The Potassium *t*-Butoxide Catalyzed Addition of Carbonyl Derivatives to Styrenes

Supporting Information

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Spectral data for compounds **5a, 5b, 5c, 5d, 5e, 5f, 5g, 6a, 6b, 6c, 6d** and **9:**

2-ethyl-2,4-diphenylbutanenitrile (5a):
^{1}H NMR (300 MHz, $CDCl_3$): δ 7.65-7.40 (m, 10H), 2.89 (dt, J = 13, 4 Hz, 1H), 2.60-2.00 (m, 5H), 1.04 (t, 3H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 141.3, 138.5, 129.5, 129.0, 128.8, 128.3, 126.7, 16.5, 122.6, 49.5, 43.2, 34.8, 32.3, 10.2.

2-ethyl-2-phenyl-4-(4-fluorophenyl)butanenitrile (5b):
^{1}H NMR (300 MHz, $CDCl_3$): δ 7.36-7.17, 6.95-6.87 and 6.84-6.75 (each m, 9H), 2.62 (dt, J = 13, 4.4 Hz, 1H), 2.30-1.76 (m, 5H), 0.81 (t, J = 7.4 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 163.4, 160.2, 138.3, 136.9, 130.1, 130.0, 129.5, 128.3, 126.4, 122.5, 115.8, 115.5, 49.4, 43.2, 34.7, 31.4, 10.1.

2,2-dimethyl-4-phenylbutanenitrile (5c):
^{1}H NMR (300 MHz, $CDCl_3$): δ 7.50-7.25 (m, 5H), 2.69-2.60 and 1.73-1.65 (each m, 4H), 1.24 (s, 6H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 141.3, 129.0, 128.8, 126.7, 125.2, 43.4, 32.6, 32.9, 27.1.

2,2-dimethyl-4-(4-fluorophenyl)butanenitrile (5d):
^{1}H NMR (300 MHz, $CDCl_3$): δ 7.06-6.98 and 6.89-6.79 (each m, 4H), 2.68-2.59 and 1.70-1.61 (each m, 4H), 1.26 (s, 6H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 163.4, 160.2, 137, 130.2, 130.1, 125.1, 115.8, 115.5, 43.4, 32.8, 31.3, 26.9.

2,2-dimethyl-4-(4-methoxyphenyl)butanenitrile (5e):
^{1}H NMR (300 MHz, $CDCl_3$): δ 7.00 and 6.75 (each d, J = 9 Hz, 4H), 3.68 (s, 3H), 2.69-2.60 and 1.74-1.65 (each m, 4H), 1.29 (s, 6H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 158.5, 133.3, 129.6, 125.3, 114.4, 55.6, 43.7, 32.8, 31.3, 27.1.

2,2-dimethyl-4-(2-bromophenyl)butanenitrile (5f):
^{1}H NMR (300 MHz, $CDCl_3$): δ 7.43 (dt, J = 9 Hz, 1H), 7.19-7.11 and 7.03-6.93 (each m, 3H), 2.86-2.79 and 1.75-1.67 (each m, 4H), 1.34 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 140.5, 133.3, 130.8, 128.5, 128.2, 125.1, 124.6, 41.5, 32.7, 32.6.

2-(2-phenylethyl)cyclohexanecarbonitrile (5g):
^{1}H NMR (300 MHz, $CDCl_3$): δ 7.30-7.00 (m, 5H), 2.80-2.65 (m, 2H), 2.10-1.90 (m, 2H), 1.80-1.40 and 1.30-1.00 (each m, 10H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 141.5, 128.9, 128.7, 126.6, 123.9, 43.0, 39.5, 36.1, 31.3, 25.8, 23.5.

2-methyl-1,3-diphenylpropanone (6a):
^{1}H NMR (300 MHz, $CDCl_3$): δ 7.96-7.90, 7.62-7.55, 7.52-7.45 and 7.37-7.18 (each m, 10H), 3.53 (q, J = 7 Hz, 1H), 2.71 (t, J = 7.5 Hz, 2H), 2.31-2.18 and 1.89-1.75 (each m, 2H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 204.4, 142.2, 137.0, 133.3, 129, 128.9, 28.8, 128.6, 126.3, 40.2, 35.6, 33.9, 17.7.

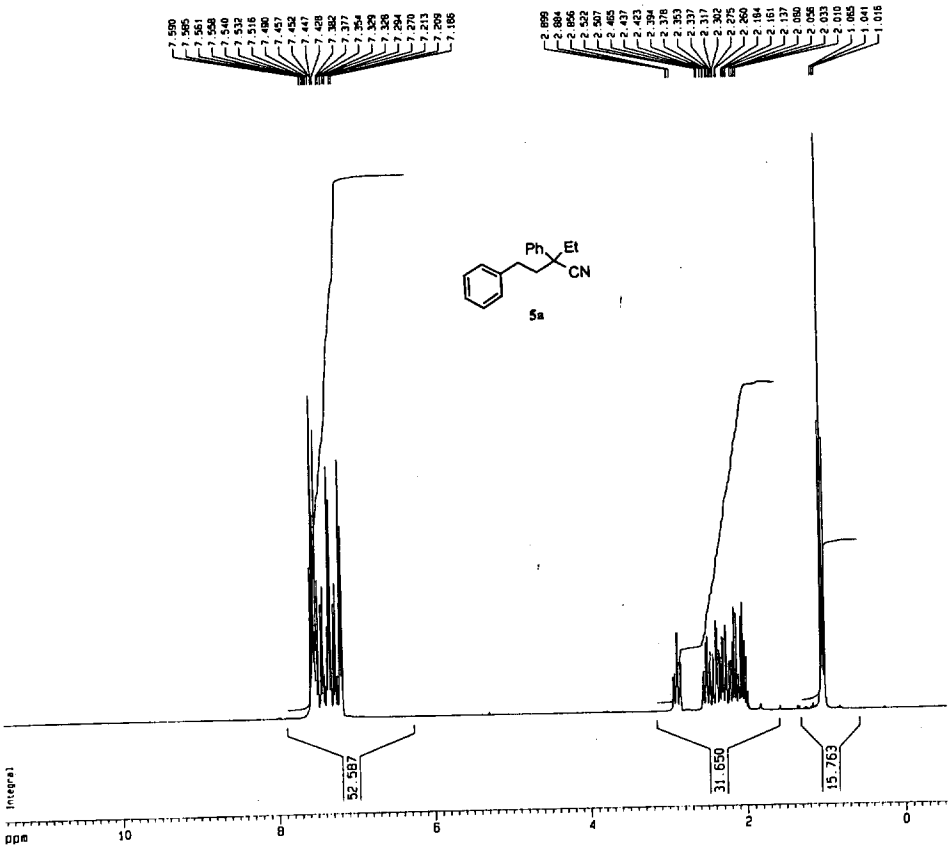
2-(2-phenylethyl)cyclohexanone (6b):
^{1}H NMR (200 MHz, $CDCl_3$): δ 7.22-7.16 and 7.13-7.06 (each m, 5H), 2.64 (t, J = 12 Hz, 2H), 2.44-1.36 (m, 11H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 213.5, 142.6, 128.8, 128.7, 126.2, 50.3, 42.5, 34.4, 33.6, 31.6, 28.5, 25.3.

2-(2-phenylethyl)-3,4-dihydro-2*H*-naphthalen-1-one (6c):
^{1}H NMR (300 MHz, $CDCl_3$): δ 7.94-7.89 (m, 1H), 7.3 (dt, J = 7.4, 1.5 Hz, 1H), 7.18-7.10 (m, 7H), 2.87-2.80, 2.72-2.53, 2.41-2.30, 2.26-2.08 and 1.85-1.59 (each m, 9H). ^{13}C NMR(75 MHz, $CDCl_3$): δ 198.9, 142.8, 141.3, 141.0, 132.1, 131.5, 127.6, 127.4, 127.3, 126.3, 125.4, 124.7, 45.7, 32.1, 30.3, 27.4.

3-(2-phenylethyl)-1,7,7-trimethyl-bicyclo[2.2.1]heptan-2-one (6d):
^{1}H NMR (300 MHz, $CDCl_3$): δ 7.30-7.00 (m, 5H), 2.70-2.50, 2.35-2.25, 2.05-1.90, 1.80-1.35 and 1.30-1.10 (each m, 10H), 1.00-0.70 (m, 9H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 221.7, 142.2, 128.8, 128.7, 126.3, 49.4, 46.6, 46.2, 34.5, 31.6, 31.4, 29.5, 20.4, 19.8, 19.7, 10, 9.8.

Compound 7a:
Compound **7a** was converted by acidic hydrolysis to the ketone **(6b)**.

2-(2-phenylethyl)cyclopentanenitrile (9):
^{1}H NMR (300 MHz, $CDCl_3$): δ 7.50-6.90 (m, 5H), 2.80-2.55, 2.50-2.35 and 2.30-1.00 (each m, 12H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 140.7, 139.7, 129.4, 129.1, 128.9, 126.9, 126.7, 47.7, 45.8, 40.3, 38.5, 34.2, 34.1, 31.5, 30.7, 30.6, 24.1, 23.2.



