

Supplementary Information

Ferrocene modified analogues of imatinib and nilotinib as potent anti-cancer agents

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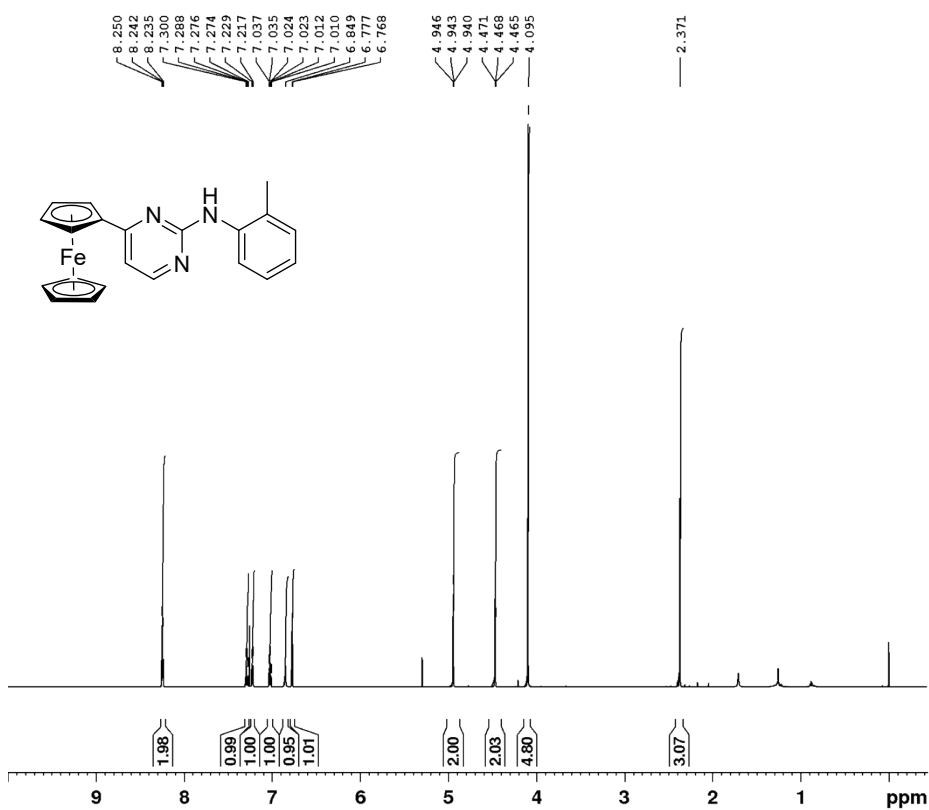
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Copies of ¹H and ¹³C NMR spectra of the target compounds.

¹H NMR monitoring of 15a stability in DMSO-*d*₆ (80%) / PBS in D₂O (20%)

Compound 3

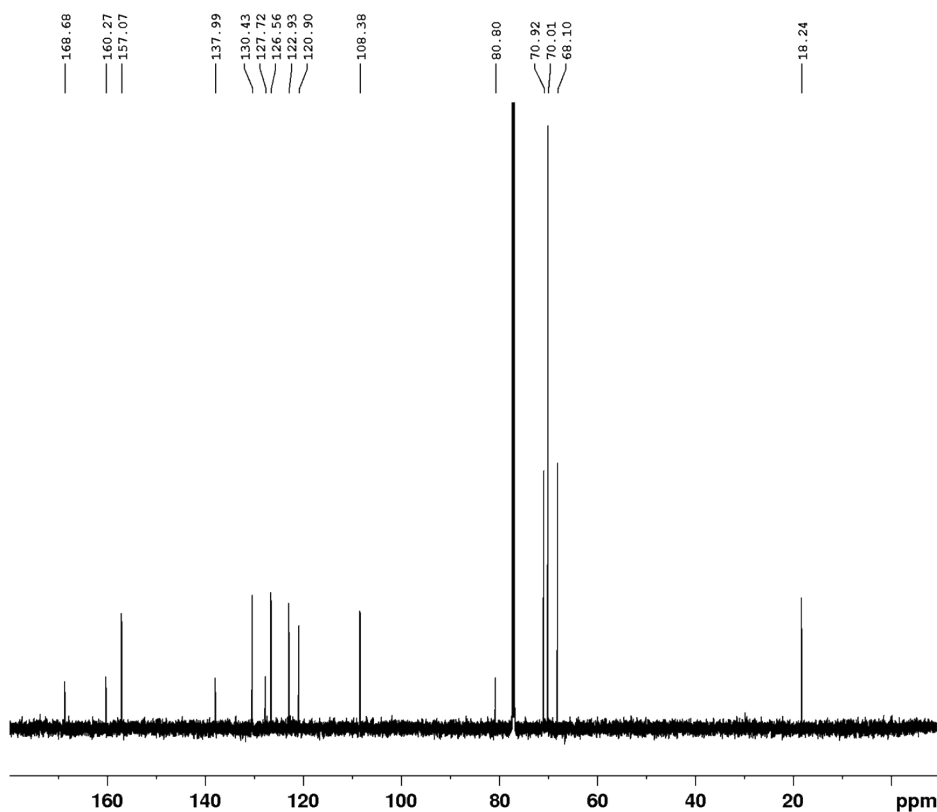


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Current Data Parameters
NAME          FL07603
EXPNO         11
PROCNO        1

F2 - Acquisition Parameters
Date_         20220318
Time          4.33 h
INSTRUM       spect
PROBHD        Z847801_0047 (
PULPROG       zg30
TD            65536
SOLVENT       CDCl3
NS            16
DS            0
SWH           9615.385 Hz
FIDRES        0.293438 Hz
AQ            3.4078720 sec
RG            203
DW            52.000 usec
DE            14.38 usec
TE            293.0 K
D1            2.00000000 sec
TD0           1
SF01          599.9845606 MHz
NUC1          1H
P0            3.60 usec
P1            10.80 usec
PLW1          20.00000000 W

