Supplementary Information for:

A Practical Synthesis of Cabergoline

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¹H NMR Spectrum for **1** (cabergoline) in CDCl₃

¹³C NMR Spectrum for **1** (cabergoline) in CDCl₃

¹H NMR Spectrum for **1** (cabergoline) in DMSO-*d*₆

¹³C NMR Spectrum for **1** (cabergoline) in DMSO-*d*₆

¹H NMR Spectrum for **2**

¹³C NMR Spectrum for **2**

¹H NMR Spectrum for **9**

¹³C NMR Spectrum for **9**

¹H NMR Spectrum for **10**

¹³C NMR Spectrum for **10**

¹H NMR Spectrum for **11**

¹³C NMR Spectrum for **11**

cabergoline 34385-swa-53

Current Data Parameters
 NAME: cabergoline 34385-swa-53
 EXPNO: 1
 PROCNO: 1
 F2: Acquisition Parameters
 Date_ : 5000
 Time : 7.12
 INSTRUM: amx4
 PROBHD: 5 mm Dual
 PULPROG: zgpg30
 TD: 65536
 SOLVENT: DMSO
 NS: 1024
 DS: 4
 SWH: 8333.3 Hz
 FIDRES: 0.5086 Hz
 AQ: 0.98309 sec
 RG: 327.68
 DW: 60.000000 sec
 DE: 85.000000 sec
 TE: 300.2 K
 HL1: 11.000000 Hz
 PL: 11.000000 Hz
 DE: 85.000000 sec
 SFO1: 400.132400 MHz
 NUC1: 1H
 F2: Processing parameters
 SI: 16
 SF: 400.13001 MHz
 WDW: EM
 SSB: 0
 LB: 0.5 Hz
 GB: 0
 PC: 5.00
 ID: NMR plot parameters
 CX: 15.000000 Hz
 FLIP: 10.000000 Hz
 F1: 420.13001 MHz
 F2: 420.13001 MHz
 F3: 420.13001 MHz
 PPMCH: 0.311000 ppm
 HZCM: 135.751467 Hz

Current Data Parameters
NAME: sep01
EXPNO: 1
PROCNO: 1

F2 - Acquisition Parameters
Date_: 5900
Time: 7.
INSTRUM: amx4
PROBHD: 5 mm Dual
PULPROG: zgpg30
TD: 327
SOLVENT: CDC
NS: 2

DS: 3333.3
SWH: 1.0172
FIDRES: 0.49157
RG: 327
DW: 15.0
DE: 21.0
TE: 300

H1: 1.000000
D1: 10.0
S1: 10.0
P3: 10.0
SFO2: 400.13160
DECNUC: 13
D2: 0.003571
P4: 21.0
P1: 5.0
P2: 11.0
D13: 0.000004
S2: 21.0
DE: 21.0
SFO1: 100.62543
NUCLEUS: 1
CPDPRG: waltz
P11: 185.0

F2 - Processing Parameters
SI: 327
SF: 100.61277
WDW: EM
SSB: 0
LB: 0
GB: 0
PC: 0

1D NMR plot parameters
CX: 35.0
F1P: 228.0
F1: 226.37
F2P: 50.0
F2: 49.50
PRCM: 6.570
HZCM: 66.169

Cabergoline

cabergoline 34385-swa-53

Formula	C28 H37 N5 O2	FW	451	Primary Name	Cabergoline	Secondary Name(s)	Dostinex, Sogilen
IUPAC Name	N-[(8β)-6-allylergolin-8-yl]carbonyl]-N-[3-(dimethylamino)propyl]-N-ethylurea						PNU # 142779
Spectrum Notebook	50	Solvent	DMSO	Solvent ref	2.49	Chemist	SASHford
Lab Notebook ID	34385-SWA-53	Structure Lab Report	01-054				
Acquisition Time (sec)	0.7799	Comment	apr1151	Date	11 Apr 2001 12:52:52		
File Name	\uspofers02\RMOWERY\NMR\AMX500\apr1151_1.esp						Frequency (MHz) 500.13
Nucleus	1H	Number of Transients	16	Original Points Count	16384	Points Count	16384
Solvent	DMSO-D6	Sweep Width (Hz)	10504.20	Temperature (degree C)	27.000

