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Synthesis, Characterization, Antimicrobial and Antibiofilm Activity, Molecular Docking Analysis of NHC Precursors and Their Ag-NHC Complexes

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Supplementary Files

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Figure S1. ¹H and ¹³C{¹H} NMR spectrums of 1



Figure S2. FT-IR spectrum of 1



Figure S3. ¹H and ¹³C{¹H} NMR spectrums of 1a



Figure S4. FT-IR spectrum of 1a



Figure S5. ¹H and ¹³C{¹H} NMR spectrums of **1b**



Figure S6. FT-IR spectrum of 1b



Figure S7. ¹H and ¹³C{¹H} NMR spectrums of **1**c



Figure S8. FT-IR spectrum of 1c







Figure S10. FT-IR spectrum of 1d







Figure S12. FT-IR spectrum of 2a



Figure S13. LC-MS spectrum of 2a







Figure S15. FT-IR spectrum of 2b



Figure S16. LC-MS spectrum of 2b



Figure S17. ¹H and ¹³C{¹H} NMR spectrums of 2c



Figure S18. FT-IR spectrum of 2c



Figure S19. LC-MS spectrum of 2c



Figure S20. ¹H and ¹³C{¹H} NMR spectrums of 2d



Figure S21. FT-IR spectrum of 2d



Figure S22. LC-MS spectrum of 2d

Parameters	2b	2c	2d
Bond lengths (Å)			
Ag1–Cl1	2.382	2.367	2.371
Ag1–C1	2.144	2.138	2.138
N1C1	1.366	1.361	1.362
N1-C2	1.402	1.402	1.402
N1-C10	1.478	1.472	1.464
N2-C1	1.361	1.365	1.364
N2–C9	1.402	1.402	1.403
N2-C13	1.464	1.474	1.475
Bond angles (°)			
Cl1-Ag1-C1	170.5	169.5	169.6
Ag1-C1-N1	125.3	124.3	128.3
Ag1-C1-N2	127.7	128.7	124.8
N1-C1-N2	107.0	106.9	106.9
C1-N1-C2	110.3	110.4	110.5
C1-N1-C10	125.8	124.2	124.2
C2-N1-C10	123.8	125.4	125.3
C1-N2-C9	110.5	110.4	110.4
C1-N2-C13	124.4	125.7	125.8
C9–N2–C13	125.2	123.9	123.8

Table S1. Selected optimization results for 2b, 2c and 2d.



Atom(labe	x	У	Z
)			
H(1)	-0.5369	-0.8091	-1.8930
N(2)	-0.6675	0.4587	-0.1464
N(3)	1.1842	-0.6792	-0.5704
C(4)	0.2332	0.7596	0.8846
C(5)	1.4141	0.0287	0.6180
C(6)	-0.0679	-0.4019	-0.9907
C(7)	-2.7616	0.5215	-1.5097
C(8)	0.1315	1.5959	2.0080
H(9)	-0.7842	2.1668	2.2191
C(10)	2.5274	0.1076	1.4689
H(11)	3.4407	-0.4717	1.2719
C(12)	-2.0435	1.0092	-0.2733
H(13)	-1.9451	2.1143	-0.2749
H(14)	-2.5889	0.7205	0.6489
C(15)	2.4421	0.9404	2.5972
C(16)	1.2391	1.6892	2.8675
C(17)	-2.6675	1.2423	-2.7205
C(18)	-3.5209	-0.6685	-1.4711
C(19)	-4.0665	-0.4126	-3.8294
C(20)	2.1222	-1.5943	-1.2324
H(21)	3.1198	-1.1038	-1.2332
H(22)	1.8232	-1.6649	-2.2999
C(23)	-4.1692	-1.1338	-2.6268
H(24)	-4.7652	-2.0579	-2.5857
C(25)	-3.3178	0.7766	-3.8747
H(26)	-3.2489	1.3502	-4.8113
C(27)	3.6170	1.0480	3.5366
H(28)	4.4682	0.4270	3.2006
H(29)	3.3445	0.7250	4.5636
H(30)	3.9730	2.0961	3.6232
H(31)	-3.6184	-1.2283	-0.5267
C(32)	1.1705	2.5811	4.0814
H(33)	0.1900	3.0859	4.1651
H(34)	1.9561	3.3654	4.0513
H(35)	1.3381	2.0070	5.0168
H(36)	-2.0947	2.1829	-2.7567
H(37)	-4.5804	-0.7734	-4.7331
C(38)	2.2055	-2.9695	-0.6125
H(39)	2.9687	-3.6158	-1.0805
C(40)	1.4584	-3.4367	0.4001
H(41)	0.6894	-2.8259	0.9010
H(42)	1.5954	-4.4623	0.7736

Table S3. Calculated Cartesian Coordinates of 1b



Atom(label)	х	У	Z
N(1)	-0.0652	0.4421	0.2988
N(2)	1.7475	-0.7746	-0.0746
C(3)	0.8572	0.7788	1.2985
C(4)	2.0137	-0.0010	1.0643
C(5)	0.4974	-0.4862	-0.4960
C(6)	-2.1765	0.4664	-1.0468
C(7)	0.7935	1.6835	2.3704
H(8)	-0.1045	2.2906	2.5558
C(9)	3.1398	0.0982	1.8962
H(10)	4.0338	-0.5184	1.7251
C(11)	-1.4315	1.0198	0.1449
H(12)	-1.2979	2.1173	0.0742
H(13)	-1.9643	0.8120	1.0940
C(14)	3.0921	1.0000	2.9725
C(15)	1.9136	1.7966	3.2110
C(16)	-2.0725	1.1144	-2.3113
C(17)	-2.9814	-0.6973	-0.8999
C(18)	-3.5776	-0.5761	-3.2896
C(19)	2.6476	-1.7574	-0.6896
H(20)	3.6605	-1.3010	-0.7314
H(21)	2.3328	-1.8826	-1.7474
C(22)	-3.6637	-1.1948	-2.0274
H(23)	-4.2913	-2.0934	-1.9133
C(24)	-2.7759	0.5786	-3.4055
H(25)	-2.7025	1.0852	-4.3816
C(26)	4.2817	1.1305	3.8908
H(27)	5.1123	0.4688	3.5817
H(28)	4.0142	0.8746	4.9381
H(29)	4.6659	2.1721	3.9126
C(30)	-3.1412	-1.3950	0.4348
H(31)	-3.7549	-2.3095	0.3314
H(32)	-3.6498	-0.7463	1.1805
H(33)	-2.1712	-1.7025	0.8800
C(34)	1.8823	2.7577	4.3723
H(35)	0.9157	3.2916	4.4374
H(36)	2.6867	3.5190	4.2903
H(37)	2.0463	2.2338	5.3375
C(38)	-1.2496	2.3728	-2.4970
H(39)	-1.6617	3.2236	-1.9122
H(40)	-1.2397	2.6874	-3.5577
H(41)	-0.1914	2.2475	-2.1835
C(42)	-4.3127	-1.1298	-4.4861
H(43)	-4.8602	-0.3314	-5.0272
H(44)	-5.0403	-1.9119	-4.1961
H(45)	-3.6052	-1.5821	-5.2141
C(46)	2.6951	-3.0953	0.0105
H(47)	3.4135	-3.8017	-0.4414
C(48)	1.9663	-3.4673	1.0744
H(49)	1.2432	-2.7928	1.5621
H(50)	2.0728	-4.4736	1.5060
H(51)	-0.0002	-0.9307	-1.3656

Table S4. Calculated	rtesian Coordinates of 1c
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	60		
Atom(label)	х	y	Z
H(1)	-0.7279	1.3572	0.1074
N(2)	0.1404	-0.6137	-0.0301
N(3)	-0.0263	0.3986	1.9333
C(4)	0.6754	-1.4921	0.9211
C(5)	0.5735	-0.8458	2.1756
C(6)	1.2258	-2.7786	0.8056
H(7)	1.3048	-3.2836	-0.1679
C(8)	-0.2652	0.4990	0.6084
C(9)	1.6769	-3.4155	1.9740
C(10)	-0.5823	0.2796	-2.2618
C(11)	0.2628	1.3010	-2.7835
C(12)	0.0319	-0.8715	-1.4919
H(13)	-0.5621	-1.7991	-1.6041
H(14)	1.0544	-1.0993	-1.8501
C(15)	1.5735	-2.7569	3.2528
C(16)	1.0215	-1.4682	3.3517
H(17)	0.9560	-0.9633	4.3249
C(18)	-0.3164	2.3384	-3.5620
C(19)	-2.5573	1.3387	-3.2542
C(20)	-1.9925	0.2984	-2.4697
C(21)	-0.3344	1.4380	2.9369
H(22)	-0.9629	0.9791	3.7280
H(23)	-0.9609	2.1936	2.4168
C(24)	-1.7055	2.3279	-3.7780
H(25)	-2.1474	3.1327	-4.3887
C(26)	2.0654	-3.4543	4.4965
H(27)	1.5300	-4.4122	4.6637
H(28)	3.1431	-3.7094	4.4193
H(29)	1.9285	-2.8276	5.3977
C(30)	1.7609	1.3218	-2.5623
H(31)	2.1213	0.5909	-1.8146
H(32)	2.3116	1.1226	-3.5074
H(33)	2.1002	2.3221	-2.2220
C(34)	2.2743	-4./979	1.8884
H(35)	1.7008	-5.525/	2.4999
H(36)	2.2951	-5.1/16	0.8474
H(37)	3.3142	-4.8134	2.2758
U(38)	-2.9069	-U.//18	-1.9093
П(39) П(40)	-2.4779	-1.3138	-1.0492
П(4U) Ц(41)	-3.8052	-0.3384	-1.3020
⊓(4⊥) C(42)	-3.1/13	-1.52/4	-2.001/
U(42)	-4.0392 1 6115	1.2023 1 1001	-3.3433
п(45) ц(44)	-4.0445 1 2002	1.4004 2.2176	-2.019U
П(44) Ц(ЛЕ)	-4.2892 1 2027	2.24/0	-4.1985
r1(45) C(46)	-4.3927	0.40/3	-4.0540
U(40)	0.535/	3.4283 2.0054	-4.10/3
П(47) Ц(48)	1.0986	3.9954	-3.3940
H(48)	1.2959	3.018/	-4.8663
H(49)	-0.0807	4.1542	-4./313
C(50)	0.9000	2.0783	3.5228
H(51)	1.6209	2.4936	2.7963
C(52)	1.1200	2.2059	4.8423
H(53)	0.4123	1.8138	5.5925
H(54)	2.0124	2.7253	5.2242

 Table S5. Calculated Cartesian Coordinates of 1d

	6. ⁰		
	e e		
Atom(label)	x	у	Z
C(1)	0.9347	-0.0302	-0.3728
C(2)	2.2588	1.6414	0.2768
C(3)	3.2890	2.5719	0.4853
H(4)	4.2263	2.5284	-0.0880
C(5)	3.0890	3.5804	1.4430
C(6)	4.1743	4.5979	1.6913
H(7)	5.0605	4.4161	1.0547
H(8)	4.5090	4.5846	2.7500
H(9)	3.8168	5.6297	1.4890
C(10)	1.8550	3.0532	2.1850
U(12)	1.0093	4.7438	3.2089
П(12) Ц(12)	2.4520	4.0902	4.0050
П(13) Ц(14)	1 7/56	4.0738 5 7517	2 7506
C(15)	0.8310	2 7158	1 9631
H(16)	-0 1096	2.7150	2 5281
C(17)	1 0478	1 7126	1 0046
C(18)	3.1499	0.0683	-1.5381
H(19)	4.1419	0.1122	-1.0380
H(20)	2.9600	-1.0097	-1.7283
C(21)	3.1742	0.8378	-2.8379
H(22)	3.9643	0.5012	-3.5321
C(23)	2.3504	1.8365	-3.1921
H(24)	1.5528	2.2102	-2.5290
H(25)	2.4491	2.3274	-4.1716
C(26)	-1.1185	0.3184	1.0570
H(27)	-1.7431	1.2123	0.8680
H(28)	-1.0373	0.2108	2.1557
C(29)	-1.7047	-0.9203	0.4134
C(30)	-2.4934	-0.7918	-0.7658
U(31)	-2.7034 2 E 0 2 7	0.5544	-1.4303
п(32) ц(22)	-2.5827	0.4814	-2.3333
H(33)	-1.9927	1.5500	-1.0558
C(35)	-3 0971	-1 9489	-1 3185
C(36)	-3.9973	-1.8514	-2.5329
H(37)	-3.5127	-2.2712	-3.4421
H(38)	-4.2941	-0.8151	-2.7684
H(39)	-4.9315	-2.4297	-2.3877
C(40)	-2.8736	-3.2286	-0.7328
C(41)	-3.5029	-4.4309	-1.4036
H(42)	-4.6063	-4.4442	-1.2625
H(43)	-3.1149	-5.3920	-1.0270
H(44)	-3.3303	-4.4147	-2.4986
C(45)	-2.0839	-3.3495	0.4417
C(46)	-1.8679	-4.6759	1.1398
H(47)	-2.4517	-5.5000	0.6973
H(48)	-2.1585	-4.6163	2.2093
п(49) С(50)	-0./995	-4.9829 _2 1010	1.1203
C(51)	-1.4022	-2.1910	2 2520
H(52)	-0.0680	-1.4560	2.5390
H(53)	0.1076	-3,1748	2.1255
H(54)	-1.2525	-2.6486	3.1308
H(55)	0.5481	-0.9158	-0.8901
N(56)	2.1478	0.5295	-0.5704
N(57)	0.2497	0.6478	0.5650



