Supporting Information

1,3-Dipolar Cycloaddition Chemistry for the Preparation of Novel Indolizinone-Based Compounds

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Supporting Information Available: ^1H and ^{13}C -NMR spectra for new compounds lacking elemental analyses. This material is available free of charge *via* the Internet at <http://pubs.acs.org>.

General Experimental Section Paragraph: Melting points are uncorrected. Mass spectra were determined at an ionizing voltage of 70eV. Unless otherwise noted, all reactions were performed in flame dried glassware under an atmosphere of dry nitrogen. Solutions were evaporated under reduced pressure with a rotary evaporator and the residue was chromatographed on a silica gel column using an ethyl acetate-hexane mixture as the eluent unless specified otherwise.

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S3	^1H -NMR spectrum of compound 16a
S4	^1H -NMR spectrum of compound 19a
S5	^1H -NMR spectrum of compound 20a
S6	^1H -NMR spectrum of compound 23a
S7	^1H -NMR spectrum of compound 25a
S8	^1H -NMR spectrum of compound 17b
S9	^1H -NMR spectrum of compound 19b

- S10 ¹H-NMR spectrum of compound **20b**
- S11 ¹H-NMR spectrum of compound **16c**
- S12 ¹H-NMR spectrum of compound **17c**
- S13 ¹H-NMR spectrum of compound **18c**
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13C SENSITIVITY
ASTM SAMPLE

Pulse Sequence: zgpg30

Solvent: cdcl3

Ambient temperature

User: 1-15-87

INNOVA-600 "innova600"

PULSE SEQUENCE

Relax. delay 2.000 sec

Pulse 22.5 degrees

Acq. time 0.443 sec

Width 33984.7 Hz

2256 repetitions

OBSERVE C13, 150.8055560 MHz

DECOUPLE H1, 599.7458205 MHz

Power 40 dB

continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 2.0 Hz

FI size 32768

Total time 6 hr, 43 min, 38 sec

**13C SENSITIVITY
ASTM SAMPLE**

Pulse Sequence: szpul
Solvent: cdcl3
Ambient Temperature
User: 1-15-87
INOVA-600 "Inova600"

PULSE SEQUENCE
Relax: delay 2.00 sec
Pulse 22.5 degrees
Acq. time 0.443 sec
Width 33384.7 Hz
36 repetitions
ORFRAVE C13, 150.3055581 MHz
DECOUPLE H1, 599.7458205 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
F1 size 32768
Total time 6 hr, 48 min, 39 sec

STANDARD CARBON PARAMETERS

Pulse Sequence: szpul

Solvent: cdc13
Ambient temperature
INOVA-600 "Inova600"

PULSE SEQUENCE

Relax. delay 1.000 sec

Pulse 43.3 degrees

Acq. time 1.598 sec

Width 4830.0 Hz

16 repetitions

USERVE H1 598.7432086 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FI size 16384

Total time 0 min, 41 sec

STANDARD 1H OBSERVE

Pulse Sequence: szpu1
 Solvent: cdcl3
 Ambient temperature
 INOVA-400 "INOVA-400"
 PULSE SEQUENCE
 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 2.201 sec
 Width 3213.6 Hz
 16 repetitions
 OBSERVE H1, 399.9393025 MHz
 DATA PROCESSING
 Line broadening 0.2 Hz
 FT size 16384
 Total time 0 min, 51 sec

STANDARD 1H OBSERVE

Pulse Sequence: zgpg30
 Solvent: cdcl3
 Ambient temperature:
 INOVA-400 "INOVA400"
 PULSE SEQUENCE
 Relax: delay 1.000 sec
 Pulse: 45.0 degrees
 Acq. time 2.205 sec
 Width 3425.5 Hz
 16 repetitions
 OBSERVE H1, 399.939025 MHz
 DATA PROCESSING
 Line broadening 0.2 Hz
 FT size 16394
 Total time 0 min, 51 sec

STANDARD CARBON PARAMETERS

Pulse Sequence: szpu1

Solvent: cdc13

Ambient temperature

INNOVA-600 "Inova600"

PULSE SEQUENCE

Relax. delay 1.000 sec

Pulse 43.3 degrees

Acq. time 1.598 sec

Width 4819.9 Hz

16 repetitions

OBSERVE H1 599.7432086 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 16384

Total time 0 min, 41 sec

STANDARD CARBON PARAMETERS

Pulse Sequence: szpu1

Solvent: cdcl3

Ambient temperature

INOVA-600 "Inova600"

