Supplementary material

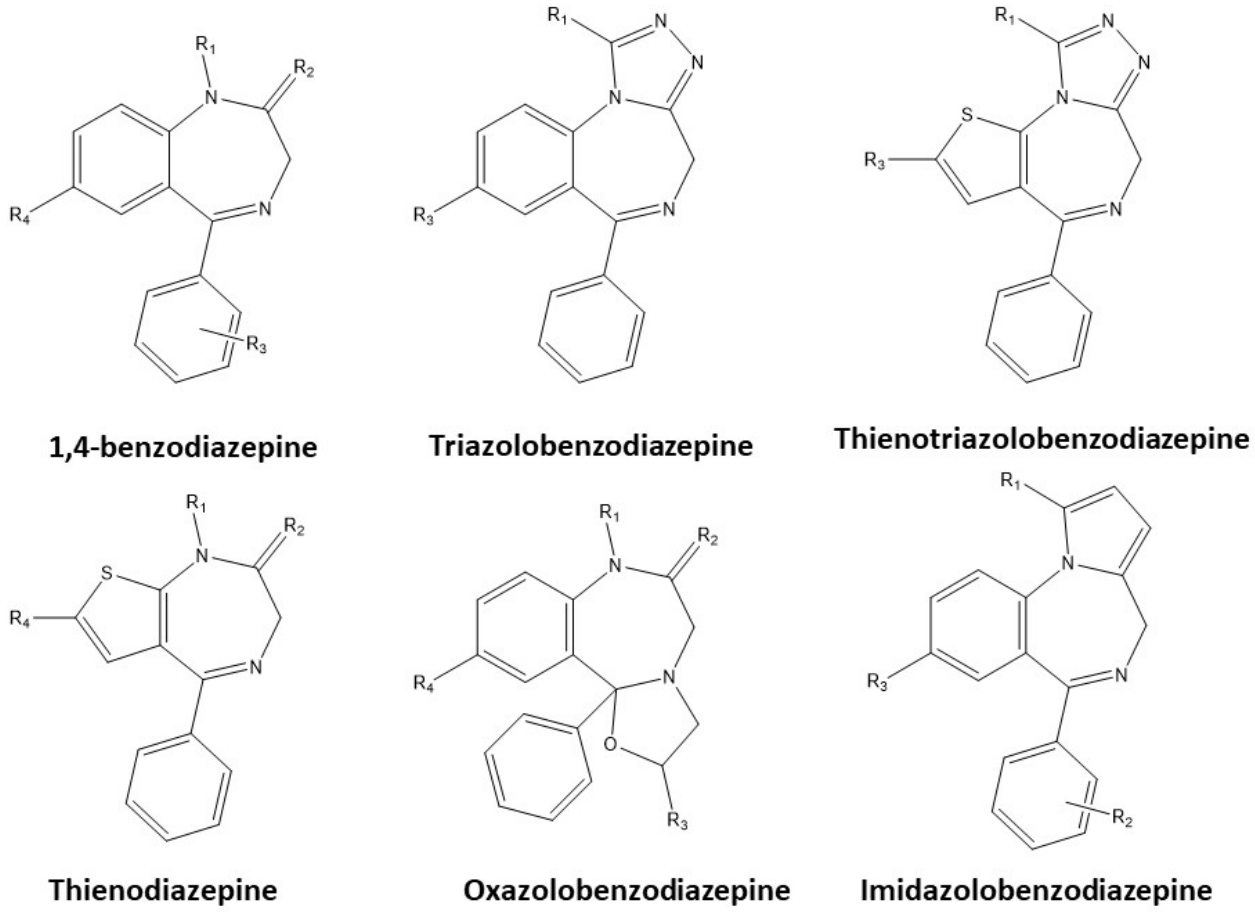

Figure S1 The six different substructural groups of designer benzodiazepines

Table S1 Experimental log1/c values reported for the training and test sets.

Molecule	SMILES	log 1/c
Training set		
Brotizolam	Brc1cc2c(s1)-n3c(nnc3CN=C2c4ccccc4Cl)C	8.92
Meclonazepam	Clc1ccccc1C=2c3cc([N+]([O-])=O)ccc3NC(=O)[C@@H](N2)C	8.92
Ro 11-1465	Clc1cc2c(s1)-n3c(nnc3CN=C2c4ccccc4Cl)C	8.85
Ro 05-4435	Fc1ccccc1C=2c3cc([N+]([O-])=O)ccc3NC(=O)CN2	8.82
Clonazepam	Clc1ccccc1C=2c3cc([N+]([O-])=O)ccc3NC(=O)CN2	8.74
Delorazepam	Clc1ccc2c(C(=NCC(=O)N2)c3ccccc3Cl)c1	8.74
Ro 05-4082	Clc1ccccc1C=2c3cc([N+]([O-])=O)ccc3N(C)C(=O)CN2	8.66
Ro 07-9957	Ic1ccc2c(C(=NCC(=O)N2C)c3ccccc3F)c1	8.54
Etizolam	Clc1ccccc1C=2c3cc(sc3-n4c(nnc4CN2)C)CC	8.51
Ro 11-5073	Clc1ccc-2c(C(=N[C@@H](c3nnc(n23)C)C)c4ccccc4F)c1	8.48
Ro 11-5074	Clc1ccccc1C=2c3cc([N+]([O-])=O)ccc3-n4c(nnc4[C@@H](SC)N2)C	8.47
Lorazepam	Clc1ccc2c(C(=N[C@@H](O)C(=O)N2)c3ccccc3Cl)c1	8.46
Ro 11-4878	Clc1ccc2c(C(=N[C@H](C(=O)N2)C)c3ccccc3F)c1	8.46
Ro 17-4582	Clc1ccccc1C=2c3ccsc3-n4c(nnc4CN2)C	8.46
Flunitrazepam	Fc1ccccc1C=2c3cc([N+]([O-])=O)ccc3N(C)C(=O)CN2	8.42
Ro 11-6679	Fc1ccccc1C=2c3cc([N+]([O-])=O)ccc3-n4c(nnc4[C@@H](SC)N2)C	8.40

