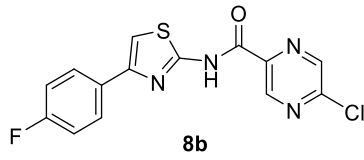


Supplementary Material 3

Design, synthesis and antimycobacterial activity of hybrid molecules combining pyrazinamide with 4-phenylthiazol-2-amine scaffold

Jan Zitko, Ondřej Jand'ourek, Pavla Paterová, Lucie Navrátilová, Jiří Kuneš, Jarmila Vinšová, Martin Doležal

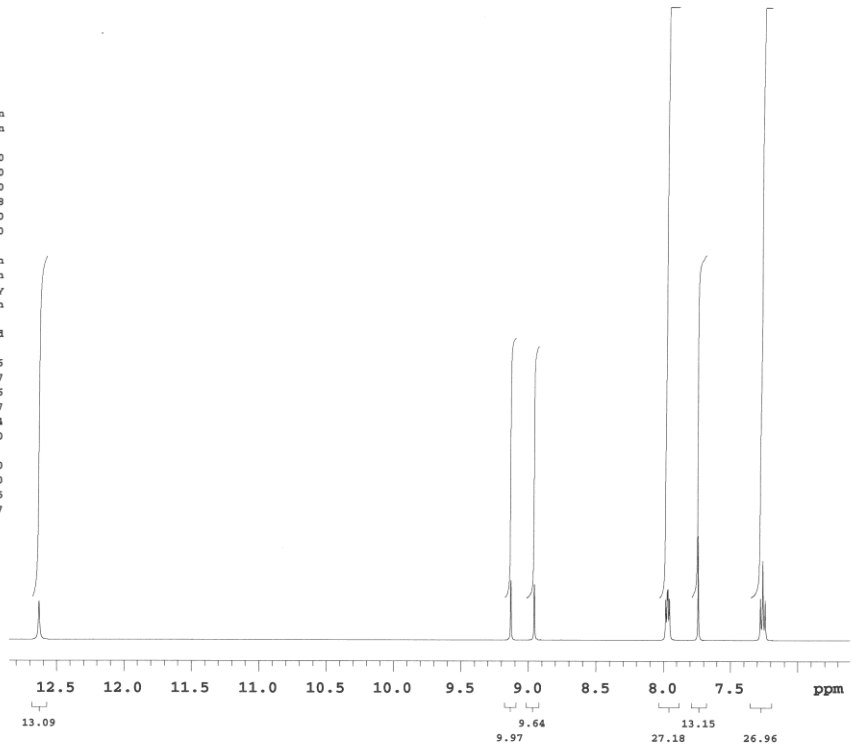
Representative NMR spectra of selected compounds



JZ-141

exp1 PROTON

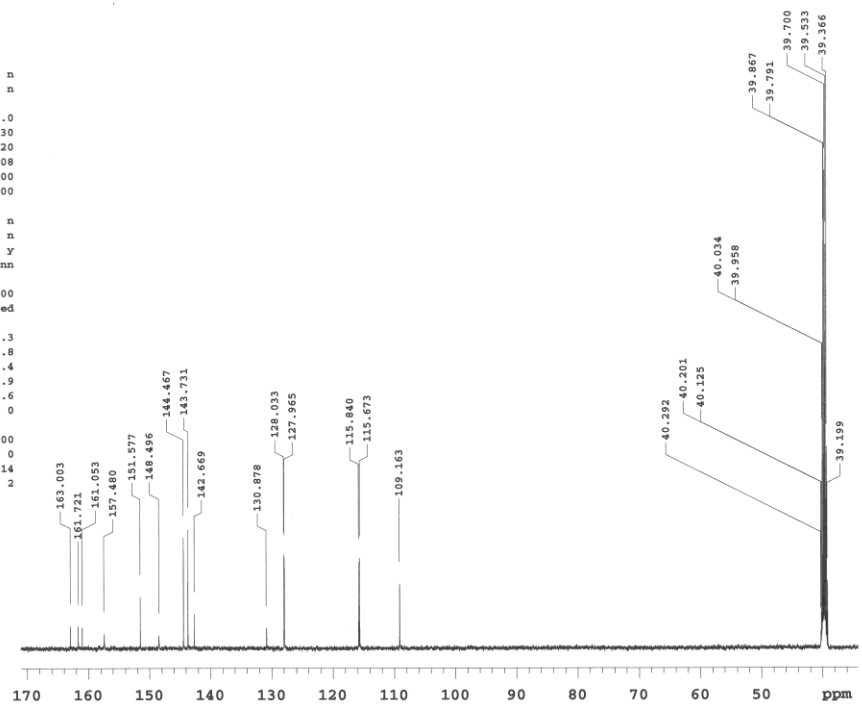
SAMPLE		PRESATURATION	
date	Jan 27 2014	satmode	n
solvent	dmsd	wet	n
file	exp	SPECIAL	
ACQUISITION		temp	25.0
sw	8012.8	gain	30
at	2.045	spin	20
np	32768	hst	0.008
fb	4000	pw90	9.100
bs	32	alfa	10.000
d1	1.000	FLAGS	
nt	8	il	n
ct	8	in	n
TRANSMITTER		dp	y
tn	H1	hs	nn
sfrq		499.869	PROCESSING
tof	499.8	fn	not used
tpwr	60	DISPLAY	
pw	4.550	sp	3305.6
DECOUPLER		wp	3119.7
dn	C13	rfl	2254.6
dof	0	rfp	1244.7
dm	nnn	rp	47.4
decwave	W40_OneNMR-	lp	0
	_W018	PLOT	
dpwr	37	wc	200
dmf	32258	sc	0
		vs	45
		th	7
		ai	cdc ph

