Supplementary Material for

Synthesis and Evaluation of 5-(Heteroarylmethylene)hydantoins as Glycogen Synthase Kinase-3β Inhibitors

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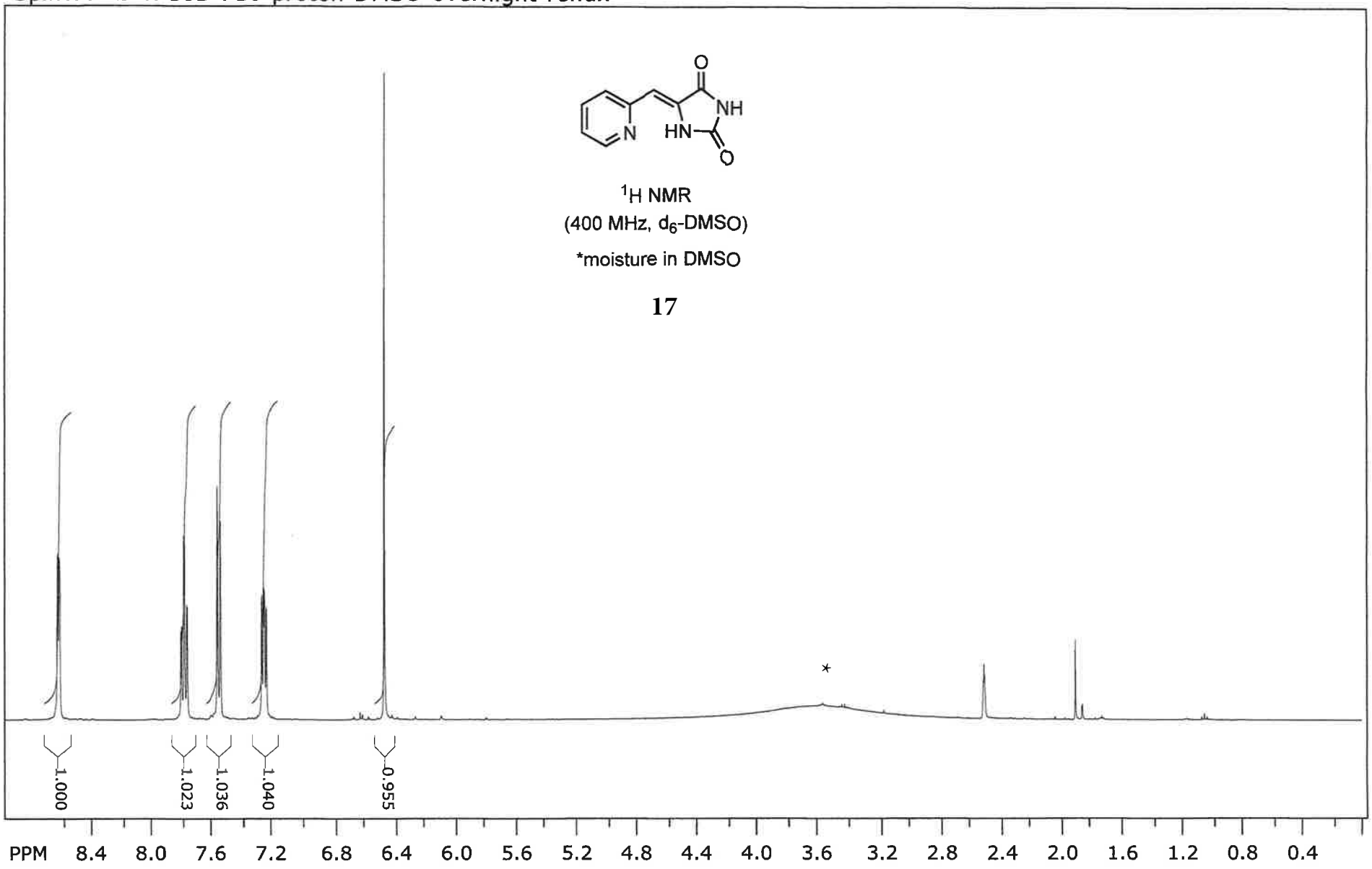
This document includes:

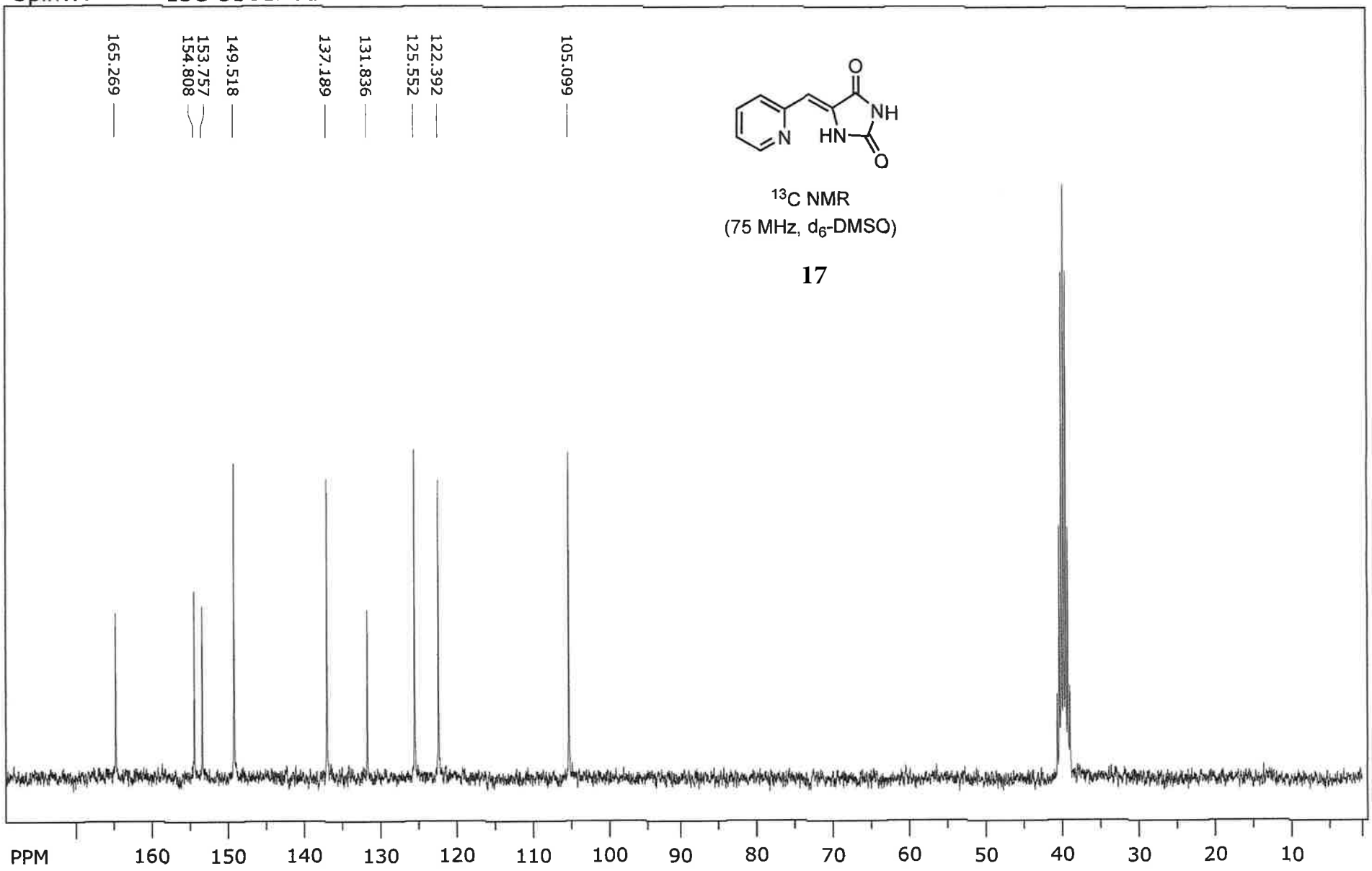
SpinWorks 4: DJB-710-proton-DMSO-overnight-reflux



file: ...oton-DMSO-reflux-overnight.fid\fid block# 1 expt: "s2pul"
transmitter freq.: 399.732139 MHz
time domain size: 32768 points
width: 6410.26 Hz = 16.0364 ppm = 0.195626 Hz/pt
number of scans: 8

freq. of 0 ppm: 399.729732 MHz
processed size: 32768 complex points
LB: 0.500 GF: 0.0000
Hz/cm: 143.875 ppm/cm: 0.35993

SpinWorks 4: 13C OBSERVE



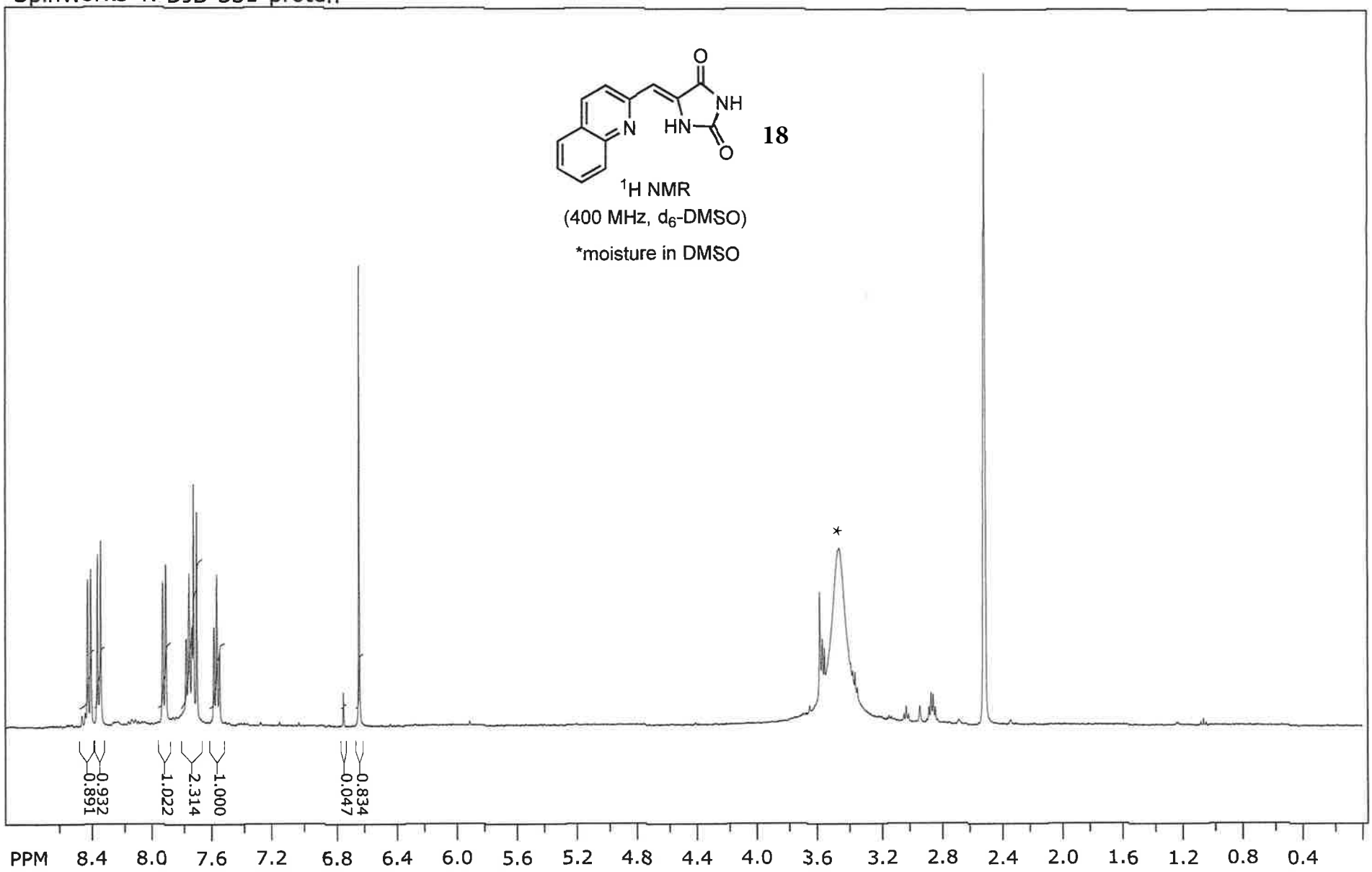
^{13}C NMR
(75 MHz, d_6-DMSO)

17

file: ...ldsonw\Desktop\DJB-234-13C.fid\fid block# 1 expt: "s2pul"
transmitter freq.: 75.476694 MHz
time domain size: 68492 points
width: 18867.92 Hz = 249.9835 ppm = 0.275476 Hz/pt
number of scans: 256

freq. of 0 ppm: 75.468435 MHz
processed size: 131072 complex points
LB: 2.500 GF: 0.0000
Hz/cm: 543.396 ppm/cm: 7.19952