Hydroxytriazolam	Clc1ccc-2c(C(=NCc3nnc(n32)CO)c4ccccc4Cl)c1	8.38
Midazolam	Clc1ccc-2c(C(=NCc3cnc(n32)C)c4ccccc4F)c1	8.32
Ro 05-6822	Fc1ccc2c(C(=NCC(=O)N2C)c3ccccc3F)c1	8.29
Ro 14-3074	Fc1ccccc1C=2c3cc(/N=[N+]=[N-])ccc3NC(=O)CN2	8.28
Ro 20-7078	Clc1ccc2c(C(=N[C@H](Cl)C(=O)N2)c3ccccc3F)c1	8.28
Ro 05-6820	Fc1ccc2c(C(=NCC(=O)N2)c3ccccc3F)c1	8.13
Ro 21-5205	Clc1ccc-2c(C(=NCc3c(ncn32)C(OC)=O)c4ccccc4F)c1	8.13
Diazepam	Clc1ccc2c(C(=NCC(=O)N2C)c3ccccc3)c1	8.09
Ro 07-1986	ClN1C(=O)CN=C(c2c1ccc(CC[NH3+])c2)c3ccccc3F	8.08
Estazolam	Clc1ccc-2c(C(=NCc3nncn32)c4ccccc4)c1	8.07
Nordiazepam	Clc1ccc2c(C(=NCC(=O)N2)c3ccccc3)c1	8.03
Ro 22-1892	Clc1ccc-2c(C(=NCc3c(ncn32)C(OC(C)C)=O)c4ccccc4)c1	7.92
Ro 05-2904	FC(F)(F)c1ccc2c(C(=NCC(=O)N2)c3ccccc3)c1	7.89
Ro 16-0529	Clc1cccc-2c1C(=NCc3c(ncn32)C(OCC)=O)c4ccccc4	7.85
Flurazepam	Clc1ccc2c(C(=NCC(=O)N2CC[NH+](CC)CC)c3ccccc3F)c1	7.83
Ro 15-8670	Clc1ccc-2c(C(=NCc3c(ncn32)C(OCC)=O)c4ccccc4)c1	7.82
Ro 05-4865	Fc1ccc2c(C(=NCC(=O)N2C)c3ccccc3)c1	7.77
Oxazepam	Clc1ccc2c(C(=N[C@@H](O)C(=O)N2)c3ccccc3)c1	7.74
Ro 20-3053	Fc1ccccc1C=2c3cc(ccc3NC(=O)CN2)C(=O)C	7.74
Alprazolam	Clc1ccc-2c(C(=NCc3nnc(n32)C)c4ccccc4)c1	7.70
Ro 20-5747	O=C1CN=C(c2cc(ccc2N1)C=C)c3ccccc3	7.62
Ro 07-2750	Clc1ccc2c(C(=NCC(=O)N2CCO)c3ccccc3F)c1	7.61
Ro 20-2541	Fc1ccccc1C=2c3cc(ccc3N(C)C(=O)CN2)C#N	7.52
Desmethyltetrazepam	Clc1ccc2c(C(=NCC(=O)N2)C3=CCCCC3)c1	7.47
Tetrazepam	Clc1ccc2c(C(=NCC(=O)N2C)C3=CCCCC3)c1	7.47
Ro 20-2533	O=C1CN=C(c2cc(CC)ccc2N1)c3ccccc3	7.44
Ro 08-9013	ClN1C(=O)CN=C(c2c1ccc(CCOCC(=O)N)c2)c3ccccc3F	7.37
Ro 06-7263	ClN1C(=O)[C@@H](N=C(c2cc(Cl)ccc21)c3ccccc3)C	7.31
Ro 08-3026	Clc1ccccc1C=2c3c(NC(=O)CN2)ccc(COCC[NH3+])c3	7.20
Ro 20-1815	Fc1ccccc1C=2c3cc(N)ccc3N(C)C(=O)CN2	7.19
Ro 05-4619	Clc1ccccc1C=2c3cc(N)ccc3NC(=O)CN2	7.12
Halazepam	Clc1ccc2c(C(=NCC(=O)N2CC(F)(F)F)c3ccccc3)c1	7.04
Pinazepam	Clc1ccc2c(C(=NCC(=O)N2CC#C)c3ccccc3)c1	7.03
Ro 20-7736	Fc1ccccc1C=2c3cc(NO)ccc3N(C)C(=O)CN2	7.02
Adinazolam	Clc1ccc-2c(C(=NCc3nnc(n32)C[NH+](C)C)c4ccccc4)c1	6.87
Ro 22-4683	Fc1ccccc1C=2c3cc([N+]([O-])=O)ccc3N(C(C)(C)C)C(=O)CN2	6.52
Ro 05-4528	O=C1CN=C(c2cc(ccc2N1C)C#N)c3ccccc3	6.42
Ro 12-6377	Fc1ccccc1C=2c3cc(NC(=O)NC)ccc3N(C)C(=O)CN2	6.34
Ro 20-1310	Clc1ccc2c(C(=NCC(=O)N2C(C)(C)C)c3ccccc3)c1	6.21
Camazepam	Clc1ccc2c(C(=N[C@@H](OC(=O)N(C)C)C(=O)N2C)c3ccccc3)c1	6.05
Prazepam	Clc1ccc2c(C(=NCC(=O)N2CC3CC3)c4ccccc4)c1	6.96
Ro 05-2921	O=C1CN=C(c2ccccc2N1)c3ccccc3	6.45
7-Aminonitrazepam	O=C1CN=C(c2cc(N)ccc2N1)c3ccccc3	6.41
Norfludiazepam	Clc1ccc2c(C(=NCC(=O)N2)c3ccccc3F)c1	8.70
Ro 05-4336	Fc1ccccc1C=2c3ccccc3NC(=O)CN2	6.51
Ro 05-4520	Fc1ccccc1C=2c3ccccc3N(C(=O)CN2)C	7.47