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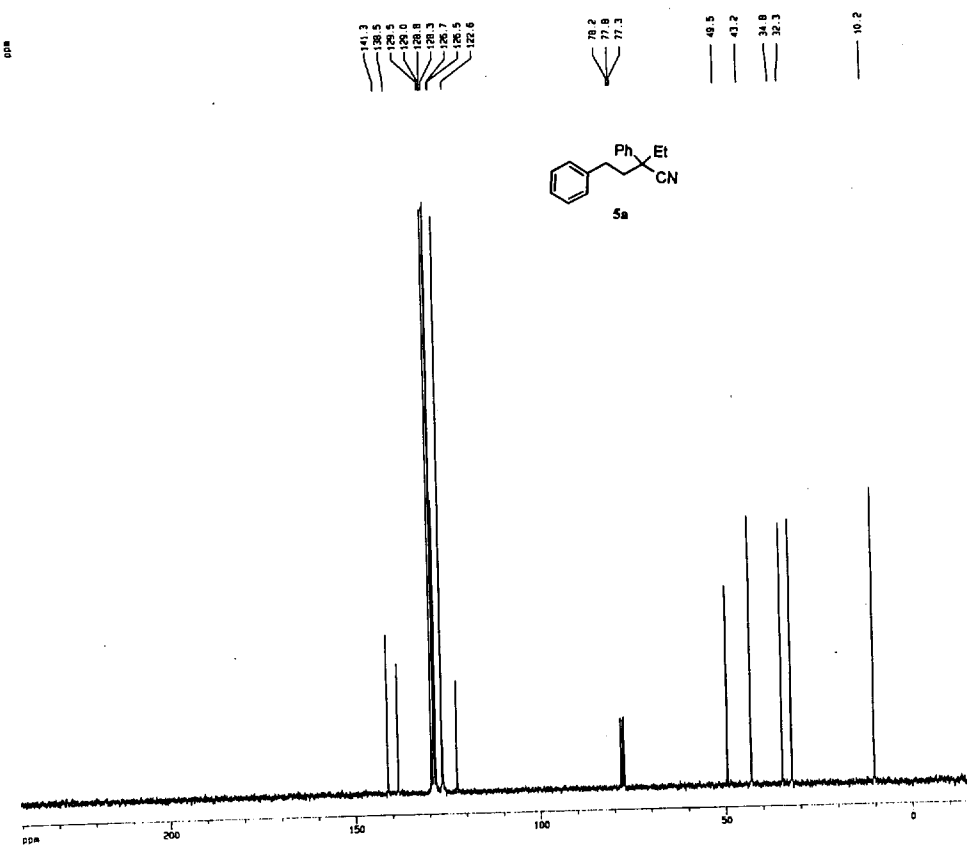

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1D NMR plot parameters
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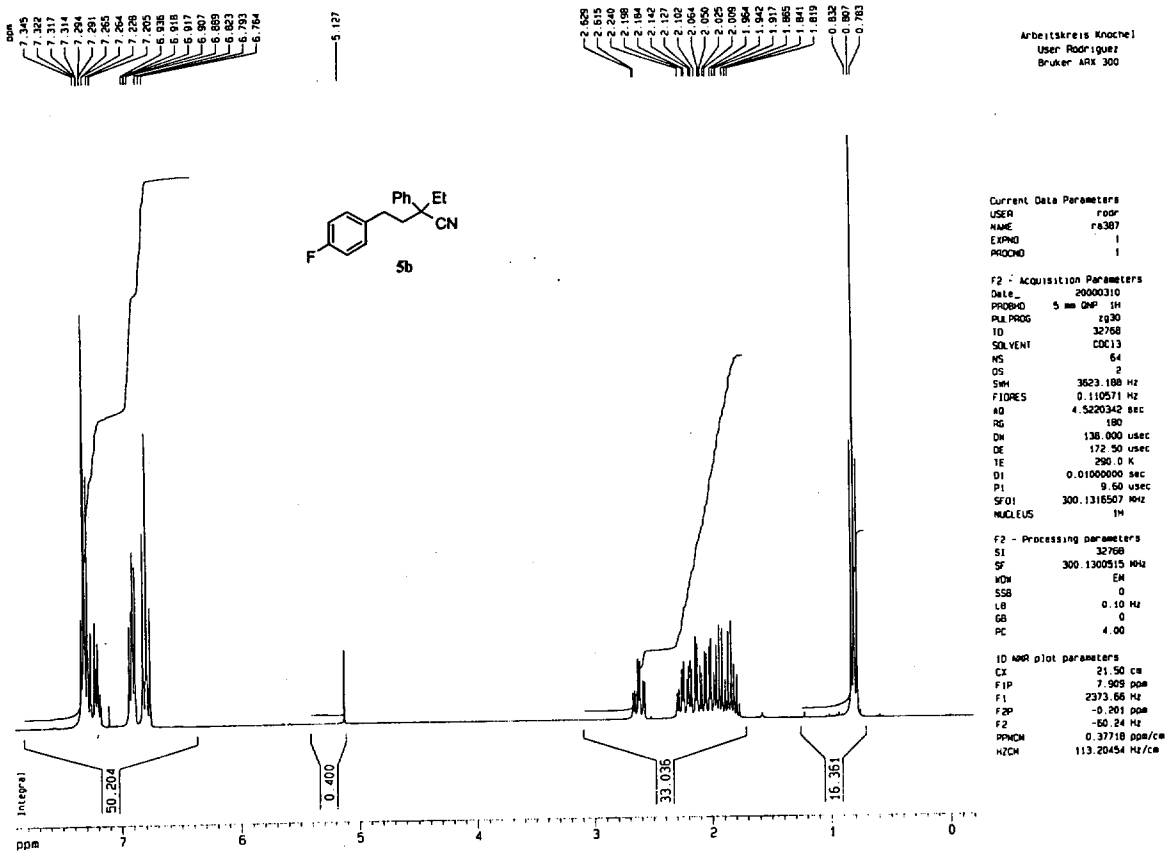

