Supporting Information

N-Heterocyclic Carbene-Catalyzed [4+1] Annulation of Phthalaldehyde and Imines

Fang-Gang Sun and Song Ye *

Beijing National Laboratory for Molecular Sciences, CAS Key Laboratory of Molecular Recognition and Function, Institute of Chemistry, Chinese Academy of Sciences, Beijing 100190, China

songye@iccas.ac.cn

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Part I Experimental part

General Information

All reactions were carried out under an argon atmosphere in oven-dried glassware with magnetic stirring. CH_2Cl_2 and CH_3CN were distilled from CaH_2. Phthalaldehyde was used after recrystallization from petroleum ether. tert-Butyl aryl(phenylsulfonyl)methylcarbamate was prepared according to the literatures. Column chromatograph was performed on silica gel 200 ~ 300 mesh. All ^1^H NMR (300 MHz), ^1^C NMR (75 MHz) spectra were recorded in CDCl_3, with tetramethylsilane as an internal standard and reported in parts per million (ppm, δ). ^1^H NMR Spectroscopy splitting patterns were designated as singlet (s), doublet (d), triplet (t). Splitting patterns that could not be interpreted or easily visualized were designated as multiplet (m) or broad (br). Infrared spectra were reported as wavenumber (cm⁻¹).

1.1 Synthesis of cis-indanones via a Cascade Stetter-Aldol Reaction Catalyzed by NHC 4a

Typical procedure. To an oven-dried 50 mL Schlenk tube equipped with a stir bar was charged with thiazolium salt (26.9 mg, 0.1 mmol) and Cs_2CO_3 (32.6 mg, 0.1 mmol). The tube was closed with a septum, evacuated, and back-filled with argon. To
this mixture was added distilled solvent 5 mL, then stirred for 10 min at room

temperature. DIPEA (173.9 μL, 1 mmol), tert-butyl phenyl(phenylsulfonyl)
methylcarbamate (173.5 mg, 0.5 mmol), and phthalaldehyde (100.5 mg, 0.75 mmol)
was added to the tube. The mixture was further stirred for overnight, then diluted with
ethyl acetate and passed through a short silica pad. The solvent was removed under
reduced pressure and the residue was purified by chromatography on silica gel (ethyl
acetate/petroleum ether) to give the desired product.

tert-butyl-1-hydroxy-3-oxo-2-phenyl-2,3-dihydro-1H-inden-2-ylcarbamate

Purified with petroleum ether/ethyl acetate (3/1), yielding 78.5 mg (76%) of cis-3a as
a white solid, Rf = 0.17 (petroleum ether/ethyl acetate = 3/1), mp: 125-127 °C. 1H
NMR (300 MHz, CDCl3) δ 7.82-7.74 (m, 3H), 7.57-7.52 (m, 1H), 7.30-7.22 (m, 5H),
5.78 (b, 1H), 5.65 (d, J = 6.6 Hz, 1H), 3.94 (b, 1H), 1.45 (s, 9H); 13C NMR (75 MHz,
CDCl3) δ 200.3, 156.8, 152.2, 138.7, 136.1, 133.7, 130.0, 128.6, 127.7, 126.8, 125.5, 124.7, 80.8,
77.6, 70.3, 28.0; IR (KBr) ν 1723, 1696, 1163, 699; EIMS m/z: 339 (10.0), 222 (100);
HRMS-(EI) (m/z): M+ calcd for C20H21NO4, 339.1471; found 339.1474.