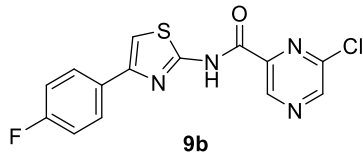


1-AH-82

exp2 CARBON

SAMPLE		PRESATURATION	
date	Jan 27 2014	satmode	n
solvent	dmsd	wet	n
file	exp	SPECIAL	
ACQUISITION		temp	25.0
sw	31250.0	gain	30
at	1.049	spin	20
np	65536	hst	0.008
fb	17000	pw90	11.300
bs	1	alfa	10.000
d1	3.000	FLAGS	
nt	1000	il	n
ct	216	in	n
TRANSMITTER		dp	y
tn	C13	hs	nn
sfrq		125.705	PROCESSING
tof	1913.9	lb	1.00
tpwr	55	fn	not used
pw	5.650	DISPLAY	
DECOUPLER		sp	4304.3
dn	H1	wp	17193.8
dof	0	rfl	6826.4
dm	YYY	rfp	4989.9
decwave	w	rp	134.6
dpwr	41	lp	0
dmf	12346	PLOT	
		wc	200
		sc	0
		vs	114
		th	2
		nm	cdc ph

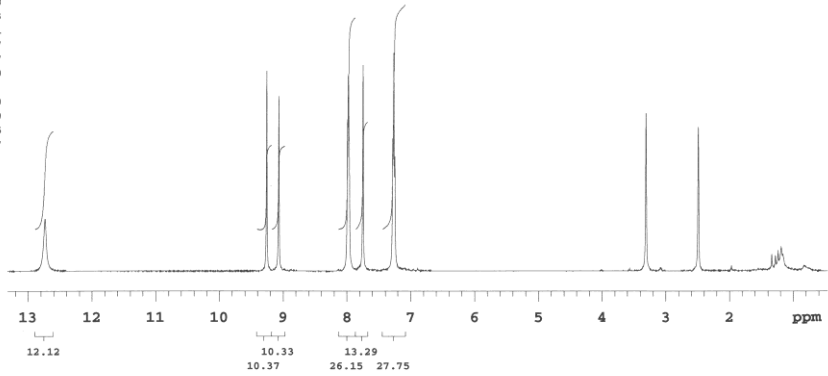




BS-J2-4F

exp1 PROTON

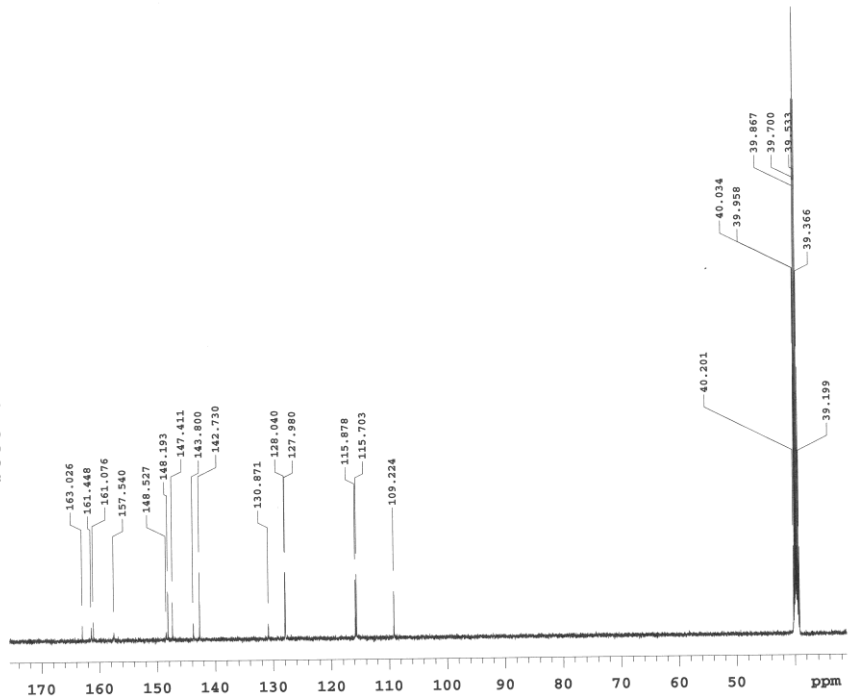
SAMPLE		PRESATURATION	
date	Apr 8 2014	satmode	n
solvent	dmsc	wet	n
file	exp	SPECIAL	
ACQUISITION		temp	25.0
sw	8012.8	gain	30
at	2.045	spin	20
np	32768	hst	0.008
fb	4000	pw90	9.100
bs	32	alfa	10.000