Atom(label)	х	У	Z
Ag(1)	0.0235	-0.5481	-2.9358
CI(2)	-0.2187	-1.5172	-5.0916
N(3)	0.1272	0.8660	-0.1310
N(4)	1.9552	-0.3021	-0.4515
C(5)	0.9031	1.0376	1.0215
C(6)	2.0782	0.2721	0.8189
C(7)	0.7841	0.0791	-1.0322
C(8)	-2.0717	0.7524	-1.3094
C(9)	0.7229	1.7965	2.1882
H(10)	-0.1778	2.4072	2.3467
C(11)	3.0972	0.2345	1.7817
H(12)	4.0048	-0.3672	1.6301
C(13)	-1.1691	1.5318	-0.3745
H(14)	-0.9759	2.5499	-0.7739
H(15)	-1.6609	1.6504	0.6102
C(16)	2.9249	0.9738	2.9653
C(17)	1.7298	1.7621	3.1690
C(18)	-2.0005	0.9650	-2.7201
C(19)	-2.9943	-0.1849	-0.8143
C(20)	-3.7610	-0.6881	-3.0842
C(21)	2.9269	-1.2086	-1.0685
H(22)	3.9454	-0.8204	-0.8497
H(23)	2.8029	-1.1198	-2.1699
C(24)	-3.8349	-0.8956	-1.6941
H(25)	-4.5601	-1.6163	-1.2858
C(26)	-2.8485	0.2423	-3.6014
H(27)	-2.7999	0.4377	-4.6830
C(28)	3.9901	0.9423	4.0296
H(29)	4.8437	0.3024	3.7385
H(30)	3.5904	0.5602	4.9928
H(31)	4.3835	1.9596	4.2397
H(32)	-3.0696	-0.3600	0.2706
C(33)	1.5628	2.5531	4.4399
H(34)	0.5985	3.0946	4.4628
H(35)	2.3760	3.2998	4.5629
H(36)	1.6077	1.8982	5.3356
H(37)	-1.3847	1.7908	-3.1181
H(38)	-4.4248	-1.2442	-3.7627
C(39)	2.8051	-2.6516	-0.6398
H(40)	3.5779	-3.3095	-1.0752
C(41)	1.8705	-3.1650	0.1770
H(42)	1.0846	-2.5449	0.6378
H(43)	1.8633	-4.2377	0.4224



Atom(label)xyzAg(1)7.96294.37764.4876Cl(2)7.42233.53662.3255N(3)8.14635.82087.2673N(4)9.97494.66656.9138C(5)8.96316.03318.3872C(6)10.13685.27988.1641C(7)8.77495.00706.3689C(8)5.96935.78406.0306C(9)8.80756.81089.5461H(10)7.90227.41039.7211C(11)11.18445.27369.0966H(12)12.09304.67728.9298C(13)6.82806.46307.0781H(14)6.99407.53156.8304H(15)6.31946.44218.0602C(16)11.04166.039810.2678C(17)9.84686.813410.4931C(18)6.09786.15434.6443C(19)5.03274.79156.4033C(20)4.35974.48574.0289C(21)10.95043.78016.2762H(22)11.95394.25276.3610
Ag(1)7.96294.37764.4876 $Cl(2)$ 7.42233.53662.3255 $N(3)$ 8.14635.82087.2673 $N(4)$ 9.97494.66656.9138 $C(5)$ 8.96316.03318.3872 $C(6)$ 10.13685.27988.1641 $C(7)$ 8.77495.00706.3689 $C(8)$ 5.96935.78406.0306 $C(9)$ 8.80756.81089.5461 $H(10)$ 7.90227.41039.7211 $C(11)$ 11.18445.27369.0966 $H(12)$ 12.09304.67728.9298 $C(13)$ 6.82806.46307.0781 $H(14)$ 6.99407.53156.8304 $H(15)$ 6.31946.44218.0602 $C(16)$ 11.04166.039810.2678 $C(17)$ 9.84686.813410.4931 $C(18)$ 6.09786.15434.6443 $C(19)$ 5.03274.79156.4033 $C(20)$ 4.35974.48574.0289 $C(21)$ 10.95043.78016.2762 $H(22)$ 11.95394.25276.3610
Cl(2)7.42233.53662.3255 $N(3)$ 8.1463 5.8208 7.2673 $N(4)$ 9.9749 4.6665 6.9138 $C(5)$ 8.9631 6.0331 8.3872 $C(6)$ 10.1368 5.2798 8.1641 $C(7)$ 8.7749 5.0070 6.3689 $C(8)$ 5.9693 5.7840 6.0306 $C(9)$ 8.8075 6.8108 9.5461 $H(10)$ 7.9022 7.4103 9.7211 $C(11)$ 11.1844 5.2736 9.0966 $H(12)$ 12.0930 4.6772 8.9298 $C(13)$ 6.8280 6.4630 7.0781 $H(14)$ 6.9940 7.5315 6.8304 $H(15)$ 6.3194 6.4421 8.0602 $C(16)$ 11.0416 6.0398 10.2678 $C(17)$ 9.8468 6.8134 10.4931 $C(18)$ 6.0978 6.1543 4.6443 $C(19)$ 5.0327 4.7915 6.4033 $C(20)$ 4.3597 4.4857 4.0289 $C(21)$ 10.9504 3.7801 6.2762 $H(22)$ 11.9539 4.2527 6.3610
N(3) 8.1463 5.8208 7.2673 $N(4)$ 9.9749 4.6665 6.9138 $C(5)$ 8.9631 6.0331 8.3872 $C(6)$ 10.1368 5.2798 8.1641 $C(7)$ 8.7749 5.0070 6.3689 $C(8)$ 5.9693 5.7840 6.0306 $C(9)$ 8.8075 6.8108 9.5461 $H(10)$ 7.9022 7.4103 9.7211 $C(11)$ 11.1844 5.2736 9.0966 $H(12)$ 12.0930 4.6772 8.9298 $C(13)$ 6.8280 6.4630 7.0781 $H(14)$ 6.9940 7.5315 6.8304 $H(15)$ 6.3194 6.4421 8.0602 $C(16)$ 11.0416 6.0398 10.2678 $C(17)$ 9.8468 6.8134 10.4931 $C(18)$ 6.0978 6.1543 4.6443 $C(19)$ 5.0327 4.7915 6.4033 $C(20)$ 4.3597 4.4857 4.0289 $C(21)$ 10.9504 3.7801 6.2762 $H(22)$ 11.9539 4.2527 6.3610
N(4)9.97494.66656.9138C(5)8.96316.03318.3872C(6)10.13685.27988.1641C(7)8.77495.00706.3689C(8)5.96935.78406.0306C(9)8.80756.81089.5461H(10)7.90227.41039.7211C(11)11.18445.27369.0966H(12)12.09304.67728.9298C(13)6.82806.46307.0781H(14)6.99407.53156.8304H(15)6.31946.44218.0602C(16)11.04166.039810.2678C(17)9.84686.813410.4931C(18)6.09786.15434.6443C(19)5.03274.79156.4033C(20)4.35974.48574.0289C(21)10.95043.78016.2762H(22)11.95394.25276.3610
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C(6)10.13685.27988.1641 $C(7)$ 8.77495.00706.3689 $C(8)$ 5.96935.78406.0306 $C(9)$ 8.80756.81089.5461 $H(10)$ 7.90227.41039.7211 $C(11)$ 11.18445.27369.0966 $H(12)$ 12.09304.67728.9298 $C(13)$ 6.82806.46307.0781 $H(14)$ 6.99407.53156.8304 $H(15)$ 6.31946.44218.0602 $C(16)$ 11.04166.039810.2678 $C(17)$ 9.84686.813410.4931 $C(18)$ 6.09786.15434.6443 $C(19)$ 5.03274.79156.4033 $C(20)$ 4.35974.48574.0289 $C(21)$ 10.95043.78016.2762 $H(22)$ 11.95394.25276.3610
C(7) 8.7749 5.0070 6.3689 $C(8)$ 5.9693 5.7840 6.0306 $C(9)$ 8.8075 6.8108 9.5461 $H(10)$ 7.9022 7.4103 9.7211 $C(11)$ 11.1844 5.2736 9.0966 $H(12)$ 12.0930 4.6772 8.9298 $C(13)$ 6.8280 6.4630 7.0781 $H(14)$ 6.9940 7.5315 6.8304 $H(15)$ 6.3194 6.4421 8.0602 $C(16)$ 11.0416 6.0398 10.2678 $C(17)$ 9.8468 6.8134 10.4931 $C(18)$ 6.0978 6.1543 4.6443 $C(19)$ 5.0327 4.7915 6.4033 $C(20)$ 4.3597 4.4857 4.0289 $C(21)$ 10.9504 3.7801 6.2762 $H(22)$ 11.9539 4.2527 6.3610
C(8)5.96935.78406.0306 $C(9)$ 8.80756.81089.5461 $H(10)$ 7.90227.41039.7211 $C(11)$ 11.18445.27369.0966 $H(12)$ 12.09304.67728.9298 $C(13)$ 6.82806.46307.0781 $H(14)$ 6.99407.53156.8304 $H(15)$ 6.31946.44218.0602 $C(16)$ 11.04166.039810.2678 $C(17)$ 9.84686.813410.4931 $C(18)$ 6.09786.15434.6443 $C(19)$ 5.03274.79156.4033 $C(20)$ 4.35974.48574.0289 $C(21)$ 10.95043.78016.2762 $H(22)$ 11.95394.25276.3610
C(9) 8.8075 6.8108 9.5461 $H(10)$ 7.9022 7.4103 9.7211 $C(11)$ 11.1844 5.2736 9.0966 $H(12)$ 12.0930 4.6772 8.9298 $C(13)$ 6.8280 6.4630 7.0781 $H(14)$ 6.9940 7.5315 6.8304 $H(15)$ 6.3194 6.4421 8.0602 $C(16)$ 11.0416 6.0398 10.2678 $C(17)$ 9.8468 6.8134 10.4931 $C(18)$ 6.0978 6.1543 4.6443 $C(19)$ 5.0327 4.7915 6.4033 $C(20)$ 4.3597 4.4857 4.0289 $C(21)$ 10.9504 3.7801 6.2762 $H(22)$ 11.9539 4.2527 6.3610
H(10)7.90227.41039.7211 $C(11)$ 11.18445.27369.0966 $H(12)$ 12.09304.67728.9298 $C(13)$ 6.82806.46307.0781 $H(14)$ 6.99407.53156.8304 $H(15)$ 6.31946.44218.0602 $C(16)$ 11.04166.039810.2678 $C(17)$ 9.84686.813410.4931 $C(18)$ 6.09786.15434.6443 $C(19)$ 5.03274.79156.4033 $C(20)$ 4.35974.48574.0289 $C(21)$ 10.95043.78016.2762 $H(22)$ 11.95394.25276.3610
C(11) 11.1844 5.2736 9.0966 $H(12)$ 12.0930 4.6772 8.9298 $C(13)$ 6.8280 6.4630 7.0781 $H(14)$ 6.9940 7.5315 6.8304 $H(15)$ 6.3194 6.4421 8.0602 $C(16)$ 11.0416 6.0398 10.2678 $C(17)$ 9.8468 6.8134 10.4931 $C(18)$ 6.0978 6.1543 4.6443 $C(19)$ 5.0327 4.7915 6.4033 $C(20)$ 4.3597 4.4857 4.0289 $C(21)$ 10.9504 3.7801 6.2762 $H(22)$ 11.9539 4.2527 6.3610
H(12)12.09304.67728.9298 $C(13)$ 6.8280 6.4630 7.0781 $H(14)$ 6.9940 7.5315 6.8304 $H(15)$ 6.3194 6.4421 8.0602 $C(16)$ 11.0416 6.0398 10.2678 $C(17)$ 9.8468 6.8134 10.4931 $C(18)$ 6.0978 6.1543 4.6443 $C(19)$ 5.0327 4.7915 6.4033 $C(20)$ 4.3597 4.4857 4.0289 $C(21)$ 10.9504 3.7801 6.2762 $H(22)$ 11.9539 4.2527 6.3610
C(13)6.82806.46307.0781H(14)6.99407.53156.8304H(15)6.31946.44218.0602C(16)11.04166.039810.2678C(17)9.84686.813410.4931C(18)6.09786.15434.6443C(19)5.03274.79156.4033C(20)4.35974.48574.0289C(21)10.95043.78016.2762H(22)11.95394.25276.3610
H(14)6.99407.53156.8304H(15)6.31946.44218.0602C(16)11.04166.039810.2678C(17)9.84686.813410.4931C(18)6.09786.15434.6443C(19)5.03274.79156.4033C(20)4.35974.48574.0289C(21)10.95043.78016.2762H(22)11.95394.25276.3610
H(15)6.31946.44218.0602C(16)11.04166.039810.2678C(17)9.84686.813410.4931C(18)6.09786.15434.6443C(19)5.03274.79156.4033C(20)4.35974.48574.0289C(21)10.95043.78016.2762H(22)11.95394.25276.3610
C(16)11.04166.039810.2678C(17)9.84686.813410.4931C(18)6.09786.15434.6443C(19)5.03274.79156.4033C(20)4.35974.48574.0289C(21)10.95043.78016.2762H(22)11.95394.25276.3610
C(17) 9.8468 6.8134 10.4931 C(18) 6.0978 6.1543 4.6443 C(19) 5.0327 4.7915 6.4033 C(20) 4.3597 4.4857 4.0289 C(21) 10.9504 3.7801 6.2762 H(22) 11.9539 4.2527 6.3610
C(17) 5.0400 6.0514 10.4511 C(18) 6.0978 6.1543 4.6443 C(19) 5.0327 4.7915 6.4033 C(20) 4.3597 4.4857 4.0289 C(21) 10.9504 3.7801 6.2762 H(22) 11.9539 4.2527 6.3610
C(10) 5.0327 4.7915 6.4033 C(20) 4.3597 4.4857 4.0289 C(21) 10.9504 3.7801 6.2762 H(22) 11.9539 4.2527 6.3610
C(12) 3.021 4.7515 6.4035 C(20) 4.3597 4.4857 4.0289 C(21) 10.9504 3.7801 6.2762 H(22) 11.9539 4.2527 6.3610
C(20) 10.9504 3.7801 6.2762 H(22) 11.9539 4.2527 6.3610
H(22) 11.9539 4.2527 6.3610
H(22) 11.9539 4.2527 0.3010
H(23) 10./151 3.//00 5.1889
C(24) 4.2382 4.1799 5.3973
H(25) 3.5058 3.4163 5.7061
C(26) 5.2939 5.4758 3.6694
H(27) 5.3844 5.7828 2.6161
C(28) 12.1455 6.0484 11.2951
H(29) 12.9980 5.4152 10.9857
H(30) 11.7881 5.6792 12.2797
H(31) 12.5311 7.0752 11.4692
C(32) 4.8616 4.3562 7.8396
H(33) 4.1236 3.5364 7.9241
H(34) 4.5019 5.1884 8.4828
H(35) 5.8151 3.9942 8.2780
C(36) 9.7114 7.6346 11.7510
H(37) 8.7391 8.1608 11.7944
H(38) 10.5142 8.3985 11.8263
H(39) 9.7968 7.0038 12.6607
C(40) 6.8945 7.3591 4.1983
H(41) 6.2856 8.2797 4.3471
H(42) 7.1324 7.3033 3.1189
H(43) 7.8425 7.5023 4.7510
C(44) 3.5603 3.7647 2.9774
H(45) 3.1293 4.4700 2.2388
H(46) 2.7362 3.1708 3.4156
H(47) 4.2268 3.0759 2.4151
C(48) 10.9837 2.3710 6.8181
H(49) 11.7848 1.7478 6.3826
C(50) 10 1493 1 8473 7 7309
H(51) 9 3409 2 4361 8 1938
H(52) 10.2520 0.8011 8.0553