3b

tert-butyl-2-(4-chlorophenyl)-1-hydroxy-3-oxo-2,3-dihydro-1H-inden-2-ylcarbamate

Purified with petroleum ether/ethyl acetate (3/1), yielding 78.5 mg (83%) of cis-3a as
a waxy solid, $R_f = 0.30$ (petroleum ether/ethyl acetate = 3/1). $^1$H NMR (300 MHz, CDCl$_3$) $\delta$ 7.80-7.75 (m, 3H), 7.57-7.52 (m, 1H), 7.26-7.22 (m, 2H), 7.15 (d, $J = 8.7$ Hz, 2H), 5.81 (b, 1H), 5.64 (d, $J = 5.7$ Hz, 1H), 3.85 (b, 1H), 1.44 (s, 9H); $^{13}$C NMR (75 MHz, CDCl$_3$) $\delta$ 200.0, 156.8, 152.3, 137.3, 136.6, 134.0, 133.7, 130.5, 129.0, 127.1, 126.0, 125.2, 81.3, 77.3, 70.2, 28.2; IR (KBr) $\nu$ 1722, 1703, 1165; EIMS $m/z$: 373 (4.0), 256 (100); HRMS-(EI) ($m/z$): M$^+$ calcd for C$_{20}$H$_{20}$NO$_4$Cl, 373.1081; found 373.1086.

tert-butyl-1-hydroxy-3-oxo-2-p-tolyl-2,3-dihydro-1H-inden-2-ylcarbamate

Purified with petroleum ether/ethyl acetate (3/1), yielding 78.5 mg (56%) of cis-3a as a waxy solid, $R_f = 0.23$ (petroleum ether/ethyl acetate = 3/1). $^1$H NMR (300 MHz, CDCl$_3$) $\delta$ 7.79-7.71 (m, 3H), 7.53-7.48 (m, 1H), 7.13-7.04 (m, 4H), 5.79 (b, 1H), 5.63 (d, $J = 6.9$ Hz, 1H), 3.96 (b, 1H), 2.25 (s, 3H), 1.44 (s, 9H); $^{13}$C NMR (75 MHz, CDCl$_3$) $\delta$ 200.7, 157.2, 152.4, 137.9, 136.3, 135.9, 134.0, 130.3, 129.6, 127.1, 125.6, 124.9, 81.1, 78.0, 70.3, 28.2, 20.9; IR (KBr) $\nu$ 1727, 1702, 704; EIMS $m/z$: 353 (8.0), 226 (100); HRMS-(EI) ($m/z$): M$^+$ calcd for C$_{21}$H$_{23}$NO$_4$, 353.1627; found 353.1630.

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$^3$d

tert-butyl-1-hydroxy-2-(4-methoxyphenyl)-3-oxo-2,3-dihydro-1H-inden-2-ylcarbamate

Purified with petroleum ether/ethyl acetate (3/1), yielding 78.5 mg (40%) of cis-3a as
a waxy solid, R$_f$ = 0.20 (petroleum ether/ethyl acetate = 3/1). $^1$H NMR (300 MHz, CDCl$_3$) $\delta$ 7.81-7.72 (m, 3H), 7.55-7.50 (m, 1H), 7.16 (d, $J = 8.7$ Hz, 2H), 6.79 (d, $J = 9.0$ Hz, 2H), 5.74 (b, 1H), 5.63 (d, $J = 6.3$ Hz, 1H), 3.92 (b, 1H), 3.73 (s, 3H), 1.44 (s, 9H); $^{13}$C NMR (75 MHz, CDCl$_3$) $\delta$ 200.7, 159.3, 157.3, 152.3, 136.3, 134.0, 130.8, 130.3, 127.1, 127.0, 124.9, 81.2, 78.0, 70.0, 55.3, 28.2; IR (KBr) $\nu$ 1723, 1701, 1162; EIMS $m/z$: 369 (50.0), 251 (100); HRMS-(EI) ($m/z$): M$^+$ calcd for C$_{21}$H$_{23}$NO$_5$, 369.1576; found 369.1581.