d1	1.000	FLAGS	
nt	8	il	n
ct	8	in	n
TRANSMITTER		dp	y
tn	H1	hs	nn
sfrq	499.869	PROCESSING	
tof	499.8	fn	not used
tpwr	60	DISPLAY	
pw	4.550	sp	230.8
DECOUPLER		vp	6427.3
dn	C13	rfl	2254.1
dof	0	rfp	1244.7
dm	mnn	rp	122.7
decwave	W40_OneMR-	lp	0
		W018	
PLOT			
dpwr	37	wc	200
dmf	32258	sc	0
		vs	325
		th	7
		ai	cdc ph

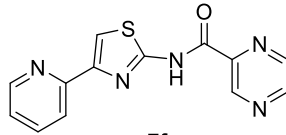


MGB-108

exp2 CARBON

SAMPLE		PRESATURATION	
date	Apr 8 2014	satmode	n
solvent	dmsc	wet	n
file	exp	SPECIAL	
ACQUISITION		temp	25.0
sw	31250.0	gain	30
at	1.049	spin	20
np	65536	hst	0.008
fb	17000	pw90	11.300
bs	1	alfa	10.000
d1	3.000	FLAGS	
nt	1000	il	n
ct	790	in	n
TRANSMITTER		dp	y
tn	C13	hs	nn
sfrq	125.705	PROCESSING	
tof	1913.9	lb	0.50
tpwr	55	fn	not used
pw	5.650	DISPLAY	
DECOUPLER		sp	3912.3
dn	H1	vp	18156.1
dof	0	rfl	6826.4
dm	yyy	rfp	4989.9
decwave	w	rp	44.8
dpwr	41	lp	0
dmf	12346	PLOT	
		wc	200
		sc	0
		vs	149
		th	44
		nm	cdc ph





