An Improved Procedure for the Three-Component Synthesis of Highly Substituted Pyridines Using Ionic Liquid

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Supporting Information

Table of Contents

Spectroscopic (IR, ¹ H NMR, ¹³ C NMR and HRMS) Data of All Products in Table 1	Page no. S2-S6
¹³ C NMR Spectra of All Products in Table 1	S7-S16

IR, ^1H , ^{13}C and melting points of all compounds and HRMS data of unknown compounds in table 1 are given below according to their entries

2-Amino-4-phenyl-6-phenylsulfanyl-pyridine-3,5-dicarbonitrile (Entry 1, Table 1):

Colourless solid, mp (CH_3CN) 216-218 $^\circ\text{C}$; IR (KBr): 3479, 3350, 3213, 2218, 1622, 1579, 1548, 1521, 1263, 758, 692 cm^{-1} ; ^1H NMR (300 MHz, DMSO-d_6): δ 7.27 (broad, 2H), 7.38-7.47 (m, 10H); ^{13}C NMR (75 MHz): δ 87.3, 94.0, 115.3 (2C), 127.5, 128.5 (2C), 128.9 (2C), 129.4, 129.7, 130.6 (2C), 133.9, 135.3 (2C), 158.4, 160.0, 167.4.

2-Amino-6-(4-chloro-phenylsulfanyl)-4-phenyl-pyridine-3,5-dicarbonitrile (Entry 2, Table 1):

White solid, mp (CH_3CN) 228-230 $^\circ\text{C}$; IR (KBr): 3481, 3352, 3214, 2218, 1621, 1570, 1548, 1262, 756, 693 cm^{-1} ; ^1H NMR (300 MHz, DMSO-d_6): δ 6.34 (broad, 2H), 7.21-7.40 (m, 9H); ^{13}C NMR (75 MHz): δ 87.0, 94.3, 114.5, 114.8, 125.5, 128.0 (2C), 128.4 (2C), 128.9 (2C), 130.3, 133.0, 135.6, 136.5 (2C), 158.0, 159.3, 167.2.

2-Amino-6-benzylsulfanyl-4-phenyl-pyridine-3,5-dicarbonitrile (Entry 3, Table 1):

Colourless solid, mp (CH_3CN) 193-195 $^\circ\text{C}$; IR (KBr): 3450, 3334, 3211, 2956, 2191, 1633, 1348, 734 cm^{-1} ; ^1H NMR (300 MHz, DMSO-d_6): δ 3.77 (s, 2H), 7.33-7.42 (m, 10H), 7.57 (broad, 2H); ^{13}C NMR (75 MHz): δ 42.2, 86.4, 93.7, 114.4, 115.7, 127.0, 128.6 (2C), 128.8 (2C), 129.0, 129.3 (2C), 130.7 (2C), 131.7, 134.3, 137.7, 160.0, 166.7.

2-Amino-6-(2-amino-phenylsulfanyl)-4-phenyl-pyridine-3,5-dicarbonitrile (Entry 4, Table 1):

Colourless solid, mp (CH_3CN) 224-225 $^\circ\text{C}$; IR (KBr): 3392, 3327, 3220, 2923, 2212, 1637, 1542, 1523, 754, 704 cm^{-1} ; ^1H NMR (300 MHz, DMSO-d_6): δ 5.36 (broad, 2H), 6.55 (t, $J = 6.9$ Hz, 1H), 6.77 (d, $J = 7.7$ Hz, 1H), 7.08-7.33 (m, 5H), 7.50-7.53 (m, 2H), 7.62 (broad, 2H); ^{13}C NMR (75 MHz): δ 86.7, 93.9, 107.9, 116.7, 116.2, 117.7, 126.2, 128.2 (2C), 128.7 (2C), 129.0, 129.9, 134.4, 137.5, 151.5, 158.7, 159.9, 167.1.

2-Amino-4-(4-chloro-phenyl)-6-phenylsulfanyl-pyridine-3,5-dicarbonitrile (Entry 5, Table 1):

Colourless solid, mp (CH_3CN) 222-224 $^\circ\text{C}$; IR (KBr): 3485, 3344, 3220, 2925,

2214, 1633, 1544, 1494, 1257, 1093 cm^{-1} ; ^1H NMR (300 MHz, DMSO-d_6): δ 7.48-7.55 (m, 3H), 7.57-7.64 (m, 6H), 7.79 (broad, 2H); ^{13}C NMR (75 MHz): δ 87.4, 93.6, 115.2, 115.5, 127.3, 129.2 (2C), 129.5 (2C), 129.8, 130.8 (2C), 133.1, 135.2 (2C), 135.7, 157.8, 159.9, 166.6.