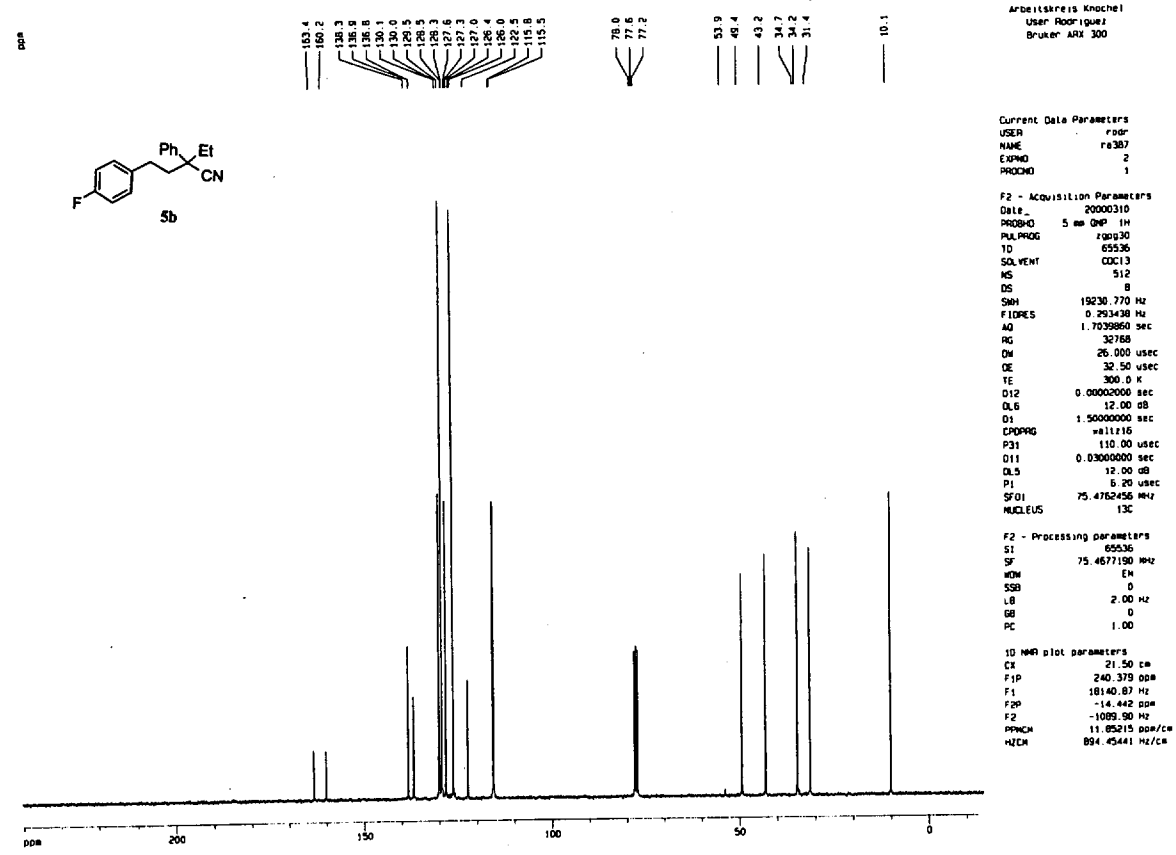

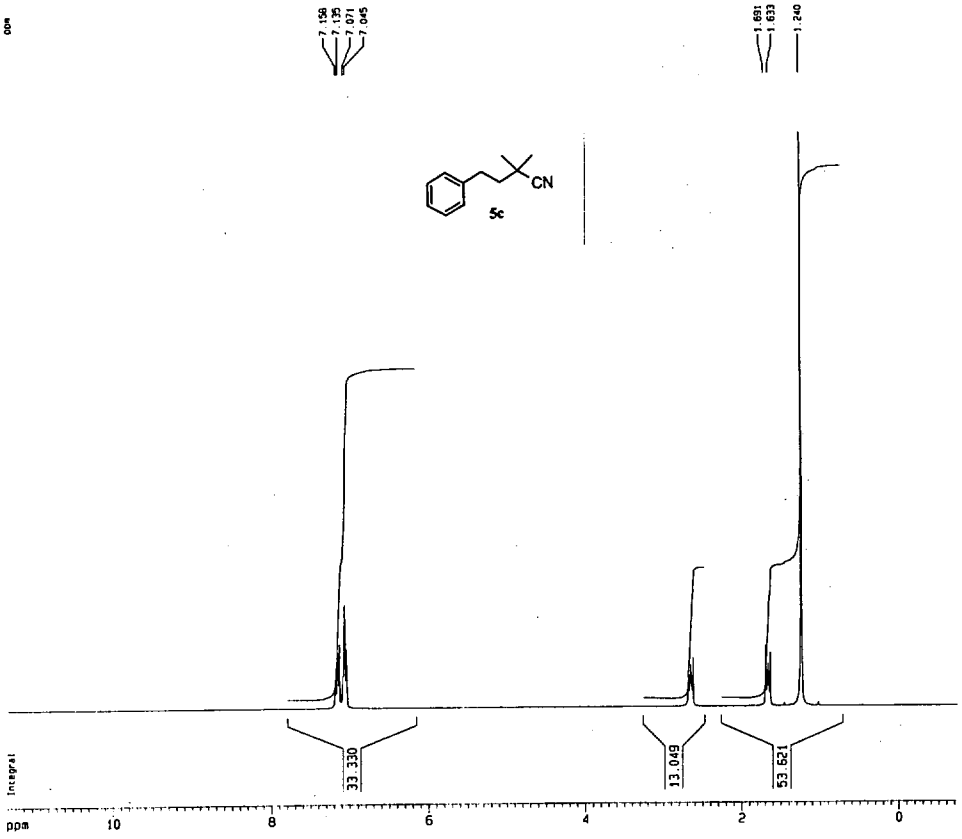

Arbeitskreis Knochel
User Rodriguez
Bruker ARX 300

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NAME ra392
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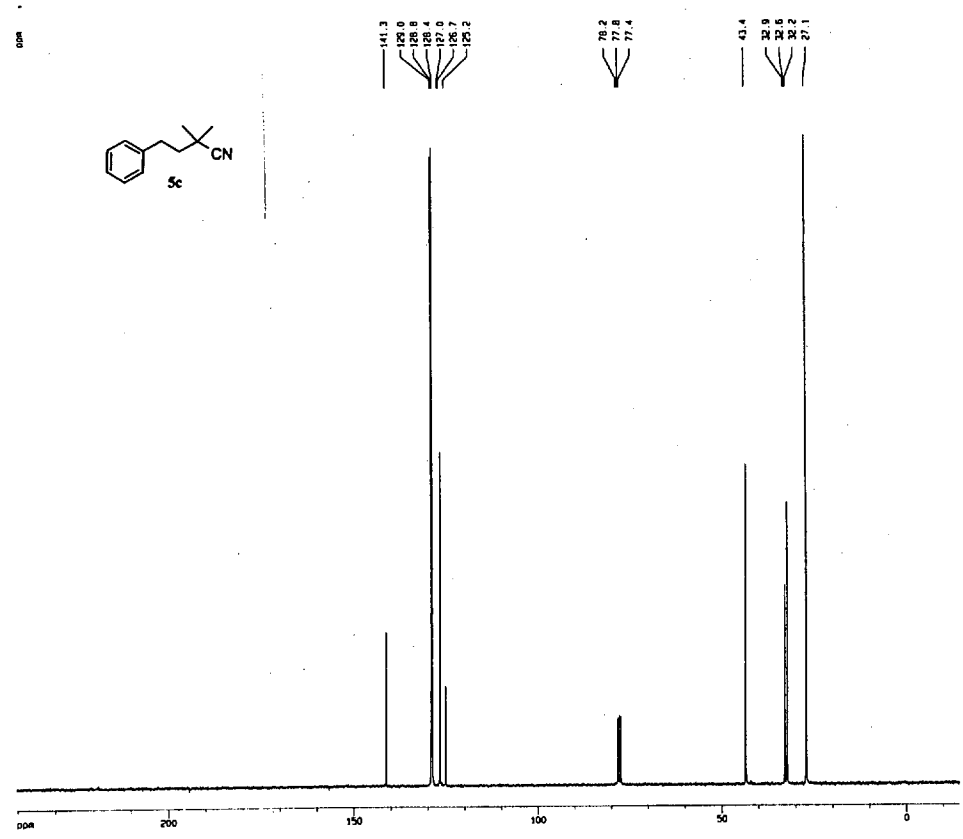

Arbeitskreis Knochel
User Rodriguez
Bruker ARX 300

Current Data Parameters
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NAME ra392
EXPNO 2
PROCNO 1

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F2 - Processing parameters
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1D NMR plot parameters
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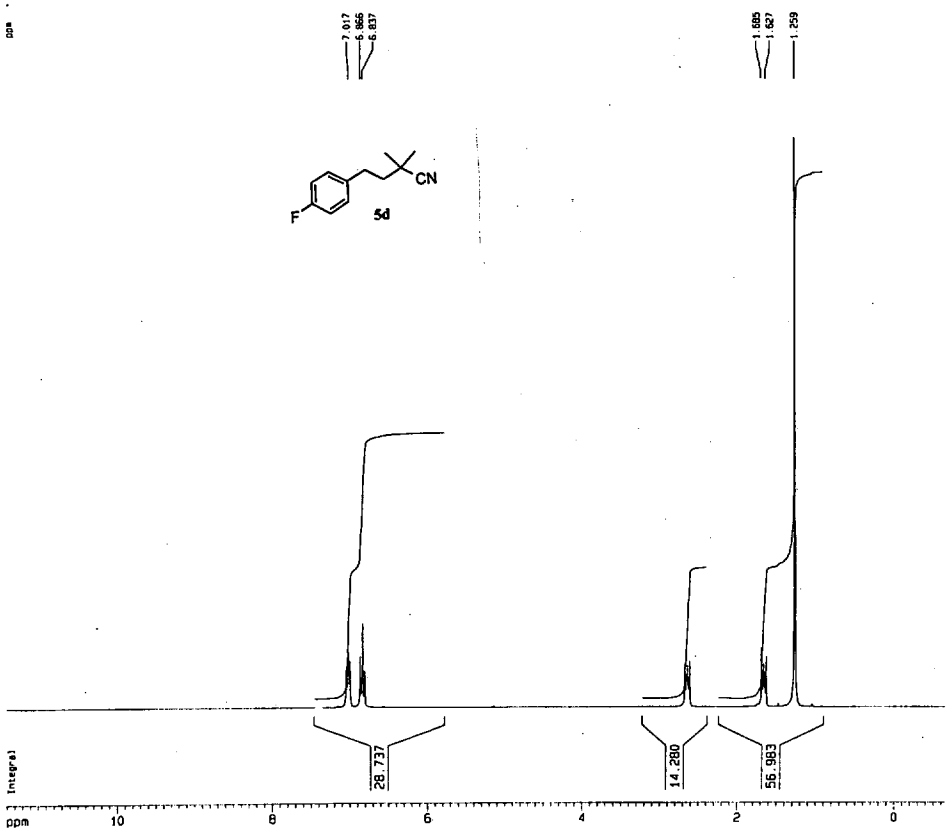

Arbeitskreis Knochel
User Rodriguez
Bruker ARX 300

Current Data Parameters
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NAME ra391
EXPNO 1
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NUCLEUS 1H

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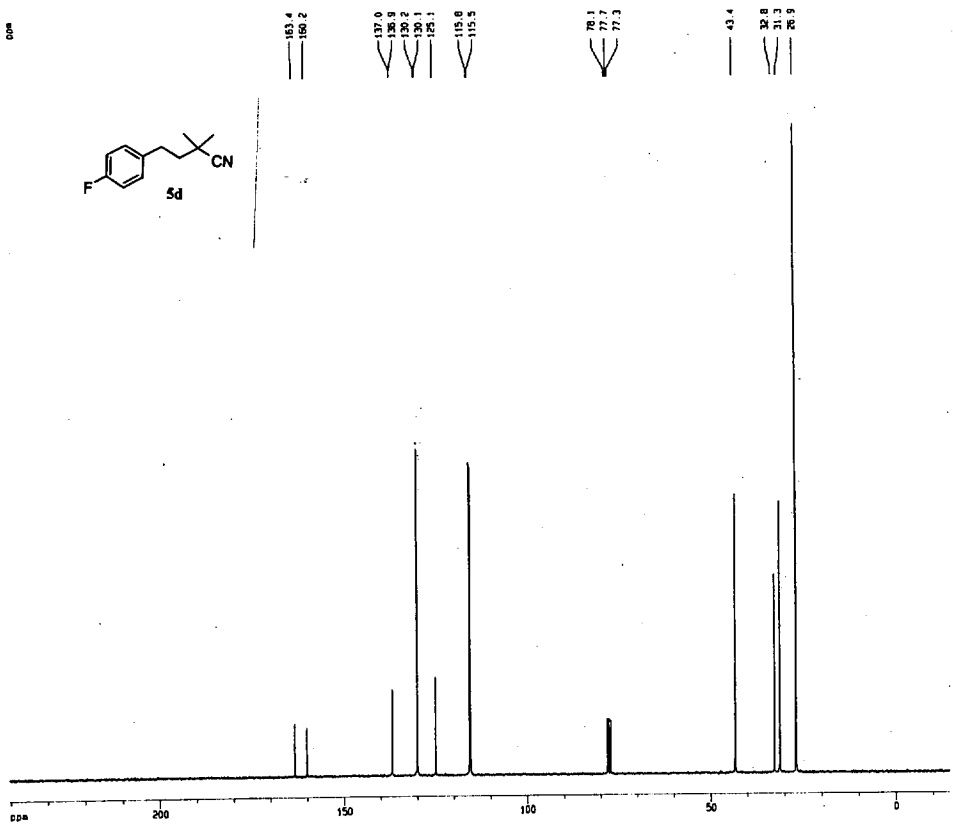