F2 - Processing parameters
SI            65536
SF            599.9800169 MHz
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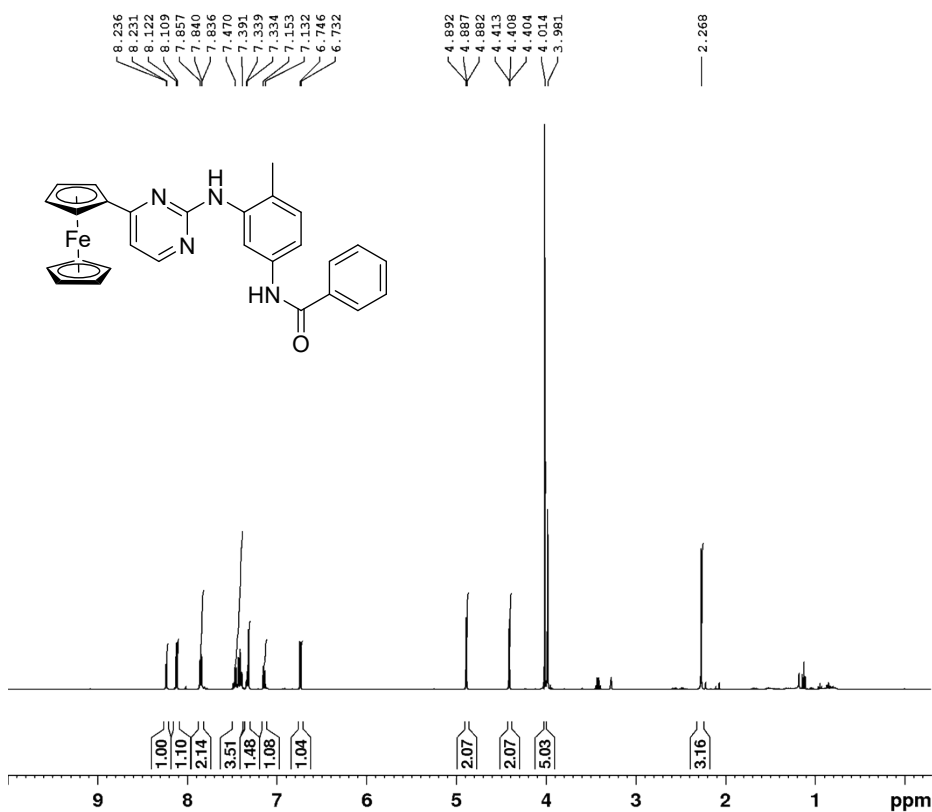
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Current Data Parameters
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EXPNO         12
PROCNO        1

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Time          4.38 h
INSTRUM       spect
PROBHD        Z847801_0047 (
PULPROG       zgdc30
TD            32768
SOLVENT       CDCl3
NS            128
DS            0
SWH           36057.691 Hz
FIDRES        2.200787 Hz
AQ            0.4543829 sec
RG            2050
DW            13.867 usec
DE            6.50 usec
TE            293.1 K
D1            1.50000000 sec
D11           0.03000000 sec
TD0           1
SF01          150.8816889 MHz
NUC1          13C
P0            3.27 usec
P1            9.80 usec
PLW1          40.00000000 W
SF02          599.9824003 MHz
NUC2          1H
CPDPRG[2]     waltz16
PCPD2         70.00 usec
PLW2          20.00000000 W
PLW12         0.53044999 W

F2 - Processing parameters
SI            65536
SF            150.8650910 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
    
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Compound 9



Current Data Parameters

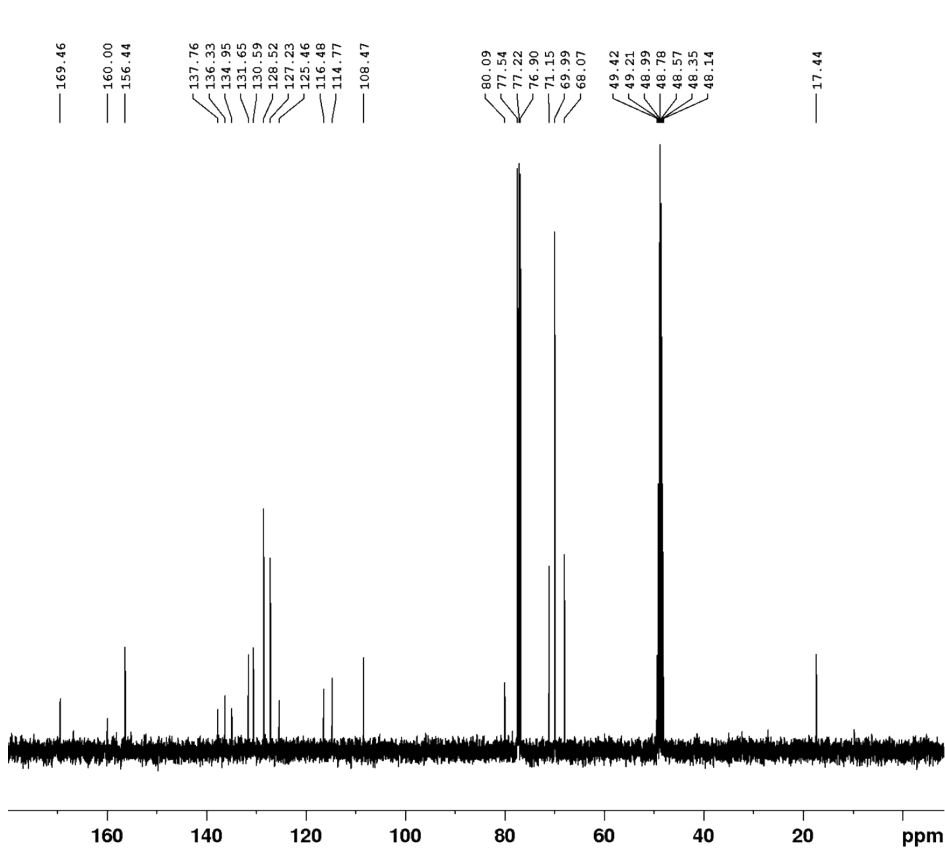
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 EXPNO 17
 PROCNO 1

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 PULPROG zg30
 TD 65536
 SOLVENT MeOD
 NS 32
 DS 0
 SWH 6578.947 Hz
 FIDRES 0.200774 Hz
 AQ 4.9807358 sec
 RG 101
 DW 76.000 usec
 DE 7.79 usec
 TE 298.0 K
 D1 2.00000000 sec
 TD0 1
 SFO1 400.1330415 MHz
 NUC1 1H
 P0 3.33 usec
 P1 10.00 usec
 PLW1 20.07200050 W