2-Amino-4-(4-nitro-phenyl)-6-phenylsulfanyl-pyridine-3,5-dicarbonitrile (Entry 6, Table 1): Colourless solid, mp (CH_3CN) 287-289 $^\circ\text{C}$; IR (KBr): 3406, 3328, 3234, 2227, 2214, 1645, 1552, 1350, 756 cm^{-1} ; ^1H NMR (300 MHz, DMSO-d_6): δ 7.46-7.48 (m, 3H), 7.56-7.59 (m, 2H), 7.85 (d, $J = 8.6$ Hz, 2H), 7.90 (broad, 2H), 8.39 (d, $J = 8.6$ Hz, 2H); ^{13}C NMR (75 MHz): δ 87.2, 93.3, 114.9, 115.3, 124.2 (2C), 127.2, 129.8 (2C), 130.1, 130.5 (2C), 135.1 (2C), 140.5, 148.9, 157.0, 159.8, 166.5.

2-Amino-4-(4-methylsulfanyl-phenyl)-6-phenylsulfanyl-pyridine-3,5-dicarbonitrile (Entry 7, Table 1): Colourless solid; mp (CH_3CN) 254-256 $^\circ\text{C}$; IR (KBr): 3408, 3332, 3247, 3151, 2218, 2215, 1651, 1573, 1552, 1481, 1294 cm^{-1} ; ^1H NMR (300 MHz, DMSO-d_6): δ 2.55 (s, 3H), 7.43 (d, $J = 8.3$ Hz, 2H), 7.48-7.50 (m, 4H), 7.58-7.61 (m, 3H), 7.78 (broad, 2H); ^{13}C NMR (75 MHz): δ 14.4, 87.4, 93.7, 115.5, 115.8, 125.6 (2C), 127.6, 129.4 (2C), 129.8 (2C), 130.1, 130.2, 135.2 (2C), 142.2, 158.5, 160.1, 166.5.
HRMS Calcd for $\text{C}_{20}\text{H}_{14}\text{N}_4\text{S}_2$: $[\text{M}+\text{H}]^+$, 375.0738; Found: 375.0728.

2-Amino-4-(4-hydroxy-phenyl)-6-phenylsulfanyl-pyridine-3,5-dicarbonitrile (Entry 8, Table 2): Colourless solid, mp (CH_3CN) 315-316 $^\circ\text{C}$; IR (KBr): 3648, 3496, 3367, 3236, 2222, 2216, 1631, 1609, 1552, 758 cm^{-1} ; ^1H NMR (300 MHz, DMSO-d_6): δ 6.93 (d, $J = 8.5$ Hz, 2H), 7.39 (d, $J = 8.5$ Hz, 2H), 7.50 (m, 3H), 7.60 (m, 2H), 7.69 (broad, 2H), 10.04 (bs, 1H); ^{13}C NMR (75 MHz): δ 93.7, 96.9, 115.5 (2C), 115.8, 116.0, 124.5, 127.6, 129.8 (2C), 130.0, 130.7 (2C), 135.2 (2C), 159.0, 159.8, 160.2, 166.5.

2-Amino-4-benzo[1,3]dioxol-5-yl-6-phenylsulfanyl-pyridine-3,5-dicarbonitrile (Entry 9, Table 1): Colourless solid, mp (CH_3CN) 234-236 $^\circ\text{C}$; IR (KBr): 3479, 3350, 3213, 2218, 1622, 1548, 1263, 758, 692, 451 cm^{-1} ; ^1H NMR (300 MHz, DMSO-d_6): δ 6.14 (s, 2H), 7.01-7.16 (m, 3H), 7.47-7.49 (m, 3H), 7.57-7.60 (m, 2H), 7.74 (broad, 2H);

^{13}C NMR (75 MHz): δ 88.0, 94.4, 102.6, 109.4, 109.7, 116.0, 116.2, 123.9, 128.0, 128.1, 130.3 (2C), 130.5, 135.6 (2C), 148.2, 149.8, 159.0, 160.5, 166.9.

2-Amino-4-(4-methoxy-phenyl)-6-phenylsulfanyl-pyridine-3,5-dicarbonitrile (Entry 10, Table 1): Colourless solid, mp (CH_3CN) 238-240 $^\circ\text{C}$; IR (KBr): 3440, 3330, 3226, 2227, 2214, 1641, 1548, 1512, 1259, 1190, 1018, 756 cm^{-1} ; ^1H NMR (300 MHz, DMSO-d_6): δ 3.82 (s, 3H), 7.94 (d, J = 8.4 Hz, 2H), 7.47-7.56 (m, 7H), 7.68 (broad, 2H); ^{13}C NMR (75 MHz): δ 55.5, 87.1, 93.5, 114.2 (2C), 115.7, 125.9, 127.3, 129.6 (2C), 129.8, 130.4 (2C), 134.9 (2C), 158.5, 159.9, 161.0, 166.3.

