

Investigation of quinoline-4-carboxylic acid as a highly potent scaffold for the development of alkaline phosphatase inhibitors: Synthesis, SAR analysis and molecular modelling studies

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^d*Centre de Recherche du CHU de Québec – Université Laval, Québec, QC, Canada*

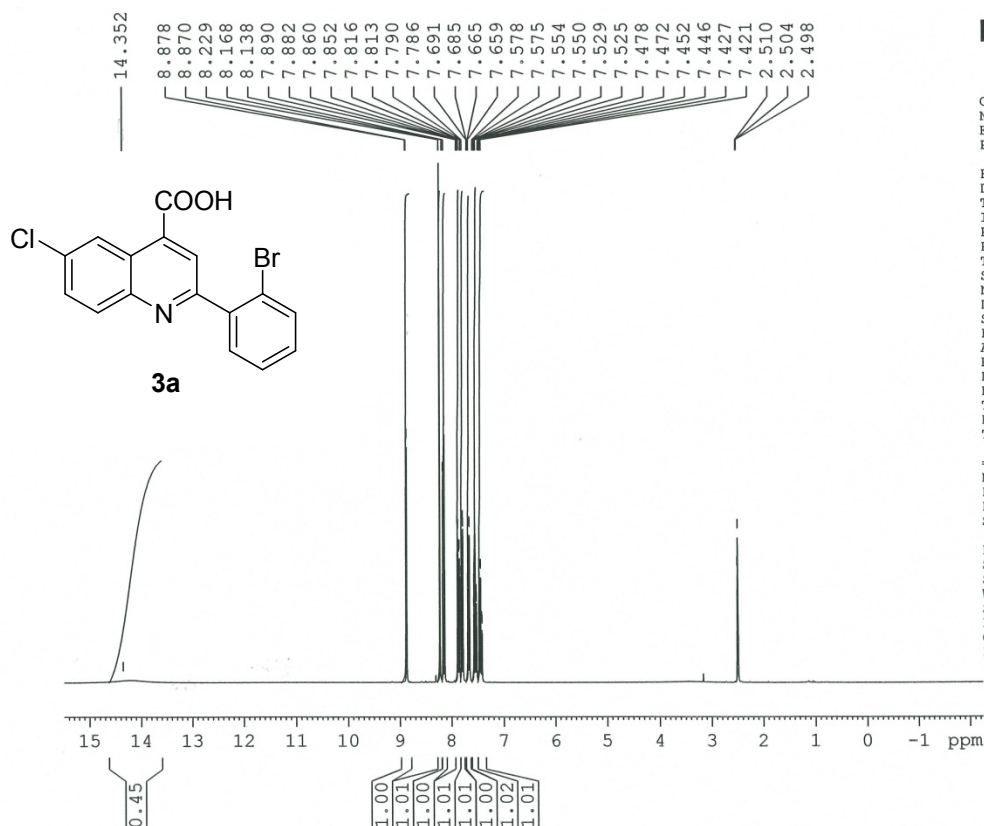
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Supporting Information

¹H and ¹³C NMR spectra of synthesized compounds



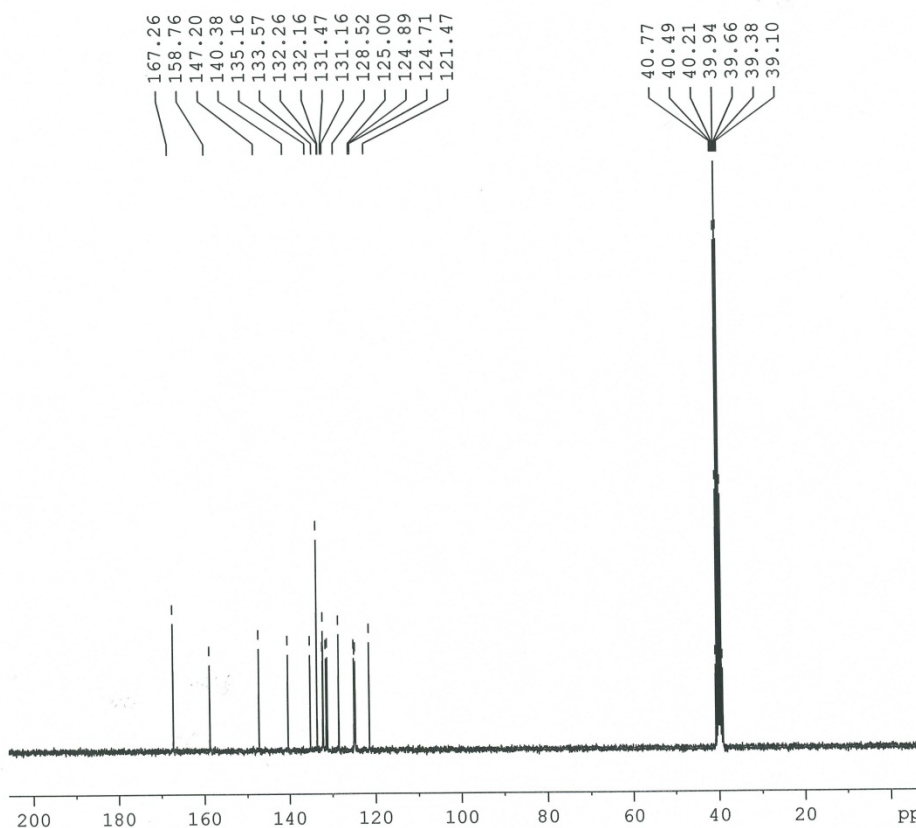
BRÜKER

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PROCNO 1

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SOLVENT DMSO
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FIDRES 0.094190 Hz
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D1 1.00000000 sec
TD0 1

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F2 - Processing parameters
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SF 300.1300000 MHz
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PC 1.00



BRÜKER

Current Data Parameters
NAME RXN-29_13CNMR DMSO
EXPNO 1
PROCNO 1

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Time 10.13
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SOLVENT DMSO
NS 437
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NUC1 13C
P1 6.00 usec
PL1 -5.00 dB
SFO1 75.4752953 MHz