PULSE SEQUENCE

Relax. delay 1.000 sec

Pulse 43.3 degrees

Acc. time 1.598 sec

Width 4963.4 Hz

16 repetitions

OBSERVE H1, 599.7432076 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 16384

Total time 0 min, 41 sec

STANDARD 1H OBSERVE

Pulse Sequence: szpu
 Solvent: cdcl3
 Ambient temperature:
 INOVA-400 "Inova400"
 PULSE SEQUENCE
 Relax delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 2.201 sec
 Width 3227.2 Hz
 16 repetitions
 OBSERVE H1, 399.939025 MHz
 DATA PROCESSING
 Line broadening 0.2 Hz
 FI size 16384
 Total time 0 min, 51 sec

STANDARD 1H OBSERVE

Pulse Sequence: s2pu1
Solvent: cdcl3
Ambient temperature:
INOVA-400 "INOVA400"

PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.202 sec
Width 3857.1 Hz
16 repetitions
OBSERVE H1, 399.9399023 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 16384
Total time 0 min, 51 sec

¹³C SENSITIVITY
ASTM SAMPLE
 Pulse Sequence: szpul
 Solvent: c6cl3
 Ambient temperature
 User: 1-15-87
 INOVA-600 "Inova600"
PULSE SEQUENCE
 Relax. delay 2.000 sec
 Pulse 22.5 degrees
 Acq. time 0.443 sec
 Width 33984.7 Hz
 1040 repetitions
 OBSERVE C13, 150.805518 MHz
 DECOUPLE H1, 599.7458205 MHz
 Power 40 dB
 continuously on
 WALTZ-16 modulated
DATA PROCESSING
 Line broadening 2.0 Hz
 FT size 32768
 Total time 6 hr, 48 min, 36 sec

STANDARD PROTON PARAMETERS

Pulse Sequence: szpul
 Solvent: DMSO
 Ambient temperature
 INOVA-600 "Inova600"
 PULSE SEQUENCE
 Pulse 45.0 degrees
 Acq. time 1.892 sec
 Width 5795.8 Hz
 16 repetitions
 OBSERVE H1: 509.7460462 MHz
 DATA PROCESSING
 FT size 32768
 Total time 0 min, 30 sec

STANDARD CARBON PARAMETERS

Pulse Sequence: szpul

Solvent: cdc13

Ambient temperature

INOVA-600 "INOVA600"

PULSE SEQUENCE

Relax. delay 1.000 sec

Pulse 43.3 degrees

Acq. time 1.593 sec

Width 4953.3 Hz

18 repetitions

OBSERVE H1: 599.7432006 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 16384

Total time 0 min, 41 sec

Solvent: cdcl₃
Ambient temperature

AMBIENTE Lempriere
INOVA-600 "inova600"

PULSE SEQUENCE

Relax. delay 1.000 sec
Pulse 43.3 degrees

Acq. time 1.598 sec

16 repetitions

OBSERVE H1, 599.7432086 MHz
DATA PROCESSING

Line broadening 0.2 Hz

FT size 16384
Total time 0

Total time 0 min, 41 sec

STANDARD 1H OBSERVE

Pulse Sequence: s2pu1
 Solvent: cdcl3
 Ambient temperature:
 INOVA-400 "Inova400"
 PULSE SEQUENCE
 Relax delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 2.202 sec
 Width 5203.3 Hz
 16 repetitions
 OBSERVE H1, 399.9389025 MHz
 DATA PROCESSING
 Line broadening 0.2 Hz
 FT size 32768
 Total time 0 min, 51 sec

STANDARD CARBON PARAMETERS

Pulse Sequence: szpu1

Solvent: cdc13

Ambient Temperature

INOVA-600 "Inova600"

PULSE SEQUENCE

Relax. delay 1.000 sec

Pulse 43.3 degrees

Acq. time 1.508 sec

Width 7804.1 Hz

Single scan

Observe H1, 509.7432076 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 32768

