Application of Monte Carlo Algorithm to Explore Simplified Molecular-Input Line-Entry System based Molecular Descriptors of BACE1 inhibitors for Therapeutic Application in Alzheimer's Disease

Md Lutful Islam
Research Scholar, Department of Computer Science and Engineering, Shri Jagdish Prasad Jhabarmal Tibrewala University, Vidyanagari, Jhunjhunu - 333 001, Rajasthan, India

Gulabchand K. Gupta
Seva Sadan College of Arts, Science & Commerce (Affiliated to University of Mumbai), Seva Sadan Marg, Ulhasnagar - 421 003, Dist. Thane, Maharashtra, India

ABSTRACT
Application of computer science and algorithms are now become an integral part of the drug discovery research. In the current work, well known Monte Carlo (MC) algorithm was used to develop quantitative structure-activity relationship (QSAR) models with molecular descriptors derived from simplified molecular-input line-entry system (SMILES) representation of beta-site APP cleaving enzyme1 (BACE1) inhibitors. A set of BACE1 inhibitors was obtained from the binding database and subsequently divided into training, test, calibration and external sets. The QSAR models were developed from the training set compounds while other sets used to assess the quality of developed models. With- and without-influence of cyclic rings on inhibitory activity were considered to develop the QSAR models. Best QSAR models were selected based on statistical parameters of final models. High correlation and low standard error values of training, test, calibration and external sets undoubtedly suggested that the selected models were robust and efficient enough to predict the inhibitory activity of the molecules. On evaluation of statistical parameters it was revealed that cyclic rings of molecular scaffold significantly contributed to the inhibition of BACE1. The molecular fragments were found to be crucial to increase or decrease the inhibitory activity of the molecules which indicated that models have mechanistic interpretation. Therefore, important molecular fragments explained by the QSAR models can be used to design new and novel BACE1 inhibitors for therapeutic application in Alzheimer's disease.

Keywords
Alzheimer's disease; BACE1 inhibitors; QSAR; Monte Carlo algorithm; SMILES

1. INTRODUCTION
Alzheimer's disease (AD) is severe and a progressive neurodegenerative disease categorized by two histopathological hallmarks, namely β-amyloid plaques and neurofibrillary tangles [1-4]. AD is common cause of senile dementia, accounts for 60–70% of all dementias and clinically characterized by impairment of memory, disorientation, difficulty in speaking or writing, loss of reasoning skills, and delusions among other symptoms [5]. Direct reason of the AD progression is still doubtful but some studies reported that both genetic and environmental factors are play major role for the AD [6] development. About 44 million people worldwide are suffering from AD or related dementia in 2017. As per reports, AD most prominently found in Western Europe and least prevalent in Sub-Saharan Africa. World Health Organization (WHO) data explained that there is about 5.7 million people living in United States of America in 2018 with AD. More than 4 million people have some form of dementia and AD in India, and it will be double in India by 2030 (The Indian Express, September 21, 2016). With development of AD, there is high risk of several age related diseases including hypertension, dyslipidemia, metabolic syndrome and diabetes. There is no approved chemical agents to treat such devastating disease rather management of the symptoms.

The extracellular accumulation of amyloid plaques collected of the β-amyloid (Aβ) peptide characterizes the main reason of AD [7]. The Aβ formed due to sequential breakdown of β-amyloid precursor protein (APP) by two aspartyl protease, beta-site APP cleaving enzyme1 (BACE1) followed by γ secretase [8]. Stop or decrease of Aβ production by inhibition of BACE1 enzyme is an ideal approach to control the AD. Researchers from worldwide already proved that BACE1 inhibitors hold great potential as a potential strategy in decreasing Aβ brain concentrations which lead to stop the progression of AD [9, 10]. It has been established by the experimental approach that BACE1 enzyme could be clinically feasible with few mechanistic side effects [11-13]. Hence, control production of Aβ through by the inhibition of BACE1 may represent modifying treatment for AD.

In order to develop promising chemical agents for the proper treatment of AD, the present research was deliberated the Monte Carlo (MC) algorithm based quantitative structure activity relationship (QSAR) study to explore critical chemical functionalities and design new lead chemical agents for therapeutic application of AD. The QSAR can be expressed as the statistically validated and mathematical relationship between biological activity and chemical structures in terms of molecular descriptors. Numerical values of chemical or physical properties of the small molecules are called molecular descriptors and used in QSAR model development. Statistically robust QSAR models can give instincts into the decisive structural information of the small molecules which contribute to biological activity [14]. Major division of the molecular descriptors are physico-chemical, topological and electronic, geometric and structural, and simple indicator parameter. Moreover, descriptors are also be characterized on the basis dimensionality such as 0D, 1D, 2D or 3D [15]. Obtaining molecular descriptors based on geometry are usually tough and need high computational costs and long computational calculation time. Then 0D, 1D and 2D are termed as the conformation-independent descriptors based on the constitutional and topological molecular features of small molecules have been established as a substitute method

[16, 17]. In most cases the descriptors based on molecular graph are used to develop QSAR models [18-20]. But molecules in simplified molecular input-line entry system (SMILES) representation can also be used [21-23] for molecular descriptor generation followed by development of QSAR models. Without any information 3D structure of the molecules the SMILES notation can derived descriptors based on both on the molecular structure and the property under analysis[14]. Therefore, QSAR models can be progressed with SMILES based molecular descriptors [24-26]. Several research groups from industry and academia have already been successfully used SMILES based descriptors to develop robust QSAR models [27-33].

2. MATERIALS AND METHODS

2.1 Dataset

A set of more than thousand reported BACE1 inhibitors were downloaded from Binding DB (http://www.bindingdb.org/) with inhibition constant (K_i) activity in nM range. Initially duplicate and without activity molecules were identified and removed. Remaining compounds were considered to verify the Lipinski's rule of five [34] and Viber's [35] rules and only considered molecules those satisfied the above two rules. Finally, 411 molecules were found to be satisfied above criteria and considered for for the study. To QSAR model development the experimental inhibitory activity (K_i) of dataset were converted into logarithm value [pK_i = $\log((1/K_i)x10^7)$]. Molecules in the entire dataset were randomly divided into training, calibration, test and external sets. Each of the set has specific role during the model development. Compounds present in the training set were considered to develop the model and calibration and test sets used to assess the predictive quality of selected models. Compounds of the external set were unseen during model generation that is no information of validation set was involved for model development. External set finally was used to calculate final estimation of the model. Molecules of all fours sets (training, test, calibration and external) are given in Supplementary file (Table S1 and S2) in SMILES representation with pK_i.

2.2 Optimal descriptors

The SMILES representation of the dataset was used to calculate the molecular descriptor. The SMILES format of chemical structures is one of the widely accepted and helpful molecular file format to calculate the optimal molecular descriptors which are mathematical functions of so-called correlation weights (CW) that is "Descriptors of Correlation Weights" (DCW). The Monte Carlo algorithm was adopted to derive the DCW from the set of BACE1 inhibitors. In the current work, DCW was calculated using two approaches viz. without and with considering the influence of cyclic rings to the pK_i. For calculation of DCW following expression was used and influence of cyclic rings on inhibitory activity not considered.

$$DCW_1(SMILES,T,N_{epoch}) = \alpha\sum CW(S_k) + \beta\sum CW(SS_k) + \gamma\sum CW(SSS_k) + x\cdot CW(NOSP) + y\cdot CW(HALO) + z\cdot CW(BOND) + t\cdot CW(PAIR) \quad (1)$$

Where, T indicates threshold and defines as coefficient for classifying various molecular features extracted from SMILES into two classes such as active, in which CW is involved in the modelling process and rare, where CW is not involved in the modelling process. N_{epoch} signifies the number of epochs in Monte Carlo optimization which gives the best statistical results of the calibration set. S_k denotes the one symbol separately of the SMILES representation while, the SS_k and SSS_k are represented for combination of two or three respectively. NOSP, HALO, BOND and PAIR explain the descriptors based on presence or absence of different elements. NOSP explain the nitrogen, oxygen, sulphur and phosphorus; HALO represents halogen atoms such as fluorine, chlorine, bromine and iodine; BOND offers double (=), triple (#) or stereochemical bonds (@ or @@); and PAIR refers the probable grouping of pair atoms and/or SMILES attributes (for example double, triple, and stereochemical bonds) that takes place in the structure together. The α, β, γ, x, y and t are discrete coefficient with values 0 and 1. Detail calculation of the above descriptors with example can be found in some where else. [31].

The optimal descriptors with influence of cyclic rings can be calculated using following equation (2).

$$DCW_2(SMILES,T,N_{epoch}) = \alpha\sum CW(S_k) + \beta\sum CW(SS_k) + \gamma\sum CW(SSS_k) + x\cdot CW(NOSP) + y\cdot CW(HALO) + z\cdot CW(BOND) + t\cdot CW(PAIR) + CW(C3) + CW(C4) + CW(C5) + CW(C6) + CW(C7) \quad (2)$$

Where, C3, C4, C5, C6 and C7 are denoted by three-, four-, five-, six- and seven-membered cyclic rings. Details explanation of such descriptors are can be found somewhere else[36].

The well known and widely used MC algorithm was adopted to calculate the CW which must give the best statistical results for the test set. In order to get preferable threshold (T*) and number of epochs (N*), range of T and N_{epoch} were selected from 1 to 10 and 1 to 20 respectively. The statistical results were analysed and the best (N*, T*) selected for final model development. The selected best statistics of calibration set makes possible to obtain the endpoint value using numerical values of correlation weights from the training set as follows:

$$\text{Endpoint} = C_0 + C_1 \times \text{DCW(SMILES, T, } N_{epoch}) \quad (3)$$

The endpoint represents the biological activity and, C_0 and C_1 are constant.

2.3 Validation

Validation of any *in-silico* model is essential step to assess the quality of the model. In this research the QSAR models were validated with the help of a) internal validation using training set compounds; b) external validation using test compounds; and c) **Y**-scrambling or randomization of data. Several studies [26, 27, 29, 30, 33] already used these validation methodologies on SMILES notation optimal descriptor based QSAR models. The cross-validated correlation coefficient (Q^2) was also derived from the predicted activity of training compounds. Model can be explained robust with Q^2 >0.5[37]. Further to verify the significant predictive capability of the training set molecules, the modified r^2 ($r^2_{m(LOO)}$) [38, 39] that is r^2_m was calculated which the measure of the degree of deviation of the predicted activity from the observed ones. In order to check the chance correlation, **Y**-scrambling given by Ojha and Roy [40] was also performed in which ten probes of calculation were carried out. In one probe of calculation, X and Y represent the vectors of experiment and the vector of prediction. First of all, exchange of random N1 and random N2 from row X (Y is not modified) were performed thousand times. Further, from above probes the $R^2_{(X,Y)}$ was calculated and represented as R^2_r. The ${}^C R^2_p$ was finally calculated according to the equation (3).

$$^{C}R^{2}_{p} = R \times (R^{2} - R^{2}_{r})^{1/2} \quad (3)$$

Where R^2 and R^2_r were utilized from the non-randomized and randomized model respectively. For acceptance of QSAR model the threshold value of $^{C}R^{2}_{p}$ should be greater than 0.5.

3. RESULTS AND DISCUSSION

The SMILES format of 411 BACE1 inhibitors were used to calculate the molecular descriptor followed by QSAR model development using MC algorithm based CORAL software (http://www.insilico.eu/coral/). The pK_i was considered as dependent variable and molecular descriptors as independent variables. In this manuscript, two approaches were implemented to calculate the descriptors such as descriptor generation with- and without-considering the influence of cyclic rings of the molecular systems. During the model development 3 compounds were found to be outlier. Subsequently these three molecules were discarded from the dataset for further study.

3.1 Selection of optimal T and N_{epoch}

Optimal T and N_{epoch} were identified with help of the "Search for preferable model" option of the CORAL. The threshold values in the range of 1 to 10 and the number of epochs ranging from 1 to 30 were used. The statistical parameters, epoch numbers and corresponding threshold values are given in Tables 1 and 2 in case without- and with-considering the influence of cyclic rings on inhibitory activity respectively. On detailed analysis of the correlation coefficient of training, calibration and test sets, optimal T and N_{epoch} (T* and N^*_{epoch}) were found to be (6, 7) and (6, 6) in case of without- and with-considering the influence of cyclic rings on inhibitory activity respectively.

Table 1: Statistical parameters of training, calibration and test sets to search T* and N^*_{epoch} for without influence of cyclic rings on inhibitory activity

Epoch no.	R_{tr}^2	s_{tr}	R_c^2	s_c	R_{ts}^2	s_{ts}	$R_{m}^2{}_{av}$	T
2	0.622	0.689	0.607	0.864	0.610	0.779	0.574	5
3	0.667	0.647	0.673	0.807	0.620	0.765	0.595	6
4	0.665	0.649	0.674	0.802	0.617	0.768	0.602	9
5	0.700	0.614	0.714	0.756	0.601	0.783	0.587	7
6	0.716	0.597	0.728	0.742	0.585	0.797	0.576	7
7	0.719	0.594	0.729	0.738	0.566	0.817	0.552	7
8	0.723	0.590	0.745	0.728	0.569	0.814	0.555	7
9	0.727	0.586	0.751	0.713	0.536	0.845	0.521	7
10	0725	0.587	0.756	0.719	0.527	0.822	0.547	7
11	0.731	0.581	0.754	0.719	0.554	0.830	0.533	7
12	0.730	0.583	0.745	0.710	0.543	0.840	0.516	8
13	0.734	0.578	0.750	0.712	0.537	0.849	0.508	8
14	0.737	0.575	0.761	0.710	0.552	0.831	0.538	7
15	0.729	0.58	0.776	0.701	0.517	0.866	0.492	7
16	0.737	0.575	0.769	0.705	0.534	0.848	0.514	7
17	0.735	0.577	0.779	0.703	0.517	0.863	0.494	7
18	0.735	0.577	0.774	0.702	0.515	0.866	0.494	8
19	0.736	0.575	0.769	0.704	0.527	0.856	0.506	7
20	0.740	0572	0.780	0.700	0.499	0.885	0.463	7
21	0.738	0.573	0.772	0.704	0.519	0.865	0.488	9
22	0.735	0.577	0.769	0.702	0.513	0.872	0.486	8
23	0.747	0.564	0.771	0.704	0.525	0.858	0.505	7
24	0.739	0.572	0.781	0.700	0.513	0.871	0.483	7
25	0.737	0.575	0.777	0.687	0.507	0.880	0.464	8
26	0.745	0.566	0.787	0.691	0.520	0.863	0.490	8
27	0.742	0.569	0.774	0.690	0.497	0.889	0.463	8
28	0.740	0.571	0.775	0.695	0.794	0.888	0.464	8
29	0.740	0.571	0.777	0.696	0.501	0.883	0.466	8

30	0.737	0.574	0.773	0.704	0.514	0.872	0.479	9

R_{tr}^2: Correlation coefficient of training set; s_{tr}: standard error of training set; R^2_c: Correlation coefficient of calibration set; s_c: standard error of calibration set; R_{ts}^2: Correlation coefficient of test set; s_{ts}: standard error of test set; $R_{m}^2{}_{av}$: Modified correlation coefficient; *T*: Threshold

Table 2: Statistical parameters of training, calibration and test sets to search T* and N*$_{epoch}$ for with influence of cyclic rings on inhibitory activity

Epoch no.	R_{tr}^2	s_{tr}	R_c^2	s_c	R_{ts}^2	s_{ts}	$R_{m}^2{}_{av}$	*T*
2	0.670	0.644	0.653	0.821	0.590	0.794	0.573	3
3	0.664	0.650	0.662	0.809	0.615	0.770	0.596	6
4	0.688	0.626	0.696	0.780	0.597	0.787	0.587	6
5	0.688	0.626	0.699	0.779	0.596	0.787	0.593	9
6	0.721	0.592	0.732	0.729	0.584	0.799	0.569	6
7	0.707	0.606	0.740	0.738	0.558	0.825	0.537	9
8	0.718	0.595	0.738	0.732	0.555	0.282	0.543	9
9	0.713	0.600	0.748	0.730	0.548	0.836	0.519	9
10	0.729	0.583	0.761	0.712	0.553	0.830	0.531	7
11	0.725	0.588	0.765	0.704	0.534	0.849	0.509	7
12	0.734	0.578	0.763	0.708	0.531	0.851	0.508	7
13	0.736	0.576	0.765	0.705	0.545	0.837	0.531	7
14	0.737	0.575	0.764	0.707	0.533	0.849	0.511	7
15	0.739	0.573	0.762	0.700	0.537	0.847	0.510	8
16	0.736	0.576	0.759	0.704	0.526	0.85	0.502	8
17	0.731	0.581	0.769	0.709	0.523	0.860	0.491	7
18	0.738	0.573	0.781	0.694	0.501	0.881	0.474	7
19	0.740	0.571	0.460	0.715	0.514	0.869	0.488	7
20	0.740	0.572	0.780	0.700	0.499	0.885	0.463	7
21	0.737	0.574	0.777	0.695	0.505	0.877	0.481	9
22	0.738	0.574	0.781	0.699	0.536	0.849	0.508	7
23	0.735	0.577	0.769	0.701	0.513	0.869	0.484	7
24	0.751	0.559	0.760	0.698	0.516	0.875	0.461	6
25	0.743	0.568	0.776	0.696	0.503	0.881	0.478	7
26	0.744	0.567	0.782	0.692	0.518	0.864	0.487	7
27	0.742	0.569	0.774	0.690	0.497	0.889	0.463	8
28	0.739	0.573	0.781	0.688	0.505	0.876	0.479	7
29	0.745	0.566	0.774	0.693	0.518	0.866	0.479	6
30	0.738	0.573	0.785	0.692	0.500	0.882	0.471	7

R_{tr}^2: Correlation coefficient of training set; s_{tr}: standard error of training set; R^2_c: Correlation coefficient of calibration set; s_c: standard error of calibration set; R_{ts}^2: Correlation coefficient of test set; s_{ts}: standard error of test set; $R_{m}^2{}_{av}$: Modified correlation coefficient; *T*: Threshold

3.2 Without considering influence of various cyclic rings

Influence of cyclic ring on the inhibitory activity was not considered and the DCW derived. Subsequently the QSAR model was developed. The best model was selected based on best MC optimization runs.

$$pK_i = 0.727(\pm 0.008) + 0.024(\pm 0.00007) \times DCW(7,6) \quad (4)$$

Training set: n = 204; R^2 = 0.711; s = 0.729; F = 498; Q^2 = 0.706; R_m^2 = 0.584; $^{C}R^2_p$ = 0.709

Calibration set: n = 64; R^2 = 0.729; s = 0.742; F = 167; R_m^2 =0.612; ${}^{C}R^2_p$ = 0.720

Test set: n = 70; R^2 = 0.590; s = 0.792, F = 98; R_m^2 =0.573; ${}^{C}R^2_p$ = 0.577

External set: n = 70; R^2 =0.775; s = 0.575, F = 234; R_m^2 = 0.600

The statistical value of the model developed without considering impact of cyclic rings on the inhibitory activity clearly suggested that model was statically robust in nature and capable enough to predict the inhibitory activity of the external set of molecules.

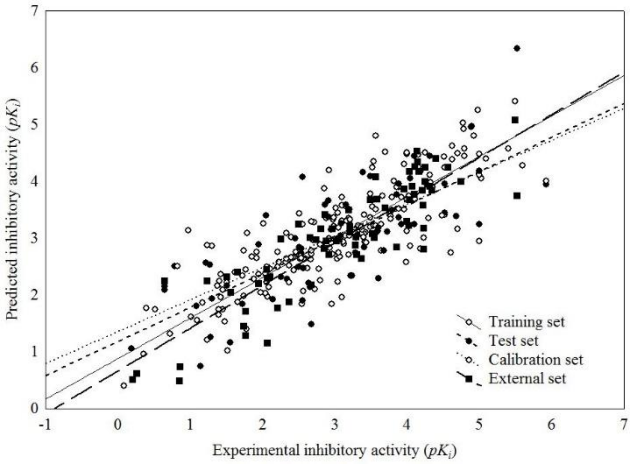

Figure 1: Observed and predicted inhibitory activity as per model developed without considering cyclic rings

The experimental and predicted inhibitory activity according the model are portrayed in the Figure 1 and Table S1 (Supplementary file). To check the closeness between experimental and predicted activity the radar plot was developed and given in Figure 2. The radar plot clearly exhibited the closeness between the experimental and predicted activity.

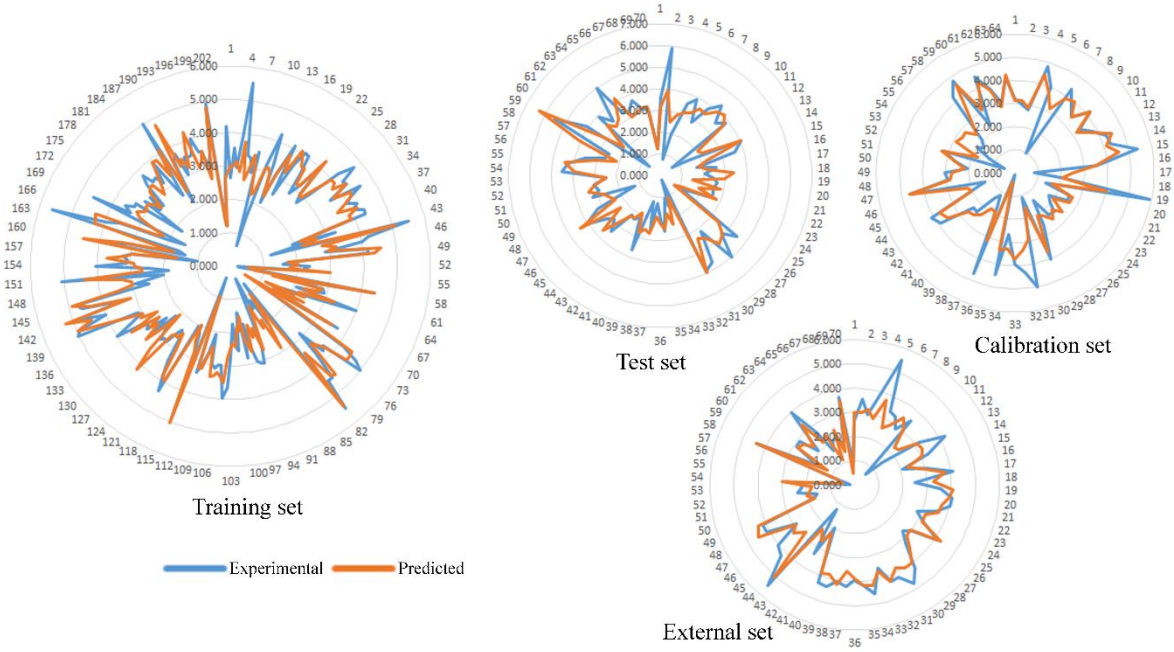

Figure 2: Radar plot showing fitness of observed and predicted inhibitory activity of training, test, calibration and external sets per model developed without considering cyclic rings

The detailed exploration of DCW from the best model developed without considering any influence of cyclic rings on the inhibitory activity explained that components "+ + + +B2- -B3= =", "+ + + +Cl- -B2= =" and "+ + + +S-- -B2= =" were found to be positive impact, while ++++F---B2==", "+ + + +F- - -S= = =" and "+ + + +O- - -B2= =" showed negative impact on the inhibitory activity. The "BOND10000000", "BOND10100000" and "BOND11100000" components were also showed negative influence towards the inhibition of BACE1. The components "HALO00000000", "HALO01000000", "HALO01100000" and "HALO11000000" decrease the pK_i but "HALO00100000" showed no significance on pK_i. On other hand impact of nitrogen, oxygen and sulphur together ("NOSP11100000") showed negative impact towards the pK_i.

3.3 With considering influence of various cyclic rings

The best QSAR model with the influence of cycling rings on inhibitory activity was developed and given below. The best model was selected based on best Monte Carlo optimization runs.

$$pK_i = 0.645(\pm 0.008) + 0.025(\pm 0.0001) \times DCW(6,6) \quad (5)$$

Training set: n = 204; R^2 = 0.717; s = 0.597; F = 511; Q^2 = 0.712; $R_m{}^2$ = 0.581; ${}^C R^2{}_p$= 0.715

Calibration set: n = 64; R^2 = 0.723; s = 0.734; F = 162; $R_m{}^2$ = 0.598; ${}^C R^2{}_p$ = 0.712

Test set: n = 70; R^2 = 0.539; s = 0.843; F = 79; $R_m{}^2$ = 0.512; ${}^C R^2{}_p$ = 0.535

External set: n = 70; R^2 =0.660; s = 0.621; F = 52; $R_m{}^2$ = 0.532

The best model was developed with considering the impact of cyclic rings on inhibitory activity with threshold and N_{epoch} of 6 and 6 respectively. Values of statistical parameters were recorded and it observed that correlation coefficient of all training, calibration, test and external sets found to be 0.714, 0.723, 0.539 and 0.660 respectively. The $R_m{}^2$ and ${}^C R^2{}_p$ were also found to be more than 0.5 for all sets. The cross-validated correlation coefficient (Q^2) of training set was also found to be 0.712. Therefore, above statistical outcome undoubtedly explained that selected model robust in nature and efficient to predict the biological activity of molecules outside the training set. Experimental and predicted activity as per above model are given in Figure 3 and Table S2 (Supplementary file). Radar plot between the experimental and predicted activity also plotted and given in Figure 4. Radar plot clearly explained the closeness between experimental and predicted activity which substantiated the predictive capability of the model.

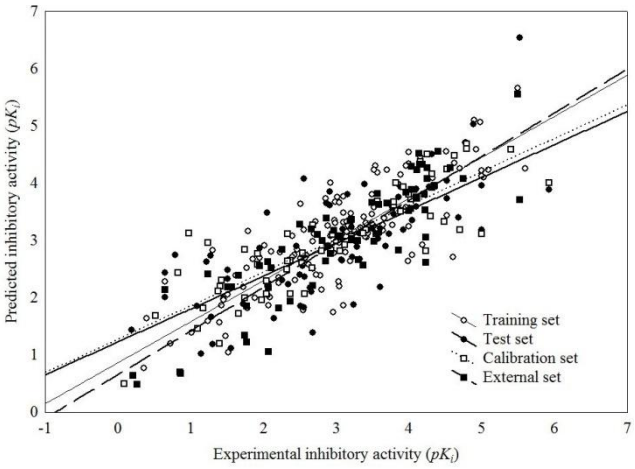

Figure 3: Observed and predicted inhibitory activity as per model developed with considering cyclic rings

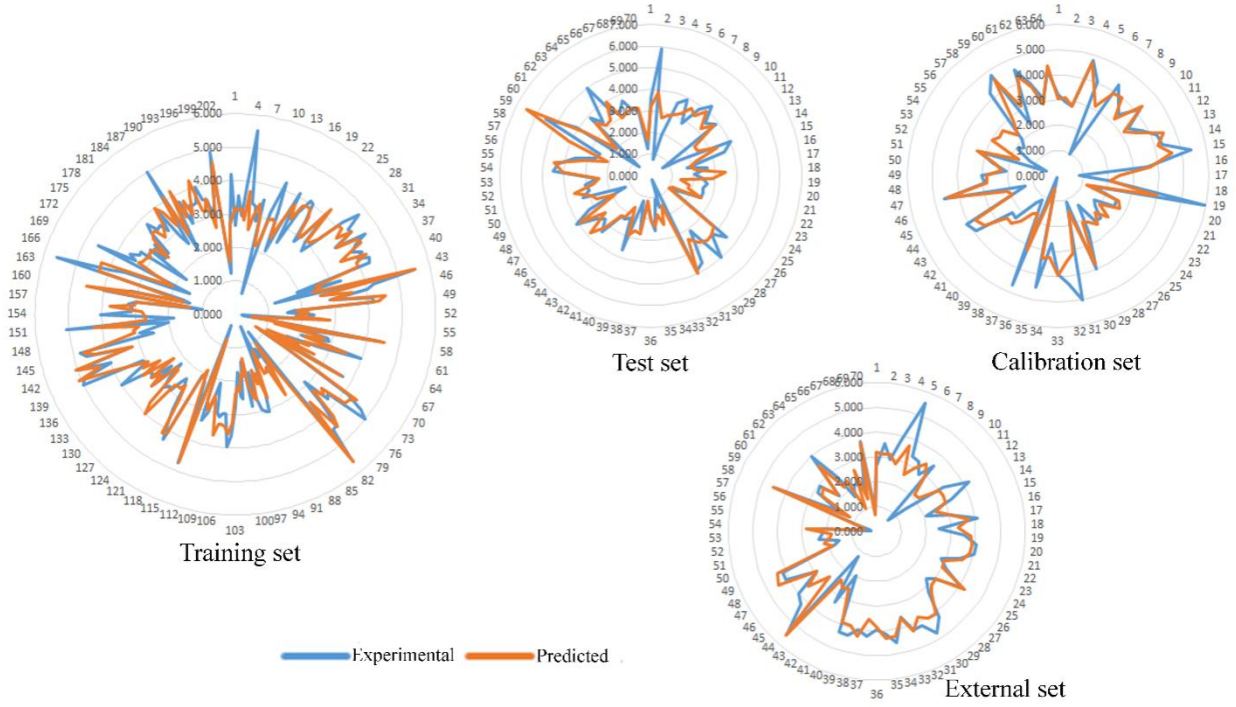

Figure 4: Radar plot showing fitness of observed and predicted inhibitory activity of training, test, calibration and external sets per model developed with considering cyclic rings

To explore the mechanistic interpretation of the model DCW were analysed. The molecular fragments including "+ + + +F- - -N= = =", "+ + + +CL- -N= = =", "+ + + +N- - -B3= =" and "+ + + +S- - -B3= =" were found to be crucial for the inhibition of the BACE1 enzyme. Conversly, "+ + + +F- - -B2= =", "+ + + +F- - -S= = =", "+ + + +CL- -S= = =" and "+ + + +O- - -B2= =" were given negative impact for the inhibitory activity. In case of bonding parameters the "BOND10000000" was found critical for pK_i but remaining two parmeters "BOND10100000" and "BOND11100000" not significant to increase or decrease the pK_i. Presence or absence of halogen atoms were also explored and found that "HALO10000000" (presence of fluorine) and "HALO11000000" (presence of both fluorine and clrorine) give negative influnece for the inhibition of BACE1.

The influence of cyclic rings of the molecular systems for the inhibition was explored. The statistical parameters of models developed without (Equation 4) and with (Equation 5) considering the cyclic rings were analyses. It was observed improved statistical parameters for the model developed with influence of cyclic ring on the pK_i. Above observation clearly suggested that cyclic rings in the BACE1 inhibitors were crucial for potential inhibition.

4. CONCLUSION

A large dataset of BACE1 inhibiotors was considered to develop the QSAR models with SMILES based molecular descriptors. The descriptors were calculated using the MC algoritm based CORAL software tool. Two approches such as without and with considering the impact of cyclic rings on the inhibitory activity were considered to develop QSAR model. Both models were assessed using the differentent statitical parameters including R^2, s, Q^2, R_m^2, ${}^C R_p$ etc. All statistical parameters clearly suggested that both models were statitically robust in nature. Predictive cabalibity was adjudged using the external set molcules by predicting the inhibitory activity. High correlation value between experimental and predicted activity of external set explained that models were capable enough to predict the pK_i of molecules outside the training set. Statistical parameters obtained from the both models also explained that cyclic rings were crucial of the BACE1 inhihibitors for the potential inhibition of BACE1 enzyme. Different molecular fragments were found to be important either increase or decrease the inhibitory activity which explain that both have mechanistic interpretation. Therefore, important molecular fragmanets explained by both models can play crucial role to identify new potential BACE1 inhibitors for the therapeutic application in Alzheimer's disease.

5. ACKNOWLEDGEMENT

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7. APPENDIX

Application of Monte Carlo Algorithm to Explore Simplified Molecular-Input Line-Entry System based Molecular Descriptors of BACE1 inhibitors for Therapeutic Application in Alzheimer's Disease

Supplementary data

Table S1: SMILES, experimental and predicted inhibitory activity of training, test, calibration and external sets used in QSAR model without considering cycling rings

Set	SMILES	Pk_i	
		[1]Obs	[2]Pred
Training set			
Tr1	O=C1OC([H])([H])C([H])([H])C([H])([H])C([H])([H])N([H])C(=O)C([H])([H])[C@]([H])(N([H])C(=O)[C@@]([H])(N1[H])C([H])(C([H])([H])[H])C([H])([H])[H])C(=O)N([H])[C@@]([H])(C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])[C@@]([H])(O[H])C([H])([H])[C@]([H])(	2.662	3.003
Tr2	O=C1OC([H])([H])C([H])([H])C([H])=C([H])C([H])([H])N([H])C(=O)C([H])([H])[C@]([H])(N([H])C(=O)[C@@]([H])(N1[H])C([H])(C([H])([H])[H])C([H])([H])[H])C(=O)N([H])[C@@]([H])(C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])[C@@]([H])(O[H])C([H])([H])[C@]([H]	3.547	3.009
Tr3	O=C2N([H])[C@]([H])(C(=O)N([H])[C@@]([H])(C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])[C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C=1C([H])=C([H])C([H])=C([H])C=1[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H]	2.966	3.165
Tr4	O=C(OC([H])([H])N1N=C(C([H])=C1C([H])([H])[H])C([H])([H])[H])N([H])[C@]([H])(C(=O)N([H])[C@@]([H])(C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])[C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C=2C([H])=C([H])C([H])=C([	3.854	2.836
Tr5	O=C(OC([H])([H])N1N=C(C([H])=C1C([H])([H])[H])C([H])([H])[H])N([H])[C@]([H])(C(=O)N([H])[C@@]([H])(C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])[C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H	5.523	3.748
Tr6	[F]/C1=C(\[H])C([H])=C(C([H])=C1[H])[C@]([H])(N([H])C(=O)C2=C([H])C(=C([H])C(=C2[H])C3=NN=C(O3)[C@@](C([H])([H])[H])(C([H])([H])C=4C([H])=C([H])C([H])=C([H])C=4[H])[N]([H])([H])[H])N(C([H])([H])[H])[S](=O)(=O)C([H])([H])[H])C([H])([H])[H]	3.373	2.634
Tr7	O=[S](=O)(N(C=2C([H])=C(C([H])=C([H])[C@@]1([H])C([H])([H])[C@]1([H])C([H])([H])[H])C([H])=C(C=2[H])C3=NN=C(O3)[C@@](C([H])([H])[H])(C([H])([H])C=4C([H])=C([H])C([H])=C([H])C=4[H])[N]([H])([H])[H])C([H])([H])C([H])([H])C([H])([H])[H])C([H])([H])[H]	3.285	2.874
Tr8	O=C(C=1C([H])=C(C([H])=C(C=1[H])C(=O)N([H])[C@@]([H])(C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])[C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([	2.866	3.413

Tr9	O=C(N(C([H])([H])[H])[C@@]1([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C1([H])[H])C([H])([H])C([H])([H])[C@@]([H])(N4C(=NC=3C([H])=C([H])C(OC=2C([H])=C([H])C([H])=C([H])C=2[H])=C([H])C=3C4([H])[H])N([H])[H])[C@]5([H])C([H])([H])C([H])([H])C([H])([H	3.523	3.079
Tr10	O=C(N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])[C@@]([H])(N([H])C(=O)OC(C([H])([H])[H])[H])	0.649	2.248
Tr11	O=C(N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])[C@@]([H])(N([H])C	1.504	2.320
Tr12	O=C(N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])[C@@]([H])(N([H])C(=O)[C@@]([H])(N([H])C	3.212	3.106
Tr13	O=C(N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])[C@@]([H])(N([H])C	4.229	3.178
Tr14	O=C(N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])[C@@]([H])(N([H])C	3.300	3.016
Tr15	O=C(C=1C([H])=C([H])C([H])=C(C=1[H])C(=O)N([H])[C@@]([H])(C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])[C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H	2.103	2.320
Tr16	O=C1OC([H])([H])C([H])=C([H])C([H])([H])N([H])C(=O)C([H])([H])[C@]([H])(N([H])C(=O)[C@@]([H])(N1[H])C([H])(C([H])([H])[H])C([H])([H])[H])C(=O)N([H])[C@@]([H])(C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])[C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H	3.059	2.985
Tr17	O=C(N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])[C@@]([H])(N([H])C	4.097	3.772
Tr18	O=C(C=1C([H])=C(C([H])=C(C=1[H])C(=O)N([H])[C@@]([H])(C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])[C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([	2.502	3.244
Tr19	O=C(C=1C([H])=C(C([H])=C(C=1[H])C(=O)N([H])[C@@]([H])(C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])[C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([	3.569	4.073
Tr20	O=C2N(C(=N[C@]4(C=1C([F])=C([H])C([H])=C([F])C=1[H])[C@@]2([H])C([H])([H])N(/C3=N/C(=C(/[F])C(=N3)OC([H])([H])[H])C([H])([H])[H])C4([H])[H])N([H])[H])C([H])([H])[H]	4.071	3.913