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NUC2 1H
PCPD2 80.00 usec
PL2 2.00 dB
PL12 20.98 dB
PL13 20.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
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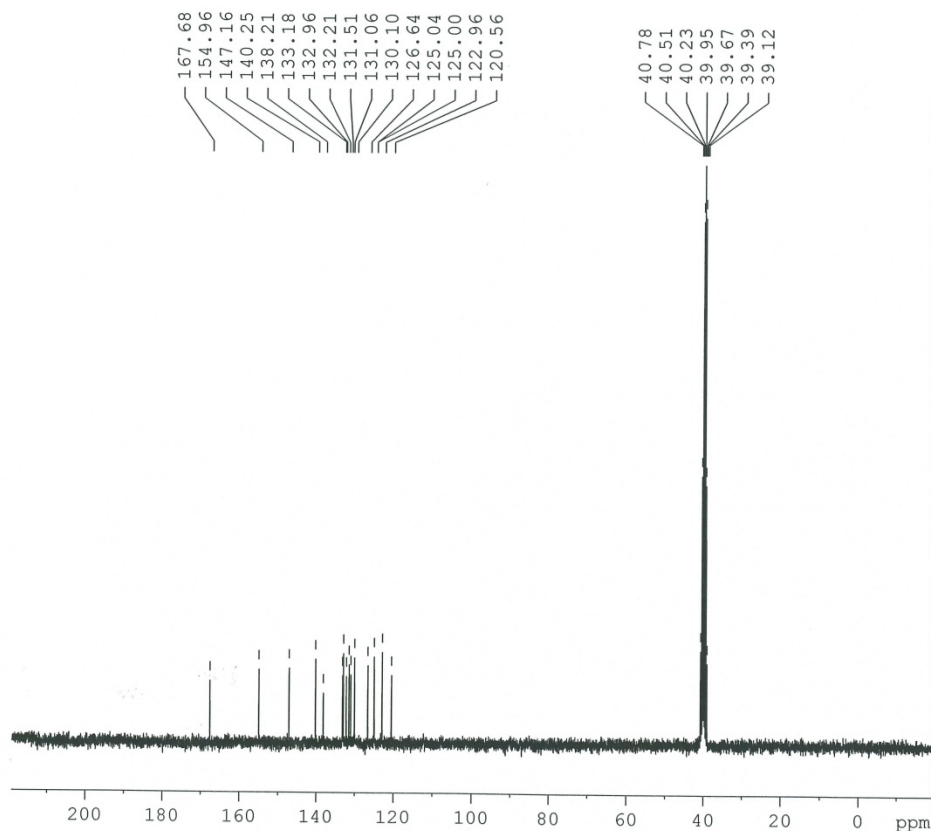
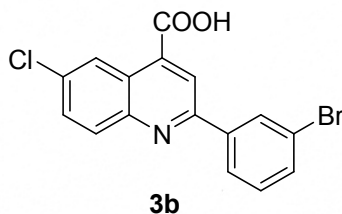
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NUC1                1H
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PL1                 2.00 dB
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F2 - Processing parameters
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Current Data Parameters
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EXPNO     1
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Time_      15.24
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TD          35968
SOLVENT    DMSO
NS          118
DS          0
SWH         17985.611 Hz
FIDRES     0.500045 Hz
AQ          0.99999604 sec
RG          1625.5
DE          27.800 umsec
TE          6.00 K
TW          294.3 K
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d11         0.03000000 sec
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TD0         1

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SFO1               75.4752953 MHz
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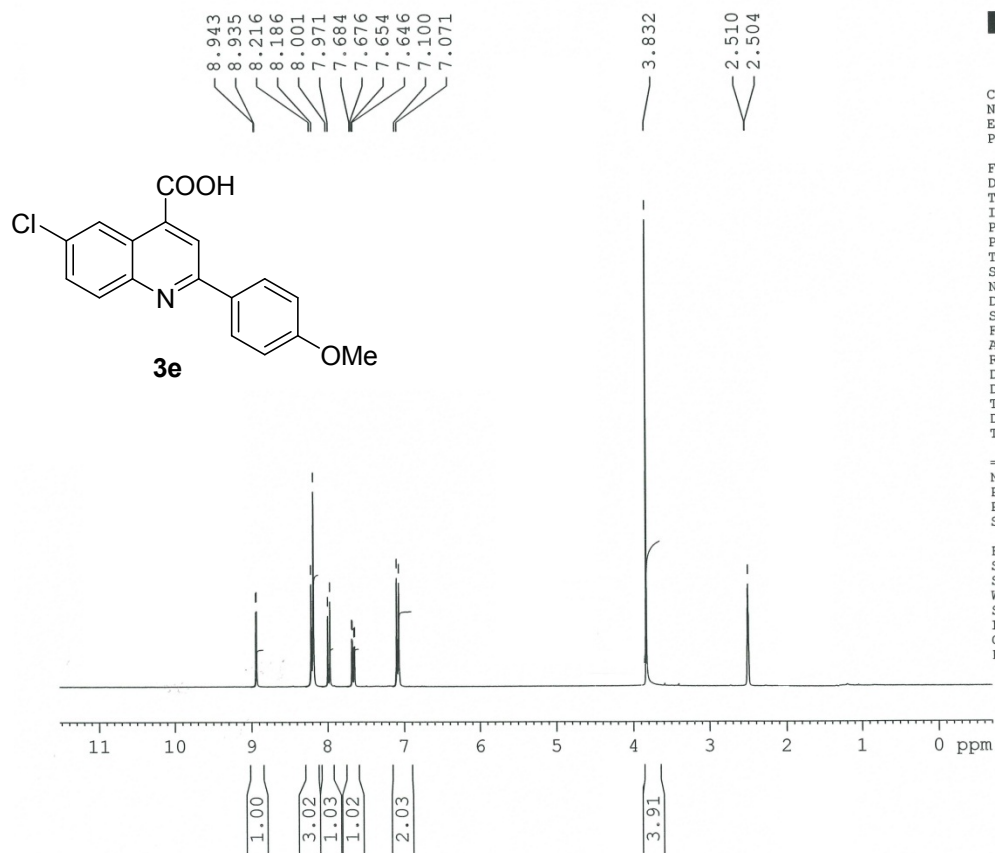
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PL13             20.00 dB
SFO2            300.1312005 MHz

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F2 - Processing parameters
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PC                      1.40

