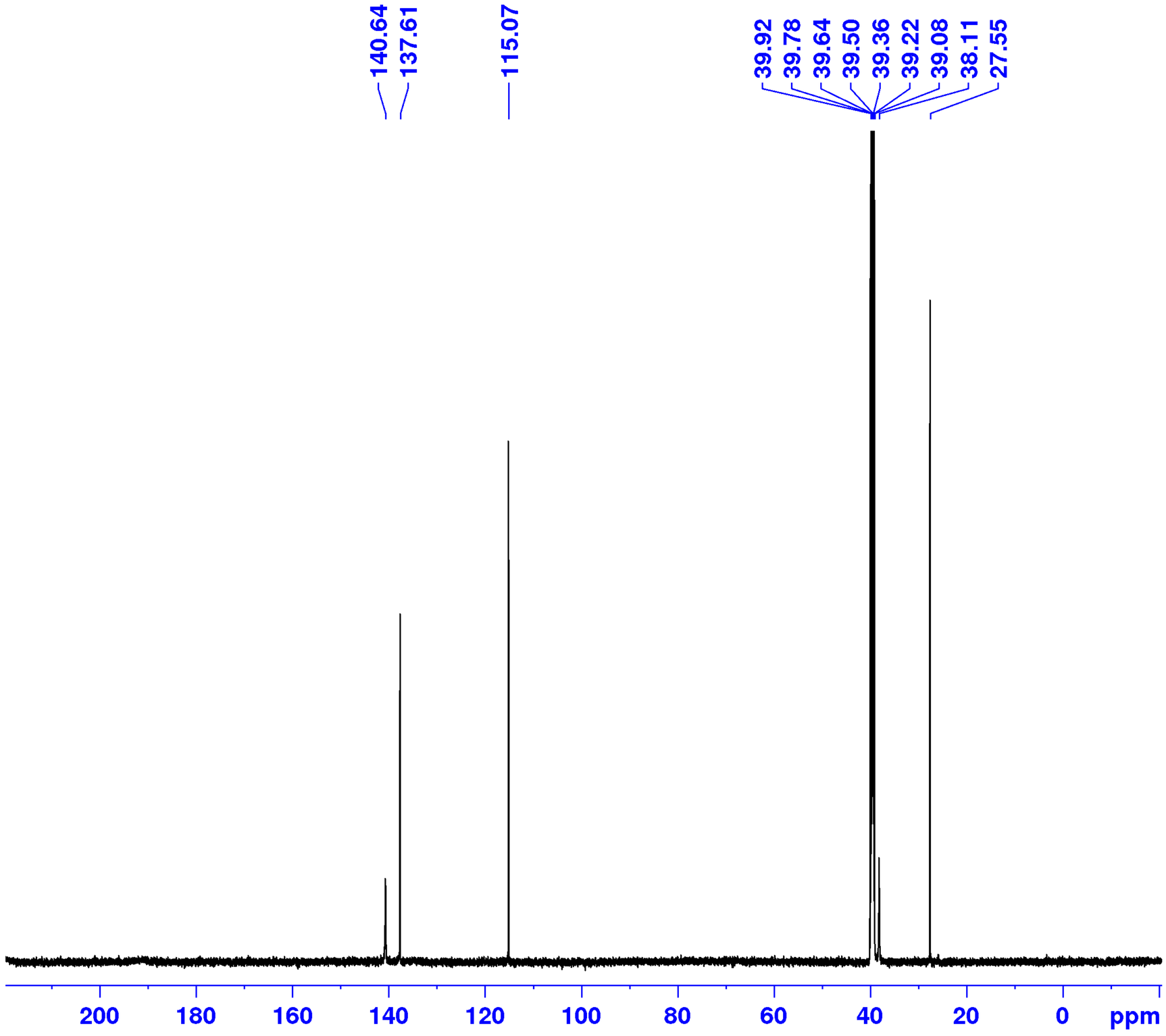
1-(5-Iodo-1H-imidazole-4-yl)pent-4-en-1-one 13C NMR



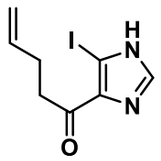
Current Data Parameters
NAME TCG-AC-L1-023-DMSO-13C-2-3-21
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210204
Time 6.52 h
INSTRUM spect
PROBHD Z148658_0003 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 5000
DS 4
SWH 36231.883 Hz
FIDRES 1.105709 Hz
AQ 0.9043968 sec
RG 199.73
DW 13.800 usec
DE 6.50 usec
TE 305.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 150.8864644 MHz
NUC1 13C
P1 12.00 usec
PLW1 77.65699768 W
SFO2 600.0074000 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 70.00 usec
PLW2 13.23200035 W
PLW12 0.64876997 W
PLW13 0.32633001 W