Tr21	O=C2N(C(=N[C@]4(C=1C([F])=C([H])C([H])=C([H])C=1[H])[C@@]2([H])C([H])([H])N(/C3=N/C(=C(/[Cl])C(=N3)OC([H])([H])[H])C([H])([H])[H])C4([H])[H])N([H])[H])C([H])([H])[H]	4.032	3.673
Tr22	O=C2N(C(=N[C@]4(C=1C([F])=C([H])C([H])=C([H])C=1[F])[C@@]2([H])C([H])([H])N(/C3=N/C(=C(/[F])C(=N3)OC([H])([H])[H])C([H])([H])[H])C4([H])[H])N([H])[H])C([H])([H])[H]	3.495	3.673
Tr23	O=C2N(C(=N[C@]4(C=1C([H])=C([H])C([H])=C([H])C=1[H])[C@@]2([H])C([H])([H])N(/C3=N/C(=C(/[F])C(=N3)C([H])([H])[H])C([H])([H])[H])C4([H])[H])N([H])[H])C([H])([H])[H]	2.812	3.157
Tr24	O=C2N(C(=N[C@]4(C=1C([H])=C([H])C([H])=C([H])C=1[H])[C@@]2([H])C([H])([H])N(/C3=N/C(=C(/[F])C(=N3)C([H])([H])C([H])([H])[H])C([H])([H])[H])C4([H])[H])N([H])[H])C([H])([H])[H]	3.215	3.181
Tr25	O=C2N(C(=N[C@]4(C=1C([F])=C([H])C([F])=C([F])C=1[H])[C@@]2([H])C([H])([H])N(/C3=N/C(=C(/[F])C(=N3)OC([H])([H])[H])C([H])([H])[H])C4([H])[H])N([H])[H])C([H])([H])[H]	4.114	4.250
Tr26	O=C2N(C(=N[C@]5(C=1C([H])=C([H])C([H])=C([H])C=1[H])[C@@]2([H])C([H])([H])N(/C3=N/C(=C(/[Cl])C(=N3)[C@@]4([H])C([H])([H])C4([H])[H])C([H])([H])[H])C5([H])[H])N([H])[H])C([H])([H])[H]	3.027	2.953
Tr27	O=C2N(C(=N[C@]5(C=1C([H])=C([H])C([H])=C([H])C=1[H])[C@@]2([H])C([H])([H])N(/C3=N/C(=C(/[Cl])C(=N3)[C@@]4([H])C([H])([H])C4([H])[H])C([H])([H])C([H])([H])[H])C5([H])[H])N([H])[H])C([H])([H])[H]	2.745	2.977
Tr28	O=C2N(C(=N[C@]4(C=1C([H])=C([H])C([F])=C([H])C=1[H])[C@@]2([H])C([H])([H])N(/C3=N/C(=C(/[F])C(=N3)C([H])([H])[H])C([H])([H])[H])C4([H])[H])N([H])[H])C([H])([H])[H]	3.194	3.493
Tr29	O=C2N(C(=N[C@]4(C=1C([H])=C([F])C([H])=C([H])C=1[F])[C@@]2([H])C([H])([H])N(/C3=N/C(OC([H])([H])[H])=C([F])C(=N3)OC([H])([H])[H])C4([H])[H])N([H])[H])C([H])([H])[H]	4.252	3.992
Tr30	O=C2N(C(=N[C@]4(C=1C([H])=C([H])C([F])=C([H])C=1[F])[C@@]2([H])C([H])([H])N(/C3=N/C(OC([H])([H])[H])=C([F])C(=N3)OC([H])([H])[H])C4([H])[H])N([H])[H])C([H])([H])[H]	4.745	3.992
Tr31	O=C2N(C(=N[C@]4(C=1C([H])=C([H])C([F])=C([H])C=1[H])[C@@]2([H])C([H])([H])N(/C3=N/C(OC([H])([H])[H])=C([F])C(=N3)C([H])([H])C([H])([H])[H])C4([H])[H])N([H])[H])C([H])([H])[H]	4.215	3.836
Tr32	O=C2N(C(=N[C@]5(C=1C([F])=C([H])C([H])=C([F])C=1[H])[C@@]2([H])C([H])([H])N(/C3=N/C(OC([H])([H])[H])=C([F])C(=N3)[C@]4([H])C([H])([H])C4([H])[H])C5([H])[H])N([H])[H])C([H])([H])[H]	4.252	4.244
Tr33	O=C2N(C(=N[C@]5(C=1C([H])=C([F])C([H])=C([H])C=1[F])[C@@]2([H])C([H])([H])N(/C3=N/C(=C(/[F])C(=N3)[C@]4([H])C([H])([H])C4([H])[H])C([H])([H])[H])C5([H])[H])N([H])[H])C([H])([H])[H]	3.585	3.686
Tr34	O=C2N(C(=N[C@]5(C=1C([F])=C([H])C([F])=C([H])C=1[H])[C@@]2([H])C([H])([H])N(/C3=N/C(OC([H])([H])[H])=C([F])C(=N3)[C@]4([H])C([H])([H])C4([H])[H])C5([H])[H])N([H])[H])C([H])([H])[H]	4.569	4.244
Tr35	O=C2N(C(=N[C@]5(C=1C([F])=C([H])C([F])=C([H])C=1[H])[C@@]2([H])C([H])([H])N(/C3=N/C(OC([H])([H])[H])=C([Cl])C(=N3)[C@]4([H])C([H])([H])C4([H])[H])C5([H])[H])N([H])[H])C([H])([H])[H]	4.167	4.166

Tr36	[F]C=1C([H])=C([F])C(=C([H])C=1[H])[C@@]24N=C(N(C(=O)[C@]2([H])C([H])([H])N(/C3=N/C(=C(/[F])C(=N3)OC([H])([H])[H])C([F])([F])C([H])([H])[H])C4([H])[H])C([H])([H])[H])N([H])[H]	3.959	3.865
Tr37	O=C2N(C(=N[C@]4(C=1C([F])=C([H])C([H])=C([H])C=1[H])[C@@]2([H])C([H])([H])N(/C3=N/C(=C(/[F])C(=N3)OC([H])([H])[H])C([H])([H])[H])C4([H])[H])N([H])[H])C([H])([H])[H]	4.222	3.577
Tr38	O=C2N(C(=N[C@]4(C=1C([F])=C([Cl])C([F])=C([H])C=1[H])[C@@]2([H])C([H])([H])N(/C3=N/C(=C(/[F])C(=N3)OC([H])([H])[H])C([H])([H])[H])C4([H])[H])N([H])[H])C([H])([H])[H]	4.036	4.171
Tr39	O=C2N(C(=N[C@]4(C=1C([Cl])=C([H])C([F])=C([H])C=1[H])[C@@]2([H])C([H])([H])N(/C3=N/C(=C(/[F])C(=N3)OC([H])([H])[H])C([H])([H])[H])C4([H])[H])N([H])[H])C([H])([H])[H]	4.347	3.835
Tr40	O=C2N(C(=N[C@]5(C=1C([H])=C([H])C([F])=C([H])C=1[H])[C@@]2([H])C([H])([H])N(/C3=N/C(OC([H])([H])[H])=C([F])C(=N3)[C@]4([H])C([H])([H])C4([H])[H])C5([H])[H])N([H])[H])C([H])([H])[H]	4.319	3.908
Tr41	O=[S](=O)(C([H])([H])[C@]([H])(N([H])C(=O)OC(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])C(=O)C([H])([H])N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])(C([H])([H]	1.947	2.199
Tr42	O=C(N([H])[C@@]([H])(C(=O)N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[	3.301	2.715
Tr43	O=C(OC(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])N([H])[C@@]([H])(C(=O)N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])	1.236	2.247
Tr44	O=C(N([H])[C@]([H])(C(=O)C([H])([H])[C@]([H])(C(=O)O[H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])([H])C([H])([H])C(=O)O[H])[C@@]([H])(N([H])C(=O)[C@@]([H])(C([H])([H])[C@]([H])(O[H])[C@@]([H])(N([H])C(=O)[C@@]([H])(N([H])C(=O)[C@@]([H])(N([H]	5.495	5.079
Tr45	O=C(N([H])[C@]([H])(C(=O)N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])([H])[H])C([H])([H])[H])[H]	4.229	2.805
Tr46	O=[S](=O)(C([H])([H])[C@@]([H])(C(=O)N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])(C([H])([H])[H])C	4.027	3.219
Tr47	N#C/C1=C(\[F])C([H])=C([H])C(=C1[H])C=2[S]/C(=C(/[H])C=2[H])[C@@]35N=C(N(C(=O)[C@]3([H])C([H])([H])N(/C4=C(\[H])C([H])=C([F])C([H])=C4[H])C5([H])[H])C([H])([H])[H])N([H])[H]	2.879	2.953
Tr48	O=[S]3(=O)N(C=2C([H])=C(C([H])=C1/C(=C(/[H])N(C1=2)C([H])([H])C3([H])[H])C([H])([H])C([H])([H])[H])C(=O)N([H])[C@]([H])(C([H])([H])N([H])[C@]([H])(C(=O)N([H])C([H])([H])C([H])(C([H])([H])[H])[H])C([H])([H])[H])[C@@]([H])(O[H])C([H])([H])[H])C([H])([H])C4=C(	4.137	4.524

Tr49	O=[S]3(=O)N(C=2C([H])=C(C([H])=C1/C(=C(/[H])N(C1=2)C([H])([H])[C@]34C([H])([H])C4([H])[H])C([H])([H])C([H])([H])[H])C(=O)N([H])[C@]([H])(C([H])([H])N([H])[C@]([H])(C(=O)N([H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])[C@@]([H])(O[H])C([H])([H])[H]	4.143	4.337
Tr50	O=C(N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])([H])C(=O)O[H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])([H])[C@]([H])(N([H])C(=O)C([H])([H])C([H])(C([H])([H])	1.770	1.714
Tr51	O=C(N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])([H])OC(=O)C([H])([H])[H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])([H])[C@]([H])(N([H])C(=O)C([H])([H])C([H])	1.569	2.044
Tr52	O=C(N([H])[C@@]([H])(C=1C([H])=C([H])C([H])=C([H])C=1[H])C([H])([H])[H])C2=C([H])C(=C([H])C(=C2[H])N(C([H])([H])[H])[S](=O)(=O)C([H])([H])[H])C(=O)N([H])[C@]([H])([C@]([H])([H])(O[H])C([H])([H])N([H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])C3=C([H])C	2.372	1.883
Tr53	O=C(N([H])[C@]([H])(C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])([H])[H])C2=C([H])C(=C([H])C(=C2[H])N(C([H])([H])[H])[S](=O)(=O)C([H])([H])[H])C(=O)N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])N([H])C([H])([H])C3=C([H])C(OC([H])([H])[H])=C([H])C([H])=C3[H])C(	2.210	1.770
Tr54	O=C(N([H])C([H])([H])C=1N=C(OC=1C([H])([H])[H])C([H])([H])[H])C2=C([H])C(=C([H])C(=C2[H])N(C([H])([H])[H])[S](=O)(=O)C([H])([H])[H])C(=O)N([H])[C@]([H])([C@]([H])([H])(O[H])C([H])([H])N([H])C([H])([H])C3=C([H])C(OC([H])([H])[H])=C([H])C([H])=C3[H])C([H])([H]	2.258	2.988
Tr55	O=C3O/C2=C(\OC([H])([H])C([H])=C(C([H])([H])C([H])([H])C([H])=C(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C=1OC([H])=C([H])C=1C([H])=C2C([H])=C3[H]	0.208	0.512
Tr56	O=C3OC=2C(OC([H])([H])[C@@]([H])(O[H])C(O[H])(C([H])([H])[H])C([H])([H])[H])=C1OC([H])=C([H])C1=C(OC([H])([H])[H])C=2C([H])=C3[H]	0.260	0.613
Tr57	O=C3OC=2C(OC([H])([H])[H])=C1OC([H])=C([H])C1=C(OC([H])([H])C([H])=C(C([H])([H])C([H])([H])C([H])=C(C([H])([H])[H])C([H])([H])C([H])([H])[H])C([H])([H])[H])C=2C([H])=C3[H]	0.863	0.740
Tr58	O=C(N([H])C(=NC([H])([H])C1=C([H])C([Cl])=C(C([Cl])=C1[H])N([H])C(=O)C([H])([H])N2C([H])([H])C([H])([H])C2([H])[H])N([H])[H])C=3C(=N[S]C=3C([H])([H])[H])C4=C([H])C([H])=C(OC([H])([H])[H])C([H])=C4[H]	4.398	4.400
Tr59	O=C(N([H])C(=NC([H])([H])C=1C([H])=C([H])C([H])=C2C=1C([H])=C([H])C([H])=C2[H])N([H])[H])C=3C(=NOC=3C([H])([H])[H])C4=C([H])C([H])=C(OC([H])([H])[H])C([H])=C4[H]	1.770	1.286
Tr60	O=C(N([H])C(=NC([H])([H])C1=C([H])C(=C([H])C([Cl])=C1[H])C([H])=C([H])C([H])([H])C([H])([H])O[H])N([H])[H])C=2C(=NOC=2C([H])([H])[H])C3=C([H])C([H])=C(OC([H])([H])[H])[H])C([H])=C3[H]	2.854	2.816
Tr61	O=C(N([H])C(=NC([H])([H])C1=C([H])C([Cl])=C(C([Cl])=C1[H])N([H])[H])N([H])[H])C=2C(=NOC=2C([H])([H])[H])C3=C([H])C([H])=C(OC([H])([H])[H])C([H])=C3[H]	2.921	2.713
Tr62	O=C(N([H])C(=NC([H])([H])C1=C([H])C(=C([H])C([Cl])=C1[H])C([H])=C([H])C([H])([H])C([H])([H])C([H])([H])[H])N([H])[H])C=2C(=NOC=2C([H])([H])[H])C3=C([H])C([H])=C(OC([H])([H])[H])C([H])=C3[H]	2.071	2.293
Tr63	O=C(N([H])C(=NC([H])([H])C1=C([H])C(=C(C([Cl])=C1[H])N([H])C(=O)C([H])([H])N([H])C([H])([H])C2=C([H])C([H])=C([H])C([H])=C2[H])C([H])([H])N([H])[H])C=3C(=N[S]	4.000	3.296

	C=3C([H])([H])[H])C4=C([H])C([H])=C(OC([H])([H])[H])C([H])=C4[H]		
Tr64	O=C(N([H])C(=NC([H])([H])C1=C([H])C([Cl])=C([H])C([Cl])=C1[H])N([H])[H])C=2C(=NN([H])C=2C([H])([H])[H])C3=C([H])C([H])=C(OC([H])([H])[H])C([H])=C3[H]	2.678	2.179
Tr65	O=C(N([H])C(=NC([H])([H])C1=C([H])C([Cl])=C([H])C([Cl])=C1[H])N([H])[H])C=2C(=NOC=2C([H])([H])[H])C3=C([H])C([H])=C([F])C([H])=C3[H]	1.658	2.395
Tr66	O=C(N([H])C(=NC([H])([H])C1=C([H])C([Cl])=C([H])C([Cl])=C1[H])N([H])[H])C2=C(O/N=C2/C([H])([H])[H])C3=C([H])C([H])=C(OC([H])([H])[H])C([H])=C3[H]	2.066	1.147
Tr67	O=C(N([H])C(=NC([H])([H])C1=C([H])C=2C(C([H])=C1[H])=C([H])C([H])=C([H])C=2[H])N([H])[H])C=3C(=N[S]C=3C([H])([H])[H])C4=C([H])C([H])=C(OC([H])([H])[H])C([H])=C4[H]	2.060	2.445
Tr68	O=C(N([H])C(=NC([H])([H])C=1C([H])=C([H])C([H])=C2C=1C([H])=C([H])C([H])=C2[H])N([H])[H])C=3C(=NOC=3C([H])([H])[H])C4=C([H])C([H])=C([F])C([H])=C4[H]	1.745	1.448
Tr69	O=C(N([H])C(=NC([H])([H])C1=C([H])C(=C(C([Cl])=C1[H])N([H])C(=O)C([H])([H])N([H])C([H])([H])C([H])([H])[H])C([H])([H])[H])N([H])[H])C=2C(=N[S]C=2C([H])([H])[H])C3=C([H])C([H])=C(OC([H])([H])[H])C([H])=C3[H]	3.699	3.530
Tr70	O=C2C=1C(O[H])=C([H])C(O[H])=C([H])C=1O/C(=C2/O[H])C3=C([H])C([H])=C(O[H])C(O[H])=C3[H]	0.854	0.488
Tr71	[H]C=2C(O[H])=C1OC=6C(OC1=C3C=2OC=4/C3=C(/O[H])C([H])=C(O[H])C=4O/C5=C(\[H])C(O[H])=C([H])C(O[H])=C5[H])=C(O[H])C([H])=C(O[H])C=6OC=7C([H])=C(O[H])C([H])=C(O[H])C=7[H]	1.886	2.278
Tr72	O=C(/C1=C(\[H])C(=C([H])C(=C1[H])C(=O)N2[C@]([H])(C([H])([H])C([H])([H])C2([H])[H])C([H])([H])OC([H])([H])[H])C([H])([H])[H])N([H])[C@]([H])([C@]([H])(O[H])[C@]3([H])N([H])C([H])([H])C([H])([H])N(C3([H])[H])[S](=O)(=O)[C@@]4([H])C([H])([H])C4([H])[H])C(	4.155	4.463
Tr73	[F]C=1C([H])=C(C([H])=C([F])C=1[H])C([H])([H])[C@]([H])(N([H])C(=O)C2=C([H])C(=C([H])C(=C2[H])C(=O)N3[C@]([H])(C([H])([H])C([H])([H])C3([H])[H])C([H])([H])OC([H])([H])[H])C([H])([H])[H])[C@]([H])(O[H])[C@]4([H])N([H])C([H])([H])C([H])([H])N(C4([H])[H])[	4.699	4.487
Tr74	[F]C=1C([H])=C(C([H])=C([F])C=1[H])C([H])([H])[C@]([H])(N([H])C(=O)C2=C([H])C(=C([H])C(=C2[H])C(=O)N3[C@]([H])(C([H])([H])C([H])([H])C3([H])[H])C([H])([H])OC([H])([H])[H])C([H])([H])[H])[C@]([H])(O[H])[C@]4([H])N([H])C([H])([H])C([H])([H])N(C4([H])[H])[	5.000	4.481
Tr75	O=C3N(C([H])([H])C([H])([H])C=4C([H])=C(OC=2C([H])=C([H])C=1N=C(N(C([H])([H])C=1C=2[H])[C@@]([H])(C([H])([H])C3([H])[H])C([H])(C([H])([H])[H])C([H])([H])[H])N([H])[H])C([H])=C([H])C=4[H])[C@]5([H])C([H])([H])C([H])([H])OC([H])([H])C5([H])[H]	3.658	3.747
Tr76	O=C3N(C([H])([H])C([H])([H])C=5C([H])=C(O/C2=C(\[H])C([H])=C1N=C(N(C([H])([H])C1=C2[H])[C@@]([H])(C([H])([H])C3([H])[H])[C@@]4([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C4([H])[H])N([H])[H])C([H])=C([H])C=5[H])[C@@]6([H])C([H])([H])C([H])([H])OC([	3.770	3.475
Tr77	O=C(N([H])[C@@]([H])(C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])([H])[H])C2=C([H])C(=C([H])C(=C2[H])N(C([H])([H])[H])[S](=O)(=O)C([H])([H])[H])C(=O)N([H])[C@]([H])(C([H])([H])C([H])([H])[H])[C@@]([H])(OC([H])([H])[H])C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H]	2.886	3.348
Tr78	O=C(N([H])[C@@]([H])(C=1C([H])=C([H])C([H])=C([H])C=1[H])C([H])([H])[H])C=2C([H])=C(C([H])=C(C=2[H])N(C([H])([H])[H])[S](=O)(=O)C([H])([H])[H])C(=O)N([H])[C@]([H	3.699	4.519

	])([C@@]([H])(O[H])C([H])([H])[C@@]([H])(OC([H])([H])C3=C([H])C([H])=C([H])C([H])=C3[H])C(=O		
Tr79	O=C(N([H])[C@@]([H])(C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])([H])[H])C=2C([H])=C(C([H])=C(C=2[H])N(C([H])([H])[H])[S](=O)(=O)C([H])([H])[H])C(=O)N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])[C@@]([H])(OC([H])([H])C([H])([H])OC([H])([H])[H])C(=O)N([H])[C	4.509	4.434
Tr80	O=C(N([H])[C@@]([H])(C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])([H])[H])C2=C([H])C(=C([H])C(=C2[H])N(C([H])([H])[H])[S](=O)(=O)C([H])([H])[H])C(=O)N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])[C@@]([H])(OC([H])([H])C([H])([H])C([H])([H])[H])C(=O)N([H])[C@]	4.523	3.413
Tr81	O=C(N([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)O[H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])([H])C([H])([H])C(=O)O[H])[C@@]([H])(N([H])C(=O)[C@@]([H])(C([H])([H])[C@]([H])(O[H])[C@@]([H])(N([H])C(=O)[C@@]([H])(N([H])C(=O)[C@@]([H])(N([H])C(=O	5.495	5.409
Tr82	O=C(OC(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])N([H])[C@]([H])(C(=O)N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])(C	0.649	2.241
Tr83	O=C3N([H])[C@]([H])(C(=O)N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])N([H])C([H])([H])C1=C([H])C(=C([H])C([H])=C1[H])N(C([H])([H])[H])C([H])([H])[H])C([H])([H])C2=C([H])C([H])=C([H])C([H])=C2[H])C([H])([H])[C@@]3([H])C([H])([H])C4=C([H])C([H])=C([H])C([H]	1.522	1.019
Tr84	O=C3N([H])[C@]([H])(C(=O)N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])N([H])C([H])([H])C1=C([H])C(=C([H])C([H])=C1[H])N(C([H])([H])[H])C([H])([H])[H])C([H])([H])C2=C([H])C([H])=C([H])C([H])=C2[H])C([H])([H])N3C([H])([H])C4=C([H])C([H])=C([F])C([H])=C4[H]	2.087	2.135
Tr85	O=C3N([H])[C@]([H])(C(=O)N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])N([H])C([H])([H])C1=C([H])C(=C([H])C([H])=C1[H])N(C([H])([H])[H])C([H])([H])[H])C([H])([H])C2=C([H])C([H])=C([H])C([H])=C2[H])C([H])([H])N3C([H])([H])C4=C([H])C([H])=C(C([H])=C4[H])C([F]	1.305	2.861
Tr86	O=C3N([H])[C@](C(=O)N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])N([H])C([H])([H])C1=C([H])C(=C([H])C([H])=C1[H])N(C([H])([H])[H])C([H])([H])[H])C([H])([H])C2=C([H])C([H])=C([H])C([H])=C2[H])(C([H])([H])N3C([H])([H])C4=C([H])C([H])=C([H])C([H])=C4[H])C([H]	1.170	1.871
Tr87	O=C3N([H])[C@]([H])(C(=O)N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])N([H])C([H])([H])C1=C([H])C(=C([H])C([H])=C1[H])N(C([H])([H])[H])C([H])([H])[H])C([H])([H])C2=C([H])C([H])=C([H])C([H])=C2[H])C([H])([H])N3C([H])([H])C([H])([H])O/C4=C(\[H])C([H])=C([H])	1.454	2.093
Tr88	O=C3N([H])[C@]([H])(C(=O)N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])N([H])C([H])([H])C1=C([H])C(=C([H])C([H])=C1[H])N(C([H])([H])[H])C([H])([H])[H])C([H])([H])C2=C([H])C([H])=C([H])C([H])=C2[H])C([H])([H])N3/C4=C(\[H])C([Br])=C([H])C([Br])=C4[H]	1.456	1.744
Tr89	O=C3N([H])[C@]([H])(C(=O)N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])N([H])C([H])([H])C1=C([H])C(=C([H])C([H])=C1[H])N(C([H])([H])[H])C([H])([H])[H])C([H])([H])C2=C([H])C([H])=C([H])C([H])=C2[H])C([H])([H])N3[H]	0.721	1.318
Tr90	O=C3N([H])[C@]([H])(C(=O)N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])N([H])C([H])([H])C1=C([H])C(=C([H])C([H])=C1[H])N(C([H])([H])[H])C([H])([H])[H])C([H])([H])C2=C([H])C([H])=C([H])C([H])=C2[H])C([H])([H])N3C([H])([H])C([H])([H])C([H])([H])C([H])([H	0.398	1.774

	])[H]		
Tr91	O=C1N(C(=N[C@@]1(C=2C([H])=C([H])C([H])=C([H])C=2[H])C3=C([H])C(=C([H])C([H])=C3[H])C=4/N=C(/[H])C([H])=NC=4[H])N([H])[H])C([H])([H])[H]	2.509	2.696
Tr92	O=C1N(C(=N[C@]1(C=2C([H])=C([H])C([H])=C([H])C=2[H])C3=C([H])C(=C([H])C([H])=C3[H])C4=C([H])C(OC([H])([H])[H])=C([H])C([H])=C4[H])N([H])[H])C([H])([H])[H]	3.097	1.964
Tr93	O=C1N(C(=N[C@]1(C=2C([H])=C([H])C([H])=C([H])C=2[H])C3=C([H])C(=C([H])C([H])=C3[H])C4=C([H])N=C([H])C([Cl])=C4[H])N([H])[H])C([H])([H])[H]	3.046	2.239
Tr94	O=C1N(C(=N[C@]1(C=2C([H])=C([H])C([H])=C([H])C=2[H])C3=C([H])C(=C([H])C([H])=C3[H])C4=C([H])N=C([H])C([H])=C4[H])N([H])[H])C([H])([H])[H]	2.959	1.844
Tr95	O=C1N(C(=N[C@@]1(C=2C([H])=C([H])C([H])=C([H])C=2[H])C3=C([H])C([Cl])=C([H])C([H])=C3[H])N([H])[H])C([H])([H])[H]	2.523	2.636
Tr96	O=C1N(C(=N[C@@]1(C=2C([H])=C([H])C([H])=C([H])C=2[H])C3=C([H])C(=C([H])C([H])=C3[H])C4=C([H])N=C([H])C([H])=C4[H])N([H])[H])C([H])([H])[H]	1.770	2.444
Tr97	O=C1N(C(=N[C@@]1(/C2=C(\[H])C(=C([H])C([H])=C2[H])C3=C([H])N=C([H])C([F])=C3[H])[C@@]4([H])C([H])([H])C4([H])[H])N([H])[H])C([H])([H])[H]	2.796	2.257
Tr98	O=C1N(C(=N[C@]1(/C2=C(\[H])C([H])=C([H])C([H])=C2[H])C3=C([H])C(=C([H])C([H])=C3[H])C4=C([H])C([H])=C([H])C([H])=C4[H])N([H])[H])C([H])([H])[H]	1.481	1.532
Tr99	O=C1N(C(=N[C@]1(C=2C([H])=C([H])C([H])=C([H])C=2[H])C3=C([H])C(=C([H])C([H])=C3[H])C4=C([H])C([H])=C(OC([H])([H])[H])C([H])=C4[H])N([H])[H])C([H])([H])[H]	1.420	1.964
Tr100	O=C3N([H])[C@]([H])(C(=O)N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])N([H])C([H])([H])C1=C([H])C(=C([H])C([H])=C1[H])N(C([H])([H])[H])C([H])([H])[H])C([H])([H])C2=C([H])C([H])=C([H])C([H])=C2[H])C([H])([H])N3C([H])([H])C4=C([H])C([H])=C([H])C([H])=C4[H]	2.547	1.847
Tr101	O=C1N(C(=N[C@@]1(/C2=C(\[H])C([H])=C([H])C([H])=C2[H])C3=C([H])C(C#N)=C([H])C([H])=C3[H])N([H])[H])C([H])([H])[H]	2.432	2.432
Tr102	O=C1N(C(=N[C@]1(C=2C([H])=C([H])C([H])=C([H])C=2[H])C3=C([H])C(=C([H])C([H])=C3[H])C4=NC([H])=C([H])C([H])=C4[H])N([H])[H])C([H])([H])[H]	1.721	2.336
Tr103	O=C(N([C@@]1([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C1([H])[H])C([H])([H])[H])C([H])([H])C([H])([H])[C@]([H])(N4C(=N/C3=C(\[H])C([H])=C(O/C2=C(\[H])C([H])=C([H])C([H])=C2[H])C([H])=C3C4([H])[H])N([H])[H])C5=C([H])C([H])=C([H])C([H])=C5[H]	2.785	2.466
Tr104	O=C(N([C@@]1([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C1([H])[H])C([H])([H])C2=C([H])N([H])N=C2[H])C([H])([H])C([H])([H])[C@]([H])(N5C(=NC=4C([H])=C([H])C(O/C3=C(\[H])C([H])=C([H])C([H])=C3[H])=C([H])C=4C5([H])[H])N([H])[H])[C@@]6([H])C([H])([H])	3.638	2.778
Tr105	O=C(N([C@@]1([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C1([H])[H])C([H])([H])C2=C([H])N(/N=C2/[H])C([H])([H])[H])C([H])([H])C([H])([H])[C@]([H])(N5C(=NC=4C([H])=C([H])C(O/C3=C(\[H])C([H])=C([H])C([H])=C3[H])=C([H])C=4C5([H])[H])N([H])[H])[C@@]6([H	3.959	3.505
Tr106	O=C(N([C@@]1([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C1([H])[H])C([H])([H])C([H])([H])C=2N=C([S]C=2[H])C([H])([H])[H])C([H])([H])C([H])([H])[C@]([H])(N5C(=NC=4C([H])=C([H])C(O/C3=C(\[H])C([H])=C([H])C([H])=C3[H])=C([H])C=4C5([H])[H])N([H])[H])[C	2.975	3.331

Tr107	O=C(N([C@@]1([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C1([H])[H])[C@@]([H])(C=2N=C([S]C=2[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])([H])[C@]([H])(N5C(=NC=4C([H])=C([H])C(O/C3=C(\[H])C([H])=C([H])C([H])=C3[H])=C([H])C=4C5([H])[H])N([H])[H	2.983	3.211
Tr108	O=C(N([C@@]1([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C1([H])[H])C([H])([H])C=2N=C([S]C=2[H])C([H])([H])[H])C([H])([H])C([H])([H])[C@]([H])(N5C(=NC=4C([H])=C([H])C(O/C3=C(\[H])C([H])=C([H])C([H])=C3[H])=C([H])C=4C5([H])[H])N([H])[H])[C@@]6([H])C(	3.102	3.307
Tr109	O=C(OC([H])([H])[C@]([H])(N3C(=N/C2=C(\[H])C([H])=C(O/C1=C(\[H])C([H])=C([H])C([H])=C1[H])C([H])=C2C3([H])[H])N([H])[H])[C@]4([H])C([H])([H])OC([H])([H])C([H])([H])C4([H])[H])N([C@@]5([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C5([H])[H])C([H])([H]	2.983	3.368
Tr110	O=C(OC([H])([H])[C@]([H])(N3C(=N/C2=C(\[H])C([H])=C(O/C1=C(\[H])C([H])=C([H])C([H])=C1[H])C([H])=C2C3([H])[H])N([H])[H])C4=C([H])C([H])=C([H])C([H])=C4[H])N([C@@]5([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C5([H])[H])C([H])([H])[H]	2.106	2.462
Tr111	N#CC=1C([H])=C(C([H])=C([H])C=1[H])C=2[S]C([H])=C(C=2[H])[C@]3(N=C(N(C(=O)C3([H])[H])C([H])([H])[H])N([H])[H])C([H])([H])[H]	2.678	2.720
Tr112	N#CC=1C([H])=C(C([H])=C([H])C=1[H])C=2[S]/C(=C(/[H])C=2[H])[C@]3(N=C(N(C(=O)C3([H])[H])C([H])([H])[H])N([H])[H])C([H])([H])[H]	3.056	3.187
Tr113	O=C3N(C(=N[C@](C=1C([H])=C([S]C=1[H])C2=C([H])C(C#CC([H])([H])[H])=C([H])N=C2[H])(C3([H])[H])C([H])([H])[H])N([H])[H])C([H])([H])[H]	3.328	3.218
Tr114	O=C4N(C(=N[C@@](/C1=C(\[H])C([H])=C([H])C(=C1[H])C2=C([H])N=C([H])C([H])=C2[H])(C3=C([H])C([H])=C([H])C([H])=C3[H])C4([H])[H])N([H])[H])C([H])([H])[H]	0.357	0.967
Tr115	O=C3N(C(=N[C@](C=2[S]C(C=1C([H])=C(C#CC([H])([H])[H])C([H])=NC=1[H])=C([H])C=2[Cl])(C3([H])[H])C([H])([H])[H])N([H])[H])C([H])([H])[H]	4.770	5.025
Tr116	O=C(O[C@]2([H])[C@@]([H])(OC1=C(C(O[H])=C([H])C(O[H])=C1[H])C2([H])[H])C=3C([H])=C(O[H])C(O[H])=C(O[H])C=3[H])C=4C([H])=C(O[H])C(O[H])=C(O[H])C=4[H]	2.678	2.775
Tr117	O=C(N([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])N([H])C=2C=1C([H])=C([H])C([H])=C([H])C=1N=C3C=2C([H])([H])C([H])([H])C([H])([H])C3([H])[H])C=4OC=5C(C(=O)C=4[H])=C(OC([H])([H])[H])C	2.208	2.492
Tr118	O=C(N([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])N([H])C2=C1C([H])=C([H])C([H])=C([H])C1=NC3=C2C([H])([H])C([H])([H])C([H])([H])C3([H])[H])C=4OC=5C(C(=O)C=4[H])=C(O[H])C([H])=C(OC([H	2.071	1.969
Tr119	O=C(N([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])N([H])C=2C=1C([H])=C([H])C([H])=C([H])C=1N=C3C=2C([H])([H])C([H])([H])C([H])([H])C3([H])[H])C=4OC=5C(C(=O)C=4[H])=C([H])C(OC([H])([H]	2.056	2.492
Tr120	O=C2N(/C(=N\[H])N([H])[C@]4(C=1C([F])=C([H])C([F])=C([H])C=1[H])[C@@]2([H])C([H])([H])N(/C3=N/C(OC([H])([H])[H])=C([F])C(=N3)C([H])([H])[H])C4([H])[H])C([H])([H])[H]	4.328	3.980
Tr121	O=C2N(/C(=N\[H])N([H])[C@]4(C=1C([F])=C([H])C([H])=C([Cl])C=1[H])[C@@]2([H])C([H])([H])N(/C3=N/C(OC([H])([H])[H])=C([F])C(=N3)C([H])([H])[H])C4([H])[H])C([H])([H])[H]	3.886	3.901

Tr122	O=C(N([H])C3=C([H])C([H])=C2OC([C@]4([C@@]1(N=C(OC1([H])[H])N([H])[H])C2=C3[H])C([H])([H])OC4([H])[H])(C([H])([H])[H])C([H])([H])[H])C=5/N=C(/[H])C([Cl])=C([H])C=5[H]	3.418	2.935
Tr123	O=C(N([H])C3=C([H])C([H])=C2OC([H])([H])[C@]4([C@@]1(N=C(OC1([H])[H])N([H])[H])C2=C3[H])C([H])([H])C4([H])[H])C=5/N=C(/[H])C([Cl])=C([H])C=5[F]	2.620	2.473
Tr124	O=C(N([H])C3=C([H])C([H])=C2OC([H])([H])[C@]4([C@@]1(N=C(OC1([H])[H])N([H])[H])C2=C3[H])C([H])([H])C4([H])[H])C=5/N=C(/[H])C([Cl])=C([H])C=5[H]	2.423	2.659
Tr125	[H]/C4=C(/C([H])=C1C(OC([C@]3([C@@]12N=C(OC2([H])[H])N([H])[H])C([H])([H])OC3([H])[H])(C([H])([H])[H])C([H])([H])[H])=C4[H])C5=C([H])N=C([H])C(OC([H])([H])[H])=C5[H]	2.593	2.642
Tr126	[H]/C4=C(/C([H])=C1C(O[C@]([H])([C@]3([C@]12N=C(OC2([H])[H])N([H])[H])C([H])([H])OC3([H])[H])C([H])([H])C([H])([H])[H])=C4[H])C5=C([H])N=C([H])C(C#CC([H])([H])[H])=C5[H]	2.971	2.719
Tr127	[H]/C5=C(/C([H])=C1C(O[C@@]4([C@]3([C@@]12N=C(OC2([H])[H])N([H])[H])C([H])([H])OC3([H])[H])C([H])([H])C([H])([H])C4([H])[H])=C5[H])C6=C([H])N=C([H])C(C#CC([H])([H])[H])=C6[H]	2.921	4.190
Tr128	[H]/C4=C(/C([H])=C1C(OC([C@]3([C@@]12N=C(OC2([H])[H])N([H])[H])C([H])([H])OC3([H])[H])(C([H])([H])[H])C([H])([H])[H])=C4[H])C5=C([H])N=C([H])C(C#CC([H])([H])[H])=C5[H]	3.044	3.452
Tr129	[Cl]C=5C([H])=C(/C3=C(\[H])C([H])=C2OC([C@]4([C@@]1(N=C(OC1([H])[H])N([H])[H])C2=C3[H])C([H])([H])OC4([H])[H])(C([H])([H])[H])C([H])([H])[H])C([H])=C([F])C=5[H]	2.726	2.107
Tr130	O=C(N([H])C3=C([H])C([H])=C2OC([H])([H])[C@]4([C@@]1(N=C(OC1([H])[H])N([H])[H])C2=C3[H])C([H])([H])C4([H])[H])C5=NC([H])=C([Br])C([H])=N5	2.206	2.762
Tr131	O=C(N([H])C3=C([H])C([H])=C2OC([C@]4([C@@]1(N=C(OC1([H])[H])N([H])[H])C2=C3[H])C([H])([H])OC4([H])[H])(C([H])([H])[H])C([H])([H])[H])C5=NC([H])=C([Cl])C([H])=C5C([H])([H])[H]	3.190	3.356
Tr132	O=C(N([H])C3=C([H])C([H])=C2OC([H])([H])[C@]4([C@@]1(N=C(OC1([H])[H])N([H])[H])C2=C3[H])C([H])([H])C4([H])[H])C=5/N=C(/[H])C(C#N)=C([H])C=5[H]	2.466	2.762
Tr133	O=C(N([H])C3=C([H])C([H])=C2OC([C@]4([C@@]1(N=C(OC1([H])[H])N([H])[H])C2=C3[H])C([H])([H])OC4([H])[H])(C([H])([H])[H])C([H])([H])[H])C=5/N=C(/[H])C(C#N)=C([H])C=5[H]	3.143	3.038
Tr134	[H]/C5=C(/C([H])=C1C(O[C@]([H])([C@]3([C@]12N=C(OC2([H])[H])N([H])[H])C([H])([H])OC3([H])[H])C([H])([H])C4=C([H])C([H])=C([H])C([H])=C4[H])=C5[H])C6=C([H])N=C([H])N=C6[H]	3.036	2.635
Tr135	[H]/C5=C(/C([H])=C1C(O[C@]([H])([C@]3([C@]12N=C(OC2([H])[H])N([H])[H])C([H])([H])OC3([H])[H])C([H])([H])C4=C([H])C([H])=C([H])C([H])=C4[H])=C5[H])C6=C([H])N=C([H])C(C#CC([H])([H])[H])=C6[H]	3.148	3.566
Tr136	O=C(N([H])C3=C([H])C([H])=C2OC([C@]4([C@@]1(N=C(OC1([H])[H])N([H])[H])C2=C3[H])C([H])([H])OC4([H])[H])(C([H])([H])[H])C([H])([H])[H])C=5/N=C(/[H])C([Br])=C([H])C=5[H]	3.991	2.575
Tr137	O=C(N([H])C3=C([H])C([H])=C2OC([C@]4([C@@]1(N=C(OC1([H])[H])N([H])[H])C2=C3[H])C([H])([H])C4([H])[H])(C([H])([H])[H])C([H])([H])[H])C5=NC([H])=C([Cl])C([H])=C5[H]	3.423	3.097