2-Amino-6-benzylsulfanyl-4-(4-methoxy-phenyl)-pyridine-3,5-dicarbonitrile (Entry 11, Table 1): Colourless solid, mp (CH_3CN) 228-230 $^\circ\text{C}$; IR (KBr): 3450, 3334, 3211, 2956, 2191, 1633, 734 cm^{-1} ; ^1H NMR (300 MHz, DMSO-d_6): δ 3.65 (s, 3H), 4.26 (s, 2H), 6.55 (broad, 2H), 6.81 (d, J = 8.7 Hz, 2H), 7.07-7.13 (m, 3H), 7.19-7.24 (m, 2H), 7.25 (d, J = 8.7 Hz, 2H); ^{13}C NMR (75 MHz): δ 33.9, 54.8, 85.7, 94.4, 113.7 (2C), 114.9, 115.3, 125.0, 126.9, 128.0 (2C), 128.6 (2C), 129.6 (2C), 136.1, 157.3, 159.3, 160.8, 167.3.
HRMS Calcd for $\text{C}_{21}\text{H}_{16}\text{N}_4\text{OS}$: $[\text{M}+\text{H}]^+$, 373.1123; Found: 373.1108.

2-Amino-6-phenylsulfanyl-4-thiophen-2-yl-pyridine-3,5-dicarbonitrile (Entry 12, Table 1): Colourless solid, mp (CH_3CN) 208-210 $^\circ\text{C}$; IR (KBr): 3408, 3332, 3247, 3151, 2218, 2215, 1651, 1573, 1552, 1481, 1294 cm^{-1} ; ^1H NMR (300 MHz, DMSO-d_6): δ 6.40 (broad, 2H), 6.97 (t, J = 4.5 Hz, 1H), 7.20-7.22 (m, 3H), 7.29-7.32 (m, 3H), 7.43 (d, J = 4.9 Hz, 1H); ^{13}C NMR (75 MHz): δ 86.1, 93.5, 114.7, 114.9, 126.7, 127.2, 128.6 (2C), 129.1, 129.4, 130.4, 132.2, 134.8 (2C), 149.8, 159.3, 167.9.
HRMS Calcd for $\text{C}_{17}\text{H}_{10}\text{N}_4\text{S}_2$: $[\text{M}+\text{H}]^+$, 335.0425; Found: 335.0446.

2-Amino-4-(4-hydroxy-3-methoxy-phenyl)-6-phenylsulfanyl-pyridine-3,5-dicarbonitrile (Entry 13, Table 1): Colourless solid, mp (CH_3CN) 218-220 $^\circ\text{C}$; IR (KBr): 3648, 3496, 3367, 3236, 2222, 2216, 1631, 1609, 1552, 1354, 1266, 1109, 758 cm^{-1} ; ^1H NMR (300 MHz, DMSO-d_6): δ 3.88 (s, 3H), 6.64-6.78 (m, 1H), 6.90-7.01 (m, 2H), 7.17 (s, 1H), 7.33-7.43 (m, 2H), 7.58 (t, J = 3.5 Hz, 2H), 7.69 (broad, 2H), 9.69

(broad, 1H); ^{13}C NMR (75 MHz): δ 56.6, 87.7, 94.2, 113.8, 116.3, 116.5, 122.7, 125.2, 128.1, 130.2 (2C), 130.3, 131.0, 135.6 (2C), 148.2, 149.6, 159.4, 160.7, 166.9.

HRMS Calcd for $\text{C}_{20}\text{H}_{15}\text{N}_4\text{O}_2\text{S}$: $[\text{M}+\text{H}]^+$, 375.0916; Found: 375.0909.

2-Amino-4-(3-bromo-phenyl)-6-phenylsulfanyl-pyridine-3,5-dicarbonitrile (Entry 14, Table 1): Colourless solid, mp (CH_3CN) 256-258 $^\circ\text{C}$; IR (KBr): 3360, 3058, 2212, 2208, 1620, 1544, 1516, 1264, 760, 704 cm^{-1} ; ^1H NMR (300 MHz, DMSO-d_6): δ 7.46-7.48 (m, 6H), 7.56 (broad, 2H), 7.67 (s, 1H), 7.70-7.72 (m, 2H); ^{13}C NMR (75 MHz): δ 85.5, 92.0, 113.3, 113.4, 120.6, 125.8, 127.1 (2C), 128.0, 129.1, 129.5, 131.7, 131.9, 133.5 (2C), 134.3, 158.2, 159.8, 166.4.

HRMS Calcd for $\text{C}_{19}\text{H}_{11}\text{BrN}_4\text{S}$: $[\text{M}+\text{H}]^+$, 406.9966; Found: 406.9968.

2-Amino-4-(2-bromo-phenyl)-6-phenylsulfanyl-pyridine-3,5-dicarbonitrile (Entry 15, Table 1): Colourless solid, mp (CH_3CN) 242-244 $^\circ\text{C}$; IR (KBr): 3440, 3336, 3217, 2214, 1627, 1596, 1542, 1263, 758 cm^{-1} ; ^1H NMR (300 MHz, DMSO-d_6): δ 7.43-7.60 (m, 8H), 7.80 (d, $J = 7.8$ Hz, 1H), 7.91 (broad, 2H); ^{13}C NMR (75 MHz): δ 88.2, 94.2, 114.6, 114.9, 121.1, 127.2, 128.8, 129.9 (2C), 130.2, 130.5, 132.4, 133.3, 135.3 (2C), 135.5, 158.4, 159.8, 166.4.