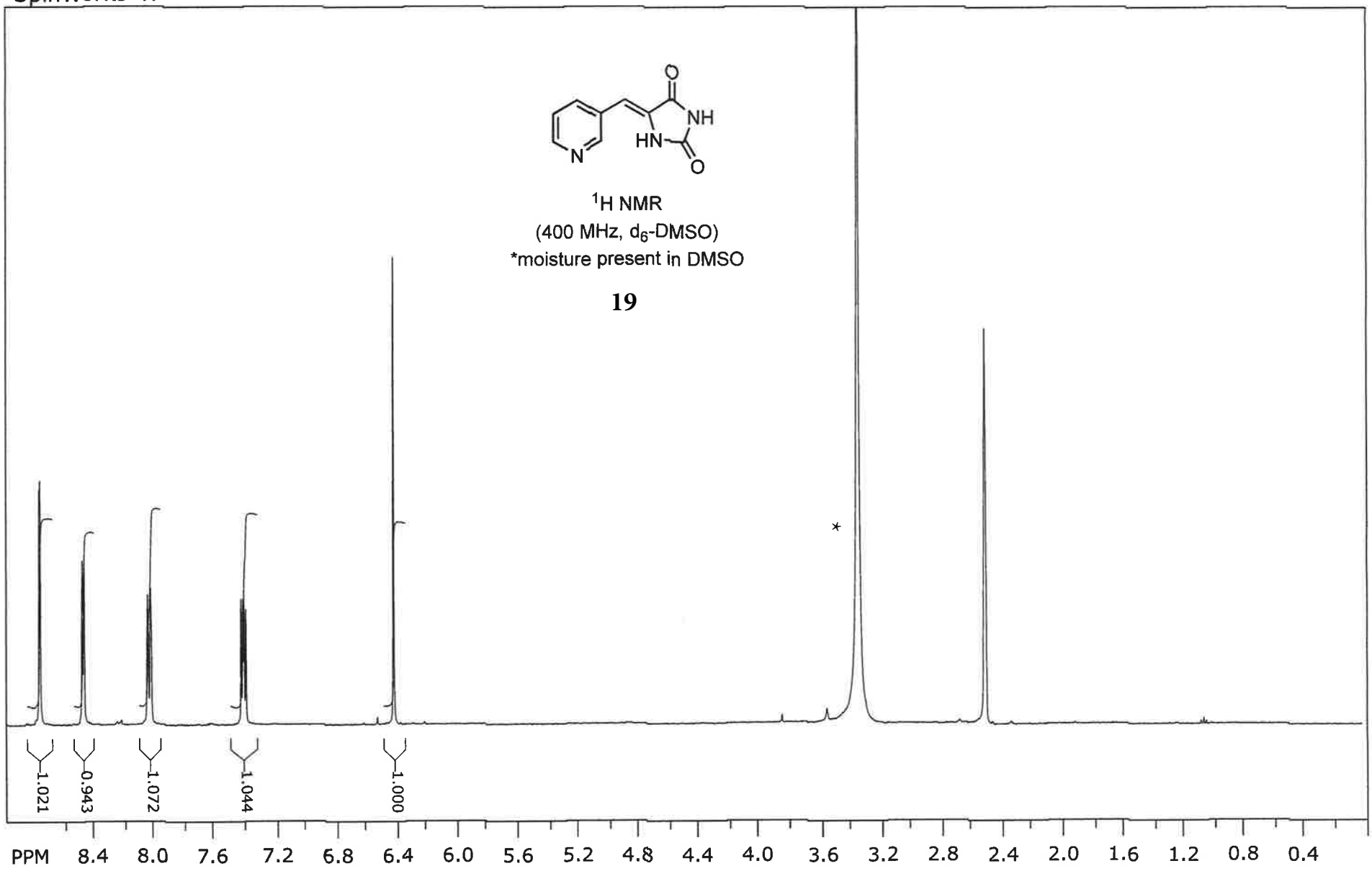
SpinWorks 4: DJB-331-proton



file: ...DJB spectra\DJB-334-proton.fid\fid block# 1 expt: "s2pul"
transmitter freq.: 399.736048 MHz
time domain size: 32768 points
width: 6410.26 Hz = 16.0362 ppm = 0.195626 Hz/pt
number of scans: 8

freq. of 0 ppm: 399.733634 MHz
processed size: 32768 complex points
LB: 0.500 GF: 0.0000
Hz/cm: 143.875 ppm/cm: 0.35992

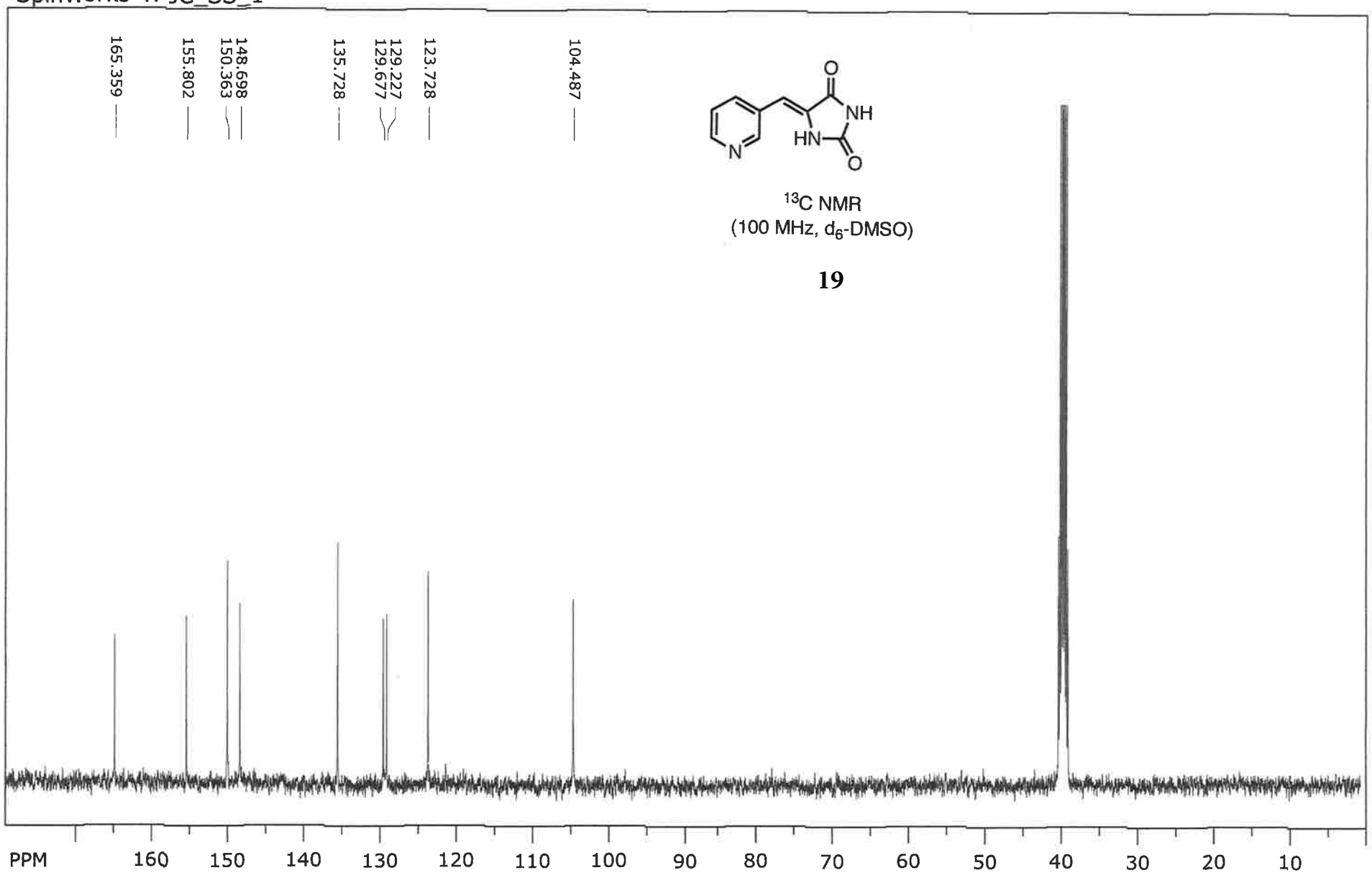
SpinWorks 4:



file: ...DJB spectra\DJB-235-proton.fid\fid block# 1 expt: "s2pul"
transmitter freq.: 399.738002 MHz
time domain size: 26264 points
width: 6410.26 Hz = 16.0361 ppm = 0.244070 Hz/pt
number of scans: 8

freq. of 0 ppm: 399.735598 MHz
processed size: 65536 complex points
LB: 0.500 GF: 0.0000
Hz/cm: 143.875 ppm/cm: 0.35992

SpinWorks 4: JC_SS_1



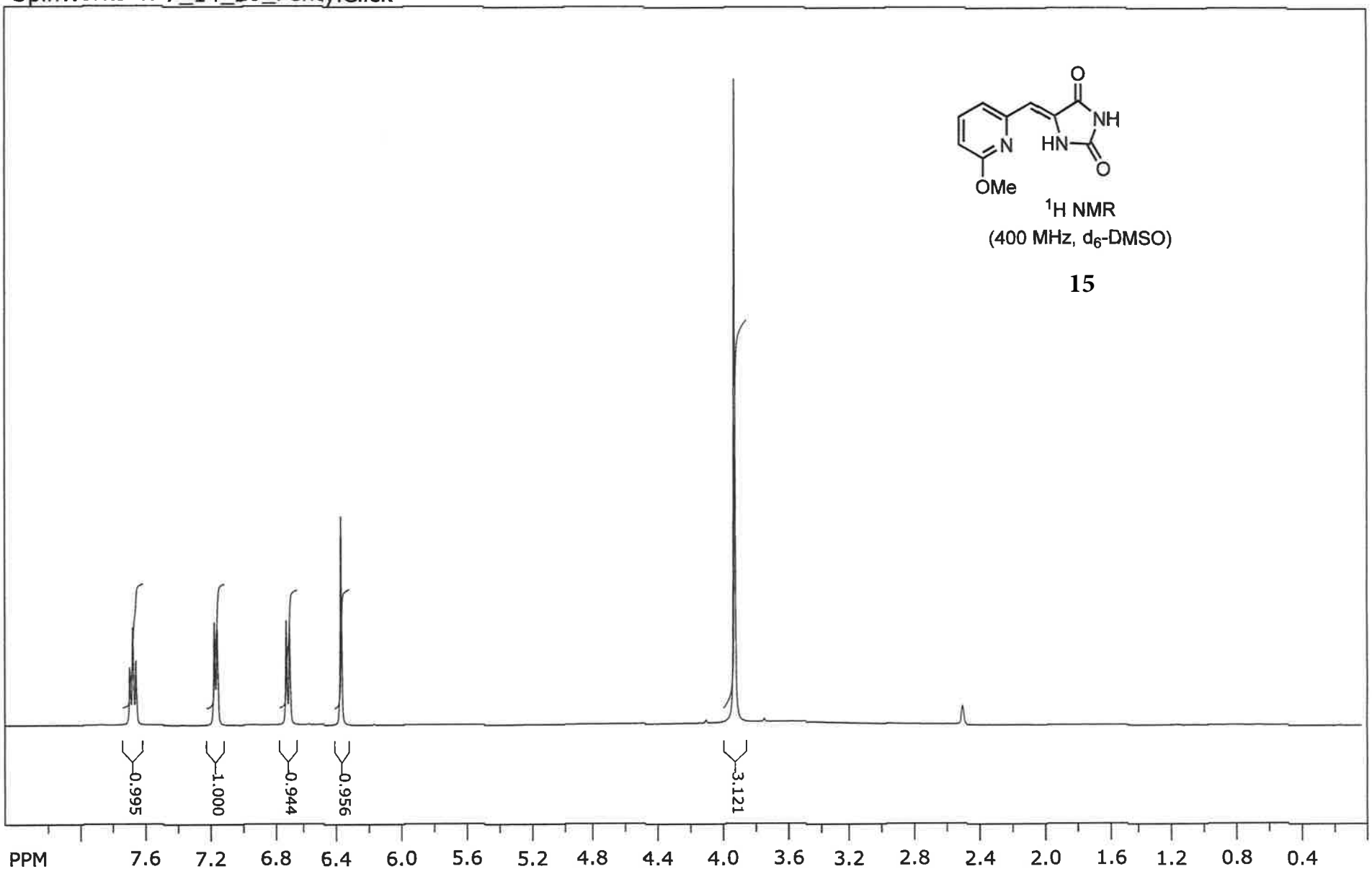
^{13}C NMR
(100 MHz, d_6-DMSO)

19

file: ...on\WD325_13C_DMSO_20240116.fid\fid block# 1 expt: "s2pul"
transmitter freq.: 100.523180 MHz
time domain size: 65536 points
width: 25000.00 Hz = 248.6989 ppm = 0.381470 Hz/pt
number of scans: 2048

freq. of 0 ppm: 100.512160 MHz
processed size: 65536 complex points
LB: 2.500 GF: 0.0000
Hz/cm: 723.333 ppm/cm: 7.19569

SpinWorks 4: 7_14_20_PentylClick



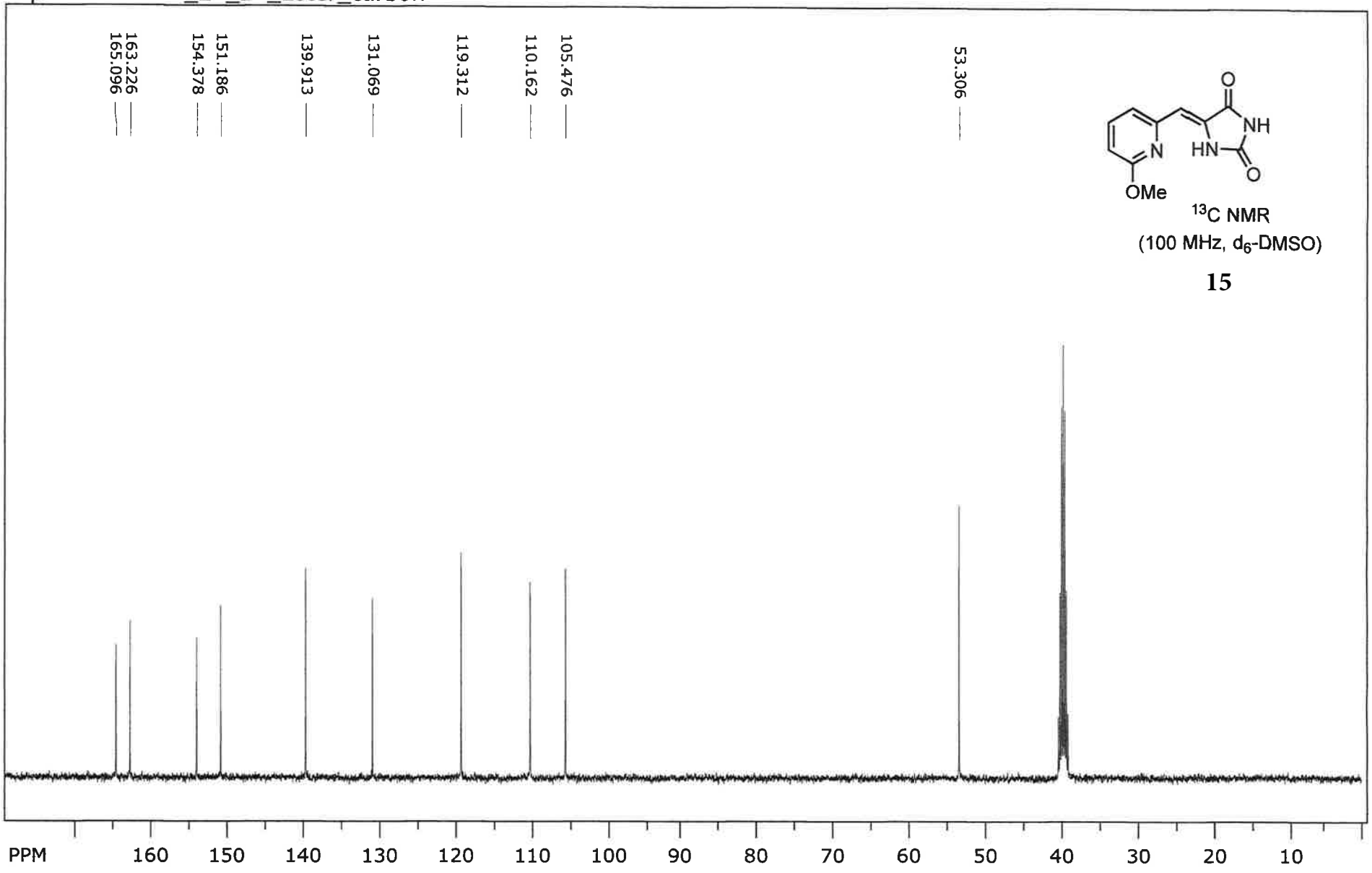
^{1}H NMR
(400 MHz, d_6-DMSO)