Tr138	O=C(N([H])C3=C([H])C([H])=C2OC([C@]4([C@@]1(N=C(OC1([H])[H])N([H])[H])C2=C3[H])C([H])([H])C4([H])[H])(C([H])([H])[H])C([H])([H])[H])C5=NC([H])=C([F])C([H])=C5[H]	3.039	2.990
Tr139	O=C(N([H])C3=C([H])C([H])=C2OC([C@]4([C@@]1(N=C(OC1([H])[H])N([H])[H])C2=C3[H])C([H])([H])OC4([H])[H])(C([H])([H])[H])C([H])([H])[H])C=5/N=C(/[H])C(=NC=5[H])OC([H])([H])[H]	3.101	3.578
Tr140	O=C(/C1=N/C([H])=C([Cl])C([H])=C1[H])N([H])C2=C([H])C(=C([F])C([H])=C2[H])[C@]3(N([H])C(=N[H])N([S](=O)(=O)C3([H])[H])C([H])([H])[H])C([H])([H])[H]	5.023	4.057
Tr141	O=C(/C1=N/C([H])=C(C([H])=C1[H])C([F])([F])[F])N([H])C2=C([H])C(=C([F])C([H])=C2[H])[C@]3(N([H])C(=N[H])N([S](=O)(=O)C3([H])[H])C([H])([H])[H])C([H])([H])[H]	4.899	4.970
Tr142	O=C(/C1=N/C([H])=C(/N=C1/[H])C([H])([H])[H])N([H])C2=C([H])C(=C([F])C([H])=C2[H])[C@]3(N([H])C(=N[H])N([S](=O)(=O)C3([H])[H])C([H])([H])[H])C([H])([H])[H]	4.000	4.478
Tr143	O=C(/C1=N/C([H])=C(/N=C1/[H])OC([H])([H])[H])N([H])C2=C([H])C(=C([F])C([F])=C2[H])[C@]3(N([H])C(=N[H])N([S](=O)(=O)C3([H])[H])C([H])([H])[H])C([H])([H])[H]	4.979	5.258
Tr144	O=[S]3(=O)N(/C(=N\[H])N([H])[C@](C=1[S]C([H])=C(C=1[H])C2=C([H])C([H])=C([F])C(C#N)=C2[H])(C3([H])[H])C([H])([H])[H])C([H])([H])[H]	3.337	3.145
Tr145	O=[S]3(=O)N(/C(=N\[H])N([H])[C@](C=1[S]/C(=C(/[H])C=1[Cl])C2=C([H])N=C([H])C(C#CC([H])([H])[H])=C2[H])(C3([H])[H])C([H])([H])[H])C([H])([H])[H]	4.622	4.388
Tr146	O=C(/C1=N/C([H])=C(/N=C1/[H])OC([H])([H])[H])N([H])C2=C([H])C(=C([F])C([H])=C2[H])[C@]3(N([H])C(=N[H])N([S](=O)(=O)C3([H])[H])C([H])([H])[H])C([H])([H])[H]	4.785	4.922
Tr147	[F]C=1C([H])=C(C([H])=C([F])C=1[H])C([H])([H])[C@]([H])(N([H])C(=O)C2=C([H])C(=C([H])C(=C2[H])C([H])([H])[H])C(=O)N(C([H])([H])C([H])([H])C([H])([H])[H])C([H])([H])C([H])([H])C([H])([H])[H])[C@]([H])(O[H])[C@]3([H])N([H])C([H])([H])C([H])([H])N(C3([H])[	2.509	3.437
Tr148	[F]C=1C([H])=C(C([H])=C([F])C=1[H])C([H])([H])[C@]([H])(N([H])C(=O)C2=C([H])C(=C([H])C(=C2[H])C([H])([H])[H])C(=O)N(C([H])([H])C([H])([H])C([H])([H])[H])C([H])([H])C([H])([H])C([H])([H])[H])[C@]([H])(O[H])[C@]3([H])N([H])C([H])([H])C([H])([H])N(C3([H])[	2.921	2.993
Tr149	[F]C=1C([H])=C(C([H])=C([F])C=1[H])C([H])([H])[C@]([H])(N([H])C(=O)C2=C([H])C(=C([H])C(=C2[H])C([H])([H])[H])C(=O)N(C([H])([H])C([H])([H])C([H])([H])[H])C([H])([H])C([H])([H])C([H])([H])[H])[C@]([H])(O[H])[C@]3([H])N([H])C([H])([H])C([H])([H])N(C3([H])[	2.398	3.017
Tr150	[F]C=1C([H])=C(C([H])=C([F])C=1[H])C([H])([H])[C@]([H])(N([H])C(=O)C2=C([H])C(=C([H])C(=C2[H])C([H])([H])[H])C(=O)N(C([H])([H])C([H])([H])C([H])([H])[H])C([H])([H])C([H])([H])C([H])([H])[H])[C@]([H])(O[H])[C@]3([H])N([H])C([H])([H])C([H])([H])N(C3([H])[	2.013	3.262
Tr151	O=C(N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])[C@@]([H])(N([H]	5.097	4.395
Tr152	O=C(N([H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])[C@]([H])(OC([H])([H])[H])C([H])([H])[C@]([H])(O[H])[C@@]([H])(N([H])C(=O)C2=C([H])C(=C([H])C(=C2[H])C(=O)N([H])[C@@]([H])(C3=C([H])C([H])=C([H])C([H])=C3[H])C([H])([H])[H])N(C([H])([H])[S](=O)(=O)	1.854	2.670

Tr153	O=C(N([H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])[C@]([H])(OC([H])([H])[H])C([H])([H])[C@]([H])(O[H])[C@@]([H])(N([H])C(=O)C1=C([H])C(=C([H])C(=C1[H])C(=O)N([H])[C@@]([H])(C2=C([H])C([H])=C([H])C([H])=C2[H])C([H])([H])[H])N(C([H])([H])[S](=O)(=	2.398	2.657
Tr154	O=C(N([H])[C@]([H])(C(=O)N([H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])(C([H])([H])[H])C([H])([H])[H])[C@]([H])(OC([H])([H])[H])C([H])([H])[C@]([H])(O[H])[C@@]([H])(N([H])C(=O)C2=C([H])C(=C([H])C(=C2[H])C(=O)N([H])[C@@]([H])(C3=C([H])C([H])=	4.046	2.867
Tr155	O=C(N([H])[C@]([H])(C(=O)N([H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])(C([H])([H])[H])C([H])([H])[H])[C@]([H])(OC([H])([H])[H])C([H])([H])[C@]([H])(O[H])[C@@]([H])(N([H])C(=O)C2=C([H])C(=C([H])C(=C2[H])C(=O)N([H])[C@@]([H])(C3=C([H])C([H])=	3.125	2.903
Tr156	O=C(N([H])[C@]([H])(C(=O)N([H])C([H])([H])C=1C([H])=C([H])C([H])=C([H])C=1[H])C([H])(C([H])([H])[H])C([H])([H])[H])[C@]([H])(OC([H])([H])[H])C([H])([H])[C@]([H])(O[H])[C@@]([H])(N([H])C(=O)C2=C([H])C(=C([H])C(=C2[H])C(=O)N([H])[C@@]([H])(C3=C([H])C([H])	3.097	3.714
Tr157	O=C(N([H])[C@]([H])(C(=O)N([H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])(C([H])([H])[H])C([H])([H])[H])[C@]([H])(OC([H])([H])[H])C([H])([H])[C@]([H])(O[H])[C@@]([H])(N([H])C(=O)C2=C([H])C(=C([H])C(=C2[H])C(=O)N([H])[C@@]([H])(C3=C([H])C([H])=	3.222	3.149
Tr158	O=C(N([H])C1=C([H])C([H])=C([F])C([H])=C1[H])[C@]([H])(OC([H])([H])[H])C([H])([H])[C@]([H])(O[H])[C@@]([H])(N([H])C(=O)C2=C([H])C(=C([H])C(=C2[H])C(=O)N([H])[C@@]([H])(C3=C([H])C([H])=C([H])C([H])=C3[H])C([H])([H])[H])N(C([H])([H])[S](=O)(=O)C([H])([H])	3.000	2.982
Tr159	O=C(N([H])C1=C([H])C(=C(C([H])=C1[H])N(C([H])([H])[H])C([H])([H])[H])C(=O)N([H])C([H])([H])C([H])([H])C([H])([H])OC([H])([H])C([H])([H])[H])N([H])C2=C([H])C([Cl])=C([H])C([H])=C2[H]	1.009	1.620
Tr160	O=C(N([H])[C@]([H])(C(=O)N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])[H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)O[H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])([H])C([H])([H])C(=O)O[H])C([H])([H])[H])C([H])([H]	4.000	4.508
Tr161	O=C(N([H])[C@]([H])(C(=O)N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])[H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)O[H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])([H])C([H])([H])C(=O)O[H])C([H])([H])[H])C([H])([H]	3.167	3.308
Tr162	O=C(N([H])C(=NC([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])N([H])[H])C=2C(=NOC=2C([H])([H])[H])C3=C([H])C([H])=C(OC([H])([H])[H])C([H])=C3[H]	1.398	1.742
Tr163	O=C(N([H])C(=NC([H])([H])C1=C([H])C([Cl])=C([Cl])C([H])=C1[H])N([H])[H])C=2C(=NOC=2C([H])([H])[H])C3=C([H])C([H])=C([F])C([H])=C3[H]	1.620	2.395
Tr164	O=C(N([H])[C@]([H])(C(=O)N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])([H])[H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H]	5.602	4.275
Tr165	O=C(N([H])[C@]([H])(C(=O)N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])([H])[H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])([H])[H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H]	3.959	4.299

Tr166	O=C(N([H])[C@]([H])(C(=O)N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H]	3.538	4.347
Tr167	O=[S](=O)(C([H])([H])[C@@]([H])(C(=O)N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])(C([H])([H])[H])C	1.947	2.361
Tr168	O=C(N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])[C@@]([H])(N([H])C(	1.504	2.224
Tr169	O=C(N([H])[C@@]([H])(C(=O)N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[	4.602	2.739
Tr170	O=C1N(/C(=N\[H])N([H])[C@]1(C([H])([H])C([H])([H])[C@@]2([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C2([H])[H])C([H])([H])[C@]4([H])C([H])([H])[C@]([H])(N([H])C(=O)C3=C([H])C([H])=NC([H])=C3[H])C([H])([H])C([H])([H])C4([H])[H])C([H])([H])[H]	3.409	3.083
Tr171	O=C1N(/C(=N\[H])N([H])[C@]1(C([H])([H])C([H])([H])[C@@]2([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C2([H])[H])C([H])([H])[C@]4([H])C([H])([H])[C@]([H])(N([H])[C@@]3([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C3([H])[H])C([H])([H])C([H])([H])C	3.638	3.244
Tr172	O=C1N(/C(=N\[H])N([H])[C@]1(C([H])([H])C([H])([H])[C@@]2([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C2([H])[H])C([H])([H])[C@]4([H])C([H])([H])[C@]([H])(N([H])[C@]3([H])C([H])([H])C([H])([H])C([H])([H])C3([H])[H])C([H])([H])C([H])([H])C4([H])[H])C(	3.367	3.076
Tr173	O=C(N([H])[C@]([H])(C(=O)N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H]	3.398	3.020
Tr174	O=C(N([H])[C@]([H])(C(=O)N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H]	1.785	3.092
Tr175	O=C(N([H])[C@]([H])(C(=O)N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H]	3.201	3.044
Tr176	O=C(N([H])[C@]([H])(C(=O)N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H]	2.697	2.966
Tr177	O=C(N([H])[C@]([H])(C(=O)N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H]	3.194	2.714

Tr178	O=[S](=O)(C([H])([H])[C@]([H])(N([H])C(=O)[C@]([H])(C([H])([H])N1N=C(C([H])=C1C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C(=O)N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C([H])(C([H])([H])[H])C([H])(	2.717	3.278
Tr179	O=C(N([H])[C@]([H])(C(=O)N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H]	3.495	3.369
Tr180	O=C(N([H])[C@]([H])(C(=O)N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H]	3.770	3.393
Tr181	O=C1N(/C(=N\[H])N([H])[C@]1(C([H])([H])C([H])([H])[C@@]2([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C2([H])[H])C([H])([H])[C@@]4([H])C([H])([H])N(C(=O)C([H])([H])[C@]3([H])C([H])([H])C([H])([H])C([H])([H])C3([H])[H])C([H])([H])C4([H])[H])C([H])([H]	3.432	2.921
Tr182	O=C1N(/C(=N/[H])N([H])[C@]1(C([H])([H])C([H])([H])[C@@]2([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C2([H])[H])C([H])([H])[C@]3([H])C([H])([H])N(C(=O)C([H])([H])C([H])([H])C([H])([H])C([H])([H])[H])C([H])([H])C([H])([H])C3([H])[H])C([H])([H])[H]	3.495	3.191
Tr183	O=[S](=O)(N3C([H])([H])[C@@]([H])(C([H])([H])[C@]1(N([H])C(=N[H])N(C1=O)C([H])([H])[H])C([H])([H])C([H])([H])[C@@]2([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C2([H])[H])C([H])([H])C([H])([H])C3([H])[H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])[	3.201	3.509
Tr184	O=C1N(/C(=N\[H])N([H])[C@]1(C([H])([H])C([H])([H])[C@@]2([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C2([H])[H])C([H])([H])[C@]5([H])C([H])([H])[C@]([H])(N([H])C(=O)N([H])C3=NC=4C(/N=C3/[H])=C([H])C([H])=C([H])C=4[H])C([H])([H])C([H])([H])C5([H])[H]	3.854	3.900
Tr185	O=C1N(/C(=N\[H])N([H])[C@]1(C([H])([H])C([H])([H])[C@@]2([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C2([H])[H])C([H])([H])[C@]4([H])C([H])([H])[C@]([H])(N([H])C(=O)N([H])[C@@]3([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C3([H])[H])C([H])([H])C	2.860	3.874
Tr186	O=C1N(/C(=N/[H])N([H])[C@]1(C([H])([H])C([H])([H])[C@@]2([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C2([H])[H])C([H])([H])[C@]4([H])C([H])([H])[C@]([H])(N([H])C(=O)N([H])C3=C(OC([H])([H])[H])C([H])=C([H])C([H])=C3[H])C([H])([H])C([H])([H])C4([H])[H	2.559	3.239
Tr187	O=C1N(/C(=N\[H])N([H])[C@]1(C([H])([H])C([H])([H])[C@]2([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C2([H])[H])C([H])([H])[C@]4([H])C([H])([H])[C@]([H])(N([H])C(=O)N([H])C3=C([H])C([H])=C([Cl])C([H])=C3[H])C([H])([H])C([H])([H])C4([H])[H])C([H])([H]	5.000	4.115
Tr188	O=C1N(/C(=N\[H])N([H])[C@]1(C([H])([H])C([H])([H])[C@@]2([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C2([H])[H])C([H])([H])[C@]4([H])C([H])([H])[C@]([H])(N([H])C(=O)C([H])([H])C3=C([H])C([H])=C([H])C([H])=C3[H])C([H])([H])C([H])([H])C4([H])[H])C([H]	2.233	2.585
Tr189	O=C1N(/C(=N\[H])N([H])[C@@]1(C([H])([H])[C@@]2([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C2([H])[H])C([H])([H])C([H])([H])[C@@]3([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C3([H])[H])C([H])([H])C4=C([H])C([H])=C(C([H])=C4[H])C([H])([H])N5C(=O	3.569	4.795
Tr190	O=C1N(/C(=N/[H])N([H])[C@]1(C([H])([H])C([H])([H])[C@@]2([H])C([H])([H])C([H])([H	3.770	3.335

	])C([H])([H])C([H])([H])C2([H])[H])C([H])([H])[C@@]3([H])C([H])([H])N(C(=O)C([H])([H])C([H])([H])C([H])([H])C([H])([H])[H])C([H])([H])C([H])([H])C3([H])[H])C([H])([H])[H]		
Tr191	O=C1N(/C(=N\[H])N([H])[C@]1(C([H])([H])C([H])([H])[C@@]2([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C2([H])[H])C([H])([H])[C@]4([H])C([H])([H])N(C(=O)C([H])([H])[C@]3([H])C([H])([H])C([H])([H])C([H])([H])C3([H])[H])C([H])([H])C([H])([H])C4([H])[H])	3.013	3.527
Tr192	O=C1N(/C(=N\[H])N([H])[C@]1(C([H])([H])C([H])([H])[C@@]2([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C2([H])[H])C([H])([H])[C@]3([H])C([H])([H])N(C(=O)OC(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])([H])C3([H])[H])C([H])([H])[H]	3.538	3.215
Tr193	O=[S]2(=O)N(/C(=N/[H])N([H])[C@]4(/C1=C(\[H])C([F])=C([F])C([H])=C1[F])[C@@]2([H])C([H])([H])N(/C3=N/C(=C(/[F])C(=N3)OC([H])([H])[H])C([H])([H])[H])C4([H])[H])C([H])([H])[H]	3.495	3.781
Tr194	O=[S]2(=O)N(/C(=N/[H])N([H])[C@]4(/C1=C(\[H])C([H])=C([F])C([H])=C1[F])[C@]2([H])C([H])([H])N(/C3=N/C(=C(/[F])C(=N3)OC([H])([H])[H])C([H])([H])[H])C4([H])[H])C([H])([H])[H]	3.523	4.249
Tr195	O=[S]2(=O)N(/C(=N/[H])N([H])[C@]4(/C1=C(\[H])C([F])=C([H])C([H])=C1[F])[C@@]2([H])C([H])([H])N(/C3=N/C(OC([H])([H])[H])=C([H])C(=C3[H])C([H])([H])OC([H])([H])[H])C4([H])[H])C([H])([H])[H]	4.000	3.121
Tr196	O=[S]2(=O)N(/C(=N/[H])N([H])[C@@]4(/C1=C(\[H])C([H])=C([H])C([H])=C1[H])[C@]2([H])C([H])([H])N(/C3=N/C(OC([H])([H])[H])=C([H])C(=C3[H])C([H])([H])OC([H])([H])[H])C4([H])[H])C([H])([H])[H]	3.569	3.223
Tr197	O=[S]2(=O)N(/C(=N/[H])N([H])[C@@]4(/C1=C(\[H])C([H])=C([H])C([H])=C1[H])[C@]2([H])C([H])([H])N(/C3=N/C(OC([H])([H])[H])=C([F])C(=N3)OC([H])([H])[H])C4([H])[H])C([H])([H])[H]	3.523	3.553
Tr198	O=[S]2(=O)N(/C(=N/[H])N([H])[C@@]4(/C1=C(\[H])C([H])=C([H])C([H])=C1[H])[C@]2([H])C([H])([H])N(/C3=N/C(OC([H])([H])[H])=C([H])C([H])=C3[H])C4([H])[H])C([H])([H])[H]	3.066	2.677
Tr199	O=[S]2(=O)N(/C(=N/[H])N([H])[C@@]5(/C1=C(\[H])C([H])=C([H])C([H])=C1[H])[C@]2([H])C([H])([H])N(/C3=N/C(=C(/[F])C(=N3)OC([H])([H])[H])[C@@]4([H])C([H])([H])C4([H])[H])C5([H])[H])C([H])([H])[H]	3.377	3.145
Tr200	O=[S]3(=O)N(/C(=N/[H])N([H])[C@]5(/C1=C(\[H])C(=C([H])C([H])=C1[F])N([H])C(=O)C2=NC([H])=C([F])C([H])=C2[H])[C@]3([H])C([H])([H])N(/C4=N/C(OC([H])([H])[H])=C([F])C(=N4)C([H])([H])[H])C5([H])[H])C([H])([H])[H]	4.921	4.802
Tr201	O=C(C=1C([H])=C(C([H])=C(C=1[H])C(=O)N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])N([H])[C@]([H])(C(=O)N([H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])[C@@]([H])(O[H])C([H])([H])[H])C([H])([H])C2=C([H])C([H])=C([H])C([H])=C2[H])C([H])([H])[H])N([C@]	1.781	1.397
Tr202	O=C(C=1C([H])=C([H])C([H])=C(C=1[H])C(=O)N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])N([H])[C@]([H])(C(=O)N([H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])[C@@]([H])(O[H])C([H])([H])[H])C([H])([H])C2=C([H])C([H])=C([H])C([H])=C2[H])N([C@]([H])(C3=C(	1.236	1.211
Tr203	O=C(C=1C([H])=C([H])C([H])=C(C=1[H])C(=O)N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])N([H])[C@]([H])(C(=O)N([H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])[C@@]([H])(O[H])C([H])([H])C([H])([H])C([H])([H])[H])C([H])([H])C2=C([H])C([H])=C([H])C([H])=C	2.573	2.627

Tr204	O=C(C=1C([H])=C(C([H])=C(C=1[H])C(=O)N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])N([H])[C@]([H])(C(=O)N([H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])[C@@]([H])(O[H])C([H])([H])C([H])([H])C([H])([H])[H])C([H])([H])C2=C([H])C([H])=C([H])C([H])=C2[H]	4.183	2.813
Test set			
Ts1	O=C2N([H])[C@]([H])(C(=O)N([H])[C@@]([H])(C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])[C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C=1C([H])=C([H])C([H])=C([H])C=1[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])C(=O)N([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])OC(=O)N([H])[C@@]2([H])C([H])(C([H])([H])[H])C([H])([H])[H]	3.600	3.189
Ts2	O=C(OC([H])([H])C=1N=C(OC=1C([H])([H])[H])C([H])([H])[H])N([H])[C@]([H])(C(=O)N([H])[C@@]([H])(C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])[C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])[S](=O)(=O)C([H])([H])[H]	5.921	3.940
Ts3	O=C(/C1=C(\[H])C(=C([H])C(=C1[H])C2=NN=C(O2)[C@@](C([H])([H])[H])(C([H])([H])C=3C([H])=C([H])C([H])=C([H])C=3[H])[N]([H])([H])[H])N(C([H])([H])[H])[S](=O)(=O)C([H])([H])[H])C([H])(C([H])([H])[H])C([H])([H])[H]	0.783	2.509
Ts4	O=C(N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])[C@@]([H])(N([H])C(=O)OC(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[S](=O)(=O)C([H])([H])[H]	1.947	2.890
Ts5	O=C(OC([H])([H])C([H])=C([H])[H])N([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])[C@@]([H])(C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])[C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C=1C([H])=C([H])C([H])=C([H])C=1[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])C(=O)N([H])C([H])([H])C([H])=C([H])[H])C([H])(C([H])([H])[H])C([H])([H])[H]	3.575	3.106
Ts6	O=C2N(C(=N[C@]4(C=1C([H])=C([H])C([H])=C([H])C=1[H])[C@@]2([H])C([H])([H])N(/C3=N/C(=C(/[F])C(=N3)OC([H])([H])[H])C([H])([H])[H])C4([H])[H])N([H])[H])C([H])([H])[H]	3.921	3.241
Ts7	O=C2N(C(=N[C@]4(C=1C([H])=C([H])C([H])=C([H])C=1[H])[C@@]2([H])C([H])([H])N(/C3=N/C(OC([H])([H])C([H])([H])[H])=C([F])C(=N3)OC([H])([H])[H])C4([H])[H])N([H])[H])C([H])([H])[H]	2.863	3.584
Ts8	O=C2N(C(=N[C@]4(C=1C([H])=C([H])C([H])=C([H])C=1[H])[C@@]2([H])C([H])([H])N(/C3=N/C(OC([H])([H])[H])=C([F])C(=N3)C([H])([H])C([H])([H])[H])C4([H])[H])N([H])[H])C([H])([H])[H]	3.796	3.500
Ts9	O=C2N(C(=N[C@]4(C=1C([H])=C([H])C([F])=C([H])C=1[F])[C@@]2([H])C([H])([H])N(/C3=N/C(OC([H])([H])[H])=C([F])C(=N3)C([H])([H])C([H])([H])[H])C4([H])[H])N([H])[H])C([H])([H])[H]	4.276	3.932
Ts10	[F]/C1=C(/N=C(/N=C1/OC([H])([H])[H])N3C([H])([H])[C@@]2(N=C(N(C(=O)[C@]2([H])C3([H])[H])C([H])([H])[H])N([H])[H])C4=C([H])C([H])=C([F])C([H])=C4[F])C([F])([F])[F]	3.495	4.088
Ts11	O=C2N(C(=N[C@]4(C=1C([H])=C(CN)C([H])=C([H])C=1[H])[C@@]2([H])C([H])([H])N(/C3=N/C(=C(/[F])C(=N3)OC([H])([H])[H])C([H])([H])[H])C4([H])[H])N([H])[H])C([H])([H])[H]	3.854	3.763
Ts12	O=C(OC(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])N([H])[C@]([H])(C(=O)C([H])([H])N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N	0.649	2.091

	([H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])C(=O)N([H])[H]		
Ts13	O=C(OC(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])N([H])[C@]([H])(C(=O)C([H])([H])N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])C(=O)N([H])[H]	1.504	2.163
Ts14	NC/C1=C(\[H])C(=C([H])C([H])=C1[H])C2=C([H])[S]/C(=C2/[H])[C@@]35N=C(N(C(=O)[C@]3([H])C([H])([H])N(/C4=N/C([H])=C(C([H])=N4)C([H])([H])[H])C5([H])[H])C([H])([H])[H])N([H])[H]	4.046	4.058
Ts15	O=[S](=O)(N(C=1C([H])=C(C([H])=C(C=1[H])C(=O)N([H])[C@]([H])(C([H])([H])N([H])[C@]([H])(C(=O)N([H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])C2=C([H])C([H])=C([H])C([H])=C2[H])C(=O)N([H])[C@@]([H])(C3=C([H])C([H])=C([H])C([H])=C3[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])[H]	3.602	2.291
Ts16	O=C(N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])([H])[C@]([H])(N([H])C(=O)C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])C(=O)O[H]	1.721	1.846
Ts17	O=C(N([H])[C@@]([H])(C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])([H])[H])C2=C([H])C(=C([H])C(=C2[H])N(C([H])([H])[H])[S](=O)(=O)C([H])([H])[H])C(=O)N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])N([H])C([H])([H])C3=C([H])C4=C(C([H])=C3[H])C([H])=C([H])N4[H])C([H])([H])C5=C([H])C([H])=C([H])C([H])=C5[H]	2.638	2.214
Ts18	O=C(N([H])[C@]([H])(C=1N=C(OC=1C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C=2C([H])=C(C([H])=C(C=2[H])N(C([H])([H])[H])[S](=O)(=O)C([H])([H])[H])C(=O)N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])N([H])C([H])([H])C3=C([H])C(OC([H])([H])[H])=C([H])C([H])=C3[H])C([H])([H])C4=C([H])C([H])=C([H])C([H])=C4[H]	2.049	3.397
Ts19	O=C2N([H])C1=C([H])C([H])=C([H])C([H])=C1N([H])C3=C2C([H])=C([H])C(=C3[H])C(=O)N([H])C4=N/C(=C(/[H])N4[H])C5=C([H])C([H])=NC([H])=C5[H]	2.458	2.990
Ts20	O=C2N([H])C1=C([H])C([H])=C([H])C([H])=C1N([H])C3=C2C([H])=C([H])C(=C3[H])C(=O)N([H])C4=C([H])C([H])=C([F])C([H])=C4[H]	2.676	1.490
Ts21	O=C2N([H])C1=C([H])C([H])=C([H])C([H])=C1N([H])C=3/C2=C(/[H])C([H])=C(C=3[H])C(=O)N([H])C4=NC=5C(N4[H])=C([H])N=C([H])C=5[H]	2.510	2.846
Ts22	O=C(N([H])C(=NC([H])([H])C1=C([H])C(=C([H])C(=C1[H])C([H])([H])[H])C([H])([H])[H])N([H])[H])C=2C(=NOC=2C([H])([H])[H])C3=C([H])C([H])=C(OC([H])([H])[H])C([H])=C3[H]	2.553	1.898
Ts23	O=C(N([H])C(=NC([H])([H])C1=C([H])C([Cl])=C([H])C([Cl])=C1[H])N([H])[H])C=2C(=N[S]C=2C([H])([H])[H])C3=C([H])C([H])=C(OC([H])([H])[H])C([H])=C3[H]	2.538	2.816
Ts24	O=C(N([H])C(=NC([H])([H])C=1C([H])=C([H])C([H])=C2C=1C([H])=C([H])C([H])=C2[H])N([H])[H])C=3C(=NOC=3C([H])([H])[H])C4=C([H])C([H])=C([H])C([H])=C4[H]	1.553	1.160
Ts25	[H]C=5C(O[H])=C(O/C2=C(\[H])C(O[H])=C1OC3=C(O/C1=C2\[H])C(O[H])=C([H])C(O[H])=C3O/C4=C(\[H])C(O[H])=C([H])C(O[H])=C4[H])C(O[H])=C([H])C=5O[H]	1.143	0.753
Ts26	[F]C=1C([H])=C(C([H])=C([F])C=1[H])C([H])([H])[C@]([H])(N([H])C(=O)C=2C([H])=C(C([H])=C(C=2[H])C([H])([H])[H])C(=O)N(C([H])([H])C([H])([H])C([H])([H])[H])C([H])([H])C([H])([H])C([H])([H])[H])[C@]([H])(O[H])[C@]3([H])N([H])C([H])([H])C([H])([H])N(C3(	4.523	3.444

	[H])[H])[S](=O)(=O)C4=C([H])C([H])=C([H])C([H])=C4[H]		
Ts27	[F]C=1C([H])=C(C([H])=C([F])C=1[H])C([H])([H])[C@]([H])(N([H])C(=O)C2=C([H])C(=C([H])C(=C2[H])C(=O)N3[C@]([H])(C([H])([H])C([H])([H])C3([H])[H])C([H])([H])OC([H])([H])[H])C([H])([H])[H])[C@]([H])(O[H])[C@]4([H])N([H])C([H])([H])C([H])([H])N(C4([H])[H])[S](=O)(=O)C([H])([H])[H]	3.886	3.959
Ts28	[F]C=1C([H])=C(C([H])=C([F])C=1[H])C([H])([H])[C@]([H])(N([H])C(=O)C2=C([H])C(=C([H])C(=C2[H])C(=O)N3[C@]([H])(C([H])([H])C([H])([H])C3([H])[H])C([H])([H])OC([H])([H])[H])C([H])([H])[H])[C@]([H])(O[H])[C@]4([H])N([H])C([H])([H])C([H])([H])N(C4([H])[H])[S](=O)(=O)C([H])([H])C5=C([H])C([H])=C([H])C([H])=C5[H]	5.000	4.187
Ts29	O=C(N([H])[C@@]([H])(C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])([H])[H])C2=C([H])C(=C([H])C(=C2[H])N(C([H])([H])[H])[S](=O)(=O)C([H])([H])[H])C(=O)N([H])[C@]([H])([C@@]([H])(N=[N]=[N])C([H])([H])[C@@]([H])(OC([H])([H])[H])C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C3=C([H])C([H])=C([H])C([H])=C3[H])C([H])(C([H])([H])[H])[H])C([H])([H])[H])C([H])([H])O/C4=C(\[H])C([F])=C([H])C([F])=C4[H]	3.155	3.587
Ts30	O=C(N([H])[C@@]([H])(C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])([H])[H])C2=C([H])C(=C([H])C(=C2[H])N(C([H])([H])[H])[S](=O)(=O)C([H])([H])[H])C(=O)N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])[C@@]([H])(OC([H])([H])C([H])([H])[H])C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C3=C([H])C([H])=C([H])C([H])=C3[H])C([H])(C([H])([H])[H])[H])C([H])([H])[H])C([H])([H])O/C4=C(\[H])C([F])=C([H])C([F])=C4[H]	4.678	3.390
Ts31	O=C(N([H])[C@@]([H])(C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])([H])[H])C=2C([H])=C(C([H])=C(C=2[H])N(C([H])([H])[H])[S](=O)(=O)C([H])([H])[H])C(=O)N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])[C@@]([H])(OC([H])([H])[C@@]3([H])C([H])([H])C3([H])[H])C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C4=C([H])C([H])=C([H])C([H])=C4[H])C([H])(C([H])([H])[H])[H])C([H])([H])[H])C([H])([H])O/C5=C(\[H])C([F])=C([H])C([F])=C5[H]	4.886	4.950
Ts32	O=C1C4=C(O/C(=C1/C([H])([H])C([H])=C(C([H])([H])[H])C([H])([H])[H])C=2C([H])=C([H])C(O[H])=C([H])C=2O[H])C3=C(OC(C([H])=C3[H])(C([H])([H])[H])C([H])([H])[H])C([H])=C4O[H]	0.193	1.058
Ts33	O=C(OC(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])N([H])[C@]([H])(C(=O)N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])(C([H])([H])[H])[H])C([H])([H])[H])C([H])([H])C([H])(C([H])([H])[H])[H])C([H])([H])[H])C([H])([H])C(=O)N([H])[H]	1.504	2.313
Ts34	O=C3N([H])[C@]([H])(C(=O)N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])N([H])C([H])([H])C1=C([H])C(=C([H])C([H])=C1[H])N(C([H])([H])[H])C([H])([H])[H])C([H])([H])C2=C([H])C([H])=C([H])C([H])=C2[H])C([H])([H])N3/C4=C(\[H])C([H])=C([H])C([H])=C4[H]	1.087	1.805
Ts35	O=C3N([H])[C@]([H])(C(=O)N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])N([H])C([H])([H])C1=C([H])C(=C([H])C([H])=C1[H])N(C([H])([H])[H])C([H])([H])[H])C([H])([H])C2=C([H])C([H])=C([H])C([H])=C2[H])C([H])([H])N3C([H])([H])C4=C([H])C([H])=C([F])C([F])=C4[H]	2.565	2.471
Ts36	O=C3N([H])[C@]([H])(C(=O)N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])N([H])C([H])([H])C1=C([H])C(=C([H])C([H])=C1[H])N(C([H])([H])[H])C([H])([H])[H])C([H])([H])C2=C([H])C([H])=C([H])C([H])=C2[H])C([H])([H])N3C([H])([H])C4=C([H])C([H])=C([F])C([H])=C4[F]	2.062	2.231
Ts37	O=C(N([H])[C@@]([H])(C([H])([H])[H])C1=C([H])C([H])=C([H])C([H])=C1[H])[C@]([H])(O[H])C([H])([H])N([H])C([H])([H])C2=C([H])C([H])=C([H])C(=C2[H])N(C([H])([H])[H])C([H])([H])[H])[C@]3(N([H])C(=O)N(C3([H])[H])C([H])([H])C4=C([H])C([H])=C([H])C([H])=C4[H])C([H])([H])C=5C([H])=C([H])C([H])=C([H])C=5[H]	1.301	1.932
Ts38	O=C1N(C(=N[C@@]1(C=2C([H])=C([H])C([H])=C([H])C=2[H])C3=C([H])C(=C([H])C([H]	2.538	2.732