![Chemical Structure 3e](image)

**3e**

*tert*-butyl-2-(3-chlorophenyl)-1-hydroxy-3-oxo-2,3-dihydro-1H-inden-2-ylcarbamate

Purified with petroleum ether/ethyl acetate (3/1), yielding 78.5 mg (87%) of cis-3a as a white solid, Rf = 0.24 (petroleum ether/ethyl acetate = 3/1), mp: 132-134 °C. $^1$H NMR (300 MHz, CDCl$_3$) $\delta$ 7.80-7.76 (m, 3H), 7.57-7.53 (m, 1H), 7.26-7.15 (m, 3H), 7.05 (d, $J = 6.6$ Hz, 1H), 5.84 (b, 1H), 5.64 (d, $J = 5.1$ Hz, 1H), 3.91 (b, 1H), 1.45 (s, 9H); $^{13}$C NMR (75 MHz, CDCl$_3$) $\delta$ 199.9, 156.9, 152.3, 140.8, 136.7, 135.0, 133.7, 130.6, 130.1, 128.3, 127.2, 125.9, 125.2, 123.8, 81.5, 77.3, 70.2, 28.2; IR (KBr) $\nu$ 1720, 1694, 1161, 696; EIMS $m/z$: 373 (4.0), 256 (100); HRMS-(EI) ($m/z$): M$^+$ calcd for C$_{20}$H$_{20}$NO$_4$Cl, 373.1081; found 373.1084.

![Chemical Structure 3f](image)

**3f**

*tert*-butyl-1-hydroxy-2-(3-nitrophenyl)-3-oxo-2,3-dihydro-1H-inden-2-ylcarbamate
Purified with petroleum ether/ethyl acetate (3/1), yielding 78.5 mg (91%) of \textit{cis}-3a as a white solid, \( R_f = 0.17 \) (petroleum ether/ethyl acetate = 3/1), mp: 99-100 °C. \( ^1\text{H} \) NMR (300 MHz, CDCl\(_3\)) \( \delta \) 8.14-8.09 (m, 2H), 7.91-7.81 (m, 3H), 7.63-7.58 (m, 1H), 7.45 (d, \( J = 7.2 \) Hz, 2H), 5.93 (b, 1H), 5.76 (d, \( J = 5.4 \) Hz, 1H), 3.74 (b, 1H), 1.48 (s, 9H); \( ^{13}\text{C} \) NMR (75 MHz, CDCl\(_3\)) \( \delta \) 199.0, 156.4, 152.1, 148.5, 140.9, 136.9, 133.3, 131.4, 130.7, 129.7, 127.1, 125.4, 122.9, 120.7, 81.7, 77.4, 70.2, 28.2; IR (KBr) \( \nu \) 1719, 1703, 1159, 702; EIMS \( m/z \): 384 (4.0), 267 (100); HRMS-(EI) \( (m/z) \): \( M^+ \) calcd for C\(_{20}\)H\(_{20}\)N\(_2\)O\(_6\), 384.1321; found 384.1326.

\[
\text{tert-butyl-1-hydroxy-3-oxo-2-(pyridin-2-yl)-2,3-dihydro-1H-inden-2-ylcarbamate}
\]

Purified with petroleum ether/ethyl acetate (3/1), yielding 78.5 mg (87%) of \textit{cis}-3a as a waxy solid, \( R_f = 0.17 \) (petroleum ether/ethyl acetate = 3/1). \( ^1\text{H} \) NMR (300 MHz, CDCl\(_3\)) \( \delta \) 8.52 (d, \( J = 4.2 \) Hz, 1H), 7.87-7.77 (m, 3H), 7.57 (t, \( J = 7.5 \) Hz, 2H), 7.37 (b, 1H), 7.21-7.17 (m, 1H), 6.84 (d, \( J = 7.8 \) Hz, 1H), 5.41 (d, \( J = 10.2 \) Hz, 1H), 4.04 (d, \( J = 10.2 \) Hz, 1H), 1.46 (s, 9H); \( ^{13}\text{C} \) NMR (75 MHz, CDCl\(_3\)) \( \delta \) 200.7, 158.1, 155.7, 153.7, 148.3, 137.5, 136.4, 134.4, 130.2, 127.3, 124.7, 123.0, 119.8, 81.1, 78.3, 70.4, 28.2; IR (KBr) \( \nu \) 1725, 1697, 1165, 701; EIMS \( m/z \): 340 (5.0), 223 (100); HRMS-(EI) \( (m/z) \): \( M^+ \) calcd for C\(_{19}\)H\(_{20}\)N\(_2\)O\(_4\), 340.1423; found 340.1425.
**tert-butyl-1-hydroxy-3-oxo-2-(thiophen-2-yl)-2,3-dihydro-1H-inden-2-ylcarbamate**

