=O	-0.844
mol1960	OCCNC1CCN(CC1)C	-0.91
mol1961	S1(=O)(=O)CC(NC(CC)C(O)=O)C(O)C1	-0.939
mol1962	S(O)(=O)(=O)c1cc2nc([nH]c2cc1)C(O)C	-0.985
mol1963	S(O)(=O)(=O)c1cc2nc([nH]c2cc1)C(O)C	-0.988
mol1964	S1(=O)(=O)CC(N)C(N)C1	-1.002
mol1965	O=C1NC(=O)NC(C(O)=O)=C1CNCCO	-1.014
mol1966	FC(F)n1nc(cc1)C(O)=O	-1.022
mol1967	OC(=O)CCCNC=1NCCN=1	-1.04
mol1968	Clc1cn(nc1[N+](=O)[O-])CC(O)=O	-1.069
mol1969	s1c(nnc1NC(=O)CCC(O)=O)C	-1.076
mol1970	S1(=O)(=O)CC(N)C(N)C1	-1.095
mol1971	S1(=O)(=O)CC(NN)C(O)C1	-1.338
mol1972	S(CC(O)=O)c1nc([nH]c1[N+](=O)[O-])C	-1.349
mol1973	S1(=O)(=O)CC(NN)C(O)C1	-1.356
mol1974	S(O)(=O)(=O)c1c(n(nc1C)C)C	-1.379
mol1975	OC(=O)c1ncnnc1NC(=O)NC	-2.008
mol1976	S(=O)(CCC(O)=O)CCC(O)=O	-2.184
mol1977	S(=O)(CC(O)=O)CC(O)=O	-2.983

APPENDICE