15

file: ...spectra\WD340-349\WD340-1H.fid\fid block# 1 expt: "s2pul"
transmitter freq.: 399.732139 MHz
time domain size: 32768 points
width: 6410.26 Hz = 16.0364 ppm = 0.195626 Hz/pt
number of scans: 8

freq. of 0 ppm: 399.729734 MHz
processed size: 32768 complex points
LB: 0.500 GF: 0.0000
Hz/cm: 135.897 ppm/cm: 0.33997

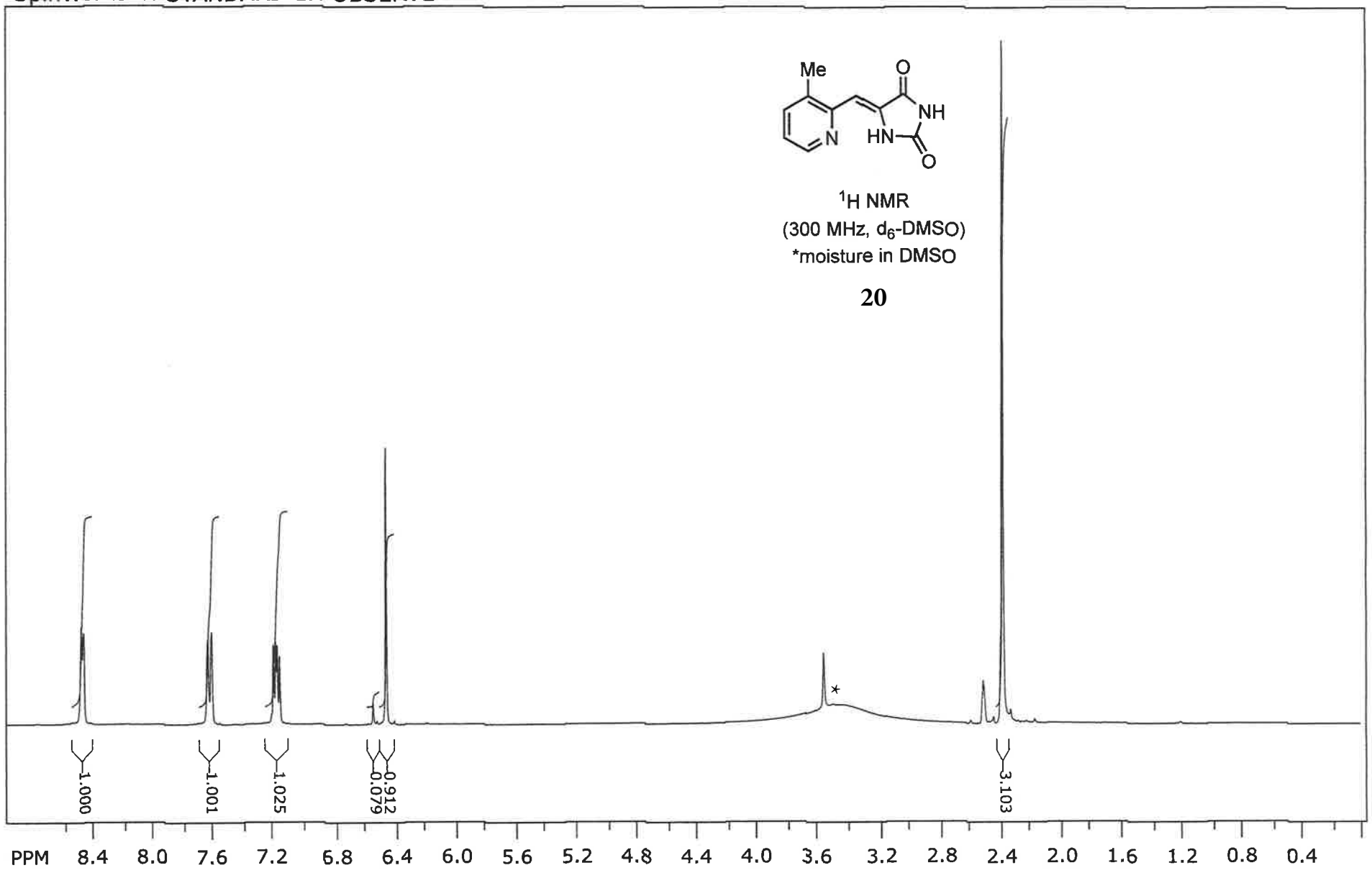
SpinWorks 4: 7_27_20_Ester_carbon



file: ...ectra\WD spectra\WD340-13C.fid\fid block# 1 expt: "s2pul"
transmitter freq.: 100.523180 MHz
time domain size: 65536 points
width: 25000.00 Hz = 248.6989 ppm = 0.381470 Hz/pt
number of scans: 256

freq. of 0 ppm: 100.512156 MHz
processed size: 65536 complex points
LB: 1.500 GF: 0.0000
Hz/cm: 723.889 ppm/cm: 7.20121

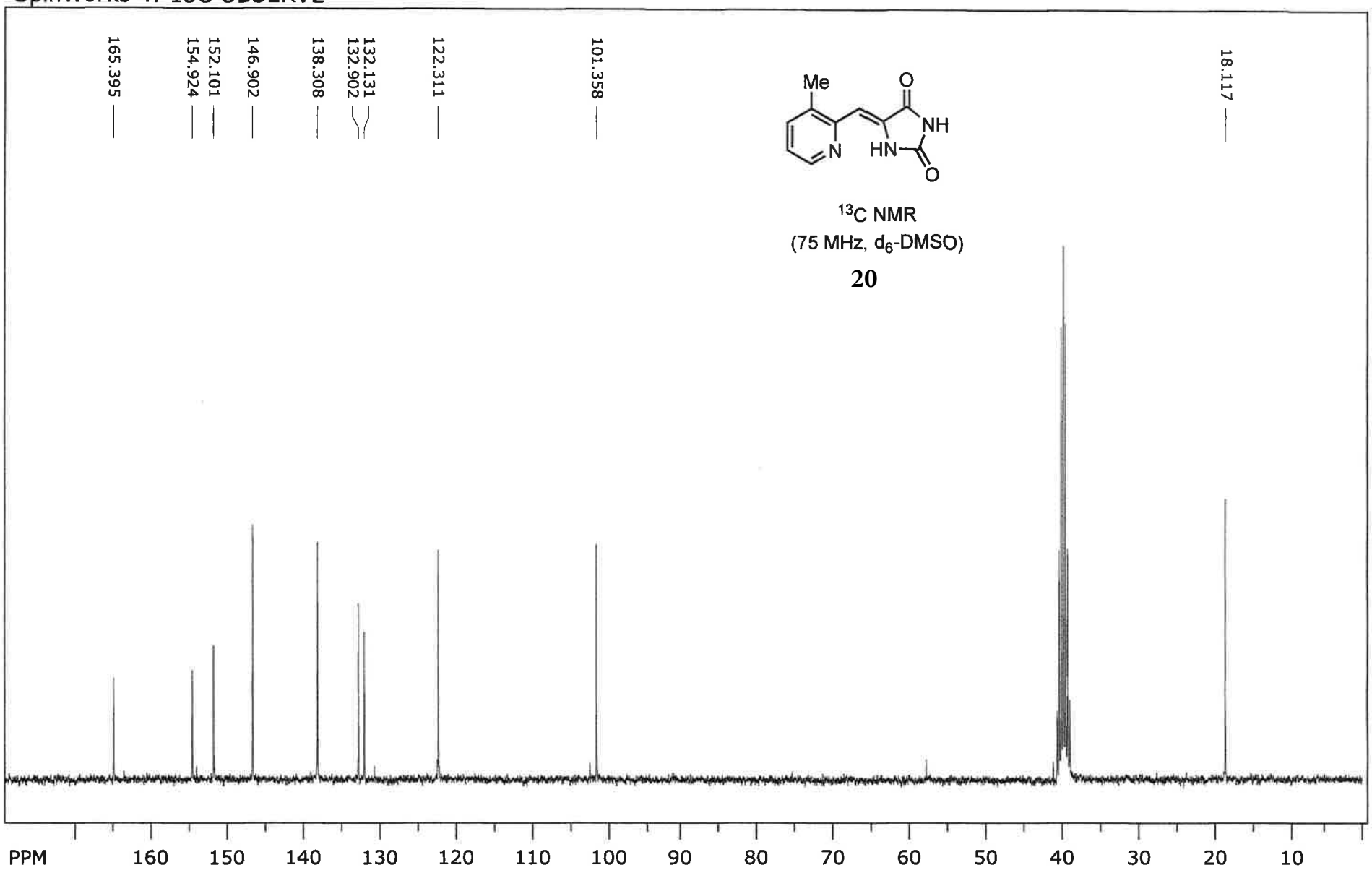
SpinWorks 4: STANDARD 1H OBSERVE



file: ...pectra\WD320-329\WD-328_1H.fid\fid block# 1 expt: "s2pul"
transmitter freq.: 300.134434 MHz
time domain size: 19192 points
width: 4803.07 Hz = 16.0031 ppm = 0.250264 Hz/pt
number of scans: 8

freq. of 0 ppm: 300.132628 MHz
processed size: 32768 complex points
LB: 0.500 GF: 0.0000
Hz/cm: 108.016 ppm/cm: 0.35989

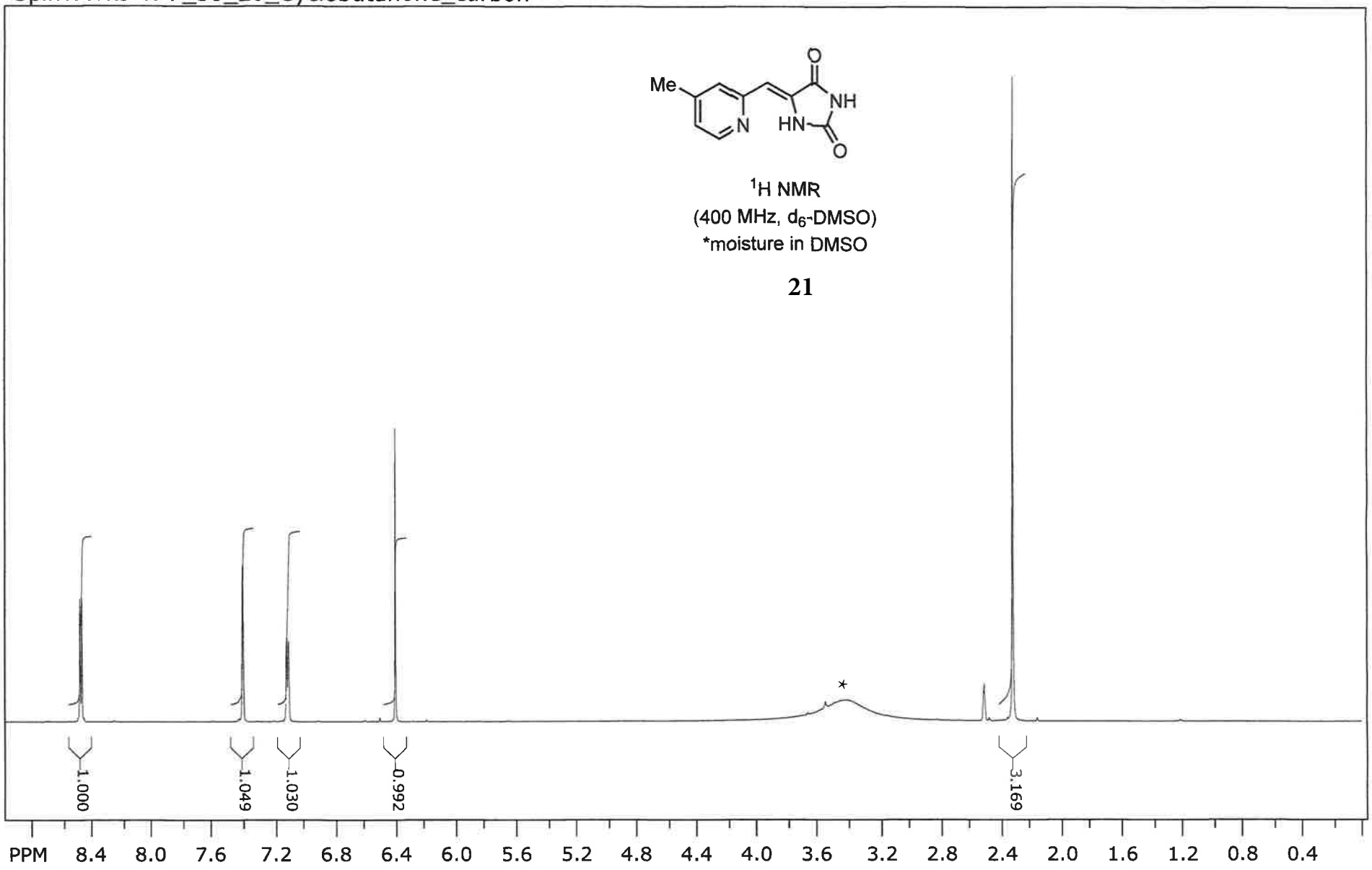
SpinWorks 4: 13C OBSERVE



file: ...ctra\WD spectra\WD-328_13C.fid\fid block# 1 expt: "s2pul"
transmitter freq.: 75.476694 MHz
time domain size: 68492 points
width: 18867.92 Hz = 249.9835 ppm = 0.275476 Hz/pt
number of scans: 384

freq. of 0 ppm: 75.468436 MHz
processed size: 131072 complex points
LB: 1.500 GF: 0.0000
Hz/cm: 543.396 ppm/cm: 7.19952

