Supporting Information

Design and Synthesis of novel fluconazole analogues

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¹ H and ¹³ C NMR Spectra of compounds 4 to 13	2-65
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Figure S-1 ^MH MNR spectrum of 4a



Figure S-2¹³C NMR spectrum of 4a



Figure S-3 ¹H MNR spectrum of 4b



Figure S-4¹³C NMR spectrum of 4b



Figure S-5 1 H MNR spectrum of 4c



Figure S-6¹³C NMR spectrum of 4c



Figure S-7¹H MNR spectrum of 4d



Figure S-8¹³C NMR spectrum of 4d



Figure S-⁹ 1H MNR spectrum of 4e



Figure S-10¹³C NMR spectrum of 4e



Figure S-11 ¹H MNR spectrum of 5a



Figure S-12 ¹³C NMR spectrum of 5a



Figure S-13 ¹H MNR spectrum of 5b



Figure S-14 ¹³C NMR spectrum of 5b



Figure S-15 ¹H MNR spectrum of 5c



Figure S-16 $^{\rm 13}{\rm C}$ NMR spectrum of 5c



Figure S-17 ¹H MNR spectrum of 5d



Figure S-18¹³C NMR spectrum of 5d



Figure S-19 ¹H MNR spectrum of 5e



Figure S-20 ¹³C NMR spectrum of 5e



Figure S-21¹H MNR spectrum of 6a



Figure S-22 ¹³C NMR spectrum of 6a



Figure S-23 ¹H MNR spectrum of 6b



Figure S-24¹³C NMR spectrum of 6b



Figure S-25 ¹H MNR spectrum of 6c



Figure S-26 ¹³C NMR spectrum of 6c



Figure S-27 ¹H MNR spectrum of 6d



Figure S-28¹³C NMR spectrum of 6d



Figure S-29¹H MNR spectrum of 6e



Figure S-30¹³C NMR spectrum of 6e



Figure S-31 ¹H MNR spectrum of 7



Figure S-32 ¹H MNR spectrum of 8



Figure S-33 ¹³C NMR spectrum of 8



Figure S-34 ¹H MNR spectrum of 9a



Figure S-35 ¹³C NMR spectrum of 9a


Figure S-36 ¹H MNR spectrum of 9b



Figure S-37¹³C NMR spectrum of 9b



Figure S-38 ¹H MNR spectrum of 9c



Figure S-39¹H MNR spectrum of 9d



Figure S-40 ¹³C NMR spectrum of 9d



Figure S-41 ¹H MNR spectrum of 9e



Figure S-42 ¹³C NMR spectrum of 9e



Figure S-43 ¹H MNR spectrum of 12



Figure S-44 ¹³C NMR spectrum of 12





Figure S-46¹³C NMR spectrum of 13a



Figure S-47 ¹H MNR spectrum of 13b



Figure S-48 ¹³C NMR spectrum of 13b



Figure S-49 ¹H MNR spectrum of 13c



Figure S-50 ¹³C NMR spectrum of 13c



Figure S-51 ¹H MNR spectrum of 13d



Figure S-52 ¹³C NMR spectrum of 13d



Figure S-53 ¹H MNR spectrum of 13e

54

0.00



Figure S-54 ¹³C NMR spectrum of 13e



Figure S-55 ¹H MNR spectrum of 13f



Figure S-56¹³C NMR spectrum of 13f



Figure S-57 ¹H MNR spectrum of 13g





Figure S-59 ¹H MNR spectrum of 13h



Figure S-60 ¹³C NMR spectrum of 13h



Figure S-61 ¹H MNR spectrum of 13i









Figure S-65 ¹³C NMR spectrum of 13j

Analyzed: 04/20/15 09:09 AM

Reported: 04/21/15 04:45 PM Processed: 04/21/15 04:44 PM

Data Path: C:\WIN32APP\HSM\HPLC\DATA\7855\ Processing Method: SANTOSHH

System(acquisition): Sys 1 Application: HPLC Sample Name: 6a Injection from this vial: 1 of 1 Sample Description: MEOH:H2O(60:40) Series:7855 Volume: 10.0 ul