Arbeitskreis Knochel
User Rodriguez
Bruker ARX 300

Current Data Parameters
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NAME ra391
EXPNO 2
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1D NMR plot parameters
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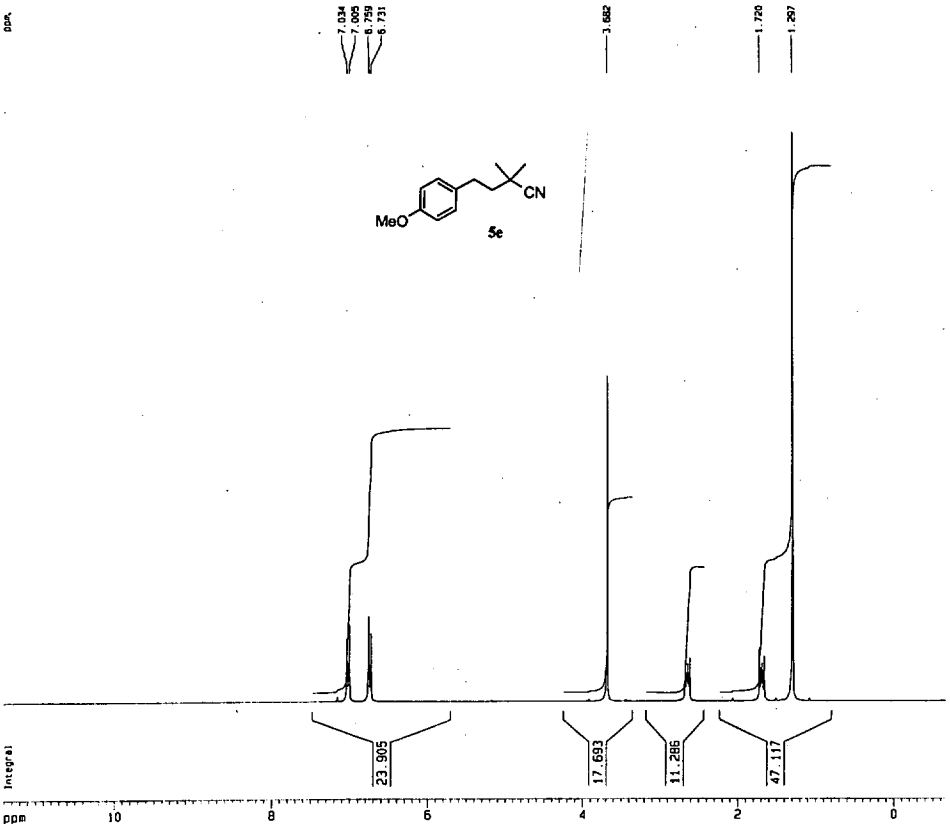

Arbeitskreis Knochel
User Rodriguez
Bruker ARX 300

Current Data Parameters
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NAME ra395
EXPNO 1
PROCNO 1

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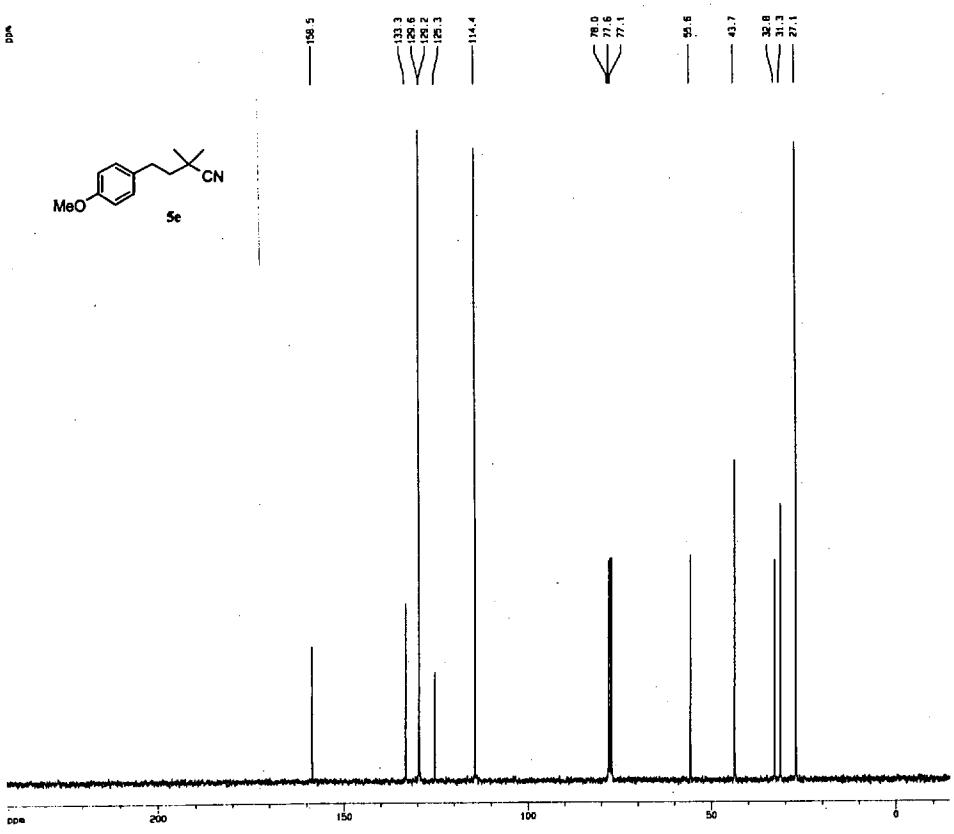

Arbeitskreis Knochel
User Rodriguez
Bruker ARX 300

Current Data Parameters
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NAME ra395
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PROCNO 1

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NUCLEUS 13C

F2 - Processing parameters
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1D NMR plot parameters
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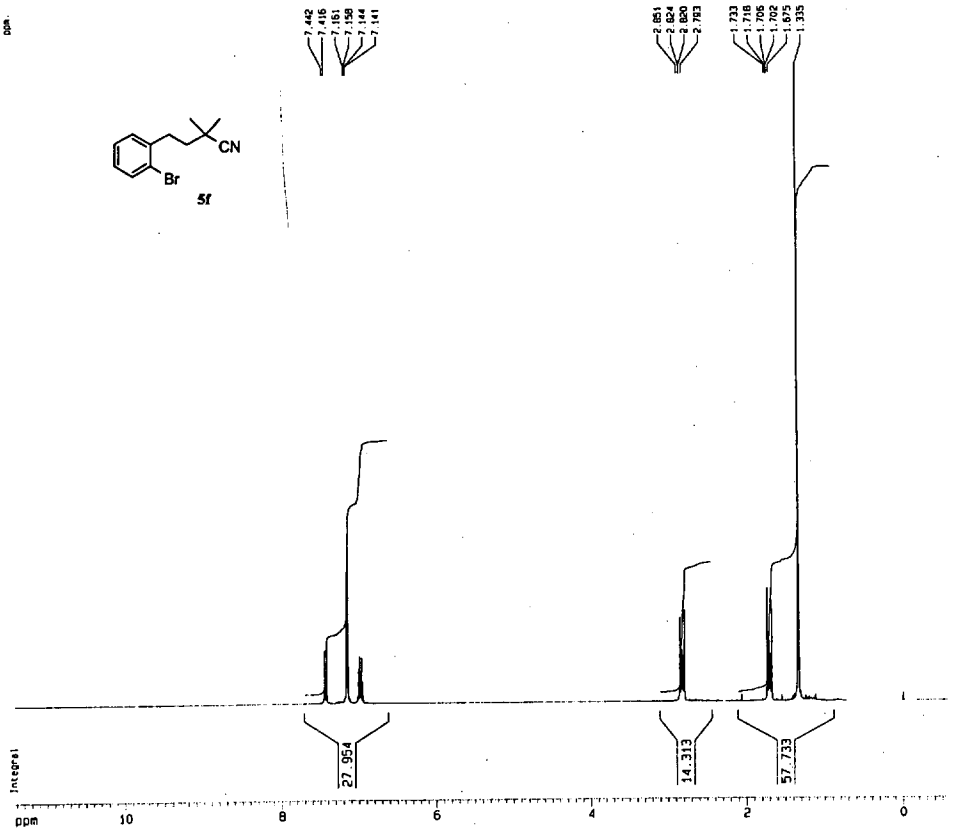