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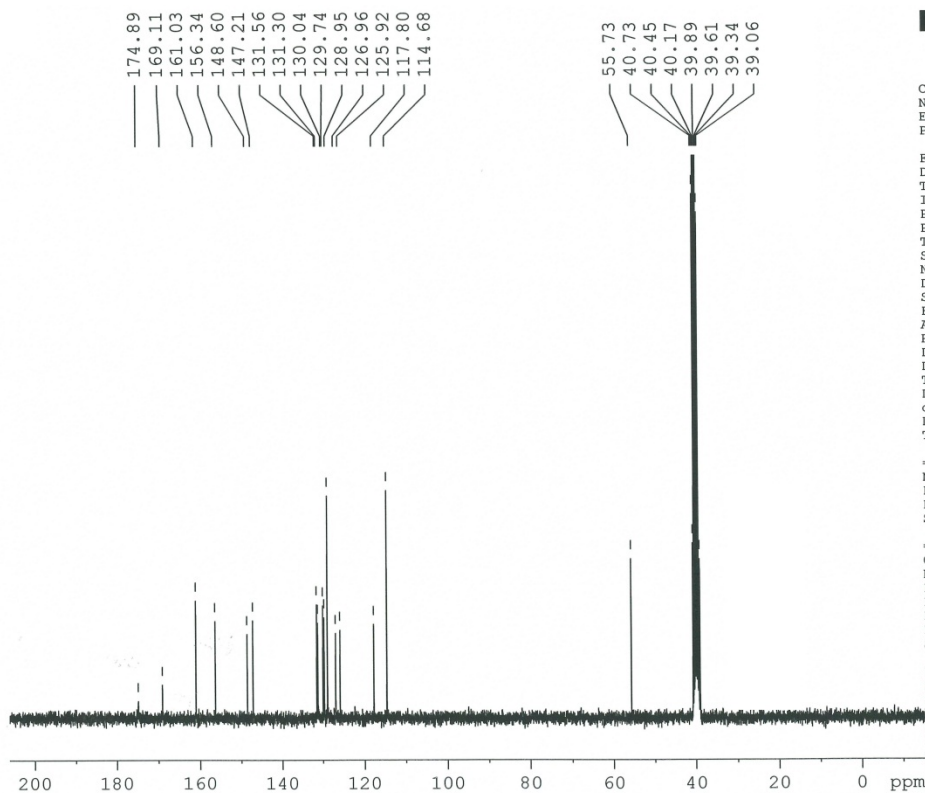
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PULPROG zg30
TD 65536
SOLVENT DMSO
NS 4
DS 0
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FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 143.7
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DE 6.00 usec
TE 294.3 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
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P1 9.00 usec
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SFO1 300.1318534 MHz

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PC 1.00



BRÜKER

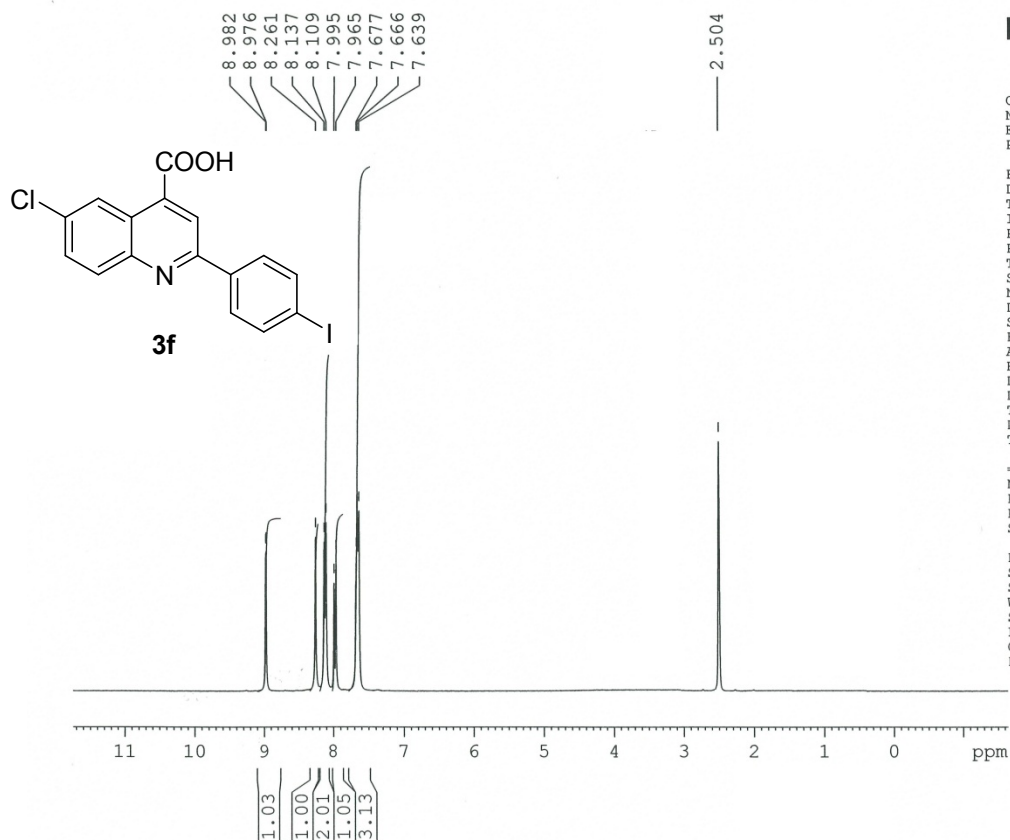
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PULPROG zgpg30
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SOLVENT DMSO
NS 455
DS 0
SWH 17985.611 Hz
FIDRES 0.500045 Hz
AQ 0.9999604 sec
RG 2580.3
DW 27.800 usec
DE 6.00 usec
TE 294.7 K
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DELTA 1.89999998 sec
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===== CHANNEL f1 =====
NUC1 13C
P1 6.00 usec
PL1 -5.00 dB
SFO1 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.00 dB
PL12 20.98 dB
PL13 20.00 dB
SFO2 300.1312005 MHz