HRMS Calcd for $\text{C}_{19}\text{H}_{11}\text{BrN}_4\text{S}$: $[\text{M}+\text{H}]^+$, 406.9966; Found: 406.9961.

2-Amino-6-phenylsulfanyl-4-p-tolyl-pyridine-3,5-dicarbonitrile (Entry 16, Table 1): Colourless solid, mp (CH_3CN) 208-211 $^\circ\text{C}$; IR (KBr): 3441, 3337, 3217, 2214, 1627, 1542, 1521, 1263, 1095, 758 cm^{-1} ; ^1H NMR (300 MHz, DMSO-d_6): δ 2.52 (s, 3H), 7.32-7.74 (m, 6H), 7.45-7.55 (m, 3H), 7.63 (broad, 2H); ^{13}C NMR (75 MHz): δ 14.9, 87.6, 94.1, 115.9, 116.0, 126.0 (2C), 128.1, 129.7 (2C), 130.1 (2C), 130.3, 130.5, 135.6 (2C), 142.7, 158.6, 160.6 (2C).

2-Amino-6-(4-chloro-phenylsulfanyl)-4-(2-methoxy-naphthalen-1-yl)-pyridine-3,5-dicarbonitrile (Entry 17, Table 1): Colourless solid, mp (CH_3CN) 257-260 $^\circ\text{C}$; IR (KBr): 3440, 3328, 3217, 2221, 2206, 1627, 1544, 1521, 1494, 1263, 696 cm^{-1} ; ^1H NMR (300 MHz, DMSO-d_6): δ 3.92 (s, 3H), 7.36 (d, $J = 8.1$ Hz, 1H), 7.42-7.62 (m, 5H), 7.62-

7.69 (m, 2H), 7.81 (broad, 2H), 7.99 (d, $J = 7.8$ Hz, 1H), 8.20 (d, $J = 7.8$ Hz, 1H); ^{13}C NMR (75 MHz): δ 56.1, 88.7, 94.4, 113.1, 114.0, 114.2, 122.4, 123.6, 125.4, 127.4, 127.7, 127.9, 128.0 (2C), 130.3, 131.7, 134.3, 136.0, 136.2 (2C), 153.1, 155.1, 159.2, 165.0.

HRMS Calcd for $\text{C}_{20}\text{H}_{14}\text{N}_4\text{S}$: $[\text{M}+\text{Na}]^+$, 465.0553; Found: 464.6729.

2-Amino-4-(2,6-dichloro-phenyl)-6-phenylsulfanyl-1,4-dihydro-pyridine-3,5-dicarbonitrile (Entry 18, Table 1): Colourless solid, mp (CH_3CN) 319-320 $^\circ\text{C}$; IR (KBr): 3460, 3359, 2208, 2171, 1647, 1490, 1438, 1249, 779 cm^{-1} ; ^1H NMR (300 MHz, DMSO-d_6): δ 5.64 (s, 1H), 5.99 (broad, 2H), 7.37 (q, $J = 7.0$ Hz, 7.49-7.60 (m, 8H), 9.21 (bs, 1H); ^{13}C NMR (75 MHz): δ 39.7, 53.0, 88.8, 118.3, 120.7, 129.5, 130.5, 130.7 (2C), 131.1, 131.5 (2C), 135.9, 136.0 (2C), 143.6 (2C), 152.3 (2C).

2-Amino-6-(4-chloro-phenylsulfanyl)-4-(2,6-dichloro-phenyl)-1,4-dihydro-pyridine-3,5-dicarbonitrile (Entry 19, Table 1): Colourless solid, mp (CH_3CN) 334-335 $^\circ\text{C}$; IR (KBr): 3448, 3361, 2208, 2165, 1647, 1488, 1481, 1436, 1251, 1093, 819, 781; ^1H NMR (300 MHz, DMSO-d_6): δ 5.61 (s, 1H), 5.98 (broad, 2H), 7.33-7.38 (m, 2H), 7.48-7.53 (m, 4H), 9.19 (broad, 2H); ^{13}C NMR (75 MHz): δ 38.4, 51.7, 87.5, 116.8, 119.2, 128.1, 129.3 (2C), 129.7, 132.0 (2C), 132.1, 133.1, 134.6 (2C), 142.0 (2C), 150.9 (2C).

HRMS Calcd for $\text{C}_{19}\text{H}_{11}\text{N}_4\text{SCl}_3$: $[\text{M}+\text{Na}]^+$, 454.9668; Found: 454.9662.