	)=C3[H])C4=C([H])N=C([H])C([F])=C4[H])N([H])[H])C([H])([H])[H]		
Ts39	O=C1N(C(=N[C@@]1(C=2C([H])=C([H])C([H])=C([H])C=2[H])C3=C([H])C(=C([H])C([H])=C3[H])C4=C([H])C(OC([H])([H])[H])=C([H])C([H])=C4[H])N([H])[H])C([H])([H])[H]	1.222	2.565
Ts40	O=C1N(C(=N[C@@]1(C=2C([H])=C(C([H])=C([H])C=2[H])C3=C([H])C([Cl])=C([H])N=C3[H])[C@@]4([H])C([H])([H])C4([H])[H])N([H])[H])C([H])([H])[H]	3.678	2.779
Ts41	O=C1N(C(=N[C@]1(C=2C([H])=C([H])C([H])=C([H])C=2[H])C3=C([H])C([F])=C([H])C([H])=C3[H])N([H])[H])C([H])([H])[H]	2.143	1.927
Ts42	O=C1N(C(=N[C@@]1(/C2=C(\[H])C([H])=C([H])C([H])=C2[H])C3=C([H])C(=C([H])C([H])=C3[H])C4=C([H])C(OC([H])([H])C([H])([H])[H])=C([H])C([H])=C4[H])N([H])[H])C([H])([H])[H]	2.337	2.282
Ts43	O=C1N(C(=N[C@@]1(C=2C([H])=C([H])C([H])=C([H])C=2[H])C3=C([H])C(=C([H])C([H])=C3[H])C([H])([H])[H])N([H])[H])C([H])([H])[H]	2.260	2.318
Ts44	O=C(N([C@@]1([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C1([H])[H])C([H])([H])C2=C(N([H])N=C2[H])C([H])([H])[H])C([H])([H])C([H])([H])[C@](H])(N5C(=NC=4C([H])=C([H])C(O/C3=C(\[H])C([H])=C([H])C([H])=C3[H])=C([H])C=4C5([H])[H])N([H])[H])[C@@]6([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C6([H])[H]	3.409	2.844
Ts45	O=C(N([C@@]1([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C1([H])[H])C([H])([H])[H])C([H])([H])C([H])([H])[C@](H])(N4C(=N/C3=C(\[H])C([H])=C(OC=2C([H])=C([H])C([H])=C([H])C=2[H])C([H])=C3C4([H])[H])N([H])[H])[C@]5([H])C([H])([H])OC([H])([H])C([H])([H])C5([H])[H]	2.914	3.655
Ts46	O=C(OC([H])([H])[C@](H])(N3C(=N/C2=C(\[H])C([H])=C(O/C1=C(\[H])C([H])=C([H])C([H])=C1[H])C([H])=C2C3([H])[H])N([H])[H])[C@@]4([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C4([H])[H])N([H])[C@@]5([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C5([H])[H]	3.222	2.341
Ts47	O=C3N(C(=N[C@](C=1C([H])=C([S]C=1[Cl])C=2C([H])=C(CCC([H])([H])[H])C([H])=NC=2[H])(C3([H])[H])C([H])([H])[H])N([H])[H])C([H])([H])[H]	4.097	4.443
Ts48	NCC=1C([H])=C(C([H])=C([H])C=1[H])C=2C([H])=C([S]C=2[H])[C@]3(N=C(N(C(=O)C3([H])[H])C([H])([H])[H])N([H])[H])C([H])([H])[H]	3.244	2.341
Ts49	O=C(O[C@]2([H])[C@@]([H])(OC1=C(C(O[H])=C([H])C(O[H])=C1[H])C2([H])[H])C3=C([H])C(O[H])=C(O[H])C([H])=C3[H])C=4C([H])=C(O[H])C(O[H])=C(O[H])C=4[H]	1.276	2.529
Ts50	O=C(N([H])C3=C([H])C([H])=C2OC([C@]4([C@@]1(N=C(OC1([H])[H])N([H])[H])C2=C3[H])C([H])([H])OC4([H])[H])(C([H])([H])[H])C([H])([H])[H])C=5/N=C(/[H])C([Cl])=C([H])C=5[F]	3.288	2.749
Ts51	[H]/C4=C(/C([H])=C1C(OC([H])([H])[C@]3([C@@]12N=C(OC2([H])[H])N([H])[H])C([H])([H])OC3([H])[H])=C4[H])C5=C([H])N=C([H])C(CCC([H])([H])[H])=C5[H]	2.910	3.381
Ts52	O=C(N([H])C3=C([H])C([H])=C2OC([C@]4([C@@]1(N=C(OC1([H])[H])N([H])[H])C2=C3[H])C([H])([H])OC4([H])[H])(C([H])([H])[H])C([H])([H])[H])C5=NC([H])=C([Br])C([H])=N5	3.078	3.038
Ts53	O=C(N([H])C3=C([H])C([H])=C2OC([H])([H])[C@@]4([C@@]1(N=C(OC1([H])[H])N([H])[H])C2=C3[H])C([H])([H])C4([H])[H])C5=NC([H])=C([Cl])C([H])=C5C([H])([H])[H]	2.504	2.498
Ts54	O=C(/C1=N/C([H])=C(C([H])=C1[H])C([H])([H])[H])N([H])C2=C([H])C(=C([F])C([H])=C2[H])[C@]3(N([H])C(=N[H])N([S](=O)(=O)C3([H])[H])C([H])([H])[H])C([H])([H])[H]	4.523	3.961

Ts55	O=C(/C1=N/C([H])=C([F])C([H])=C1[H])N([H])C2=C([F])C(=C([F])C([H])=C2[H])[C@]3(N([H])C(=N[H])N([S](=O)(=O)C3([H])[H])C([H])([H])[H])C([H])([H])[H]	4.312	4.448
Ts56	O=[S]3(=O)N(/C(=N\[H])N([H])[C@](C=1[S]C([H])=C(C=1[H])C2=C([H])C([H])=C([H])C(CN)=C2[H])(C3([H])[H])C([H])([H])[H])C([H])([H])[H]	3.592	3.122
Ts57	O=C(N([H])[C@]1([H])C([H])([H])C1([H])[H])[C@](OC([H])([H])[H])C([H])([H])[C@]([H])(O[H])[C@@]([H])(N([H])C(=O)C=2C([H])=C([H])C([H])=C(C=2[H])C(=O)N(C([H])([H])C([H])([H])C([H])([H])[H])C([H])([H])C([H])([H])C([H])([H])[H])C([H])([H])O/C3=C(\[H])C([F])=C([H])C([F])=C3[H]	2.658	2.141
Ts58	O=C(N([H])C(=NC([H])([H])C1=C([H])C([Cl])=C(C([Cl])=C1[H])N([H])[S](=O)(=O)C([H])([H])[H])N([H])[H])C=2C(=N[S]C=2C([H])([H])[H])C3=C([H])C([H])=C(OC([H])([H])[H])C([H])=C3[H]	2.553	4.082
Ts59	O=C(N([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)O[H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])([H])C([H])([H])C(=O)O[H])[C@@]([H])(N([H])C(=O)[C@@]([H])(N([H])C([H])([H])[C@@]([H])(O[H])C(=O)[C@@]([H])(N([H])C(=O)[C@@]([H])(N([H])C(=O)[C@@]([H])(N([H])C(=O)[C@@]([H])(N([H])[H])C([H])([H])C([H])([H])C(=O)O[H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])C(=O)O[H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])(C([H])([H])[H])C([H])([H])[H]~	5.523	6.340
Ts60	O=[S](=O)(C([H])([H])C([H])([H])[C@@]([H])(C(=O)N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])(C([H])([H])[H])C([H])([H])[H])N([H])C(=O)[C@@]([H])(N([H])C(=O)OC(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H]	4.097	3.243
Ts61	O=C(N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])([H])[H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])[C@@]([H])(N([H])C(=O)OC(C([H])([H])[H])([H])C([H])([H])[H])C([H])([H])[H])C(=O)N([H])[H]	0.649	2.152
Ts62	O=C1N(/C(=N\[H])N([H])[C@]1(C([H])([H])C([H])([H])[C@]2([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C2([H])[H])C([H])([H])[C@]4([H])C([H])([H])[C@]([H])(N([H])C(=O)C3=C([H])C([H])=C([H])C([H])=C3[H])C([H])([H])C([H])([H])C4([H])[H])C([H])([H])[H]	3.886	3.365
Ts63	O=C1N(/C(=N\[H])N([H])[C@]1(C([H])([H])C([H])([H])[C@@]2([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C2([H])[H])C([H])([H])[C@]4([H])C([H])([H])[C@]([H])(N([H])C([H])([H])[C@]3([H])C([H])([H])C3([H])[H])C([H])([H])C([H])([H])C4([H])[H])C([H])([H])[H]	3.319	3.052
Ts64	O=C1N(/C(=N/[H])N([H])[C@]1(C([H])([H])C([H])([H])[C@@]2([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C2([H])[H])C([H])([H])[C@]4([H])C([H])([H])[C@]([H])(N([H])C(=O)N([H])C3=C([H])C([H])=C(OC([H])([H])[H])C([H])=C3[H])C([H])([H])C([H])([H])C4([H])[H])C([H])([H])[H]	5.000	3.239
Ts65	O=C1N(/C(=N\[H])N([H])[C@]1(C([H])([H])C([H])([H])[C@]2([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C2([H])[H])C([H])([H])[C@@]3([H])C([H])([H])N(C(=O)OC(C([H])([H])[H])([H])C([H])([H])[H])C([H])([H])C([H])([H])[H])C([H])([H])C([H])([H])[H]	3.387	4.164
Ts66	O=[S]2(=O)N(/C(=N/[H])N([H])[C@]4(/C1=C(\[H])C([H])=C([H])C([H])=C1[H])[C@@]2([H])C([H])([H])N(/C3=N/C(=C(/[F])C(=N3)OC([H])([H])[H])C([H])([H])[H])C4([H])[H])C([H])([H])[H]	3.292	3.012
Ts67	O=[S]2(=O)N(/C(=N/[H])N([H])[C@]4(/C1=C(\[H])C([H])=C([H])C([H])=C1[F])[C@@]2([H])C([H])([H])N(/C3=N/C(=C(/[F])C(=N3)OC([H])([H])[H])C([H])([H])[H])C4([H])[H])C([H])([H])[H]	3.721	3.108

Ts68	O=[S]2(=O)N(/C(=N/[H])N([H])[C@@]4(/C1=C(\[H])C([H])=C([H])C([H])=C1[H])[C@]2([H])C([H])([H])N(/C3=N/C(OC([H])([H])[H])=C([H])C(=C3[H])C([H])([H])OC([H])([H])C([H])([H])[H])C4([H])[H])C([H])([H])[H]	3.215	3.247
Ts69	O=[S]2(=O)N(/C(=N/[H])N([H])[C@@]4(/C1=C(\[H])C([H])=C([H])C([H])=C1[H])[C@]2([H])C([H])([H])N(/C3=N/C(=C(/[F])C(=N3)OC([H])([H])[H])C([H])([H])C([H])([H])[H])C4([H])[H])C([H])([H])[H]	3.086	3.259
Ts70	O=C(C=1C([H])=C([H])C([H])=C(C=1[H])C(=O)N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])N([H])[C@]([H])(C(=O)N([H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])[C@@]([H])(O[H])C([H])([H])C([H])([H])C([H])([H])[H])C([H])([H])C2=C([H])C([H])=C([H])C([H])=C2[H])N([C@]([H])(C3=C([H])C([H])=C([H])C([H])=C3[H])C([H])([H])[H])C([H])([H])[H]	1.280	1.258
Calibration set			
Calib1	O=C(OC([H])([H])C([H])([H])C([H])=C([H])[H])N([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])[C@@]([H])(C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])[C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C=1C([H])=C([H])C([H])	3.212	3.130
Calib2	O=C(OC([H])([H])C([H])([H])C([H])([H])C([H])=C([H])[H])N([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])[C@@]([H])(C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])[C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C=1C([H])=C	2.950	3.154
Calib3	O=C(/C1=C(\[H])C([H])=C([H])C(=C1[H])C([H])([H])N4C(=NC=3C([H])=C([H])C(OC=2C([H])=C([H])C([H])=C([H])C=2[H])=C([H])C=3C4([H])[H])N([H])[H])N(C([H])([H])[H])C5([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C5([H])[H]	2.801	2.889
Calib4	O=C(O[H])C([H])([H])C([H])([H])[C@@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)O[H])C([H])([H])C1=C([H])C([H])=C([H])C([H]	4.796	4.442
Calib5	O=C(N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])[C@@]([H])(N([H])C	4.027	3.748
Calib6	O=C(N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])(C([H])([H])[H])[H])	0.979	3.135
Calib7	O=C2N(C(=N[C@]4(C=1C([H])=C([H])C([F])=C([H])C=1[H])[C@@]2([H])C([H])([H])N(/C3=N/C(OC([H])([H])[H])=C([F])C(=N3)OC([H])([H])[H])C4([H])[H])N([H])[H])C([H])([H])[H])[H]	4.357	3.896
Calib8	O=C2N(C(=N[C@]4(C=1C([F])=C([H])C([F])=C([H])C=1[F])[C@@]2([H])C([H])([H])N(/C3=N/C(=C(/[F])C(=N3)OC([H])([H])[H])C([H])([H])[H])C4([H])[H])N([H])[H])C([H])([H])[H]	3.824	4.010
Calib9	O=C2N(C(=N[C@]4(/C1=C(\[H])C([Cl])=C([H])C([H])=C1[H])[C@@]2([H])C([H])([H])N(/C3=N/C(OC([H])([H])[H])=C([F])C(=N3)C([H])([H])[H])C4([H])[H])N([H])[H])C([H])([H])[H]	3.409	3.409
Calib10	O=C2N(C(=N[C@]5(C=1C(=C([H])C([H])=C([F])C=1[H])[C@@]2([H])C([H])([H])N(/C3=N/C(OC([H])([H])[H])=C([Cl])C(=N3)[C@]4([H])C([H])([H])C4([H])[H])C5([H])[H])N([	4.187	4.166

	H])[H])C([H])([H])[H]		
Calib11	O=C2N(C(=N[C@]5(C=1C([H])=C(C#N)C([H])=C([H])C=1[H])[C@@]2([H])C([H])([H])N(/C3=N/C(=C(/[F])C(=N3)[C@@]4([H])C([H])([H])C4([H])[H])C([H])([H])[H])C5([H])[H])N([H])[H])C([H])([H])[H]	3.367	3.193
Calib12	[F]C=1C([H])=C([F])C(=C([H])C=1[H])[C@@]24N=C(N(C(=O)[C@]2([H])C([H])([H])N(/C3=N/C(=C(/[F])C(=N3)OC([H])([H])[H])C([H])([H])O[H])C4([H])[H])C([H])([H])[H])N([H])[H]	3.796	3.715
Calib13	O=C2N(C(=N[C@]4(C=1C([F])=C([H])C([F])=C([F])C=1[H])[C@@]2([H])C([H])([H])N(/C3=N/C(OC([H])([H])[H])=C([F])C(=N3)C([H])([H])C([H])([H])[H])C4([H])[H])N([H])[H])C([H])([H])[H]	4.252	4.508
Calib14	O=C(/C1=N/C([H])=C([F])C([H])=C1[H])N([H])C2=C([H])C(=C([F])C([H])=C2[H])[C@]3(N([H])C(=N[H])N([S](=O)(=O)C3([H])[H])C([H])([H])[H])C([H])([H])[H]	4.312	4.112
Calib15	O=[S]3(=O)N(C=2C([H])=C(C([H])=C1/C(=C(/[H])N(C1=2)C([H])([H])C3([H])[H])C([H])([H])C([H])([H])[H])C(=O)N([H])[C@]([H])(C([H])([H])N([H])[C@]([H])(C(=O)N([H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])[C@@]([H])(O[H])C([H])([H])C([H])([H])C([H])([H])[H])C([H])([H])[H])([H	5.398	4.572
Calib16	O=C(N([H])[C@@]([H])(C=1C([H])=C([H])C([H])=C([H])C=1[H])C([H])([H])[H])C2=C([H])C(=C([H])C(=C2[H])N(C([H])([H])[H])[S](=O)(=O)C([H])([H])[H])C(=O)N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])N([H])C([H])([H])C3=C([H])C4=C(C([H])=C3[H])C([H])=C([H])N4[S](=	3.569	3.504
Calib17	O=C(OC([H])([H])C=1N=C(OC=1C([H])([H])[H])C([H])([H])[H])N([H])[C@]([H])(C(=O)N([H])[C@@]([H])(C([H])([H])C2=C([H])C([H])=C([H])C([H])=C2[H])[C@]([H])(O[H])C([H])([H])N([H])C([H])([H])C3=C([H])C(OC([H])([H])[H])=C([H])C([H])=C3[H])C([H])([H])[S](=O)(=O)	0.824	2.502
Calib18	O=C(N([H])[C@@]([H])(C=1C([H])=C([H])C([H])=C([H])C=1[H])C([H])([H])[H])C2=C([H])C(=C([H])C(=C2[H])N(C([H])([H])[H])[S](=O)(=O)C([H])([H])[H])C(=O)N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])N([H])C([H])([H])C3=C([H])C(OC([H])([H])[H])=C([H])C([H])=C3[H])	2.038	2.033
Calib19	O=C(OC([H])([H])C=1N=C(OC=1C([H])([H])[H])C([H])([H])[H])N([H])[C@]([H])(C(=O)N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H]	5.921	4.006
Calib20	O=C(N([H])C(=NC([H])([H])C1=C([H])C([Cl])=C([H])C([Cl])=C1[H])N([H])[H])C2=C(N(/N=C2/C([H])([H])[H])C([H])([H])[H])C3=C([H])C([H])=C(OC([H])([H])[H])C([H])=C3[H]	1.398	1.656
Calib21	O=C2N([H])C1=C([H])C([H])=C([H])C([H])=C1N([H])C=3/C2=C(/[H])C([H])=C(C=3[H])C(=O)N([H])C4=C([H])C([H])=NC([H])=C4[H]	2.530	2.691
Calib22	O=C2N([H])C=1C([H])=C([H])C([H])=C([H])C=1N([H])C3=C2C([H])=C([H])C(=C3[H])C(=O)N([H])C4=N/C(=C(/[H])N4[H])C5=C([H])C([H])=C([F])C([H])=C5[H]	2.533	2.654
Calib23	O=C(N([H])C(=NC([H])([H])C1=C([H])C(=C([H])C([Cl])=C1[H])C2=C([H])N=C([H])C([H])=C2[H])N([H])[H])C=3C(=NOC=3C([H])([H])[H])C4=C([H])C([H])=C(OC([H])([H])[H])C([H])=C4[H]	1.745	1.988
Calib24	O=C(N([H])C(=NC([H])([H])C1=C([H])C(=C([H])C([Cl])=C1[H])C=2C([H])=C([H])[S]C=2[H])N([H])[H])C=3C(=NOC=3C([H])([H])[H])C4=C([H])C([H])=C(OC([H])([H])[H])C([H])=C4[H]	1.921	2.654

Calib25	O=C(N([H])C(=NC([H])([H])C1=C([H])C(=C([H])C([Cl])=C1[H])C([H])=C([H])[H])N([H])[H])C=2C(=NOC=2C([H])([H])[H])C3=C([H])C([H])=C(OC([H])([H])[H])C([H])=C3[H]	2.367	2.222
Calib26	O=C(N([H])C(=NC([H])([H])C1=C([H])C([Cl])=C(O[H])C([Cl])=C1[H])N([H])[H])C=2C(=NOC=2C([H])([H])[H])C3=C([H])C([H])=C(OC([H])([H])[H])C([H])=C3[H]	2.319	2.575
Calib27	O=C(N([H])C(=NC([H])([H])C1=C([H])C([Cl])=C([H])C([Cl])=C1[H])N([H])[H])C=2C(=NOC=2C([H])([H])[H])C3=C([H])C([H])=C([H])C([H])=C3[H]	1.409	2.245
Calib28	O=C(N([H])C(=NC([H])([H])C1=C([H])C([Br])=C([H])C([Cl])=C1[H])N([H])[H])C=2C(=NOC=2C([H])([H])[H])C3=C([H])C([H])=C(OC([H])([H])[H])C([H])=C3[H]	2.569	2.071
Calib29	O=C(N([H])C(=NC([H])([H])C1=C([H])C([Cl])=C(C([Cl])=C1[H])N([H])C(=O)C([H])([H])N([H])C([H])([H])C([H])([H])[H])N([H])[H])C=2C(=N[S]C=2C([H])([H])[H])C3=C([H])C([H])=C(OC([H])([H])[H])C([H])=C3[H]	4.000	3.685
Calib30	[H]C=2C(O[H])=C([H])C=1OC=3C(OC=1C=2O[H])=C([H])C(O[H])=C4OC5=C(OC=34)C(O[H])=C([H])C(O[H])=C5[H]	1.097	1.557
Calib31	[F]C=1C([H])=C(C([H])=C([F])C=1[H])C([H])([H])[C@]([H])(N([H])C(=O)C2=C([H])C(=C([H])C(=C2[H])C([H])([H])[H])C(=O)N(C([H])([H])C([H])([H])C([H])([H])[H])C([H])([H])C([H])([H])C([H])([H])[H])[C@]([H])(O[H])[C@]3([H])N([H])C([H])([H])C([H])([H])N(C3([H])[	5.000	2.945
Calib32	[F]C=1C([H])=C(C([H])=C([F])C=1[H])C([H])([H])[C@]([H])(N([H])C(=O)C2=C([H])C(=C([H])C(=C2[H])C([H])([H])[H])C(=O)N(C([H])([H])C([H])([H])C([H])([H])[H])C([H])([H])C([H])([H])C([H])([H])[H])[C@]([H])(O[H])[C@]3([H])N([H])C([H])([H])C([H])([H])N(C3([H])[	4.301	3.353
Calib33	O=C3N(C([H])([H])C([H])([H])C=5C([H])=C(OC=2C(OC([H])([H])[H])=C([H])C=1N=C(N(C([H])([H])C=1C=2[H])[C@@]([H])(C([H])([H])C3([H])[H])[C@@]4([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C4([H])[H])N([H])[H])C([H])=C([H])C=5[H])[C@]6([H])C([H])([H])C([H	3.921	3.715
Calib34	O=C(N([H])[C@@]([H])(C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])([H])[H])C2=C([H])C(=C([H])C(=C2[H])N(C([H])([H])[H])[S](=O)(=O)C([H])([H])[H])C(=O)N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])[C@@]([H])(OC([H])([H])[H])C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])	2.678	3.293
Calib35	O=C(N([H])[C@@]([H])(C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])([H])[H])C2=C([H])C(=C([H])C(=C2[H])N(C([H])([H])[H])[S](=O)(=O)C([H])([H])[H])C(=O)N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])[C@@]([H])(OC([H])([H])C([H])=C([H])[H])C(=O)N([H])[C@]([H])(C(=	4.481	3.396
Calib36	O=C1C([H])=C(OC=2/C1=C(/O[H])C([H])=C(O[H])C=2[H])C3=C(O[H])C([H])=C(O[H])C([H])=C3[H]	0.083	0.404
Calib37	O=C3N([H])[C@]([H])(C(=O)N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])N([H])C([H])([H])C1=C([H])C(=C([H])C([H])=C1[H])C(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])C2=C([H])C([F])=C([H])C([F])=C2[H])C([H])([H])N3C([H])([H])C4=C([H])C([F])=C([H	4.699	3.156
Calib38	O=C3N(C([H])([H])[C@@]([H])(C(=O)N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])N([H])C([H])([H])C1=C([H])C(=C([H])C([H])=C1[H])N(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C2=C([H])C([H])=C([H])C([H])=C2[H])C3([H])[H])C([H])([H])C4=C([H])C([H])=C([H])C([H])=C	1.659	1.872
Calib39	O=C3N([H])[C@]([H])(C(=O)N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])N([H])C([H])([H])C1=C([H])C(=C([H])C([H])=C1[H])N(C([H])([H])[H])C([H])([H])[H])C([H])([H])C2=C([H])C([H])=C([H])C([H])=C2[H])C([H])([H])N3C([H])([H])C([H])([H])C4=C([H])C([H])=C([	1.167	1.871

	H])C([		
Calib40	O=C1N(C(=N[C@]1(C=2C([H])=C([H])C([H])=C([H])C=2[H])C3=C([H])C(=C([H])C([H])=C3[H])C4=C([H])C([H])=NC([H])=C4[H])N([H])[H])C([H])([H])[H]	1.420	2.360
Calib41	O=C1N(C(=N[C@@]1(C=2C([H])=C([H])C([H])=C([H])C=2[H])C3=C([H])C(=C([H])C([H])=C3[H])C4=C([H])N=C([H])C(=C4[H])C([H])([H])[H])N([H])[H])C([H])([H])[H]	2.367	2.522
Calib42	O=C1N(C(=N[C@@]1(/C2=C(\[H])C([H])=C([H])C([H])=C2[H])C3=C([H])C(=C([H])C([H])=C3[H])C4=C([H])N=C([H])C(C#N)=C4[H])N([H])[H])C([H])([H])[H]	2.328	2.636
Calib43	O=C(N([C@]1([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C1([H])[H])C([H])([H])C=2N=C([S]C=2[H])C([H])([H])OC([H])([H])[H])C([H])([H])C([H])([H])[C@]([H])(N5C(=N/C4=C(\[H])C([H])=C(O/C3=C(\[H])C([H])=C([H])C([H])=C3[H])C([H])=C4C5([H])[H])N([H])[H])[	3.886	3.516
Calib44	O=C3N(C(=N[C@](C=2[S]C([H])=C(/C1=C(\[H])C(C#CC([H])([H])[H])=C([H])N=C1[H])C=2[H])(C3([H])[H])C([H])([H])[H])N([H])[H])C([H])([H])[H]	4.108	3.680
Calib45	O=C(N([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])N([H])C2=C1C([H])=C([H])C([H])=C([H])C1=NC3=C2C([H])([H])C([H])([H])C([H])([H])C3([H])[H])C=4OC=5C(C(=O)C=4[H])=C(O[H])C([H])=C(O[H])	1.975	2.047
Calib46	O=C(N([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])N([H])C2=C1C([H])=C([H])C([Cl])=C([H])C1=NC3=C2C([H])([H])C([H])([H])C([H])([H])C3([H])[H])C=4OC=5C(C(=O)C=4[H])=C([H])C(OC([H])([H])	1.374	2.160
Calib47	O=[S]3(=O)N(C(=N[C@@](C=1[S]/C(=C(/[H])C=1[Cl])C2=C([H])C(C#CC([H])([H])[H])=C([H])N=C2[H])(C([H])([H])[H])C3([H])[H])N([H])[H])C([H])([H])[H]	4.620	4.628
Calib48	O=C(N([H])C3=C([H])C([H])=C2OC([C@]4([C@@]1(N=C(OC1([H])[H])N([H])[H])C2=C3[H])C([H])([H])OC4([H])[H])(C([H])([H])[H])C([H])([H])[H])C=5/N=C(/[H])C([F])=C([H])C=5[H]	2.932	2.828
Calib49	[H]/C4=C(/C([H])=C1C(O[C@]([H])([C@]3([C@]12N=C(OC2([H])[H])N([H])[H])C([H])([H])OC3([H])[H])C([H])([H])C([H])([H])C([H])([H])[H])=C4[H])C5=C([H])N=C([H])C(C#CC([H])([H])[H])=C5[H]	3.056	2.743
Calib50	[F]C([F])([F])C([H])([H])C([H])([H])[C@]3([H])O/C1=C(\[H])C([H])=C(C([H])=C1[C@@]2(N=C(OC2([H])[H])N([H])[H])[C@]34C([H])([H])OC4([H])[H])C5=C([H])N=C([H])C(C#CC([H])([H])[H])=C5[H]	2.061	2.221
Calib51	O=C(N([H])C3=C([H])C([H])=C2OC([H])([H])[C@@]4([C@@]1(N=C(OC1([H])[H])N([H])[H])C2=C3[H])C([H])([H])C4([H])[H])C5=NC([H])=C(C#N)C([H])=C5C([H])([H])[H]	2.668	2.624
Calib52	O=C(N([H])C3=C([H])C([H])=C2OC([C@]4([C@@]1(N=C(OC1([H])[H])N([H])[H])C2=C3[H])C([H])([H])C4([H])[H])(C([H])([H])[H])C([H])([H])[H])C5=NC([H])=C(/N=C5/[H])OC([H])([H])[H]	3.213	3.326
Calib53	O=C(N([H])C3=C([H])C([H])=C2OC([C@@]4([C@]1(N=C(OC1([H])[H])N([H])[H])C2=C3[H])C([H])([H])OC4([H])[H])(C([H])([H])[H])C([H])([H])[H])C=5/N=C(/[H])C([Cl])=C([H])C=5[H]	0.520	1.753
Calib54	[F]C=1C([H])=C(C([H])=C([F])C=1[H])C([H])([H])[C@]([H])(N([H])C(=O)C2=C([H])C(=C([H])C(=C2[H])C([H])([H])[H])[H])C(=O)N(C([H])([H])C([H])([H])C([H])([H])[H])C([H])([H])C([H])([H])C([H])([H])[H])[C@]([H])(O[H])[C@]3([H])N([H])C([H])([H])C([H])([H])N(C3([H])[	1.237	2.873

Calib55	[F]C=1C([H])=C(C([H])=C([F])C=1[H])C([H])([H])[C@]([H])(N([H])C(=O)C2=C([H])C(=C([H])C(=C2[H])C([H])([H])[H])C(=O)N(C([H])([H])C([H])([H])C([H])([H])[H])C([H])([H])C([H])([H])C([H])([H])[H])[C@]([H])(O[H])[C@]3([H])N([H])C([H])([H])C([H])([H])N(C3([H])[	1.921	2.753
Calib56	O=C(N([H])[C@]1([H])C([H])([H])C1([H])[H])[C@]([H])(OC([H])([H])[H])C([H])([H])[C@]([H])(O[H])[C@@]([H])(N([H])C(=O)C2=C([H])C(=C([H])C(=C2[H])C(=O)N([H])[C@@]([H])(C3=C([H])C([H])=C([H])C([H])=C3[H])C([H])([H])[H])N(C([H])([H])[S](=O)(=O)C([H])([H])[H]	1.745	2.783
Calib57	O=C(N([H])C(=NC([H])([H])C1=C([H])C([Cl])=C([Cl])C([H])=C1[H])N([H])[H])C=2C(=NOC=2C([H])([H])[H])C3=C([H])C([H])=C(OC([H])([H])[H])C([H])=C3[H]	2.041	2.371
Calib58	O=C(N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])[C@]([H])(N([H])C(=	4.229	3.009
Calib59	O=C(O[H])C([H])([H])C([H])([H])[C@]([H])(N([H])[H])C(=O)N([H])[C@@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])[C@@]([H])(C(=O)O[H])C([H])([H])C1=C([H])C([H])=	4.796	4.574
Calib60	O=C(N([H])[C@]([H])(C(=O)N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H]	2.327	3.092
Calib61	O=C1N(/C(=N\[H])N([H])[C@]1(C([H])([H])C([H])([H])[C@]2([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C2([H])[H])C([H])([H])[C@]4([H])C([H])([H])[C@]([H])(N([H])C(=O)N([H])C3=C([H])C([H])=C(C#N)C([H])=C3[H])C([H])([H])C([H])([H])C4([H])[H])C([H])([H])	4.523	4.241
Calib62	O=C1N(/C(=N\[H])N([H])[C@]1(C([H])([H])C([H])([H])[C@]2([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C2([H])[H])C([H])([H])[C@]4([H])C([H])([H])[C@]([H])(N([H])C(=O)N([H])C3=C([H])C([H])=C([H])C([H])=C3[H])C([H])([H])C([H])([H])C4([H])[H])C([H])([H])	3.796	3.719
Calib63	O=C1N(/C(=N/[H])N([H])[C@]1(C([H])([H])C([H])([H])[C@@]2([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C2([H])[H])C([H])([H])[C@]3([H])C([H])([H])N(C([H])([H])C([H])([H])C3([H])[H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])[H])C([H])([H])	3.119	2.939
Calib64	O=[S]2(=O)N(/C(=N/[H])N([H])[C@]4(/C1=C(\[H])C([F])=C([F])C([H])=C1[F])[C@]2([H])C([H])([H])N(/C3=N/C(OC([H])([H])[H])=C([H])C(=C3[H])C([H])([H])OC([H])([H])[H])C4([H])[H])C([H])([H])[H]	4.155	4.261
External set			
Ext1	C004O=C2N([H])[C@]([H])(C(=O)N([H])[C@@]([H])(C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])[C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C=1C([H])=C([H])C([H])=C([H])C=1[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])C(=O)N([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])OC(=O)N([H])[C@@]2([H])C([H])(C([H])([H])[H])C([H])([H])[H]	2.966	3.084
Ext2	C005O=C(OC([H])([H])C([H])([H])C([H])([H])C([H])=C([H])[H])N([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])[C@@]([H])(C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])[C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C=1C([H])=C([H])C([H])=C([H])C=1[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])C(=O)N([H])C([H])([H])C([H])=C([H])[H])C([H])(C([H])([H])[H])C([H])([H	2.950	3.093

	])[H]		
Ext3	C006O=C1OC([H])([H])C([H])([H])C([H])([H])C([H])=C([H])C([H])([H])N([H])C(=O)C([H])([H])[C@](H])(N([H])C(=O)[C@@]([H])(N1[H])C([H])(C([H])([H])[H])C([H])([H])[H])C(=O)N([H])[C@@]([H])(C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])[C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C=2C([H])=C([H])C([H])=C([H])C=2[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H]	3.848	3.684
Ext4	C015O=C(C=1C([H])=C(C([H])=C(C=1[H])C(=O)N([H])[C@@]([H])(C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])[C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])N(C([H])([H])[H])[S](=O)(=O)C([H])([H])[H])N([H])C([H])([H])C=2N=C(OC=2C([H])([H])[H])C([H])([H])[H]	4.745	3.570
Ext5	C020O=C(N(C([H])([H])[H])[C@@]1([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C1([H])[H])C([H])([H])C([H])([H])[C@@]([H])(N4C(=NC=3C([H])=C([H])C(OC=2C([H])=C([H])C([H])=C([H])C=2[H])=C([H])C=3C4([H])[H])N([H])[H])[C@]5([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C5([H])[H]	3.523	3.030
Ext6	C028O=C(N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])[C@@]([H])(N([H])C(=O)[C@@]([H])(N([H])C(=O)OC(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])C(=O)N([H])[H]	4.229	3.904
Ext7	C109O=C(N([H])[C@@]([H])(C=1C([H])=C([H])C([H])=C([H])C=1[H])C([H])([H])[H])C2=C([H])C(=C([H])C(=C2[H])N(C([H])([H])[H])[S](=O)(=O)C([H])([H])[H])C(=O)N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])N([H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])C3=C([H])C([H])=C([H])C([H])=C3[H]	2.372	1.766
Ext8	C115O=C(N([H])C(=NC([H])([H])C1=C([H])C([Cl])=C([H])C([Cl])=C1[H])N([H])[H])C2=C(N(/N=C2/C([H])([H])[H])C([H])([H])[H])C3=C([H])C([H])=C(OC([H])([H])[H])C([H])=C3[H]	1.398	1.712
Ext9	C117O=C3OC=2C(OC([H])([H])[C@@]([H])(O[H])C(O[H])(C([H])([H])[H])C([H])([H])[H])=C1OC([H])=C([H])C1=C(OC([H])([H])[H])C=2C([H])=C3[H]	0.260	0.995
Ext10	C123O=C2N([H])C1=C([H])C([H])=C([H])C([H])=C1N([H])C3=C2C([H])=C([H])C(=C3[H])C(=O)N([H])C4=C([H])C([H])=C([F])C([H])=C4[H]	2.676	2.639
Ext11	C124O=C(N([H])[C@@]([H])(C1=C([H])C([H])=C([F])C([H])=C1[H])C([H])([H])[H])C=2C([H])=C(C([H])=C(C=2[H])N([H])[S](=O)(=O)C([H])([H])[H])C(=O)N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])N([H])[C@@]3([H])C([H])([H])C3([H])[H])C([H])([H])C4=C([H])C([H])=C([H])C([H])=C4[H]	4.000	2.982
Ext12	C134O=C(N([H])C(=NC([H])([H])C1=C([H])C(=C([H])C([Cl])=C1[H])C([H])=C([H])C([H])([H])OC([H])([H])[H])N([H])[H])C=2C(=NOC=2C([H])([H])[H])C3=C([H])C([H])=C(OC([H])([H])[H])C([H])=C3[H]	2.824	2.037
Ext13	C140O=C(N([H])C(=NC([H])([H])C1=C([H])C([Cl])=C([H])C([Cl])=C1[H])N([H])[H])C=2C(=N[S]C=2C([H])([H])[H])C3=C([H])C([H])=C(OC([H])([H])[H])C([H])=C3[H]	2.538	2.601
Ext14	C153[H]C=2C(O[H])=C1OC=6C(OC1=C3C=2OC=4/C3=C(/O[H])C([H])=C(O[H])C=4O/C5=C(\[H])C(O[H])=C([H])C(O[H])=C5[H])=C(O[H])C([H])=C(OC=7C([H])=C(O[H])C([H])=C(O[H])C=7[H]	1.886	1.258
Ext15	C158O=C(/C1=C(\[H])C(=C([H])C(=C1[H])C(=O)N2[C@]([H])(C([H])([H])C([H])([H])C2([H])[H])C([H])([H])OC([H])([H])[H])C([H])([H])[H])N([H])[C@]([H])([C@]([H])(O[H])[C@]3([H])N([H])C([H])([H])C([H])([H])N(C3([H])[H])[S](=O)(=O)[C@@]4([H])C([H])([H])C4	4.155	4.345