Purified with petroleum ether/ethyl acetate (3/1), yielding 78.5 mg (93%) of *cis-3a* as a white solid, *R*<sub>f</sub> = 0.16 (petroleum ether/ethyl acetate = 3/1), mp: 135-136 °C. ¹H NMR (300 MHz, CDCl<sub>3</sub>) δ 7.83-7.73 (m, 3H), 7.55 (t, *J* = 6.9 Hz, 1H), 7.18 (d, *J* = 4.5 Hz, 1H), 6.85-6.73 (m, 2H), 5.89 (b, 1H), 5.73 (d, *J* = 4.5 Hz, 1H), 3.96 (b, 1H), 1.46 (s, 9H); ¹³C NMR (75 MHz, CDCl<sub>3</sub>) δ 198.5, 156.8, 151.7, 142.8, 136.4, 133.1, 130.5, 127.4, 127.2, 125.6, 125.3, 125.1, 81.4, 78.3, 68.4, 28.2; IR (KBr) ν 1727, 1694, 1163, 703; EIMS *m/z*: 345 (4.0), 228 (100); HRMS-(EI) (*m/z*): M⁺ calcd for C<sub>18</sub>H<sub>19</sub>NO<sub>4</sub>S, 345.1035; found 345.1039.

**benzyl-1-hydroxy-3-oxo-2-phenyl-2,3-dihydro-1H-inden-2-ylcarbamate**

Purified with petroleum ether/ethyl acetate (3/1), yielding 78.5 mg (66%) of *cis-3a* as a waxy solid, *R*<sub>f</sub> = 0.19 (petroleum ether/ethyl acetate = 3/1). ¹H NMR (300 MHz, CDCl<sub>3</sub>) δ 7.82-7.74 (m, 3H), 7.54 (t, *J* = 7.2 Hz, 1H), 7.35-7.23 (m, 11H), 6.07 (b, 1H), 5.72 (d, *J* = 5.7 Hz, 1H), 5.13 (s, 2H), 3.66 (d, *J* = 5.7 Hz, 1H); ¹³C NMR (75 MHz, CDCl<sub>3</sub>) δ 200.0, 157.4, 152.3, 138.4, 136.5, 135.8, 133.9, 130.5, 129.0, 128.6, 128.4, 128.2, 128.0, 127.1, 125.6, 125.1, 77.7, 70.6, 67.6; IR (KBr) ν 1718, 1700,
N-(1-hydroxy-3-oxo-2-p-tolyl-2,3-dihydro-1H-inden-2-yl)benzamide