Atom(label)	x	у	Z
Ag(1)	1.1503	7.6964	3.1859
CI(2)	-0.1518	9.5720	2.5625
N(3)	2.8124	5.0704	3.4488
N(4)	2.5753	5.9679	5.4328
C(5)	3.4617	4.2094	4.3443
C(6)	3.3166	4.7934	5.6229
C(7)	4.1539	3.0009	4.1693
H(8)	4.2618	2.5359	3.1784
C(9)	2.2802	6.1365	4.1146
C(10)	4.7065	2.3773	5.3030
C(11)	2.2099	6.0002	1.1867
C(12)	3.1372	6.8236	0.5083
C(13)	2.6913	4.8121	2.0028
H(14)	2.0099	3.9475	1.8612
H(15)	3.6830	4.4798	1.6432
C(16)	4.5639	2.9751	6.6056
C(17)	3.8698	4.1885	6.7621
H(18)	3.7738	4.6498	7.7547
C(19)	2.6481	7.8548	-0.3655
C(20)	0.3139	7.2811	0.1864
C(21)	0.7880	6.2294	1.0668
C(22)	2.1805	6.9077	6.4948
H(23)	1.6257	6.3483	7.2772
H(24)	1.4603	7.6090	6.0171
C(25)	1.2630	8.0512	-0.5012
H(26)	0.9049	8.8442	-1.1759
C(27)	5.1622	2.2958	7.8128
H(28)	4.7516	1.2735	7.9506
H(29)	6.2619	2.1788	7.7110
H(30)	4.9665	2.8663	8.7401
C(31)	4.6309	6.6743	0.6658
H(32)	4.9265	5.9920	1.4823
H(33)	5.1041	6.3080	-0.2711
H(34)	5.1007	7.6560	0.8811
C(35)	5.4498	1.0729	5.1514
H(36)	4.9837	0.2662	5.7557
H(37)	5.4740	0.7354	4.0979
H(38)	6.4992	1.1597	5.5039
C(39)	-0.2247	5.2631	1.6370
H(40)	0.1405	4.7006	2.5146
H(41)	-1.1597	5.7760	1.9317
H(42)	-0.5119	4.5200	0.8584
C(43)	-1.1545	7.4723	-0.0744
H(44)	-1.7195	7.6488	0.8625
H(45)	-1.3286	8.3387	-0.7386
H(46)	-1.5921	6.5736	-0.5615
C(47)	3.6030	8.7342	-1.1222
H(48)	4.2372	9.3301	-0.4297
H(49)	4.3045	8.1404	-1.7459
H(50)	3.0686	9.4424	-1.7822
C(51)	3.3421	7.6653	7.0874
H(52)	4.0075	8.1674	6.3622
C(53)	3.5621	7.7932	8.4072
H(54)	2.9082	7.3144	9.1558



	6 6	6 0 0 0 0 0	
		64 4 8	
Atom(label)	x	у	Ζ
C(1)	8.1841	6.9123	4.5136
C(2)	9.3756	8.7673	5.0591
C(3)	10.3305	9.7862	5.2008
H(4)	11.2999	9.7375	4.6844
C(5)	10.0171	10.8888	6.0156
C(6)	11.0249	11.9981	6.1915
H(7)	11.9497	11.8053	5.6162
H(8)	11.3097	12.1250	7.2570
H(9)	10.6162	12.9750	5.8577
C(10)	8.7417	10.9672	6.6792
C(11)	8.4196	12.1558	7.5509
H(12)	9.1427	12.2559	8.3875
H(13)	7.4061	12.0801	7.9877
H(14)	8.4729	13.1061	6.9789
C(15)	7.7914	9.9417	6.5189
H(16)	6.8192	10.0067	7.0290
C(17)	8.1226	8.8471	5.7047
C(18)	10.4716	7.0603	3.5218
H(19)	11.4172	7.1797	4.0955
H(20)	10.3209	5.9633	3.4119
C(21)	10.5942	7,7084	2.1638
H(22)	11.4791	7.3766	1.5920
C(23)	9.7447	8.5986	1.6262
H(24)	8 8515	8 9565	2 1635
H(25)	9 9166	9.0075	0.6196
C(26)	6 0710	7 3572	5 8268
H(27)	5 4579	8 2731	5 7424
H(28)	6 1429	7 1326	6 9114
C(29)	5 3991	6 2078	5.0950
C(30)	4 4 4 5 0	6.4578	4 0875
C(31)	1 1837	7 8577	3 5775
H(32)	1 0989	7.8577	2 / 729
H(33)	4.0505	8 5662	2.4723
П(33) Ц(24)	4.9097	0.J002 9.J717	2 0712
C(35)	3 71/2	5 2505	3 5125
C(35)	2 61/2	5.6456	2 5217
L(30)	2.0143	5.0450	1 1719
H(38)	2.3881	6 6573	2 6/05
L(20)	2.1809	0.0373	2.0405
C(40)	1.7040	4.9190	2.0119
C(40)	4.0551	4.0145	3.0309 3.143E
U(41)	2.2022	2.0009	3.1425
H(42)	2.0433	2.3207	3.7994
H(43)	4.1305	2.1210	2.8239
П(44) С(45)	2.8201	3.1/14	2.2309
C(45)	4.395/	3./323	4.00// E 2720
C(40)	J.2331	2.3300	J.J/JO
H(47)	4.0746	1.5948	4.8072
H(48)	4.9202	2.2/6/	6.43/8
H(49)	6.3049	2.0804	5.3237
C(50)	5.6948	4.8534	5.4922
C(51)	6.5522	4.5590	6.7012
H(52)	7.2552	5.3/14	6.9542
H(53)	7.1394	3.6303	6.5769
H(54)	5.8990	4.3912	7.5882

Ag(55)	7.5736	5.0337	3.6963
CI(56)	7.2700	2.9662	2.5759
N(57)	9.3718	7.5581	4.3495
N(58)	7.4218	7.6888	5.3365

 Table S10.
 Analysis of the docking of all molecules, Ciprofloxacin, and Fluconazole in the active site of receptors.