Proflazepam	Clc1ccc2c(C(=NCC(=O)N2C[C@@H](O)CO)c3ccccc3F)c1	6.85
Triazolam	Clc1ccc-2c(C(=NCc3nnc(n32)C)c4ccccc4Cl)c1	8.40
4-hydroxymidazolam	Clc1ccc-2c(C(=NCc3cnc(n32)CO)c4ccccc4F)c1	8.35
Test set		
Ro 14-1636	Ic1cc2c(s1)-n3c(nnc3CN=C2c4ccccc4Cl)C	8.82
Ro 11-7800	Clc1cc2c(s1)-n3c(nnc3C[NH3+])CN=C2c4ccccc4Cl	8.54
Ro 05-3590	FC(F)(F)c1ccccc1C=2c3cc([N+]([O-])=O)ccc3NC(=O)CN2	8.46
U-35005	Clc1ccc-2c(C(=NCc3nnc(n32)C)c4ccccc4Cl)c1	8.37
Ro 11-6896	Fc1ccccc1C=2c3cc([N+]([O-])=O)ccc3N(C(=O)[C@@H](N2)C)C	8.15
Nitrazepam	O=C1CN=C(c2cc([N+]([O-])=O)ccc2N1)c3ccccc3	8.00
Temazepam	Clc1ccc2c(C(=N[C@@H](O)C(=O)N2C)c3ccccc3)c1	7.80
Ro 21-8482	Clc1ccc-2c(C(=NCc3c(nc(n32)C)C(=O)N)c4ccccc4Cl)c1	7.59
Ro 05-3061	Fc1ccc2c(C(=NCC(=O)N2)c3ccccc3)c1	7.40
Ro 05-3328	Clc1ccc2c(C(=NCC(=O)N2C)C3CCCCC3)c1	7.06
Ro 17-2221	O=C1CN=C(c2c(N1)ccc(CC[NH3+])c2)c3ccccc3	6.59
Ro 06-9098	O=C1CN=C(c2cc([N+]([O-])=O)ccc2N1COC)c3ccccc3	6.37