	([H])[H])C([H])([H])C5=C([H])C([F])=C([H])C([F])=C5[H]		
Ext16	C167O=C(N([H])[C@@]([H])(C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])([H])[H])C2=C([H])C(=C([H])C(=C2[H])N(C([H])([H])[H])[S](=O)(=O)C([H])([H])[H])C(=O)N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])[C@@]([H])(OC([H])([H])[H])C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C3=C([H])C([H])=C([H])C([H])=C3[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])O/C4=C(\[H])C([F])=C([H])C([F])=C4[H]	2.678	3.169
Ext17	C172O=C(N([H])[C@@]([H])(C=1C([H])=C([H])C([H])=C([H])C=1[H])C([H])([H])[H])C=2C([H])=C(C([H])=C(C=2[H])N(C([H])([H])[H])[S](=O)(=O)C([H])([H])[H])C(=O)N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])[C@@]([H])(OC([H])([H])C3=C([H])C([H])=C([H])C([H])=C3[H])C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C4=C([H])C([H])=C([H])C([H])=C4[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])OC=5C([H])=C([F])C([H])=C([F])C=5[H]	3.699	3.899
Ext18	C177O=C(N([H])C1=C([H])C([H])=C([H])C([H])=C1[H])[C@]([H])(OC([H])([H])[H])C([H])([H])[C@]([H])(O[H])[C@@]([H])(N([H])C(=O)C2=C([H])C(=C([H])C(=C2[H])C(=O)N([H])[C@@]([H])(C3=C([H])C([H])=C([H])C([H])=C3[H])C([H])([H])[H])N(C([H])([H])[S](=O)(=O)C([H])([H])[H])C([H])([H])[H])C([H])([H])O/C4=C(\[H])C([F])=C([H])C([F])=C4[H]	2.699	2.405
Ext19	C184O=C(OC(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])N([H])[C@]([H])(C(=O)N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])C(=O)N([H])[H]	1.504	2.150
Ext20	C201O=C3N([H])[C@]([H])(C(=O)N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])N([H])C([H])([H])C1=C([H])C(=C([H])C([H])=C1[H])N(C([H])([H])[H])C([H])([H])[H])C([H])([H])C2=C([H])C([H])=C([H])C([H])=C2[H])C([H])([H])N3C([H])([H])C([H])([H])C([H])([H])C([H])([H])[H]	0.398	0.564
Ext21	C202O=C1N(C(=N[C@]1(C=2C([H])=C([H])C([H])=C([H])C=2[H])C3=C([H])C(=C([H])C([H])=C3[H])C4=C([H])C([H])=NC([H])=C4[H])N([H])[H])C([H])([H])[H]	1.420	2.498
Ext22	C208O=C1N(C(=N[C@]1(C=2C([H])=C([H])C([H])=C([H])C=2[H])C3=C([H])C(=C([H])C([H])=C3[H])C4=C([H])N=C([H])C([Cl])=C4[H])N([H])[H])C([H])([H])[H]	3.046	2.972
Ext23	C212O=C1N(C(=N[C@@]1(C=2C([H])=C([H])C([H])=C([H])C=2[H])C3=C([H])C(=C([H])C([H])=C3[H])C4=C([H])N=C([H])C([H])=C4[H])N([H])[H])C([H])([H])[H]	1.770	2.372
Ext24	C213O=C1N(C(=N[C@@]1(/C2=C(\[H])C(=C([H])C([H])=C2[H])C3=C([H])N=C([H])C([F])=C3[H])[C@@]4([H])C([H])([H])C4([H])[H])N([H])[H])C([H])([H])[H]	2.796	2.549
Ext25	C219O=C1N(C(=N[C@]1(C=2C([H])=C([H])C([H])=C([H])C=2[H])C3=C([H])C([F])=C([H])C([H])=C3[H])N([H])[H])C([H])([H])[H]	2.143	2.174
Ext26	C224O=C1N(C(=N[C@@]1(C=2C([H])=C([H])C([H])=C([H])C=2[H])C3=C([H])C(=C([H])C([H])=C3[H])C4=C([H])N=C([H])C([H])=C4[H])N([H])[H])C([H])([H])[H]	2.276	2.372
Ext27	C229O=C(N([C@@]1([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C1([H])[H])C([H])([H])C2=C([H])N(/N=C2/[H])C([H])([H])[H])C([H])([H])C([H])([H])[H])[C@]([H])(N5C(=NC=4C([H])=C([H])C(O/C3=C(\[H])C([H])=C([H])C([H])=C3[H])=C([H])C=4C5([H])[H])N([H])[H])[C@@]6([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C6([H])[H]	3.959	3.832
Ext28	C234O=C(N([C@@]1([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C1([H])[H])C([H])([H])C=2N=C([S]C=2[H])C([H])([H])[H])C([H])([H])C([H])([H])C([H])([H])[C@]([H])(N5C(=NC=4C([H])=C([H])C(O/C3=C(\[H])C([H])=C([H])C([H])=C3[H])=C([H])C=4C5([H])[H])N([H])[H])[C@@]6([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C6([H])[H]	3.102	3.256
Ext29	C239O=C(OC([H])([H])[C@]([H])(N3C(=N/C2=C(\[H])C([H])=C(O/C1=C(\[H])C([H])=C([H])C([H])=C1[H])C([H])=C2C3([H])[H])N([H])[H])[C@@]4([H])C([H])([H])C([H])([H])C([H])([H])C([	3.420	2.813

	H])([H])C([H])([H])C4([H])[H])N([C@@]5([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C5([H])[H])C([H])([H])[H]		
Ext30	C240O=C(OC([H])([H])[C@]([H])(N3C(=N/C2=C(\[H])C([H])=C(O/C1=C(\[H])C([H])=C([H])C([H])=C1[H])C([H])=C2C3([H])[H])N([H])[H])C4=C([H])C([H])=C([H])C([H])=C4[H])N([C@@]5([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C5([H])[H])C([H])([H])[H]	2.106	2.360
Ext31	C246O=C4N(C(=N[C@@](C=1C([H])=C([H])C([H])=C(C=1[H])C2=C([H])C(CN)=C([H])C([H])=C2[H])(C3=C([H])C([H])=C([H])C([H])=C3[H])C4([H])[H])N([H])[H])C([H])([H])[H]	1.022	1.487
Ext32	C252O=C(O[C@]2([H])[C@@]([H])(OC1=C(C(O[H])=C([H])C(O[H])=C1[H])C2([H])[H])C=3C([H])=C(O[H])C(O[H])=C(O[H])C=3[H])C=4C([H])=C(O[H])C(O[H])=C(O[H])C=4[H]	2.678	1.075
Ext33	C257O=C(N([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])N([H])C=2C=1C([H])=C([H])C([H])=C([H])C=1N=C3C=2C([H])([H])C([H])([H])C([H])([H])C3([H])[H])C=4OC=5C(C(=O)C=4[H])=C([H])C(OC([H])([H])[H])=C(OC([H])([H])[H])C=5[H]	2.056	2.215
Ext34	C262O=C2N(/C(=N\[H])N([H])[C@]4(C=1C([Cl])=C([H])C([H])=C([F])C=1[H])[C@@]2([H])C([H])([H])N(/C3=N/C(OC([H])([H])[H])=C([F])C(=N3)C([H])([H])[H])C4([H])[H])C([H])([H])[H]	4.051	4.094
Ext35	C266O=C(N([H])C3=C([H])C([H])=C2OC([C@]4([C@@]1(N=C(OC1([H])[H])N([H])[H])C2=C3[H])C([H])([H])OC4([H])[H])(C([H])([H])[H])C([H])([H])[H])C=5/N=C(/[H])C([Cl])=C([H])C=5[F]	3.288	2.905
Ext36	C270[H]/C4=C(/C([H])=C1C(OC([C@]3([C@@]12N=C(OC2([H])[H])N([H])[H])C([H])([H])OC3([H])[H])(C([H])([H])[H])C([H])([H])[H])=C4[H])C5=C([H])N=C([H])C(OC([H])([H])[H])=C5[H]	2.593	2.329
Ext37	C275[H]/C4=C(/C([H])=C1C(OC([C@]3([C@@]12N=C(OC2([H])[H])N([H])[H])C([H])([H])OC3([H])[H])(C([H])([H])[H])C([H])([H])[H])=C4[H])C5=C([H])N=C([H])C(CCC([H])([H])[H])=C5[H]	3.044	3.163
Ext38	C283O=C(N([H])C3=C([H])C([H])=C2OC([C@]4([C@@]1(N=C(OC1([H])[H])N([H])[H])C2=C3[H])C([H])([H])OC4([H])[H])(C([H])([H])[H])C([H])([H])[H])C5=NC([H])=C([Cl])C([H])=C5C([H])([H])[H]	3.190	3.442
Ext39	C289O=C(N([H])C3=C([H])C([H])=C2OC([C@]4([C@@]1(N=C(OC1([H])[H])N([H])[H])C2=C3[H])C([H])([H])OC4([H])[H])(C([H])([H])[H])C([H])([H])[H])C=5/N=C(/[H])C([Cl])=C([H])C=5[H]	3.987	2.848
Ext40	C294O=C(N([H])C3=C([H])C([H])=C2OC([C@]4([C@@]1(N=C(OC1([H])[H])N([H])[H])C2=C3[H])C([H])([H])C4([H])[H])(C([H])([H])[H])C([H])([H])[H])C5=NC([H])=C(/N=C5/[H])OC([H])([H])[H]	3.213	3.098
Ext41	C295O=C(N([H])C3=C([H])C([H])=C2OC([C@]4([C@@]1(N=C(OC1([H])[H])N([H])[H])C2=C3[H])C([H])([H])C4([H])[H])(C([H])([H])[H])C([H])([H])[H])C5=NC([H])=C(/N=C5/[H])C([F])([F])[H]	3.278	3.192
Ext42	C301O=C(/C1=N/C([H])=C(/N=C1/[H])OC([H])([H])[H])N([H])C2=C([H])C(=C([F])C([F])=C2[H])[C@]3(N([H])C(=N[H])N([S](=O)(=O)C3([H])[H])C([H])([H])[H])C([H])([H])[H]	4.979	4.840
Ext43	C304O=[S]3(=O)N(/C(=N\[H])N([H])[C@](C=1[S]C([H])=C(C=1[H])C2=C([H])C([H])=C([H])C(CN)=C2[H])(C3([H])[H])C([H])([H])[H])C([H])([H])[H]	3.592	3.245
Ext44	C308O=C(N([H])[C@]([H])(C(=O)N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])C(=O)N([H])C([H])([H])C([H])=C([H])[H])[C@]([H])(N([H])C(=O)	3.569	2.098

	OC([H])([H])C([H])=C([H])[H])C([H])(C([H])([H])[H])C([H])([H])[H]		
Ext45	C312[F]C=1C([H])=C(C([H])=C([F])C=1[H])C([H])([H])[C@]([H])(N([H])C(=O)C2=C([H])C(=C([H])C(=C2[H])C([H])([H])[H])C(=O)N(C([H])([H])C([H])([H])C([H])([H])[H])C([H])([H])C([H])([H])C([H])([H])[H])[C@]([H])(O[H])[C@]3([H])N([H])C([H])([H])C([H])([H])N(C3([H])[H])[S](=O)(=O)C4=C([H])C([H])=C([H])N=C4[H]	1.237	1.453
Ext46	C316O=C(N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])(C([H])([H])[H])[C@@]([H])(N([H])C(=O)[C@@]([H])(N([H])C(=O)OC(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])([H])[S]C([H])([H])[H]	5.097	3.649
Ext47	C321O=C(N([H])[C@]([H])(C(=O)N([H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])(C([H])([H])[H])C([H])([H])[H])[C@]([H])(OC([H])([H])[H])C([H])([H])[C@]([H])(O[H])[C@@]([H])(N([H])C(=O)C2=C([H])C(=C([H])C(=C2[H])C(=O)N([H])[C@@]([H])(C3=C([H])C([H])=C([H])C([H])=C3[H])C([H])([H])[H])N(C([H])([H])[S](=O)(=O)C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])O/C4=C(\[H])C([H])=C([Br])C([H])=C4[H]	3.125	2.623
Ext48	C325O=C(N([H])C1=C([H])C([H])=C([F])C([H])=C1[H])[C@]([H])(OC([H])([H])[H])C([H])([H])[C@]([H])(O[H])[C@@]([H])(N([H])C(=O)C2=C([H])C(=C([H])C(=C2[H])C(=O)N([H])[C@@]([H])(C3=C([H])C([H])=C([H])C([H])=C3[H])C([H])([H])[H])N(C([H])([H])[S](=O)(=O)C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])O/C4=C(\[H])C([F])=C([H])C([F])=C4[H]	3.000	2.540
Ext49	C328O=C(N([H])[C@]([H])(C(=O)N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)O[H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])([H])C([H])([H])C(=O)O[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])C(=O)N([H])[H])[C@@]([H])(N([H])C(=O)[C@@]([H])(N([H])[H])C([H])([H])C(=O)O[H])C([H])(C([H])([H])[H])C([H])([H])[H]	4.000	4.150
Ext50	C332O=C(N([H])C(=NC([H])([H])C1=C([H])C([Cl])=C([Cl])C([H])=C1[H])N([H])[H])C=2C(=NOC=2C([H])([H])[H])C3=C([H])C([H])=C([F])C([H])=C3[H]	1.620	2.016
Ext51	C334O=C(N([H])C(=NC([H])([H])C1=C([H])C([Cl])=C([Cl])C([H])=C1[H])N([H])[H])C=2C(=NOC=2C([H])([H])[H])C3=C([H])C([H])=C([H])C([H])=C3[H]	1.056	1.861
Ext52	C337O=C(N([H])[C@]([H])(C(=O)N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])N([H])C(=O)OC(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])[C@]([H])(C([H])([H])C=1[S]C([H])=C(N=1)C([H])([H])[H])C([H])(C([H])([H])[H])C([H])([H])[H])[H]	3.538	4.335
Ext53	C341O=C(N([H])[C@@]([H])(C(=O)N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])C([H])([H])[S]C([H])([H])[H])[C@@]([H])(N([H])C(=O)OC(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])C([H])(C([H])([H])[H])C([H])([H])[H]	0.979	2.564
Ext54	C344O=C(N([H])[C@@]([H])(C(=O)N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])[S]C([H])([H])[H])[C@@]([H])(N([H])C(=O)OC(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])C([H])(C([H])([H])[H])C([H])([H])[H]	3.301	2.442
Ext55	C348O=C(OC(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])N([H])[C@@]([H])(C(=O)N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H]	3.229	2.094

	)C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])([H])[S]C([H])([H])[H]		
Ext56	C351O=C1N(/C(=N\[H])N([H])[C@]1(C([H])([H])C([H])([H])[C@@]2([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C2([H])[H])C([H])([H])[C@]4([H])C([H])([H])[C@]([H])(N([H])C(=O)C3=C([H])C([H])=NC([H])=C3[H])C([H])([H])C([H])([H])C4([H])[H])C([H])([H])[H]	3.409	3.545
Ext57	C355O=C1N(/C(=N\[H])N([H])[C@]1(C([H])([H])C([H])([H])[C@@]2([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C2([H])[H])C([H])([H])[C@]4([H])C([H])([H])[C@]([H])(N([H])[C@]3([H])C([H])([H])C([H])([H])C([H])([H])C3([H])[H])C([H])([H])C([H])([H])C4([H])[H])C([H])([H])[H]	3.367	3.801
Ext58	C359O=C(N([H])[C@]([H])(C(=O)N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])N([H])C(=O)OC(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])[C@@]([H])(C([H])([H])N1N=C(C([H])=C1C([H])([H])[H])C([H])([H])[H])C([H])([H])[H]	1.785	3.338
Ext59	C363O=C(N([H])[C@]([H])(C(=O)N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])N([H])C(=O)OC(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])[C@]([H])(C([H])([H])N1N=C(C([H])=C1[H])C([H])([H])[H])C([H])([H])[H]	2.697	3.251

[1]Experimental inhibitory activity; [2]Predicted inhibitory activity

Table S2: SMILES, experimental and predicted inhibitory activity of training, test, calibration and external sets used in QSAR model with considering cycling rings

Set	**SMILES**	Pk_i	
		[1]Obs	**[2]Pred**
Training set			
Tr1	O=C1OC([H])([H])C([H])([H])C([H])([H])C([H])([H])N([H])C(=O)C([H])([H])[C@]([H])(N([H])C(=O)[C@@]([H])(N1[H])C([H])(C([H])([H])[H])C([H])([H])[H])C(=O)N([H])[C@@]([H])(C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])[C@@]([H])(O[H])C([H])([H])[C@]([H])(	2.662	3.194
Tr2	O=C1OC([H])([H])C([H])([H])C([H])=C([H])C([H])([H])N([H])C(=O)C([H])([H])[C@]([H])(N([H])C(=O)[C@@]([H])(N1[H])C([H])(C([H])([H])[H])C([H])([H])[H])C(=O)N([H])[C@@]([H])(C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])[C@@]([H])(O[H])C([H])([H])[C@]([H]	3.547	3.119
Tr3	O=C2N([H])[C@]([H])(C(=O)N([H])[C@@]([H])(C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])[C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C=1C([H])=C([H])C([H])=C([H])C=1[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H]	2.966	3.168

Tr4	O=C(OC([H])([H])N1N=C(C([H])=C1C([H])([H])[H])C([H])([H])[H])N([H])[C@]([H])(C(=O)N([H])[C@@]([H])(C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])[C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C=2C([H])=C([H])C([H])=C([	3.854	2.834
Tr5	O=C(OC([H])([H])N1N=C(C([H])=C1C([H])([H])[H])C([H])([H])[H])N([H])[C@]([H])(C(=O)N([H])[C@@]([H])(C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])[C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C([H])(C([H])([H])[H])C([H	5.523	3.702
Tr6	[F]/C1=C(\[H])C([H])=C(C([H])=C1[H])[C@]([H])(N([H])C(=O)C2=C([H])C(=C([H])C(=C2[H])C3=NN=C(O3)[C@@](C([H])([H])[H])(C([H])([H])C=4C([H])=C([H])C([H])=C([H])C=4[H])[N+]([H])([H])[H])N(C([H])([H])[H])[S](=O)(=O)C([H])([H])[H])C([H])([H])[H]	3.373	2.564
Tr7	O=[S](=O)(N(C=2C([H])=C(C([H])=C([H])[C@@]1([H])C([H])([H])[C@]1([H])C([H])([H])[H])C([H])=C(C=2[H])C3=NN=C(O3)[C@@](C([H])([H])[H])(C([H])([H])C=4C([H])=C([H])C([H])=C([H])C=4[H])[N+]([H])([H])[H])C([H])([H])C([H])([H])C([H])([H])[H])C([H])([H])[H]	3.285	2.999
Tr8	O=C(C=1C([H])=C(C([H])=C(C=1[H])C(=O)N([H])[C@@]([H])(C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])[C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([	2.866	3.390
Tr9	O=C(N(C([H])([H])[H])[C@@]1([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C1([H])[H])C([H])([H])C([H])([H])[C@@]([H])(N4C(=NC=3C([H])=C([H])C(OC=2C([H])=C([H])C([H])=C([H])C=2[H])=C([H])C=3C4([H])[H])N([H])[H])[C@]5([H])C([H])([H])C([H])([H])C([H])([H	3.523	2.984
Tr10	O=C(N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])[C@@]([H])(N([H])C(=O)OC(C([H])([H])[H])[H])	0.649	2.144
Tr11	O=C(N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])[C@@]([H])(N([H])C	1.504	2.192
Tr12	O=C(N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])[C@@]([H])(N([H])C(=O)[C@@]([H])(N([H])C	3.212	3.001
Tr13	O=C(N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])[C@@]([H])(N([H])C	4.229	3.049
Tr14	O=C(N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])[C@@]([H])(N([H])C	3.300	3.000

Tr15	O=C(C=1C([H])=C([H])C([H])=C(C=1[H])C(=O)N([H])[C@@](H])(C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])[C@@](H])(O[H])C([H])([H])[C@](H])(C(=O)N([H])[C@](H])(C(=O)N([H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H	2.103	2.525
Tr16	O=C1OC([H])([H])C([H])=C([H])C([H])([H])N([H])C(=O)C([H])([H])[C@](H])(N([H])C(=O)[C@@](H])(N1[H])C([H])(C([H])([H])[H])C([H])([H])[H])C(=O)N([H])[C@@](H])(C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])[C@@](H])(O[H])C([H])([H])[C@](H])(C(=O)N([H	3.059	3.082
Tr17	O=C(N([H])[C@](H])([C@@](H])(O[H])C([H])([H])[C@](H])(C(=O)N([H])[C@](H])(C(=O)N([H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])[C@@](H])(N([H])C	4.097	3.753
Tr18	O=C(C=1C([H])=C(C([H])=C(C=1[H])C(=O)N([H])[C@@](H])(C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])[C@@](H])(O[H])C([H])([H])[C@](H])(C(=O)N([H])[C@](H])(C(=O)N([H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([	2.502	3.283
Tr19	O=C(C=1C([H])=C(C([H])=C(C=1[H])C(=O)N([H])[C@@](H])(C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])[C@@](H])(O[H])C([H])([H])[C@](H])(C(=O)N([H])[C@](H])(C(=O)N([H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([	3.569	3.819
Tr20	O=C2N(C(=N[C@]4(C=1C([F])=C([H])C([H])=C([F])C=1[H])[C@@]2([H])C([H])([H])N(/C3=N/C(=C(/[F])C(=N3)OC([H])([H])[H])C([H])([H])[H])C4([H])[H])N([H])[H])C([H])([H])[H]	4.071	3.883
Tr21	O=C2N(C(=N[C@]4(C=1C([F])=C([H])C([H])=C([H])C=1[H])[C@@]2([H])C([H])([H])N(/C3=N/C(=C(/[Cl])C(=N3)OC([H])([H])[H])C([H])([H])[H])C4([H])[H])N([H])[H])C([H])([H])[H]	4.032	3.883
Tr22	O=C2N(C(=N[C@]4(C=1C([F])=C([H])C([H])=C([H])C=1[F])[C@@]2([H])C([H])([H])N(/C3=N/C(=C(/[F])C(=N3)OC([H])([H])[H])C([H])([H])[H])C4([H])[H])N([H])[H])C([H])([H])[H]	3.495	3.658
Tr23	O=C2N(C(=N[C@]4(C=1C([H])=C([H])C([H])=C([H])C=1[H])[C@@]2([H])C([H])([H])N(/C3=N/C(=C(/[F])C(=N3)C([H])([H])[H])C([H])([H])[H])C4([H])[H])N([H])[H])C([H])([H])[H]	2.812	2.996
Tr24	O=C2N(C(=N[C@]4(C=1C([H])=C([H])C([H])=C([H])C=1[H])[C@@]2([H])C([H])([H])N(/C3=N/C(=C(/[F])C(=N3)C([H])([H])C([H])([H])[H])C([H])([H])[H])C4([H])[H])N([H])[H])C([H])([H])[H]	3.215	3.032
Tr25	O=C2N(C(=N[C@]4(C=1C([F])=C([H])C([F])=C([F])C=1[H])[C@@]2([H])C([H])([H])N(/C3=N/C(=C(/[F])C(=N3)OC([H])([H])[H])C([H])([H])[H])C4([H])[H])N([H])[H])C([H])([H])[H]	4.114	4.233
Tr26	O=C2N(C(=N[C@]5(C=1C([H])=C([H])C([H])=C([H])C=1[H])[C@@]2([H])C([H])([H])N(/C3=N/C(=C(/[Cl])C(=N3)[C@@]4([H])C([H])([H])C4([H])[H])C([H])([H])[H])C5([H])[H])N([H])[H])C([H])([H])[H]	3.027	3.062
Tr27	O=C2N(C(=N[C@]5(C=1C([H])=C([H])C([H])=C([H])C=1[H])[C@@]2([H])C([H])([H])N(/C3=N/C(=C(/[Cl])C(=N3)[C@@]4([H])C([H])([H])C4([H])[H])C([H])([H]	2.745	3.099

	)C([H])([H])[H])C5([H])[H])N([H])[H])C([H])([H])[H]		
Tr28	O=C2N(C(=N[C@]4(C=1C([H])=C([H])C([F])=C([H])C=1[H])[C@@]2([H])C([H])([H])N(/C3=N/C(=C(/[F])C(=N3)C([H])([H])[H])C([H])([H])[H])C4([H])[H])N([H])[H])C([H])([H])[H]	3.194	3.346
Tr29	O=C2N(C(=N[C@]4(C=1C([H])=C([F])C([H])=C([H])C=1[F])[C@@]2([H])C([H])([H])N(/C3=N/C(OC([H])([H])[H])=C([F])C(=N3)OC([H])([H])[H])C4([H])[H])N([H])[H])C([H])([H])[H]	4.252	4.082
Tr30	O=C2N(C(=N[C@]4(C=1C([H])=C([H])C([F])=C([H])C=1[F])[C@@]2([H])C([H])([H])N(/C3=N/C(OC([H])([H])[H])=C([F])C(=N3)OC([H])([H])[H])C4([H])[H])N([H])[H])C([H])([H])[H]	4.745	4.082
Tr31	O=C2N(C(=N[C@]4(C=1C([H])=C([H])C([F])=C([H])C=1[H])[C@@]2([H])C([H])([H])N(/C3=N/C(OC([H])([H])[H])=C([F])C(=N3)C([H])([H])C([H])([H])[H])C4([H])[H])N([H])[H])C([H])([H])[H]	4.215	3.806
Tr32	O=C2N(C(=N[C@]5(C=1C([F])=C([H])C([H])=C([F])C=1[H])[C@@]2([H])C([H])([H])N(/C3=N/C(OC([H])([H])[H])=C([F])C(=N3)[C@]4([H])C([H])([H])C4([H])[H])C5([H])[H])N([H])[H])C([H])([H])[H]	4.252	4.268
Tr33	O=C2N(C(=N[C@]5(C=1C([H])=C([F])C([H])=C([H])C=1[F])[C@@]2([H])C([H])([H])N(/C3=N/C(=C(/[F])C(=N3)[C@]4([H])C([H])([H])C4([H])[H])C([H])([H])[H])C5([H])[H])N([H])[H])C([H])([H])[H]	3.585	3.619
Tr34	O=C2N(C(=N[C@]5(C=1C([F])=C([H])C([F])=C([H])C=1[H])[C@@]2([H])C([H])([H])N(/C3=N/C(OC([H])([H])[H])=C([F])C(=N3)[C@]4([H])C([H])([H])C4([H])[H])C5([H])[H])N([H])[H])C([H])([H])[H]	4.569	4.268
Tr35	O=C2N(C(=N[C@]5(C=1C([F])=C([H])C([F])=C([H])C=1[H])[C@@]2([H])C([H])([H])N(/C3=N/C(OC([H])([H])[H])=C([Cl])C(=N3)[C@]4([H])C([H])([H])C4([H])[H])C5([H])[H])N([H])[H])C([H])([H])[H]	4.167	4.330
Tr36	[F]C=1C([H])=C([F])C(=C([H])C=1[H])[C@@]24N=C(N(C(=O)[C@]2([H])C([H])([H])N(/C3=N/C(=C(/[F])C(=N3)OC([H])([H])[H])C([F])([F])C([H])([H])[H])C4([H])[H])C([H])([H])[H])N([H])[H]	3.959	3.845
Tr37	O=C2N(C(=N[C@]4(C=1C([F])=C([H])C([H])=C([H])C=1[H])[C@@]2([H])C([H])([H])N(/C3=N/C(=C(/[F])C(=N3)OC([H])([H])[H])C([H])([H])[H])C4([H])[H])N([H])[H])C([H])([H])[H]	4.222	3.533
Tr38	O=C2N(C(=N[C@]4(C=1C([F])=C([Cl])C([F])=C([H])C=1[H])[C@@]2([H])C([H])([H])N(/C3=N/C(=C(/[F])C(=N3)OC([H])([H])[H])C([H])([H])[H])C4([H])[H])N([H])[H])C([H])([H])[H]	4.036	4.295
Tr39	O=C2N(C(=N[C@]4(C=1C([Cl])=C([H])C([F])=C([H])C=1[H])[C@@]2([H])C([H])([H])N(/C3=N/C(=C(/[F])C(=N3)OC([H])([H])[H])C([H])([H])[H])C4([H])[H])N([H])[H])C([H])([H])[H]	4.347	3.945
Tr40	O=C2N(C(=N[C@]5(C=1C([H])=C([H])C([F])=C([H])C=1[H])[C@@]2([H])C([H])([H])N(/C3=N/C(OC([H])([H])[H])=C([F])C(=N3)[C@]4([H])C([H])([H])C4([H])[H])C5([H])[H])N([H])[H])C([H])([H])[H]	4.319	3.918

Tr41	O=[S](=O)(C([H])([H])[C@]([H])(N([H])C(=O)OC(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])C(=O)C([H])([H])N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])(C([H])([H	1.947	2.559
Tr42	O=C(N([H])[C@@]([H])(C(=O)N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[	3.301	2.668
Tr43	O=C(OC(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])N([H])[C@@]([H])(C(=O)N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])	1.236	2.416
Tr44	O=C(N([H])[C@]([H])(C(=O)C([H])([H])[C@]([H])(C(=O)O[H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])([H])C([H])([H])C(=O)O[H])[C@@]([H])(N([H])C(=O)[C@@]([H])(C([H])([H])[C@]([H])(O[H])[C@@]([H])(N([H])C(=O)[C@@]([H])(N([H])C(=O)[C@@]([H])(N([H]	5.495	5.547
Tr45	O=C(N([H])[C@]([H])(C(=O)N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H	4.229	2.618
Tr46	O=[S](=O)(C([H])([H])[C@@]([H])(C(=O)N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])(C([H])([H])[H])C	4.027	3.555
Tr47	N#C/C1=C(\[F])C([H])=C([H])C(=C1[H])C=2[S]/C(=C(/[H])C=2[H])[C@@]35N=C(N(C(=O)[C@]3([H])C([H])([H])N(/C4=C(\[H])C([H])=C([F])C([H])=C4[H])C5([H])[H])C([H])([H])[H])N([H])[H]	2.879	2.896
Tr48	O=[S]3(=O)N(C=2C([H])=C(C([H])=C1/C(=C(/[H])N(C1=2)C([H])([H])C3([H])[H])C([H])([H])C([H])([H])[H])C(=O)N([H])[C@]([H])(C([H])([H])N([H])[C@]([H])(C(=O)N([H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])[C@@]([H])(O[H])C([H])([H])[H])C([H])([H])C4=C(	4.137	4.520
Tr49	O=[S]3(=O)N(C=2C([H])=C(C([H])=C1/C(=C(/[H])N(C1=2)C([H])([H])[C@]34C([H])([H])C4([H])[H])C([H])([H])C([H])([H])[H])C(=O)N([H])[C@]([H])(C([H])([H])N([H])[C@]([H])(C(=O)N([H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])[C@@]([H])(O[H])C([H])([H])[H]	4.143	4.331
Tr50	O=C(N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])([H])C(=O)O[H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])([H])[C@]([H])(N([H])C(=O)C([H])([H])C([H])(C([H])([H	1.770	1.859
Tr51	O=C(N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])([H])OC(=O)C([H])([H])[H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])([H])[C@]([H])(N([H])C(=O)C([H])([H])C([H]	1.569	2.189

Tr52	O=C(N([H])[C@@]([H])(C=1C([H])=C([H])C([H])=C([H])C=1[H])C([H])([H])[H])C2=C([H])C(=C([H])C(=C2[H])N(C([H])([H])[H])[S](=O)(=O)C([H])([H])[H])C(=O)N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])N([H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])C3=C([H])C	2.372	1.934
Tr53	O=C(N([H])[C@]([H])(C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])([H])[H])C2=C([H])C(=C([H])C(=C2[H])N(C([H])([H])[H])[S](=O)(=O)C([H])([H])[H])C(=O)N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])N([H])C([H])([H])C3=C([H])C(OC([H])([H])[H])=C([H])C([H])=C3[H])C(	2.210	1.820
Tr54	O=C(N([H])C([H])([H])C=1N=C(OC=1C([H])([H])[H])C([H])([H])[H])C2=C([H])C(=C([H])C(=C2[H])N(C([H])([H])[H])[S](=O)(=O)C([H])([H])[H])C(=O)N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])N([H])C([H])([H])C3=C([H])C(OC([H])([H])[H])=C([H])C([H])=C3[H])C([H])([H]	2.258	2.839
Tr55	O=C3O/C2=C(\OC([H])([H])C([H])=C(C([H])([H])C([H])([H])C([H])=C(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C=1OC([H])=C([H])C=1C([H])=C2C([H])=C3[H]	0.208	0.646
Tr56	O=C3OC=2C(OC([H])([H])[C@@]([H])(O[H])C(O[H])(C([H])([H])[H])C([H])([H])[H])=C1OC([H])=C([H])C1=C(OC([H])([H])[H])C=2C([H])=C3[H]	0.260	0.486
Tr57	O=C3OC=2C(OC([H])([H])[H])=C1OC([H])=C([H])C1=C(OC([H])([H])C([H])=C(C([H])([H])C([H])([H])C([H])=C(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C=2C([H])=C3[H]	0.863	0.677
Tr58	O=C(N([H])C(=NC([H])([H])C1=C([H])C([Cl])=C(C([Cl])=C1[H])N([H])C(=O)C([H])([H])N2C([H])([H])C([H])([H])C2([H])[H])N([H])[H])C=3C(=N[S]C=3C([H])([H])[H])C4=C([H])C([H])=C(OC([H])([H])[H])C([H])=C4[H]	4.398	4.548
Tr59	O=C(N([H])C(=NC([H])([H])C=1C([H])=C([H])C([H])=C2C=1C([H])=C([H])C([H])=C2[H])N([H])[H])C=3C(=NOC=3C([H])([H])[H])C4=C([H])C([H])=C(OC([H])([H])[H])C([H])=C4[H]	1.770	1.221
Tr60	O=C(N([H])C(=NC([H])([H])C1=C([H])C(=C([H])C([Cl])=C1[H])C([H])=C([H])C([H])([H])C([H])([H])O[H])N([H])[H])C=2C(=NOC=2C([H])([H])[H])C3=C([H])C([H])=C(OC([H])([H])[H])C([H])=C3[H]	2.854	2.644
Tr61	O=C(N([H])C(=NC([H])([H])C1=C([H])C([Cl])=C(C([Cl])=C1[H])N([H])[H])N([H])[H])C=2C(=NOC=2C([H])([H])[H])C3=C([H])C([H])=C(OC([H])([H])[H])C([H])=C3[H]	2.921	2.765
Tr62	O=C(N([H])C(=NC([H])([H])C1=C([H])C(=C([H])C([Cl])=C1[H])C([H])=C([H])C([H])([H])C([H])([H])C([H])([H])[H])N([H])[H])C=2C(=NOC=2C([H])([H])[H])C3=C([H])C([H])=C(OC([H])([H])[H])C([H])=C3[H]	2.071	2.180
Tr63	O=C(N([H])C(=NC([H])([H])C1=C([H])C(=C(C([Cl])=C1[H])N([H])C(=O)C([H])([H])N([H])C([H])([H])C2=C([H])C([H])=C([H])C([H])=C2[H])C([H])([H])[H])N([H])[H])C=3C(=N[S]C=3C([H])([H])[H])C4=C([H])C([H])=C(OC([H])([H])[H])C([H])=C4[H]	4.000	3.521
Tr64	O=C(N([H])C(=NC([H])([H])C1=C([H])C([Cl])=C([H])C([Cl])=C1[H])N([H])[H])C=2C(=NN([H])C=2C([H])([H])[H])C3=C([H])C([H])=C(OC([H])([H])[H])C([H])=C3[H]	2.678	2.215