F2 - Processing parameters
SI 32768
SF 150.8714523 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Submitter's data

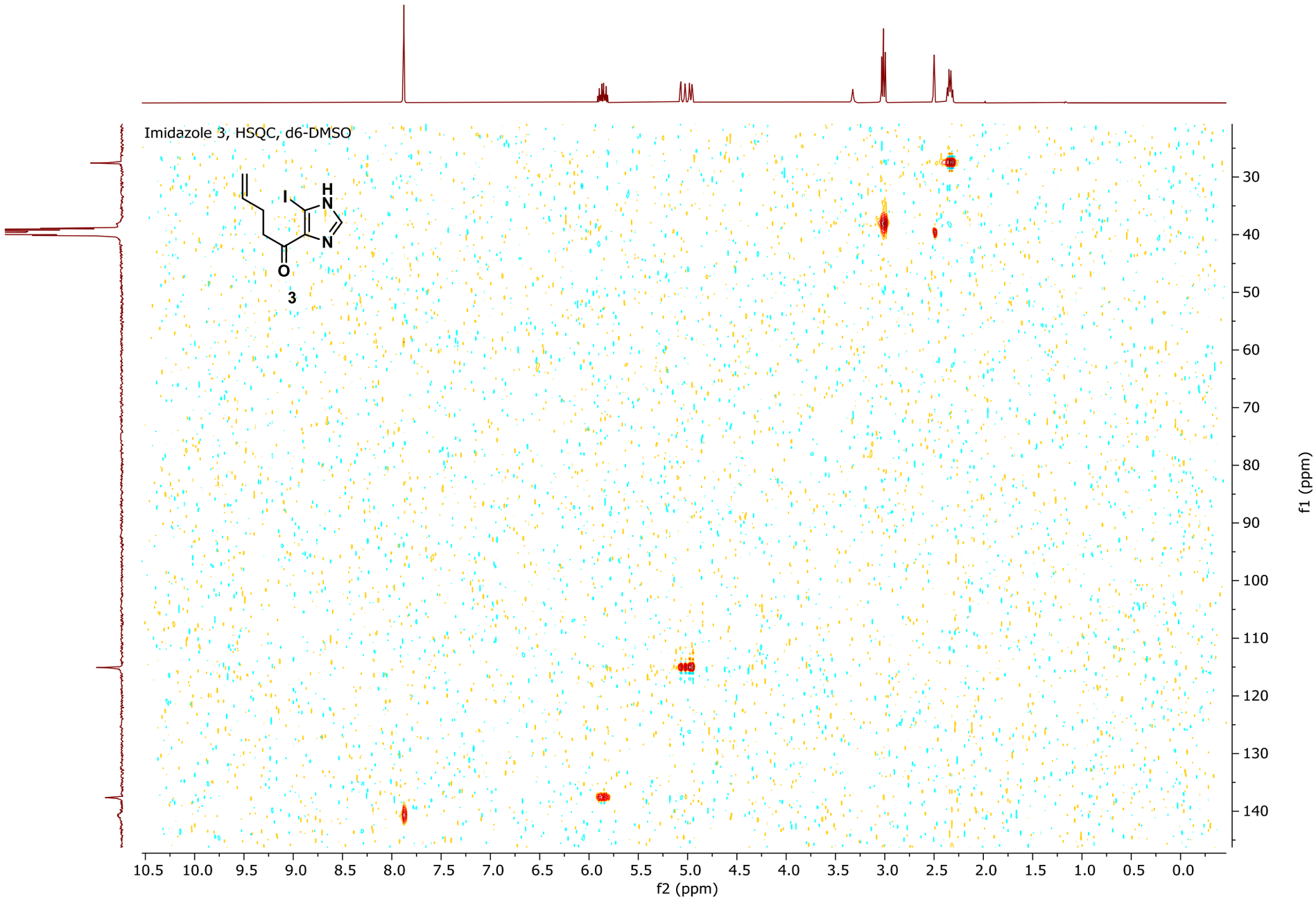
Imidazole 3, 13C, d6-DMSO



3

13C NMR (101 MHz, d6-DMSO) δ (194.6 exchanging with 188.5), 140.6, (140.2 exchanging with 132.1), 137.6, 115.1, (92.2 exchanging with 72.6), 38.0, 27.6 ppm. Two very broad signals were observed for each quaternary carbon due to imidazole-N1/3-H tautomers. Because of the broad peaks, these signals could only be observed in an HMBC spectrum (see spectrum below).

Submitter's data



Submitter's data