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



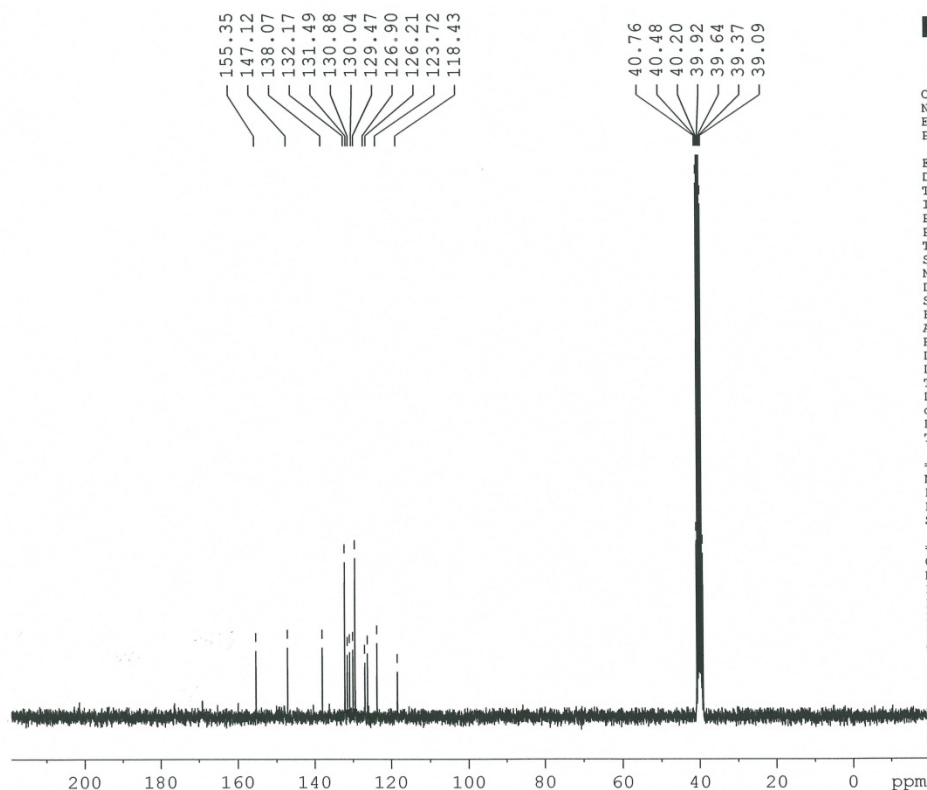
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Current Data Parameters
NAME RXN-31_1HNMR_DMSO
EXPNO 1
PROCNO 1

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Time_ 11.56
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PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
DS 0
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 181
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DE 6.00 usec
TE 293.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 9.00 usec
PL1 2.00 dB
SFO1 300.1318534 MHz

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SI 32768
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WDW EM
SSB 0
LB 0.30 Hz
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PC 1.00



BRUKER

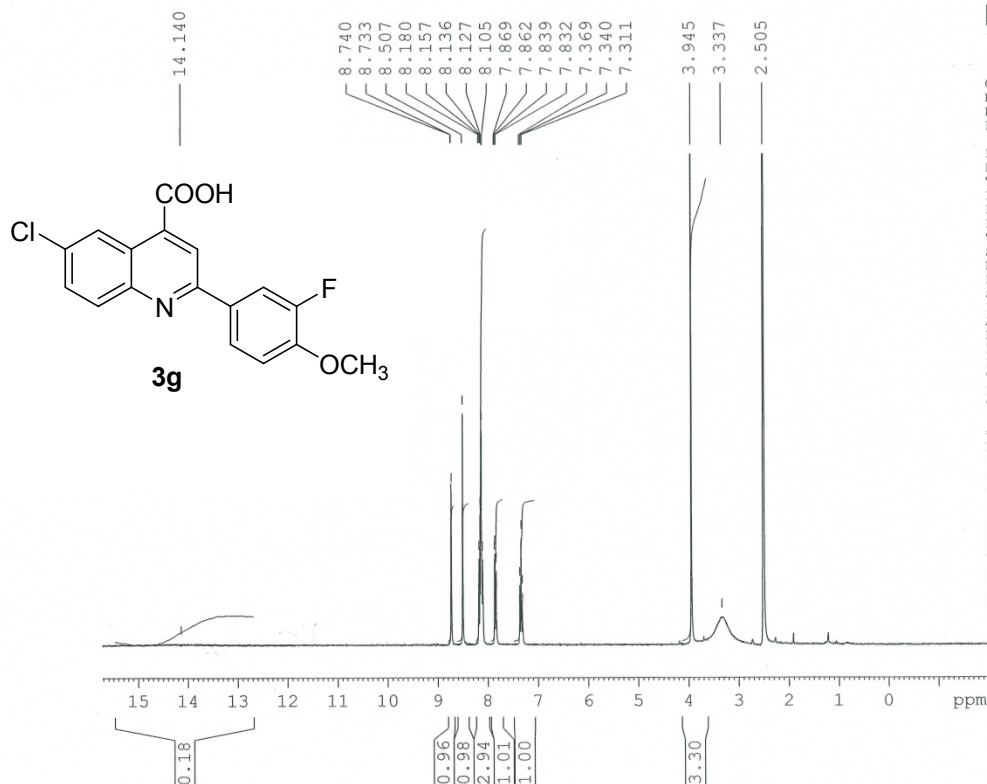
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EXPNO 1
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PULPROG zgpg30
TD 35968
SOLVENT DMSO
NS 409
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FIDRES 0.500045 Hz
AQ 0.9999604 sec
RG 3649.1
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DE 6.00 usec
TE 293.7 K
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DELTA 1.89999998 sec
TD0 1

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NUC1 13C
P1 6.00 usec
PL1 -5.00 dB
SFO1 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.00 dB
PL12 20.98 dB
PL13 20.00 dB
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F2 - Processing parameters
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WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



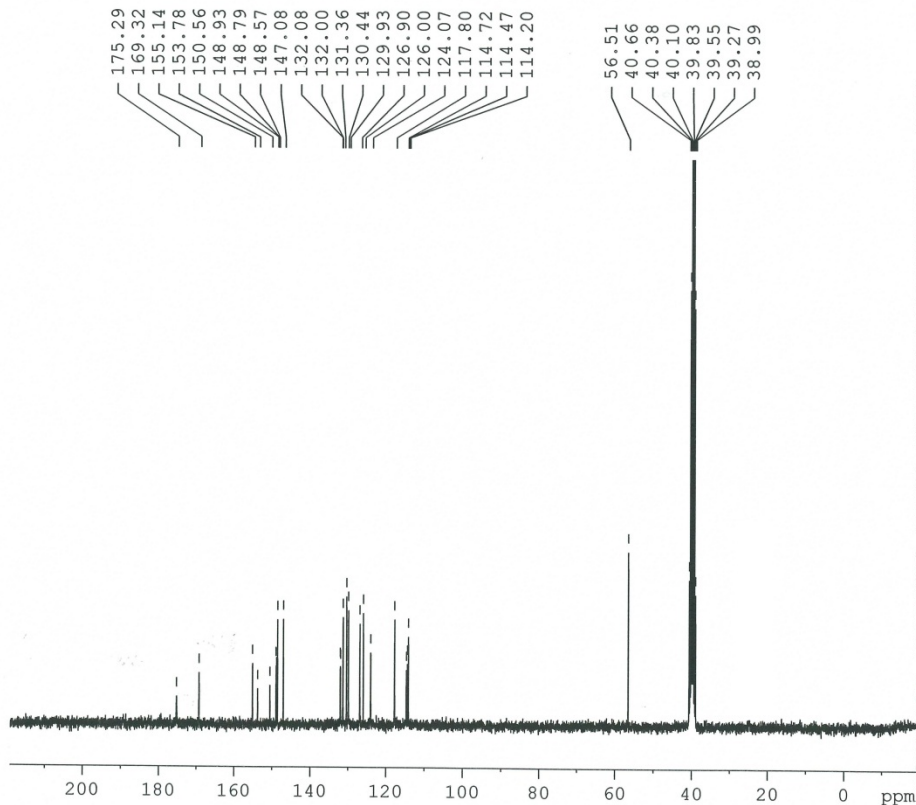
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EXPNO 1
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Time 17.56
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PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 0
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 812.7
DW 81.000 usec
DE 6.00 usec
TE 298.7 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 9.00 usec
PL1 2.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