Purified with petroleum ether/ethyl acetate (3/1), yielding 78.5 mg (53%) of cis-3a as a white solid, R$_f$ = 0.20 (petroleum ether/ethyl acetate = 3/1), mp: 107-108 °C. $^1$H NMR (300 MHz, CDCl$_3$) δ 7.92-7.76 (m, 5H), 7.57 (t, $J$ = 7.2 Hz, 2H), 7.48 (t, $J$ = 7.2 Hz, 2H), 7.30 (s, 1H), 7.19 (d, $J$ = 8.4 Hz, 2H), 7.09 (d, $J$ = 8.4 Hz, 2H), 5.89 (d, $J$ = 6.9 Hz, 1H), 3.90 (d, $J$ = 6.9 Hz, 1H), 2.27 (s, 3H); $^{13}$C NMR (75 MHz, CDCl$_3$) δ 200.6, 169.1, 152.3, 138.2, 136.5, 135.3, 133.9, 133.1, 132.4, 130.4, 129.8, 128.8, 127.4, 127.2, 125.7, 125.0, 78.0, 71.3, 21.0; IR (KBr) ν 1729, 1700, 1644, 1385, 696; EIMS m/z: 357 (4.0), 105 (100); HRMS-(EI) (m/z): M$^+$ calcd for C$_{23}$H$_{19}$NO$_3$, 357.1365; found 357.1370.

1.2 Synthesis of isoquinolinone 6

![Synthesis of isoquinolinone 6](image)

2-benzoyl-3-p-tolylisoquinolin-1(2H)-one (6)
To an oven-dried 25 mL Schlenk tube equipped with a stir bar was charged with the indanone (76 mg, 0.213 mmol) and PPh₃ (83.6 mg, 0.319 mmol). The tube was closed with a septum, evacuated, and back-filled with argon. To this mixture was added distilled solvent THF(2 mL), then the mixture was cooled to 0°C. DEAD(55.6 mg, 0.319 mmol) was added to the tube. The mixture was further stirred for 1h at 0°C, then 2h at room temperature. The solvent was removed under reduced pressure and the residue was purified by chromatography on silica gel (ethyl acetate/petroleum ether) to give the desired product.

Purified with petroleum ether/ethyl acetate (10/1), yielding 59.9 mg (83%) as a waxy solid, Rᵣ = 0.35 (petroleum ether/ethyl acetate = 10/1). ¹H NMR (300 MHz, CDCl₃) δ 8.37 (d, J = 7.2 Hz, 2H), 8.03-7.91 (m, 5H), 7.71 (t, J = 7.5 Hz, 1H), 7.61-7.51 (m, 3H), 7.28 (d, J = 8.1 Hz, 2H), 2.41 (s, 3H); ¹³C NMR (75 MHz, CDCl₃) δ 165.0, 155.6, 149.6, 139.9, 138.8, 135.7, 134.0, 131.1, 130.6, 129.5, 129.1, 128.7, 127.5, 127.2, 126.9, 123.7, 120.6, 115.5, 21.3; IR (KBr) ν 1654, 1364, 613; EIMS m/z: 339 (50.0), 235 (100); HRMS-(EI) (m/z): M⁺ calcd for C₂₃H₁₇NO₂, 339.1259; found 339.1264.

3-p-tolylisoquinolin-1(2H)-one (7)

To an 10mL rounded-bottom flask equipped with a stir bar was added isoquinolinone (40mg, 0.118 mmol) and CH₃OH (1mL). Then, K₂CO₃(32.6 mg, 0.236 mmol) was added to the mixture. The stirring was continuing for 3h. The solvent was removed under reduced pressure and the residue was purified by chromatography on silica gel...
(ethyl acetate/petroleum ether) to give the desired product.

Purified with petroleum ether/ethyl acetate (3/1-1/1), yielding 26.4 mg (95%) as a white solid, Rf = 0.23 (petroleum ether/ethyl acetate = 3/1), mp: 239-240°C. 1H NMR (300 MHz, CDCl₃) δ 10.06 (s, 1H), 8.41 (d, J = 8.1 Hz, 1H), 7.70-7.57 (m, 4H), 7.50-7.45 (m, 1H), 7.32 (d, J = 8.1 Hz, 2H), 6.76 (s, 1H), 2.43 (s, 3H); 13C NMR (75 MHz, CDCl₃) δ 163.9, 139.8, 139.5, 138.4, 132.8, 131.5, 129.9, 127.5, 126.5, 126.0, 124.9, 103.8, 21.3; IR (KBr) ν 1739, 1154, 810.