No.	RT	Height	Area	Area %
1	1.40	2353	20447	0.117
2	2.36	3092	24051	0.137
3	3.58	1271	11579	0.066
4	6.05	606272	17401992	99.443
5	8.28	2372	41365	0.236
		615360	17499434	100.000

Peak rejection level: 0

Group Leader :- Dr. V. S. Pore COLUMN :-Kromasil C18 (150 X 4.6mm) MOBILE PHASE :-MEOH:H20(60:40) WAVELENGTH :- 254nm FLOW RATE :- 1 ml/min (1730psi) SAMPLE CONC :- 1 mg/1ml Injection vol:5ul

Analyzed: 04/24/15 04:54 PM

Data Path: C:\WIN32APP\HSM\HPLC\DATA\7901\ Processing Method: SANTOSHH

System(acquisition): Sys 1 Application: HPLC Sample Name: 6B Injection from this vial: 1 of 1 Sample Description: MEOH:H2O(60:40) Reported: 04/24/15 05:22 PM Processed: 04/24/15 05:22 PM

Series:7901 Volume: 10.0 ul



No.	RT	Height	Area	Area %
1	2.38	8480	62488	0.190
2	5.85	3754	42425	0.129
3	7.94	1842	70535	0.214
4	11.58	365890	32364016	98.393
5	22.65	10888	353237	1.074
		390854	32892701	100.000

Peak rejection level: 0

Group Leader :- DR.V. S. PORE COLUMN :-KROMASIL C-18 (150 X 4.6mm) MOBILE PHASE :-MEOH:H20(60:40) WAVELENGTH :- 254nm FLOW RATE :- 1 ml/min (1715psi) SAMPLE CONC :- 1mg/1ml Injection vol:20ul

Analyzed: 04/24/15 03:25 PM

Reported: 04/24/15 03:52 PM Processed: 04/24/15 03:52 PM

Data Path: C:\WIN32APP\HSM\HPLC\DATA\7897\ Processing Method: SANTOSHH

System(acquisition): Sys 1 Application: HPLC Sample Name: 6C Injection from this vial: 1 of 1 Sample Description: MEOH:H2O(60:40) Series:7897 Volume: 10.0 ul