F2 - Processing parameters

SI 65536
 SF 400.1300230 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00



Current Data Parameters

NAME FL09402
 EXPNO 18
 PROCNO 1

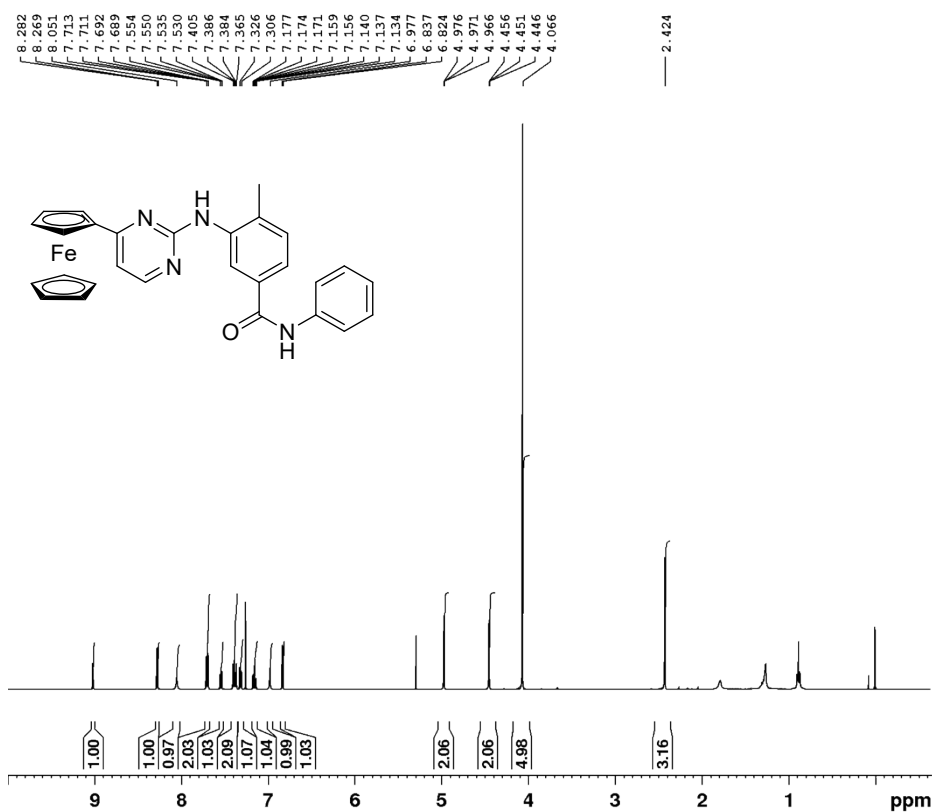
F2 - Acquisition Parameters

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 Time 14.06 h
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 PULPROG zgdc30
 TD 32768
 SOLVENT MeOD
 NS 128
 DS 0
 SWH 23809.523 Hz
 FIDRES 1.453218 Hz
 AQ 0.6881280 sec
 RG 32
 DW 21.000 usec
 DE 6.50 usec
 TE 298.0 K
 D1 1.50000000 sec
 D11 0.03000000 sec
 TD0 1
 SFO1 100.6238383 MHz
 NUC1 13C
 P0 3.33 usec
 P1 10.00 usec
 PLW1 58.46900177 W
 SFO2 400.1316008 MHz
 NUC2 1H
 CPDPRG2 waltz16
 FCPD2 90.00 usec
 PLW2 20.07200050 W
 PLW12 0.24781001 W

F2 - Processing parameters

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 SSB 0
 LB 1.00 Hz
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 PC 1.40

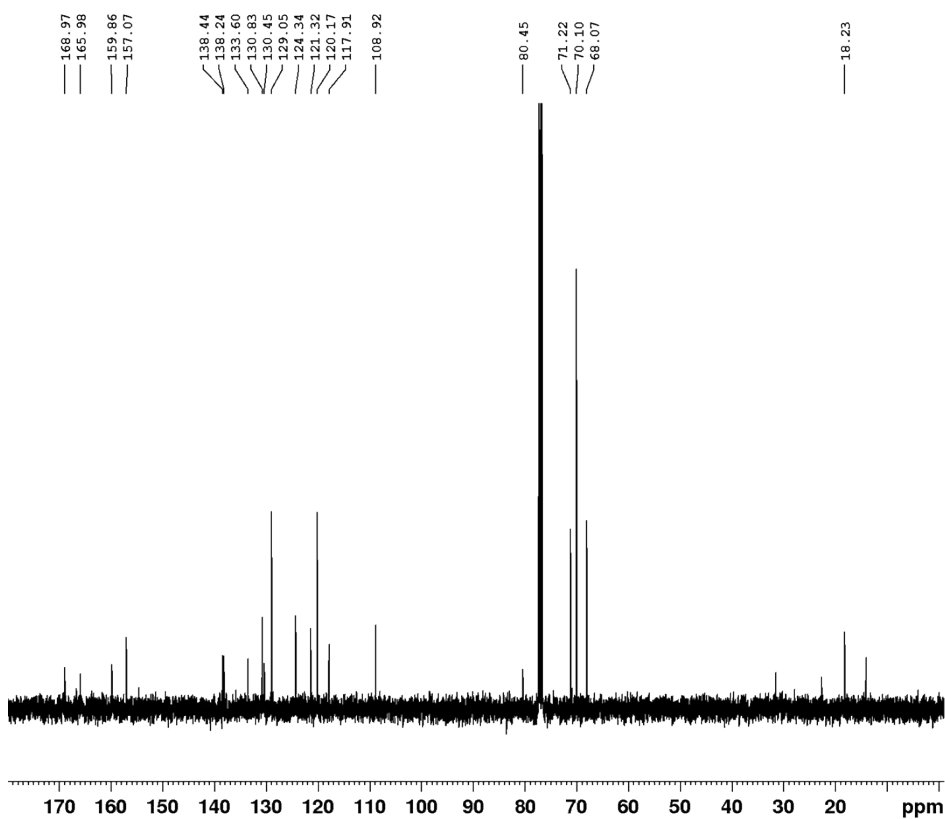
Compound 15a



Current Data Parameters
 NAME FL08402
 EXPNO 11
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20220411
 Time 17.57 h
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 PROBHD z175272.0007 ()
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 32
 DS 0
 SWH 6578.947 Hz
 FIDRES 0.401547 Hz
 AQ 2.4903679 sec
 RG 101
 DW 76.000 usec
 DE 7.79 usec
 TE 298.0 K
 D1 2.00000000 sec
 TD0 1
 SFO1 400.1330415 MHz
 NUC1 1H
 P0 3.33 usec
 P1 10.00 usec
 PLW1 20.07200050 W