Notes. The 75 are listed in decreasing order of log1/c

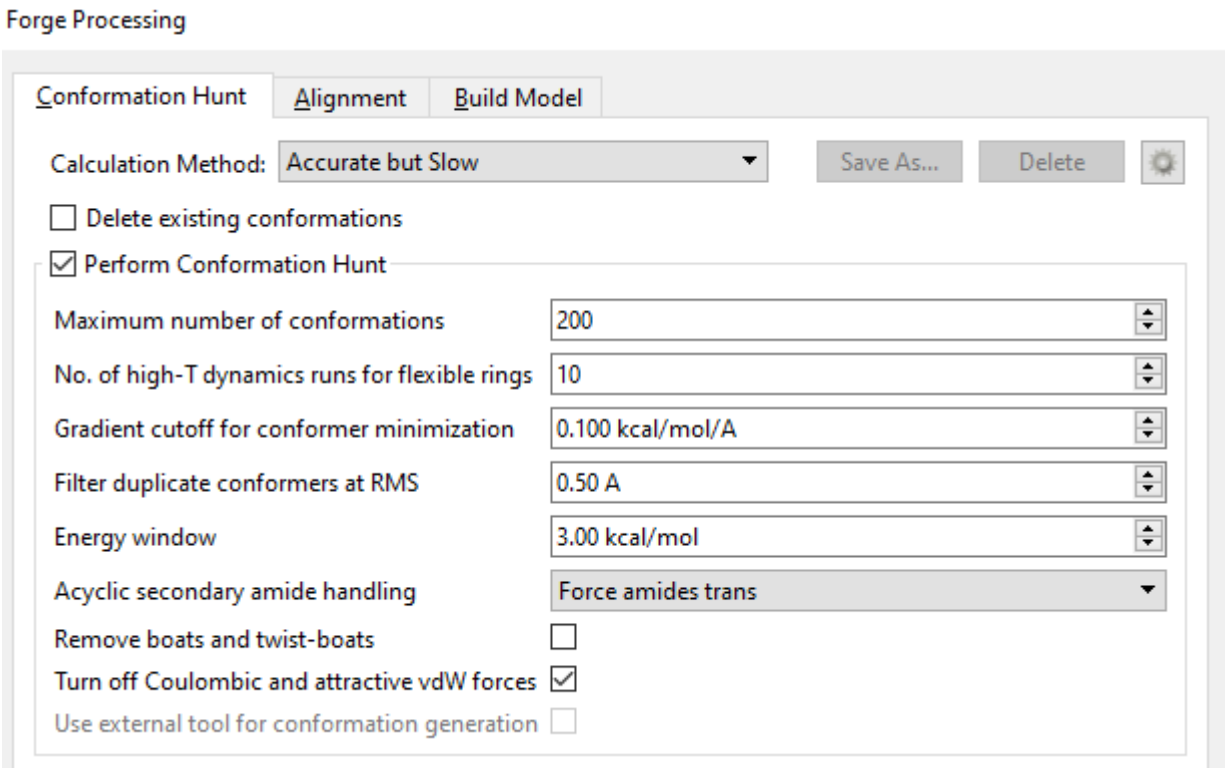

Figure S2 Parameters used for the Conformational hunt in Forge™

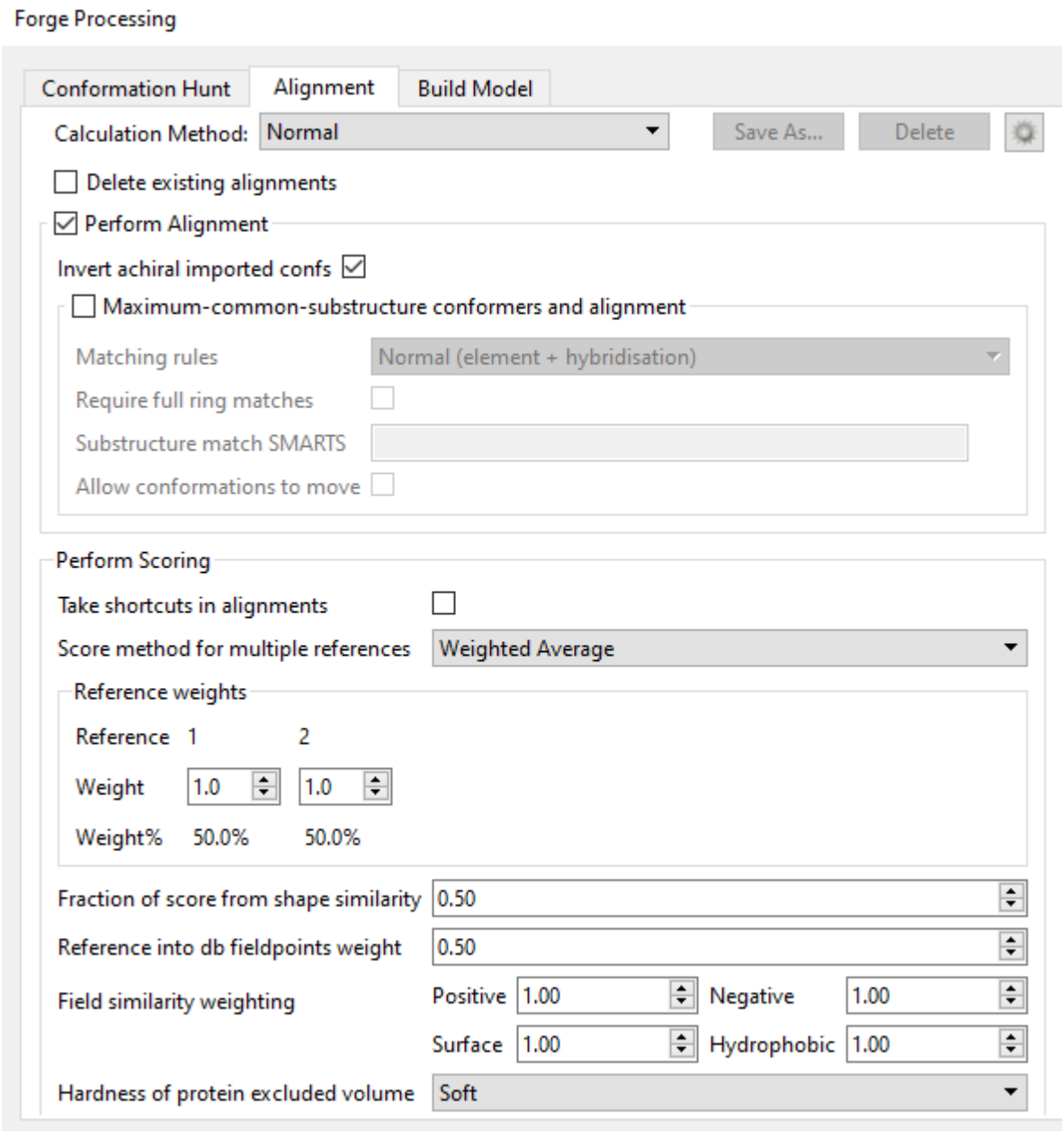

Figure S3 Parameters used for the alignment process in Forge™

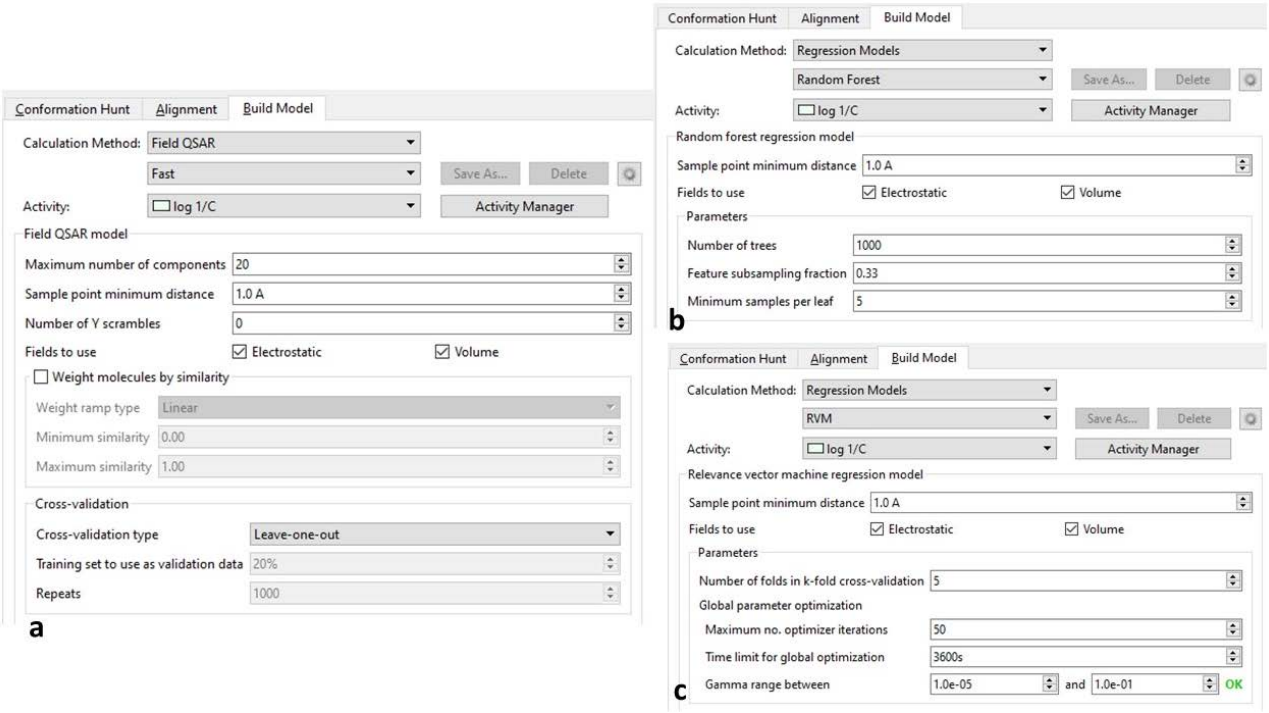

Figure S4 Parameters used for the model building process in Forge™

Table S2 Statistics for the 20 3D Field QSAR models generated.

Comps	r^2	q^2	r^2 Test	RMSE	Tau
0	0.00	-0.03	0.00	0.77	-0.99
1	0.64	0.39	0.55	0.59	0.46
2	0.80	0.61	0.71	0.47	0.62
3	0.85	0.64	0.78	0.46	0.65
4	0.92	0.69	0.81	0.43	0.67
5	0.96	0.70	0.80	0.42	0.70
6	0.97	0.73	0.80	0.39	0.71
7	0.97	0.75	0.79	0.38	0.72
8*	0.98	0.75	0.82	0.38	0.72
9	0.99	0.75	0.81	0.38	0.71
10	0.99	0.73	0.82	0.39	0.71
11	0.99	0.74	0.82	0.39	0.71
12	1.00	0.73	0.84	0.39	0.71
13	1.00	0.73	0.83	0.39	0.71
14	1.00	0.73	0.83	0.40	0.70
15	1.00	0.71	0.83	0.41	0.70
16	1.00	0.70	0.82	0.42	0.69
17	1.00	0.69	0.81	0.42	0.68
18	1.00	0.69	0.81	0.43	0.69
19	1.00	0.68	0.81	0.03	0.43
20	1.00	0.68	0.81	0.02	0.43