1.3 X-ray Crystal Structure

Figure S1. X-Ray crystal structure of cis-3a

A colorless solution of 3a in EtOAc was prepared. Crystals suitable for X-ray structural analysis were obtained by slow evaporation of the solvents at room temperature.
References


Part II Copy of NMR Spectra

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EXPNO                30
PROCNO                1
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SWH           8992.806 Hz
FIDRES         0.137219 Hz
AQ            3.6438515 sec
RG                322.5
DW               55.600 usec
DE                 8.00 usec
TE                300.3 K
D1           1.00000000 sec

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PL1                3.00 dB
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F2 - Processing parameters
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WDW                  EM
SSB                   0
LB                 0.30 Hz
PC                 1.00

NEW 16
F1          10.80 usec
FA              3.00 dB
SF01 300.1324010 MHz

0 1 2 3 4 5 6 7 8 ppm

--- CHANNEL f2 ---
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PL12              22.33 dB
PL13              23.00 dB
SFO2        300.1312005 MHz

F2 - Processing parameters
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PC                 1.40

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PROCNO                1
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RG               5160.6
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DE                 8.00 usec
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D11          0.03000000 sec

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P1                12.50 usec
PL1               2.00 dB
SFO1         75.4752953 MHz

== CHANNEL f2 ========
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NUC2                 1H
PCPD2            100.00 usec
PL2                1.00 dB
PL12              22.33 dB
PL13              23.30 dB
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F2 - Processing parameters
SI                32768
SF           75.4477768 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
PC                 1.40
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Current Data Parameters
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PROCNO: 1

F2 - Acquisition Parameters
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FIDRES: 0.137219 Hz
AQ: 3.6438515 sec
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DI: 0.00

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PC: 1.00

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NS: 420
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SWH: 17985.611 Hz
FIDRES: 0.274439 Hz
AQ: 1.8219508 sec
RG: 5792.6
TE: 297.9 K
D1: 0.0000000 sec
D11: 0.0300000 sec
TD0: 1

======== CHANNEL f1 ========
NUC1: 1H
P1: 12.50 usec
PL1: 2.00 dB
SFO1: 75.4752953 MHz

======== CHANNEL f2 ========
NUC2: 13C
PCPD: 100.00 usec
PL2: 2.00 dB
PL12: 22.33 dB
PL13: 23.00 dB
SFO2: 300.1322005 MHz

F2 - Processing parameters
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SF: 75.4677490 MHz
WDW: EM
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LB: 1.00 Hz
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Current Data Parameters
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EXPNO                20
PROCNO                1

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PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                 16
DS                    0
SWH           8992.806 Hz
FIDRES         0.137219 Hz
AQ            3.6438515 sec
RG                  512
DW              55.600 usec
DE                 8.00 usec
TE                297.9 K
DI       1.00000000 sec
TOO                   1

======== CHANNEL f1 ========
NUC1                1H
P1                10.80 usec
PL1                3.00 dB
SFO1        300.1324010 MHz

F2 - Processing parameters
SI                32768
SF           300.1300066 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
PC                 1.00

Current Data Parameters
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EXPNO                31
PROCNO                1

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TD                65536
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NS                 171
DS                    4
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FIDRES         0.274439 Hz
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RG             11585.2
DW              27.800 usec
DE                 8.00 usec
TE                292.4 K
D1           2.00000000 sec
D11          0.03000000 sec
TOO                   1

======== CHANNEL f1 ========
NUC1                13C
P1                12.50 usec
PL1                2.00 dB
SFO1         75.4752953 MHz

======== CHANNEL f2 ========
NUC2                 1H
PCPD2            100.00 usec
PL2                3.00 dB
PL12              22.33 dB
PL13              23.00 dB
SFO2        300.1312055 MHz

F2 - Processing parameters
SI                32768
SF           75.4677490 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
PC                 1.40