¹³C NMR spectra of all compounds in Table 1 are given below

RJ-7L-13C (SR)

Current Data Parameters
NAME RJ-7L-13C
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 500000
Time 19.49
INSTRUM dpx300
PROBHD 5 mm Multinu
PULPROG zgpg
TD 109152
SOLVENT DMSO
NS 1096
DS 0
SWH 19841.270 Hz
FIDRES 0.181777 Hz
AQ 2.7506804 sec
RG 8192
DW 25.200 usec
DE 4.50 usec
TE 300.0 K
d11 0.0300000 sec
PL12 16.00 dB
CPDPRG2 waltz16
PCPD2 100.00 usec
SF02 300.1314795 MHz
NUC2 1H
PL2 120.00 dB
D1 1.0000000 sec
P1 10.50 usec
DE 4.50 usec
SF01 75.4766447 MHz
NUC1 13C
PL1 -1.00 dB

F2 - Processing parameters
SI 65536
SF 75.4677517 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 22.00 cm
F1P 181.205 ppm
F1 13675.12 Hz
F2P -5.787 ppm
F2 -437.51 Hz
PPMCM 8.50010 ppm/cm
HZCM 641.48303 Hz/cm

RJ-14L-13C (SR)

Current Data Parameters
NAME RJ-14L-13C
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 500000
Time 9.03
INSTRUM dpx300
PROBHD 5 mm Multinu
PULPROG zgpg
TD 39680
SOLVENT DMSO
NS 21852
DS 0
SWH 19841.270 Hz
FIDRES 0.500032 Hz
AQ 0.9999860 sec
RG 8192
DW 25.200 usec
DE 4.50 usec
TE 300.0 K
d11 0.0300000 sec
PL12 16.00 dB
CPDPRG2 waltz16
PCPD2 100.00 usec
SF02 300.1314795 MHz
NUC2 1H
PL2 120.00 dB
D1 1.0000000 sec
P1 10.50 usec
DE 4.50 usec
SF01 75.4766447 MHz
NUC1 13C
PL1 -1.00 dB

F2 - Processing parameters
SI 65536
SF 75.4677571 MHz
WDW EM
SSB 0
LB 4.00 Hz
GB 0
PC 0.50

1D NMR plot parameters
CX 22.00 cm
F1P 180.807 ppm
F1 13645.08 Hz
F2P -6.521 ppm
F2 -482.13 Hz
PPMCM 8.51490 ppm/cm
HZCM 642.60059 Hz/cm

RJ-56K-13C (SR)

Entry 5, Table 1

Current Data Parameters
NAME RJ-56K-13C
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 500000
Time 19.09
INSTRUM dp3300
PROBHD 5 mm Multinu
PULPROG zgpg
TO 109152
SOLVENT CDCl3
NS 1181
DS 0
SWH 19841.270 Hz
FIDRES 0.181777 Hz
AQ 2.7506804 sec
RG 8192
DW 25.200 usec
DE 4.50 usec
TE 300.0 K
d11 0.0300000 sec
PL12 16.00 dB
CPDPRG2 waltz16
PCPD2 100.00 usec
SF02 300.1314795 MHz
NUC2 1H
PL2 120.00 dB
D1 1.00000000 sec
P1 10.50 usec
DE 4.50 usec
SF01 75.4766447 MHz
NUC1 13C
PL1 -1.00 dB

F2 - Processing parameters
SI 65536
SF 75.4677550 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 22.00 cm
F1P 194.353 ppm
F1 14667.40 Hz
F2P -6.385 ppm
F2 -481.85 Hz
PPMCM 9.12445 ppm/cm
HZCM 688.60211 Hz/cm

RJ-92K-13C (SR)

Entry 6, Table 1

Current Data Parameters
NAME RJ-92K-13C
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 500000
Time 17.03
INSTRUM dp3300
PROBHD 5 mm Multinu
PULPROG zgpg
TO 109152
SOLVENT DMSO
NS 1024
DS 0
SWH 19841.270 Hz
FIDRES 0.181777 Hz
AQ 2.7506804 sec
RG 8192
DW 25.200 usec
DE 4.50 usec
TE 300.0 K
d11 0.0300000 sec
PL12 16.00 dB
CPDPRG2 waltz16
PCPD2 100.00 usec
SF02 300.1314795 MHz
NUC2 1H
PL2 120.00 dB
D1 1.00000000 sec
P1 10.50 usec
DE 4.50 usec
SF01 75.4766447 MHz
NUC1 13C
PL1 -1.00 dB

F2 - Processing parameters
SI 65536
SF 75.4677595 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 22.00 cm
F1P 186.208 ppm
F1 14052.69 Hz
F2P -7.907 ppm
F2 -596.70 Hz
PPMCM 8.82339 ppm/cm
HZCM 665.88129 Hz/cm

RJ-93K-13C (SR)