Notes. Here are presented the statistic of the 3D Field QSAR models generated in the form of : the coefficient of determination (r2) which indicates the goodness of fit; the cross-validated coefficient of determination (q2) which

indicates the robustness ; the coefficient of determination for the test set (r2 test), which indicates the predictive power; the root mean square error (RMSE) as reliability measure; and Tau as a further parameter to assess the predictivity of the model. The chosen model is highlighted in red.

Table S3 Predicted values for 99 classified/ unclassified DBZDs identified on-line.

Molecule	SMILES	pred log1/c
Flubrotizolam	Brc1cc2c(s1)-n3c(nnc3CN=C2c4ccccc4F)C	9.6
Clonazolam	Clc1ccccc1C=2c3cc([N+]([O-])=O)ccc3-n4c(nnc4CN2)C	9.5
Pynazolam	[O-][N+](=O)c1ccc-2c(C(=NCc3nnc(n32)C)c4ccccn4)c1	9.4
Fluclotizolam	Clc1cc2c(s1)-n3c(nnc3CN=C2c4ccccc4F)C	9.1
MP-III-022	Fc1ccccc1C=2c3cc(ccc3-n4cnc(c4[C@@H](N2)C)C(=O)NC)C#C	9.1
Ro 09-9212	Clc1cc2c(s1)NC(=O)CN=C2c3ccccc3Cl	9.0
Desmethylnitrazolam	[O-][N+](=O)c1ccc-2c(C(=NCc3nncn32)c4ccccc4)c1	8.8
Imidazenil	Brc1ccccc1C=2c3cc(F)ccc3-n4cnc(c4CN2)C(=O)N	8.8
Flunitrazolam	Fc1ccccc1C=2c3cc([N+]([O-])=O)ccc3-n4c(nnc4CN2)C	8.8
Zapizolam	Clc1ccccc1C=2c3c(-n4cnnc4CN2)ccc(Cl)n3	8.8
Fluetizolam	Fc1ccccc1C=2c3cc(sc3-n4c(nnc4CN2)C)CC	8.8
Flubromazolam	Brc1ccc-2c(C(=NCc3nnc(n32)C)c4ccccc4F)c1	8.8
Etizolam	Clc1ccccc1C=2c3cc(sc3-n4c(nnc4CN2)C)CC	8.7
3-Hydroxyphenazepam	Brc1ccc2c(C(=N[C@@H](O)C(=O)N2)c3ccccc3Cl)c1	8.7
Cinolazepam	Clc1ccc2c(C(=N[C@H](O)C(=O)N2CCC#N)c3ccccc3F)c1	8.7
Methyl Clonazepam	Clc1ccccc1C=2c3cc([N+]([O-])=O)ccc3N(C)C(=O)CN2	8.7
Ro 15-9270	Clc1ccccc1C2=CCc3nnc(n3-c4ccc([N+]([O-])=O)cc42)C	8.6
Metizolam	Clc1ccccc1C=2c3cc(sc3-n4cnnc4CN2)CC	8.6
Mexazolam	Clc1ccc2c([C@@]3([NH+]([C@H](CO3)C)CC(=O)N2)c4ccccc4Cl)c1	8.6
Nifoxipam	Fc1ccccc1C=2c3cc([N+]([O-])=O)ccc3NC(=O)[C@H](O)N2	8.5
Nitrazolam	[O-][N+](=O)c1ccc-2c(C(=NCc3nnc(n32)C)c4ccccc4)c1	8.5
Estazolam	Clc1ccc-2c(C(=NCc3nncn32)c4ccccc4)c1	8.5
Deschloroetizolam	Cc1nnc2CN=C(c3cc(sc3-n12)CC)c4ccccc4	8.5
Bromazolam	Brc1ccc-2c(C(=NCc3nnc(n32)C)c4ccccc4)c1	8.5
Bentazepam	O=C1CN=C(c2c(sc3CCCCc23)N1)c4ccccc4	8.5
Ro 20-8552	Clc1c(cc2c(NC(=O)CN=C2c3ccccc3F)c1)C	8.4
Phenazepam	Brc1ccc2c(C(=NCC(=O)N2)c3ccccc3Cl)c1	8.4
Triflubazam	FC(F)(F)c1ccc2c(N(C(=O)CC(=O)N2C)c3ccccc3)c1	8.4