Tr65	O=C(N([H])C(=NC([H])([H])C1=C([H])C([Cl])=C([H])C([Cl])=C1[H])N([H])[H])C=2C(=NOC=2C([H])([H])[H])C3=C([H])C([H])=C([F])C([H])=C3[H]	1.658	2.386
Tr66	O=C(N([H])C(=NC([H])([H])C1=C([H])C([Cl])=C([H])C([Cl])=C1[H])N([H])[H])C2=C(O/N=C2/C([H])([H])[H])C3=C([H])C([H])=C(OC([H])([H])[H])C([H])=C3[H]	2.066	1.054
Tr67	O=C(N([H])C(=NC([H])([H])C1=C([H])C=2C(C([H])=C1[H])=C([H])C([H])=C([H])C=2[H])N([H])[H])C=3C(=N[S]C=3C([H])([H])[H])C4=C([H])C([H])=C(OC([H])([H])[H])C([H])=C4[H]	2.060	2.632
Tr68	O=C(N([H])C(=NC([H])([H])C=1C([H])=C([H])C([H])=C2C=1C([H])=C([H])C([H])=C2[H])N([H])[H])C=3C(=NOC=3C([H])([H])[H])C4=C([H])C([H])=C([F])C([H])=C4[H]	1.745	1.347
Tr69	O=C(N([H])C(=NC([H])([H])C1=C([H])C(=C(C([Cl])=C1[H])N([H])C(=O)C([H])([H])N([H])C([H])([H])C([H])([H])[H])C([H])([H])[H])N([H])[H])C=2C(=N[S]C=2C([H])([H])[H])C3=C([H])C([H])=C(OC([H])([H])[H])C([H])=C3[H]	3.699	3.653
Tr70	O=C2C=1C(O[H])=C([H])C(O[H])=C([H])C=1O/C(=C2/O[H])C3=C([H])C([H])=C(O[H])C(O[H])=C3[H]	0.854	0.696
Tr71	[H]C=2C(O[H])=C1OC=6C(OC1=C3C=2OC=4/C3=C(/O[H])C([H])=C(O[H])C=4O/C5=C(\[H])C(O[H])=C([H])C(O[H])=C5[H])=C(O[H])C([H])=C(O[H])C=6OC=7C([H])=C(O[H])C([H])=C(O[H])C=7[H]	1.886	1.992
Tr72	O=C(/C1=C(\[H])C(=C([H])C(=C1[H])C(=O)N2[C@](H)(C([H])([H])C([H])([H])C2([H])[H])C([H])([H])OC([H])([H])[H])C([H])([H])[H])N([H])[C@]([H])([C@]([H])(O[H])[C@]3([H])N([H])C([H])([H])C([H])([H])N(C3([H])[H])[S](=O)(=O)[C@@]4([H])C([H])([H])C4([H])[H])C(	4.155	4.452
Tr73	[F]C=1C([H])=C(C([H])=C([F])C=1[H])C([H])([H])[C@]([H])(N([H])C(=O)C2=C([H])C(=C([H])C(=C2[H])C(=O)N3[C@]([H])(C([H])([H])C([H])([H])C3([H])[H])C([H])([H])OC([H])([H])[H])C([H])([H])[H])[C@]([H])(O[H])[C@]4([H])N([H])C([H])([H])C([H])([H])N(C4([H])[H])[	4.699	4.251
Tr74	[F]C=1C([H])=C(C([H])=C([F])C=1[H])C([H])([H])[C@]([H])(N([H])C(=O)C2=C([H])C(=C([H])C(=C2[H])C(=O)N3[C@]([H])(C([H])([H])C([H])([H])C3([H])[H])C([H])([H])OC([H])([H])[H])C([H])([H])[H])[C@]([H])(O[H])[C@]4([H])N([H])C([H])([H])C([H])([H])N(C4([H])[H])[	5.000	4.214
Tr75	O=C3N(C([H])([H])C([H])([H])C=4C([H])=C(OC=2C([H])=C([H])C=1N=C(N(C([H])([H])C=1C=2[H])[C@@]([H])(C([H])([H])C3([H])[H])C([H])(C([H])([H])[H])C([H])([H])[H])N([H])[H])C([H])=C([H])C=4[H])[C@]5([H])C([H])([H])C([H])([H])OC([H])([H])C5([H])[H]	3.658	3.393
Tr76	O=C3N(C([H])([H])C([H])([H])C=5C([H])=C(O/C2=C(\[H])C([H])=C1N=C(N(C([H])([H])C1=C2[H])[C@@]([H])(C([H])([H])C3([H])[H])[C@@]4([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C4([H])[H])N([H])[H])C([H])=C([H])C=5[H])[C@@]6([H])C([H])([H])C([H])([H])OC([	3.770	3.579
Tr77	O=C(N([H])[C@@]([H])(C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])([H])[H])C2=C([H])C(=C([H])C(=C2[H])N(C([H])([H])[H])[S](=O)(=O)C([H])([H])[H])C(=O)N([H])[C@]([H])(C([H])([H])C([H])([H])[C@@]([H])(OC([H])([H])[H])C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H]	2.886	3.251

Tr78	O=C(N([H])[C@@]([H])(C=1C([H])=C([H])C([H])=C([H])C=1[H])C([H])([H])[H])C=2C([H])=C(C([H])=C(C=2[H])N(C([H])([H])[H])[S](=O)(=O)C([H])([H])[H])C(=O)N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])[C@@]([H])(OC([H])([H])C3=C([H])C([H])=C([H])C([H])=C3[H])C(=O	3.699	4.228
Tr79	O=C(N([H])[C@@]([H])(C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])([H])[H])C=2C([H])=C(C([H])=C(C=2[H])N(C([H])([H])[H])[S](=O)(=O)C([H])([H])[H])C(=O)N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])[C@@]([H])(OC([H])([H])C([H])([H])OC([H])([H])[H])C(=O)N([H])[C	4.509	4.554
Tr80	O=C(N([H])[C@@]([H])(C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])([H])[H])C2=C([H])C(=C([H])C(=C2[H])N(C([H])([H])[H])[S](=O)(=O)C([H])([H])[H])C(=O)N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])[C@@]([H])(OC([H])([H])C([H])([H])C([H])([H])[H])C(=O)N([H])[C@]	4.523	3.437
Tr81	O=C(N([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)O[H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])([H])C([H])([H])C(=O)O[H])[C@@]([H])(N([H])C(=O)[C@@]([H])(C([H])([H])[C@]([H])(O[H])[C@@]([H])(N([H])C(=O)[C@@]([H])(N([H])C(=O)[C@@]([H])(N([H])C(=O	5.495	5.660
Tr82	O=C(OC(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])N([H])[C@]([H])(C(=O)N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])C([H])(C(=O)N([H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])(C	0.649	2.281
Tr83	O=C3N([H])[C@]([H])(C(=O)N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])N([H])C([H])([H])C1=C([H])C(=C([H])C([H])=C1[H])N(C([H])([H])[H])C([H])([H])[H])C([H])([H])C2=C([H])C([H])=C([H])C([H])=C2[H])C([H])([H])[C@@]3([H])C([H])([H])C4=C([H])C([H])=C([H])C([H]	1.522	1.049
Tr84	O=C3N([H])[C@]([H])(C(=O)N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])N([H])C([H])([H])C1=C([H])C(=C([H])C([H])=C1[H])N(C([H])([H])[H])C([H])([H])[H])C([H])([H])C2=C([H])C([H])=C([H])C([H])=C2[H])C([H])([H])N3C([H])([H])C4=C([H])C([H])=C([F])C([H])=C4[H]	2.087	2.011
Tr85	O=C3N([H])[C@]([H])(C(=O)N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])N([H])C([H])([H])C1=C([H])C(=C([H])C([H])=C1[H])N(C([H])([H])[H])C([H])([H])[H])C([H])([H])C2=C([H])C([H])=C([H])C([H])=C2[H])C([H])([H])N3C([H])([H])C4=C([H])C([H])=C(C([H])=C4[H])C([F]	1.305	2.829
Tr86	O=C3N([H])[C@](C(=O)N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])N([H])C([H])([H])C1=C([H])C(=C([H])C([H])=C1[H])N(C([H])([H])[H])C([H])([H])[H])C([H])([H])C2=C([H])C([H])=C([H])C([H])=C2[H])(C([H])([H])N3C([H])([H])C4=C([H])C([H])=C([H])C([H])=C4[H])C([H]	1.170	1.823
Tr87	O=C3N([H])[C@]([H])(C(=O)N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])N([H])C([H])([H])C1=C([H])C(=C([H])C([H])=C1[H])N(C([H])([H])[H])C([H])([H])[H])C([H])([H])C2=C([H])C([H])=C([H])C([H])=C2[H])C([H])([H])N3C([H])([H])C([H])([H])O/C4=C(\[H])C([H])=C([H])	1.454	1.979
Tr88	O=C3N([H])[C@]([H])(C(=O)N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])N([H])C([H])([H])C1=C([H])C(=C([H])C([H])=C1[H])N(C([H])([H])[H])C([H])([H])[H])C([H])([H])C2=C([H])C([H])=C([H])C([H])=C2[H])C([H])([H])N3/C4=C(\[H])C([Br])=C([H])C([Br])=C4[H]	1.456	1.956

Tr89	O=C3N([H])[C@]([H])(C(=O)N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])N([H])C([H])([H])C1=C([H])C(=C([H])C([H])=C1[H])N(C([H])([H])[H])C([H])([H])[H])C([H])([H])C2=C([H])C([H])=C([H])C([H])=C2[H])C([H])([H])N3[H]	0.721	1.197
Tr90	O=C3N([H])[C@]([H])(C(=O)N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])N([H])C([H])([H])C1=C([H])C(=C([H])C([H])=C1[H])N(C([H])([H])[H])C([H])([H])[H])C([H])([H])C2=C([H])C([H])=C([H])C([H])=C2[H])C([H])([H])N3C([H])([H])C([H])([H])C([H])([H])C([H])([H])[H]	0.398	1.636
Tr91	O=C1N(C(=N[C@@]1(C=2C([H])=C([H])C([H])=C([H])C=2[H])C3=C([H])C(=C([H])C([H])=C3[H])C=4/N=C(/[H])C([H])=NC=4[H])N([H])[H])C([H])([H])[H]	2.509	2.685
Tr92	O=C1N(C(=N[C@]1(C=2C([H])=C([H])C([H])=C([H])C=2[H])C3=C([H])C(=C([H])C([H])=C3[H])C4=C([H])C(OC([H])([H])[H])=C([H])C([H])=C4[H])N([H])[H])C([H])([H])[H]	3.097	1.864
Tr93	O=C1N(C(=N[C@]1(C=2C([H])=C([H])C([H])=C([H])C=2[H])C3=C([H])C(=C([H])C([H])=C3[H])C4=C([H])N=C([H])C([Cl])=C4[H])N([H])[H])C([H])([H])[H]	3.046	2.197
Tr94	O=C1N(C(=N[C@]1(C=2C([H])=C([H])C([H])=C([H])C=2[H])C3=C([H])C(=C([H])C([H])=C3[H])C4=C([H])N=C([H])C([H])=C4[H])N([H])[H])C([H])([H])[H]	2.959	1.747
Tr95	O=C1N(C(=N[C@@]1(C=2C([H])=C([H])C([H])=C([H])C=2[H])C3=C([H])C([Cl])=C([H])C([H])=C3[H])N([H])[H])C([H])([H])[H]	2.523	2.630
Tr96	O=C1N(C(=N[C@@]1(C=2C([H])=C([H])C([H])=C([H])C=2[H])C3=C([H])C(=C([H])C([H])=C3[H])C4=C([H])N=C([H])C([H])=C4[H])N([H])[H])C([H])([H])[H]	1.770	2.515
Tr97	O=C1N(C(=N[C@@]1(/C2=C(\[H])C(=C([H])C([H])=C2[H])C3=C([H])N=C([H])C([F])=C3[H])[C@@]4([H])C([H])([H])C4([H])[H])N([H])[H])C([H])([H])[H]	2.796	2.135
Tr98	O=C1N(C(=N[C@]1(/C2=C(\[H])C([H])=C([H])C([H])=C2[H])C3=C([H])C(=C([H])C([H])=C3[H])C4=C([H])C([H])=C([H])C([H])=C4[H])N([H])[H])C([H])([H])[H]	1.481	1.335
Tr99	O=C1N(C(=N[C@]1(C=2C([H])=C([H])C([H])=C([H])C=2[H])C3=C([H])C(=C([H])C([H])=C3[H])C4=C([H])C([H])=C(OC([H])([H])[H])C([H])=C4[H])N([H])[H])C([H])([H])[H]	1.420	1.864
Tr100	O=C3N([H])[C@]([H])(C(=O)N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])N([H])C([H])([H])C1=C([H])C(=C([H])C([H])=C1[H])N(C([H])([H])[H])C([H])([H])[H])C([H])([H])C2=C([H])C([H])=C([H])C([H])=C2[H])C([H])([H])N3C([H])([H])C4=C([H])C([H])=C([H])C([H])=C4[H]	2.547	1.786
Tr101	O=C1N(C(=N[C@@]1(/C2=C(\[H])C([H])=C([H])C([H])=C2[H])C3=C([H])C(C#N)=C([H])C([H])=C3[H])N([H])[H])C([H])([H])[H]	2.432	2.299
Tr102	O=C1N(C(=N[C@]1(C=2C([H])=C([H])C([H])=C([H])C=2[H])C3=C([H])C(=C([H])C([H])=C3[H])C4=NC([H])=C([H])C([H])=C4[H])N([H])[H])C([H])([H])[H]	1.721	2.184
Tr103	O=C(N([C@@]1([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C1([H])[H])C([H])([H])[H])C([H])([H])C([H])([H])[C@]([H])(N4C(=N/C3=C(\[H])C([H])=C(O/C2=C(\[H])C([H])=C([H])C([H])=C2[H])C([H])=C3C4([H])[H])N([H])[H])C5=C([H])C([H])=C([H])C([H])=C5[H]	2.785	2.388
Tr104	O=C(N([C@@]1([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C1([H])[H])C([	3.638	3.271

	H])([H])C2=C([H])N([H])N=C2[H])C([H])([H])C([H])([H])[C@]([H])(N5C(=NC=4C([H])=C([H])C(O/C3=C(\[H])C([H])=C([H])C([H])=C3[H])=C([H])C=4C5([H])[H])N([H])[H])[C@@]6([H])C([H])([H])		
Tr105	O=C(N([C@@]1([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C1([H])[H])C([H])([H])C2=C([H])N(/N=C2/[H])C([H])([H])[H])C([H])([H])C([H])([H])[C@]([H])(N5C(=NC=4C([H])=C([H])C(O/C3=C(\[H])C([H])=C([H])C([H])=C3[H])=C([H])C=4C5([H])[H])N([H])[H])[C@@]6([H	3.959	3.583
Tr106	O=C(N([C@@]1([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C1([H])[H])C([H])([H])C([H])([H])C=2N=C([S]C=2[H])C([H])([H])[H])C([H])([H])C([H])([H])[C@]([H])(N5C(=NC=4C([H])=C([H])C(O/C3=C(\[H])C([H])=C([H])C([H])=C3[H])=C([H])C=4C5([H])[H])N([H])[H])[C	2.975	3.351
Tr107	O=C(N([C@@]1([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C1([H])[H])[C@@]([H])(C=2N=C([S]C=2[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])([H])[C@]([H])(N5C(=NC=4C([H])=C([H])C(O/C3=C(\[H])C([H])=C([H])C([H])=C3[H])=C([H])C=4C5([H])[H])N([H])[H	2.983	3.308
Tr108	O=C(N([C@@]1([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C1([H])[H])C([H])([H])C=2N=C([S]C=2[H])C([H])([H])[H])C([H])([H])C([H])([H])[C@]([H])(N5C(=NC=4C([H])=C([H])C(O/C3=C(\[H])C([H])=C([H])C([H])=C3[H])=C([H])C=4C5([H])[H])N([H])[H])[C@@]6([H])C(	3.102	3.315
Tr109	O=C(OC([H])([H])[C@]([H])(N3C(=N/C2=C(\[H])C([H])=C(O/C1=C(\[H])C([H])=C([H])C([H])=C1[H])C([H])=C2C3([H])[H])N([H])[H])[C@]4([H])C([H])([H])OC([H])([H])C([H])([H])C4([H])[H])N([C@@]5([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C5([H])[H])C([H])([H]	2.983	3.667
Tr110	O=C(OC([H])([H])[C@]([H])(N3C(=N/C2=C(\[H])C([H])=C(O/C1=C(\[H])C([H])=C([H])C([H])=C1[H])C([H])=C2C3([H])[H])N([H])[H])C4=C([H])C([H])=C([H])C([H])=C4[H])N([C@@]5([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C5([H])[H])C([H])([H])[H]	2.106	2.807
Tr111	N#CC=1C([H])=C(C([H])=C([H])C=1[H])C=2[S]C([H])=C(C=2[H])[C@]3(N=C(N(C(=O)C3([H])[H])C([H])([H])[H])N([H])[H])C([H])([H])[H]	2.678	2.504
Tr112	N#CC=1C([H])=C(C([H])=C([H])C=1[H])C=2[S]/C(=C(/[H])C=2[H])[C@]3(N=C(N(C(=O)C3([H])[H])C([H])([H])[H])N([H])[H])C([H])([H])[H]	3.056	2.986
Tr113	O=C3N(C(=N[C@](C=1C([H])=C([S]C=1[H])C2=C([H])C(C#CC([H])([H])[H])=C([H])N=C2[H])(C3([H])[H])C([H])([H])[H])N([H])[H])C([H])([H])[H]	3.328	2.672
Tr114	O=C4N(C(=N[C@@](/C1=C(\[H])C([H])=C([H])C(=C1[H])C2=C([H])N=C([H])C([H])=C2[H])(C3=C([H])C([H])=C([H])C([H])=C3[H])C4([H])[H])N([H])[H])C([H])([H])[H]	0.357	0.772
Tr115	O=C3N(C(=N[C@](C=2[S]C(C=1C([H])=C(C#CC([H])([H])[H])C([H])=NC=1[H])=C([H])C=2[Cl])(C3([H])[H])C([H])([H])[H])N([H])[H])C([H])([H])[H]	4.770	4.708
Tr116	O=C(O[C@]2([H])[C@@]([H])(OC1=C(C(O[H])=C([H])C(O[H])=C1[H])C2([H])[H])C=3C([H])=C(O[H])C(O[H])=C(O[H])C=3[H])C=4C([H])=C(O[H])C(O[H])=C(O[H])C=4[H]	2.678	2.978

Tr117	O=C(N([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])N([H])C=2C=1C([H])=C([H])C([H])=C([H])C=1N=C3C=2C([H])([H])C([H])([H])C([H])([H])C3([H])[H])C=4OC=5C(C(=O)C=4[H])=C(OC([H])([H])[H])C	2.208	2.264
Tr118	O=C(N([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])N([H])C2=C1C([H])=C([H])C([H])=C([H])C1=NC3=C2C([H])([H])C([H])([H])C([H])([H])C3([H])[H])C=4OC=5C(C(=O)C=4[H])=C(O[H])C([H])=C(OC([H	2.071	1.860
Tr119	O=C(N([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])N([H])C=2C=1C([H])=C([H])C([H])=C([H])C=1N=C3C=2C([H])([H])C([H])([H])C([H])([H])C3([H])[H])C=4OC=5C(C(=O)C=4[H])=C([H])C(OC([H])([H]	2.056	2.264
Tr120	O=C2N(/C(=N\[H])N([H])[C@]4(C=1C([F])=C([H])C([F])=C([H])C=1[H])[C@@]2([H])C([H])([H])N(/C3=N/C(OC([H])([H])[H])=C([F])C(=N3)C([H])([H])[H])C4([H])[H])C([H])([H])[H]	4.328	4.088
Tr121	O=C2N(/C(=N\[H])N([H])[C@]4(C=1C([F])=C([H])C([H])=C([Cl])C=1[H])[C@@]2([H])C([H])([H])N(/C3=N/C(OC([H])([H])[H])=C([F])C(=N3)C([H])([H])[H])C4([H])[H])C([H])([H])[H]	3.886	4.151
Tr122	O=C(N([H])C3=C([H])C([H])=C2OC([C@]4([C@@]1(N=C(OC1([H])[H])N([H])[H])C2=C3[H])C([H])([H])OC4([H])[H])(C([H])([H])[H])C([H])([H])[H])C=5/N=C(/[H])C([Cl])=C([H])C=5[H]	3.418	3.050
Tr123	O=C(N([H])C3=C([H])C([H])=C2OC([H])([H])[C@]4([C@@]1(N=C(OC1([H])[H])N([H])[H])C2=C3[H])C([H])([H])C4([H])[H])C=5/N=C(/[H])C([Cl])=C([H])C=5[F]	2.620	2.584
Tr124	O=C(N([H])C3=C([H])C([H])=C2OC([H])([H])[C@]4([C@@]1(N=C(OC1([H])[H])N([H])[H])C2=C3[H])C([H])([H])C4([H])[H])C=5/N=C(/[H])C([Cl])=C([H])C=5[H]	2.423	2.746
Tr125	[H]/C4=C(/C([H])=C1C(OC([C@]3([C@@]12N=C(OC2([H])[H])N([H])[H])C([H])([H])OC3([H])[H])(C([H])([H])[H])C([H])([H])[H])=C4[H])C5=C([H])N=C([H])C(OC([H])([H])[H])=C5[H]	2.593	2.733
Tr126	[H]/C4=C(/C([H])=C1C(O[C@]([H])([C@]3([C@]12N=C(OC2([H])[H])N([H])[H])C([H])([H])OC3([H])[H])C([H])([H])C([H])([H])[H])=C4[H])C5=C([H])N=C([H])C(C#CC([H])([H])[H])=C5[H]	2.971	2.777
Tr127	[H]/C5=C(/C([H])=C1C(O[C@@]4([C@]3([C@@]12N=C(OC2([H])[H])N([H])[H])C([H])([H])OC3([H])[H])C([H])([H])C([H])([H])C4([H])[H])=C5[H])C6=C([H])N=C([H])C(C#CC([H])([H])[H])=C6[H]	2.921	4.001
Tr128	[H]/C4=C(/C([H])=C1C(OC([C@]3([C@@]12N=C(OC2([H])[H])N([H])[H])C([H])([H])OC3([H])[H])(C([H])([H])[H])C([H])([H])[H])=C4[H])C5=C([H])N=C([H])C(C#CC([H])([H])[H])=C5[H]	3.044	3.664
Tr129	[Cl]C=5C([H])=C(/C3=C(\[H])C([H])=C2OC([C@]4([C@@]1(N=C(OC1([H])[H])N([H])[H])C2=C3[H])C([H])([H])OC4([H])[H])(C([H])([H])[H])C([H])([H])[H])C([H])=C([F])C=5[H]	2.726	2.396

Tr130	O=C(N([H])C3=C([H])C([H])=C2OC([H])([H])[C@]4([C@@]1(N=C(OC1([H])[H])N([H])[H])C2=C3[H])C([H])([H])C4([H])[H])C5=NC([H])=C([Br])C([H])=N5	2.206	2.352
Tr131	O=C(N([H])C3=C([H])C([H])=C2OC([C@]4([C@@]1(N=C(OC1([H])[H])N([H])[H])C2=C3[H])C([H])([H])OC4([H])[H])(C([H])([H])[H])C([H])([H])[H])C5=NC([H])=C([Cl])C([H])=C5C([H])([H])[H]	3.190	3.293
Tr132	O=C(N([H])C3=C([H])C([H])=C2OC([H])([H])[C@]4([C@@]1(N=C(OC1([H])[H])N([H])[H])C2=C3[H])C([H])([H])C4([H])[H])C=5/N=C(/[H])C(C#N)=C([H])C=5[H]	2.466	2.846
Tr133	O=C(N([H])C3=C([H])C([H])=C2OC([C@]4([C@@]1(N=C(OC1([H])[H])N([H])[H])C2=C3[H])C([H])([H])OC4([H])[H])(C([H])([H])[H])C([H])([H])[H])C=5/N=C(/[H])C(C#N)=C([H])C=5[H]	3.143	3.150
Tr134	[H]/C5=C(/C([H])=C1C(O[C@]([H])([C@]3([C@]12N=C(OC2([H])[H])N([H])[H])C([H])([H])OC3([H])[H])C([H])([H])C4=C([H])C([H])=C([H])C([H])=C4[H])=C5[H])C6=C([H])N=C([H])N=C6[H]	3.036	2.277
Tr135	[H]/C5=C(/C([H])=C1C(O[C@]([H])([C@]3([C@]12N=C(OC2([H])[H])N([H])[H])C([H])([H])OC3([H])[H])C([H])([H])C4=C([H])C([H])=C([H])C([H])=C4[H])=C5[H])C6=C([H])N=C([H])C(C#CC([H])([H])[H])=C6[H]	3.148	3.325
Tr136	O=C(N([H])C3=C([H])C([H])=C2OC([C@]4([C@@]1(N=C(OC1([H])[H])N([H])[H])C2=C3[H])C([H])([H])OC4([H])[H])(C([H])([H])[H])C([H])([H])[H])C=5/N=C(/[H])C([Br])=C([H])C=5[H]	3.991	2.644
Tr137	O=C(N([H])C3=C([H])C([H])=C2OC([C@]4([C@@]1(N=C(OC1([H])[H])N([H])[H])C2=C3[H])C([H])([H])C4([H])[H])(C([H])([H])[H])C([H])([H])[H])C5=NC([H])=C([Cl])C([H])=C5[H]	3.423	3.188
Tr138	O=C(N([H])C3=C([H])C([H])=C2OC([C@]4([C@@]1(N=C(OC1([H])[H])N([H])[H])C2=C3[H])C([H])([H])C4([H])[H])(C([H])([H])[H])C([H])([H])[H])C5=NC([H])=C([F])C([H])=C5[H]	3.039	2.963
Tr139	O=C(N([H])C3=C([H])C([H])=C2OC([C@]4([C@@]1(N=C(OC1([H])[H])N([H])[H])C2=C3[H])C([H])([H])OC4([H])[H])(C([H])([H])[H])C([H])([H])[H])C=5/N=C(/[H])C(=NC=5[H])OC([H])([H])[H]	3.101	3.481
Tr140	O=C(/C1=N/C([H])=C([Cl])C([H])=C1[H])N([H])C2=C([H])C(=C([F])C([H])=C2[H])[C@]3(N([H])C(=N[H])N([S](=O)(=O)C3([H])[H])C([H])([H])[H])C([H])([H])[H]	5.023	4.097
Tr141	O=C(/C1=N/C([H])=C(C([H])=C1[H])C([F])([F])[F])N([H])C2=C([H])C(=C([F])C([H])=C2[H])[C@]3(N([H])C(=N[H])N([S](=O)(=O)C3([H])[H])C([H])([H])[H])C([H])([H])[H]	4.899	5.095
Tr142	O=C(/C1=N/C([H])=C(/N=C1/[H])C([H])([H])[H])N([H])C2=C([H])C(=C([F])C([H])=C2[H])[C@]3(N([H])C(=N[H])N([S](=O)(=O)C3([H])[H])C([H])([H])[H])C([H])([H])[H]	4.000	4.340
Tr143	O=C(/C1=N/C([H])=C(/N=C1/[H])OC([H])([H])[H])N([H])C2=C([H])C(=C([F])C([F])=C2[H])[C@]3(N([H])C(=N[H])N([S](=O)(=O)C3([H])[H])C([H])([H])[H])C([H])([H])[H]	4.979	5.058

Tr144	O=[S]3(=O)N(/C(=N\[H])N([H])[C@](C=1[S]C([H])=C(C=1[H])C2=C([H])C([H])=C([F])C(C#N)=C2[H])(C3([H])[H])C([H])([H])[H])C([H])([H])[H]	3.337	3.223
Tr145	O=[S]3(=O)N(/C(=N\[H])N([H])[C@](C=1[S]/C(=C(/[H])C=1[Cl])C2=C([H])N=C([H])C(C#CC([H])([H])[H])=C2[H])(C3([H])[H])C([H])([H])[H])C([H])([H])[H]	4.622	4.353
Tr146	O=C(/C1=N/C([H])=C(/N=C1/[H])OC([H])([H])[H])N([H])C2=C([H])C(=C([F])C([H])=C2[H])[C@]3(N([H])C(=N[H])N([S](=O)(=O)C3([H])[H])C([H])([H])[H])C([H])([H])[H]	4.785	4.708
Tr147	[F]C=1C([H])=C(C([H])=C([F])C=1[H])C([H])([H])[C@]([H])(N([H])C(=O)C2=C([H])C(=C([H])C(=C2[H])C([H])([H])[H])C(=O)N(C([H])([H])C([H])([H])C([H])([H])[H])C([H])([H])C([H])([H])C([H])([H])[H])[C@]([H])(O[H])[C@]3([H])N([H])C([H])([H])C([H])([H])N(C3([H])[	2.509	3.632
Tr148	[F]C=1C([H])=C(C([H])=C([F])C=1[H])C([H])([H])[C@]([H])(N([H])C(=O)C2=C([H])C(=C([H])C(=C2[H])C([H])([H])[H])C(=O)N(C([H])([H])C([H])([H])C([H])([H])[H])C([H])([H])C([H])([H])C([H])([H])[H])[C@]([H])(O[H])[C@]3([H])N([H])C([H])([H])C([H])([H])N(C3([H])[	2.921	3.082
Tr149	[F]C=1C([H])=C(C([H])=C([F])C=1[H])C([H])([H])[C@]([H])(N([H])C(=O)C2=C([H])C(=C([H])C(=C2[H])C([H])([H])[H])C(=O)N(C([H])([H])C([H])([H])C([H])([H])[H])C([H])([H])C([H])([H])C([H])([H])[H])[C@]([H])(O[H])[C@]3([H])N([H])C([H])([H])C([H])([H])N(C3([H])[	2.398	3.082
Tr150	[F]C=1C([H])=C(C([H])=C([F])C=1[H])C([H])([H])[C@]([H])(N([H])C(=O)C2=C([H])C(=C([H])C(=C2[H])C([H])([H])[H])C(=O)N(C([H])([H])C([H])([H])C([H])([H])[H])C([H])([H])C([H])([H])C([H])([H])[H])[C@]([H])(O[H])[C@]3([H])N([H])C([H])([H])C([H])([H])N(C3([H])[	2.013	2.912
Tr151	O=C(N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])[C@@]([H])(N([H]	5.097	4.235
Tr152	O=C(N([H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])[C@]([H])(OC([H])([H])[H])C([H])([H])[C@]([H])(O[H])[C@@]([H])(N([H])C(=O)C2=C([H])C(=C([H])C(=C2[H])C(=O)N([H])[C@@]([H])(C3=C([H])C([H])=C([H])C([H])=C3[H])C([H])([H])[H])N(C([H])([H])[S](=O)(=O)	1.854	2.675
Tr153	O=C(N([H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])[C@]([H])(OC([H])([H])[H])C([H])([H])[C@]([H])(O[H])[C@@]([H])(N([H])C(=O)C1=C([H])C(=C([H])C(=C1[H])C(=O)N([H])[C@@]([H])(C2=C([H])C([H])=C([H])C([H])=C2[H])C([H])([H])[H])N(C([H])([H])[S](=O)(=	2.398	2.712
Tr154	O=C(N([H])[C@]([H])(C(=O)N([H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])(C([H])([H])[H])C([H])([H])[H])[C@]([H])(OC([H])([H])[H])C([H])([H])[C@]([H])(O[H])[C@@]([H])(N([H])C(=O)C2=C([H])C(=C([H])C(=C2[H])C(=O)N([H])[C@@]([H])(C3=C([H])C([H])=	4.046	2.750
Tr155	O=C(N([H])[C@]([H])(C(=O)N([H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])(C([H])([H])[H])C([H])([H])[H])[C@]([H])(OC([H])([H])[H])C([H])([H])[C@]([H])(O[H])[C@@]([H])(N([H])C(=O)C2=C([H])C(=C([H])C(=C2[H])C(=O)N([H])[C@@]([H])(C3=C([H])C([H])=	3.125	2.794

Tr156	O=C(N([H])[C@]([H])(C(=O)N([H])C([H])([H])C=1C([H])=C([H])C([H])=C([H])C=1[H])C([H])(C([H])([H])[H])C([H])([H])[H])[C@]([H])(OC([H])([H])[H])C([H])([H])[C@]([H])(O[H])[C@@]([H])(N([H])C(=O)C2=C([H])C(=C([H])C(=C2[H])C(=O)N([H])[C@@]([H])(C3=C([H])C([H])	3.097	3.773
Tr157	O=C(N([H])[C@]([H])(C(=O)N([H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])(C([H])([H])[H])C([H])([H])[H])[C@]([H])(OC([H])([H])[H])C([H])([H])[C@]([H])(O[H])[C@@]([H])(N([H])C(=O)C2=C([H])C(=C([H])C(=C2[H])C(=O)N([H])[C@@]([H])(C3=C([H])C([H])=	3.222	3.042
Tr158	O=C(N([H])C1=C([H])C([H])=C([F])C([H])=C1[H])[C@]([H])(OC([H])([H])[H])C([H])([H])[C@]([H])(O[H])[C@@]([H])(N([H])C(=O)C2=C([H])C(=C([H])C(=C2[H])C(=O)N([H])[C@@]([H])(C3=C([H])C([H])=C([H])C([H])=C3[H])C([H])([H])[H])N(C([H])([H])[S](=O)(=O)C([H])([H])	3.000	2.988
Tr159	O=C(N([H])C1=C([H])C(=C(C([H])=C1[H])N(C([H])([H])[H])C([H])([H])[H])C(=O)N([H])C([H])([H])C([H])([H])C([H])([H])OC([H])([H])C([H])([H])[H])N([H])C2=C([H])C([Cl])=C([H])C([H])=C2[H]	1.009	1.393
Tr160	O=C(N([H])[C@]([H])(C(=O)N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)O[H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])([H])C([H])([H])C(=O)O[H])C([H])([H])[H])C([H])([H]	4.000	4.545
Tr161	O=C(N([H])[C@]([H])(C(=O)N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)O[H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])([H])C([H])([H])C(=O)O[H])C([H])([H])[H])C([H])([H]	3.167	3.262
Tr162	O=C(N([H])C(=NC([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])N([H])[H])C=2C(=NOC=2C([H])([H])[H])C3=C([H])C([H])=C(OC([H])([H])[H])C([H])=C3[H]	1.398	1.566
Tr163	O=C(N([H])C(=NC([H])([H])C1=C([H])C([Cl])=C([Cl])C([H])=C1[H])N([H])[H])C=2C(=NOC=2C([H])([H])[H])C3=C([H])C([H])=C([F])C([H])=C3[H]	1.620	2.386
Tr164	O=C(N([H])[C@]([H])(C(=O)N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H]	5.602	4.260
Tr165	O=C(N([H])[C@]([H])(C(=O)N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H]	3.959	4.297
Tr166	O=C(N([H])[C@]([H])(C(=O)N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H]	3.538	4.308
Tr167	O=[S](=O)(C([H])([H])[C@@]([H])(C(=O)N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])(C([H])([H])[H])C	1.947	2.697

Tr168	O=C(N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])[C@@]([H])(N([H])C(	1.504	2.056
Tr169	O=C(N([H])[C@@]([H])(C(=O)N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[	4.602	2.705
Tr170	O=C1N(/C(=N\[H])N([H])[C@]1(C([H])([H])C([H])([H])[C@@]2([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C2([H])[H])C([H])([H])[C@]4([H])C([H])([H])[C@]([H])(N([H])C(=O)C3=C([H])C([H])=NC([H])=C3[H])C([H])([H])C([H])([H])C4([H])[H])C([H])([H])[H]	3.409	3.300
Tr171	O=C1N(/C(=N\[H])N([H])[C@]1(C([H])([H])C([H])([H])[C@@]2([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C2([H])[H])C([H])([H])[C@]4([H])C([H])([H])[C@]([H])(N([H])[C@@]3([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C3([H])[H])C([H])([H])C([H])([H])C	3.638	3.178
Tr172	O=C1N(/C(=N\[H])N([H])[C@]1(C([H])([H])C([H])([H])[C@@]2([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C2([H])[H])C([H])([H])[C@]4([H])C([H])([H])[C@]([H])(N([H])[C@]3([H])C([H])([H])C([H])([H])C([H])([H])C3([H])[H])C([H])([H])C4([H])[H])C(	3.367	3.160
Tr173	O=C(N([H])[C@]([H])(C(=O)N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H]	3.398	3.067
Tr174	O=C(N([H])[C@]([H])(C(=O)N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H]	1.785	3.167
Tr175	O=C(N([H])[C@]([H])(C(=O)N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H]	3.201	3.103
Tr176	O=C(N([H])[C@]([H])(C(=O)N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H]	2.697	3.117
Tr177	O=C(N([H])[C@]([H])(C(=O)N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H]	3.194	2.633
Tr178	O=[S](=O)(C([H])([H])[C@]([H])(N([H])C(=O)[C@]([H])(C([H])([H])N1N=C(C([H])=C1C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C(=O)N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])[C@]([H])([H])C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C([H])(C([H])([H])[H])C([H])(	2.717	3.325