Area	Height	RT	No.
347793	22443	4.47	1
18396192	832929	5.82	2
20568	758	9.83	3
18764553	856130		
	Area 347793 18396192 20568 18764553	Height Area 22443 347793 832929 18396192 758 20568 856130 18764553	RT Height Area 4.47 22443 347793 5.82 832929 18396192 9.83 758 20568 856130 18764553

```
Group Leader :- DR.V. S. PORE

COLUMN :-KROMASIL C-18 (150 X 4.6mm)

MOBILE PHASE :-MEOH:H20(60:40)

WAVELENGTH :- 254nm

FLOW RATE :- 1 ml/min (1715psi)

SAMPLE CONC :- 1mg/1ml Injection vol:20ul
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Reported: 04/24/15 04:37 PM Processed: 04/24/15 04:37 PM

Data Path: C:\WIN32APP\HSM\HPLC\DATA\7899\ Processing Method: SANTOSHH

System(acquisition): Sys 1 Application: HPLC Sample Name: 6D Injection from this vial: 1 of 1 Sample Description: MEOH:H2O(60:40) Series:7899 Volume: 10.0 ul



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Group Leader :- DR.V. S. PORE

COLUMN :-KROMASIL C-18 (150 X 4.6mm)

MOBILE PHASE :-MEOH:H20(60:40)

WAVELENGTH :- 254nm

FLOW RATE :- 1 ml/min (1715psi)

SAMPLE CONC :- 1mg/1ml Injection vol:20ul
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D-7000 HPLC System Manager Report

Analyzed: 04/21/15 02:18 PM

Data Path: C:\WIN32APP\HSM\HPLC\DATA\7859\ Processing Method: SANTOSHH

System(acquisition): Sys 1 Application: HPLC Sample Name: 6e Injection from this vial: 1 of 1 Sample Description: MEOH:H2O(60:40) Reported: 04/21/15 04:40 PM Processed: 04/21/15 04:37 PM

Series:7859 Volume: 10.0 ul



No.	RT	Height	Area	Area %
1	0.12	2270	11795	0.060
2	1.80	2477	27969	0.143
3	2.96	2976	37502	0.192
4	3.60	2593	44737	0.228
5	4.53	4187	202061	1.032
6	7.63	463710	19193753	98.027
7	10.51	2435	62315	0.318
		480648	19580132	100.000

Peak rejection level: 0

Group Leader :- Dr. V. S. Pore COLUMN :-Kromasil C18 (150 X 4.6mm) MOBILE PHASE :-MEOH:H20(60:40) WAVELENGTH :- 254nm FLOW RATE :- 1 ml/min (1730psi) SAMPLE CONC :- 1 mg/1ml Injection vol:5ul



Group Leader	:- DR.V. S. PORE
COLUMN	:-KROMASIL 100 RP-18 (150 X 4.6mm)
MOBILE PHASE	:-MEOH;H20(50:50)
WAVELENGTH	:- 254nm
FLOW RATE	;- 1 ml/min (2240psi)
SAMPLE CONC	:- 1 mg/1ml Injection vol:10ul



Group Leader	;- DR.V. S. PORE
COLUMN	:-KROMASIL 100 RP-18 (150 X 4.6mm)
MOBILE PHASE	:-MEOH:H20(50:50)
WAVELENGTH	:- 254nm
FLOW RATE	:- 1 ml/min (2240psi)
SAMPLE CONC	:- 1 mg/1m) Injection vol:10ul
Analyzed: 04/24/15 02:56 PM

Reported: 04/24/15 04:34 PM Processed: 04/24/15 04:33 PM

Data Path: C:\WIN32APP\HSM\HPLC\DATA\7895\ Processing Method: SANTOSHH

System(acquisition): Sys 1 Application: HPLC Sample Name: 9A Injection from this vial: 1 of 1 Sample Description: MEOH:H2O [60:40] Series:7895 Volume: 10.0 ul



No.	RT	Height	Area	Area %
1	2.34	3169	24918	0.174
2	3.53	1557	36124	0.253
3	5.88	540776	14212252	99.339
4	7.96	2114	33538	0.234
		547616	14306832	100.000

Peak rejection level: 0



Peak rejection level: 0



Peak rejection level: 0

00w11vï└üß☺└011vï└üß☺└0Dw7090HPLCeSoten MangeerBCPPIt2vï└üГ@♥012vï└üГ@♥00w12vï└üГ@♥

Analyzed: 04/24/15 04:28 PM

Data Path: C:\WIN32APP\HSM\HPLC\DATA\7900\ Processing Method: SANTOSHH