Arbeitskreis Knochel
User Rodriquez
Bruker ARX 300

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PROCNO 1

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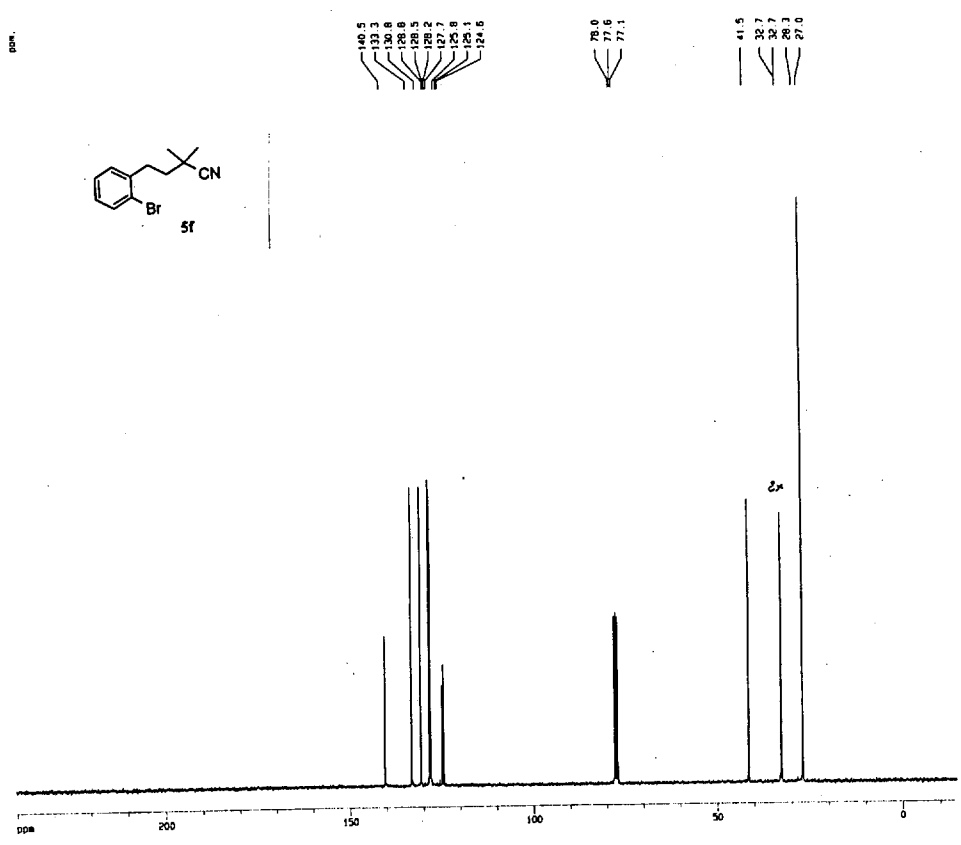

Arbeitskreis Knochel
User Rodriquez
Bruker ARX 300

Current Data Parameters
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PROCNO 1

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1D NMR plot parameters
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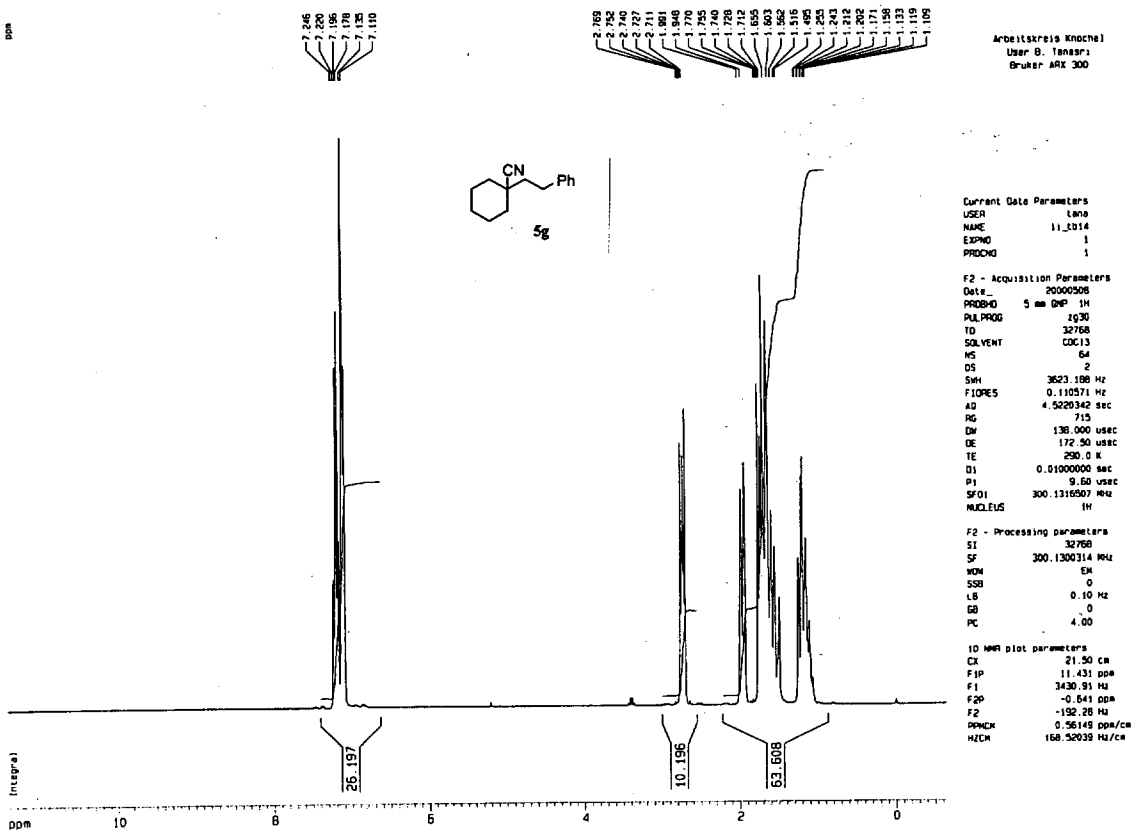