Dete 1a 6.55 ApdD8, HistD6, Mett38, GluI36, HistD6, LeuI6, Tyr134, Ala206, His235, Ile73, LeuI05, Phei07, Tyr137, Apj31, GlyQ07 1b -6.56 Met138, HistD6, Ile73, Phe107, HistD9, Tyr134, Ala206, His235, Asp108, GluI36, Tyr137, Apj313, GlyQ17 1c -6.75 Asp108, HistD6, GlyQ27, Phe208 1d -6.37 Mett38, GlyZ16, Phe208 2a -6.77 Mett38, GlyZ16, Sert20, Apj10, GlyZ27, Phe208 2a -6.37 Mett38, GlyZ16, Sert20, Apj10, GlyZ27, Phe208 2b -6.33 Asp108, HistD6, Phe107, Tyr134, HistD6, Phe208 2c -6.55 Mett38, GlyZ44, Ile73, HistD6, Phe107, Tyr137, HistB18, Tyr137, Mett38, Cys141, HistB19, Tyr134, HistB28, Sert20, Apj101, GlyZ07, Phe208 2c -6.54 Mett38, GlyZ4, GluZ4, LeuI5, Ile73, Tyr137, Tyr134, Hist235, LeuI5, Asp108, Arg134, GluZ6, Asp131, LeuI6, Ile73, Tyr137, Tyr194, His235, LeuI05, Asp108, Arg134, GluZ6, GlyZ07, Phe208 2c -6.54 Mett38, Cys14, Ile73, Hist06, Asp131, LeuI6, Ile73, Tyr137, Tyr134, Hist235, LeuI5, Asp108, Arg134, Hist39, Asp131, Ile20, GlyZ07, Phe208 2d -6.64 Hist37, Firt24, GluZ6, GlyZ07, Phe208 Hist235, Cys14, LeuI5, Ile73, Cys14, Ser20, Leu33, Val35, Ile73, Phe137, Ala218, Tyr132, Tyr132, Tyr132, Tyr132, Tyr132, Tyr132, Tyr132, Tyr132, Tyr132, Tyr132, Tyr132, Tyr132, Tyr132, Tyr132, Tyr132, Tyr132, Tyr132, Tyr132, T	Compounds	Bind. Aff.*	Amino Acids Residue	
1a -6.55 Asp108, Histöß, Mett38, Giul36, Histöß, Leulő, Tyrl34, Ala206, His235, Ile73, Leulös, Phelo7, Tyrl37, Gly207 1b -6.56 Mett38, Histöß, Ile73, Phel07, Histö9, Tyrl34, Ala206, His235, Asp108, Giul36, Tyrl37, Asp131, Gly207 1c -6.75 Asp108, Histöß, Ile73, Phel07, Histö9, Tyrl34, Ala206, His235, Leuló, Giul36, Tyrl37, Asp131, Gly207, Phe208 1d -6.37 Mett38, Giul36, Cys14, Ile73, Histö6, Phel07, Tyrl34, Ala206, His235, Leul6, Asp108, Arg134, Tyrl37, Asp131, Gly207, Phe208 2a -6.57 Mett38, Giul36, Cys14, Ile73, Histö6, Phel07, Tyrl34, His235, Leul6, Asp108, Arg134, Fyrl337, Histö9, Fyrl30, App131, Gly207, Phe208 2b -6.33 Asp108, Histö6, Phel07, Giul36, Cys14, Leul5, Ile73, Tyrl37, Tyrl34, His235, Leul6, Leul08, Asp108, Arg134, Giul36, Asp191, Gly207, Phe208 2d -6.64 Histö9, Serl20, Histö6, Phel07, Tyrl37, Histö9, Tyrl34, His235, Leul5, Leul08, Asp108, Histö6, Phel07, Asp108, Kistö9, Asp191, Leul6, Ala206, Cys14, Ser20, Leu33, Val35, Ile73, Phel27, Histö9, Giy207, Phe208 Cipro -4.93 Histö9, App191, Ala206, Giy207, Phe208 Cipro -4.93 Histö9, App191, Ala206, Giy207, Phe208 Cipro -4.93 Histö8, Ser20, Histö9 1a -5.09 Ala38, Phe137, Tyrl42, Phe134, Leu160, Tyrl52, Thrl41, Giu145, Hist59, Asn161 1b -5.34			2br6	
Phetal07, Tyr137, Gly207 1b 4.5.6 Met138, Histolo, Iler37, Phet07, Hist09, Hist09, Tyr194, Ala206, His235, Asp108, Glu136, Tyr137, Asp113, Gly207 1c -6.7.5 Asp108, Histol6, Met138, Leu16, Iler37, Hist06, Phet07, Tyr137, Tyr194, Ala206, His235, Leu105, Glu136, Gly207, Phe208 1d -6.37 Met138, Glu36, Gly207, Phe208 2a -6.27 Met138, Glu36, Gly213, Iler37, Hist06, Phe107, Tyr194, His235, Leu16, Asp108, Arg134, Tyr137, Hist05, Ser107, Asp113, Gly207, Phe208 2b -5.31 Asp108, Hist05, Phe107, Glu136, Cyr14, Leu16, Iler3, Tyr137, Met138, Cys141, Hist06, Tyr194, His235, Ileu16, Leu105, Asp108, Arg134, Glu36, Asp1019, Gly207, Phe208 2d -6.64 Hist06, Phe107, Met138, Cys14, Leu16, Iler3, Tyr137, Tyr194, His235, Leu16, Leu105, Asp108, Arg134, Hist09, Asp131, Ja206, Gly207, Phe208 Cipro -4.93 Hist09, Fibr07, Asp108, Tyr144, Glu136, Asp191, Leu16, Ala206, Cys14, Ser20, Leu33, Val35, Iler3, Phe107, Hist09, Gly207, Phe208, His235 Filu -5.51 Hist09, Fibr07, Asp108, Tyr144, Glu136, Asp191, Hist235, Cys14, Leu16, Iler3, Cys14, Ala206, Leu33, Val35, Iler3, Phe137, Liu26, Gly207, Phe208, Hist29 1a -5.09 Ala138, Phe137, Leu22, Lys123, Ile126, Ala138, Tyr142, Tyr142, Mist161 1b -5.31 Phe134, Leu160, Tyr162, Thr141, Glu145, Hist59, Asn161 1c -5.64 Phe134, Leu2	1a	-6.55	Asp108, His169, Met138, Glu136, His106, Leu16, Tyr194, Ala206, His235, Ile73, Leu105,	
1b -6.56 Met138, Histöb, Ile72, Phe107, Histöb, Tyr194, Ala206, His225, Asp108, Glu136, Tyr137, Asp113, Gly207 1c -6.75 Asp108, Hist69, Met138, Leu16, Ile73, Hist06, Phe107, Tyr137, Tyr194, Ala206, His235, Leu105, Glu136, Gly207, Phe208 1d -6.37 Met138, Hist06, Ile73, Phe107, Hist09, Hist69, Tyr194, Ala206, His235, Asp108, Glu136, Tyr137, Asp131, Gly207, Phe208 2a -6.57 Met138, Glu36, Cys14, Ile73, Hist06, Phe107, Tyr194, His235, Leu16, Asp108, Arg134, Tyr137, Hist69, Ser120, Asp191, Gly207, Phe208 2b -6.53 Met138, Guy14, Ile73, Hist06, Phe107, Tyr137, Hist69, Tyr194, His235, Leu105, Asp108, Arg134, Hist06, Phe107, Tyr137, Hist69, Tyr194, His235, Leu105, Asp108, Arg134, Hist06, Phe107, Tyr137, Hist69, Tyr194, His235, Leu105, Asp108, Arg134, Hist06, Phe107, Hist08, Gly201, Phe208 2d -6.64 Hist06, Phe107, Met138, Cys14, Leu16, Ile73, Tyr137, Tyr194, His235, Leu105, Asp108, Arg134, Hist09, Gly207, Phe208 Cipro -4.93 Hist06, Phe107, Asp108, Asp101, Leu16, Ala206, Cys14, Ser20, Leu3, Val5, Ile73, Phe107, Hist09, Gly207, Phe208 Cipro -5.04 Hist06, Phe107, Asp108, Tyr134, Glu136, Hist69, Asp191, Hs235, Cys14, Leu16, Ile73, Cys14, Ala206, Leu33, Ser217, Leu22, Leu32, Xiz21, Ile124, Ala138, Tyr142, Tir144, Ile145, Hist59, Asp161 1b -5.04 Phe134, Phe137, Tyr124, Phe134, Ala138, Vil211, Ile215, Thr141, Tyr142, Glu145, Leu160, Tyr162, Leu208, Asp121 1c -5.64			Phe107, Tyr137, Gly207	
1c 6.75 Asp108, HistoB, Met138, Leul5, IIe73, Hist06, Phe107, Tyr137, Tyr194, Ala206, His235, Leul5, Glu136, Gly207, Phe208 1d -6.37 Met138, Hist06, IIe73, Phe107, Hist09, Hist69, Tyr194, Ala206, His235, Asp108, Glu136, Tyr137, Asp131, Gly207, Phe208 2a -6.27 Met138, Glu136, Gys11, Gly207, Phe208 2b -6.33 Asp108, Hist06, Phe107, Glu136, Cys14, Leu16, IIe73, Tyr137, Met138, Cys141, Hist69, Tyr139, His255 2c -6.55 Met138, Cys14, IIe73, Hist06, Phe107, Tyr137, Tir137, Tyr194, His235, Leu16, Leu105, Asp108, Arg134, Glu136, Asp131, Leu16, Glu207, Phe208 2d -6.64 Hist06, Phe107, Met138, Cys14, Leu16, IIe73, Tyr137, Tyr194, His235, Leu16, Leu105, Asp108, Arg134, Hist09, Asp131, Lau66, Giy207, Phe208 2d -6.64 Hist06, Fhe107, VT194, Asp104, Glu136, Asp131, Leu16, Ala206, Cys14, Ser20, Leu33, Val35, IIe73, Phe107, Hist09, Gly207, Phe208, His235 Flu -5.81 Hist06, Fhe137, Tyr142, Phe134, Leu160, Tyr162, Thr141, Glu145, Hist59, Asp161 1a -5.09 Ala138, Phe137, Tyr142, Phe134, Leu160, Tyr162, Thr141, Glu145, Hist59, Asp161 1a -5.09 Ala138, Phe137, Tyr142, Phe134, Leu160, Tyr162, Thr141, Glu145, Hist59, Asp161 1a -5.09 Ala138, Phe137, Tyr142, Phe134, Leu160, Tyr162, Thr141, Glu145, Hist59, Asp161 1a -5.04 Phe134, Ph	1b	-6.56	Met138, His106, Ile73, Phe107, His109, His169, Tyr194, Ala206, His235, Asp108, Glu136,	
1c -6.75 Asp108, His169, Met138, Leu15, IIe73, His106, Phe107, Tyr137, Tyr194, Ala206, His235, Leu105, Guil36, Gy207, Phe208 1d -6.37 Met138, Guil36, Cys14, IIe73, His109, His169, Tyr194, Ala206, His235, Leu16, Asp108, Arg134, Tyr137, Tis169, Ser170, Asp191, Gly207, Phe208 2a -6.27 Met138, Guil36, Cys14, IIe73, His106, Phe107, Tyr194, His235, Leu16, Asp108, Arg134, Tyr137, His169, Ser170, Asp191, Gly207, Phe208 2b -6.33 Met138, Cys14, IIe73, His106, Phe107, Tyr137, Tyr194, His235, Leu16, Leu105, Asp108, Arg134, His166, Asp191, Gly207, Phe208 2c -6.54 Met138, Cys14, IIe73, His106, Gly207, Phe208 2d -6.64 His106, Phe107, Met138, Cys14, Leu5, IIe73, Tyr137, Tyr194, His235, Leu105, Asp108, Arg134, His169, Asp191, Ja206, Gly207, Phe208 Cipro -4.93 His106, Fhe107, Asp108, Apr191, Ala206, Gly207, Phe208 Flu -5.81 His106, Fhe107, Asp108, Tyr194, Gli36, His169, Asp191, Hs235, Cys14, Leu16, IIe73, Cys14, Ala206, Leu33, Ser20, His109 <i>Zrp</i> 1a -5.09 Ala138, Phe137, Leu122, Lys123, IIe126, Ala138, Tyr142, Leu160, Tyr162, Ala119, Thr141, Hie159, Asn161 1b -5.34 Glu145, His159, Asn212 IIe164, Ala206, Cys127, Har14, Glu145, His159, Asn161 1c -5.46 Phe134, Lys123, IIe126, Ala138, Tyr142, Thr141, Glu145, His159, Asn161 1c -5.46			Tyr137, Asp191, Gly207	
Leui05, Glui26, Giy207, Phe208 1d -6.37 Met138, Hitslö, Hor27, Phe208 2a -6.27 Met138, Glui26, Cyst4, Hor37, Hitslo9, Try194, Ala206, Hits235, Asp108, Glui36, Tyr137, Asp191, Gly207, Phe208 2a -6.27 Met138, Glui36, Cyst4, Hor37, Hitslo6, Phe107, Tyr194, Hits235, Leui6, Asp108, Arg134, Tyr137, Hits235 2c -6.55 Met138, Cyst4, Hor37, Hitslö6, Phe107, Glui36, Cyst4, Leui5, Hir23, Tyr137, Met138, Cyst41, Hitsl69, Tyr134, Hits236 2d -6.64 Hitsl06, Phe107, Met138, Cyst4, Leui5, Hir23, Tyr137, Tyr194, Hits235, Leui16, Leui05, Asp108, Arg134, Glui36, Cyst41, Leui6, Hir27, Tyr137, Tyr194, Hits235, Leui16, Leui05, Asp108, Arg134, Glui36, Cyst41, Leui6, Hir27, Tyr137, Tyr194, Hits235, Leui05, Asp108, Arg134, Hits169, Asp191, Ala206, Gly207, Phe208 2d -6.64 Hitsl06, Phe107, Met138, Cyst4, Leui6, Hir23, Tyr137, Tyr194, Hits25, Leui05, Asp108, Arg134, Hits196, Asp191, Ala206, Gly207, Phe208 Clpro -4.93 Hits109, Hits109, Hits109, Hits235 Flu -5.81 Hits106, Phe107, Aps108, Tyr194, Glui36, Hits194, Asp101, Hits25, Cyst4, Leui6, He73, Cyst4, Ala206, Leui33, Ser20, Hits109 -200 -201 -201 -20 -201 -20 -201 -20 -201 -201	1c	-6.75	Asp108, His169, Met138, Leu16, Ile73, His106, Phe107, Tyr137, Tyr194, Ala206, His235,	