Tr179	O=C(N([H])[C@]([H])(C(=O)N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H]	3.495	3.455
Tr180	O=C(N([H])[C@]([H])(C(=O)N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H]	3.770	3.491
Tr181	O=C1N(/C(=N\[H])N([H])[C@]1(C([H])([H])C([H])([H])[C@@]2([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C2([H])[H])C([H])([H])[C@@]4([H])C([H])([H])N(C(=O)C([H])([H])[C@]3([H])C([H])([H])C([H])([H])C([H])([H])C3([H])[H])C([H])([H])C4([H])[H])C([H])([H]	3.432	3.124
Tr182	O=C1N(/C(=N/[H])N([H])[C@]1(C([H])([H])C([H])([H])[C@@]2([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C2([H])[H])C([H])([H])[C@]3([H])C([H])([H])N(C(=O)C([H])([H])C([H])([H])C([H])([H])C([H])([H])[H])C([H])([H])C([H])([H])C3([H])[H])C([H])([H])[H]	3.495	3.287
Tr183	O=[S](=O)(N3C([H])([H])[C@@]([H])(C([H])([H])[C@]1(N([H])C(=N[H])N(C1=O)C([H])([H])[H])C([H])([H])C([H])([H])[C@@]2([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C2([H])[H])C([H])([H])C([H])([H])C3([H])[H])C([H])([H])C([H])([H])C([H])([H])[	3.201	3.474
Tr184	O=C1N(/C(=N\[H])N([H])[C@]1(C([H])([H])C([H])([H])[C@@]2([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C2([H])[H])C([H])([H])[C@]5([H])C([H])([H])[C@]([H])(N([H])C(=O)N([H])C3=NC=4C(/N=C3/[H])=C([H])C([H])=C([H])C=4[H])C([H])([H])C([H])([H])C5([H])[H]	3.854	3.985
Tr185	O=C1N(/C(=N\[H])N([H])[C@]1(C([H])([H])C([H])([H])[C@@]2([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C2([H])[H])C([H])([H])[C@]4([H])C([H])([H])[C@]([H])(N([H])C(=O)N([H])[C@@]3([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C3([H])[H])C([H])([H])C	2.860	3.727
Tr186	O=C1N(/C(=N/[H])N([H])[C@]1(C([H])([H])C([H])([H])[C@@]2([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C2([H])[H])C([H])([H])[C@]4([H])C([H])([H])[C@]([H])(N([H])C(=O)N([H])C3=C(OC([H])([H])[H])C([H])=C([H])C([H])=C3[H])C([H])([H])C([H])([H])C4([H])[H	2.559	3.179
Tr187	O=C1N(/C(=N\[H])N([H])[C@]1(C([H])([H])C([H])([H])[C@]2([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C2([H])[H])C([H])([H])[C@]4([H])C([H])([H])[C@]([H])(N([H])C(=O)N([H])C3=C([H])C([H])=C([Cl])C([H])=C3[H])C([H])([H])C([H])([H])C4([H])[H])C([H])([H]	5.000	4.123
Tr188	O=C1N(/C(=N\[H])N([H])[C@]1(C([H])([H])C([H])([H])[C@@]2([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C2([H])[H])C([H])([H])[C@]4([H])C([H])([H])[C@]([H])(N([H])C(=O)C([H])([H])C3=C([H])C([H])=C([H])C([H])=C3[H])C([H])([H])C([H])([H])C4([H])[H])C([H]	2.233	2.792
Tr189	O=C1N(/C(=N\[H])N([H])[C@@]1(C([H])([H])[C@@]2([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C2([H])[H])C([H])([H])C([H])([H])[C@@]3([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C3([H])[H])C([H])([H])C4=C([H])C([H])=C(C([H])=C4[H])C([H])([H])N5C(=O	3.569	4.181

Tr190	O=C1N(/C(=N/[H])N([H])[C@]1(C([H])([H])C([H])([H])[C@@]2([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C2([H])[H])C([H])([H])[C@@]3([H])C([H])([H])N(C(=O)C([H])([H])C([H])([H])C([H])([H])C([H])([H])[H])C([H])([H])C([H])([H])C3([H])[H])C([H])([H])[H]	3.770	3.269
Tr191	O=C1N(/C(=N\[H])N([H])[C@]1(C([H])([H])C([H])([H])[C@@]2([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C2([H])[H])C([H])([H])[C@]4([H])C([H])([H])N(C(=O)C([H])([H])[C@]3([H])C([H])([H])C([H])([H])C([H])([H])C3([H])[H])C([H])([H])C([H])([H])C4([H])[H])	3.013	3.754
Tr192	O=C1N(/C(=N\[H])N([H])[C@]1(C([H])([H])C([H])([H])[C@@]2([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C2([H])[H])C([H])([H])[C@]3([H])C([H])([H])N(C(=O)OC(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])([H])C3([H])[H])C([H])([H])[H]	3.538	3.231
Tr193	O=[S]2(=O)N(/C(=N/[H])N([H])[C@]4(/C1=C(\[H])C([F])=C([F])C([H])=C1[F])[C@@]2([H])C([H])([H])N(/C3=N/C(=C(/[F])C(=N3)OC([H])([H])[H])C([H])([H])[H])C4([H])[H])C([H])([H])[H]	3.495	3.809
Tr194	O=[S]2(=O)N(/C(=N/[H])N([H])[C@]4(/C1=C(\[H])C([H])=C([F])C([H])=C1[F])[C@]2([H])C([H])([H])N(/C3=N/C(=C(/[F])C(=N3)OC([H])([H])[H])C([H])([H])[H])C4([H])[H])C([H])([H])[H]	3.523	4.227
Tr195	O=[S]2(=O)N(/C(=N/[H])N([H])[C@]4(/C1=C(\[H])C([F])=C([H])C([H])=C1[F])[C@@]2([H])C([H])([H])N(/C3=N/C(OC([H])([H])[H])=C([H])C(=C3[H])C([H])([H])OC([H])([H])[H])C4([H])[H])C([H])([H])[H]	4.000	3.250
Tr196	O=[S]2(=O)N(/C(=N/[H])N([H])[C@@]4(/C1=C(\[H])C([H])=C([H])C([H])=C1[H])[C@]2([H])C([H])([H])N(/C3=N/C(OC([H])([H])[H])=C([H])C(=C3[H])C([H])([H])OC([H])([H])[H])C4([H])[H])C([H])([H])[H]	3.569	3.199
Tr197	O=[S]2(=O)N(/C(=N/[H])N([H])[C@@]4(/C1=C(\[H])C([H])=C([H])C([H])=C1[H])[C@]2([H])C([H])([H])N(/C3=N/C(OC([H])([H])[H])=C([F])C(=N3)OC([H])([H])[H])C4([H])[H])C([H])([H])[H]	3.523	3.583
Tr198	O=[S]2(=O)N(/C(=N/[H])N([H])[C@@]4(/C1=C(\[H])C([H])=C([H])C([H])=C1[H])[C@]2([H])C([H])([H])N(/C3=N/C(OC([H])([H])[H])=C([H])C([H])=C3[H])C4([H])[H])C([H])([H])[H]	3.066	2.664
Tr199	O=[S]2(=O)N(/C(=N/[H])N([H])[C@@]5(/C1=C(\[H])C([H])=C([H])C([H])=C1[H])[C@]2([H])C([H])([H])N(/C3=N/C(=C(/[F])C(=N3)OC([H])([H])[H])[C@@]4([H])C([H])([H])C4([H])[H])C5([H])[H])C([H])([H])[H]	3.377	3.414
Tr200	O=[S]3(=O)N(/C(=N/[H])N([H])[C@]5(/C1=C(\[H])C(=C([H])C([H])=C1[F])N([H])C(=O)C2=NC([H])=C([F])C([H])=C2[H])[C@]3([H])C([H])([H])N(/C4=N/C(OC([H])([H])[H])=C([F])C(=N4)C([H])([H])[H])C5([H])[H])C([H])([H])[H]	4.921	4.586
Tr201	O=C(C=1C([H])=C(C([H])=C(C=1[H])C(=O)N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])N([H])[C@]([H])(C(=O)N([H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])[C@@]([H])(O[H])C([H])([H])[H])C([H])([H])C2=C([H])C([H])=C([H])C([H])=C2[H])C([H])([H])[H])N([C@]	1.781	1.825
Tr202	O=C(C=1C([H])=C([H])C([H])=C(C=1[H])C(=O)N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])N([H])[C@]([H])(C(=O)N([H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])[C@@]([H])(O[H])C([H])([H])[H])C([H])([H])C2=C([H])C([H])=C([	1.236	1.588

	H])C([H])=C2[H])N([C@]([H])(C3=C(		
Tr203	O=C(C=1C([H])=C([H])C([H])=C(C=1[H])C(=O)N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])N([H])[C@]([H])(C(=O)N([H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])[C@@]([H])(O[H])C([H])([H])C([H])([H])C([H])([H])[H])C([H])([H])C2=C([H])C([H])=C([H])C([H])=C	2.573	2.693
Tr204	O=C(C=1C([H])=C(C([H])=C(C=1[H])C(=O)N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])N([H])[C@]([H])(C(=O)N([H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])[C@@]([H])(O[H])C([H])([H])C([H])([H])C([H])([H])[H])C([H])([H])C2=C([H])C([H])=C([H])C([H])=C2[H]	4.183	2.930
Test set			
Ts1	O=C2N([H])[C@]([H])(C(=O)N([H])[C@@]([H])(C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])[C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C=1C([H])=C([H])C([H])=C([H])C=1[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])C(=O)N([H])C([H])([H])C([H])([H])[H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])OC(=O)N([H])[C@@]2([H])C([H])(C([H])([H])[H])C([H])([H])[H]	3.600	3.204
Ts2	O=C(OC([H])([H])C=1N=C(OC=1C([H])([H])[H])C([H])([H])[H])N([H])[C@]([H])(C(=O)N([H])[C@@]([H])(C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])[C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])[S](=O)(=O)C([H])([H])[H]	5.921	3.884
Ts3	O=C(/C1=C(\[H])C(=C([H])C(=C1[H])C2=NN=C(O2)[C@@](C([H])([H])[H])(C([H])([H])C=3C([H])=C([H])C([H])=C([H])C=3[H])[N+]([H])([H])[H])N(C([H])([H])[H])[S](=O)(=O)C([H])([H])[H])C([H])(C([H])([H])[H])C([H])([H])[H]	0.783	2.741
Ts4	O=C(N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])[C@@]([H])(N([H])C(=O)OC(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[S](=O)(=O)C([H])([H])[H]	1.947	2.860
Ts5	O=C(OC([H])([H])C([H])=C([H])[H])N([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])[C@@]([H])(C([H])([H])C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])[C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C=1C([H])=C([H])C([H])=C([H])C=1[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])C(=O)N([H])C([H])([H])C([H])=C([H])[H])C([H])(C([H])([H])[H])C([H])([H])[H]	3.575	3.030
Ts6	O=C2N(C(=N[C@]4(C=1C([H])=C([H])C([H])=C([H])C=1[H])[C@@]2([H])C([H])([H])N(/C3=N/C(=C(/[F])C(=N3)OC([H])([H])[H])C([H])([H])[H])C4([H])[H])N([H])[H])C([H])([H])[H]	3.921	3.183
Ts7	O=C2N(C(=N[C@]4(C=1C([H])=C([H])C([H])=C([H])C=1[H])[C@@]2([H])C([H])([H])N(/C3=N/C(OC([H])([H])C([H])([H])[H])=C([F])C(=N3)OC([H])([H])[H])C4([H])[H])N([H])[H])C([H])([H])[H]	2.863	3.643
Ts8	O=C2N(C(=N[C@]4(C=1C([H])=C([H])C([H])=C([H])C=1[H])[C@@]2([H])C([H])([H])N(/C3=N/C(OC([H])([H])[H])=C([F])C(=N3)C([H])([H])C([H])([H])[H])C4([	3.796	3.456

	H])[H])N([H])[H])C([H])([H])[H]		
Ts9	O=C2N(C(=N[C@]4(C=1C([H])=C([H])C([F])=C([H])C=1[F])[C@@]2([H])C([H])([H])N(/C3=N/C(OC([H])([H])[H])=C([F])C(=N3)C([H])([H])C([H])([H])[H])C4([H])[H])N([H])[H])C([H])([H])[H]	4.276	3.931
Ts10	[F]/C1=C(/N=C(/N=C1/OC([H])([H])[H])N3C([H])([H])[C@@]2(N=C(N(C(=O)[C@]2([H])C3([H])[H])C([H])([H])[H])N([H])[H])C4=C([H])C([H])=C([F])C([H])=C4[F])C([F])([F])[F]	3.495	3.203
Ts11	O=C2N(C(=N[C@]4(C=1C([H])=C(C#N)C([H])=C([H])C=1[H])[C@@]2([H])C([H])([H])N(/C3=N/C(=C(/[F])C(=N3)OC([H])([H])[H])C([H])([H])[H])C4([H])[H])N([H])[H])C([H])([H])[H]	3.854	3.758
Ts12	O=C(OC(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])N([H])[C@]([H])(C(=O)C([H])([H])N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])(C([H])([H])[H])C(=O)N([H])[H]	0.649	2.437
Ts13	O=C(OC(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])N([H])[C@]([H])(C(=O)C([H])([H])N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])C(=O)N([H])[H]	1.504	2.485
Ts14	N#C/C1=C(\[H])C(=C([H])C([H])=C1[H])C2=C([H])[S]/C(=C2/[H])[C@@]35N=C(N(C(=O)[C@]3([H])C([H])([H])N(/C4=N/C([H])=C(C([H])=N4)C([H])([H])[H])C5([H])[H])C([H])([H])[H])N([H])[H]	4.046	3.352
Ts15	O=[S](=O)(N(C=1C([H])=C(C([H])=C(C=1[H])C(=O)N([H])[C@]([H])(C([H])([H])N([H])[C@]([H])(C(=O)N([H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])[C@@]([H])(OC([H])([H])[H])C([H])([H])[H])C([H])([H])C2=C([H])C([H])=C([H])C([H])=C2[H])C(=O)N([H])[C@@]([H])(C3=C([H])C([H])=C([H])C([H])=C3[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])[H]	3.602	2.192
Ts16	O=C(N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])([H])[H])C([H])([H])O[H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])([H])[C@]([H])(N([H])C(=O)C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])C(=O)O[H]	1.721	1.884
Ts17	O=C(N([H])[C@@]([H])(C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])([H])[H])C2=C([H])C(=C([H])C(=C2[H])N(C([H])([H])[H])[S](=O)(=O)C([H])([H])[H])C(=O)N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])N([H])C([H])([H])C3=C([H])C4=C(C([H])=C3[H])C([H])=C([H])N4[H])C([H])([H])C5=C([H])C([H])=C([H])C([H])=C5[H]	2.638	2.171
Ts18	O=C(N([H])[C@]([H])(C=1N=C(OC=1C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C=2C([H])=C(C([H])=C(C=2[H])N(C([H])([H])[H])[S](=O)(=O)C([H])([H])[H])C(=O)N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])N([H])C([H])([H])C3=C([H])C(OC([H])([H])[H])=C([H])C([H])=C3[H])C([H])([H])C4=C([H])C([H])=C([H])C([H])=C4[H]	2.049	3.481
Ts19	O=C2N([H])C1=C([H])C([H])=C([H])C([H])=C1N([H])C3=C2C([H])=C([H])C(=C	2.458	2.897

	3[H])C(=O)N([H])C4=N/C(=C(/[H])N4[H])C5=C([H])C([H])=NC([H])=C5[H]		
Ts20	O=C2N([H])C1=C([H])C([H])=C([H])C([H])=C1N([H])C3=C2C([H])=C([H])C(=C3[H])C(=O)N([H])C4=C([H])C([H])=C([F])C([H])=C4[H]	2.676	1.392
Ts21	O=C2N([H])C1=C([H])C([H])=C([H])C([H])=C1N([H])C=3/C2=C(/[H])C([H])=C(C=3[H])C(=O)N([H])C4=NC=5C(N4[H])=C([H])N=C([H])C=5[H]	2.510	1.849
Ts22	O=C(N([H])C(=NC([H])([H])C1=C([H])C(=C([H])C(=C1[H])C([H])([H])[H])C([H])([H])[H])N([H])[H])C=2C(=NOC=2C([H])([H])[H])C3=C([H])C([H])=C(OC([H])([H])[H])C([H])=C3[H]	2.553	1.826
Ts23	O=C(N([H])C(=NC([H])([H])C1=C([H])C([Cl])=C([H])C([Cl])=C1[H])N([H])[H])C=2C(=N[S]C=2C([H])([H])[H])C3=C([H])C([H])=C(OC([H])([H])[H])C([H])=C3[H]	2.538	2.559
Ts24	O=C(N([H])C(=NC([H])([H])C=1C([H])=C([H])C([H])=C2C=1C([H])=C([H])C([H])=C2[H])N([H])[H])C=3C(=NOC=3C([H])([H])[H])C4=C([H])C([H])=C([H])C([H])=C4[H]	1.553	1.122
Ts25	[H]C=5C(O[H])=C(O/C2=C(\[H])C(O[H])=C1OC3=C(O/C1=C2\[H])C(O[H])=C([H])C(O[H])=C3O/C4=C(\[H])C(O[H])=C([H])C(O[H])=C4[H])C(O[H])=C([H])C=5O[H]	1.143	1.019
Ts26	[F]C=1C([H])=C(C([H])=C([F])C=1[H])C([H])([H])[C@]([H])(N([H])C(=O)C=2C([H])=C(C([H])=C(C=2[H])C([H])([H])[H])C(=O)N(C([H])([H])C([H])([H])C([H])([H])[H])C([H])([H])C([H])([H])C([H])([H])[H])[C@]([H])(O[H])[C@]3([H])N([H])C([H])([H])C([H])([H])N(C3([H])[H])[S](=O)(=O)C4=C([H])C([H])=C([H])C([H])=C4[H]	4.523	3.732
Ts27	[F]C=1C([H])=C(C([H])=C([F])C=1[H])C([H])([H])[C@]([H])(N([H])C(=O)C2=C([H])C(=C([H])C(=C2[H])C(=O)N3[C@]([H])(C([H])([H])C([H])([H])C3([H])[H])C([H])([H])OC([H])([H])[H])C([H])([H])[H])[C@]([H])(O[H])[C@]4([H])N([H])C([H])([H])C([H])([H])N(C4([H])[H])[S](=O)(=O)C([H])([H])[H]	3.886	3.934
Ts28	[F]C=1C([H])=C(C([H])=C([F])C=1[H])C([H])([H])[C@]([H])(N([H])C(=O)C2=C([H])C(=C([H])C(=C2[H])C(=O)N3[C@]([H])(C([H])([H])C([H])([H])C3([H])[H])C([H])([H])OC([H])([H])[H])C([H])([H])[H])[C@]([H])(O[H])[C@]4([H])N([H])C([H])([H])C([H])([H])N(C4([H])[H])[S](=O)(=O)C([H])([H])C5=C([H])C([H])=C([H])C([H])=C5[H]	5.000	3.962
Ts29	O=C(N([H])[C@@]([H])(C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])([H])[H])C2=C([H])C(=C([H])C(=C2[H])N(C([H])([H])[H])[S](=O)(=O)C([H])([H])[H])C(=O)N([H])[C@]([H])([C@@]([H])(N=[N+]=[N-])C([H])([H])[C@@]([H])(OC([H])([H])[H])C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C3=C([H])C([H])=C([H])C([H])=C3[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])O/C4=C(\[H])C([F])=C([H])C([F])=C4[H]	3.155	3.807
Ts30	O=C(N([H])[C@@]([H])(C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])([H])[H])C2=C([H])C(=C([H])C(=C2[H])N(C([H])([H])[H])[S](=O)(=O)C([H])([H])[H])C(=O)N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])[C@@]([H])(OC([H])([H])C([H])([H])[H])[H])C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C3=C([H])C([H])=C([H])C([H])=C3[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])O/C4=C(\[H])C([F])=C([H])C([F])=C4[H]	4.678	3.400

Ts31	O=C(N([H])[C@@]([H])(C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])([H])[H])C=2C([H])=C(C([H])=C(C=2[H])N(C([H])([H])[H])[S](=O)(=O)C([H])([H])[H])C(=O)N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])[C@@]([H])(OC([H])([H])[C@@]3([H])C([H])([H])C3([H])[H])C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C4=C([H])C([H])=C([H])C([H])=C4[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])O/C5=C(\[H])C([F])=C([H])C([F])=C5[H]	4.886	5.030
Ts32	O=C1C4=C(O/C(=C1/C([H])([H])C([H])=C(C([H])([H])[H])C([H])([H])[H])C=2C([H])=C([H])C(O[H])=C([H])C=2O[H])C3=C(OC(C([H])=C3[H])(C([H])([H])[H])C([H])([H])[H])C([H])=C4O[H]	0.193	1.433
Ts33	O=C(OC(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])N([H])[C@]([H])(C(=O)N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])C(=O)N([H])[H]	1.504	2.330
Ts34	O=C3N([H])[C@]([H])(C(=O)N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])N([H])C([H])([H])C1=C([H])C(=C([H])C([H])=C1[H])N(C([H])([H])[H])C([H])([H])[H])C([H])([H])C2=C([H])C([H])=C([H])C([H])=C2[H])C([H])([H])N3/C4=C(\[H])C([H])=C([H])C([H])=C4[H]	1.087	1.850
Ts35	O=C3N([H])[C@]([H])(C(=O)N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])N([H])C([H])([H])C1=C([H])C(=C([H])C([H])=C1[H])N(C([H])([H])[H])C([H])([H])[H])C([H])([H])C2=C([H])C([H])=C([H])C([H])=C2[H])C([H])([H])N3C([H])([H])C4=C([H])C([H])=C([F])C([F])=C4[H]	2.565	2.361
Ts36	O=C3N([H])[C@]([H])(C(=O)N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])N([H])C([H])([H])C1=C([H])C(=C([H])C([H])=C1[H])N(C([H])([H])[H])C([H])([H])[H])C([H])([H])C2=C([H])C([H])=C([H])C([H])=C2[H])C([H])([H])N3C([H])([H])C4=C([H])C([H])=C([F])C([H])=C4[F]	2.062	2.049
Ts37	O=C(N([H])[C@@]([H])(C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])[C@]([H])(O[H])C([H])([H])N([H])C([H])([H])C2=C([H])C([H])=C([H])C(=C2[H])N(C([H])([H])[H])C([H])([H])[H])[C@]3(N([H])C(=O)N(C3([H])[H])C([H])([H])C4=C([H])C([H])=C([H])C([H])=C4[H])C([H])([H])C=5C([H])=C([H])C([H])=C([H])C=5[H]	1.301	1.184
Ts38	O=C1N(C(=N[C@@]1(C=2C([H])=C([H])C([H])=C([H])C=2[H])C3=C([H])C(=C([H])C([H])=C3[H])C4=C([H])N=C([H])C([F])=C4[H])N([H])[H])C([H])([H])[H]	2.538	2.740
Ts39	O=C1N(C(=N[C@@]1(C=2C([H])=C([H])C([H])=C([H])C=2[H])C3=C([H])C(=C([H])C([H])=C3[H])C4=C([H])C(OC([H])([H])[H])=C([H])C([H])=C4[H])N([H])[H])C([H])([H])[H]	1.222	2.632
Ts40	O=C1N(C(=N[C@@]1(C=2C([H])=C(C([H])=C([H])C=2[H])C3=C([H])C([Cl])=C([H])N=C3[H])[C@@]4([H])C([H])([H])C4([H])[H])N([H])[H])C([H])([H])[H]	3.678	2.896
Ts41	O=C1N(C(=N[C@]1(C=2C([H])=C([H])C([H])=C([H])C=2[H])C3=C([H])C([F])=C([H])C([H])=C3[H])N([H])[H])C([H])([H])[H]	2.143	1.637
Ts42	O=C1N(C(=N[C@@]1(/C2=C(\[H])C([H])=C([H])C([H])=C2[H])C3=C([H])C(=C([H])C([H])=C3[H])C4=C([H])C(OC([H])([H])C([H])([H])[H])=C([H])C([H])=C4[H])N([H])[H])C([H])([H])[H]	2.337	2.238

Ts43	O=C1N(C(=N[C@@]1(C=2C([H])=C([H])C([H])=C([H])C=2[H])C3=C([H])C(=C([H])C([H])=C3[H])C([H])([H])[H])N([H])[H])C([H])([H])[H]	2.260	2.310
Ts44	O=C(N([C@@]1([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C1([H])[H])C([H])([H])C2=C(N([H])N=C2[H])C([H])([H])[H])C([H])([H])[C@]([H])(N5C(=NC=4C([H])=C([H])C(O/C3=C(\[H])C([H])=C([H])C([H])=C3[H])=C([H])C=4C5([H])[H])N([H])[H])[C@@]6([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C6([H])[H]	3.409	3.164
Ts45	O=C(N([C@@]1([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C1([H])[H])C([H])([H])[H])C([H])([H])C([H])([H])[C@]([H])(N4C(=N/C3=C(\[H])C([H])=C(OC=2C([H])=C([H])C([H])=C([H])C=2[H])C([H])=C3C4([H])[H])N([H])[H])[C@]5([H])C([H])([H])OC([H])([H])C([H])([H])C5([H])[H]	2.914	3.847
Ts46	O=C(OC([H])([H])[C@]([H])(N3C(=N/C2=C(\[H])C([H])=C(O/C1=C(\[H])C([H])=C([H])C([H])=C1[H])C([H])=C2C3([H])[H])N([H])[H])[C@@]4([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C4([H])[H])N([H])[C@@]5([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C5([H])[H]	3.222	2.706
Ts47	O=C3N(C(=N[C@](C=1C([H])=C([S]C=1[Cl])C=2C([H])=C(C#CC([H])([H])[H])C([H])=NC=2[H])(C3([H])[H])C([H])([H])[H])N([H])[H])C([H])([H])[H]	4.097	3.896
Ts48	N#CC=1C([H])=C(C([H])=C([H])C=1[H])C=2C([H])=C([S]C=2[H])[C@]3(N=C(N(C(=O)C3([H])[H])C([H])([H])[H])N([H])[H])C([H])([H])[H]	3.244	1.873
Ts49	O=C(O[C@]2([H])[C@@]([H])(OC1=C(C(O[H])=C([H])C(O[H])=C1[H])C2([H])[H])C3=C([H])C(O[H])=C(O[H])C([H])=C3[H])C=4C([H])=C(O[H])C(O[H])=C(O[H])C=4[H]	1.276	2.728
Ts50	O=C(N([H])C3=C([H])C([H])=C2OC([C@]4([C@@]1(N=C(OC1([H])[H])N([H])[H])C2=C3[H])C([H])([H])OC4([H])[H])(C([H])([H])[H])C([H])([H])[H])C=5/N=C(/[H])C([Cl])=C([H])C=5[F]	3.288	2.888
Ts51	[H]/C4=C(/C([H])=C1C(OC([H])([H])[C@]3([C@@]12N=C(OC2([H])[H])N([H])[H])C([H])([H])OC3([H])[H])=C4[H])C5=C([H])N=C([H])C(C#CC([H])([H])[H])=C5[H]	2.910	3.616
Ts52	O=C(N([H])C3=C([H])C([H])=C2OC([C@]4([C@@]1(N=C(OC1([H])[H])N([H])[H])C2=C3[H])C([H])([H])OC4([H])[H])(C([H])([H])[H])C([H])([H])[H])C5=NC([H])=C([Br])C([H])=N5	3.078	2.657
Ts53	O=C(N([H])C3=C([H])C([H])=C2OC([H])([H])[C@@]4([C@@]1(N=C(OC1([H])[H])N([H])[H])C2=C3[H])C([H])([H])C4([H])[H])C5=NC([H])=C([Cl])C([H])=C5C([H])([H])[H]	2.504	2.395
Ts54	O=C(/C1=N/C([H])=C(C([H])=C1[H])C([H])([H])[H])N([H])C2=C([H])C(=C([F])C([H])=C2[H])[C@]3(N([H])C(=N[H])N([S](=O)(=O)C3([H])[H])C([H])([H])[H])C([H])([H])[H]	4.523	4.046
Ts55	O=C(/C1=N/C([H])=C([F])C([H])=C1[H])N([H])C2=C([F])C(=C([F])C([H])=C2[H])[C@]3(N([H])C(=N[H])N([S](=O)(=O)C3([H])[H])C([H])([H])[H])C([H])([H])[H]	4.312	4.509
Ts56	O=[S]3(=O)N(/C(=N\[H])N([H])[C@](C=1[S]C([H])=C(C=1[H])C2=C([H])C([H])=C([H])C(C#N)=C2[H])(C3([H])[H])C([H])([H])[H])C([H])([H])[H]	3.592	3.122

Ts57	O=C(N([H])[C@]1([H])C([H])([H])C1([H])[H])[C@]([H])(OC([H])([H])[H])C([H])([H])[C@]([H])(O[H])[C@@]([H])(N([H])C(=O)C=2C([H])=C([H])C([H])=C(C=2[H])C(=O)N(C([H])([H])C([H])([H])C([H])([H])[H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])O/C3=C(\[H])C([F])=C([H])C([F])=C3[H]	2.658	2.105
Ts58	O=C(N([H])C(=NC([H])([H])C1=C([H])C([Cl])=C(C([Cl])=C1[H])N([H])[S](=O)(=O)C([H])([H])[H])N([H])[H])C=2C(=N[S]C=2C([H])([H])[H])C3=C([H])C([H])=C(OC([H])([H])[H])C([H])=C3[H]	2.553	4.081
Ts59	O=C(N([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)O[H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])([H])C([H])([H])C(=O)O[H])[C@@]([H])(N([H])C(=O)[C@@]([H])(N([H])C([H])([H])[C@@]([H])(O[H])C(=O)[C@@]([H])(N([H])C(=O)[C@@]([H])(N([H])C(=O)[C@@]([H])(N([H])C(=O)[C@@]([H])(N([H])[H])C([H])([H])C([H])([H])C(=O)O[H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])C(=O)O[H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])(C([H])([H])[H])C([H])([H])[H]~	5.523	6.540
Ts60	O=[S](=O)(C([H])([H])C([H])([H])[C@@]([H])(C(=O)N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])N([H])C(=O)[C@@]([H])(N([H])C(=O)OC(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H]	4.097	3.591
Ts61	O=C(N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])[C@@]([H])(N([H])C(=O)OC(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])C([H])(C([H])([H])[H])C(=O)N([H])[H]	0.649	2.008
Ts62	O=C1N(/C(=N\[H])N([H])[C@]1(C([H])([H])C([H])([H])[C@]2([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C2([H])[H])C([H])([H])[C@]4([H])C([H])([H])[C@]([H])(N([H])C(=O)C3=C([H])C([H])=C([H])C([H])=C3[H])C([H])([H])C([H])([H])C4([H])[H])C([H])([H])[H]	3.886	3.523
Ts63	O=C1N(/C(=N\[H])N([H])[C@]1(C([H])([H])C([H])([H])[C@@]2([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C2([H])[H])C([H])([H])[C@]4([H])C([H])([H])[C@]([H])(N([H])C([H])([H])[C@]3([H])C([H])([H])C3([H])[H])C([H])([H])C([H])([H])C4([H])[H])C([H])([H])[H]	3.319	3.124
Ts64	O=C1N(/C(=N/[H])N([H])[C@]1(C([H])([H])C([H])([H])[C@@]2([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C2([H])[H])C([H])([H])[C@]4([H])C([H])([H])[C@]([H])(N([H])C(=O)N([H])C3=C([H])C([H])=C(OC([H])([H])[H])C([H])=C3[H])C([H])([H])C([H])([H])C4([H])[H])C([H])([H])[H]	5.000	3.179
Ts65	O=C1N(/C(=N\[H])N([H])[C@]1(C([H])([H])C([H])([H])[C@]2([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C2([H])[H])C([H])([H])[C@@]3([H])C([H])([H])N(C(=O)OC(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])([H])C3([H])[H])C([H])([H])[H]	3.387	3.981
Ts66	O=[S]2(=O)N(/C(=N/[H])N([H])[C@]4(/C1=C(\[H])C([H])=C([H])C([H])=C1[H])[C@@]2([H])C([H])([H])N(/C3=N/C(=C(/[F])C(=N3)OC([H])([H])[H])C([H])([H])[H])C4([H])[H])C([H])([H])[H]	3.292	2.984
Ts67	O=[S]2(=O)N(/C(=N/[H])N([H])[C@]4(/C1=C(\[H])C([H])=C([H])C([H])=C1[F])[	3.721	3.109

	C@@]2([H])C([H])([H])N(/C3=N/C(=C(/[F])C(=N3)OC([H])([H])[H])C([H])([H])[H])C4([H])[H])C([H])([H])[H]		
Ts68	O=[S]2(=O)N(/C(=N/[H])N([H])[C@@]4(/C1=C(\[H])C([H])=C([H])C([H])=C1[H])[C@]2([H])C([H])([H])N(/C3=N/C(OC([H])([H])[H])=C([H])C(=C3[H])C([H])([H])OC([H])([H])C([H])([H])[H])C4([H])[H])C([H])([H])[H]	3.215	3.236
Ts69	O=[S]2(=O)N(/C(=N/[H])N([H])[C@@]4(/C1=C(\[H])C([H])=C([H])C([H])=C1[H])[C@]2([H])C([H])([H])N(/C3=N/C(=C(/[F])C(=N3)OC([H])([H])[H])C([H])([H])C([H])([H])[H])C4([H])[H])C([H])([H])[H]	3.086	3.195
Ts70	O=C(C=1C([H])=C([H])C([H])=C(C=1[H])C(=O)N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])N([H])[C@]([H])(C(=O)N([H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])[C@@]([H])(O[H])C([H])([H])C([H])([H])C([H])([H])[H])C([H])([H])C2=C([H])C([H])=C([H])C([H])=C2[H])N([C@]([H])(C3=C([H])C([H])=C([H])C([H])=C3[H])C([H])([H])[H])C([H])([H])[H]	1.280	1.661
Calibration set			
Calib1	O=C(OC([H])([H])C([H])([H])C([H])=C([H])[H])N([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])[C@@]([H])(C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])[C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C=1C([H])=C([H])C([H])	3.212	3.066
Calib2	O=C(OC([H])([H])C([H])([H])C([H])([H])C([H])=C([H])[H])N([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])[C@@]([H])(C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])[C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C=1C([H])=C	2.950	3.103
Calib3	O=C(/C1=C(\[H])C([H])=C([H])C(=C1[H])C([H])([H])N4C(=NC=3C([H])=C([H])C(OC=2C([H])=C([H])C([H])=C([H])C=2[H])=C([H])C=3C4([H])[H])N([H])[H])N(C([H])([H])[H])C5([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C5([H])[H]	2.801	2.815
Calib4	O=C(O[H])C([H])([H])C([H])([H])[C@@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)O[H])C([H])([H])C1=C([H])C([H])=C([H])C([H]	4.796	4.688
Calib5	O=C(N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])[C@@]([H])(N([H])C	4.027	3.717
Calib6	O=C(N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])(C([H])([H])[H])	0.979	3.121
Calib7	O=C2N(C(=N[C@]4(C=1C([H])=C([H])C([F])=C([H])C=1[H])[C@@]2([H])C([H])([H])N(/C3=N/C(OC([H])([H])[H])=C([F])C(=N3)OC([H])([H])[H])C4([H])[H])N([H])[H])C([H])([H])[H]	4.357	3.957
Calib8	O=C2N(C(=N[C@]4(C=1C([F])=C([H])C([F])=C([H])C=1[F])[C@@]2([H])C([H])([H])N(/C3=N/C(=C(/[F])C(=N3)OC([H])([H])[H])C([H])([H])[H])C4([H])[H])N([H]	3.824	4.008

	)[H])C([H])([H])[H]		
Calib9	O=C2N(C(=N[C@]4(/C1=C(\[H])C([Cl])=C([H])C([H])=C1[H])[C@@]2([H])C([H])([H])N(/C3=N/C(OC([H])([H])[H])=C([F])C(=N3)C([H])([H])[H])C4([H])[H])N([H])[H])C([H])([H])[H]	3.409	3.183
Calib10	O=C2N(C(=N[C@]5(C=1C([F])=C([H])C([H])=C([F])C=1[H])[C@@]2([H])C([H])([H])N(/C3=N/C(OC([H])([H])[H])=C([Cl])C(=N3)[C@]4([H])C([H])([H])C4([H])[H])C5([H])[H])N([H])[H])C([H])([H])[H]	4.187	4.330
Calib11	O=C2N(C(=N[C@]5(C=1C([H])=C(C#N)C([H])=C([H])C=1[H])[C@@]2([H])C([H])([H])N(/C3=N/C(=C(/[F])C(=N3)[C@@]4([H])C([H])([H])C4([H])[H])C([H])([H])[H])C5([H])[H])N([H])[H])C([H])([H])[H]	3.367	3.126
Calib12	[F]C=1C([H])=C([F])C(=C([H])C=1[H])[C@@]24N=C(N(C(=O)[C@]2([H])C([H])([H])N(/C3=N/C(=C(/[F])C(=N3)OC([H])([H])[H])C([H])([H])O[H])C4([H])[H])C([H])([H])[H])N([H])[H]	3.796	3.608
Calib13	O=C2N(C(=N[C@]4(C=1C([F])=C([H])C([F])=C([F])C=1[H])[C@@]2([H])C([H])([H])N(/C3=N/C(OC([H])([H])[H])=C([F])C(=N3)C([H])([H])C([H])([H])[H])C4([H])[H])N([H])[H])C([H])([H])[H]	4.252	4.506
Calib14	O=C(/C1=N/C([H])=C([F])C([H])=C1[H])N([H])C2=C([H])C(=C([F])C([H])=C2[H])[C@]3(N([H])C(=N[H])N([S](=O)(=O)C3([H])[H])C([H])([H])[H])C([H])([H])[H]	4.312	4.159
Calib15	O=[S]3(=O)N(C=2C([H])=C(C([H])=C1/C(=C(/[H])N(C1=2)C([H])([H])C3([H])[H])C([H])([H])C([H])([H])[H])C(=O)N([H])[C@]([H])(C([H])([H])N([H])[C@]([H])(C(=O)N([H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])[C@@]([H])(O[H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])[H]	5.398	4.593
Calib16	O=C(N([H])[C@@]([H])(C=1C([H])=C([H])C([H])=C([H])C=1[H])C([H])([H])[H])C2=C([H])C(=C([H])C(=C2[H])N(C([H])([H])[H])[S](=O)(=O)C([H])([H])[H])C(=O)N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])N([H])C([H])([H])C3=C([H])C4=C(C([H])=C3[H])C([H])=C([H])N4[S](=	3.569	3.680
Calib17	O=C(OC([H])([H])C=1N=C(OC=1C([H])([H])[H])C([H])([H])[H])N([H])[C@]([H])(C(=O)N([H])[C@@]([H])(C([H])([H])C2=C([H])C([H])=C([H])C([H])=C2[H])[C@]([H])(O[H])C([H])([H])N([H])C([H])([H])C3=C([H])C(OC([H])([H])[H])=C([H])C([H])=C3[H])C([H])([H])[S](=O)(=O)	0.824	2.441
Calib18	O=C(N([H])[C@@]([H])(C=1C([H])=C([H])C([H])=C([H])C=1[H])C([H])([H])[H])C2=C([H])C(=C([H])C(=C2[H])N(C([H])([H])[H])[S](=O)(=O)C([H])([H])[H])C(=O)N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])N([H])C([H])([H])C3=C([H])C(OC([H])([H])[H])=C([H])C([H])=C3[H])	2.038	2.070
Calib19	O=C(OC([H])([H])C=1N=C(OC=1C([H])([H])[H])C([H])([H])[H])N([H])[C@]([H])(C(=O)N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H]	5.921	4.009
Calib20	O=C(N([H])C(=NC([H])([H])C1=C([H])C([Cl])=C([H])C([Cl])=C1[H])N([H])[H])C2=C(N(/N=C2/C([H])([H])[H])C([H])([H])[H])C3=C([H])C([H])=C(OC([H])([H])[H])C([H])=C3[H]	1.398	1.196