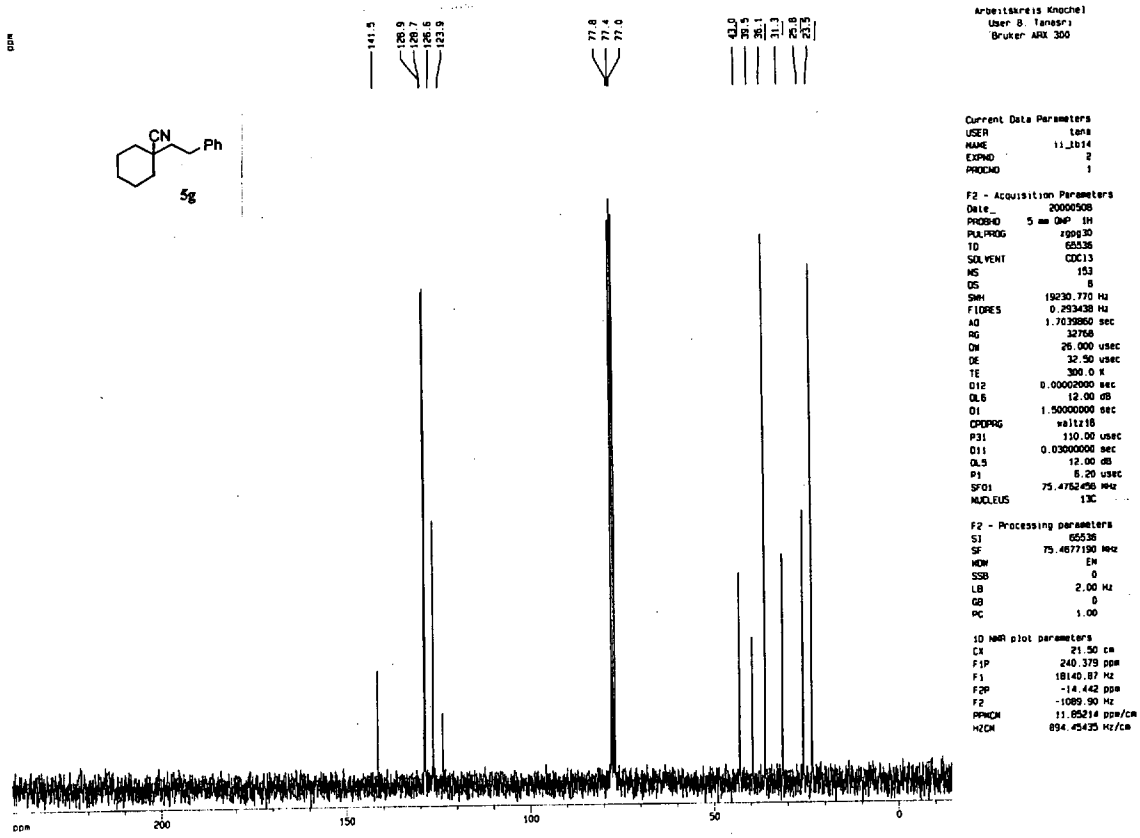

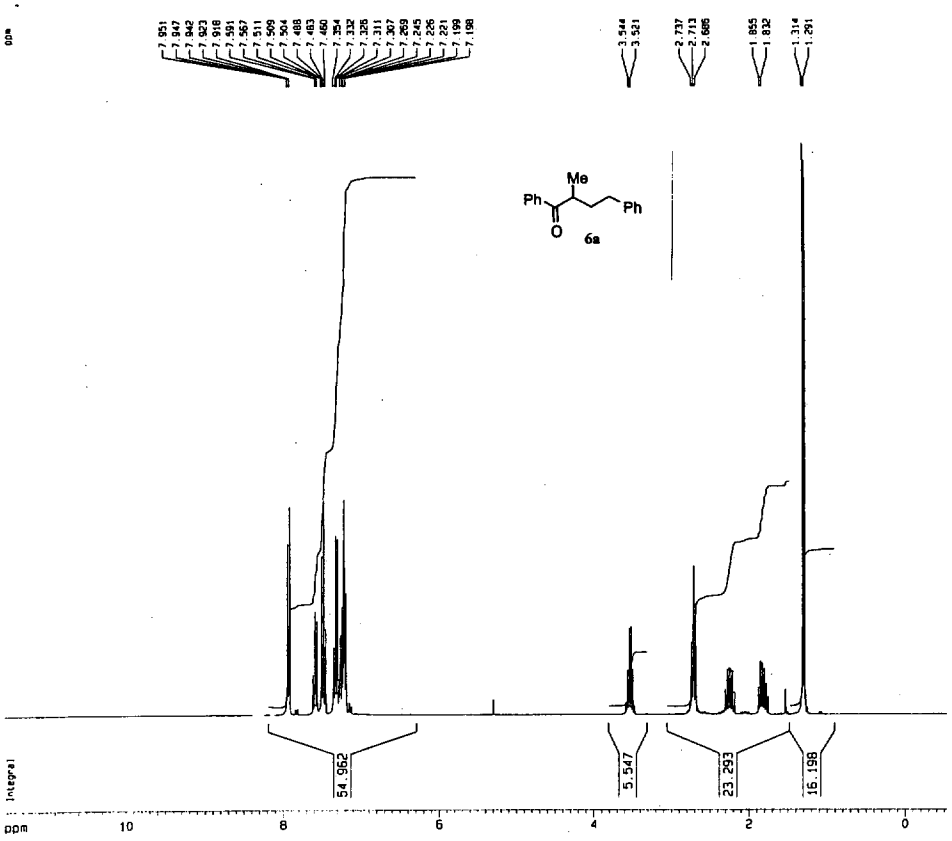

Arbeitskreis Knochel
User Rodriguez
Bruker ARX 300

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1D NMR plot parameters
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F2P -0.535 ppm
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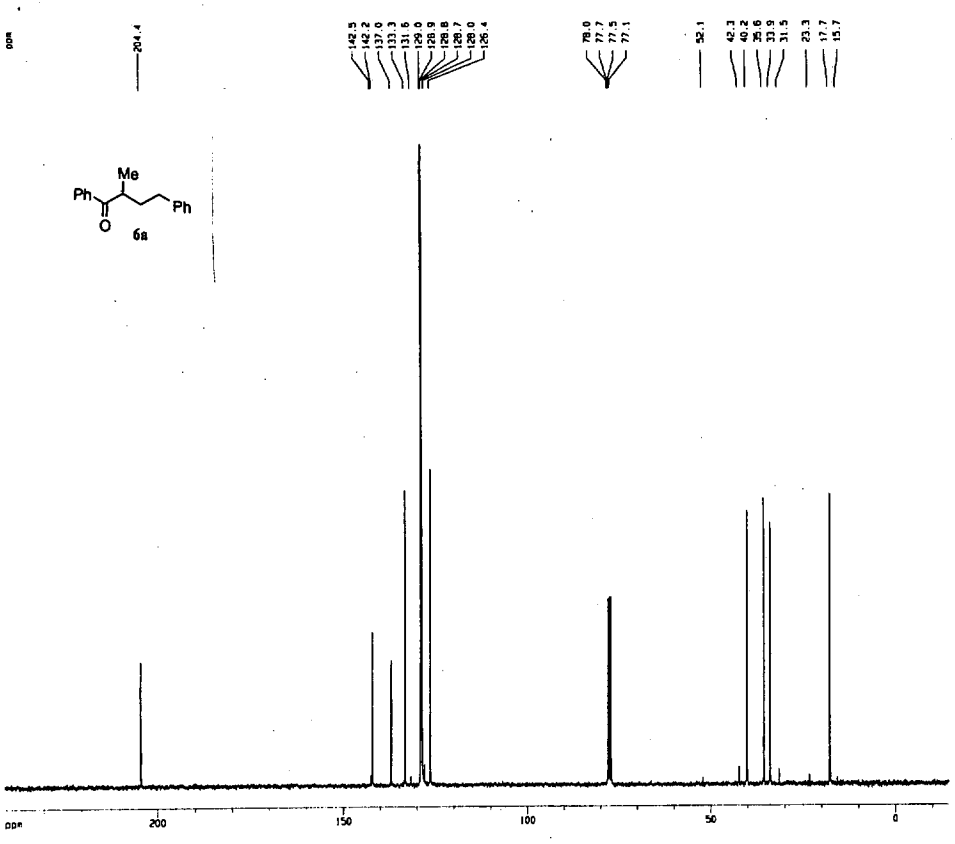

Arbeitskreis Knochel
User Rodriguez
Bruker ARX 300

Current Data Parameters
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PROCNO 1

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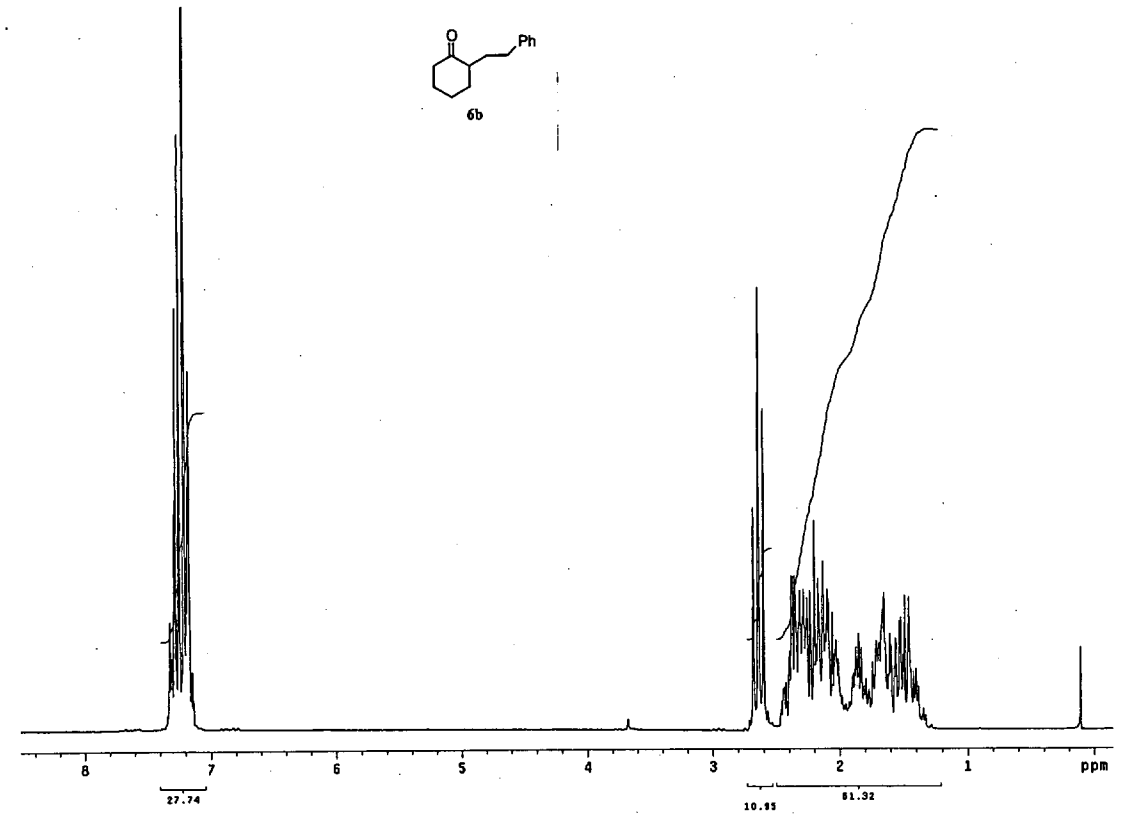
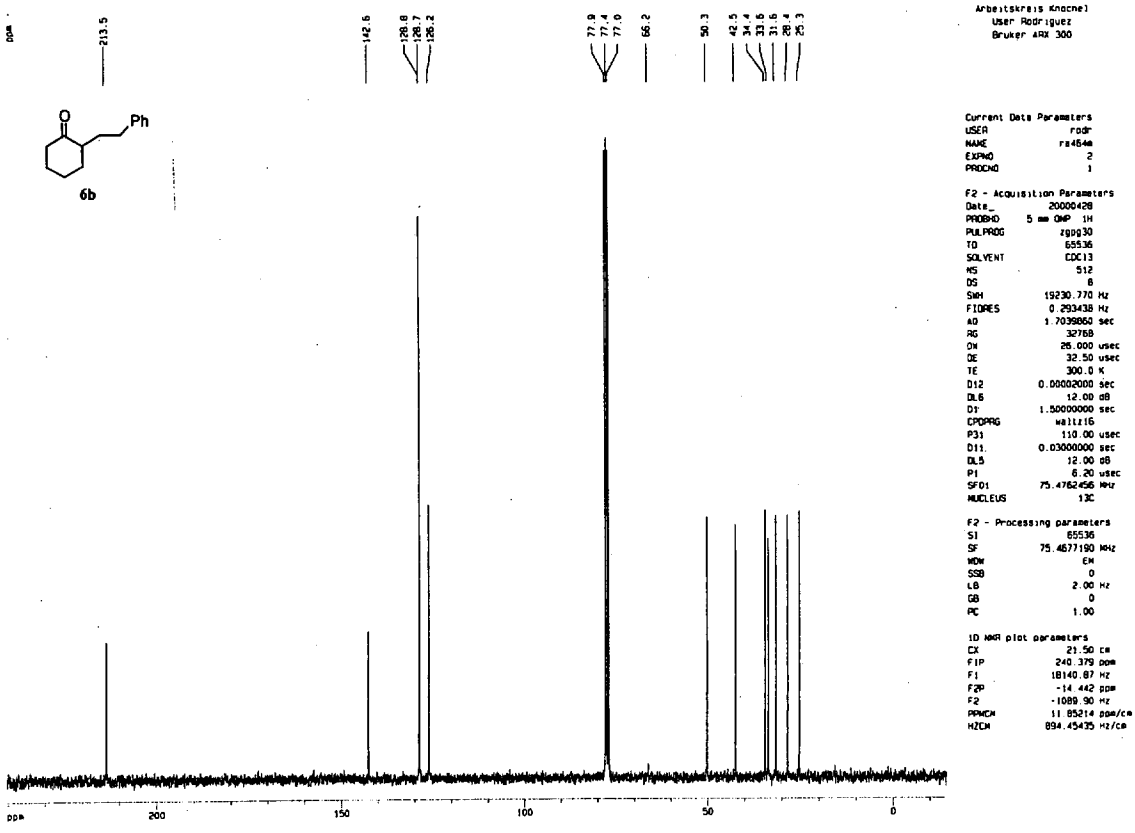
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 8
SWH 19230.770 Hz
FIDRES 0.293438 Hz
AQ 1.7039880 sec
RG 32768
DW 26.000 usec
DE 32.50 usec
TE 300.0 K
D12 0.00002000 sec
DL6 12.00 dB
D1 1.50000000 sec
CPDPRG waltz16
P31 110.00 usec
D11 0.03000000 sec
DL5 12.00 dB
P1 6.20 usec
SFO1 75.4762456 MHz
NUCLEUS 13C