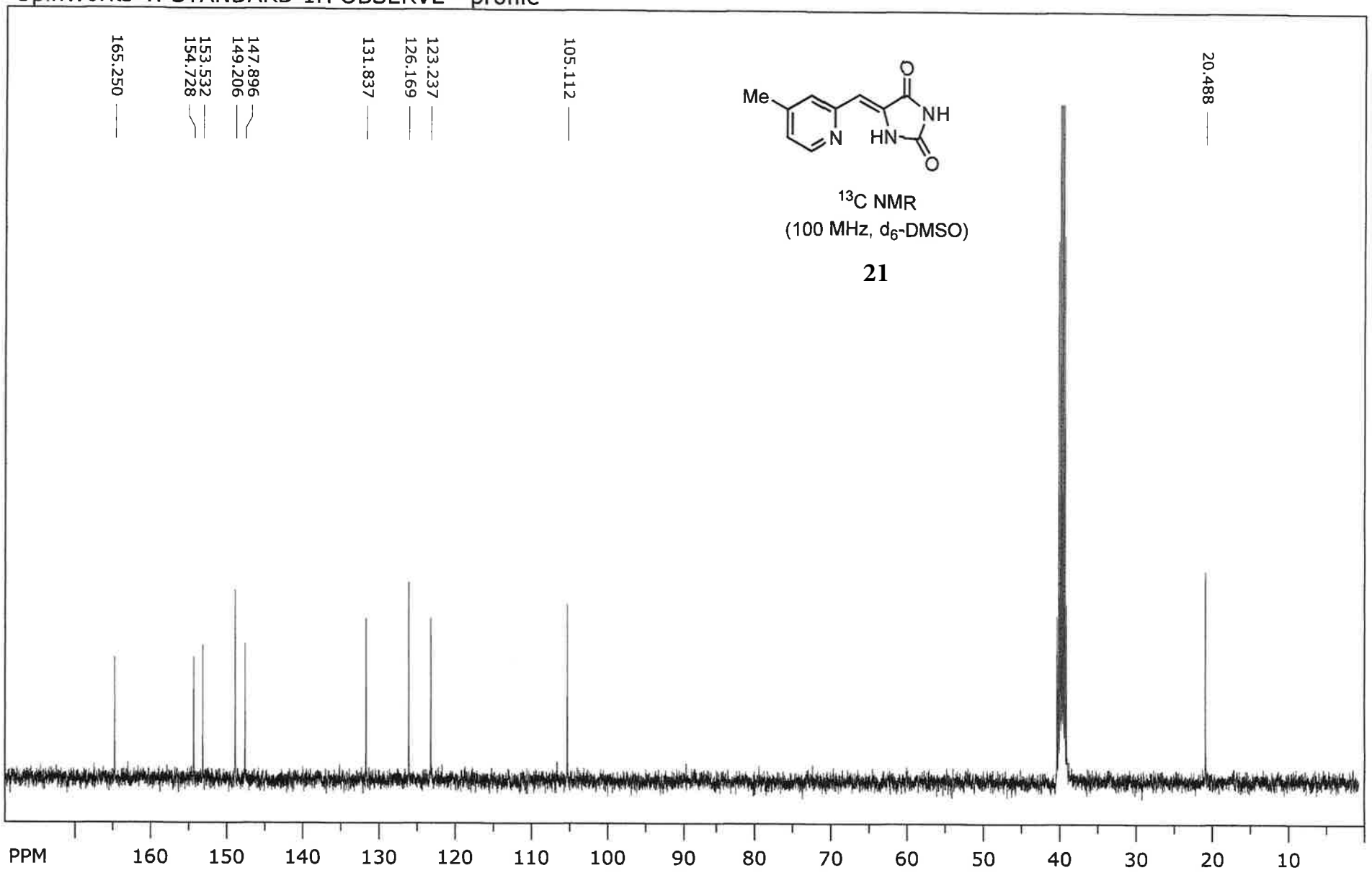
SpinWorks 4: 7_30_20_Cyclobutanone_carbon



file: ...pectra\WD spectra\WD342_1H.fid\fid block# 1 expt: "s2pul"
transmitter freq.: 399.732139 MHz
time domain size: 32768 points
width: 6410.26 Hz = 16.0364 ppm = 0.195626 Hz/pt
number of scans: 8

freq. of 0 ppm: 399.729733 MHz
processed size: 32768 complex points
LB: 0.051 GF: 0.0000
Hz/cm: 144.017 ppm/cm: 0.36028

SpinWorks 4: STANDARD 1H OBSERVE - profile



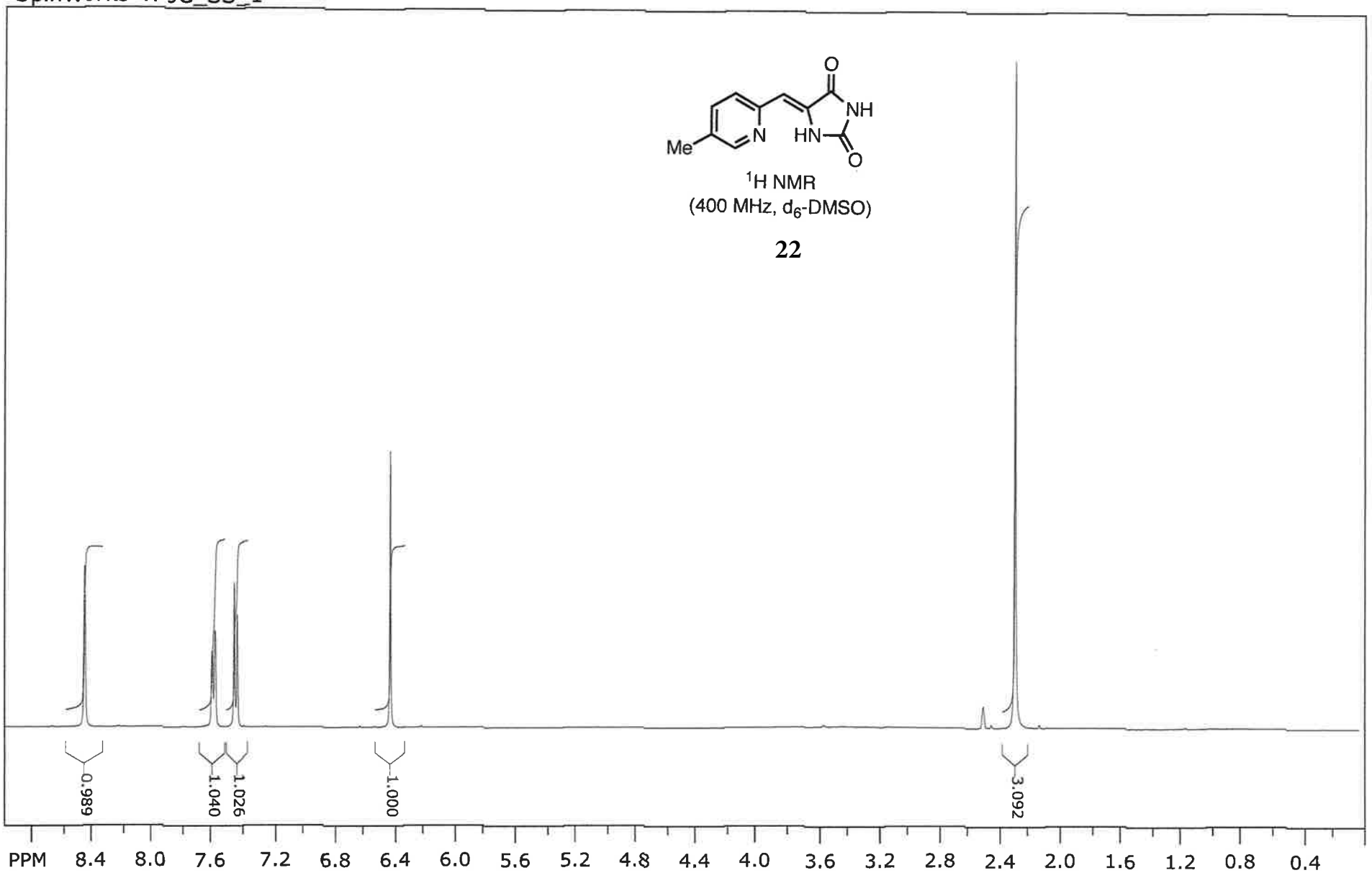
^{13}C NMR
(100 MHz, d_6-DMSO)

21

file: ...ectra\WD spectra\WD342_13C.fid\fid block# 1 expt: "s2pul"
transmitter freq.: 100.523180 MHz
time domain size: 65536 points
width: 25000.00 Hz = 248.6989 ppm = 0.381470 Hz/pt
number of scans: 512

freq. of 0 ppm: 100.512160 MHz
processed size: 65536 complex points
LB: 1.500 GF: 0.0000
Hz/cm: 723.333 ppm/cm: 7.19569

SpinWorks 4: JC_SS_1



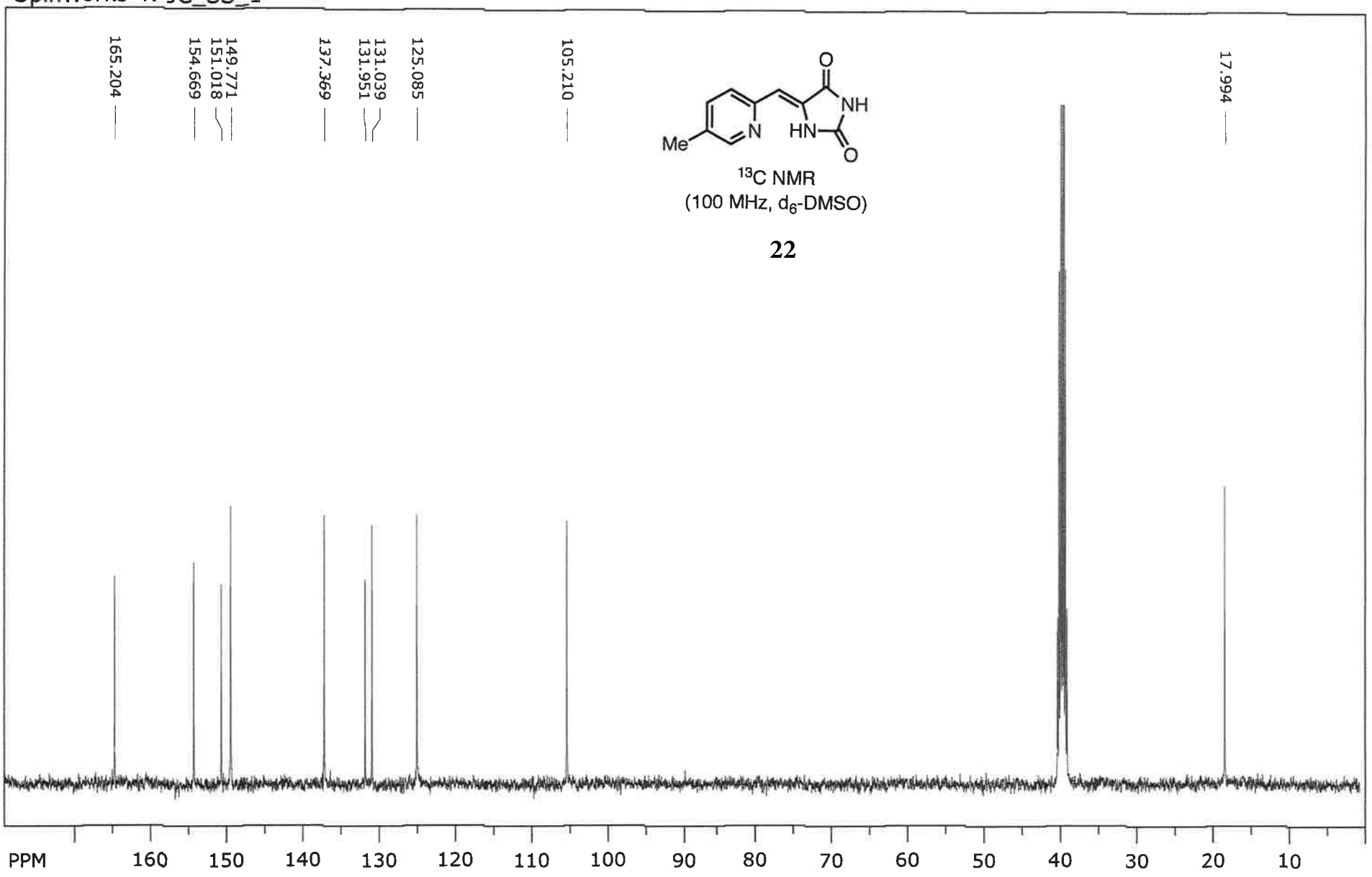
^{1}H NMR
(400 MHz, d_6-DMSO)

22

file: ...son\WD348_1H_DMSO_20240118.fid\fid block# 1 expt: "s2pul"
transmitter freq.: 399.732139 MHz
time domain size: 32768 points
width: 6410.26 Hz = 16.0364 ppm = 0.195626 Hz/pt
number of scans: 16

freq. of 0 ppm: 399.729733 MHz
processed size: 32768 complex points
LB: 0.500 GF: 0.0000
Hz/cm: 143.875 ppm/cm: 0.35993

SpinWorks 4: JC_SS_1



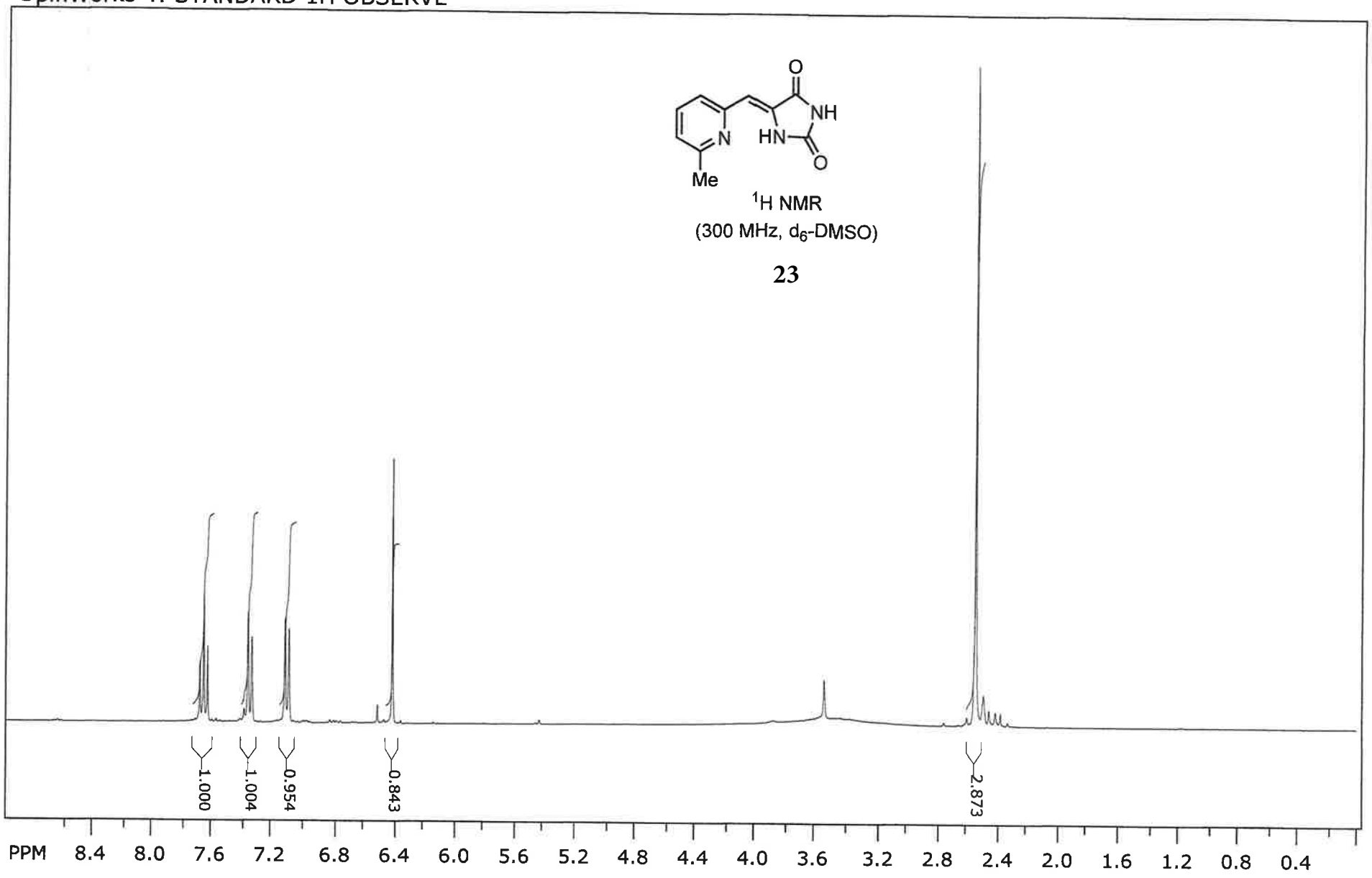
^{13}C NMR
(100 MHz, d_6-DMSO)