Calib21	O=C2N([H])C1=C([H])C([H])=C([H])C([H])=C1N([H])C=3/C2=C(/[H])C([H])=C(C=3[H])C(=O)N([H])C4=C([H])C([H])=NC([H])=C4[H]	2.530	2.605
Calib22	O=C2N([H])C=1C([H])=C([H])C([H])=C([H])C=1N([H])C3=C2C([H])=C([H])C(=C3[H])C(=O)N([H])C4=N/C(=C(/[H])N4[H])C5=C([H])C([H])=C([F])C([H])=C5[H]	2.533	2.778
Calib23	O=C(N([H])C(=NC([H])([H])C1=C([H])C(=C([H])C([Cl])=C1[H])C2=C([H])N=C([H])C([H])=C2[H])N([H])[H])C=3C(=NOC=3C([H])([H])[H])C4=C([H])C([H])=C(OC([H])([H])[H])C([H])=C4[H]	1.745	1.995
Calib24	O=C(N([H])C(=NC([H])([H])C1=C([H])C(=C([H])C([Cl])=C1[H])C=2C([H])=C([H])[S]C=2[H])N([H])[H])C=3C(=NOC=3C([H])([H])[H])C4=C([H])C([H])=C(OC([H])([H])[H])C([H])=C4[H]	1.921	2.576
Calib25	O=C(N([H])C(=NC([H])([H])C1=C([H])C(=C([H])C([Cl])=C1[H])C([H])=C([H])[H])N([H])[H])C=2C(=NOC=2C([H])([H])[H])C3=C([H])C([H])=C(OC([H])([H])[H])C([H])=C3[H]	2.367	2.071
Calib26	O=C(N([H])C(=NC([H])([H])C1=C([H])C([Cl])=C(O[H])C([Cl])=C1[H])N([H])[H])C=2C(=NOC=2C([H])([H])[H])C3=C([H])C([H])=C(OC([H])([H])[H])C([H])=C3[H]	2.319	2.491
Calib27	O=C(N([H])C(=NC([H])([H])C1=C([H])C([Cl])=C([H])C([Cl])=C1[H])N([H])[H])C=2C(=NOC=2C([H])([H])[H])C3=C([H])C([H])=C([H])C([H])=C3[H]	1.409	2.198
Calib28	O=C(N([H])C(=NC([H])([H])C1=C([H])C([Br])=C([H])C([Cl])=C1[H])N([H])[H])C=2C(=NOC=2C([H])([H])[H])C3=C([H])C([H])=C(OC([H])([H])[H])C([H])=C3[H]	2.569	2.072
Calib29	O=C(N([H])C(=NC([H])([H])C1=C([H])C([Cl])=C(C([Cl])=C1[H])N([H])C(=O)C([H])([H])N([H])C([H])([H])C([H])([H])[H])N([H])[H])C=2C(=N[S]C=2C([H])([H])[H])C3=C([H])C([H])=C(OC([H])([H])[H])C([H])=C3[H]	4.000	3.805
Calib30	[H]C=2C(O[H])=C([H])C=1OC=3C(OC=1C=2O[H])=C([H])C(O[H])=C4OC5=C(OC=34)C(O[H])=C([H])C(O[H])=C5[H]	1.097	1.459
Calib31	[F]C=1C([H])=C(C([H])=C([F])C=1[H])C([H])([H])[C@]([H])(N([H])C(=O)C2=C([H])C(=C([H])C(=C2[H])C([H])([H])[H])C(=O)N(C([H])([H])C([H])([H])C([H])([H])[H])C([H])([H])C([H])([H])C([H])([H])[H])[C@]([H])(O[H])[C@]3([H])N([H])C([H])([H])C([H])([H])N(C3([H])[	5.000	3.113
Calib32	[F]C=1C([H])=C(C([H])=C([F])C=1[H])C([H])([H])[C@]([H])(N([H])C(=O)C2=C([H])C(=C([H])C(=C2[H])C([H])([H])[H])C(=O)N(C([H])([H])C([H])([H])C([H])([H])[H])C([H])([H])C([H])([H])C([H])([H])[H])[C@]([H])(O[H])[C@]3([H])N([H])C([H])([H])C([H])([H])N(C3([H])[	4.301	3.425
Calib33	O=C3N(C([H])([H])C([H])([H])C=5C([H])=C(OC=2C(OC([H])([H])[H])=C([H])C=1N=C(N(C([H])([H])C=1C=2[H])[C@@]([H])(C([H])([H])C3([H])[H])[C@@]4([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C4([H])[H])N([H])[H])C([H])=C([H])C=5[H])[C@]6([H])C([H])([H])C([H	3.921	3.938
Calib34	O=C(N([H])[C@@]([H])(C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])([H])[H])C2=C([H])C(=C([H])C(=C2[H])N(C([H])([H])[H])[S](=O)(=O)C([H])([H])[H])C(=O)N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])[C@@]([H])(OC([H])([H])[H])C(=O	2.678	3.264

	)N([H])[C@]([H])(C(=O)N([H])C([H])		
Calib35	O=C(N([H])[C@@]([H])(C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])([H])[H])C2=C([H])C(=C([H])C(=C2[H])N(C([H])([H])[H])[S](=O)(=O)C([H])([H])[H])C(=O)N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])[C@@]([H])(OC([H])([H])C([H])=C([H])[H])C(=O)N([H])[C@]([H])(C(=	4.481	3.325
Calib36	O=C1C([H])=C(OC=2/C1=C(/O[H])C([H])=C(O[H])C=2[H])C3=C(O[H])C([H])=C(O[H])C([H])=C3[H]	0.083	0.503
Calib37	O=C3N([H])[C@]([H])(C(=O)N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])N([H])C([H])([H])C1=C([H])C(=C([H])C([H])=C1[H])C(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])C2=C([H])C([F])=C([H])C([F])=C2[H])C([H])([H])N3C([H])([H])C4=C([H])C([F])=C([H	4.699	3.185
Calib38	O=C3N(C([H])([H])[C@@]([H])(C(=O)N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])N([H])C([H])([H])C1=C([H])C(=C([H])C([H])=C1[H])N(C([H])([H])[H])C([H])([H])[H])C([H])([H])C2=C([H])C([H])=C([H])C([H])=C2[H])C3([H])[H])C([H])([H])C4=C([H])C([H])=C([H])C([H])=C	1.659	1.724
Calib39	O=C3N([H])[C@]([H])(C(=O)N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])N([H])C([H])([H])C1=C([H])C(=C([H])C([H])=C1[H])N(C([H])([H])[H])C([H])([H])[H])C([H])([H])C2=C([H])C([H])=C([H])C([H])=C2[H])C([H])([H])N3C([H])([H])C([H])([H])C4=C([H])C([H])=C([H])C([	1.167	1.823
Calib40	O=C1N(C(=N[C@]1(C=2C([H])=C([H])C([H])=C([H])C=2[H])C3=C([H])C(=C([H])C([H])=C3[H])C4=C([H])C([H])=NC([H])=C4[H])N([H])[H])C([H])([H])[H]	1.420	2.309
Calib41	O=C1N(C(=N[C@@]1(C=2C([H])=C([H])C([H])=C([H])C=2[H])C3=C([H])C(=C([H])C([H])=C3[H])C4=C([H])N=C([H])C(=C4[H])C([H])([H])[H])N([H])[H])C([H])([H])[H]	2.367	2.645
Calib42	O=C1N(C(=N[C@@]1(/C2=C(\[H])C([H])=C([H])C([H])=C2[H])C3=C([H])C(=C([H])C([H])=C3[H])C4=C([H])N=C([H])C(C#N)=C4[H])N([H])[H])C([H])([H])[H]	2.328	2.634
Calib43	O=C(N([C@]1([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C1([H])[H])C([H])([H])C=2N=C([S]C=2[H])C([H])([H])OC([H])([H])[H])C([H])([H])C([H])([H])[C@]([H])(N5C(=N/C4=C(\[H])C([H])=C(O/C3=C(\[H])C([H])=C([H])C([H])=C3[H])C([H])=C4C5([H])[H])N([H])[H])[	3.886	3.501
Calib44	O=C3N(C(=N[C@](C=2[S]C([H])=C(/C1=C(\[H])C(C#CC([H])([H])[H])=C([H])N=C1[H])C=2[H])(C3([H])[H])C([H])([H])[H])N([H])[H])C([H])([H])[H]	4.108	3.728
Calib45	O=C(N([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])N([H])C2=C1C([H])=C([H])C([H])=C([H])C1=NC3=C2C([H])([H])C([H])([H])C([H])([H])C3([H])[H])C=4OC=5C(C(=O)C=4[H])=C(O[H])C([H])=C(O[H])	1.975	1.955
Calib46	O=C(N([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])N([H])C2=C1C([H])=C([H])C([Cl])=C([H])C1=NC3=C2C([H])([H])C([H])([H])C([H])([H])C3([H])[H])C=4OC=5C(C(=O)C=4[H])=C([H])C(OC([H])([H])	1.374	2.116
Calib47	O=[S]3(=O)N(C(=N[C@@](C=1[S]/C(=C(/[H])C=1[Cl])C2=C([H])C(C#CC([H])([	4.620	4.484

	H])[H])=C([H])N=C2[H])(C([H])([H])[H])C3([H])[H])N([H])[H])C([H])([H])[H]		
Calib48	O=C(N([H])C3=C([H])C([H])=C2OC([C@]4([C@@]1(N=C(OC1([H])[H])N([H])[H])C2=C3[H])C([H])([H])OC4([H])[H])(C([H])([H])[H])C([H])([H])[H])C=5/N=C(/[H])C([F])=C([H])C=5[H]	2.932	2.825
Calib49	[H]/C4=C(/C([H])=C1C(O[C@]([H])([C@]3([C@]12N=C(OC2([H])[H])N([H])[H])C([H])([H])OC3([H])[H])C([H])([H])C([H])([H])C([H])([H])[H])=C4[H])C5=C([H])N=C([H])C(C#CC([H])([H])[H])=C5[H]	3.056	2.813
Calib50	[F]C([F])([F])C([H])([H])C([H])([H])[C@]3([H])O/C1=C(\[H])C([H])=C(C([H])=C1[C@@]2(N=C(OC2([H])[H])N([H])[H])[C@]34C([H])([H])OC4([H])[H])C5=C([H])N=C([H])C(C#CC([H])([H])[H])=C5[H]	2.061	2.233
Calib51	O=C(N([H])C3=C([H])C([H])=C2OC([H])([H])[C@@]4([C@@]1(N=C(OC1([H])[H])N([H])[H])C2=C3[H])C([H])([H])C4([H])[H])C5=NC([H])=C(C#N)C([H])=C5C([H])([H])[H]	2.668	2.520
Calib52	O=C(N([H])C3=C([H])C([H])=C2OC([C@]4([C@@]1(N=C(OC1([H])[H])N([H])[H])C2=C3[H])C([H])([H])C4([H])[H])(C([H])([H])[H])C([H])([H])[H])C5=NC([H])=C(/N=C5/[H])OC([H])([H])[H]	3.213	3.362
Calib53	O=C(N([H])C3=C([H])C([H])=C2OC([C@@]4([C@]1(N=C(OC1([H])[H])N([H])[H])C2=C3[H])C([H])([H])OC4([H])[H])(C([H])([H])[H])C([H])([H])[H])C=5/N=C(/[H])C([Cl])=C([H])C=5[H]	0.520	1.689
Calib54	[F]C=1C([H])=C(C([H])=C([F])C=1[H])C([H])([H])[C@]([H])(N([H])C(=O)C2=C([H])C(=C([H])C(=C2[H])C([H])([H])[H])C(=O)N(C([H])([H])C([H])([H])C([H])([H])[H])C([H])([H])C([H])([H])C([H])([H])[H])[C@]([H])(O[H])[C@]3([H])N([H])C([H])([H])C([H])([H])N(C3([H])[	1.237	2.964
Calib55	[F]C=1C([H])=C(C([H])=C([F])C=1[H])C([H])([H])[C@]([H])(N([H])C(=O)C2=C([H])C(=C([H])C(=C2[H])C([H])([H])[H])C(=O)N(C([H])([H])C([H])([H])C([H])([H])[H])C([H])([H])C([H])([H])C([H])([H])[H])[C@]([H])(O[H])[C@]3([H])N([H])C([H])([H])C([H])([H])N(C3([H])[	1.921	2.770
Calib56	O=C(N([H])[C@]1([H])C([H])([H])C1([H])[H])[C@]([H])(OC([H])([H])[H])C([H])([H])[C@]([H])(O[H])[C@@]([H])(N([H])C(=O)C2=C([H])C(=C([H])C(=C2[H])C(=O)N([H])[C@@]([H])(C3=C([H])C([H])=C([H])C([H])=C3[H])C([H])([H])[H])N(C([H])([H])[S](=O)(=O)C([H])([H])[H]	1.745	2.845
Calib57	O=C(N([H])C(=NC([H])([H])C1=C([H])C([Cl])=C([Cl])C([H])=C1[H])N([H])[H])C=2C(=NOC=2C([H])([H])[H])C3=C([H])C([H])=C(OC([H])([H])[H])C([H])=C3[H]	2.041	2.297
Calib58	O=C(N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])[C@]([H])(N([H])C(=	4.229	2.813
Calib59	O=C(O[H])C([H])([H])C([H])([H])[C@]([H])(N([H])[H])C(=O)N([H])[C@@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])[C@@]([H])(C(=O)O[H])C([H])([H])C1=C([H])C([H])=	4.796	4.594

Calib60	O=C(N([H])[C@]([H])(C(=O)N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H]	2.327	3.115
Calib61	O=C1N(/C(=N\[H])N([H])[C@]1(C([H])([H])C([H])([H])[C@]2([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C2([H])[H])C([H])([H])[C@]4([H])C([H])([H])[C@]([H])(N([H])C(=O)N([H])C3=C([H])C([H])=C(C#N)C([H])=C3[H])C([H])([H])C([H])([H])C4([H])[H])C([H])([H])	4.523	4.248
Calib62	O=C1N(/C(=N\[H])N([H])[C@]1(C([H])([H])C([H])([H])[C@]2([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C2([H])[H])C([H])([H])[C@]4([H])C([H])([H])[C@]([H])(N([H])C(=O)N([H])C3=C([H])C([H])=C([H])C([H])=C3[H])C([H])([H])C([H])([H])C4([H])[H])C([H])([H])	3.796	3.673
Calib63	O=C1N(/C(=N/[H])N([H])[C@]1(C([H])([H])C([H])([H])[C@@]2([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C2([H])[H])C([H])([H])[C@]3([H])C([H])([H])N(C([H])([H])C([H])([H])C3([H])[H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])[H])C([H])([H])	3.119	2.925
Calib64	O=[S]2(=O)N(/C(=N/[H])N([H])[C@]4(/C1=C(\[H])C([F])=C([F])C([H])=C1[F])[C@]2([H])C([H])([H])N(/C3=N/C(OC([H])([H])[H])=C([H])C(=C3[H])C([H])([H])OC([H])([H])[H])C4([H])[H])C([H])([H])[H]	4.155	4.368
External set			
Ext1	O=C2N([H])[C@]([H])(C(=O)N([H])[C@@]([H])(C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])[C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C=1C([H])=C([H])C([H])=C([H])C=1[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])C(=O)N([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])OC(=O)N([H])[C@@]2([H])C([H])(C([H])([H])[H])C([H])([H])[H]	3.600	3.204
Ext2	O=C(OC([H])([H])C=1N=C(OC=1C([H])([H])[H])C([H])([H])[H])N([H])[C@]([H])(C(=O)N([H])[C@@]([H])(C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])[C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C([H])([H])C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])[S](=O)(=O)C([H])([H])[H]	5.921	3.884
Ext3	O=C(/C1=C(\[H])C(=C([H])C(=C1[H])C2=NN=C(O2)[C@@]([H])([H])[H])(C([H])([H])C=3C([H])=C([H])C([H])=C([H])C=3[H])[N+]([H])([H])[H])N(C([H])([H])[H])[S](=O)(=O)C([H])([H])[H])C([H])(C([H])([H])[H])C([H])([H])[H]	0.783	2.741
Ext4	O=C(N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])[C@@]([H])(N([H])C(=O)OC(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])([H])[S](=O)(=O)C([H])([H])[H]	1.947	2.860
Ext5	O=C(OC([H])([H])C([H])=C([H])[H])N([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])[C@@]([H])(C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])[C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C=1C([H])=C([H])C([H])=C([H])C=1[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])C(=O)N([H])C([H])([H])C([H])=C([H])[H])C([H])(C([H])(	3.575	3.030

	[H])[H])C([H])([H])[H]		
Ext6	O=C2N(C(=N[C@]4(C=1C([H])=C([H])C([H])=C([H])C=1[H])[C@@]2([H])C([H])([H])N(/C3=N/C(=C(/[F])C(=N3)OC([H])([H])[H])C([H])([H])[H])C4([H])[H])N([H])[H])C([H])([H])[H]	3.921	3.183
Ext7	O=C2N(C(=N[C@]4(C=1C([H])=C([H])C([H])=C([H])C=1[H])[C@@]2([H])C([H])([H])N(/C3=N/C(OC([H])([H])C([H])([H])[H])=C([F])C(=N3)OC([H])([H])[H])C4([H])[H])N([H])[H])C([H])([H])[H]	2.863	3.643
Ext8	O=C2N(C(=N[C@]4(C=1C([H])=C([H])C([H])=C([H])C=1[H])[C@@]2([H])C([H])([H])N(/C3=N/C(OC([H])([H])[H])=C([F])C(=N3)C([H])([H])C([H])([H])[H])C4([H])[H])N([H])[H])C([H])([H])[H]	3.796	3.456
Ext9	O=C2N(C(=N[C@]4(C=1C([H])=C([H])C([F])=C([H])C=1[F])[C@@]2([H])C([H])([H])N(/C3=N/C(OC([H])([H])[H])=C([F])C(=N3)C([H])([H])C([H])([H])[H])C4([H])[H])N([H])[H])C([H])([H])[H]	4.276	3.931
Ext10	[F]/C1=C(/N=C(/N=C1/OC([H])([H])[H])N3C([H])([H])[C@@]2(N=C(N(C(=O)[C@]2([H])C3([H])[H])C([H])([H])[H])N([H])[H])C4=C([H])C([H])=C([F])C([H])=C4[F])C([F])([F])[F]	3.495	3.203
Ext11	O=C2N(C(=N[C@]4(C=1C([H])=C(C#N)C([H])=C([H])C=1[H])[C@@]2([H])C([H])([H])N(/C3=N/C(=C(/[F])C(=N3)OC([H])([H])[H])C([H])([H])[H])C4([H])[H])N([H])[H])C([H])([H])[H]	3.854	3.758
Ext12	O=C(OC(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])N([H])[C@]([H])(C(=O)C([H])([H])N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])(C(=O)N([H])[H]	0.649	2.437
Ext13	O=C(OC(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])N([H])[C@]([H])(C(=O)C([H])([H])N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])C(=O)N([H])[H]	1.504	2.485
Ext14	N#C/C1=C(\[H])C(=C([H])C([H])=C1[H])C2=C([H])[S]/C(=C2/[H])[C@@]35N=C(N(C(=O)[C@]3([H])C([H])([H])N(/C4=N/C([H])=C(C([H])=N4)C([H])([H])[H])C5([H])[H])C([H])([H])[H])N([H])[H]	4.046	3.352
Ext15	O=[S](=O)(N(C=1C([H])=C(C([H])=C(C=1[H])C(=O)N([H])[C@]([H])(C([H])([H])N([H])[C@]([H])(C(=O)N([H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])[C@@]([H])(OC([H])([H])[H])C([H])([H])[H])C([H])([H])C2=C([H])C([H])=C([H])C([H])=C2[H])C(=O)N([H])[C@@]([H])(C3=C([H])C([H])=C([H])C([H])=C3[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])[H]	3.602	2.192
Ext16	O=C(N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])O[H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])([H])[C@]([H])(N([H])C(=O)C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])C(=O)O[H]	1.721	1.884
Ext17	O=C(N([H])[C@@]([H])(C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])([H])[H])C2=C([H])C(=C([H])C(=C2[H])N(C([H])([H])[H])[S](=O)(=O)C([H])([H])[H])C(=O)	2.638	2.171

	N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])N([H])C([H])([H])C3=C([H])C4=C(C([H])=C3[H])C([H])=C([H])N4[H])C([H])([H])C5=C([H])C([H])=C([H])C([H])=C5[H]		
Ext18	O=C(N([H])[C@]([H])(C=1N=C(OC=1C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C=2C([H])=C(C([H])=C(C=2[H])N(C([H])([H])[H])[S](=O)(=O)C([H])([H])[H])C(=O)N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])N([H])C([H])([H])C3=C([H])C(OC([H])([H])[H])=C([H])C([H])=C3[H])C([H])([H])C4=C([H])C([H])=C([H])C([H])=C4[H]	2.049	3.481
Ext19	O=C2N([H])C1=C([H])C([H])=C([H])C([H])=C1N([H])C3=C2C([H])=C([H])C(=C3[H])C(=O)N([H])C4=N/C(=C(/[H])N4[H])C5=C([H])C([H])=NC([H])=C5[H]	2.458	2.897
Ext20	O=C2N([H])C1=C([H])C([H])=C([H])C([H])=C1N([H])C3=C2C([H])=C([H])C(=C3[H])C(=O)N([H])C4=C([H])C([H])=C([F])C([H])=C4[H]	2.676	1.392
Ext21	O=C2N([H])C1=C([H])C([H])=C([H])C([H])=C1N([H])C=3/C2=C(/[H])C([H])=C(C=3[H])C(=O)N([H])C4=NC=5C(N4[H])=C([H])N=C([H])C=5[H]	2.510	1.849
Ext22	O=C(N([H])C(=NC([H])([H])C1=C([H])C(=C([H])C(=C1[H])C([H])([H])[H])C([H])([H])[H])N([H])[H])C=2C(=NOC=2C([H])([H])[H])C3=C([H])C([H])=C(OC([H])([H])[H])C([H])=C3[H]	2.553	1.826
Ext23	O=C(N([H])C(=NC([H])([H])C1=C([H])C([Cl])=C([H])C([Cl])=C1[H])N([H])[H])C=2C(=N[S]C=2C([H])([H])[H])C3=C([H])C([H])=C(OC([H])([H])[H])C([H])=C3[H]	2.538	2.559
Ext24	O=C(N([H])C(=NC([H])([H])C=1C([H])=C([H])C([H])=C2C=1C([H])=C([H])C([H])=C2[H])N([H])[H])C=3C(=NOC=3C([H])([H])[H])C4=C([H])C([H])=C([H])C([H])=C4[H]	1.553	1.122
Ext25	[H]C=5C(O[H])=C(O/C2=C(\[H])C(O[H])=C1OC3=C(O/C1=C2\[H])C(O[H])=C([H])C(O[H])=C3O/C4=C(\[H])C(O[H])=C([H])C(O[H])=C4[H])C(O[H])=C([H])C=5O[H]	1.143	1.019
Ext26	[F]C=1C([H])=C(C([H])=C([F])C=1[H])C([H])([H])[C@]([H])(N([H])C(=O)C=2C([H])=C(C([H])=C(C=2[H])C([H])([H])[H])[H])C(=O)N(C([H])([H])C([H])([H])C([H])([H])[H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])[H])[C@]([H])(O[H])[C@]3([H])N([H])C([H])([H])C([H])([H])N(C3([H])[H])[S](=O)(=O)C4=C([H])C([H])=C([H])C([H])=C4[H]	4.523	3.732
Ext27	[F]C=1C([H])=C(C([H])=C([F])C=1[H])C([H])([H])[C@]([H])(N([H])C(=O)C2=C([H])C(=C([H])C(=C2[H])C(=O)N3[C@]([H])(C([H])([H])C([H])([H])C3([H])[H])C([H])([H])OC([H])([H])[H])C([H])([H])[H])[H])[C@]([H])(O[H])[C@]4([H])N([H])C([H])([H])C([H])([H])N(C4([H])[H])[S](=O)(=O)C([H])([H])[H]	3.886	3.934
Ext28	[F]C=1C([H])=C(C([H])=C([F])C=1[H])C([H])([H])[C@]([H])(N([H])C(=O)C2=C([H])C(=C([H])C(=C2[H])C(=O)N3[C@]([H])(C([H])([H])C([H])([H])C3([H])[H])C([H])([H])OC([H])([H])[H])C([H])([H])[H])[H])[C@]([H])(O[H])[C@]4([H])N([H])C([H])([H])C([H])([H])N(C4([H])[H])[S](=O)(=O)C([H])([H])C5=C([H])C([H])=C([H])C([H])=C5[H]	5.000	3.962
Ext29	O=C(N([H])[C@@]([H])(C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])([H])[H])C2=C([H])C(=C([H])C(=C2[H])N(C([H])([H])[H])[S](=O)(=O)C([H])([H])[H])C(=O)N([H])[C@]([H])([C@@]([H])(N=[N+]=[N-	3.155	3.807

	])C([H])([H])[C@@]([H])(OC([H])([H])[H])C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C3=C([H])C([H])=C([H])C([H])=C3[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])O/C4=C(\[H])C([F])=C([H])C([F])=C4[H]		
Ext30	O=C(N([H])[C@@]([H])(C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])([H])[H])C2=C([H])C(=C([H])C(=C2[H])N(C([H])([H])[H])[S](=O)(=O)C([H])([H])[H])C(=O)N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])[C@@]([H])(OC([H])([H])C([H])([H])[H])C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C3=C([H])C([H])=C([H])C([H])=C3[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])O/C4=C(\[H])C([F])=C([H])C([F])=C4[H]	4.678	3.400
Ext31	O=C(N([H])[C@@]([H])(C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])([H])[H])C=2C([H])=C(C([H])=C(C=2[H])N(C([H])([H])[H])[S](=O)(=O)C([H])([H])[H])C(=O)N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])[C@@]([H])(OC([H])([H])[C@@]3([H])C([H])([H])C3([H])[H])C(=O)N([H])[C@]([H])(C(=O)N([H])C([H])([H])C4=C([H])C([H])=C([H])C([H])=C4[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])O/C5=C(\[H])C([F])=C([H])C([F])=C5[H]	4.886	5.030
Ext32	O=C1C4=C(O/C(=C1/C([H])([H])C([H])=C(C([H])([H])[H])C([H])([H])[H])C=2C([H])=C([H])C(O[H])=C([H])C=2O[H])C3=C(OC(C([H])=C3[H])(C([H])([H])[H])C([H])([H])[H])C([H])=C4O[H]	0.193	1.433
Ext33	O=C(OC(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])N([H])[C@]([H])(C(=O)N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])[C@]([H])(C(=O)N([H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])C(=O)N([H])[H]	1.504	2.330
Ext34	O=C3N([H])[C@]([H])(C(=O)N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])N([H])C([H])([H])C1=C([H])C(=C([H])C([H])=C1[H])N(C([H])([H])[H])C([H])([H])[H])C([H])([H])C2=C([H])C([H])=C([H])C([H])=C2[H])C([H])([H])N3/C4=C(\[H])C([H])=C([H])C([H])=C4[H]	1.087	1.850
Ext35	O=C3N([H])[C@]([H])(C(=O)N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])N([H])C([H])([H])C1=C([H])C(=C([H])C([H])=C1[H])N(C([H])([H])[H])C([H])([H])[H])C([H])([H])C2=C([H])C([H])=C([H])C([H])=C2[H])C([H])([H])N3C([H])([H])C4=C([H])C([H])=C([F])C([F])=C4[H]	2.565	2.361
Ext36	O=C3N([H])[C@]([H])(C(=O)N([H])[C@]([H])([C@]([H])(O[H])C([H])([H])N([H])C([H])([H])C1=C([H])C(=C([H])C([H])=C1[H])N(C([H])([H])[H])C([H])([H])[H])C([H])([H])C2=C([H])C([H])=C([H])C([H])=C2[H])C([H])([H])N3C([H])([H])C4=C([H])C([H])=C([F])C([H])=C4[F]	2.062	2.049
Ext37	O=C(N([H])[C@@]([H])(C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])[C@]([H])(O[H])C([H])([H])N([H])C([H])([H])C2=C([H])C([H])=C([H])C(=C2[H])N(C([H])([H])[H])C([H])([H])[H])[C@]3(N([H])C(=O)N(C3([H])[H])C([H])([H])C4=C([H])C([H])=C([H])C([H])=C4[H])C([H])([H])C=5C([H])=C([H])C([H])=C([H])C=5[H]	1.301	1.184
Ext38	O=C1N(C(=N[C@@]1(C=2C([H])=C([H])C([H])=C([H])C=2[H])C3=C([H])C(=C([H])C([H])=C3[H])C4=C([H])N=C([H])C([F])=C4[H])N([H])[H])C([H])([H])[H]	2.538	2.740
Ext39	O=C1N(C(=N[C@@]1(C=2C([H])=C([H])C([H])=C([H])C=2[H])C3=C([H])C(=C([H])C([H])=C3[H])C4=C([H])C(OC([H])([H])[H])=C([H])C([H])=C4[H])N([H])[H])	1.222	2.632

	C([H])([H])[H]		
Ext40	O=C1N(C(=N[C@@]1(C=2C([H])=C(C([H])=C([H])C=2[H])C3=C([H])C([Cl])=C([H])N=C3[H])[C@@]4([H])C([H])([H])C4([H])[H])N([H])[H])C([H])([H])[H]	3.678	2.896
Ext41	O=C1N(C(=N[C@]1(C=2C([H])=C([H])C([H])=C([H])C=2[H])C3=C([H])C([F])=C([H])C([H])=C3[H])N([H])[H])C([H])([H])[H]	2.143	1.637
Ext42	O=C1N(C(=N[C@@]1(/C2=C(\[H])C([H])=C([H])C([H])=C2[H])C3=C([H])C(=C([H])C([H])=C3[H])C4=C([H])C(OC([H])([H])C([H])([H])[H])=C([H])C([H])=C4[H])N([H])[H])C([H])([H])[H]	2.337	2.238
Ext43	O=C1N(C(=N[C@@]1(C=2C([H])=C([H])C([H])=C([H])C=2[H])C3=C([H])C(=C([H])C([H])=C3[H])C([H])([H])[H])N([H])[H])C([H])([H])[H]	2.260	2.310
Ext44	O=C(N([C@@]1([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C1([H])[H])C([H])([H])C2=C(N([H])N=C2[H])C([H])([H])[H])C([H])([H])C([H])([H])[H])[C@]([H])(N5C(=NC=4C([H])=C([H])C(O/C3=C(\[H])C([H])=C([H])C([H])=C3[H])=C([H])C=4C5([H])[H])N([H])[H])[C@@]6([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C6([H])[H]	3.409	3.164
Ext45	O=C(N([C@@]1([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C1([H])[H])C([H])([H])[H])C([H])([H])C([H])([H])[C@]([H])(N4C(=N/C3=C(\[H])C([H])=C(OC=2C([H])=C([H])C([H])=C([H])C=2[H])C([H])=C3C4([H])[H])N([H])[H])[C@]5([H])C([H])([H])OC([H])([H])C([H])([H])C5([H])[H]	2.914	3.847
Ext46	O=C(OC([H])([H])[C@]([H])(N3C(=N/C2=C(\[H])C([H])=C(O/C1=C(\[H])C([H])=C([H])C([H])=C1[H])C([H])=C2C3([H])[H])N([H])[H])[C@@]4([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C4([H])[H])N([H])[C@@]5([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C5([H])[H]	3.222	2.706
Ext47	O=C3N(C(=N[C@](C=1C([H])=C([S]C=1[Cl])C=2C([H])=C(C#CC([H])([H])[H])C([H])=NC=2[H])(C3([H])[H])C([H])([H])[H])N([H])[H])C([H])([H])[H]	4.097	3.896
Ext48	N#CC=1C([H])=C(C([H])=C([H])C=1[H])C=2C([H])=C([S]C=2[H])[C@]3(N=C(N(C(=O)C3([H])[H])C([H])([H])[H])N([H])[H])C([H])([H])[H]	3.244	1.873
Ext49	O=C(O[C@]2([H])[C@@]([H])(OC1=C(C(O[H])=C([H])C(O[H])=C1[H])C2([H])[H])C3=C([H])C(O[H])=C(O[H])C([H])=C3[H])C=4C([H])=C(O[H])C(O[H])=C(O[H])C=4[H]	1.276	2.728
Ext50	O=C(N([H])C3=C([H])C([H])=C2OC([C@]4([C@@]1(N=C(OC1([H])[H])N([H])[H])C2=C3[H])C([H])([H])OC4([H])[H])(C([H])([H])[H])C([H])([H])[H])C=5/N=C(/[H])C([Cl])=C([H])C=5[F]	3.288	2.888
Ext51	[H]/C4=C(/C([H])=C1C(OC([H])([H])[C@]3([C@@]12N=C(OC2([H])[H])N([H])[H])C([H])([H])OC3([H])[H])=C4[H])C5=C([H])N=C([H])C(C#CC([H])([H])[H])=C5[H]	2.910	3.616
Ext52	O=C(N([H])C3=C([H])C([H])=C2OC([C@]4([C@@]1(N=C(OC1([H])[H])N([H])[H])C2=C3[H])C([H])([H])OC4([H])[H])(C([H])([H])[H])C([H])([H])[H])C5=NC([H])=C([Br])C([H])=N5	3.078	2.657
Ext53	O=C(N([H])C3=C([H])C([H])=C2OC([H])([H])[C@@]4([C@@]1(N=C(OC1([H])[H])N([H])[H])C2=C3[H])C([H])([H])C4([H])[H])C5=NC([H])=C([Cl])C([H])=C5C(	2.504	2.395

	[H])([H])[H]		
Ext54	O=C(/C1=N/C([H])=C(C([H])=C1[H])C([H])([H])[H])N([H])C2=C([H])C(=C([F])C([H])=C2[H])[C@]3(N([H])C(=N[H])N([S](=O)(=O)C3([H])[H])C([H])([H])[H])C([H])([H])[H]	4.523	4.046
Ext55	O=C(/C1=N/C([H])=C([F])C([H])=C1[H])N([H])C2=C([F])C(=C([F])C([H])=C2[H])[C@]3(N([H])C(=N[H])N([S](=O)(=O)C3([H])[H])C([H])([H])[H])C([H])([H])[H]	4.312	4.509
Ext56	O=[S]3(=O)N(/C(=N\[H])N([H])[C@](C=1[S]C([H])=C(C=1[H])C2=C([H])C([H])=C([H])C(C#N)=C2[H])(C3([H])[H])C([H])([H])[H])C([H])([H])[H]	3.592	3.122
Ext57	O=C(N([H])[C@]1([H])C([H])([H])C1([H])[H])[C@]([H])(OC([H])([H])[H])C([H])([H])[C@]([H])(O[H])[C@@]([H])(N([H])C(=O)C=2C([H])=C([H])C([H])=C(C=2[H])C(=O)N(C([H])([H])C([H])([H])C([H])([H])[H])C([H])([H])C([H])([H])C([H])([H])[H])C([H])([H])O/C3=C(\[H])C([F])=C([H])C([F])=C3[H]	2.658	2.105
Ext58	O=C(N([H])C(=NC([H])([H])C1=C([H])C([Cl])=C(C([Cl])=C1[H])N([H])[S](=O)(=O)C([H])([H])[H])N([H])[H])C=2C(=N[S]C=2C([H])([H])[H])C3=C([H])C([H])=C(OC([H])([H])[H])C([H])=C3[H]	2.553	4.081
Ext59	O=C(N([H])[C@]([H])(C(=O)N([H])[C@]([H])(C(=O)O[H])C([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])([H])C([H])([H])C(=O)O[H])[C@@]([H])(N([H])C(=O)[C@@]([H])(N([H])C([H])([H])[C@@]([H])(O[H])C(=O)[C@@]([H])(N([H])C(=O)[C@@]([H])(N([H])C(=O)[C@@]([H])(N([H])C(=O)[C@@]([H])(N([H])[H])C([H])([H])C([H])([H])C(=O)O[H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])C(=O)O[H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])(C([H])([H])[H])C([H])([H])[H]~	5.523	6.540

[1]Experimental inhibitory activity; [2]Predicted inhibitory activity