F2 - Processing parameters
SI 65536
SF 75.4677190 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 21.50 cm
F1P 240.379 ppm
F1 18140.87 Hz
F2P -14.442 ppm
F2 -1089.90 Hz
PPMCM 11.85214 ppm/cm
HZCM 894.45435 Hz/cm





Arbeitskreis Knochel
User Rodriguez
Bruker ARX 300

Current Data Parameters

USER	rodr
NAME	rs464m
EXPNO	2
PROCNO	1

F2 - Acquisition Parameters

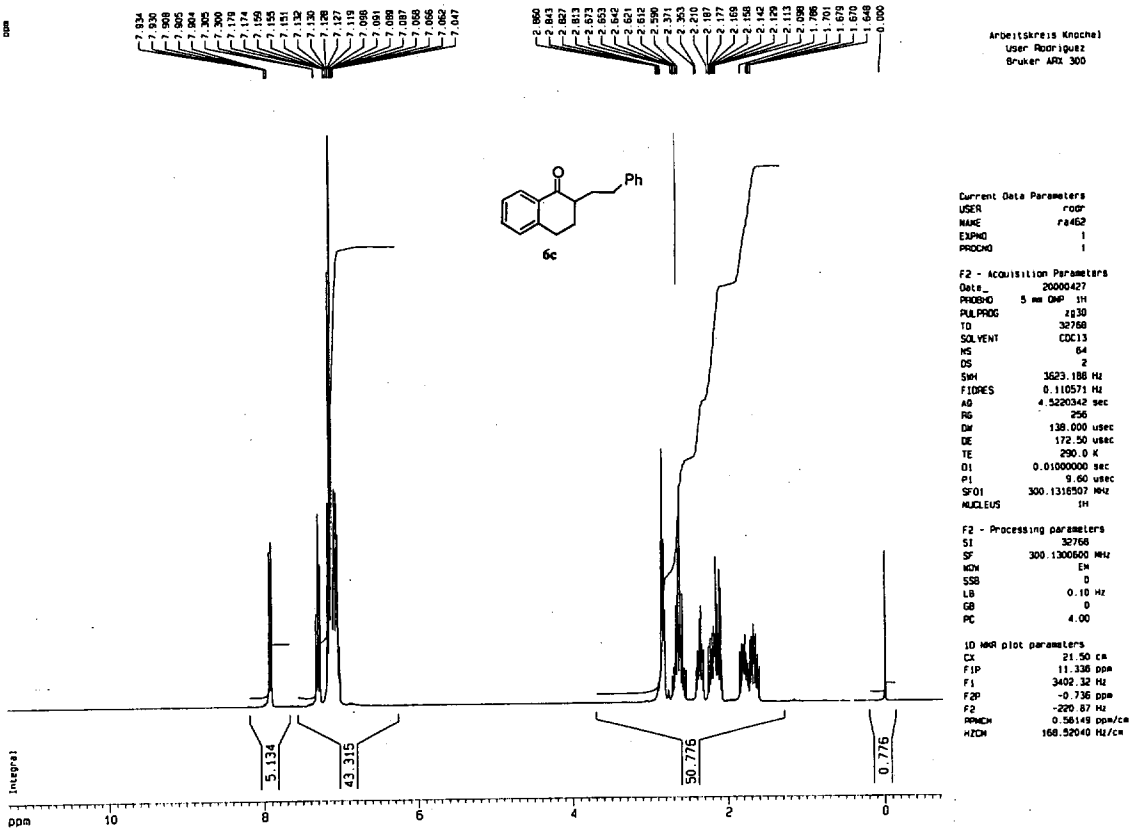
Date_	20000428
PROBHD	5 mm QNP 1H
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	512
DS	8
SWH	19230.770 Hz
FIDRES	0.293438 Hz
AQ	1.7039860 sec
RG	32768
DW	26.000 usec
DE	32.50 usec
TE	300.0 K
D12	0.00002000 sec
DL6	12.00 dB
D1	1.50000000 sec
CPDPRG	waltz16
P31	110.00 usec
D11	0.03000000 sec
DL5	12.00 dB
P1	6.20 usec
SFO1	75.4762456 MHz
NUCLEUS	13C

F2 - Processing parameters

SI	65536
SF	75.4677190 MHz
WDW	EM
SSB	0
LB	2.00 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	21.50 cm
F1P	240.379 ppm
F1	18140.87 Hz
F2P	-14.442 ppm
F2	-1089.90 Hz
PPMCM	11.85214 ppm/cm
HZCM	894.45435 Hz/cm


Arbeitskreis Knochel
User Rodriquez
Bruker ARX 300
Ph
6c
Current Data Parameters
USER rodr
NAME ra462
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20000427
PROBHD 5 mm DMP 1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 64
DS 2
SWH 3623.188 Hz
FIDRES 0.110571 Hz
AQ 4.5220342 sec
RG 256
DW 138.000 usec
DE 172.50 usec
TE 290.0 K
D1 0.01000000 sec
P1 9.60 usec
SFO1 300.1316507 MHz
NUCLEUS 1H
F2 - Processing parameters
SI 32768
SF 300.1300600 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 4.00
1D NMR plot parameters
CX 21.50 cm
F1P 11.336 ppm
F1 3402.32 Hz
F2P -0.736 ppm
F2 -220.87 Hz
PPMCM 0.56149 ppm/cm
HZCM 168.52040 Hz/cm
Integral
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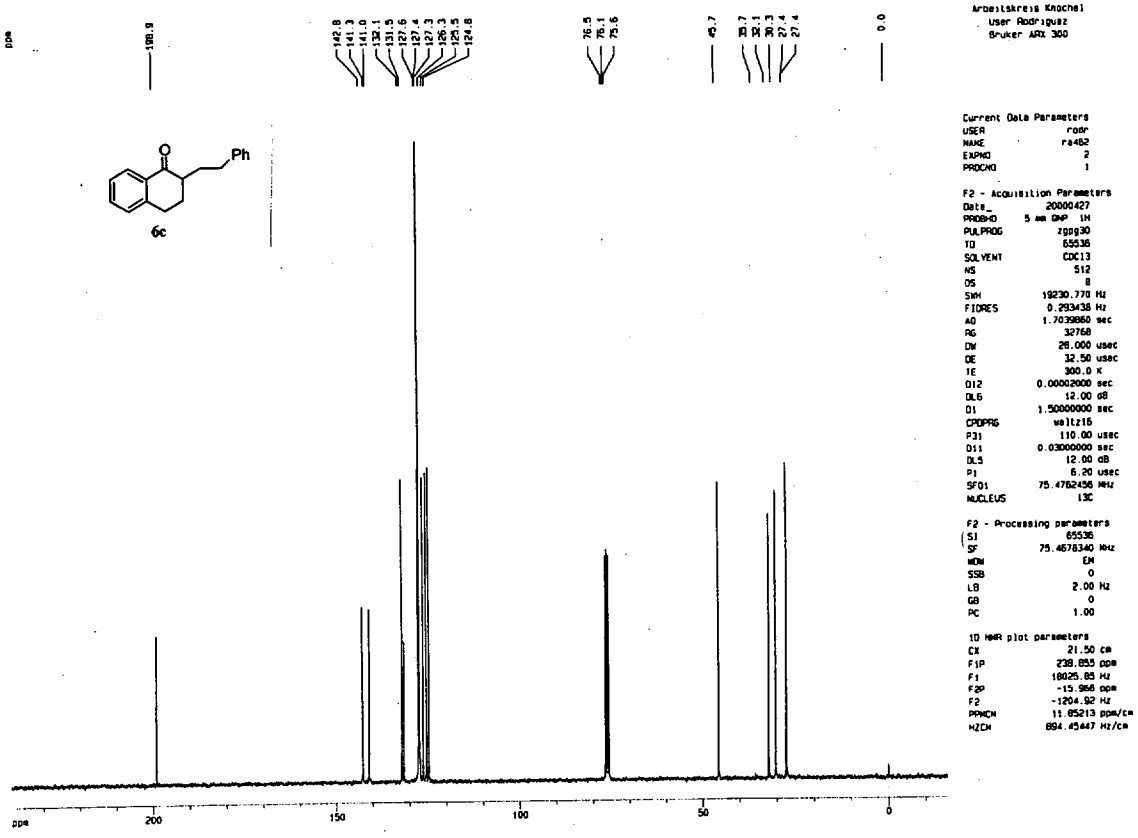
43.315
50.776
0.776
ppm