F2 - Processing parameters
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 SF 400.1300102 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00

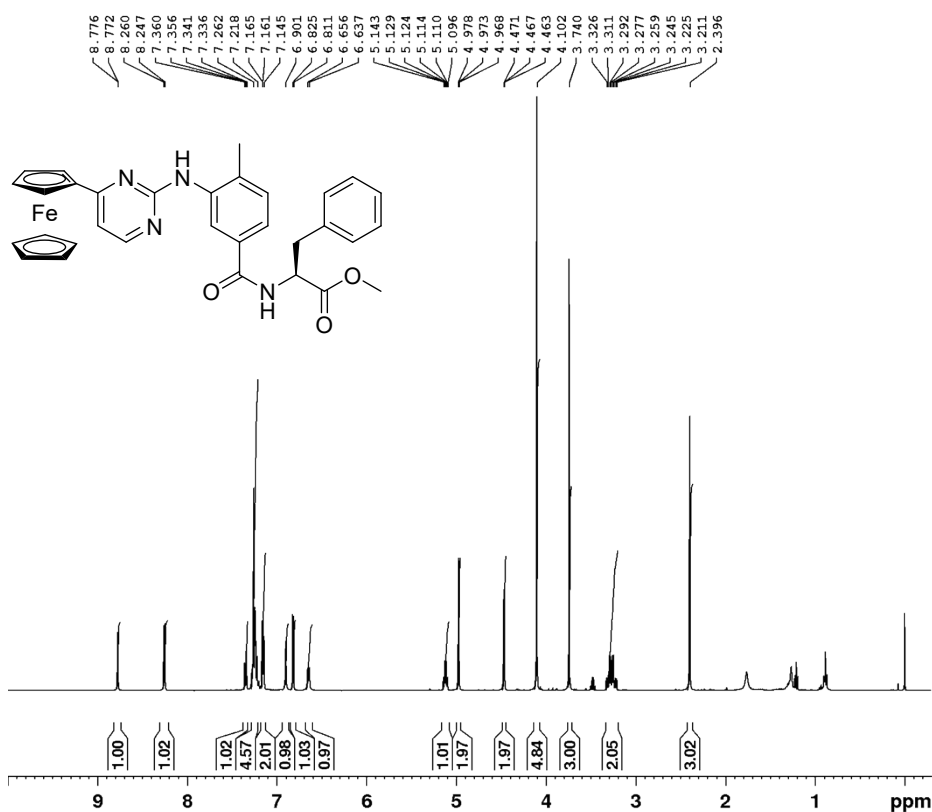


Current Data Parameters
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 EXPNO 12
 PROCNO 1

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 PULPROG zgdc30
 TD 32768
 SOLVENT CDCl3
 NS 128
 DS 0
 SWH 23809.523 Hz
 FIDRES 1.453218 Hz
 AQ 0.6881280 sec
 RG 22.6
 DW 21.000 usec
 DE 6.50 usec
 TE 298.0 K
 D1 1.50000000 sec
 D11 0.03000000 sec
 TD0 1
 SFO1 100.6238383 MHz
 NUC1 13C
 P0 3.33 usec
 P1 10.00 usec
 PLW1 58.46900177 W
 SFO2 400.1316008 MHz
 NUC2 1H
 CPDPRG2 waltz16
 FCPD2 90.00 usec
 PLW2 20.07200050 W
 PLW12 0.24781001 W

F2 - Processing parameters
 SI 65536
 SF 100.6127690 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

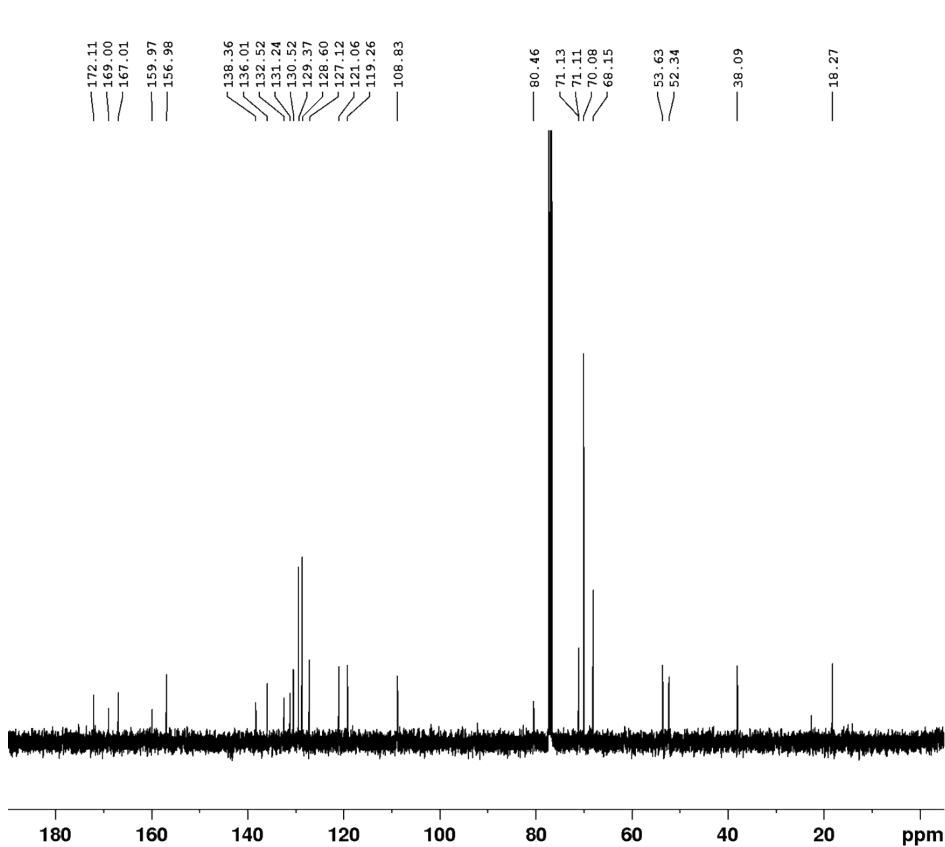
Compound 15b



Current Data Parameters
 NAME FL08802
 EXPNO 11
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20220418
 Time 16.56 h
 INSTRUM Avance Neo 400
 PROBHD z175272_0007 ()
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 32
 DS 0
 SWH 6578.947 Hz
 FIDRES 0.401547 Hz
 AQ 2.4903679 sec
 RG 101
 DW 76.000 usec
 DE 7.79 usec
 TE 298.0 K
 D1 2.00000000 sec
 TD0 1
 SFO1 400.1330415 MHz
 NUC1 1H
 P0 3.33 usec
 P1 10.00 usec
 PLW1 20.07200050 W