1d -6.37 Met138, His106, IIe73, Phe107, His109, His169, Tyr194, Als206, His235, Asp108, Glu136, Tyr137, Asp103, Glu136, Cys14, IIe73, His106, Phe107, Tyr194, His235, Leu16, Asp108, Arg134, Tyr137, His169, Ser170, Asp101, Gly207, Phe208 2a -6.53 Met138, Glu136, Cys14, IIe73, His106, Phe107, Tyr137, Tyr137, Met138, Cys141, His169, Tyr194, His235 2c -6.54 Met138, Glu136, Cys14, IIe73, Fyr137, Tyr137, Met138, Cys141, Ieu15, IIe73, Tyr137, Tyr194, His235, Leu16, Leu105, Asp108, Arg134, His169, Asp113, Alco26, Giy27, Phe208 2d -6.64 His106, Phe107, Met138, Cys14, Leu15, IIE73, Tyr137, Tyr194, His235, Leu16, Asp108, Arg134, His169, Asp191, Alco26, Giy27, Phe208 Cipro -4.93 His106, Phe107, Asp108, Tyr194, Glu136, His169, Asp191, Alco26, Giy27, Phe208 Flu -5.81 His106, Phe137, Fyr194, Glu136, His169, Asp191, Alco26, Cys14, Ser20, Leu33, Val35, IIe73, Phe107, His109, Gly20, Phe208, His25 Flu -5.81 His106, Phe137, Phe134, Leu160, Tyr162, Thr141, Glu145, His159, Asn161 1b -5.40 Phe134, Phe137, Leu122, Lys123, IIe126, Ala138, Tyr142, Leu160, Tyr162, Ala119, Thr141, His215 1c -5.46 Phe134, Phe137, Leu122, Lys123, IIe126, Ala138, Tyr142, Leu160, Tyr162, Ala119, Thr141, His219 1d -5.44 Phe134, Lys123, Phe134, Ala138, Lyr142, Thr141, Glu145, Asn161, Tyr162 2c 4.64 Tyr162, Leu100, Phe134, Ala138, Tyr142, Thr141, Glu145, Asn161, Tyr162			Leu105, Glu136, Gly207, Phe208	
Tyr137, Asp191, Giy207, Phe208 2a -6.27 Me138, Giy31, Hir27, His169, Sen170, Asp191, Giy207, Phe208 2b -6.33 Asp108, His169, Fen107, Giu136, Cys14, Leu15, Ile73, Tyr137, Met138, Cys141, His169, Tyr134, His136, Sen170, Asp191, Giy207, Phe208 2c -6.55 Me1138, Cys14, Ile73, His106, Phe107, Tyr137, His169, Tyr194, His235, Leu16, Leu105, Asp108, Arg114, Giu36, Asp1919, Giy207, Phe208 2d -6.64 His106, FPe107, Met138, Cys14, Leu16, Ile73, Tyr137, Tyr194, His235, Leu105, Asp108, Arg134, His169, Asp191, Ala206, Giy207, Phe208 Cipro -4.93 His106, FIP107, Asp108, Yap108, Asp191, Leu16, Ala206, Cys14, Ser20, Leu33, Val35, Ile73, Phe107, His109, Giy207, Phe208, His235 Flu -5.81 His106, FIP107, Asp108, Yap124, Leu160, Tyr162, Cys14, Ser20, Leu33, Val35, Ile73, Phe107, His109, Giy207, Phe208, His235 1a -5.09 1a -5.09 1a -5.04 1b -5.34 Phe134, Phe137, Leu122, Lys123, Ile126, Ala138, Tyr142, Lyr142, Cut160, Tyr162, Ala119, Tyr142, His141, Glu145, His159, Asn161 1c -5.46 Phe134, Jee137, Mie21, Phe134, Ala138, Lyr142, Tyr142, Thr141, His159, Asn161 1d -5.44 Phe134,	1d	-6.37	Met138, His106, Ile73, Phe107, His109, His169, Tyr194, Ala206, His235, Asp108, Glu136,	
2a -6.27 Met138, Giu136, Cyst4, Ile73, His106, Phe107, Tyr194, His235, Leu16, Asp108, Arg134, Tyr137, His169, Ser170, Asp191, Giy207, Phe208 2b -6.33 Asp108, Mis106, Phe107, Giu136, Cys14, Leu16, Ile73, Tyr137, Met138, Cys141, His169, Tyr194, His235, Leu16, Leu105, Asp108, Arg134, Giu136, Asp191, Giy207, Phe208 2c -6.64 His106, Ape107, Met138, Cys14, Leu16, Ile73, Tyr137, Tyr194, His235, Leu105, Asp108, Arg134, His169, Asp109, Jac206, Giy207, Phe208 2d -6.64 His106, Phe107, Met138, Cys14, Leu16, Ile73, Tyr137, Tyr194, His235, Leu105, Asp108, Arg134, His169, Asp109, Jac206, Phe208 Cipro -4.93 His106, Phe107, Met208, Hog108, His169, Asp191, He235, Cys14, Leu16, Ile73, Cys14, Ala206, Leu33, Ser20, His109 Image: Signa S			Tyr137, Asp191, Gly207, Phe208	
Tyr137, Hist69, Ser170, Asp191, Gly207, Phe208 2b -6.33 Asp108, Hist235 2c -6.55 Met138, Cys14, Hist236 2d -6.64 Hist06, Phe107, Met138, Gly14, Leu16, He73, Tyr137, Tyr194, His235, Leu105, Asp108, Asp113, Gly207, Phe208 2d -6.64 Hist06, Phe107, Met138, Gly14, Leu16, He73, Tyr137, Tyr194, His235, Leu105, Asp108, Asp113, Hal206, Gly207, Phe208 Cipro -4.93 Hist9, Hist06, Tyr194, Asp108, Asp101, Leu16, Ala206, Cys14, Ser20, Leu33, Val35, He73, Phe107, Hist09, Gly207, Phe208, His235 Flu -5.81 Hist06, Phe107, App108, Myr194, Glu136, Hist69, Asp191, Hs235, Cys14, Leu16, He73, Cys14, Ala206, Leu33, Ser20, His109 Zfp 1a -5.09 Ala138, Phe137, Tyr142, Phe134, Leu160, Tyr162, Thr141, Glu145, Hist59, Asn161 1b -5.34 Phe134, Phe137, Leu122, Lys123, Ile126, Ala138, Tyr142, Leu160, Tyr162, Kal119, Thr141, Ile215 1c -5.46 Phe134, Jis123, Leu126, Jis128, Leu160, Phe137, Thr141, Asn146, Asn161, Tyr162 Clys123, Ile126, Jis128, Leu160, Phe137, Thr141, Sis129, Asn161 Clys22, His139, Tyr142, Phe134, Ala138, Tyr142, Thr141, Glu145, Asn164, Asn161, Tyr162 Clys234, His235	2a	-6.27	Met138, Glu136, Cys14, lle73, His106, Phe107, Tyr194, His235, Leu16, Asp108, Arg134,	
2b -6.33 Asp108, His106, Phe107, Glu136, Cys14, Leu16, Ile73, Tyr137, Met138, Cys141, His169, Tyr194, His235 2c -6.55 Met138, Cys14, Ile73, His106, Phe107, Tyr137, His169, Tyr194, His235, Leu16, Leu105, Asp108, Arg134, Glu136, Asp191, Gly207, Phe208 2d -6.64 His105, Phe107, Met138, Cys14, Leu16, Ile73, Tyr137, Tyr194, His235, Leu105, Asp108, Arg134, His169, Asp108, Asp191, Leu16, Ala206, Cys14, Ser20, Leu33, Val35, Ile73, Phe107, His109, Gly207, Phe208, His235 Flu -5.81 His105, Phe107, Met138, Leu160, Tyr162, Thr141, Glu145, His159, Asp161 1b -5.09 Ala138, Phe137, Tyr142, Phe134, Leu160, Tyr162, Thr141, Glu145, His159, Asp161 1b -5.34 Phe137, Leu122, Lys123, Ile126, Ala138, Tyr142, Leu160, Tyr162, Ala119, Thr141, Ile215 1c -5.46 Phe134, Phe137, Leu122, Lys123, Ile126, Ala138, Tyr142, Thr141, His159, Asp161 1d -5.44 Phe134, Phe137, Leu122, Lys123, Ile126, Ala138, Tyr142, Thr141, His159, Asp161, Tyr162 2a -4.55 Glu145, His159, Tyr142, Phe134, Ala138, Leu160, Phe137, Thr141, Glu145, Asp161, Tyr162, Val211, Ile215, Asp161, Tyr162, Val211, Ile215, Asp161, Tyr162, Val211, Ile215, Asp161, Tyr162, Val214, Ile216, Leu160, Phe137, Tyr162, Phe134, Ala138, Tyr142, Tyr141, Glu145, His159 1d -5.44 Phe134, Leu160, Lys123, Phe134, Ala138, Tyr142, Tyr141, Glu145, His159 2d -4.64 Leu160			Tyr137, His169, Ser170, Asp191, Gly207, Phe208	
Tyr194, His235 2c -6.55 Met138, Cys14, Ile73, His166, Phe107, Tyr137, His169, Tyr194, His235, Leu16, Leu105, Asp108, Ag134, Glu136, Asp191, Gly207, Phe208 2d -6.64 His106, Phe107, Met138, Cys14, Leu16, Ile73, Tyr137, Tyr194, His235, Leu105, Asp108, Arg134, His169, Asp191, Ja206, Gly207, Phe208 Cipro -4.93 His106, Tyr194, Asp108, Asp191, Leu16, Ala206, Cys14, Ser20, Leu33, Val35, Ile73, Phe107, His108, Gly207, Phe208, His235 Flu -5.81 His106, Phe107, Ap108, Myr194, Glu136, His169, Asp191, Hs235, Cys14, Leu16, Ile73, Cys14, Ala206, Leu33, Ser20, His109 1a -5.09 Ala138, Phe137, Tyr142, Phe134, Leu160, Tyr162, Thr141, Glu145, His159, Asn161 1b -5.44 Phe134, Phe137, Leu122, Lys123, Ile126, Ala138, Tyr142, Leu160, Tyr162, Ala119, Thr141, Ile215 1c -5.46 Phe134, Phe137, Leu122, Lys123, Ile126, Ala138, Tyr142, Leu160, Tyr162, Phe134, Ala138, Val211, Ile215, Ala119, Thr141, Leu160, Leu208, Asn212 1d -5.44 Phe134, His159, Tyr142, Phe134, Ala138, Tyr142, Thr141, Glu145, Asn164, Fil559 2d -4.85 Glu145, His159, Tyr142, Phe134, Ala138, Tyr142, Thr141, Glu145, Kin159 2d -4.84 1d Tyr162, Cue106, Phe11eu160, Lys123,	2b	-6.33	Asp108, His106, Phe107, Glu136, Cys14, Leu16, lle73, Tyr137, Met138, Cys141, His169,	
2c -6.55 Met138, Cyr14, He73, His106, Phe107, Tyr137, His169, Tyr194, His235, Leu16, Leu105, Asp108, Arg134, Glu136, Asp191, Gly207, Phe208 2d -6.64 His106, Phe107, Met138, Cys14, Leu16, Ile73, Tyr137, Tyr194, His235, Leu105, Asp108, Arg134, His169, Asp103, Asp108, Asp1014, Leu16, Ala206, Cys14, Ser20, Leu33, Val35, Ile73, Phe107, His109, Gly207, Phe208, His235 Flu -5.81 His106, Phe107, Asp108, Tyr194, Glu136, His169, Asp191, Hs235, Cys14, Leu16, Ile73, Cys14, Ala206, Leu33, Ser20, His109 1a -5.09 Ala138, Phe137, Tyr142, Phe134, Leu160, Tyr162, Thr141, Glu145, His159, Asn161 1b -5.34 Phe134, Phe137, Leu122, Lys123, Ile126, Ala138, Tyr142, Leu160, Tyr162, Ala119, Thr141, Ile215 1c -5.46 Phe134, Phe137, Leu122, Lys123, Ile126, Ala138, Tyr142, Thr141, Glu145, Leu160, Tyr162, Leu208, Asn212 2a -4.55 Glu145, His159, Tyr142, Phe134, Ala138, Leu160, Phe137, Thr141, His159, Asn161, Tyr162 2b -4.87 Phe134, Lys122, Phe134, Ala138, Tyr142, Thr141, Glu145, Asn161, Tyr162 2c -4.65 Glu145, Leu160, Tyr162, Phe134, Ala138, Tyr142, Thr141, Glu145, His159 2d -4.55 Glu145, Leu160, Tyr162, Phe134, Ala138, Tyr142, Thr141, Glu145, His159 2d -4.54 Phe134, Lys122, Phe137, Ala138, Tyr142, Thr141, Glu145, His159 2d -4.54 Leu			Tyr194, His235	
Asp108, Arg134, Glu136, Asp119, Gly207, Phe208 2d -6.64 His106, Phe107, Met138, Cys14, Leu16, Ile73, Tyr137, Tyr194, His235, Leu105, Asp108, Arg134, His69, Asp101, JA206, Gly207, Phe208 Cipro -4.93 His10, Fhe107, Asp108, Tyr194, Glu136, His159, Asp191, Leu16, Ala206, Cys14, Ser20, Leu33, Val35, Ile73, Phe107, His109, Gly207, Phe208, His235 Flu -5.81 His106, Fhe107, Asp108, Tyr194, Glu136, His159, Asp191, Hs235, Cys14, Leu16, Ile73, Cys14, Ala206, Leu33, Ser20, His109 Ia -5.09 Ala138, Phe137, Tyr142, Phe134, Leu160, Tyr162, Thr141, Glu145, His159, Asn161 Ib -5.34 Phe137, Leu122, Lys123, Ile126, Ala138, Tyr142, Leu160, Tyr162, Ala119, Thr141, Ile215 Ic -5.46 Phe137, Phe137, Leu122, Lys123, Ile126, Ala138, Tyr162, Val211, Ile215, Ala119, Thr141, Ile215 Id -544 Phe134, Phe137, Tyr142, The134, Ala138, Leu160, Phe137, Thr141, Asn146, Asn161, Tyr162 2b -4.55 Glu145, His159, Tyr142, Phe134, Ala138, Leu160, Phe137, Thr141, His159, Asn161 2c -4.64 Tyr162, Leu160, Phe147, Tyr162, Phe134, Ala138, Tyr142, Tr141, Glu45, Asn161, His159 2d -4.84 Tyr162, Thr141, Ala138, Glu145, Leu160, Phe137, Ala138, Tyr142, Thr141, Glu145, His159<	2c	-6.55	Met138, Cys14, Ile73, His106, Phe107, Tyr137, His169, Tyr194, His235, Leu16, Leu105,	