Arbeitskreis Knochel
User Rodriquez
Bruker ARX 300
Ph
6c
Current Data Parameters
USER rodr
NAME ra462
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20000427
PROBHD 5 mm DMP 1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 8
SWH 19230.770 Hz
FIDRES 0.293438 Hz
AQ 1.7039860 sec
RG 32768
DW 26.000 usec
DE 32.50 usec
TE 300.0 K
D12 0.00002000 sec
DL6 12.00 dB
D1 1.50000000 sec
CPDPRG waltz16
P31 110.00 usec
D11 0.03000000 sec
DL5 12.00 dB
P1 6.20 usec
SFO1 75.4762456 MHz
NUCLEUS 13C
F2 - Processing parameters
SI 65536
SF 75.4678340 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
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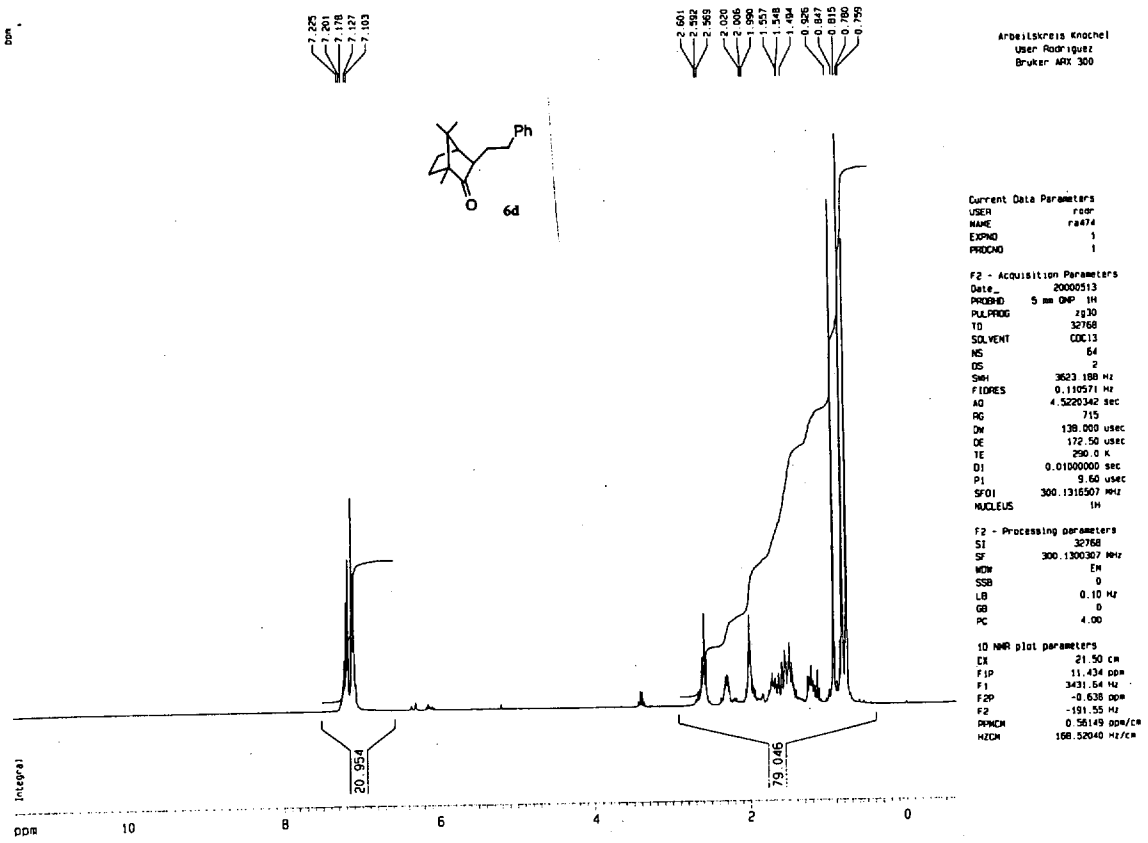
F1P 238.855 ppm
F1 18025.85 Hz
F2P -15.960 ppm
F2 -1204.92 Hz
PPMCM 11.85213 ppm/cm
HZCM 894.45447 Hz/cm
ppm


Arbeitskreis Knochel
User Rodriguez
Bruker ARX 300
Ph
O
6d
Current Data Parameters
USER rodr
NAME ra474
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20000513
PROBHD 5 mm QNP 1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 64
DS 2
SWH 3623.188 Hz
FIDRES 0.110571 Hz
AQ 4.5220342 sec
RG 715
DW 138.000 usec
DE 172.50 usec
TE 290.0 K
D1 0.01000000 sec
P1 9.60 usec
SFO1 300.1316507 MHz
NUCLEUS 1H
F2 - Processing parameters
SI 32768
SF 300.1300307 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 4.00
1D NMR plot parameters
CX 21.50 cm
F1P 11.434 ppm
F1 3431.64 Hz
F2P -0.638 ppm
F2 -191.55 Hz
PPMCM 0.56149 ppm/cm
HZCM 168.52040 Hz/cm
Integral
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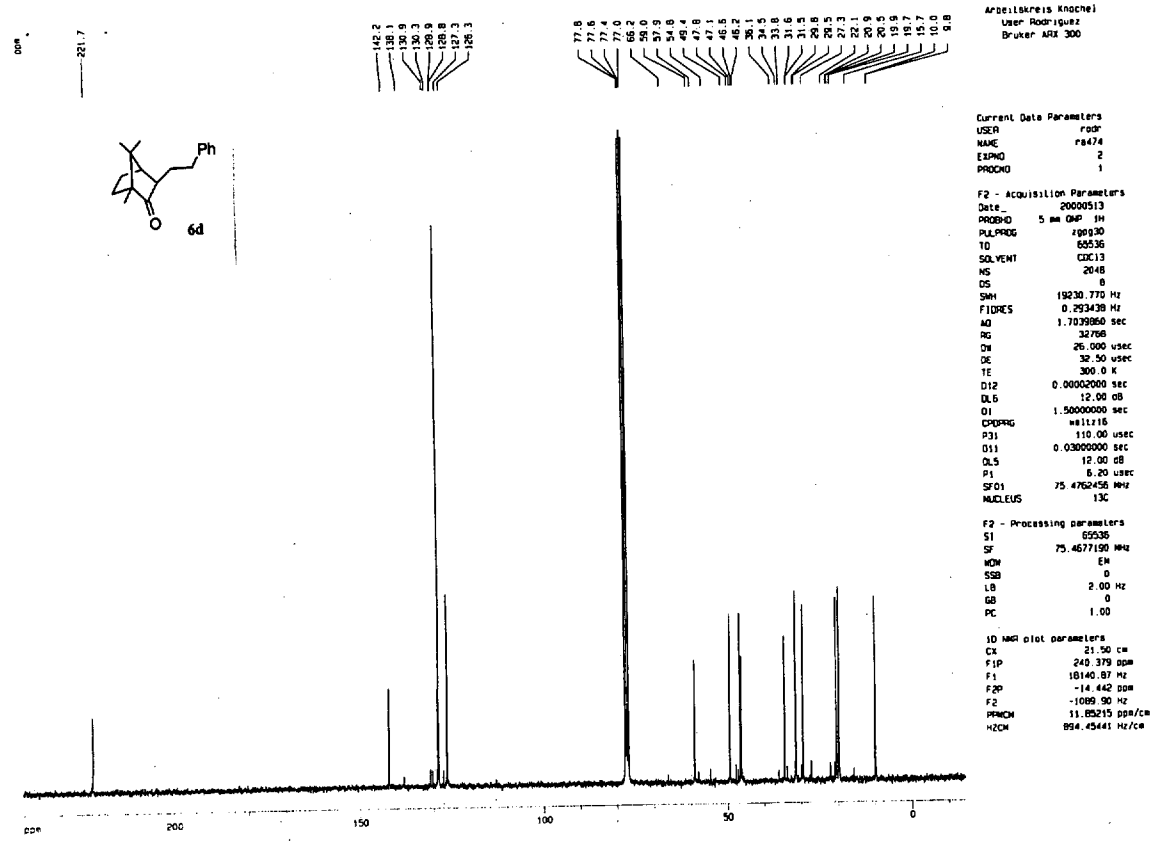
ppm


Arbeitskreis Knochel
User Rodriguez
Bruker ARX 300
Ph
O
6d
Current Data Parameters
USER rodr
NAME ra474
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20000513
PROBHD 5 mm QNP 1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 0
SWH 19230.770 Hz
FIDRES 0.293438 Hz
AQ 1.7039860 sec
RG 32768
DW 26.000 usec
DE 32.50 usec
TE 300.0 K
D12 0.00002000 sec
DL6 12.00 dB
D1 1.50000000 sec
CPDPRG waltz16
P31 110.00 usec
D11 0.03000000 sec
DL5 12.00 dB
P1 6.20 usec
SFO1 75.4762456 MHz
NUCLEUS 13C
F2 - Processing parameters
SI 65536
SF 75.4677190 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 21.50 cm
F1P 240.379 ppm
F1 18140.87 Hz
F2P -14.442 ppm
F2 -1089.90 Hz
PPMCM 11.85215 ppm/cm
HZCM 894.45441 Hz/cm
ppm