F2 - Processing parameters
 SI 65536
 SF 400.1300103 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00

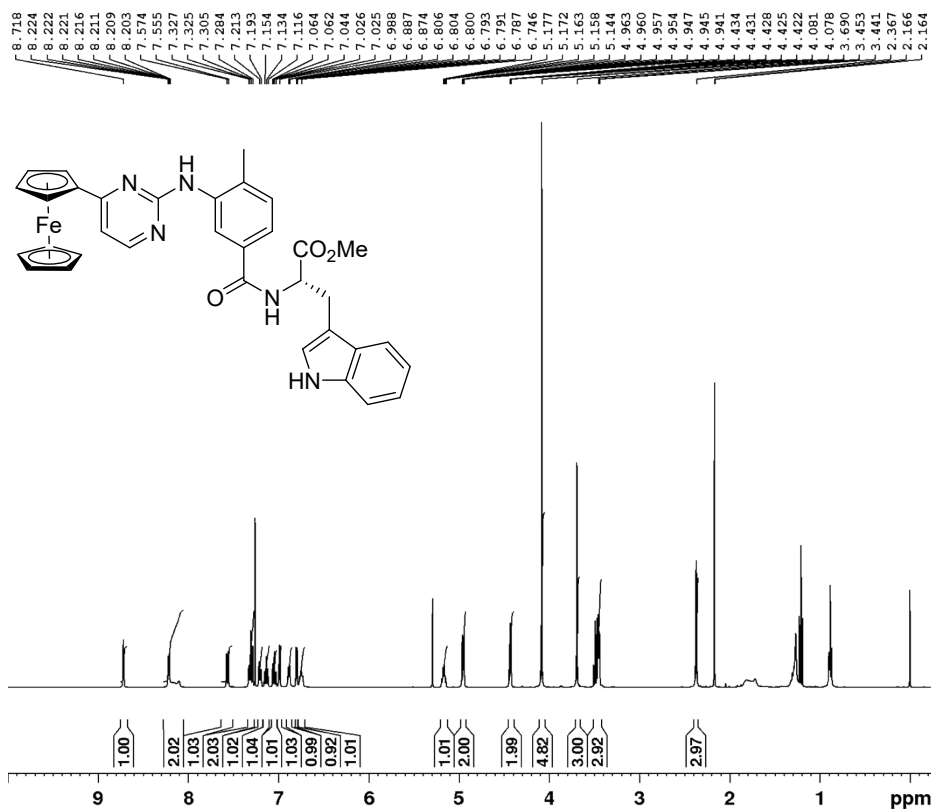


Current Data Parameters
 NAME FL08802
 EXPNO 12
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20220418
 Time 17.02 h
 INSTRUM Avance Neo 400
 PROBHD z175272_0007 ()
 PULPROG zgdc30
 TD 32768
 SOLVENT CDCl3
 NS 128
 DS 0
 SWH 23809.523 Hz
 FIDRES 1.453218 Hz
 AQ 0.6881280 sec
 RG 22.6
 DW 21.000 usec
 DE 6.50 usec
 TE 298.0 K
 D1 1.50000000 sec
 D11 0.03000000 sec
 TD0 1
 SFO1 100.6238383 MHz
 NUC1 13C
 P0 3.33 usec
 P1 10.00 usec
 PLW1 58.46900177 W
 SFO2 400.1316008 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 20.07200050 W
 PLW12 0.24781001 W

F2 - Processing parameters
 SI 65536
 SF 100.6127690 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Compound 15c



Current Data Parameters

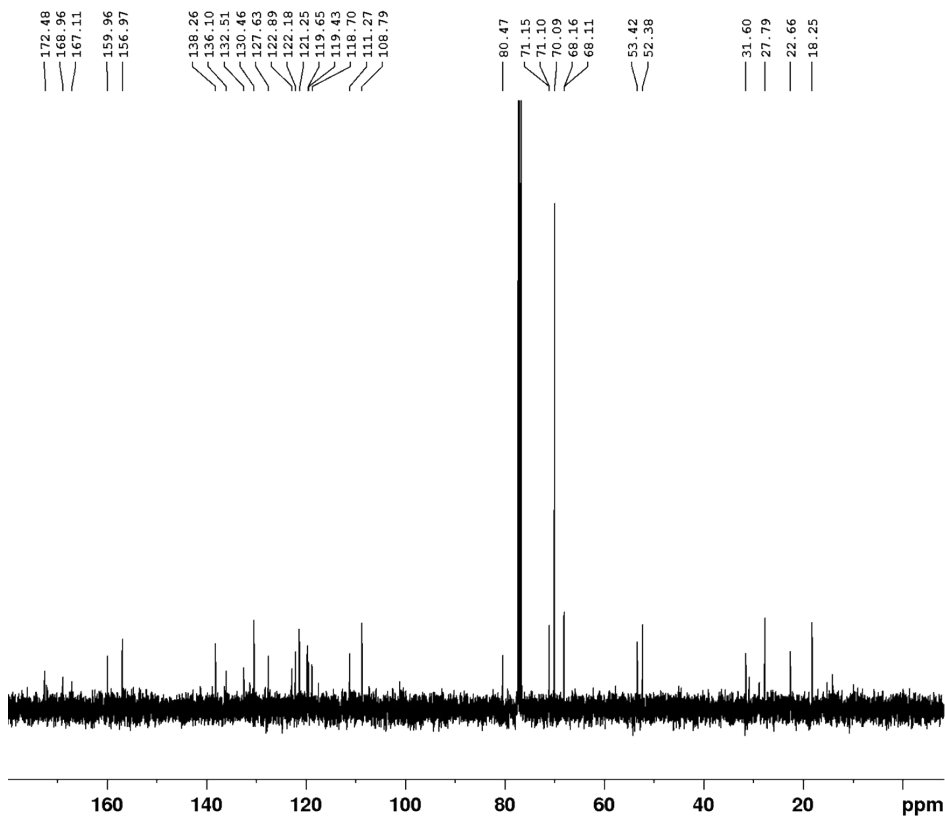
NAME FL08902
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters

Date_ 20220419
Time 16.40 h
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PROBHD Z175272_0007 (
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 6578.947 Hz
FIDRES 0.401547 Hz
AQ 2.4903679 sec
RG 101
DW 76.000 usec
DE 7.79 usec
TE 298.0 K
D1 2.00000000 sec
TDO 1
SFO1 400.1330415 MHz
NUC1 1H
PO 3.33 usec
P1 10.00 usec
PLW1 20.07200050 W

F2 - Processing parameters

SI 65536
SF 400.1300107 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



Current Data Parameters

NAME FL08902
EXPNO 12
PROCNO 1

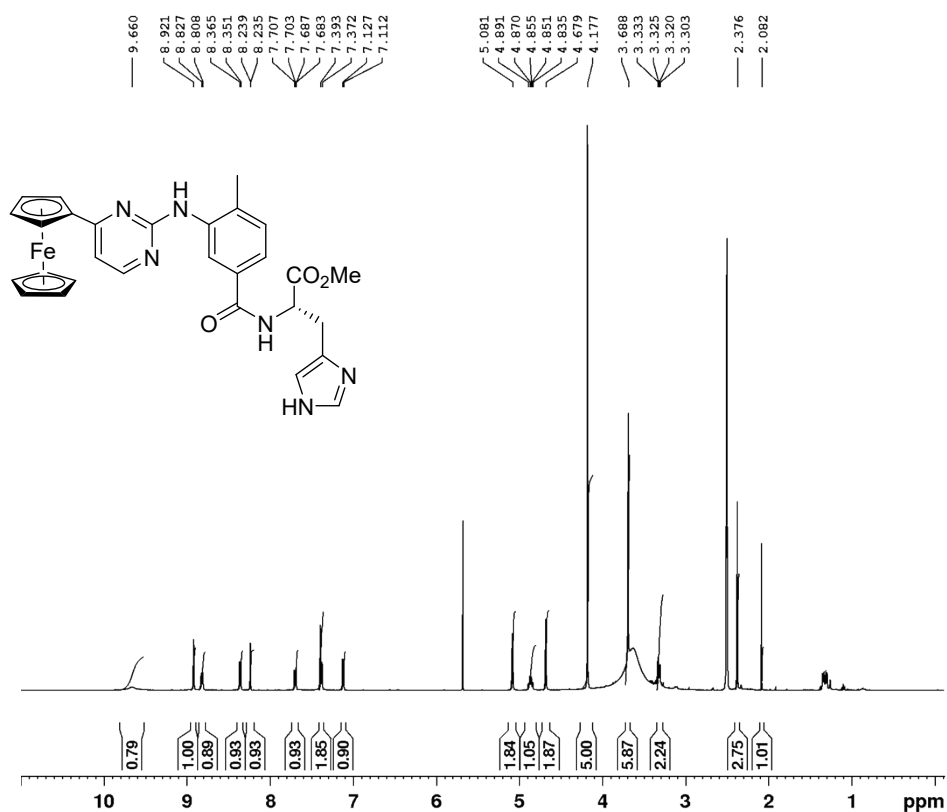
F2 - Acquisition Parameters

Date_ 20220419
Time 16.45 h
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PROBHD Z175272_0007 (
PULPROG zgdc30
TD 32768
SOLVENT CDCl3
NS 128
DS 0
SWH 23809.523 Hz
FIDRES 1.453219 Hz
AQ 0.6881280 sec
RG 22.6
DW 21.000 usec
DE 6.50 usec
TE 298.0 K
D1 1.50000000 sec
D11 0.03000000 sec
TDO 1
SFO1 100.6238383 MHz
NUC1 13C
PO 3.33 usec
P1 10.00 usec
PLW1 58.46900177 W
SFO2 400.1316008 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 20.07200050 W
PLW12 0.24781001 W

F2 - Processing parameters

SI 65536
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 0.50

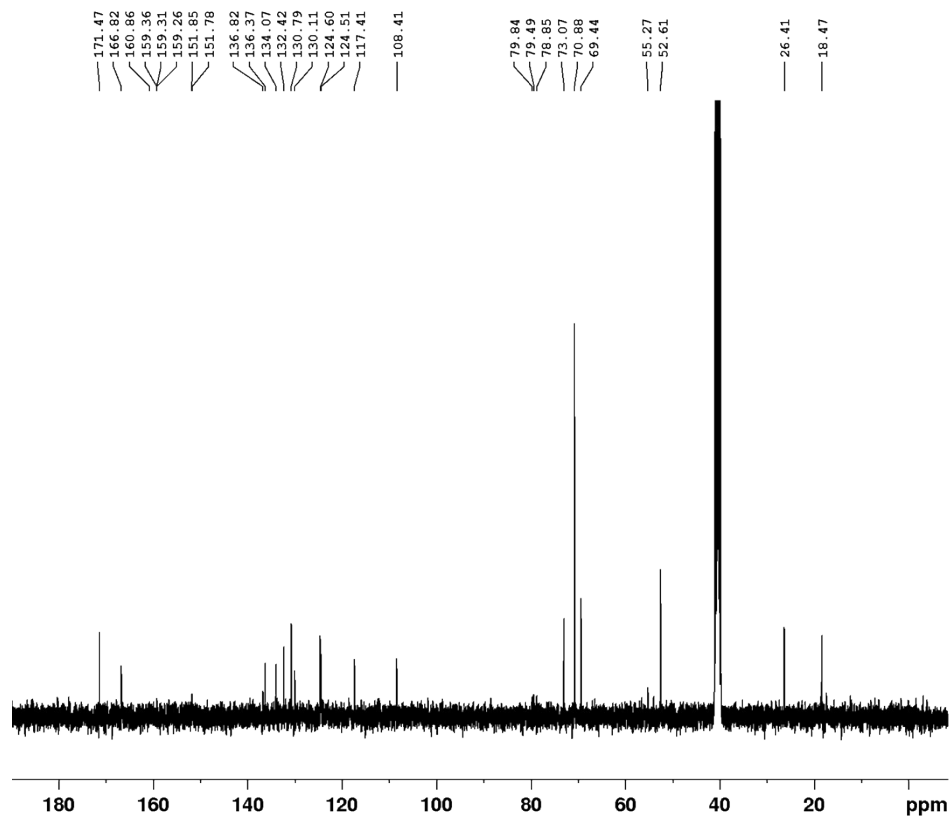
Compound 15d



Current Data Parameters
 NAME FL09204
 EXPNO 24
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20220513
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 PROBHD Z175272_0007 (
 PULPROG zg30
 TD 32768
 SOLVENT DMSO
 NS 32
 DS 0
 SWH 6578.947 Hz
 FIDRES 0.401547 Hz
 AQ 2.4903679 sec
 RG 101
 DW 76.000 usec
 DE 7.79 usec
 TE 353.0 K
 D1 2.0000000 sec
 TD0 1
 SFO1 400.1330415 MHz
 NUC1 1H
 P0 3.33 usec
 P1 10.00 usec
 PLW1 20.07200050 W