2d -6.64 His106, Phe107, Met138, Cys14, Leu16, Ile73, Tyr137, Tyr194, His235, Leu105, Asp108, Arg134, His169, Asp109, Asp103, Asp103, Ileu16, Ala206, Cys14, Ser20, Leu33, Val35, Ile73, Phe107, His109, Gly207, Phe208, His235 Fiu -5.81 His106, Fyr194, Asp108, Asp1019, Alsp101, Ala206, Cys14, Ser20, Leu33, Val35, Ile73, Phe107, His109, Gly207, Phe208, His235 Ia -5.00 Ala138, Phe137, Tyr142, Phe134, Leu160, Tyr162, Thr141, Glu145, His159, Asp161 Ib -5.34 Phe137, Phe137, Leu122, Lys123, Ile126, Ala138, Tyr142, Leu160, Tyr162, Ala119, Thr141, Ile215 Ic -5.46 Phe137, Leu122, Lys123, Ile126, Ala138, Tyr162, Val211, Ile215, Ala119, Thr141, Ile215 Id -5.44 Phe137, Leu122, Lys123, Ile126, Ala138, Tyr162, Val211, Ile215, Ala119, Thr141, Leu160, Cyr162, Leu208, Asn212 Id -5.44 Phe137, Leu122, Lys123, Ile126, Ala138, Tyr162, Val211, Ile215, Ala119, Thr141, Leu160, Cleu208, Asn212 2a -4.55 Glu145, His159, Tyr142, Phe134, Ala138, Leu160, Phe137, Thr141, Sun146, Asn161, Tyr162 2b -4.87 Phe134, Ilys123, Phe137, Tyr142, Phe134, Ala138, Tyr142, Thr141, Glu145, Asn161 2c -4.64 Leu160, Phe137, Tyr162, Lys123, Phe137, Ala138, Tyr142, Thr141, Glu145, Asn161 2c -4.86 Fyr162, Thr141, Ala138, Glu145, Leu160, Phe137, Tyr142, Asn161 71 Fur277, C			Asp108, Arg134, Glu136, Asp191, Gly207, Phe208	
Arg134, His169, Asp191, Ala206, Giy207, Phe208 Cipro -4.93 His10, Fyr134, Asp108, Asp191, Leu16, Ala206, Cys14, Ser20, Leu33, Val35, Ile73, Phe107, His109, Giy207, Phe208, His235 Flu -5.81 His106, Phe107, Asp108, Tyr194, Giu136, His169, Asp191, Hs235, Cys14, Leu16, Ile73, Cys14, Ala206, Leu33, Ser20, His109 Ite -5.81 His106, Phe107, Asp108, Tyr194, Giu136, His169, Asp191, Hs235, Cys14, Leu160, Ile73, Cys14, Ala206, Leu33, Ser20, His109 Ite -5.99 Ala138, Phe137, Tyr142, Phe134, Leu160, Tyr162, Thr141, Giu145, His159, Asn161 Ib -5.34 Phe134, Phe137, Leu122, Lys123, Ile126, Ala138, Tyr142, Leu160, Tyr162, Ala119, Thr141, Ile215 Ice -5.46 Phe134, Phe137, Leu122, Lys123, Ile126, Ala138, Tyr162, Val211, Ile215, Ala119, Thr141, Leu160, Leu208, Asn212 Id -5.47 Phe134, Lys123, Phe137, Ala138, Tyr142, Thr141, Giu145, Asn161, Tyr162 Zb -4.87 Phe134, Lys123, Phe137, Ala138, Tyr142, Thr141, Giu145, Asn161, Tyr162 Zb -4.87 Phe134, Lys123, Phe137, Ala138, Tyr142, Thr141, Giu145, His159 Cipro -5.34 Giu145, Leu160, Tyr162, Lys123, Phe134, Ala138, Tyr142, Thr141, Giu145, His159 Cipro -5.34 Giu145, Leu160, Tyr162, Lys123, Phe137, Ala138, Tyr142, Thr141, Giu145, His159 Cipro -5.34 Giu	2d	-6.64	His106, Phe107, Met138, Cys14, Leu16, Ile73, Tyr137, Tyr194, His235, Leu105, Asp108,	
Cipro -4.93 His19, His106, Tyr194, Asp108, Asp191, Leu16, Ala206, Cys14, Ser20, Leu33, Val35, Ile73, Phe107, His109, Giy207, Phe208, His235 Flu -5.81 His106, Phe107, Asp108, Tyr194, Glu136, His169, Asp191, Hs235, Cys14, Leu16, Ile73, Cys14, Ala206, Leu33, Ser20, His109 Ia -5.09 Ala138, Phe137, Tyr142, Phe134, Leu160, Tyr162, Thr141, Glu145, His159, Asn161 1b -5.34 Phe137, Leu122, Lys123, Ile126, Ala138, Tyr142, Leu160, Tyr162, Ala119, Thr141, Ile215 1c -5.46 Phe137, Leu122, Lys123, Ile126, Phe134, Ala138, Val211, Ile215, Thr141, Tyr142, Glu145, Leu160, Tyr162, Leu208, Asn212 2a -4.55 Glu145, His159, Tyr142, Phe134, Ala138, Leu160, Phe137, Thr141, Asn146, Asn161, Tyr162 2b -4.87 Phe134, Lys123, Phe137, Ala138, Tyr142, Thr141, Glu145, His159, Asn161 2c -4.64 Leu160, Phe137, Tyr162, Phe134, Ala138, Val211, Ile159, Asn161 2c -4.64 Leu160, Phe137, Tyr142, Phe134, Ala138, Thr141, His159, Asn161 2c -4.64 Leu160, Phe137, Tyr162, Phe134, Ala138, Thr141, Glu145, His159 2d -4.87 Phe134, Lys123, Phe137, Ala138, Thr141, His159, Asn161 2c -4.64 Leu160, Tyr162, Lys123, Phe134, Ala138, Thr141, His159, Asn161 2d -4.87 Tyr162, Leu248, Cig276, Met303			Arg134, His169, Asp191, Ala206, Gly207, Phe208	
Flu Phe107, His109, Gly207, Phe208, His235 Flu -5.81 His106, Phe107, Asp108, Tyr194, Glu136, His169, Asp191, Hs235, Cys14, Leu16, Ile73, Cys14, Ala206, Leu33, Ser20, His109 Ia -5.09 Ala138, Phe137, Tyr142, Phe134, Leu160, Tyr162, Thr141, Glu145, His159, Asn161 1b -5.34 Phe134, Phe137, Leu122, Lys123, Ile126, Ala138, Tyr142, Leu160, Tyr162, Ala119, Thr141, Ile215 1c -5.46 Phe137, Leu122, Lys123, Ile126, Phe134, Ala138, Val211, Ile215, Thr141, Tyr142, Glu145, Leu160, Tyr162, Leu208, Asn212 1d -5.44 Phe134, Phe137, Leu122, Lys123, Ile126, Ala138, Tyr162, Val211, Ile215, Ala119, Thr141, Leu160, Leu208, Asn212 2a -4.55 Glu145, His159, Tyr142, Phe134, Ala138, Leu160, Phe137, Thr141, Asn146, Asn161, Tyr162 2b -4.87 Phe134, Lys132, Phe137, Hal38, Tyr142, Thr141, Is159, Asn161, His159 2d -4.84 Tyr162, Leu160, Phe137, Tyr162, Phe134, Ala138, Tyr142, Thr141, Glu145, Asn161, His159 2d -4.84 Tyr162, Leu160, Tyr162, Lys123, Phe134, Phe133, Ala38, Thr141, Tyr142, Asn161 Flu -3.94 Tyr162, Thr141, Ala138, Glu145, Leu160, Phe137, Tyr124, Asn161 1c -5.846 Trp277, Cys274, Arg276, Met303, Met332, Ala332, Leu248, Glu250, Gly275, Asp278, Tyr279, Gly329, Leu444, Glu445, Glu4446, Glu446, Glu250, Gly275, Asp278, Gly329, Leu444, Glu445, Glu444	Cipro	-4.93	His19, His106, Tyr194, Asp108, Asp191, Leu16, Ala206, Cys14, Ser20, Leu33, Val35, Ile73,	
Flu -5.81 His106, Phe107, Asp108, Tyr194, Glu136, His169, Asp191, Hs235, Cys14, Leu16, Ile73, Cys14, Ala206, Leu33, Ser20, His109 Ia -5.09 Ala138, Phe137, Tyr142, Phe134, Leu160, Tyr162, Thr141, Glu145, His159, Asn161 Ib -5.34 Phe134, Phe137, Leu122, Lys123, Ile126, Ala138, Tyr142, Leu160, Tyr162, Ala119, Thr141, Ile215 1c -5.46 Phe137, Leu122, Lys123, Ile126, Phe134, Ala138, Val211, Ile215, Thr141, Tyr142, Glu145, Leu160, Tyr162, Leu208, Asn212 2a -5.44 Phe137, Leu122, Lys123, Ile126, Ala138, Tyr162, Val211, Ile215, Ala119, Thr141, Leu160, Leu208, Asn212 2a -4.55 Glu145, His159, Tyr142, Phe134, Ala138, Leu160, Phe137, Thr141, Asn146, Asn161, Tyr162 2b -4.87 Phe137, Leu122, Lys123, Ile126, Ala138, Tyr162, Thr141, His159, Asn161 2c -4.64 Leu160, Phe137, Tyr162, Phe134, Ala138, Leu160, Phe137, Thr141, Glu145, Asn161, His159 2d -4.84 Tyr162, Leu160, Phe14eu160, Lys123, Phe137, Ala138, Tyr142, Thr141, Glu145, His159 2d -5.34 Glu145, Leu160, Thr162, Lys123, Phe137, Ala138, Tyr142, Thr141, Glu145, Ala161 7bl -3.77 Trp277, Cys274, Arg276, Met303, Met332, Ala332, Leu248, Glu250, Gly275, Asp278, Tyr279, Gly329, Trp365, Leu344 1b -8.77 Trp277, Leu248, Arg276, Met303, Ala332, Leu444, Met445, Glu446, Sla449, Glu	-		Phe107, His109, Gly207, Phe208, His235	
Ala206, Leu33, Ser20, His109 Zŕnp 1a -5.09 Ala138, Phe137, Tyr142, Phe134, Leu160, Tyr162, Thr141, Giu145, His159, Asn161 1b -5.34 Phe134, Phe137, Leu122, Lys123, Ile126, Ala138, Tyr142, Leu160, Tyr162, Ala119, Thr141, Ile215 1c -5.46 Phe137, Leu122, Lys123, Ile126, Phe134, Ala138, Val211, Ile215, Thr141, Tyr142, Glu145, Leu160, Tyr162, Leu208, Asn212 1d -5.44 Phe134, Phe137, Leu122, Lys123, Ile126, Ala138, Tyr162, Val211, Ile215, Ala119, Thr141, Leu160, Leu208, Asn212 2a -4.55 Glu145, His159, Tyr142, Phe134, Ala138, Leu160, Phe137, Thr141, Asn146, Asn161, Tyr162 2b -4.87 Phe134, Lys123, Phe137, Ala138, Tyr142, Thr141, Glu145, Asn161, His159 2d -4.84 Tyr162, Leu160, Phe1124, Glu152, Phe134, Ala138, Tyr142, Thr141, Glu145, Asn161, His159 2d -4.84 Tyr162, Leu160, Phe1124, Glu152, Phe137, Ala138, Tyr142, Thr141, Glu145, Asn161 2d -4.84 Tyr162, Leu160, Phe124, Glu153, Phe137, Ala138, Tyr142, Thr141, Glu145, Asn161 2d -5.34 Glu145, Leu160, Tyr162, Lys123, Phe137, Ala138, Tyr142, Thr141, Tyr142, Asn161 Flu -3.94 Tyr162, Thr141, Ala138, Glu145, Leu30, Met332, Ala332, Leu248, Glu250, Gly275, Asp278, Tyr279, Gly329, Jeu444 1b -77 Trp277,	Flu	-5.81	His106, Phe107, Asp108, Tyr194, Glu136, His169, Asp191, Hs235, Cys14, Leu16, Ile73, Cys14,	
Image: 25.09 Ala138, Phe137, Tyr142, Phe134, Leu160, Tyr162, Thr141, Glu145, His159, Asn161 1b -5.03 Phe134, Phe137, Leu122, Lys123, Ile126, Ala138, Tyr142, Leu160, Tyr162, Ala119, Thr141, Ile215 1c -5.46 Phe137, Leu122, Lys123, Ile126, Phe134, Ala138, Val211, Ile215, Thr141, Tyr142, Glu145, Leu160, Tyr162, Leu208, Asn212 1d -5.47 Phe137, Teu122, Lys123, Ile126, Ala138, Tyr162, Val211, Ile215, Ala119, Thr141, Leu160, Leu208, Asn212 2a -4.55 Glu145, His159, Tyr142, Phe134, Ala138, Leu160, Phe137, Thr141, Asn146, Asn161, Tyr162 2b -4.87 Phe134, Lys123, Phe137, Ala138, Tyr142, Thr141, Glu145, Asn161, His159 2c -4.64 Leu160, Phe137, Tyr162, Phe134, Ala138, Tyr142, Thr141, Glu145, Asn161 2c -4.64 Leu160, Phe120, Dyr162, Lys123, Phe137, Ala138, Tyr142, Thr141, Glu145, His159 2d -4.84 Tyr162, Lru160, Lys123, Phe137, Ala138, Tyr142, Thr141, Glu145, His159 2d -4.84 Tyr162, Lru160, Var123, Phe137, Ala33, Tyr142, Thr141, Glu145, Ala161 Flu -3.94 Tyr162, Lru248, Arg276, Met303, Met332, Ala332, Leu248, Glu250, Gly275, Asp278, Tyr279, Gly329, Leu444, Glu446 1a -8.07 Trp277, Leu248, Arg276, Met303, Ala332, Leu248, Glu250, Gly275, Asp278, Gly239, Leu244, Glu250, Asp173, Gly275, Gly228, Glu350, Leu344			Ala206, Leu33, Ser20, His109	
1a -5.09 Ala138, Phe137, Tyr142, Phe134, Leu160, Tyr162, Thr141, Glu145, His159, Asn161 1b -5.34 Phe137, Leu122, Lys123, Ile126, Ala138, Tyr142, Leu160, Tyr162, Ala119, Thr141, Ile215 1c -5.46 Phe137, Leu122, Lys123, Ile126, Phe134, Ala138, Val211, Ile215, Thr141, Tyr142, Glu145, Leu160, Tyr162, Leu208, Asn212 1d -5.44 Phe137, Leu122, Lys123, Ile126, Ala138, Tyr162, Val211, Ile215, Ala119, Thr141, Leu160, Leu208, Asn212 2a -4.55 Glu145, His159, Tyr142, Phe134, Ala138, Leu160, Phe137, Thr141, Asn146, Asn161, Tyr162 2b -4.87 Phe134, Ivs123, Phe137, Ala138, Tyr142, Thr141, His159, Asn161 2c -4.64 Leu160, Phe124, Lys123, Phe137, Ala138, Tyr142, Thr141, Glu145, Asn161, His159 2d -4.87 Tyr162, Leu160, Phe134, Lys123, Phe137, Ala138, Tyr142, Thr141, Glu145, Asn161 Flu -3.94 Tyr162, Lys123, Phe137, Ala138, Tyr142, Thr141, Glu145, Asn161 Flu -3.94 Tyr162, Thr365, Leu444 1b -8.07 Trp277, Cys274, Arg276, Met303, Met332, Ala332, Leu248, Glu250, Gly275, Asp278, Tyr279, Gly329, Leu444, Glu446 1c -8.64 Trp365, Trp277, Leu248, Arg276, Met303, Ala332, Phe333, Ala449, Arg166, Glu250, Asn273, Gly275, Asp278, Gly329, Glu356, Leu444 2a -8.48 Asp447, Ar			2fnp	