BRUKER

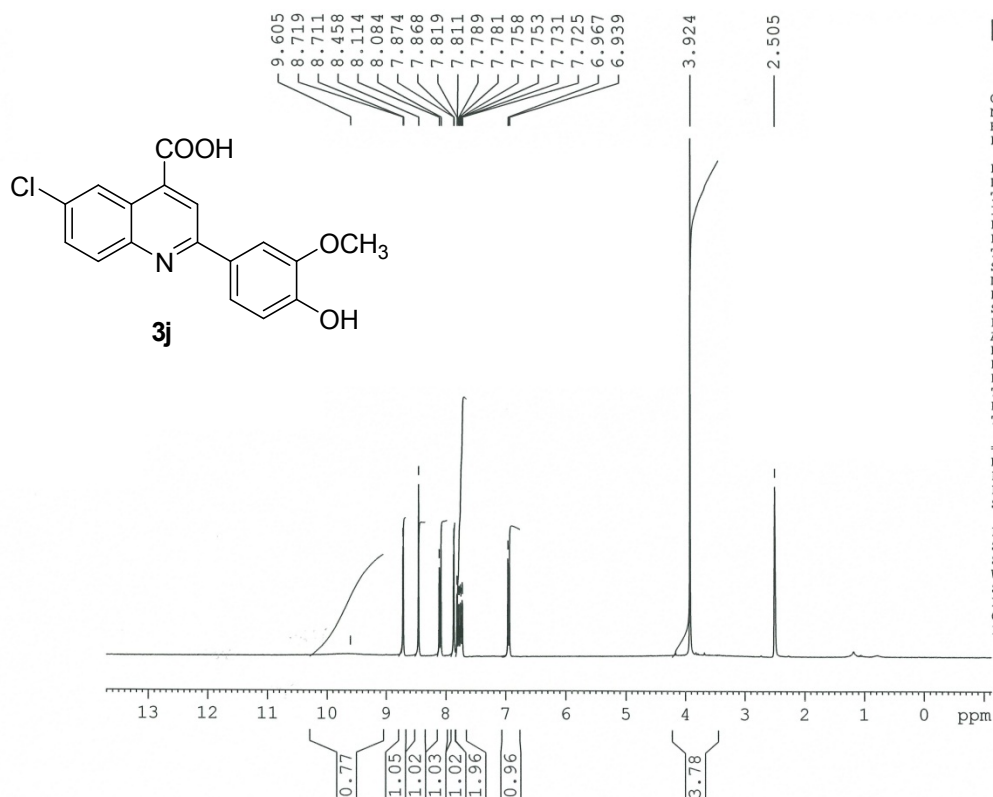
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EXPNO 1
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SOLVENT DMSO
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RG 1824.6
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DE 6.00 usec
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d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 6.00 usec
PL1 -5.00 dB
SFO1 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.00 dB
PL12 20.98 dB
PL13 20.00 dB
SFO2 300.1312005 MHz

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



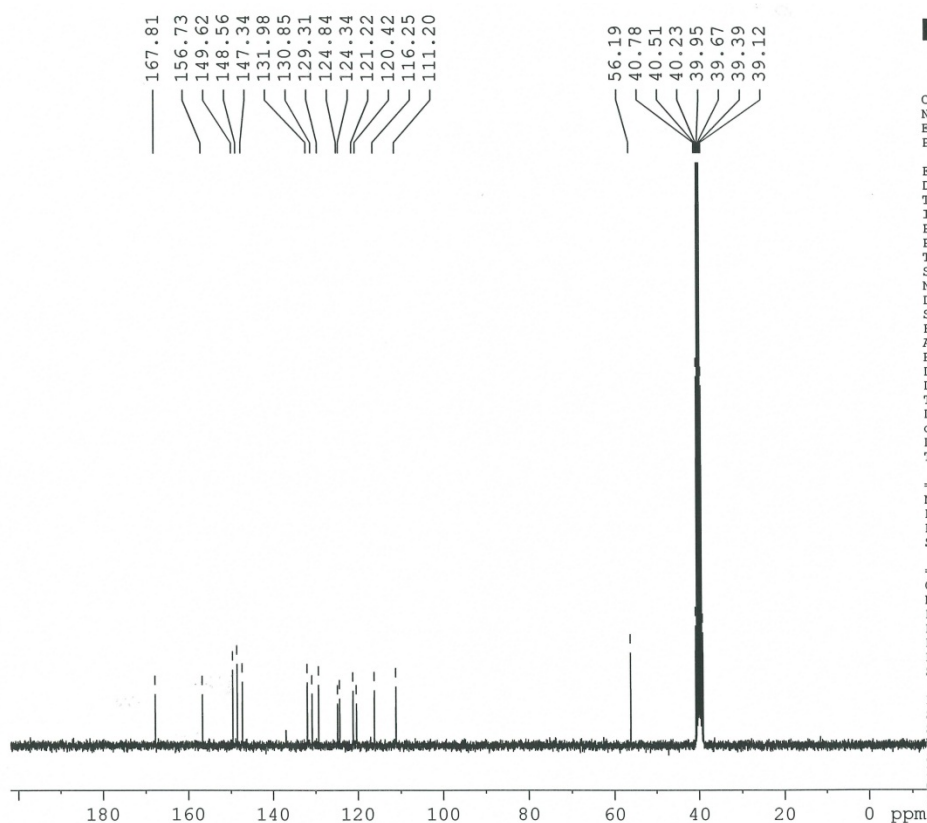
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Current Data Parameters
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EXPNO 1
PROCNO 1