F2 - Processing parameters
 SI 65536
 SF 400.1300037 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00

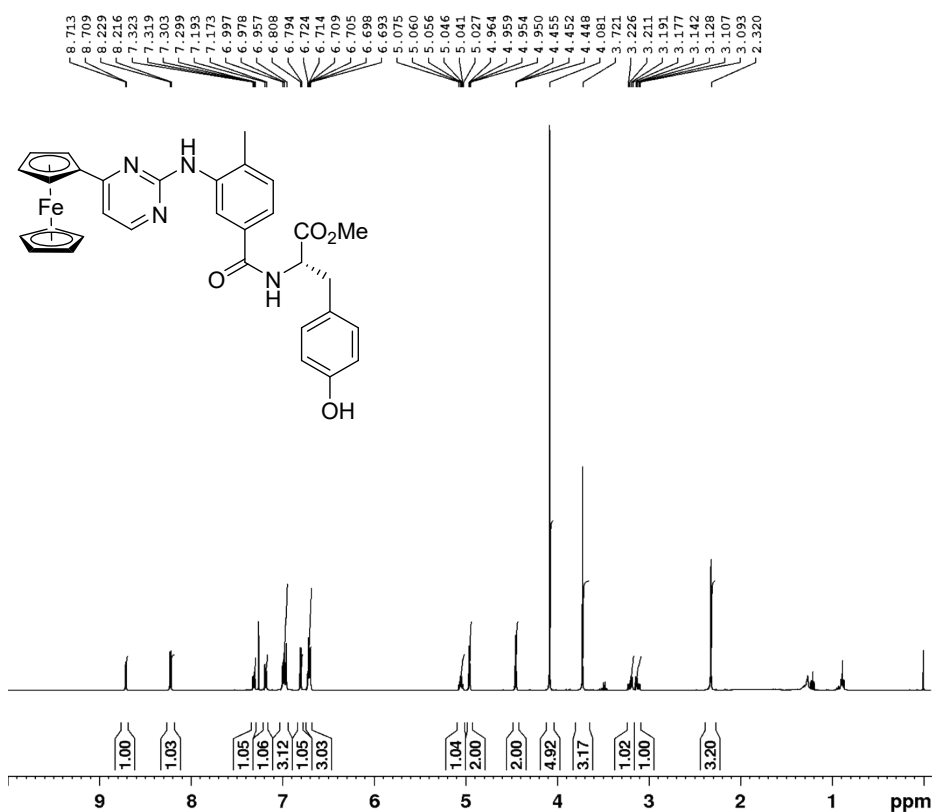


Current Data Parameters
 NAME FL09204
 EXPNO 25
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20220513
 Time 15.44 h
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 PROBHD Z175272_0007 (
 PULPROG zgdc30
 TD 32768
 SOLVENT DMSO
 NS 512
 DS 0
 SWH 23809.523 Hz
 FIDRES 1.453218 Hz
 AQ 0.6881280 sec
 RG 45.2
 DW 21.000 usec
 DE 6.50 usec
 TE 353.0 K
 D1 1.5000000 sec
 D11 0.03000000 sec
 TD0 1
 SFO1 100.6238383 MHz
 NUC1 13C
 P0 3.33 usec
 P1 10.00 usec
 PLW1 58.46900177 W
 SFO2 400.1316008 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 FCPD2 90.00 usec
 PLW2 20.07200050 W
 PLW12 0.24781001 W

F2 - Processing parameters
 SI 65536
 SF 100.6127690 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 0.50