1b -5.34 Phe134, Phe137, Leu122, Lys123, Ile126, Ala138, Tyr142, Leu160, Tyr162, Ala119, Thr141, Ile215 1c -5.46 Phe137, Leu122, Lys123, Ile126, Phe134, Ala138, Val211, Ile215, Thr141, Tyr142, Glu145, Leu160, Tyr162, Leu208, Asn212 1d -5.44 Phe134, Phe137, Leu122, Lys123, Ile126, Ala138, Tyr162, Val211, Ile215, Ala119, Thr141, Leu160, Leu208, Asn212 2a -4.55 Glu145, His159, Tyr142, Phe134, Ala138, Tyr142, Tyr162, Val211, Ile215, Ala119, Thr141, Leu160, Leu208, Asn212 2a -4.55 Glu145, His159, Tyr142, Phe134, Ala138, Tyr142, Tyr162, Thr141, Asn146, Asn161, Tyr162 2b -4.87 Phe134, Lys123, Phe137, Ala138, Tyr142, Thr141, Glu145, Asn161 2c -4.64 Leu160, Phe137, Tyr162, Phe134, Ala138, Tyr142, Thr141, Glu145, His159 2d -4.84 Tyr162, Leu160, Phe11eu160, Lys123, Phe137, Ala138, Tyr142, Thr141, Glu145, Kan160 Flu -3.94 Tyr162, Thr141, Ala138, Glu145, Leu160, Phe134, Lys123, Phe137, Tyr142, Asn161 2 -4.84 Tyr277, Cys274, Arg276, Met303, Met303, Ala332, Leu248, Glu250, Gly275, Asp278, Tyr279, Gly329, Tp365, Leu444 1b -8.77 Trp277, Leu248, Arg276, Met303, Ala332, Leu248, Glu450, Glu250, Asn273, Cys274, Gly275, Asp278, Gly329, Glu356, Leu444 1c -8.64 Trp365, Trp277, Met30, Thg365, Met303, Ala332, Ala449, Asp120,	1a	-5.09	Ala138, Phe137, Tyr142, Phe134, Leu160, Tyr162, Thr141, Glu145, His159, Asn161	
Ile215 Ile215 1c -5.46 Phe137, Leu122, Lys123, Ile126, Phe134, Ala138, Val211, Ile215, Thr141, Tyr142, Glu145, Leu160, Tyr162, Leu208, Asn212 1d -5.44 Phe134, Phe137, Leu122, Lys123, Ile126, Ala138, Tyr162, Val211, Ile215, Ala119, Thr141, Leu160, Leu208, Asn212 2a -4.55 Glu145, His159, Tyr142, Phe134, Ala138, Leu160, Phe137, Thr141, Asn146, Asn161, Tyr162 2b -4.87 Phe134, Lys123, Phe137, Ala138, Tyr142, Thr141, Glu145, Asn161, His159 2c -4.64 Leu160, Phe137, Tyr162, Phe137, Ala138, Tyr142, Thr141, Glu145, His159 2d -4.84 Tyr162, Leu160, Phe134, Phe137, Ala138, Tyr142, Thr141, Glu145, His159 Cipro -5.34 Glu145, Leu160, Tyr162, Lys123, Phe137, Ala138, Tyr142, Thr141, Glu145, His159 Flu -3.94 Tyr162, Thr141, Ala138, Glu145, Leu160, Phe134, Lys123, Phe137, Tyr142, Asn161 1z -5.07 Trp277, Cys274, Arg276, Met303, Met332, Ala332, Leu248, Glu250, Gly275, Asp278, Tyr279, Gly329, Trp365, Leu444 1b -8.07 Trp277, Leu248, Arg276, Met303, Met332, Ala332, Leu444, Glu250, Asn273, Cys274, Gly275, Asp278, Gly329, Leu444, Glu446 1c -8.64 Trp377, Leu248, Arg276, Met303, Ala332, Phe333, Ala449, Arg166, Glu250, Asn273, Cys274, Gly275, Gly328, Glu329, Leu444, Glu446, Asp447, Arg266, Lys2515, Leu248, Glu250, Asn273, Cys274, Gly275, Gly328,	1b	-5.34	Phe134. Phe137. Leu122. Lvs123. Ile126. Ala138. Tvr142. Leu160. Tvr162. Ala119. Thr141.	
1c -5.46 Phe137, Leu122, Lys123, Ile126, Phe134, Ala138, Val211, Ile215, Thr141, Tyr142, Glu145, Leu160, Tyr162, Leu208, Asn212 1d -5.44 Phe134, Phe137, Leu122, Lys123, Ile126, Ala138, Tyr162, Val211, Ile215, Ala119, Thr141, Leu160, Leu208, Asn212 2a -4.55 Glu145, His159, Tyr142, Phe134, Ala138, Leu160, Phe137, Thr141, Asn146, Asn161, Tyr162 2b -4.87 Phe134, Lys123, Phe137, Ala138, Tyr142, Tyr162, Thr141, His159, Asn161 2c -4.64 Leu160, Phe137, Tyr162, Phe137, Ala138, Tyr142, Thr141, Glu145, Asn161, His159 2d -4.84 Tyr162, Leu160, Phe1Leu160, Lys123, Phe137, Ala138, Tyr142, Thr141, Glu145, His159 Cipro -5.34 Glu145, Leu160, Phe124, Lys123, Phe137, Ala138, Tyr142, Sh161 Flu -3.94 Tyr162, Thr141, Ala138, Glu145, Leu160, Phe134, Lys123, Phe137, Tyr142, Asn161 7 Trp277, Cys274, Arg276, Met303, Met303, Ala332, Leu248, Glu250, Gly275, Asp278, Tyr279, Gly329, Trp365, Leu444 1a -8.07 Trp277, Leu248, Arg276, Met303, Met303, Ala332, Trp365, Ala449, Glu250, Cys274, Gly255, Asp278, Gly329, Leu444, Glu446 1c -8.64 Trp365, Trp277, Leu248, Cys274, Arg276, Met303, Ala332, Phe333, Ala449, Arg166, Glu250, Asn273, Cys274, Gly275, Asp278, Gly329, Glu356, Leu444 2a -8.48 Asp47, Arg276, Trp277, Met330, Trp365, Ket303, Ala332, Ala449, Sp12			lle215	
Leu160, Tyr162, Leu208, Asn212 1d -5.44 Phe134, Phe137, Leu122, Lys123, Ile126, Ala138, Tyr162, Val211, Ile215, Ala119, Thr141, Leu160, Leu208, Asn212 2a -4.55 Glu145, His159, Tyr142, Phe134, Ala138, Leu160, Phe137, Thr141, Asn146, Asn161, Tyr162 2b -4.87 Phe134, Lys123, Phe137, Ala138, Tyr142, Thr141, Glu145, Asn161, His159 2d -4.84 Tyr162, Leu160, Phe11eu160, Lys123, Phe137, Ala138, Tyr142, Thr141, Glu145, Asn161 Flu -3.94 Tyr162, Leu160, Tyr162, Lys123, Phe137, Ala138, Tyr142, Thr141, Glu145, His159 1a -8.07 Trp277, Cys274, Arg276, Met303, Met303, Ala332, Leu248, Glu250, Gly275, Asp278, Tyr279, Gly329, Trp365, Leu444 1b -8.77 Trp277, Leu248, Arg276, Met303, Met303, Ala332, Trp365, Ala449, Glu250, Cys274, Gly275, Asp278, Gly329, Leu444, Glu446 1c -8.64 Trp365, Trp277, Leu248, Arg276, Met303, Met303, Ala332, Trp365, Ala449, Arg166, Glu250, Asn273, Cys274, Gly275, Asp278, Trp277, Leu248, Arg276, Met303, Met303, Ala332, Phe333, Ala449, Arg166, Glu250, Asn273, Gly275, Asp278, Trp277, Leu248, Cys274, Arg276, Met303, Met303, Ala332, Ala449, Glu250, Cys274, Gly275, Asp278, Gly329, Leu444, Glu446 1c -8.64 Trp365, Trp277, Leu248, Cys274, Arg276, Met303, Met303, Ala332, Ala449, Glu250, Asn273, Gly275, Asp278, Trp277, Leu248, Cys274, Arg276, Met303, Met303, Ala332, Ala449, Glu250, Asn273, Gly275, Kap278, Trp277, Leu248, Cys274, Arg276, Met303, Ala332, Glu119, Asp120, Arg166, Lys215, Leu248, Glu250, Asn273, Cys274, Gly275, Gly328, Gly329, Met445, Glu446, Ala449, Thr450 2b -9.07 Trp365, Leu248, Arg276, Trp277, Met330, Trp365, Met303, Ala332, Ala449, Asp120, Arg166, Glu250, Asn273, Cys274, Gly275, Gly328, Gly329, Ala371, Leu444, Met445 2c -8.75 Met330, Trp365, Leu248, Arg276, Trp277, Met303, Ala332, Ala449, Asp120, Arg166, Glu250, Gly275, Asp278, Gly329, Asp352, Glu356, Met445, Glu446, Asp447 2d -8.78 Trp277, Met330, Leu248, Arg276, Trp277, Met303, Ala332, Ala449, Asp120, Arg166, Glu250, Gly275, Asp278, Gly329, Asp352, Glu356, Met445, Glu446, Asp447 2d -8.78 Trp277, Met330, Leu248, Arg276, Trp277,	1c	-5.46	Phe137, Leu122, Lys123, lle126, Phe134, Ala138, Val211, lle215, Thr141, Tyr142, Glu145,	
1d -5.44 Phe134, Phe137, Leu122, Lys123, Ile126, Ala138, Tyr162, Val211, Ile215, Ala119, Thr141, Leu160, Leu208, Asn212 2a -4.55 Glu145, His159, Tyr142, Phe134, Ala138, Leu160, Phe137, Thr141, Asn146, Asn161, Tyr162 2b -4.87 Phe134, Lys123, Phe137, Ala138, Tyr142, Tyr162, Thr141, His159, Asn161 2c -4.64 Leu160, Phe137, Tyr162, Phe134, Ala138, Tyr142, Thr141, Glu145, Asn161, His159 2d -4.84 Tyr162, Leu160, Phe1Leu160, Lys123, Phe137, Ala138, Tyr142, Thr141, Glu145, His159 Cipro -5.34 Glu145, Leu160, Tyr162, Lys123, Phe137, Ala138, Tyr142, Thr141, Glu145, His159 Cipro -5.34 Glu145, Leu160, Tyr162, Lys123, Phe137, Ala138, Tyr142, Asn161 Flu -3.94 Tyr162, Thr141, Ala138, Glu145, Leu160, Phe134, Lys123, Phe137, Ala138, Tyr142, Asn161 1a -8.07 Trp277, Cys274, Arg276, Met303, Met303, Ala332, Leu248, Glu250, Gly275, Asp278, Tyr279, Gly329, Trp365, Leu444, Glu444,			Leu160. Tvr162. Leu208. Asn212	
Leu160, Leu208, Asn212 2a -4.55 Glu145, His159, Tyr142, Phe134, Ala138, Leu160, Phe137, Thr141, Asn146, Asn161, Tyr162 2b -4.87 Phe134, Lys123, Phe137, Ala138, Tyr142, Tyr162, Thr141, His159, Asn161 2c -4.64 Leu160, Phe137, Tyr162, Phe134, Ala138, Tyr142, Thr141, Glu145, Asn161, His159 2d -4.84 Tyr162, Leu160, Phe1Leu160, Lys123, Phe137, Ala138, Tyr142, Thr141, Glu145, His159 Cipro -5.34 Glu145, Leu160, Tyr162, Lys123, Phe137, Ala138, Tyr142, Thr141, Glu145, His159 1a -8.07 Trp277, Cys274, Arg276, Met303, Met332, Ala332, Leu248, Glu250, Gly275, Asp278, Tyr279, Gly329, Trp365, Leu444 1b -8.77 Trp277, Leu248, Arg276, Met303, Met330, Ala332, Lrp365, Ala449, Glu250, Cys274, Gly275, Asp278, Gly329, Leu444, Glu446 1c -8.64 Trp365, Trp277, Leu248, Arg276, Met303, Ala332, Phe333, Ala449, Arg166, Glu250, Asn273, Cys274, Gly275, Asp278, Tyr279, Gly329, Glu356, Leu444 2a -8.48 Asp447, Arg276, Trp277, Leu248, Cys274, Arg276, Met303, Ala332, Glu119, Asp120, Arg166, Lys215, Leu484, Glu265, Crp277, Met330, Trp365, Clu444 2a -8.48 Asp447, Arg276, Trp277, Met330, Trp365, Met303, Ala332, Glu119, Asp120, Arg166, Lys215, Leu248, Glu250, Gly275, Gly329, Glu356, Leu444 2a -8.48 Asp447, Arg276, Trp277, Met330, Ala332, Ala449, Slu20, Arg166, Glu250, Asn273, Cys274, Gly275, Gly328, Gly329, Jaa67, Leu444, Met445, Glu446, Ala449, Glu250, Asn273, Cys274, Gly275, Gly328, Gly329, Jaa67, Leu444, Met445 2c -8.75 Met330, Trp365, Leu248, Arg276, Trp277, Met330, Ala332, Ala449, Asp120, Arg166, Glu250, Asn273, Cys274, Gly275, Gly328, Gly329, Ala367, Leu444, Met445 2c -8.75 Met330, Trp365, Leu248, Arg276, Trp277, Met330, Ala332, Ala449, Asp120, Arg166, Glu250, Asn273, Cys274, Gly275, Gly328, Gly329, Ala367, Leu444, Met445 2c -8.78 Trp277, Met330, Leu248, Arg276, Trp277, Aet333, Ala332, Ala449, Asp120, Arg166, Glu250, Asn273, Cys274, Gly275, Asp278, Gly328, Glu3250, Gly327, Trp365, Leu444, Arg166, Glu250, Gly275, Asp278, Gly329, Asp352, Glu356, Met445, Glu446, Asp447 Cipro -8.80 Asp120, Arg276, Asp278, Met330, Glu250, Gly2	1d	-5.44	Phe134, Phe137, Leu122, Lys123, Ile126, Ala138, Tyr162, Val211, Ile215, Ala119, Thr141,	
2a -4.55 Glu145, His159, Tyr142, Phe134, Ala138, Leu160, Phe137, Thr141, Asn146, Asn161, Tyr162 2b -4.87 Phe134, Lys123, Phe137, Ala138, Tyr142, Tyr162, Thr141, His159, Asn161 2c -4.64 Leu160, Phe137, Tyr162, Phe134, Ala138, Tyr142, Thr141, Glu145, Asn161, His159 2d -4.84 Tyr162, Leu160, Phe1Leu160, Lys123, Phe137, Ala138, Tyr142, Thr141, Glu145, Asn161 Flu -3.94 Tyr162, Leu160, Tyr162, Lys123, Phe134, Ala138, Tyr142, Thr141, Glu145, Asn161 Flu -3.94 Tyr162, Thr141, Ala138, Glu145, Leu160, Phe134, Lys123, Phe137, Ala138, Tyr142, Asn161 Suz 1a -8.07 Trp277, Cys274, Arg276, Met303, Met332, Ala332, Leu248, Glu250, Gly275, Asp278, Tyr279, Gly329, Trp365, Leu444 1b -8.77 Trp277, Leu248, Arg276, Met303, Met303, Ala332, Phe333, Ala449, Arg166, Glu250, Asn273, Cys274, Gly275, Asp278, Ma331, Leu444, Met445, Glu446, Asp447, Thr450 1d -9.00 Trp365, Trp277, Leu248, Cys274, Arg276, Met303, Met330, Ala332, Glu119, Asp120, Arg166, Lys215, Leu248, Glu250, Asn273, Cys274, Gly275, Gly329, Glu356, Leu444 2a -8.48 Asp447, Arg276, Trp277, Met330, Trp365, Met303, Ala332, Glu119, Asp120, Arg166, Lys215, Leu248, Glu250, Gly227, Gly227, Gly229, Met445, Glu446, Ala449, Thr450 2b -9.07 Trp365, Leu248, Arg276, Trp277, Met330, Ala332, Ala449, Asp120,			Leu160. Leu208. Asn212	