Ro 20-8065	Clc1c(Cl)cc2c(C(=NCC(=O)N2)c3ccccc3F)c1	8.3
Ro 07-3953	Clc1ccc2c(C(=NCC(=O)N2)c3c(F)cccc3F)c1	8.3
Desmethyltriazolam	Clc1ccc-2c(C(=NCc3nncn32)c4ccccc4Cl)c1	8.3
Flualprazolam	Clc1ccc-2c(C(=NCc3nnc(n32)C)c4ccccc4F)c1	8.3
Arfendazam	Clc1ccc2c(N(C(=O)CCN2C(OCC)=O)c3ccccc3)c1	8.3
Remimazolam	Brc1ccc-2c(C(=N[C@H](c3ncc(n23)C)CCC(OC)=O)c4ccccn4)c1	8.3
Ro 07-5193	Clc1ccc2c(C(=NCC(=O)N2)c3c(F)cccc3Cl)c1	8.2
Difludiazepam-	Clc1ccc2c(C(=NCC(=O)N2C)c3c(F)cccc3F)c1	8.2
Phenazolam	Brc1ccc-2c(C(=NCc3nnc(n32)C)c4ccccc4Cl)c1	8.2
Pyclazolam	Clc1ccc-2c(C(=NCc3nnc(n23)C)c4ccccn4)c1	8.2
Thionordazepam	Clc1ccc2c(C(=NCC(=S)N2)c3ccccc3)c1	8.2
Climazolam	Clc1ccc-2c(C(=NCc3cnc(n32)C)c4ccccc4Cl)c1	8.1
Pyrazolam	Brc1ccc-2c(C(=NCc3nnc(n23)C)c4ccccn4)c1	8.1
Flutemazepam	Clc1ccc2c(C(=N[C@@H](O)C(=O)N2C)c3ccccc3F)c1	8.1
Clazolam	Clc1ccc2c([C@H]3c4ccccc4CC[NH+]3CC(=O)N2C)c1	8.1
Flutazolam	Clc1ccc2c([C@@]3([NH+](CCO3)CC(=O)N2CCO)c4ccccc4F)c1	8.1
Zomebazam	O=C1CC(=O)N(c2c(N1c3ccccc3)c(nn2C)C)C	8.1
Ro 07-5220	Clc1ccc2c(C(=NCC(=O)N2C)c3c(Cl)cccc3Cl)c1	8.0
Ciclotizolam	Brc1cc2C(=NCc3nnc(n3-c2s1)C4CCCCC4)c5ccccc5Cl	8.0
Triflunordazepam	FC(F)(F)c1ccc2c(C(=NCC(=O)N2)c3ccccc3)c1	8.0
Ethyl Carfluzepate	Clc1ccc2c(C(=N[C@H](C(=O)N2C(=O)NC)C(OCC)=O)c3ccccc3F)c1	8.0
Fluloprazolam	Fc1ccccc1C=2c3cc([N+]([O-])=O)ccc3N4C(=N/C(=C/N5CC[NH+](CC5)C)C4=O)CN2	8.0
Cinazepam	Brc1ccc2c(C(=N[C@H](OC(=O)CCC([O-])=O)C(=O)N2)c3ccccc3Cl)c1	8.0
Ro 13-3780	Brc1ccc2c(C(=NCC(=O)N2C)c3c(F)cccc3F)c1	7.9
Menitrazepam	O=C1CN=C(C2=CCCCC2)c3cc([N+]([O-])=O)ccc3N1C	7.9
CP-1414s	O=C1CC(=[NH+]c2ccc([N+]([O-])=O)cc2N1c3ccccc3)N	7.9
Carburazepam	Clc1ccc2c([C@H](N(CC(=O)N2C)C(=O)N)c3ccccc3)c1	7.9
Sh-053-R-Ch3-2?F	Fc1ccccc1C=2c3cc(ccc3-n4cnc(c4[C@H](N2)C)C(OCC)=O)C#C	7.9
Pyeazolam	Cc1nnc2CN=C(c3cc(ccc3-n12)C#C)c4ccccn4	7.9
Ripazepam	O=C1CN=C(c2c(N1)c(nn2CC)C)c3ccccc3	7.9
7-BPDBD	Brc1ccc2c(C(=NCC(=O)N2)c3ccccc3)c1	7.8
Cloniprazepam	Clc1ccccc1C=2c3cc([N+]([O-])=O)ccc3N(CC4CC4)C(=O)CN2	7.8
Diclazepam	Clc1ccc2c(C(=NCC(=O)N2C)c3ccccc3Cl)c1	7.8