22

file: ...on\WD348_13C_DMSO_20240118.fid\fid block# 1 expt: "s2pul"
transmitter freq.: 100.523180 MHz
time domain size: 65536 points
width: 25000.00 Hz = 248.6989 ppm = 0.381470 Hz/pt
number of scans: 2048

freq. of 0 ppm: 100.512160 MHz
processed size: 65536 complex points
LB: 2.500 GF: 0.0000
Hz/cm: 723.333 ppm/cm: 7.19569

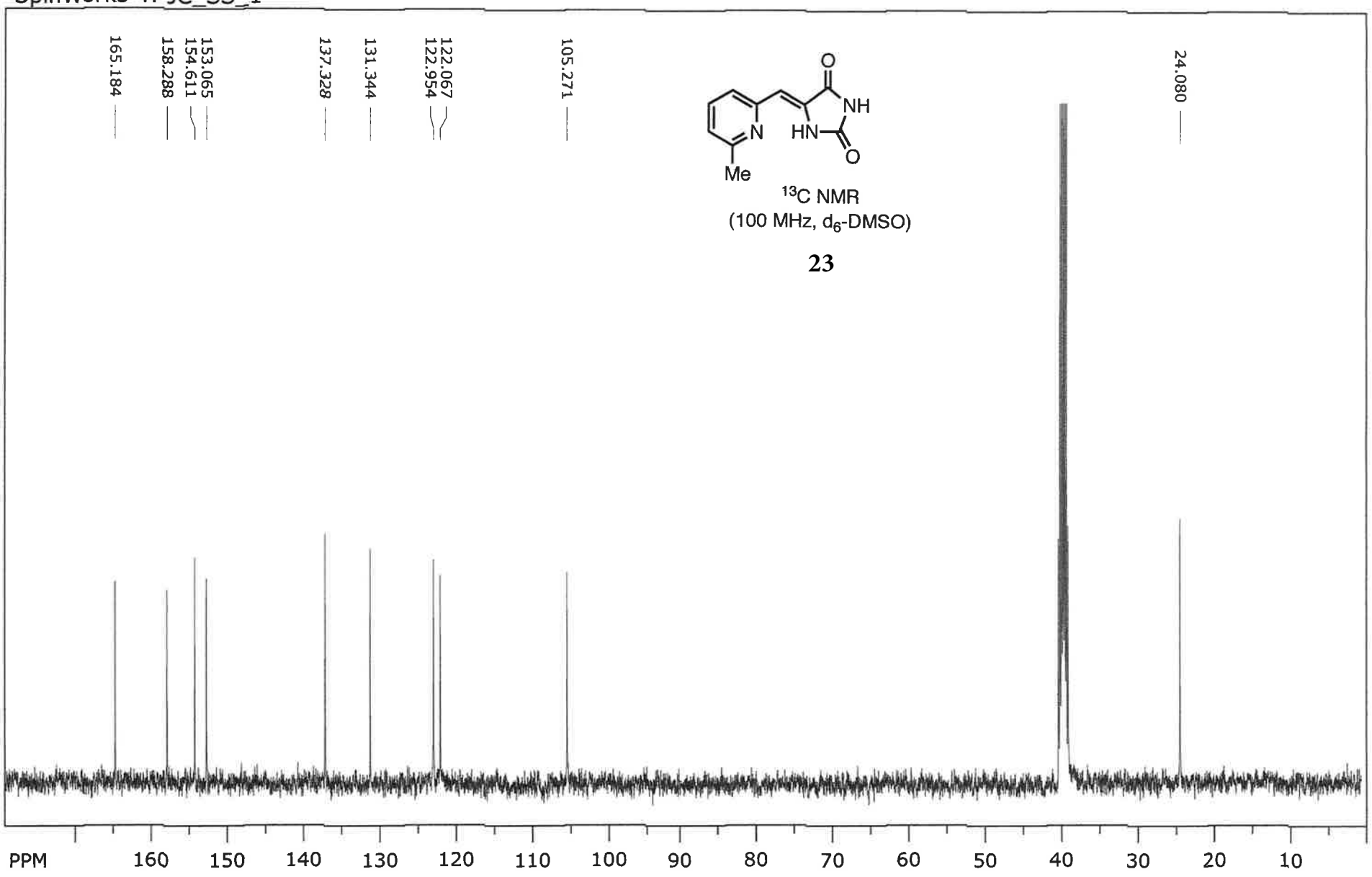
SpinWorks 4: STANDARD 1H OBSERVE



file: ...pectra\WD spectra\WD329_1H.fid\fid block# 1 expt: "s2pul"
transmitter freq.: 300.134434 MHz
time domain size: 19192 points
width: 4803.07 Hz = 16.0031 ppm = 0.250264 Hz/pt
number of scans: 8

freq. of 0 ppm: 300.132634 MHz
processed size: 32768 complex points
LB: 0.500 GF: 0.0000
Hz/cm: 108.016 ppm/cm: 0.35989

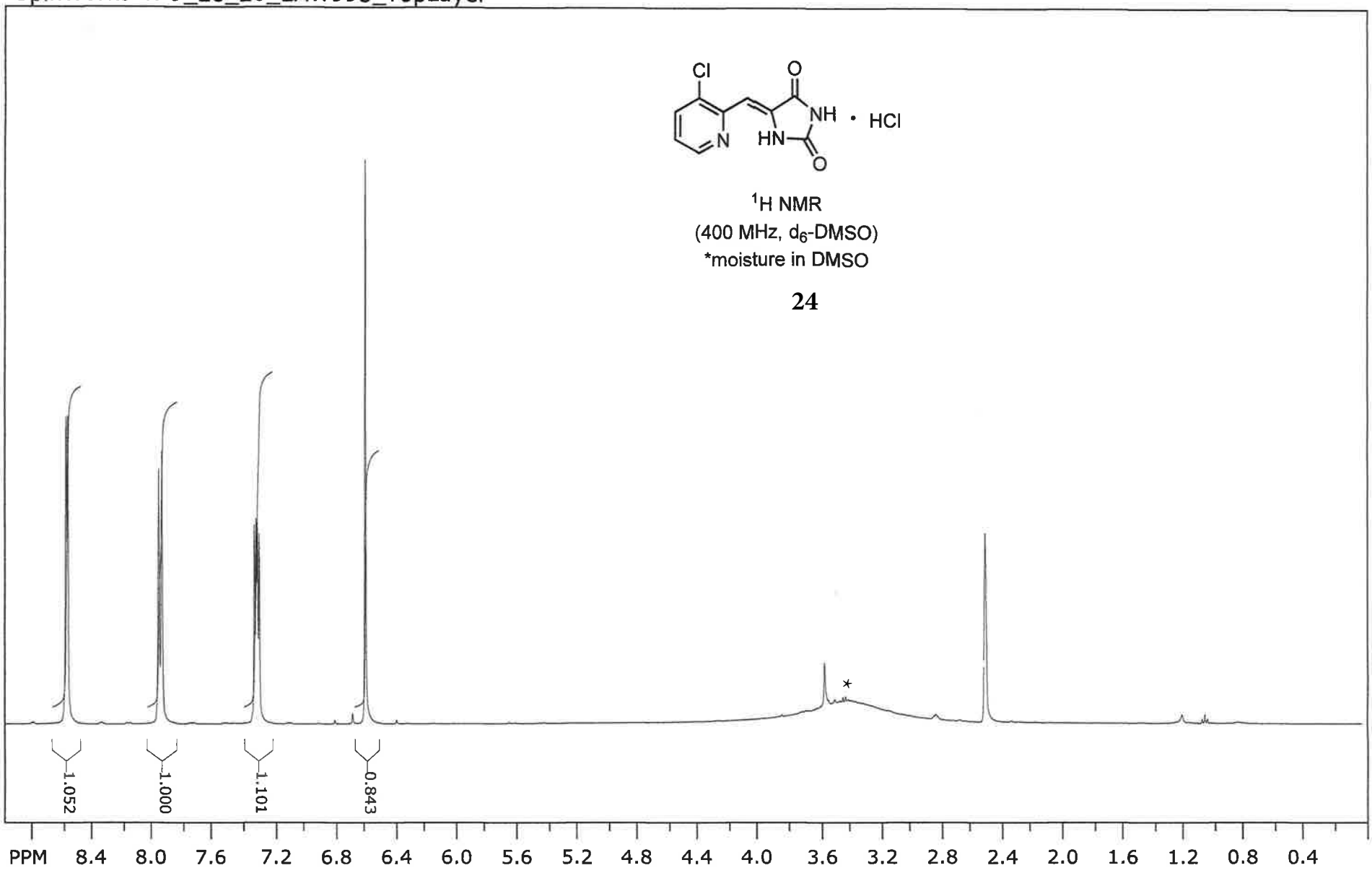
SpinWorks 4: JC_SS_1



file: ...on\WD329_13C_DMSO_20240116.fid\fid block# 1 expt: "s2pul"
transmitter freq.: 100.523180 MHz
time domain size: 65536 points
width: 25000.00 Hz = 248.6989 ppm = 0.381470 Hz/pt
number of scans: 1088

freq. of 0 ppm: 100.512161 MHz
processed size: 65536 complex points
LB: 2.500 GF: 0.0000
Hz/cm: 723.333 ppm/cm: 7.19569

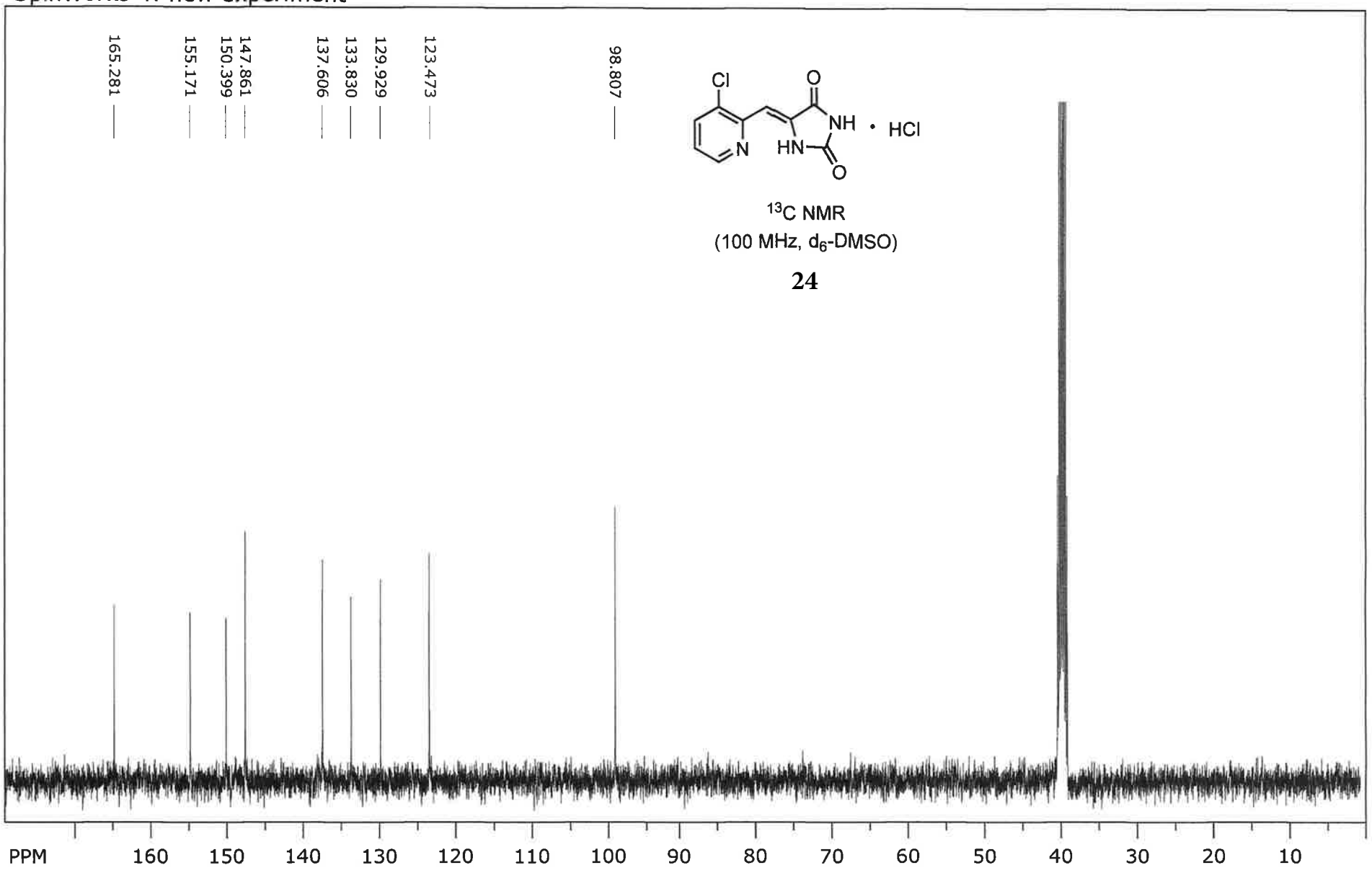
SpinWorks 4: 9_28_20_EAW995_TopLayer



file: ...spectra\WD340-349\WD346-1H.fid\fid block# 1 expt: "s2pul"
transmitter freq.: 399.732139 MHz
time domain size: 32768 points
width: 6410.26 Hz = 16.0364 ppm = 0.195626 Hz/pt
number of scans: 8

freq. of 0 ppm: 399.729734 MHz
processed size: 32768 complex points
LB: 0.510 GF: 0.0000
Hz/cm: 143.875 ppm/cm: 0.35993