Formula	C ₂₆ H ₃₇ N ₅ O ₂	FW	451	Primary Name	cabergoline	Secondary Name(s)	Dostinex, Sogilen
IUPAC Name	N-[(8R)-6-allyl(8R)-8-yl]carbonyl-N-(3-(dimethylamino)propyl)-N'-ethyleurea						142779
Spectrum Notebook	50	Solvent	DMSO	Solvent ref	39.5	Chemist	Sashford
Lab Notebook ID	34385-SWA-53	Structure Lab Report	01-054				
Acquisition Time (sec)	0.5308	Comment	apr1151	Date	11 Apr 2001 17:59:51		
File Name	\uspofers02MRMOWERYNNMR\AMX500\apr1151_2.esp						13C
Number of Transients	576	Original Points Count	32768	Frequency (MHz)	125.77	Nucleus	CHLOROFORM-D
Sweep Width (Hz)	30864.20	Temperature (degree C)	27.000	Points Count	32768	Solvent

Annotation	(ppm)
DMSO-d6	39.50

Cabergoline Int VI 33650-SWA-69

Cabergoline Int VI 33650-SWA-69

Current Data Parameters
 NAME 0514-12-KEH
 EXPNO 4
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20020514
 Time 13.37
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TO 65536
 SOLVENT DMS
 NS 64
 DS 2
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 s
 RG 1.4596.5
 DM 20.850 u
 DE 20.00 u
 TE 300.0 K
 CAGST2 145.000000
 D1 1.00000000 s
 d2 0.00344628 s
 d12 0.00002000 s
 DELTA 0.00001133 s
 ----- CHANNEL f1 -----
 NUC1 13C
 P1 8.90 u
 PL1 17.80 dB
 PS1 -2.00 dB
 SF01 100.627889 MHz
 ----- CHANNEL f2 -----
 CDPRG2 waltz16
 NUC2 1H
 P3 11.25 u
 PL3 22.50 dB
 PCPD2 98.00 u
 PL2 -2.00 dB
 PL12 15.80 dB
 SF02 400.1316005 MHz
 F2 - Processing parameters
 SI 32768
 SF 100.6127727 MHz
 MDW 0
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40
 1D NMR plot parameters
 CX 35.00
 CY 4.00
 F1P 225.000
 F1 22637.87
 F2P -5.000
 F2 -503.06
 GAMMA 6.57143
 HZCM 661.165968

Current Data Parameters
NAME jul2039
EXPNO 11
PROCNO 1

F2 - Acquisition Param
Date_ 500000
Time 11.02
INSTRUM amx400
PROBHD 5 mm Dual 13
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 16
DS 2
SWH 8333.333
FIDRES 0.508626
AQ 0.9830900
RG 256
DW 60.000
DE 85.71
TE 300.0
HL1 2
D1 1.00000000
P1 11.00
DE 85.71
SF01 400.132471800
NUCLEUS 1H

F2 - Processing param
SI 16384
SF 400.1300014
WDW GM
SSB 0
LB -0.50
GB 0.15
PC 5.00

1D NMR plot parameters
CX 35.00
FIP 10.500
F1 4201.37
F2P -0.500
F2 -200.07
FPMCM 0.31429
H2CM 125.75514

9

148550

9

148550

Current Data Parameter
 NAME jul203
 EXNO 1
 PROCNO 1
 F2 - Acquisition Param
 Date_ 50000
 Time 11.1
 INSTRUM amx40
 PROBD 5 mm Dual 1
 PULPROG dept9
 TD 3276
 SOLVENT CDCl₃
 NS 3
 DS 3333.33
 SWH 1.01725
 FIDRES 0.491570
 AQ 3276
 RG 15.00
 DW 21.4
 DE 21.4
 TE 300.
 HL1
 D1
 S¹
 P3 10.5
 SFO2 400.131600
 DECNOC 1
 D2 0.0035714
 P4 21.0
 P1 5.7
 P2 11.4
 D13 0.0000040
 S2 21.4
 DE 21.4
 SFO1 100.625435
 NUCLEUS 13
 CPDPRG waltz1
 P31 105.0
 F2 - Processing param
 SI 3276
 SF 100.612773
 WDW E
 SSB 1.0
 LB 1.4
 GB
 PC
 1D NMR plot parameters
 CX 35.0
 F1P 225.00
 F1 22637.8
 F2P 5.00
 F2 -503.0
 PPMCM 6.5714
 HZCM 661.1696