System(acquisition): Sys 1 Application: HPLC Sample Name: 9D Injection from this vial: 1 of 1 Sample Description: MEOH:H2O(60:40) Reported: 04/24/15 04:56 PM Processed: 04/24/15 04:55 PM

Series:7900 Volume: 10.0 ul



No.	RT	Height	Area	Area %
1 2 3 4	2.38 7.64 11.35 21.71	1383 5205 743629 2500	8532 242482 65950726 150462	0.013 0.365 99.395 0.227
		752717	66352202	100.000

Peak rejection level: 0



Peak rejection level: 0

Group Leader := DR.V. S. PORE COLUMN :=-KROMASTL 100 RP-18 (150 X 4.6mm) MOBILE PHASE :=-MEOH:H20:(60:40) WAVELENGTH := 254nm FLOW RATE := 1 ml/min (1480psi) SAMPLE CONC := 1 mg/lml Injection vol:10ul

Analyzed: 04/24/15 01:02 PM

Data Path: C:\WIN32APP\HSM\HPLC\DATA\7890\ Processing Method: SANTOSHH

System(acquisition): Sys 1 Application: HPLC Sample Name: 13A Injection from this vial: 1 of 1 Sample Description: ACN:H2O (40:60) Reported: 04/24/15 04:05 PM Processed: 04/24/15 04:05 PM

Series:7890 Volume: 10.0 ul



Area	Height	RT	No.
25657	1022	1.53	1
2832416	98279	4.53	2
39620	1521	12.02	3
2897693	100822		
	Area 25657 2832416 39620 2897693	HeightArea`1022256579827928324161521396201008222897693	RTHeightArea1.53`1022256574.5398279283241612.021521396201008222897693

Peak rejection level: 0

Analyzed: 04/24/15 11:49 AM

Data Path: C:\WIN32APP\HSM\HPLC\DATA\7885\ Processing Method: SANTOSHH

System(acquisition): Sys 1 Application: HPLC Sample Name: 13B Injection from this vial: 1 of 1 Sample Description: ACN:H2O (40:60) Reported: 04/24/15 03:59 PM Processed: 04/24/15 03:59 PM

100.000

Series:7885 Volume: 10.0 ul

6575491



367395

Peak rejection level: 0

Group Leader	:- DR.V. S. PORE
COLUMN	:-KROMASIL C-18 (150 X 4.6mm)
MOBILE PHASE	:-ACN:H20(40:60)
WAVELENGTH	:- 254nm
FLOW RATE	:- 1 ml/min (1715psi)
SAMPLE CONC	:- 1mg/1ml Injection vol:20ul

Analyzed: 04/21/15 04:28 PM

Data Path: C:\WIN32APP\HSM\HPLC\DATA\7867\ Processing Method: SANTOSHH

System(acquisition): Sys 1 Application: HPLC Sample Name: 13C Injection from this vial: 1 of 1 Sample Description: ACN:H2O [40:60]

Reported: 04/21/15 05:37 PM Processed: 04/21/15 05:37 PM

Series:7867 Volume: 10.0 ul



Chrom Type: HPLC Channel: 1

Retention	Time	(min)

Area %	Height	RT	No.
0.397	5401	1.42	1
0.708	6514	1.80	2
0.049	982	3.61	3
97.147	876413	4.57	4
0.267	3482	6.03	5
1.432	12651	7.91	6
100.000	905443		
	6514 982 876413 3482 12651 905443	1.80 3.61 4.57 6.03 7.91	2 3 4 5 6

Peak rejection level: 0

Analyzed: 04/21/15 05:57 PM

Reported: 04/21/15 06:18 PM Processed: 04/21/15 06:17 PM

Data Path: C:\WIN32APP\HSM\HPLC\DATA\7871_001\ Processing Method: SANTOSHH

System(acquisition): Sys 1 Application: HPLC Sample Name: 13D Injection from this vial: 1 of 1 Sample Description: ACN:H2O (40:60) Series:7871_001 Volume: 10.0 ul



No.	RT	Height	Area	Area 70
1 2 3	4.11 5.70 7.82	791033 879 858	11032604 8253 11006	99.826 0.075 0.100
		792770	11051863	100.000

Peak rejection level: 0

Analyzed: 04/21/15 04:57 PM

Reported: 04/21/15 05:40 PM Processed: 04/21/15 05:40 PM

38974

100339

13628387

0.286

0.736

100.000