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Time_ 17.36
INSTRUM spect
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PULPROG zg30
TD 65536
SOLVENT DMSO
NS 4
DS 0
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 256
DW 81.000 usec
DE 6.00 usec
TE 295.6 K
D1 1.00000000 sec
D10 1

===== CHANNEL f1 =====
NUC1 1H
P1 9.00 usec
PL1 2.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



BRÜKER

Current Data Parameters
NAME RXN-36_13CNMR_DMSO
EXPNO 1
PROCNO 1

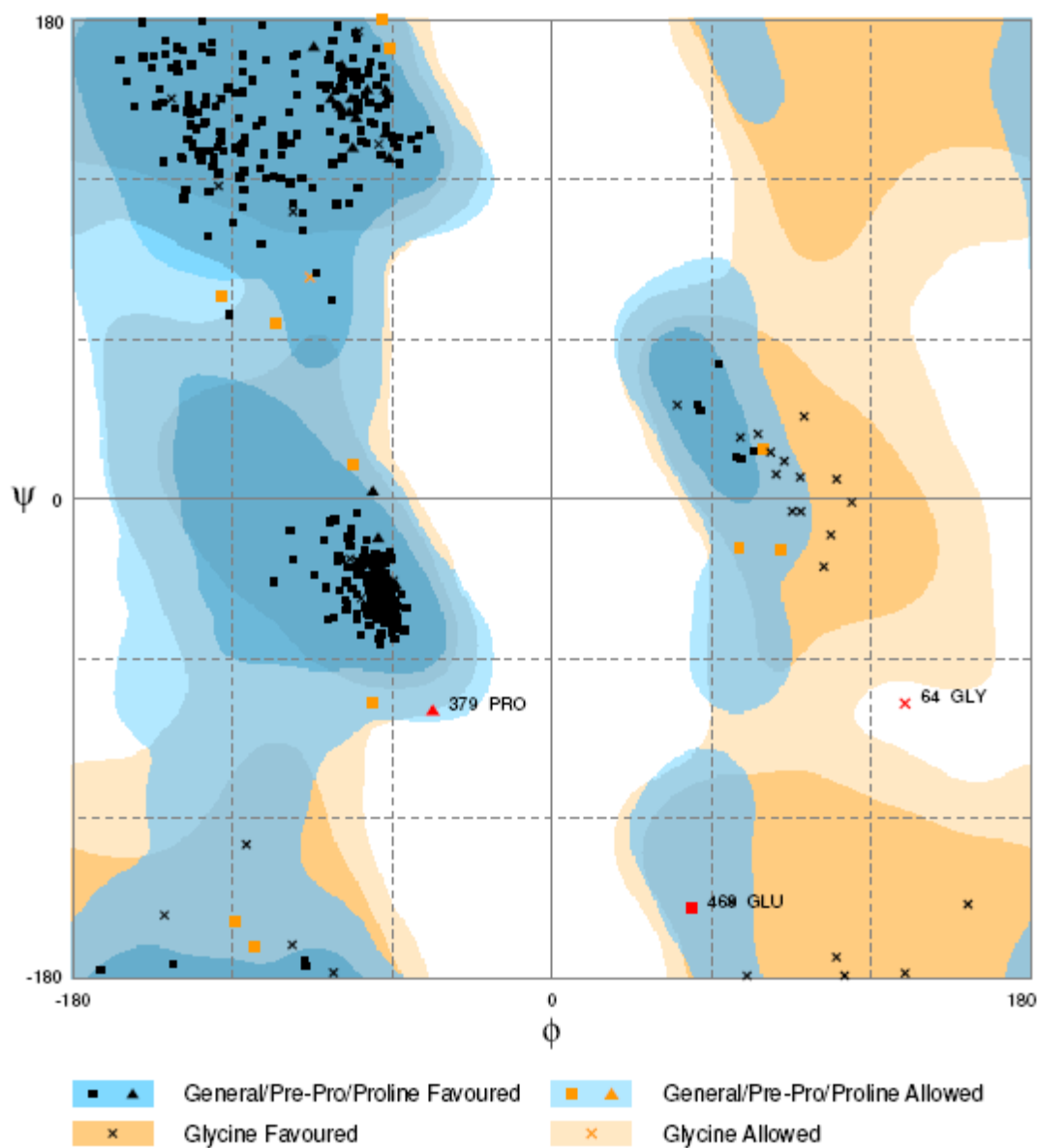
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RG 1290.2
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TE 296.1 K
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d11 0.03000000 sec
DELTA 1.89999999 sec
TD0 1

===== CHANNEL f1 =====
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P1 6.00 usec
PL1 -5.00 dB
SFO1 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.00 dB
PL12 20.98 dB
PL13 20.00 dB
SFO2 300.1312005 MHz