Current Data Parameters
NAME RJ-93K-13C
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 500000
Time 8.47
INSTRUM dpx300
PROBHD 5 mm Multinu
PULPROG zgdc
TD 39680
SOLVENT DMSO
NS 22348
DS 0
SWH 19841.270 Hz
FIDRES 0.500032 Hz
AQ 0.9999860 sec
RG 8192
DM 25.200 usec
DE 4.50 usec
TE 300.0 K
d11 0.0300000 sec
PL12 16.00 dB
CPDPRG2 waltz16
PCPD2 100.00 usec
SF02 300.1314795 MHz
NUC2 1H
PL2 120.00 dB
D1 1.00000000 sec
P1 10.50 usec
DE 4.50 usec
SF01 75.4766447 MHz
NUC1 13C
PL1 -1.00 dB

F2 - Processing parameters
SI 65536
SF 75.4677520 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 22.00 cm
F1P 175.650 ppm
F1 13255.88 Hz
F2P -6.837 ppm
F2 -516.00 Hz
PPMCM 8.29487 ppm/cm
HZCM 625.99487 Hz/cm

RJ-11L-13C (SR)

Current Data Parameters
NAME RJ-11L-13C
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 500000
Time 21.19
INSTRUM dpx300
PROBHD 5 mm Multinu
PULPROG zgdc
TD 45348
SOLVENT DMSO
NS 4341
DS 0
SWH 19841.270 Hz
FIDRES 0.437534 Hz
AQ 1.1428196 sec
RG 8192
DM 25.200 usec
DE 4.50 usec
TE 300.0 K
d11 0.0300000 sec
PL12 16.00 dB
CPDPRG2 waltz16
PCPD2 100.00 usec
SF02 300.1314105 MHz
NUC2 1H
PL2 120.00 dB
D1 0.80000001 sec
P1 10.50 usec
DE 4.50 usec
SF01 75.4766029 MHz
NUC1 13C
PL1 -1.00 dB

F2 - Processing parameters
SI 65536
SF 75.4677544 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 22.00 cm
F1P 207.330 ppm
F1 15646.70 Hz
F2P -9.319 ppm
F2 -703.30 Hz
PPMCM 8.84767 ppm/cm
HZCM 743.18158 Hz/cm

RJ91K-13C (SKD)

Current Data Parameters
NAME RJ91K-13C
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 500000
Time 14.44
INSTRUM dpx300
PROBHD 5 mm Multinu
PULPROG zgdc
TD 109152
SOLVENT CDCl3
NS 1146
DS 0
SWH 19841.270 Hz
FIDRES 0.181777 Hz
AQ 2.7506804 sec
RG 8192
DM 25.200 usec
DE 4.50 usec
TE 300.0 K
d11 0.0300000 sec
PL12 16.00 dB
CPDPRG2 waltz16
PCPD2 100.00 usec
SF02 300.1314795 MHz
NUC2 1H
PL2 120.00 dB
D1 1.00000000 sec
P1 10.50 usec
DE 4.50 usec
SF01 75.4766447 MHz
NUC1 13C
PL1 -1.00 dB

F2 - Processing parameters
SI 65536
SF 75.4677190 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 22.00 cm
F1P 173.825 ppm
F1 13118.20 Hz
F2P -5.109 ppm
F2 -385.56 Hz
PPMCM 8.13338 ppm/cm
HZCM 613.80743 Hz/cm

RJ-49K-13C (SR)

Current Data Parameters
NAME RJ-49K-13C
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 500000
Time 19.45
INSTRUM dpx300
PROBHD 5 mm Multinu
PULPROG zgdc
TD 109152
SOLVENT CDCl3
NS 1169
DS 0
SWH 19841.270 Hz
FIDRES 0.181777 Hz
AQ 2.7506804 sec
RG 8192
DM 25.200 usec
DE 4.50 usec
TE 300.0 K
d11 0.0300000 sec
PL12 16.00 dB
CPDPRG2 waltz16
PCPD2 100.00 usec
SF02 300.1314795 MHz
NUC2 1H
PL2 120.00 dB
D1 1.00000000 sec
P1 10.50 usec
DE 4.50 usec
SF01 75.4766447 MHz
NUC1 13C
PL1 -1.00 dB

F2 - Processing parameters
SI 65536
SF 75.4677113 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 22.00 cm
F1P 195.418 ppm
F1 14747.75 Hz
F2P -8.705 ppm
F2 -657.27 Hz
PPMCM 9.27850 ppm/cm
HZCM 700.22803 Hz/cm

RJ-77K-13C (SR)

Current Data Parameters
 NAME RJ-77K-13C
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 500000
 Time 19.16
 INSTRUM dpx300
 PROBHD 5 mm Multinu
 PULPROG zgpg30
 TO 109152
 SOLVENT CDCl3
 NS 1222
 DS 0
 SWH 19841.270 Hz
 FIDRES 0.181777 Hz
 AQ 2.7506804 sec
 RG 8192
 DW 25.200 usec
 DE 4.50 usec
 TE 300.0 K
 d11 0.0300000 sec
 PL12 16.00 dB
 CPDPRG2 waltz16
 PCPD2 100.00 usec
 SF02 300.1314795 MHz
 NUC2 1H
 PL2 120.00 dB
 D1 1.00000000 sec
 P1 10.50 usec
 DE 4.50 usec
 SF01 75.4766447 MHz
 NUC1 13C
 PL1 -1.00 dB