Data Path: C:\WIN32APP\HSM\HPLC\DATA\7868\ Processing Method: SANTOSHH

3.86

4.92

6.05

System(acquisition): Sys 1 Application: HPLC Sample Name: 13E Injection from this vial: 1 of 1 Sample Description: ACN:H2O [40:60] Series:7868 Volume: 10.0 ul



4614

9493

1082834

- 1		1 1	0
Peak	rejection	level:	0

3

4

5

Group Leader COLUMN MOBILE PHASE	:- Dr. V. S. Pore :-Kromasil C18 (150 X 4.6mm) :-ACN:H20(40:60)
WAVELENGTH	:- 254nm
FLOW RATE	:- 1 ml/min (1730psi)
SAMPLE CONC	:- 1 mg/1ml Injection vol:5ul

Analyzed: 04/21/15 06:25 PM

Reported: 04/21/15 06:45 PM Processed: 04/21/15 06:45 PM

Data Path: C:\WIN32APP\HSM\HPLC\DATA\7871\ Processing Method: SANTOSHH

System(acquisition): Sys 1 Application: HPLC Sample Name: 13F Injection from this vial: 1 of 1 Sample Description: ACN:H2O(40:60) Series:7871 Volume: 10.0 ul





No.	RT	Height	Area	Area %
1	2.46	2309	20044	0.217
1	2.40	763966	8907025	96.548
2	5.45	2231	27201	0.295
3	4.19	5403	59832	0.649
4	4.62	10720	141186	1.530
5	4.94	10730	70213	0.761
6	7.90	4370	70215	
		789099	9225501	100.000

Peak rejection level: 0

Analyzed: 04/21/15 05:14 PM

Reported: 04/21/15 05:54 PM Processed: 04/21/15 05:52 PM

Data Path: C:\WIN32APP\HSM\HPLC\DATA\7869\ Processing Method: SANTOSHH

System(acquisition): Sys 1 Application: HPLC Sample Name: 13G Injection from this vial: 1 of 1 Sample Description: ACN:H2O(40:60) Series:7869 Volume: 10.0 ul



No.	RT	Height	Area	Area %
1 2 3	3.11 3.88 6.04	386473 1965 8746	4193398 13040 85551	97.703 0.304 1.993
		397184	4291989	100.000

Peak rejection level: 0

Group Leader COLUMN	:- Dr. V. S. Pore :-Kromasil C18 (150 X 4.6mm)
MOBILE PHASE	:-ACN:H20(40:60)
WAVELENGTH	:- 254nm
FLOW RATE	:- 1 ml/min (1730psi)
SAMPLE CONC	:- 1 mg/1ml Injection vol:5ul

Analyzed: 04/24/15 12:05 PM

Reported: 04/24/15 04:02 PM Processed: 04/24/15 04:02 PM

Data Path: C:\WIN32APP\HSM\HPLC\DATA\7886\ Processing Method: SANTOSHH

System(acquisition): Sys 1 Application: HPLC Sample Name: 13H Injection from this vial: 1 of 1 Sample Description: ACN:H2O(40:60) Series:7886 Volume: 10.0 ul





		544995	8708348	100.000
4	5.50	1985	17703	0.203
3	4.67	1640	16249	0.187
2	3.12	540349	8657248	99.413
1	1.65	1021	1/148	0.197

Peak rejection level: 0

Analyzed: 04/24/15 11:12 AM

Data Path: C:\WIN32APP\HSM\HPLC\DATA\7882\ Processing Method: SANTOSHH

System(acquisition): Sys 1 Application: HPLC Sample Name: 13I Injection from this vial: 1 of 1 Sample Description: ACN:H2O(40:60) Reported: 04/24/15 03:56 PM Processed: 04/24/15 03:55 PM

Series:7882 Volume: 10.0 ul



No.	RT	Height	Area	Area %
1	1.94	2229	40197	0.637
2	2.62	1272	8440	0.134
3	3.61	529726	6249663	99.079
4	5.88	1032	9465	0.150
	i.	534259	6307765	100.000

Peak rejection level: 0

Analyzed: 04/24/15 01:18 PM

Data Path: C:\WIN32APP\HSM\HPLC\DATA\7891\ Processing Method: SANTOSHH

System(acquisition): Sys 1 Application: HPLC Sample Name: 13J Injection from this vial: 1 of 1 Sample Description: ACN:H2O (40:60) Reported: 04/24/15 04:07 PM Processed: 04/24/15 04:07 PM

Series:7891 Volume: 10.0 ul

Chrom Type: HPLC Channel: 1



Peak rejection level: 0