2b -4.87 Phe134, Lys123, Phe137, Ala138, Tyr142, Tyr162, Thr141, His159, Asn161 2c -4.64 Leu160, Phe137, Tyr162, Phe134, Ala138, Tyr142, Thr141, Glu145, Asn161, His159 2d -4.84 Tyr162, Leu160, Phe11eu160, Lys123, Phe137, Ala138, Tyr142, Thr141, Glu145, His159 Cipro -5.34 Glu145, Leu160, Tyr162, Lys123, Phe134, Phe137, Ala138, Thr141, Tyr142, Asn161 Flu -3.94 Tyr162, Thr141, Ala138, Glu145, Leu160, Phe134, Lys123, Phe137, Tyr142, Asn161 Suz 1a -8.07 Trp277, Cys274, Arg276, Met303, Met303, Ala332, Leu248, Glu250, Gly275, Asp278, Tyr279, Gly329, Trp365, Leu444 1b -8.77 Trp277, Leu248, Arg276, Met303, Met303, Ala332, Phe333, Ala449, Arg166, Glu250, Asn273, Cys274, Gly275, Asp278, Gly329, Leu444, Glu446 1c -8.64 Trp365, Trp277, Leu248, Arg276, Met303, Met303, Ala332, Phe333, Ala449, Arg166, Glu250, Asn273, Gly275, Asp278, Gly329, Glu356, Leu444 2a -8.64 Trp365, Trp277, Leu248, Cys274, Arg276, Met303, Met303, Ala332, Glu119, Asp120, Arg166, Lys215, Leu248, Glu250, Asn273, Cys274, Gly275, Gly328, Glu3250, Glu326, Glu3250, Glu3250, Lus444, Met445, Glu446, Asp447, Thr450 2b -9.00 Trp365, Leu248, Arg276, Trp277, Met303, Ala332, Ala449, Asp120, Arg166, Glu250, Asn273, Cys274, Gly275, Gly328, Gly329, Ala367, Leu444, Met445 2c -8.78 M	2a	-4.55	Glu145, His159, Tyr142, Phe134, Ala138, Leu160, Phe137, Thr141, Asn146, Asn161, Tyr162	
2c -4.64 Leu160, Phe137, Tyr162, Phe134, Ala138, Tyr142, Thr141, Glu145, Asn161, His159 2d -4.84 Tyr162, Leu160, Phe1Leu160, Lys123, Phe137, Ala138, Tyr142, Thr141, Glu145, His159 Cipro -5.34 Glu145, Leu160, Tyr162, Lys123, Phe134, Phe137, Ala138, Thr141, Tyr142, Asn161 Flu -3.94 Tyr162, Thr141, Ala138, Glu145, Leu160, Phe134, Lys123, Phe137, Tyr142, Asn161 Suz 1a -8.07 Trp277, Cys274, Arg276, Met303, Met332, Ala332, Leu248, Glu250, Gly275, Asp278, Tyr279, Gly329, Trp365, Leu444 1b -8.77 Trp277, Leu248, Arg276, Met303, Met303, Ala332, Trp365, Ala449, Glu250, Cys274, Gly275, Asp278, Gly329, Leu444, Glu446 1c -8.64 Trp365, Trp277, Leu248, Arg276, Met303, Ala332, Phe333, Ala449, Arg166, Glu250, Asn273, Cys274, Gly275, Asp278, Tyr279, Gly329, Glu356, Leu444 1d -9.00 Trp365, Trp277, Leu248, Cys274, Arg276, Met303, Ala332, Glu119, Asp120, Arg166, Lys215, Leu248, Glu250, Asn273, Cys274, Gly275, Gly329, Glu356, Leu444 2a -8.48 Asp447, Arg276, Trp277, Met30, Ala332, Ala449, Asp120, Arg166, Glu250, Asn273, Cys274, Gly275, Gly328, Gly329, Ala367, Leu444, Met445 2b -9.07 Trp365, Leu248, Arg276, Trp277, Met303, Ala332, Ala449, Asp120, Arg166, Glu250, Asn273, Cys274, Gly275, Gly328, Gly329, Ala337, Leu444, Met445 2c -8.75 Met330, Trp36	2b	-4.87	Phe134, Lys123, Phe137, Ala138, Tyr142, Tyr162, Thr141, His159, Asn161	
2d -4.84 Tyr162, Leu160, Phe1Leu160, Lys123, Phe137, Ala138, Tyr142, Thr141, Glu145, His159 Cipro -5.34 Glu145, Leu160, Tyr162, Lys123, Phe134, Phe137, Ala138, Thr141, Tyr142, Asn161 Flu -3.94 Tyr162, Thr141, Ala138, Glu145, Leu160, Phe134, Lys123, Phe137, Tyr142, Asn161 Suz 1a -8.07 Trp277, Cys274, Arg276, Met303, Met303, Ala332, Leu248, Glu250, Gly275, Asp278, Tyr279, Gly329, Trp365, Leu444 1b -8.77 Trp277, Leu248, Arg276, Met303, Met303, Ala332, Trp365, Ala449, Glu250, Cys274, Gly275, Asp278, Gly329, Leu444, Glu446 1c -8.64 Trp365, Trp277, Leu248, Arg276, Met330, Ala332, Phe333, Ala449, Arg166, Glu250, Asn273, Cys274, Gly275, Asp278, Tyr279, Gly329, Glu356, Leu444, Met445, Glu446, Asp447, Thr450 1d -9.00 Trp365, Trp277, Leu248, Cys274, Arg276, Met330, Ala332, Glu119, Asp120, Arg166, Lys215, Leu248, Glu250, Asn273, Cys274, Gly275, Gly329, Glu356, Leu444 2a -8.48 Asp447, Arg276, Trp277, Met330, Trp365, Met303, Ala332, Glu119, Asp120, Arg166, Glu250, Asn273, Cys274, Gly275, Gly328, Gly329, Met445, Glu446, Ala449, Thr450 2b -9.07 Trp365, Leu248, Arg276, Trp277, Met330, Ala332, Ala449, Asp120, Arg166, Glu250, Asn273, Cys274, Gly275, Gly328, Gly329, Ala337, Leu444, Met445 2c -8.75 Met330, Leu248, Arg276, Met330, Ala332, Zla449, Asp120, Arg166, Glu250, Asn273, Cys274, Gly275, Asp278, Gly328, Al	2c	-4.64	Leu160, Phe137, Tvr162, Phe134, Ala138, Tvr142, Thr141, Glu145, Asn161, His159	
Cipro -5.34 Glu145, Leu160, Tyr162, Lys123, Phe134, Phe137, Ala138, Thr141, Tyr142, Asn161 Flu -3.94 Tyr162, Thr141, Ala138, Glu145, Leu160, Phe134, Lys123, Phe137, Tyr142, Asn161 3cuz 3cuz 1a -8.07 Trp277, Cys274, Arg276, Met303, Met332, Ala332, Leu248, Glu250, Gly275, Asp278, Tyr279, Gly329, Trp365, Leu444 1b -8.77 Trp277, Leu248, Arg276, Met303, Met303, Ala332, Trp365, Ala449, Glu250, Cys274, Gly275, Asp278, Gly329, Leu444, Glu446 1c -8.64 Trp365, Trp277, Leu248, Arg276, Met330, Ala331, Leu444, Met445, Glu446, Asp447, Thr450 1d -9.00 Trp365, Trp277, Leu248, Cys274, Arg276, Met330, Ala332, Glu119, Asp120, Arg166, Lys215, Gly275, Asp278, Tyr279, Gly329, Glu356, Leu444 2a -8.48 Asp447, Arg276, Trp277, Met330, Trp365, Met303, Ala332, Glu119, Asp120, Arg166, Lys215, Leu248, Glu250, Asn273, Cys274, Gly275, Gly328, Gly329, Met445, Glu446, Ala449, Thr450 2b -9.07 Trp365, Leu248, Arg276, Trp277, Met330, Ala332, Ala449, Asp120, Arg166, Glu250, Asn273, Cys274, Gly275, Gly328, Gly329, Ala367, Leu444, Met445 2c -8.75 Met330, Trp365, Leu248, Arg276, Trp277, Met333, Ala342, Ala449, Asp120, Arg166, Glu250, Asn273, Cys274, Gly275, Gly328, Gly329, Ala367, Leu444, Met445 2c -8.75 Met330, Trp365, Leu248, Arg276, Trp277, Met333, Ala332, Ala449, Asp120, Arg166, Glu250, Asn273, Cys274, Gly275, Asp278, Gly	2d	-4.84	Tyr162, Leu160, Phe1Leu160, Lys123, Phe137, Ala138, Tyr142, Thr141, Glu145, His159	
Flu -3.94 Tyr162, Thr141, Ala138, Glu145, Leu160, Phe134, Lys123, Phe137, Tyr142, Asn161 3cuz 1a -8.07 Trp277, Cys274, Arg276, Met303, Met332, Ala332, Leu248, Glu250, Gly275, Asp278, Tyr279, Gly329, Trp365, Leu444 1b -8.77 Trp277, Leu248, Arg276, Met303, Met303, Ala332, Trp365, Ala449, Glu250, Cys274, Gly275, Asp278, Gly329, Leu444, Glu446 1c -8.64 Trp365, Trp277, Leu248, Arg276, Met330, Ala332, Phe333, Ala449, Arg166, Glu250, Asn273, Cys274, Gly275, Asp278, Ala331, Leu444, Met445, Glu446, Asp447, Thr450 1d -9.00 Trp365, Trp277, Leu248, Cys274, Arg276, Met303, Ala332, Ala439, Ala332, Ala449, Glu250, Asn273, Gly275, Asp278, Tyr279, Gly329, Glu356, Leu444 2a -8.48 Asp447, Arg276, Trp277, Met330, Trp365, Met303, Ala332, Glu119, Asp120, Arg166, Lys215, Leu248, Glu250, Asn273, Cys274, Gly275, Gly328, Gly329, Met445, Glu446, Ala449, Thr450 2b -9.07 Trp365, Leu248, Arg276, Trp277, Met330, Lau332, Ala449, Asp120, Arg166, Glu250, Asn273, Cys274, Gly275, Gly328, Gly329, Ala332, Ala449, Asp120, Arg166, Glu250, Asn273, Cys274, Gly275, Gly328, Gly329, Ala332, Ala449, Asp120, Arg166, Glu250, Asn273, Cys274, Gly275, Asp278, Gly328, Ala331, Leu444, Met445 2c -8.75 Met330, Trp365, Leu248, Arg276, Met303, Ala332, Ala449, Asp120, Arg166, Glu250, Asn273, Cys274, Gly275, Asp278, Gly328, Ala331, Glu356, Met445, Glu446, Asp447 2d -8.78 Trp277, Met330, Leu248, Arg276, Met303, Ala332, Trp365, Le	Cipro	-5.34	Glu145, Leu160, Tyr162, Lys123, Phe134, Phe137, Ala138, Thr141, Tyr142, Asn161	
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2b -9.07 Trp365, Leu248, Arg276, Trp277, Met30, Ala332, Ala449, Asp120, Arg166, Glu250, Asn273, Cys274, Gly275, Gly328, Gly329, Ala367, Leu444, Met445 2c -8.75 Met330, Trp365, Leu248, Arg276, Trp277, Met303, Ala332, Ala449, Asp120, Arg166, Glu250, Asn273, Cys274, Gly275, Asp278, Gly328, Ala331, Glu356, Met445, Glu446, Asp447 2d -8.78 Trp277, Met330, Leu248, Arg276, Met303, Ala332, Trp365, Leu444, Arg166, Glu250, Gly275, Asp278, Gly329, Ala351, Glu356, Met445, Glu446, Asp447 Cipro -8.80 Asp120, Arg276, Asp278, Met330, Glu250, Gly275, Trp277, Asp447, Ala332, Glu119, Lys215, Leu248, Gly329, Trp365, Ala331, Met445, Glu446, Ala449 Flu -6.82 Arg166, Arg276, Met330, Glu250, Cys274, Asp447, Trp365, Ala449, Leu248, Asn273, Gly275, Trp277, Asp278, Gly329			Leu248. Glu250. Asn273. Cvs274. Glv275. Glv328. Glv329. Met445. Glu446. Ala449. Thr450	
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Trp277, Asp278, Glv329	Flu	-6.82	Arg166, Arg276, Met330, Glu250, Cvs274, Asp447, Trp365, Ala449, Leu248, Asp73, Glv275	
		5.02	Trp277. Asp278. Glv329	

* Binding Affinity in kcal/mol.



Figure S23. Interaction residues of all molecules, Ciprofloxacin, and Fluconazole with Quorum-Quenching N-Acyl Homoserine Lactone Lactonase (dark green and turquoise: H-bonds; green: van der Waals; orange: pi-anion/cation; pink: alkyl and pi-alkyl; yellow: pi-sulfur; fuchsia: pi-pi stacked and pi-pi T shaped)



Figure S24. Interaction residues of all molecules, Ciprofloxacin, and Fluconazole with Crystal structure of SarA (dark green and turquoise: H-bonds; green: van der Waals; orange: pi-anion/cation; pink: alkyl and pi-alkyl; yellow: pi-sulfur; fuchsia: pi-pi stacked and pi-pi T shaped)



Figure S25. Interaction residues of all molecules, Ciprofloxacin, and Fluconazole with Atomic Resolution Structures of Escherichia coli and Bacillis anthracis Malate Synthase A (dark green and turquoise: H-bonds; green: van der Waals; orange: pi-anion/cation; pink: alkyl and pi-alkyl; yellow: pi-sulfur; fuchsia: pi-pi stacked and pi-pi T shaped).