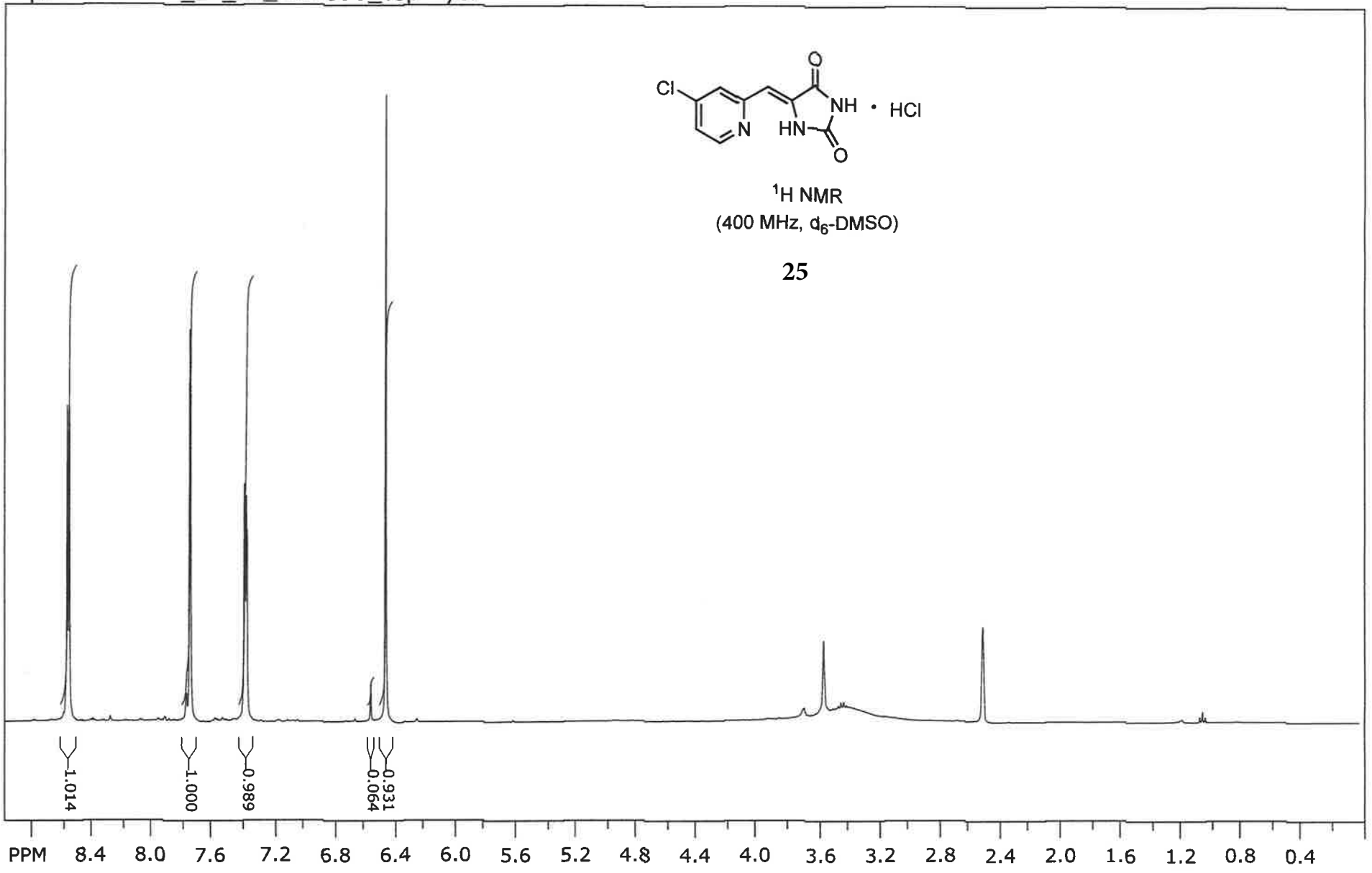
SpinWorks 4: new experiment



file: ...pectra\WD340-349\WD346-13C.fid\fid block# 1 expt: "s2pul"
transmitter freq.: 100.523180 MHz
time domain size: 65536 points
width: 25000.00 Hz = 248.6989 ppm = 0.381470 Hz/pt
number of scans: 512

freq. of 0 ppm: 100.512163 MHz
processed size: 65536 complex points
LB: 1.500 GF: 0.0000
Hz/cm: 723.333 ppm/cm: 7.19569

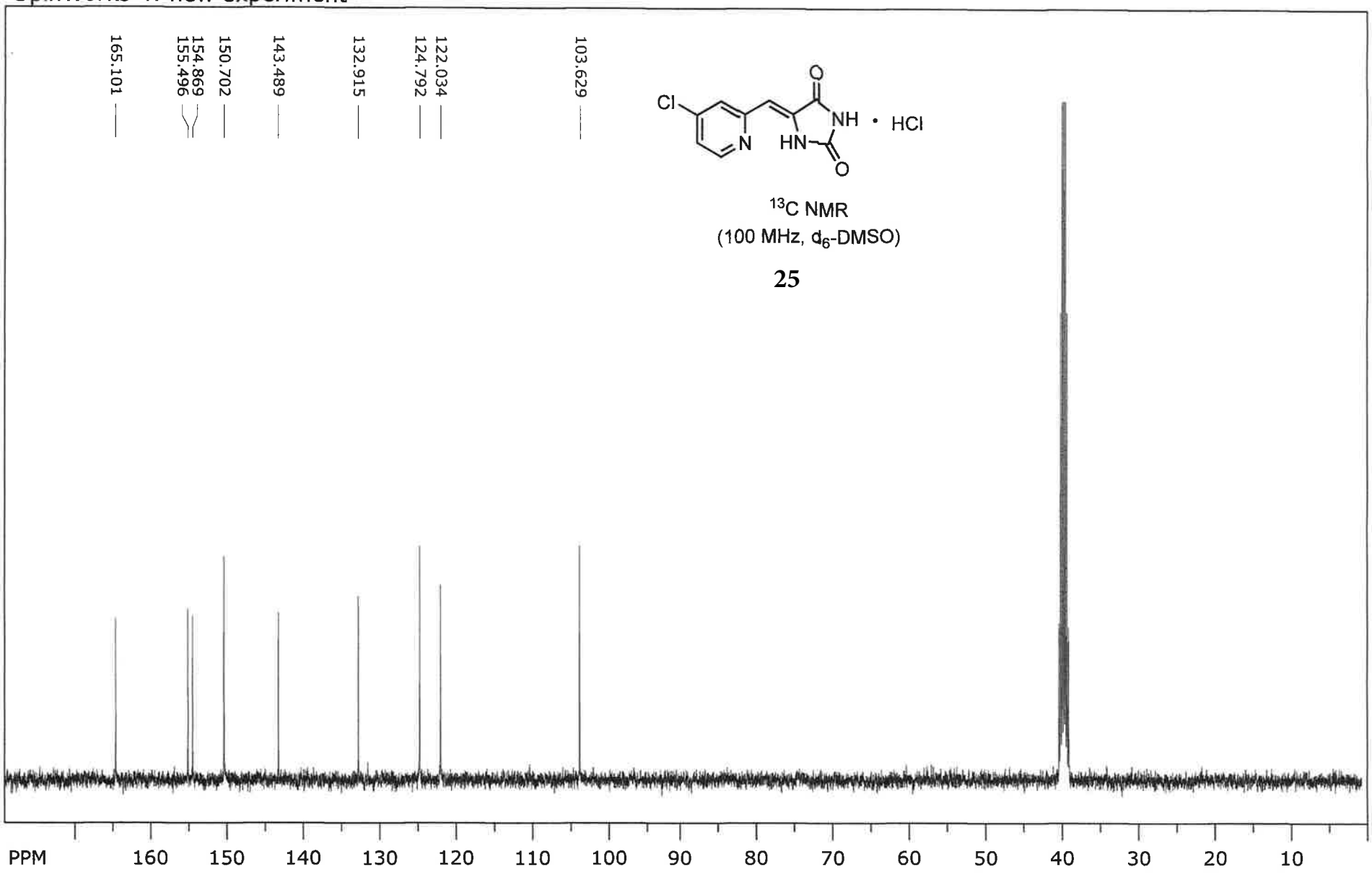
SpinWorks 4: 9_28_20_EAW995_TopLayer



file: ...spectra\WD340-349\WD347-1H.fid\fid block# 1 expt: "s2pul"
transmitter freq.: 399.732139 MHz
time domain size: 32768 points
width: 6410.26 Hz = 16.0364 ppm = 0.195626 Hz/pt
number of scans: 8

freq. of 0 ppm: 399.729734 MHz
processed size: 32768 complex points
LB: 0.610 GF: 0.0000
Hz/cm: 143.875 ppm/cm: 0.35993

SpinWorks 4: new experiment



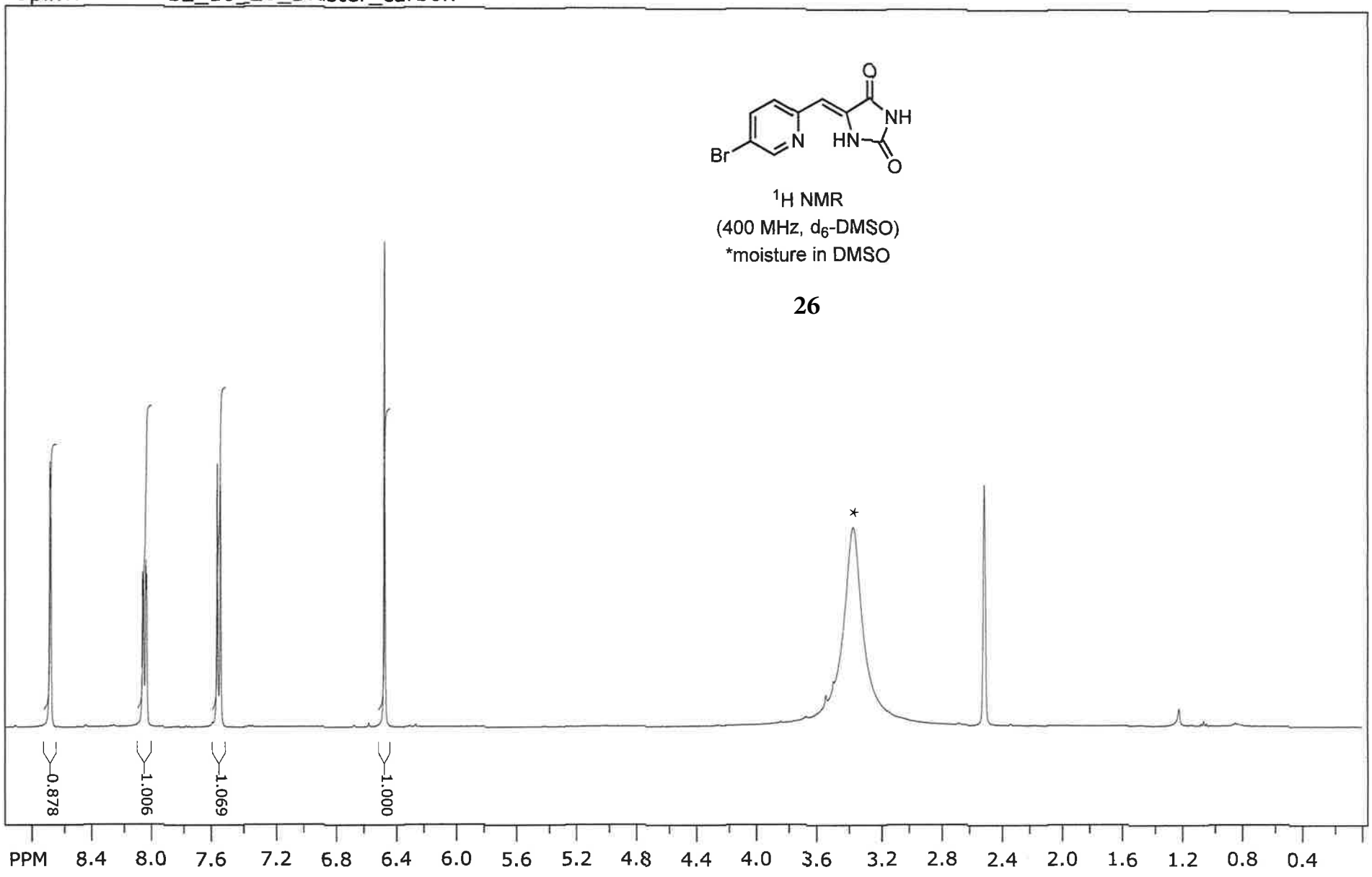
^{13}C NMR
(100 MHz, d_6-DMSO)

25

file: ...pectra\WD340-349\WD347-13C.fid\fid block# 1 expt: "s2pul"
transmitter freq.: 100.523180 MHz
time domain size: 65536 points
width: 25000.00 Hz = 248.6989 ppm = 0.381470 Hz/pt
number of scans: 512

freq. of 0 ppm: 100.512162 MHz
processed size: 65536 complex points
LB: 1.500 GF: 0.0000
Hz/cm: 723.333 ppm/cm: 7.19569