S9

S10

Current Data Parameters
 NAME jul12037
 EXPNO 11
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 500000
 Time 10.11
 INSTRUM amx400
 PROBD 5 mm Dual 13
 PULPROG zg30
 TD 16384
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8333.333
 FIDRES 0.508626
 AQ 0.9830900
 RG 256
 DW 60.000
 DE 85.71
 TE 300.0
 HL1 2
 DI 1.00000000
 P1 11.00
 DE 85.71
 SP01 400.1324710
 NUCLEUS 1H
 F2 - Processing parameters
 SI 16384
 SF 400.1300126
 WDW GM
 SSB 0
 LB -0.50
 GB 0.15
 PC 5.00
 1D NMR plot parameters
 CX 35.00
 F1P 10.500
 F1 4201.37
 F2P -0.500
 F2 -200.07
 PPMCM 0.31429
 HZCM 125.75514

148548

Current Data Parameter
 NAME jul203
 EXPNO 1
 PROCNO
 F2 - Acquisition Param's
 Date_ 50000
 Time 10.3
 INSTRUM amx40
 PROBD 5 mm Dual 1
 PULPROG deph9
 TD 3276
 SOLVENT CDCl3
 NS 3
 DS
 SWH 33333.33
 FIDRES 1.01725
 AQ 0.491570
 RG 3276
 DM 15.00
 DE 21.4
 TE 300.2
 HL1
 D1 1.0000000
 SFO2 10.5
 DECNUC 1
 D2 0.0035714
 P4 21.0
 P1 5.7
 P2 11.4
 D13 0.0000040
 S2 2
 DE 21.4
 SFO1 100.625435
 NUCLEUS 13
 CPDPRG waltz1
 P31 105.0
 F2 - Processing param's
 SI 3276
 SF 100.612773
 WDW E
 SSB 1.0
 LB 1.4
 GB
 PC
 1D NMR plot parameters
 CX 35.0
 FIP 225.00
 F1 22637.8
 P2P -5.00
 P2 -503.0
 PPMCM 6.57140
 HZCM 661.1696

S12

Current Data Parameters:
 NAME: jui2031
 EXPNO: 1
 PROCNO: 1

F2 - Acquisition Parameters
 Date_: 500001
 Time: 10.4
 INSTRUM: amx400
 PROBHD: 5 mm Dual 1
 PULPROG: zg31
 TD: 16384
 SOLVENT: CDCl₃
 NS: 11
 DS: 8333.33
 SWH: 0.508621
 FIDRES: 0.983090
 AQ: 254
 RG: 60.000
 DW: 85.7
 DE: 300.1
 HL1: 1.000000
 D1: 11.0
 P1: 85.7
 DE: 400.132471
 SFO1: 400.132471
 NUCLEUS: 11

F2 - Processing parameters
 SI: 16384
 SP: 400.130001
 WDW: GN
 SSB: 0
 LB: -0.50
 GB: 0.15
 PC: 5.00

1D NMR plot parameters
 CX: 35.00
 F1P: 10.500
 F1: 4201.37
 F2P: -0.500
 F2: -200.07
 PPMCM: 0.31429
 HZCM: 125.75514

148549

148549

11

Current Data Parameters
 NAME: EXPNO: PROCNO: F2 - Acquisition Parameters
 Date_ Time: 50001 10.1
 INSTRUM: PROBHD: 5 mm Dual
 PULPROG: DEPT: 3271
 TD: SOLVENT: CDC
 NS: DS: 33333.3
 SWH: 1.01721
 FIDRES: 0.491571
 RG: 3271
 DW: 15.01
 DE: 21.4
 TE: 300
 HL1: 1.000000
 D1: 10.3
 SF: 400.131601
 DECNUC: 13
 D2: 0.0035714
 F4: 21.4
 P1: 5.1
 P2: 11.4
 D13: 0.000004
 S2: 21.4
 DE: 100.625435
 SP01: 105.0
 NUC1EUS: waltz1
 CPDPRG: P31
 F2 - Processing parameters
 SI: 3271
 SF: 100.612773
 WDW: 1
 SSB: 1.0
 LB: 1.4
 GB: 1.4
 PC: 1.4
 ID NMR plot parameters
 CX: 35.0
 F1P: 225.00
 F1: 22637.6
 F2P: -5.00
 F2: -503.00
 PPMCH: 6.5714
 HZCH: 661.1696

S13