F2 - Processing parameters
 SI 65536
 SF 75.4677792 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 22.00 cm
 F1P 204.357 ppm
 F1 15422.39 Hz
 F2P -7.521 ppm
 F2 -567.63 Hz
 PPMCM 9.63088 ppm/cm
 HZCM 726.81885 Hz/cm

RJ-13L-13C (SR)

Current Data Parameters
 NAME RJ-13L-13C
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 500000
 Time 18.42
 INSTRUM dpx300
 PROBHD 5 mm Multinu
 PULPROG zgpg30
 TO 109152
 SOLVENT CDCl3
 NS 1598
 DS 0
 SWH 19841.270 Hz
 FIDRES 0.181777 Hz
 AQ 2.7506804 sec
 RG 8192
 DW 25.200 usec
 DE 4.50 usec
 TE 300.0 K
 d11 0.0300000 sec
 PL12 16.00 dB
 CPDPRG2 waltz16
 PCPD2 100.00 usec
 SF02 300.1314795 MHz
 NUC2 1H
 PL2 120.00 dB
 D1 1.00000000 sec
 P1 10.50 usec
 DE 4.50 usec
 SF01 75.4766447 MHz
 NUC1 13C
 PL1 -1.00 dB

F2 - Processing parameters
 SI 65536
 SF 75.4681573 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 22.00 cm
 F1P 243.918 ppm
 F1 18408.03 Hz
 F2P -18.991 ppm
 F2 -1433.24 Hz
 PPMCM 11.95042 ppm/cm
 HZCM 901.87585 Hz/cm

RJ89K-13C (SKD)

Current Data Parameters
 NAME RJ89K-13C
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 500000
 Time 12.47
 INSTRUM dpx300
 PROBNM 5 mm Multinu
 PULPROG zgpg
 TO 109152
 SOLVENT CDCl3
 NS 1734
 DS 0
 SWH 19841.270 Hz
 FIDRES 0.181777 Hz
 AQ 2.7506804 sec
 RG 8192
 DM 25.200 usec
 DE 4.50 usec
 TE 300.0 K
 d11 0.0300000 sec
 PL12 16.00 dB
 CPOPRG2 waltz16
 PCPD2 100.00 usec
 SF02 300.1314795 MHz
 NUC2 1H
 PL2 120.00 dB
 D1 1.00000000 sec
 P1 10.50 usec
 DE 4.50 usec
 SF01 75.4766447 MHz
 NUC1 13C
 PL1 -1.00 dB

F2 - Processing parameters
 SI 65536
 SF 75.4677150 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 22.00 cm
 F1P 175.783 ppm
 F1 13654.45 Hz
 F2P -9.109 ppm
 F2 -365.56 Hz
 PPMCM 8.22147 ppm/cm
 HZCM 620.45226 Hz/cm

RJ-33L-13C (SR)

Current Data Parameters
 NAME RJ-33L-13C
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 500000
 Time 16.27
 INSTRUM dpx300
 PROBNM 5 mm Multinu
 PULPROG zgpg
 TO 109152
 SOLVENT CDCl3
 NS 187
 DS 0
 SWH 19841.270 Hz
 FIDRES 0.181777 Hz
 AQ 2.7506804 sec
 RG 8192
 DM 25.200 usec
 DE 4.50 usec
 TE 300.0 K
 d11 0.0300000 sec
 PL12 16.00 dB
 CPOPRG2 waltz16
 PCPD2 100.00 usec
 SF02 300.1314795 MHz
 NUC2 1H
 PL2 120.00 dB
 D1 1.00000000 sec
 P1 10.50 usec
 DE 4.50 usec
 SF01 75.4766447 MHz
 NUC1 13C
 PL1 -1.00 dB

F2 - Processing parameters
 SI 65536
 SF 75.4682378 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 22.00 cm
 F1P 186.651 ppm
 F1 14086.24 Hz
 F2P -9.077 ppm
 F2 -685.02 Hz
 PPMCM 8.89674 ppm/cm
 HZCM 671.42108 Hz/cm

RJ-34L-13C (SR)

Current Data Parameters
NAME RJ-34L-13C
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 500000
Time 16.48
INSTRUM dpx300
PROBHD 5 mm Multinu
PULPROG zgpg30
TD 109152
SOLVENT DMSO
NS 1886
DS 0
SWH 19841.270 Hz
FIDRES 0.181777 Hz
AQ 2.7506804 sec
RG 8192
DW 25.200 usec
DE 4.50 usec
TE 300.0 K
d11 0.0300000 sec
PL12 16.00 dB
CPOPRG2 waltz16
PCPD2 100.00 usec
SFO2 300.1314795 MHz
NUC2 1H
PL2 120.00 dB
D1 1.00000000 sec
P1 10.50 usec
DE 4.50 usec
SFO1 75.4766447 MHz
NUC1 13C
PL1 -1.00 dB