Total time 0 min, 2 sec

EMO01191

expl stidh

SAMPLE

DEC. & VT

date Apr 6 2005

399.940

solvent cdcl3

h1

file exp

30

ACQUISITION

-630.7

sfrq 399.941

nmn

tn h1

c

at 2.202

200

np 22312

csdq

sw 5203.3

1.0

fb 3000

homo

bs 16

PROCESSING

tpwr 58

0.20

pw 8.0

wlfile

di 1.000

proc

tof 207.8

fn

nt 8

math

ct 8

react

alock n

procpilot

gain not used

flags

fl n

in n

dp y

hs nm

DISPLAY

sp -21.9

wp 2901.0

vs 144

sc 0

wc 250

hzmm 11.92

ts 500.00

rtf 3294.5

rtf 2903.6

th 10

ins 3.000

nm cdc ph

EMOCROTAL

expt stath

SAMPLE

DEC. 8 VI

date Dec 20 2004

399.940

solvent cdc13

H1

file exp

30

ACQUISITION

-630.7

sfrq 399.941

nm

tn H1

C

at 2.202

200

np 22912

1.0

sw 5203.3

nm

th 3000

PROCESSING

bs 16

0.20

tpwr 58

1b

pw 8.0

wtfile

dl 1.000

proc

tof 207.0

fn

nt 15

math

cl 16

react

alock not used

procplot

gain not used

react

il n

wtl

in n

wtl

dp y

wtl

hs nm

wtl

sp DISPLAY

wtl

wp -165.1

wtl

vs 3309.1

wtl

sc 144

wtl

wc 0

wtl

hzm 250

wtl

is 13.24

wtl

is 500.00

wtl

ftl 3294.2

wtl

ftl 2903.6

wtl

th 2

wtl

ins 100.000

wtl

nm cdc ph

wtl

EMOMethallyl

expl steln

SAMPLE		DEC. & VT	
date	Dec 20 2004	dfrq	399.940
solvent	cdcl3	dn	H1
file	exp	dpwr	30
ACQUISITION		do	-630.7
stfrq	399.941	dm	nm
tn	H1	dmm	c
at	2.202	dseq	200
np	22912	ures	1.0
sw	5203.3	homo	n
fb	3000	PROCESSING	
bs	16	lb	0.20
tpwr	58	wtfile	
pw	8.0	proc	ft
dl	1.000	fn	not used
tof	207.0	math	f
nt	16	werr	react
ct	16	wexp	procp1ot
alock	n	ws	
gain	not used	wrt	
flags	n		
il	n		
in	y		
dp	nm		
hs			
DISPLAY			
sp	-89.5		
wp	3158.9		
vs	144		
sc	0		
wc	250		
h2mm	12.64		
ts	500.00		
ftl	3293.8		
rfp	2903.6		
th	3		
ins	1.000		
nm	cdc	ph

EMUC:inn

expt std:th

SAMPLE 8 2005 DEC. 8 VI
 date Mar 8 2005
 solvent cdc13
 file exp
 ACQUISITION
 sfrq 399.941
 in H1
 at 2.202
 np 22912
 sw 5203.3
 fd 3000
 bs 16
 tpwr 8.0
 pw 8.0
 dl 1.000
 tof 207.0
 nl 8
 ct 8
 atlock n
 gain not used
 flags not used
 t1 n
 in n
 dp v
 hs nm
 DISPLAY -23.5
 sp 3370.7
 wp 144
 vs 0
 wc 250
 hzmm 13.48
 is 500.00
 rfi 3896.1
 rfp 2903.6
 th 20
 ins 3.000
 nm cdc ph

DEC. 8 VI
 399.940
 H1
 -680.7
 30
 nm
 c
 200
 dseq
 dres
 1.0
 n
 homo
 PROCESSING
 0.20
 lb
 wtfile
 8.0
 proc
 fn
 math
 not used
 f
 react
 procpilot
 wnt

EMCrotty\G105ad

expt stdln

SAMPLE DEC. 8 VT
date Dec 20 2004 dfrq 399.940
solvent cdcl3 dn H1
file exp 30
ACQUISITION
sfreq 399.941 dm
tn H1 dmm
at 2.202 dmf
np 22912 dseq
sw 5203.3 dres
fz 3000 homo
bs 16 PROCESSING
tpwr 58 lb 0.20
pw 8.0 wtf1e
d1 1.000 proc ft
tof 207.0 tn not used
nt 16 math f
ct 16
alock n
gain not used
FLAGS not used
il n
in n
dn y
hs nn
DISPLAY
sp -137.8
wp 3151.9
vs 144
sc 0
wc 250
hzmm 12.61
is 500.00
f1l 3294.2
r1p 2903.7
ins 2.000
nm cdc ph

SAMPLE	DEC. & VI
Jun 2 2005	300.065
cdcl3	H1
dm	
dfrq	
exp	
dpr	30
dft	0
dm	mm
dmh	C
dmt	200
2.302	
17856	
38/9.1	
2220	
lb	0.30
wetfile	
16	
proc	ft
7.0	
6.0	not used
1.000	react
215.9	procpilot
16	
WIS	
0	
WIS	
not used	
FLAGS