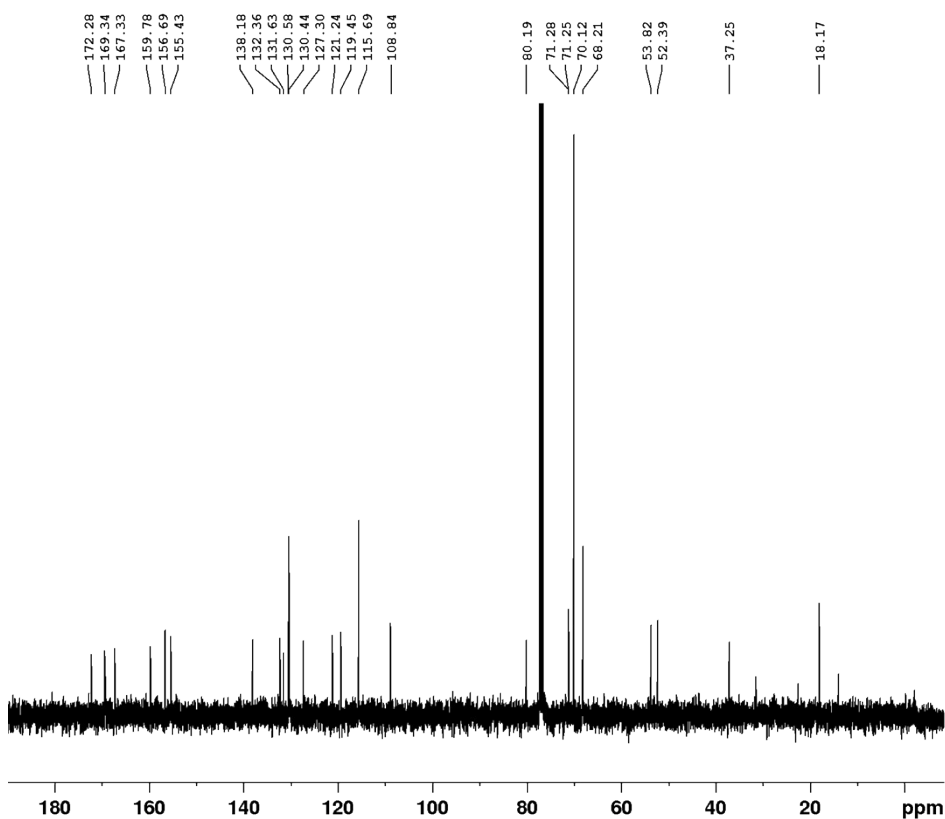
Compound 15e



Current Data Parameters
 NAME FL09302
 EXPNO 11
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20220510
 Time 18.33 h
 INSTRUM Avance Neo 400
 PROBHD Z175272_0007 (
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 32
 DS 0
 SWH 6578.947 Hz
 FIDRES 0.401547 Hz
 AQ 2.4903679 sec
 RG 101
 DW 76.000 usec
 DE 7.79 usec
 TE 298.0 K
 D1 2.0000000 sec
 TDO 1
 SFO1 400.1330415 MHz
 NUC1 1H
 P0 3.33 usec
 P1 10.00 usec
 PLW1 20.07200050 W

F2 - Processing parameters
 SI 65536
 SF 400.1300098 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00

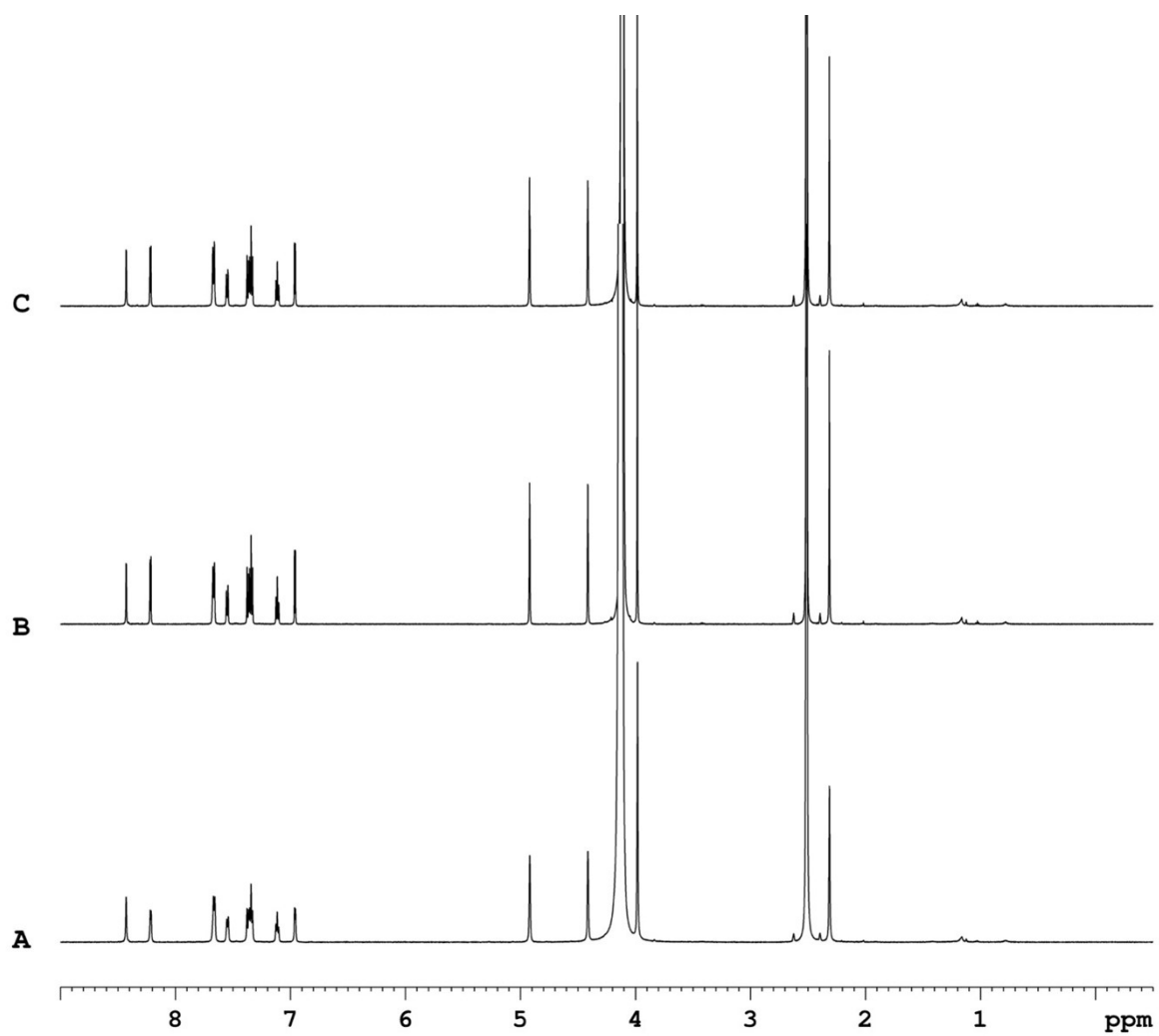


Current Data Parameters
 NAME FL09302
 EXPNO 12
 PROCNO 1

F2 - Acquisition Parameters
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 PULPROG zgdc30
 TD 32768
 SOLVENT CDCl3
 NS 128
 DS 0
 SWH 23809.523 Hz
 FIDRES 1.453219 Hz
 AQ 0.6881280 sec
 RG 22.6
 DW 21.000 usec
 DE 6.50 usec
 TE 298.0 K
 D1 1.5000000 sec
 D11 0.0300000 sec
 TDO 1
 SFO1 100.6238383 MHz
 NUC1 13C
 P0 3.33 usec
 P1 10.00 usec
 PLW1 58.46900177 W
 SFO2 400.1316008 MHz
 NUC2 1H
 CPDPRG2 waltz16
 FCPD2 90.00 usec
 PLW2 20.07200050 W
 PLW12 0.24781001 W

F2 - Processing parameters
 SI 65536
 SF 100.6127690 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

^1H NMR monitoring of 15a stability in DMSO- d_6 (80%) / PBS in D_2O (20%)



Spectra recorded at: **A** $t = 0$ min; **B** $t = 24$ h; **C** $t = 4$ d.