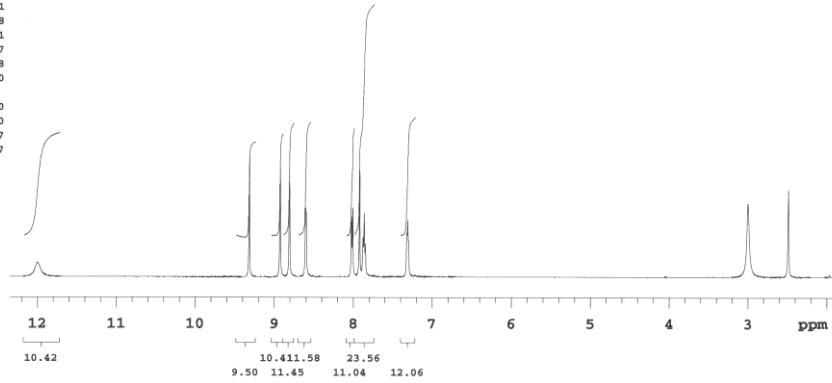
7f

JZ-155

exp62 PROTON

```

SAMPLE      PRESATURATION
date Jul 10 2014 satmode n
solvent dmsc wet n
file exp SPECIAL
ACQUISITION temp 80.0
sv 8012.8 gain 48
at 2.045 spin 20
np 32768 hst 0.008
fb 4000 pw90 9.100
hs 32 alfa 10.000
d1 1.000 FLAGS
nt 8 il n
ct 8 in n
TRANSMITTER dp y
tn H1 hs nn
sfrq 499.869 PROCESSING
tof 499.8 fn not used
tpwr 60 DISPLAY
pw 4.550 sp 956.1
DECOUPLER wp 5217.8
dn C13 rfl 2255.1
dof 0 rfp 1244.7
dm nnn rp -141.8
decwave W40_OneNMR- lp 0
_W018 PLOT
dpr 37 wc 200
dmf 32258 sc 0
vs 57
th
ai cdc ph 7
  
```

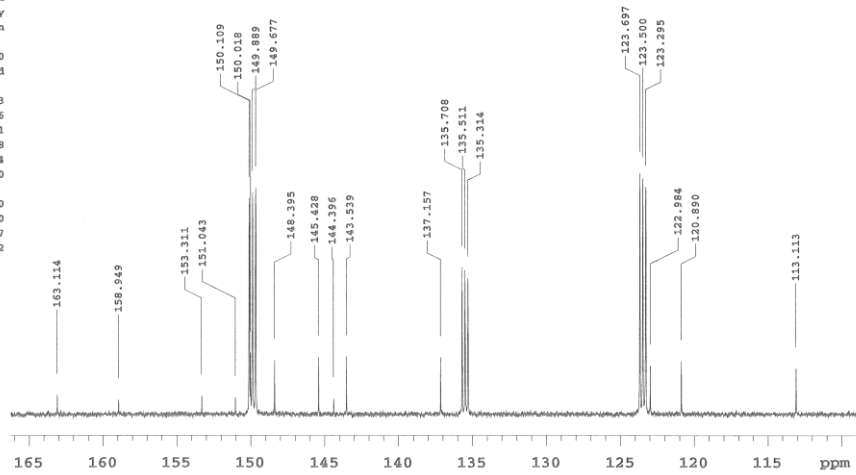


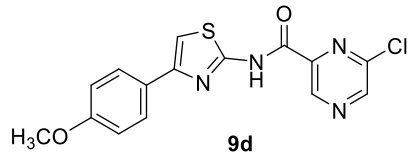
JZ-155P

exp700 CARBON

```

SAMPLE      PRESATURATION
date Sep 9 2015 satmode n
solvent pyridine wet n
file exp SPECIAL
ACQUISITION temp 25.0
sv 31250.0 gain 30
at 1.049 spin not used
np 65536 hst 0.008
fb 17000 pw90 11.300
hs 1 alfa 10.000
d1 1.000 FLAGS
nt 1500 il n
ct 129 in n
TRANSMITTER dp y
tn C13 hs nn
sfrq 125.704 PROCESSING
tof 1913.9 lb 1.00
tpwr 55 fn not used
pw 5.650 DISPLAY
DECOUPLER sp 13701.3
dn H1 vp 7193.6
dof 0 rfl 17146.1
dm yyy xfp 15522.8
decwave w xp -53.4
dpr 41 lp 0
dmf 12346 PLOT
wc 200
sc 0
vs 57
th
nm cdc ph 2
  