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

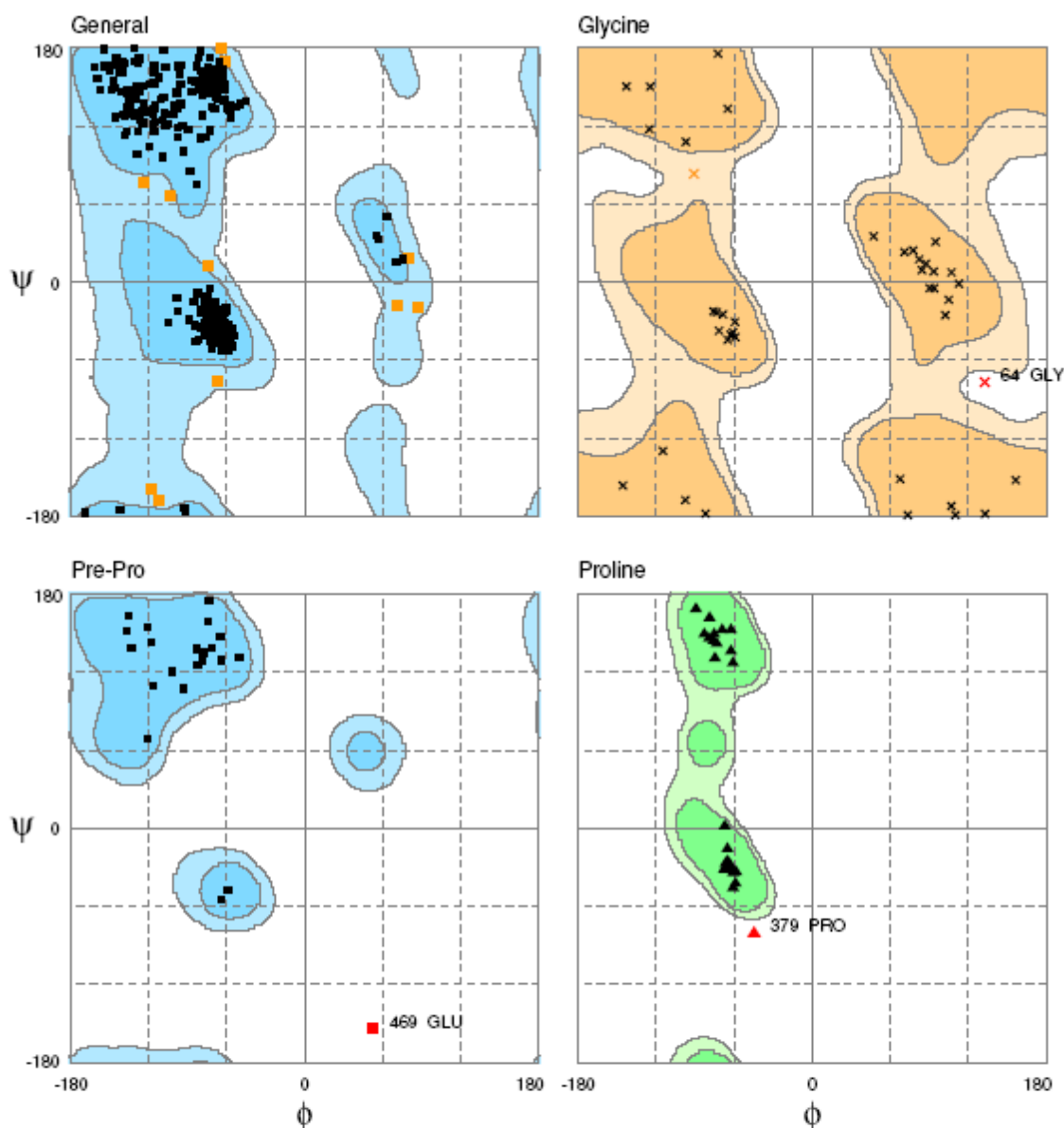
Ramachandran Plot for IAP model



Number of residues in favoured region (~98.0% expected) : 462 (96.9%)
 Number of residues in allowed region (~2.0% expected) : 12 (2.5%)
 Number of residues in outlier region : 3 (0.6%)

RAMPAGE by Paul de Bakker and Simon Lovell available at <http://www-cryst.bioc.cam.ac.uk/rampage/>

Please cite: S.C. Lovell, I.W. Davis, W.B. Aschall III, P.I.W. de Bakker, J.M. Word, M.G. Prisant, J.S. Richardson & D.C. Richardson (2002)
 Structure validation by Ca geometry: ψ/ϕ and C β deviation. *Proteins: Structure, Function & Genetics*. 50: 437-450



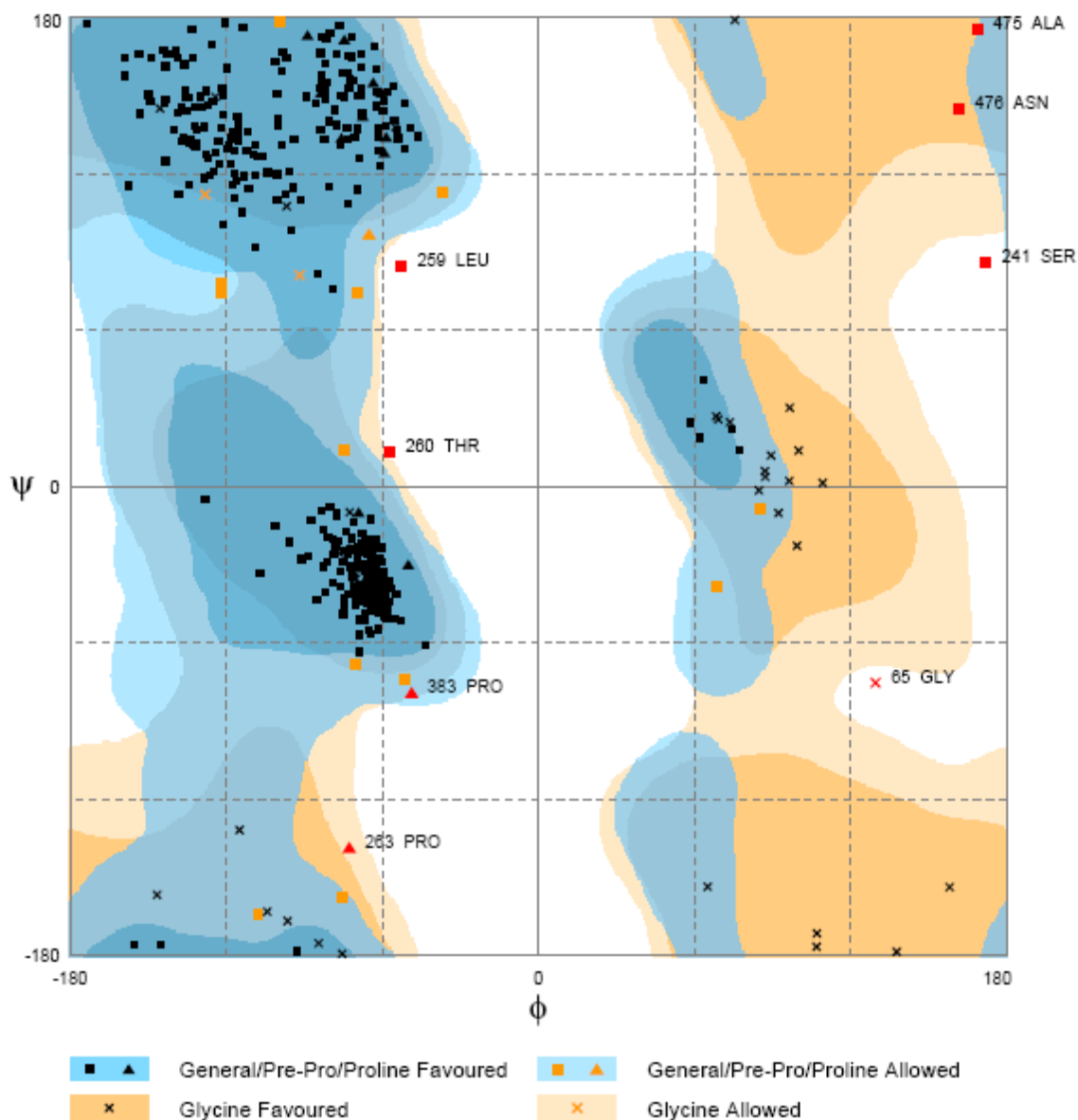
 General Favoured	 General Allowed
 Glycine Favoured	 Glycine Allowed
 Pre-Pro Favoured	 Pre-Pro Allowed
 Proline Favoured	 Proline Allowed