Ro 48-6791	Fc1ccc-2c(c1)C(=O)N(Cc3c(ncn23)-c4noc(n4)C[NH+](CCC)CCC)C	7.8
Sulazepam	Clc1ccc2c(C(=NCC(=S)N2C)c3ccccc3)c1	7.7
Tuclazepam	Clc1ccc2c(C(=NC[C@@H](N2C)CO)c3ccccc3Cl)c1	7.7
Doxefazepam	Clc1ccc2c(C(=N[C@@H](O)C(=O)N2CCO)c3ccccc3F)c1	7.7
Flupyrazapon	Fc1ccccc1C=2c3c(nn(c3N(C)C(=O)CN2)C)C	7.7
Reclazepam	Clc1ccc2c(C(=NCCN2C3=NC(=O)CO3)c4ccccc4Cl)c1	7.6
Lofendazam	Clc1ccc2c(N(C(=O)CCN2)c3ccccc3)c1	7.6
Uldazepam	Clc1ccc2c(C(=NCC(NOCC=C)=N2)c3ccccc3Cl)c1	7.6
Flubromazepam	Brc1ccc2c(C(=NCC(=O)N2)c3ccccc3F)c1	7.6
Ro 07-9749	Ic1ccc2c(C(=NCC(=O)N2)c3ccccc3F)c1	7.6
Premazepam	O=C1CN=C(c2c(N1)cn(c2C)C)c3ccccc3	7.6
Tofisopam	CC[C@@H]1C(=NN=C(c2cc(OC)c(OC)cc21)c3ccc(OC)c(OC)c3)C	7.5
Ethyl Dirazepate	Clc1ccc2c(C(=N[C@@H](C(=O)N2)C(OCC)=O)c3ccccc3Cl)c1	7.5
Ro 21-8137	Clc1ccc-2c(C(=NCc3c(ncn32)C(=O)N)c4ccccc4F)c1	7.5
FG-8205	Clc1cccc-2c1C(=O)N(Cc3c(ncn23)-c4noc(n4)C(C)C)C	7.5
Fletazepam	Clc1ccc2c(C(=NCC(=O)N2CC(F)(F)F)c3ccccc3F)c1	7.4
Lopirazepam	Clc1ccccc1C=2c3c(NC(=O)[C@H](O)N2)ccc(Cl)n3	7.4
N-Methylbromazepam	Brc1ccc2c(C(=NCC(=O)N2C)c3ccccn3)c1	7.4
QH-II-066	O=C1CN=C(c2cc(ccc2N1C)C#C)c3ccccc3	7.4
Rilmazolam	Clc1ccc-2c(C(=NCc3nc(nn32)C(=O)N(C)C)c4ccccc4Cl)c1	7.3
Fosazepam	Clc1ccc2c(C(=NCC(=O)N2CP(=O)(C)C)c3ccccc3)c1	7.3
Quazepam	Clc1ccc2c(C(=NCC(=S)N2CC(F)(F)F)c3ccccc3F)c1	7.3
Ro 05-4608	Clc1ccccc1C=2c3ccccc3N(C(=O)CN2)C	7.2
Iomazenil	Ic1cccc-2c1C(=O)N(Cc3c(ncn23)C(OCC)=O)C	7.2
4’-Chlorodiazepam	Clc1ccc2c(C(=NCC(=O)N2C)c3ccc(Cl)cc3)c1	7.2
JQ1	Clc1ccc(C=2c3c(c(sc3-n4c(nnc4[C@@H](N2)CC(OC(C)(C)C)=O)C)C)C)cc1	7.2
Ro 17-1812	Clc1cccc-2c1C(=O)N3CC[C@H]3c4c(ncn24)C(OCC5CC5)=O	7.1
Zometapine	Clc1cccc(C=2c3c(n(nc3C)C)NCCN2)c1	7.1
Fluadinazolam	Clc1ccc-2c(C(=NCc3nnc(n32)C[NH+](C)C)c4ccccc4F)c1	7.1
Pivoxazepam	Clc1ccc2c(C(=N[C@@H](OC(=O)C(C)(C)C)C(=O)N2)c3ccccc3)c1	7.0
Ro 15-4941	Clc1cccc-2c1C(=O)N3CCC[C@H]3c4c(ncn24)C(OCC)=O	7.0
Tolufazepam	Clc1ccc2c(C(=NCC(=O)N2CCS(=O)(=O)c3ccc(cc3)C)c4ccccc4Cl)c1	7.0
7-Aminoflunitrazepam	Fc1ccccc1C=2c3cc(N)ccc3N(C)C(=O)CN2	6.9

Elfazepam	Clc1ccc2c(C(=NCC(=O)N2CCS(=O)(=O)CC)c3ccccc3F)c1	6.9
Cyprazepam	Clc1ccc2c(C(=[N+]([O-])CC(NCC3CC3)=[NH+]2)c4ccccc4)c1	6.9
Ro 48-8684	Fc1ccc-2c(c1)C(=O)N(Cc3c(ncn23)-c4ncc(o4)C[NH+](CCC)CCC)C	6.8
Metaclazepam	Brc1ccc2c(C(=NC[C@@H](N2C)COC)c3ccccc3Cl)c1	6.8
Flutoprazepam	Clc1ccc2c(C(=NCC(=O)N2CC3CC3)c4ccccc4F)c1	6.6
Pwz-029	Clc1ccc-2c(c1)C(=O)N(Cc3c(ncn23)COC)C	6.6
Gidazepam	Brc1ccc2c(C(=NCC(=O)N2CC(=O)NN)c3ccccc3)c1	6.4
Devazepide	O=C1[C@@H](NC(=O)c2cc3ccccc3[nH]2)N=C(c4ccccc4N1C)c5ccccc5	6.2

The entries are ranked for decreasing values of pred log 1/c.