```

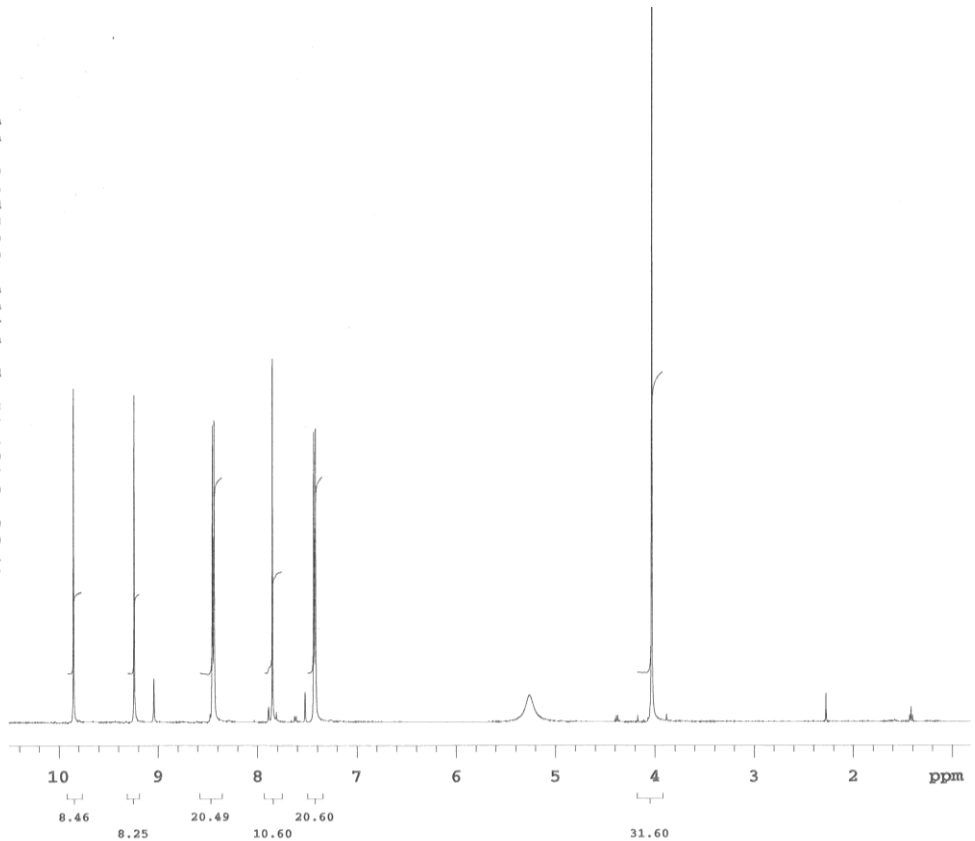




JZ-150P

exp700 PROTON

SAMPLE		PRESATURATION	
date	Sep 9 2015	satmode	n
solvent	pyridine	wet	n
file	exp	SPECIAL	
ACQUISITION		SPECIAL	
sw	8012.8	temp	25.0
at	2.045	gain	44
np	32768	spin	not used
fb	4000	hst	0.008
bs	32	pw90	9.100
dl	1.000	alfa	10.000
nt	8	il	n
ct	8	in	n
TRANSMITTER		SPECIAL	
tn	H1	hs	nn
sfrq	499.866	dp	y
PROCESSING		SPECIAL	
tof	499.9	fn	not used
tpwr	60	DISPLAY	
pw	4.550	sp	409.2
DECOUPLER		SPECIAL	
dn	C13	wp	4842.7
dof	0	rfl	1007.1
dm	nnn	rfp	0
decwave	W40_OneNMR-	rp	135.7
	_W018	lp	0
PLOT		SPECIAL	
dpwr	37	wc	200
dmf	32258	sc	0
		vs	61
		th	7
		ai	cdc ph



JZ-150P

exp700 CARBON

SAMPLE		PRESATURATION	
date	Sep 9 2015	satmode	n
solvent	pyridine	wet	n
file	exp	SPECIAL	
ACQUISITION		SPECIAL	
sw	31250.0	temp	25.0
at	1.049	gain	30
np	65536	spin	not used
fb	17000	hst	0.008
bs	1	pw90	11.300
dl	1.000	alfa	10.000
nt	1500	il	n
ct	270	in	n
TRANSMITTER		SPECIAL	
tn	C13	hs	nn
sfrq	125.704	dp	y
PROCESSING		SPECIAL	
tof	1913.9	lb	1.00
tpwr	55	fn	not used
pw	5.650	DISPLAY	
DECOUPLER		SPECIAL	
dn	H1	wp	6205.4
dof	0	rfl	14967.0
dm	YYY	rfp	17335.9
decwave	w	rp	15522.8
dpwr	41	lp	-52.1
dmf	12346	lp	0
PLOT		SPECIAL	
		wc	200
		sc	0
		vs	87
		th	3
		nm	cdc ph