Number of residues in favoured region (~98.0% expected) : 462 (96.9%)
 Number of residues in allowed region (~2.0% expected) : 12 (2.5%)
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RAMPAGE by Paul de Bakker and Simon Lovell available at <http://www-cryst.bioc.cam.ac.uk/rampage/>

Please cite: S.C. Lovell, I.W. Davis, W.B. Arendall III, P.I.W. de Bakker, J.M. Word, M.G. Prisant, J.S. Richardson & D.C. Richardson (2002)
 Structure validation by Ca geometry: ψ and ϕ deviation. *Protein: Structure, Function & Genetics*, 50: 437-450

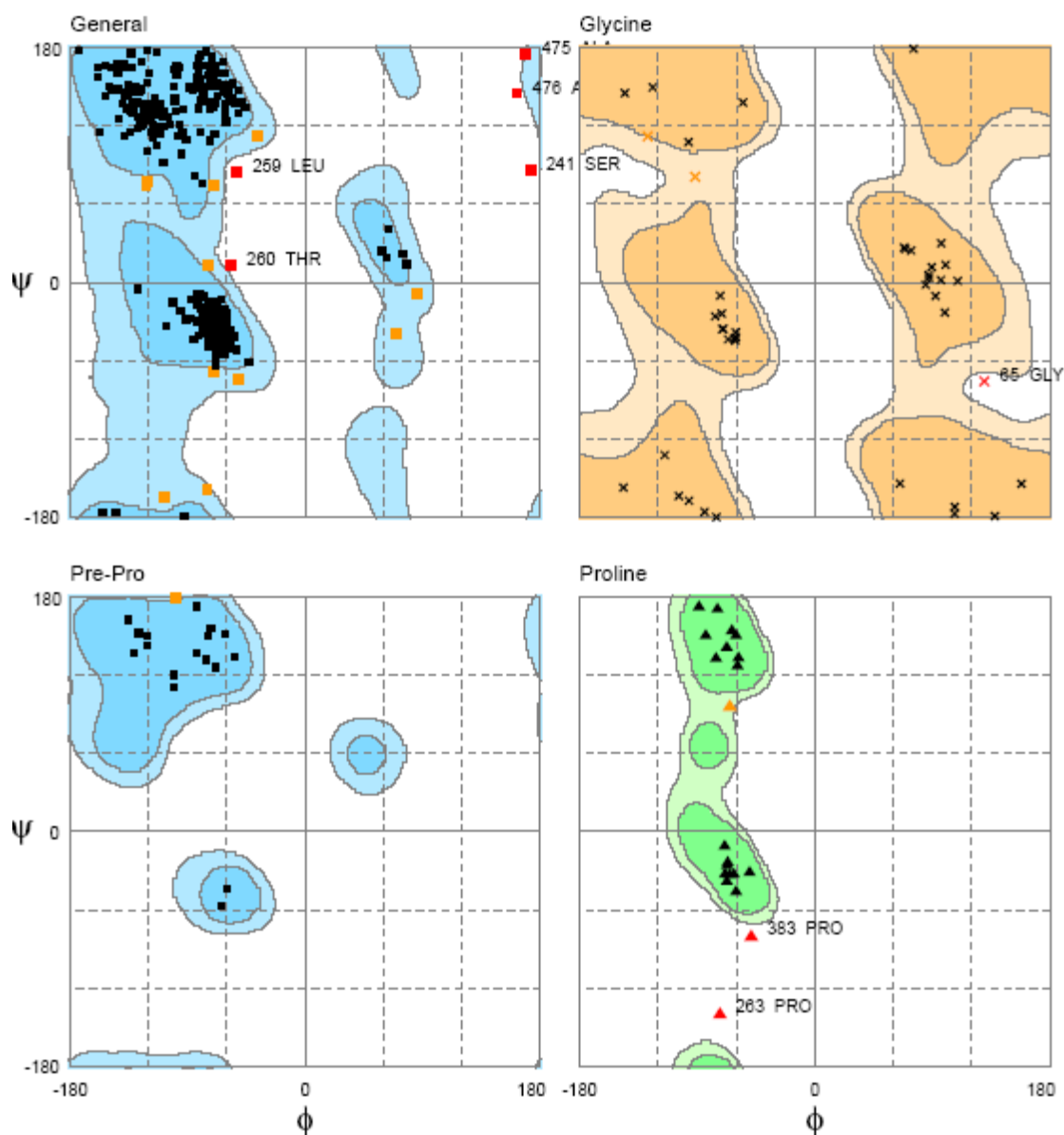
Ramachandran plot for TNAP model



Number of residues in favoured region (~98.0% expected) : 455 (95.2%)
 Number of residues in allowed region (~2.0% expected) : 15 (3.1%)
 Number of residues in outlier region : 8 (1.7%)

RAMPAGE by Paul de Bakker and Simon Lovell available at <http://www-cryst.bloc.cam.ac.uk/rampage/>

Please cite: S.C. Lovell, I.W. Davis, W.B. Arendall III, P.I.W. de Bakker, J.M. Word, M.G. Prisant, J.S. Richardson & D.C. Richardson (2002)
 Structure validation by Ca geometry: ϕ/ψ and C β deviation. *Proteins: Structure, Function & Genetics*. 60: 437-450



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RAMPAGE by Paul de Bakker and Simon Lovell available at <http://www-cryst.bloc.cam.ac.uk/rampage/>

Please cite: S.C. Lovell, I.W. Davis, W.B. Arendall III, P.I.W. de Bakker, J.M. Word, M.G. Prisant, J.S. Richardson & D.C. Richardson (2002) Structure validation by C α geometry: ϕ/ψ and C β deviation. *Proteins: Structure, Function & Genetics*. 60: 437-450