SpinWorks 4: 12_10_20_Diester_carbon



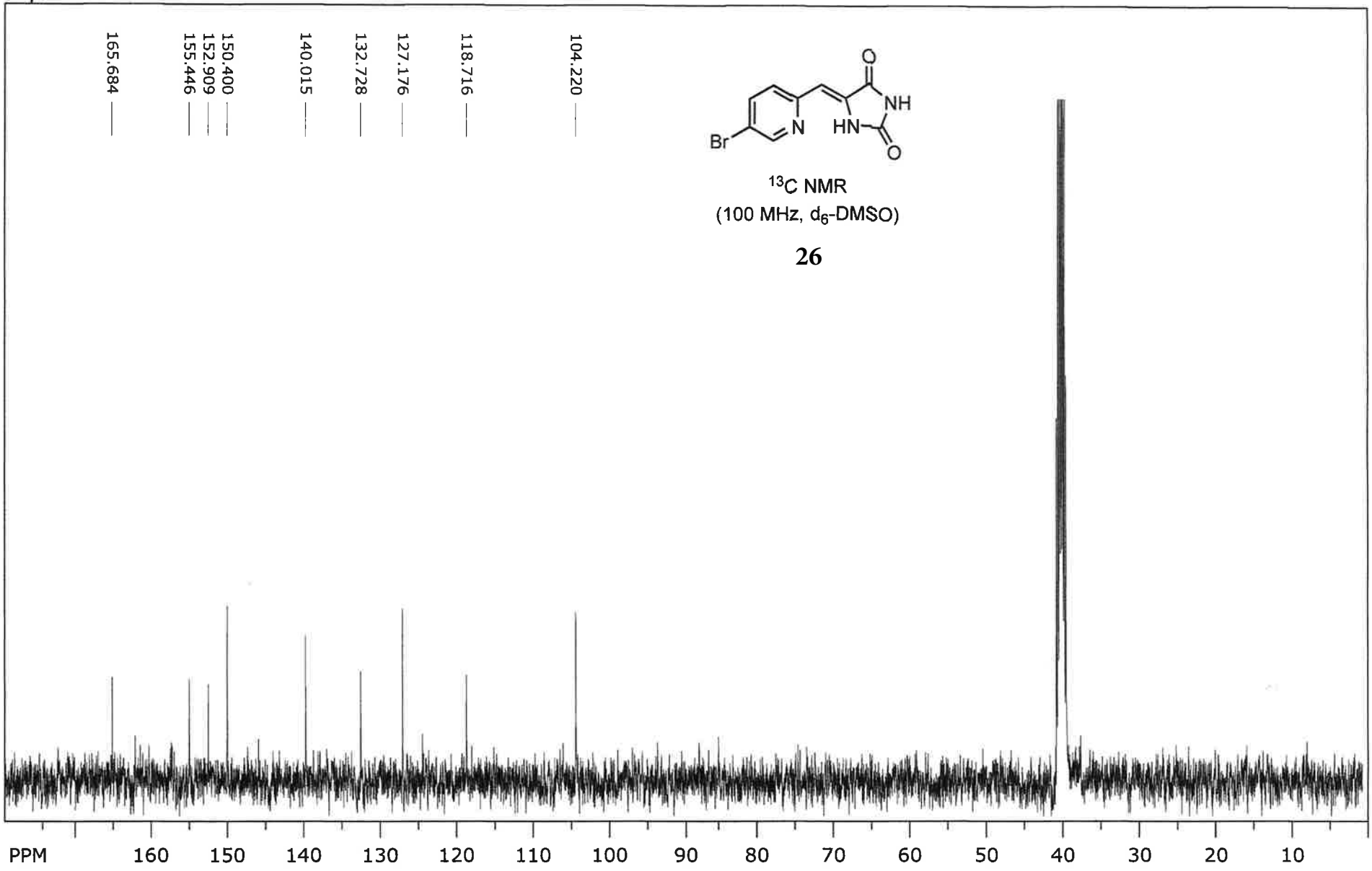
^{1}H NMR
(400 MHz, d_6-DMSO)
*moisture in DMSO

26

file: ...spectra\WD330-339\WD333-H1.fid\fid block# 1 expt: "s2pul"
transmitter freq.: 399.732139 MHz
time domain size: 32768 points
width: 6410.26 Hz = 16.0364 ppm = 0.195626 Hz/pt
number of scans: 8

freq. of 0 ppm: 399.729733 MHz
processed size: 32768 complex points
LB: 0.610 GF: 0.0000
Hz/cm: 144.017 ppm/cm: 0.36028

SpinWorks 4: wefarv



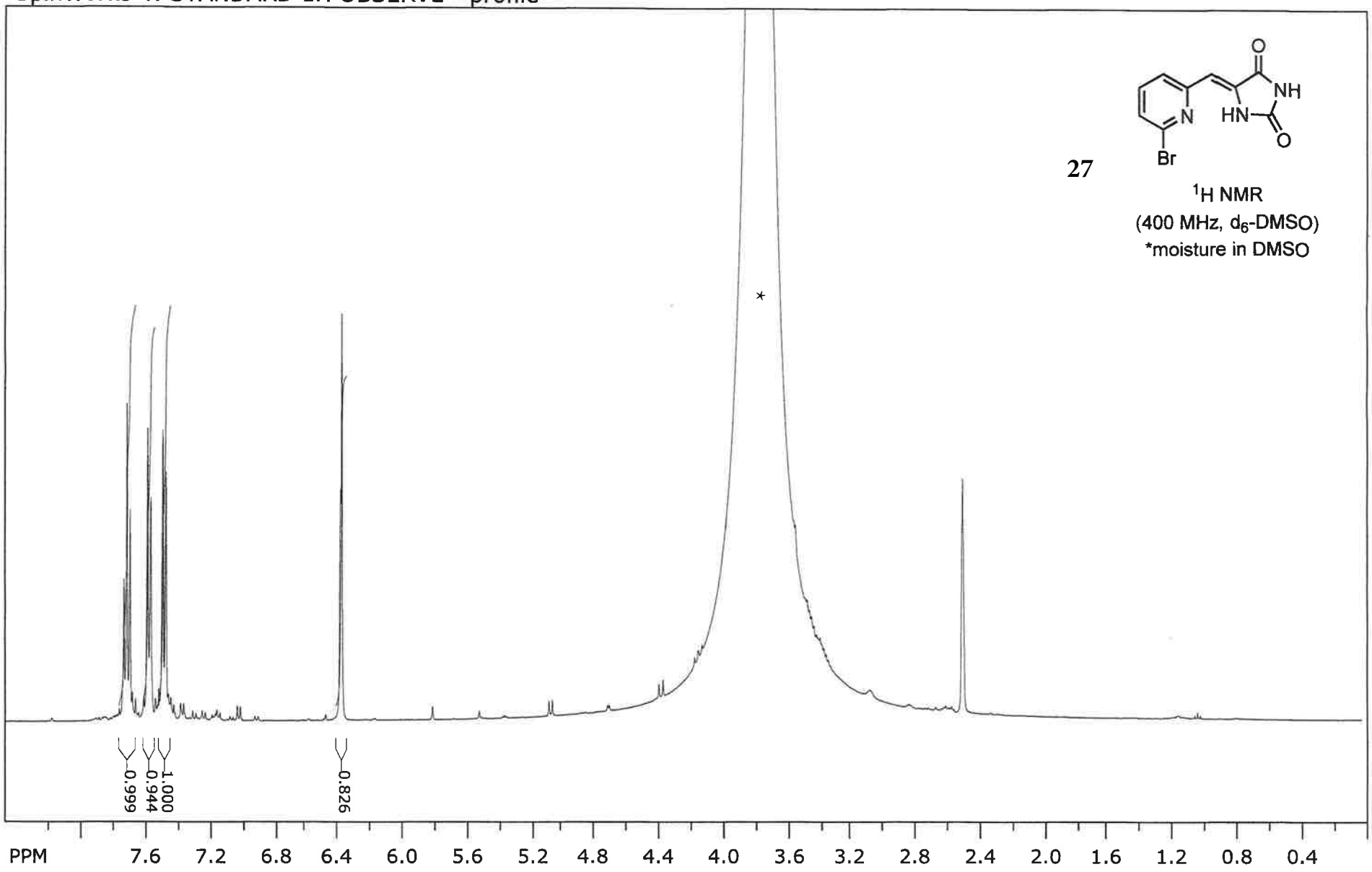
^{13}C NMR
(100 MHz, d_6-DMSO)

26

file: ...pectra\WD330-339\WD333-C13.fid\fid block# 1 expt: "s2pul"
transmitter freq.: 100.523180 MHz
time domain size: 65536 points
width: 25000.00 Hz = 248.6989 ppm = 0.381470 Hz/pt
number of scans: 256

freq. of 0 ppm: 100.512123 MHz
processed size: 65536 complex points
LB: 2.500 GF: 0.0000
Hz/cm: 723.889 ppm/cm: 7.20121

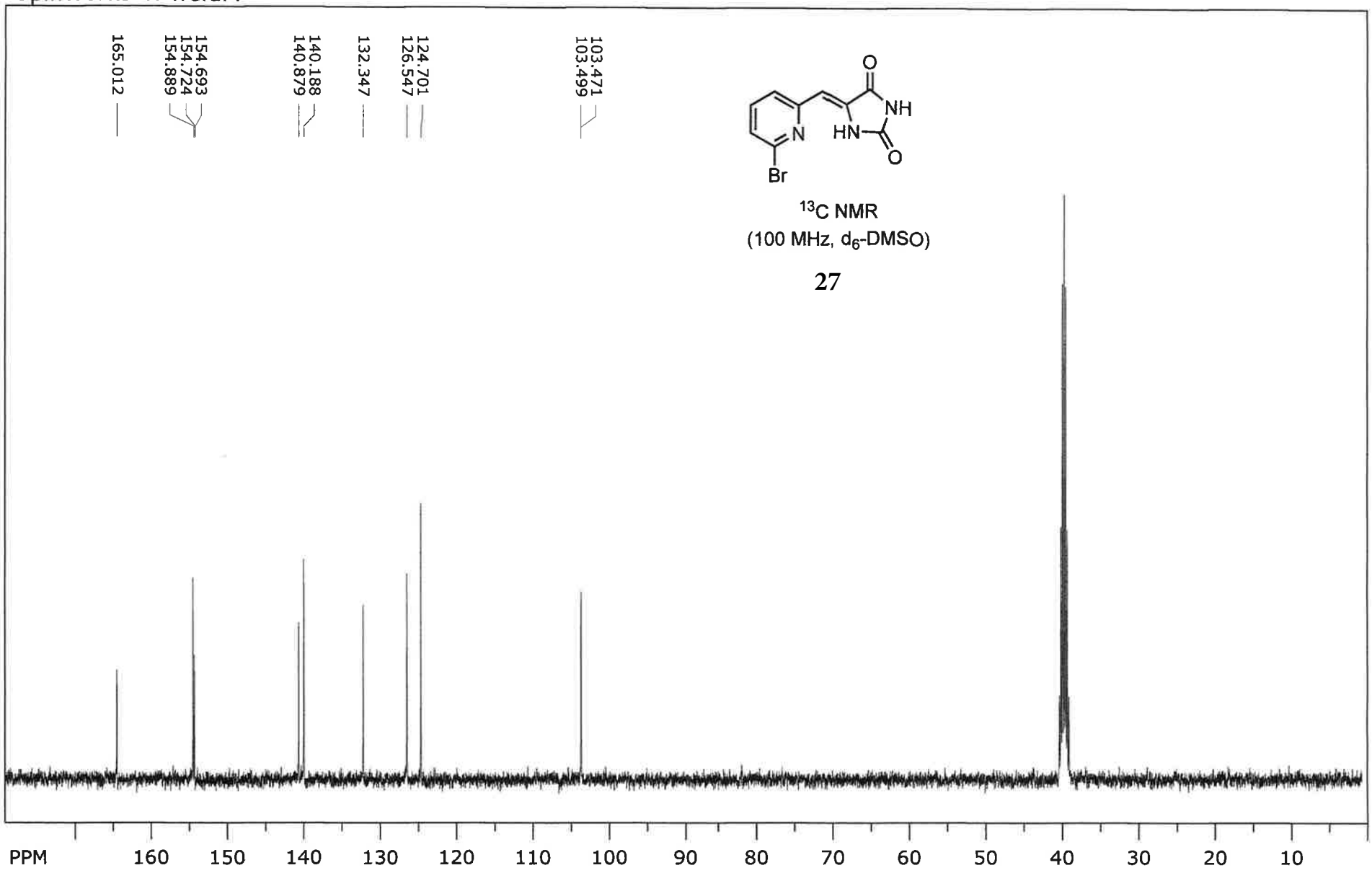
SpinWorks 4: STANDARD 1H OBSERVE - profile



file: ...pectra\WD spectra\WD326_1H.fid\fid block# 1 expt: "s2pul"
transmitter freq.: 399.732139 MHz
time domain size: 32768 points
width: 6410.26 Hz = 16.0364 ppm = 0.195626 Hz/pt
number of scans: 8

freq. of 0 ppm: 399.729734 MHz
processed size: 32768 complex points
LB: 0.506 GF: 0.0000
Hz/cm: 135.897 ppm/cm: 0.33997

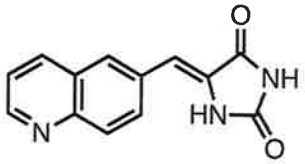
SpinWorks 4: wefarv



file: ...pectra\WD320-329\WD327-C13.fid\fid block# 1 expt: "s2pul"
transmitter freq.: 100.523180 MHz
time domain size: 65536 points
width: 25000.00 Hz = 248.6989 ppm = 0.381470 Hz/pt
number of scans: 256

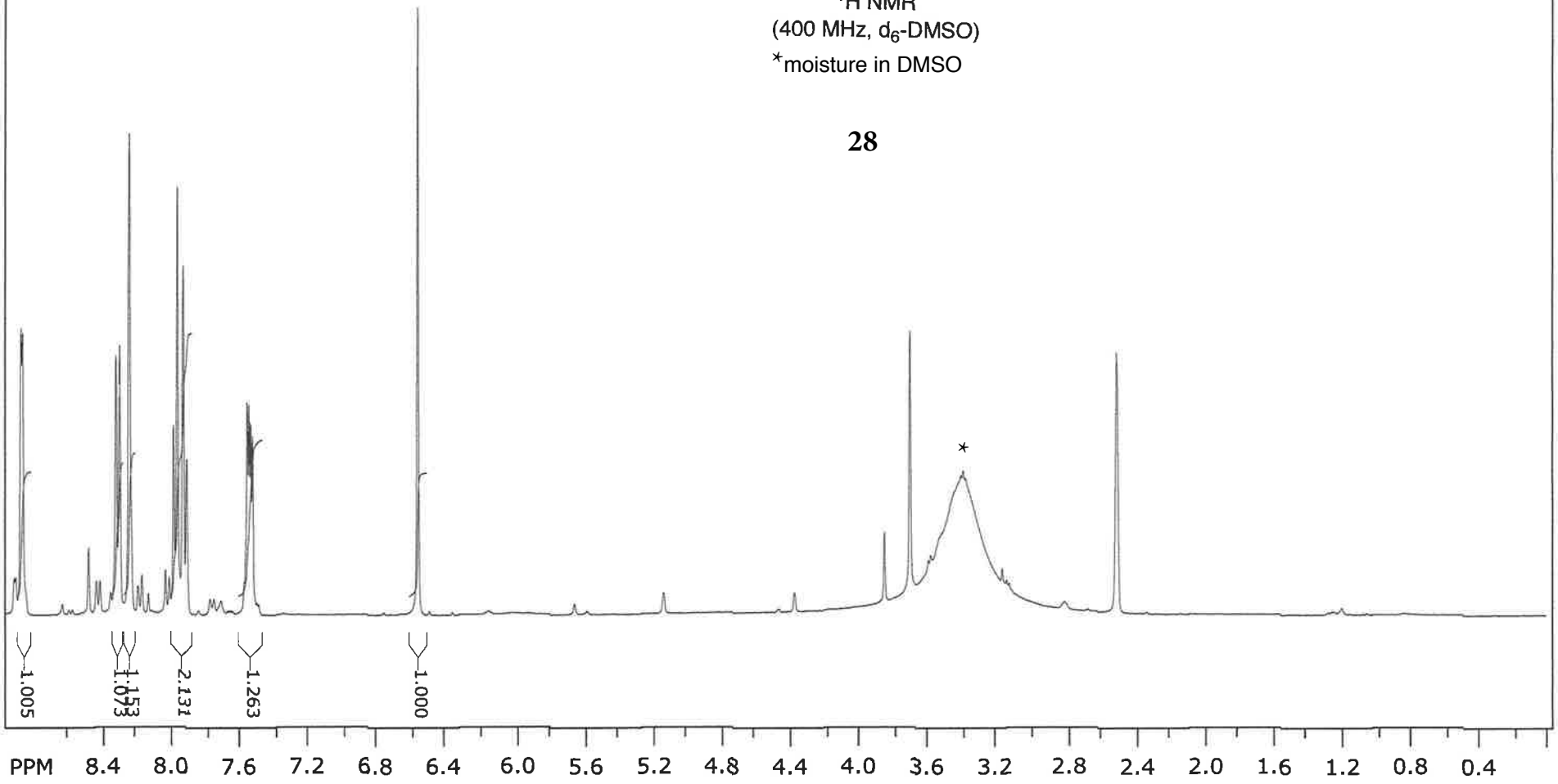
freq. of 0 ppm: 100.512160 MHz
processed size: 65536 complex points
LB: 1.500 GF: 0.0000
Hz/cm: 723.333 ppm/cm: 7.19569