F2 - Processing parameters
SI 65536
SF 75.4677507 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 22.00 cm
F1P 192.784 ppm
F1 14548.97 Hz
F2P -7.144 ppm
F2 -539.17 Hz
PPMCM 9.08765 ppm/cm
HZCM 685.62446 Hz/cm

RJ110K-13C (SKD)

Current Data Parameters
NAME RJ110K-13C
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 500000
Time 10.34
INSTRUM dpx300
PROBHD 5 mm Multinu
PULPROG zgpg30
TD 39680
SOLVENT CDCl3
NS 2766
DS 0
SWH 19841.270 Hz
FIDRES 0.500032 Hz
AQ 0.9999860 sec
RG 8192
DW 25.200 usec
DE 4.50 usec
TE 300.0 K
d11 0.0300000 sec
PL12 16.00 dB
CPOPRG2 waltz16
PCPD2 100.00 usec
SFO2 300.1314735 MHz
NUC2 1H
PL2 120.00 dB
D1 1.00000000 sec
P1 10.50 usec
DE 4.50 usec
SFO1 75.4766447 MHz
NUC1 13C
PL1 -1.00 dB

F2 - Processing parameters
SI 65536
SF 75.4677190 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 22.00 cm
F1P 168.012 ppm
F1 12679.45 Hz
F2P -6.078 ppm
F2 -458.69 Hz
PPMCM 7.91316 ppm/cm
HZCM 597.18811 Hz/cm

RJ-121K-13C (SR)

Current Data Parameters
NAME RJ-121K-13C
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 500000
Time_ 16.06
INSTRUM dpx300
PROBHD 5 mm Multinu
PULPROG zgdc
TD 39680
SOLVENT DMSO
NS 4096
DS 0
SWH 19841.270 Hz
FIDRES 0.500032 Hz
AQ 0.9999860 sec
RG 8192
DM 25.200 usec
DE 4.50 usec
TE 300.0 K
d11 0.0300000 sec
PL12 16.00 dB
CPDPRG2 waltz16
PCPD2 100.00 usec
SF02 300.1314795 MHz
NUC2 1H
PL2 120.00 dB
D1 1.00000000 sec
P1 10.50 usec
DE 4.50 usec
SF01 75.4766447 MHz
NUC1 13C
PL1 -1.00 dB

F2 - Processing parameters
SI 65536
SF 75.4678232 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 22.00 cm
F1P 182.780 ppm
F1 13794.02 Hz
F2P -7.781 ppm
F2 -587.25 Hz
PPMCH 8.66189 ppm/cm
HZCH 653.69385 Hz/cm

RJ136K-13C (SKD)

Current Data Parameters
NAME RJ136K-13C
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060901
Time_ 14.09
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgdc
TD 79362
SOLVENT DMSO
NS 537
DS 0
SWH 19841.270 Hz
FIDRES 0.250010 Hz
AQ 1.9999723 sec
RG 8192
DM 25.200 usec
DE 5.50 usec
TE 297.2 K
D1 1.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCNRK 0.01500000 sec

***** CHANNEL f1 *****
NUC1 13C
P1 10.50 usec
PL1 -1.00 dB
SF01 75.4766414 MHz

***** CHANNEL f2 *****
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 120.00 dB
PL12 16.00 dB
SF02 300.1314795 MHz

F2 - Processing parameters
SI 65536
SF 75.4677190 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 22.00 cm
CY 4.18 cm
F1P 182.273 ppm
F1 13755.73 Hz
F2P -9.194 ppm
F2 -693.87 Hz
PPMCH 8.70306 ppm/cm
HZCH 656.79999 Hz/cm

RJ-137K-13C (SR)

Current Data Parameters
 NAME RJ-137K-13C
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date 20060905
 Time 15.17
 INSTRUM spect
 PROBHD 5 mm Multinuc1
 PULPROG zgpg
 TO 109152
 SOLVENT CDCl3
 NS 148
 DS 0
 SWH 19841.270 Hz
 FIDRES 0.181777 Hz
 AQ 2.7506804 sec
 RG 8196
 DW 25.200 usec
 DE 5.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 d11 0.03000000 sec
 MCREST 0.00000000 sec
 MCWAK 0.01500000 sec

***** CHANNEL f1 *****
 NUC1 13C
 P1 10.50 usec
 PL1 -1.00 dB
 SFO1 75.4766414 MHz

***** CHANNEL f2 *****
 CPOPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 120.00 dB
 PL12 16.00 dB
 SFO2 300.1314795 MHz

F2 - Processing parameters
 SI 65536
 SF 75.4678220 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 22.00 cm
 CY 5.20 cm
 F1P 179.733 ppm
 F1 13564.04 Hz
 F2P -669.91 Hz
 F2 -669.91 Hz
 PPMCH 8.57316 ppm/cm
 HZCH 646.99792 Hz/cm