SpinWorks 4: rr



^{1}H NMR
(400 MHz, d_6-DMSO)
*moisture in DMSO

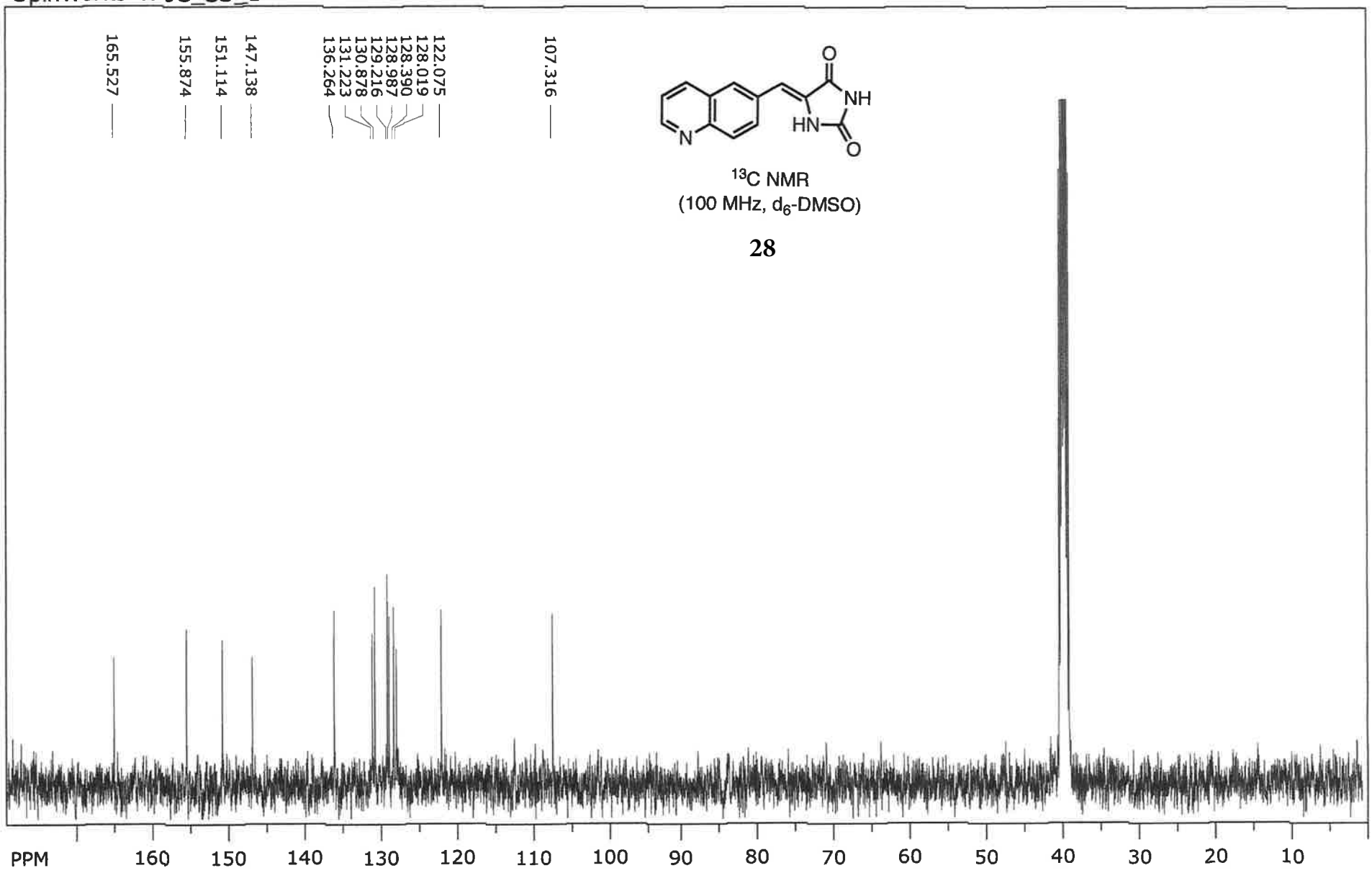
28



file: ...pectra\KG01-10\KG10-proton.fid\fid block# 1 expt: "s2pul"
transmitter freq.: 399.732139 MHz
time domain size: 32768 points
width: 6410.26 Hz = 16.0364 ppm = 0.195626 Hz/pt
number of scans: 8

freq. of 0 ppm: 399.729733 MHz
processed size: 32768 complex points
LB: 0.500 GF: 0.0000
Hz/cm: 143.732 ppm/cm: 0.35957

SpinWorks 4: JC_SS_1



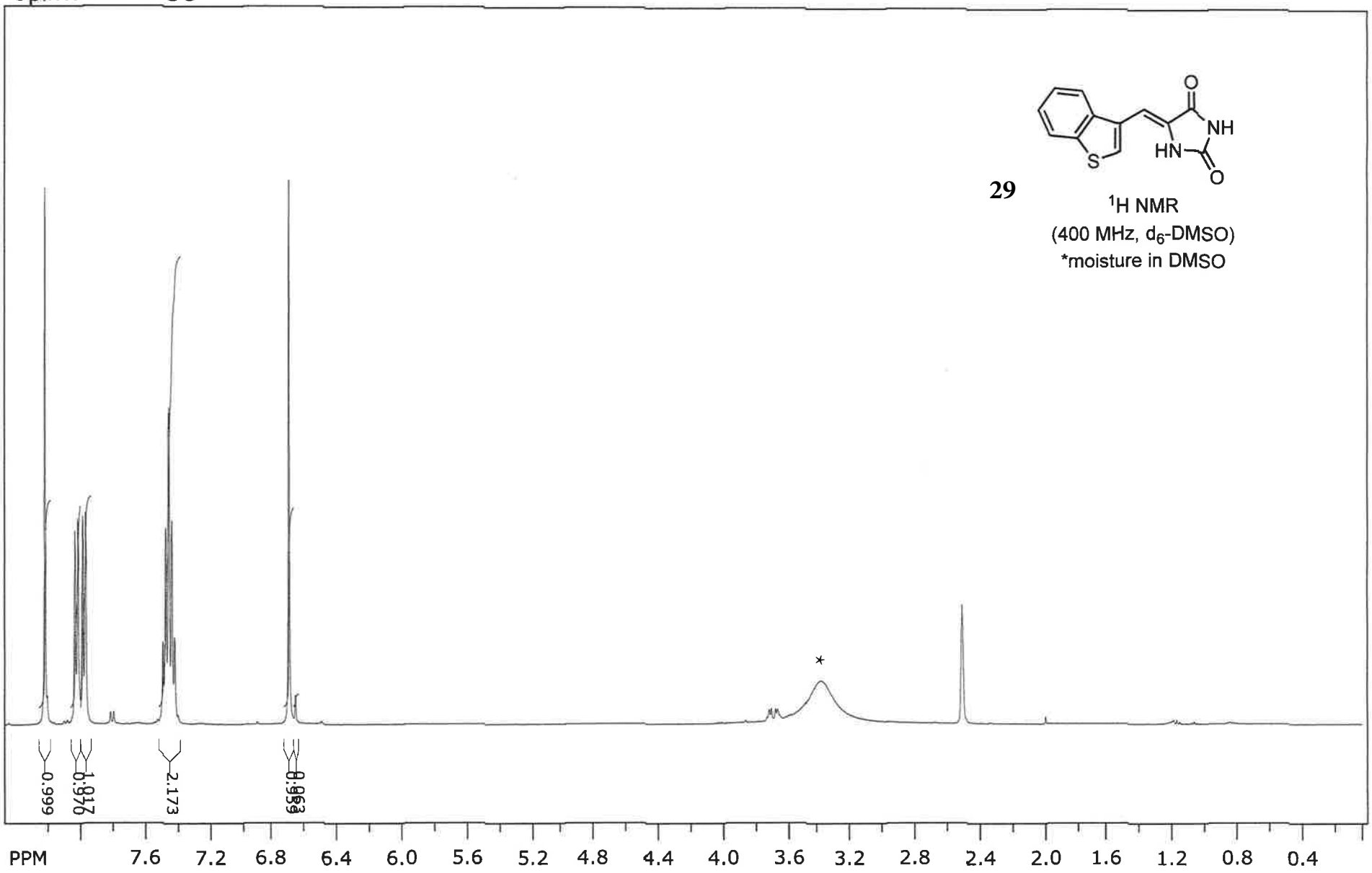
^{13}C NMR
(100 MHz, d_6-DMSO)

28

file: ...son\KG10_13C_DMSO_20240118.fid\fid block# 1 expt: "s2pul"
transmitter freq.: 100.523180 MHz
time domain size: 65536 points
width: 25000.00 Hz = 248.6989 ppm = 0.381470 Hz/pt
number of scans: 2048

freq. of 0 ppm: 100.512162 MHz
processed size: 65536 complex points
LB: 2.500 GF: 0.0000
Hz/cm: 723.333 ppm/cm: 7.19569

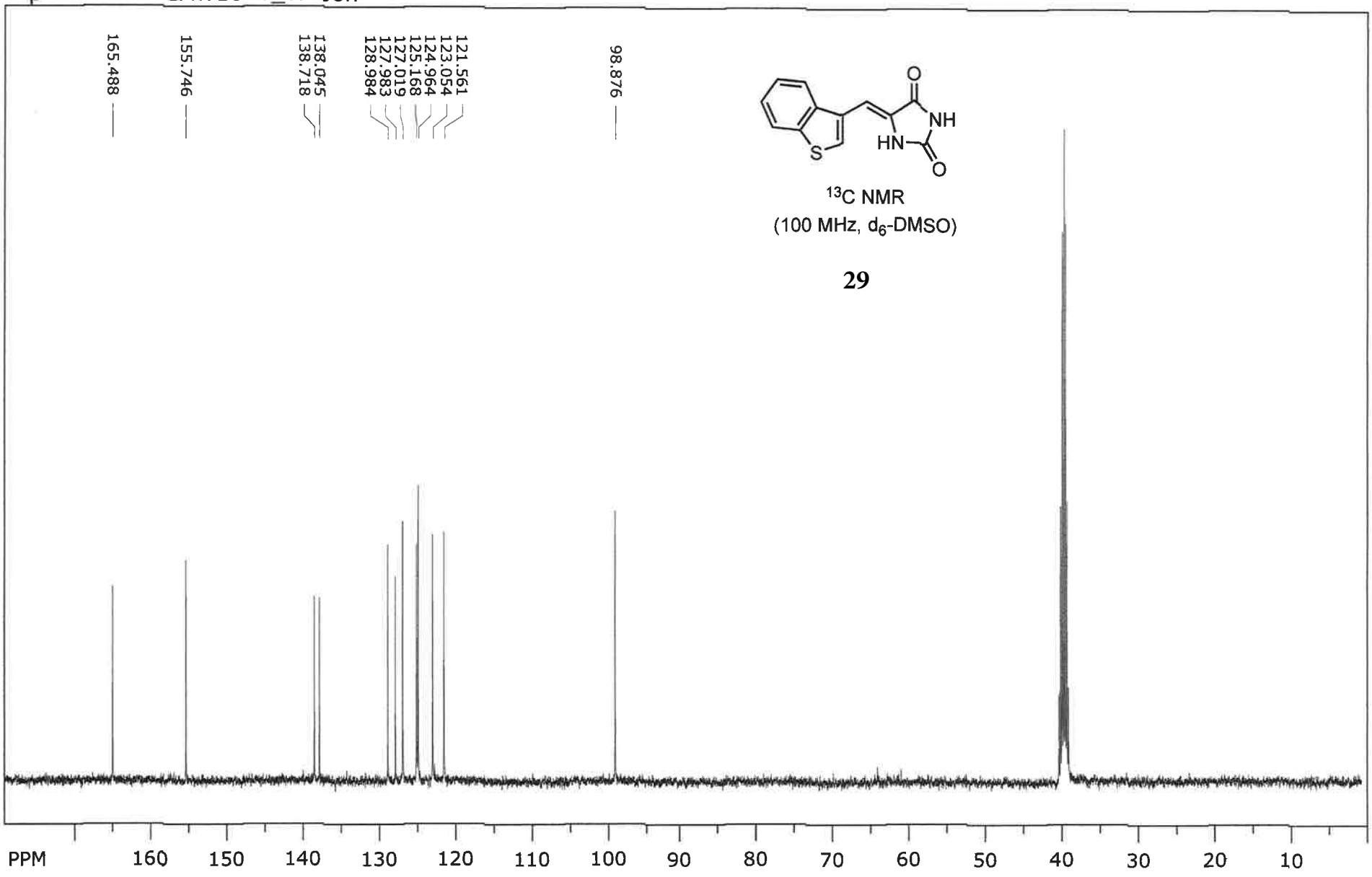
SpinWorks 4: SC



file: ...pectra\KG11-20\KG18-proton.fid\fid block# 1 expt: "s2pul"
transmitter freq.: 399.732139 MHz
time domain size: 32768 points
width: 6410.26 Hz = 16.0364 ppm = 0.195626 Hz/pt
number of scans: 8

freq. of 0 ppm: 399.729735 MHz
processed size: 32768 complex points
LB: 0.500 GF: 0.0000
Hz/cm: 135.897 ppm/cm: 0.33997

SpinWorks 4: EAW1050_carbon



^{13}C NMR
(100 MHz, d_6-DMSO)

29

file: ...ldsonw\Desktop\KG18-carbon.fid\fid block# 1 expt: "s2pul"
transmitter freq.: 100.523180 MHz
time domain size: 65536 points
width: 25000.00 Hz = 248.6989 ppm = 0.381470 Hz/pt
number of scans: 256

freq. of 0 ppm: 100.512160 MHz
processed size: 65536 complex points
LB: 1.500 GF: 0.0000
Hz/cm: 723.333 ppm/cm: 7.19569