

4-[(2,4-Dichlorophenyl)carbamoyl]butanoic Acid

Bibi Hanifa ¹, Muhammad Sirajuddin ^{1,*}, Zafran Ullah ¹, Sumera Mahboob ², Kong Mun Lo ³, See Mun Lee ³
and Edward R.T. Tiekink ^{3,*}

- 1 Department of Chemistry, University of Science and Technology, Bannu 28100, Pakistan;
bibihanifa_std@ustb.edu.pk (B.H.); zafranullah_std@ustb.edu.pk (Z.U.)
 - 2 Center of Excellence in Science and Applied Technology, Islamabad 45400, Pakistan;
anachem@desto.gov.pk
 - 3 Research Centre for Crystalline Materials, School of Medical and Life Sciences, Sunway University,
No. 5 Jalan Universiti, Bandar Sunway 47500, Selangor Darul Ehsan, Malaysia;
annieleee@sunway.edu.my (S.M.L.); kmlo@sunway.edu.my (K.M.L.)
- * Correspondence: dr.sirajuddin@ustb.edu.pk (M.S.); edwardt@sunway.edu.my (E.R.T.T.)

*** SUPPLEMENTARY MATERIALS ***

Figure S1: FTIR spectrum of 4-[(2,4-dichlorophenyl)carbamoyl]butanoic acid (**1**).

Figure S2: ¹H NMR spectrum of 4-[(2,4-dichlorophenyl)carbamoyl]butanoic acid (**1**).

Figure S3: ¹³C{¹H} NMR spectrum of 4-[(2,4-dichlorophenyl)carbamoyl]butanoic acid (**1**).

Figure S4: The COSY spectrum of 4-[(2,4-dichlorophenyl)carbamoyl]butanoic acid (**1**).

Figure S5: The HMBC spectrum of 4-[(2,4-dichlorophenyl)carbamoyl]butanoic acid (**1**).

Figure S6: UV spectrum of 4-[(2,4-dichlorophenyl)carbamoyl]butanoic acid (**1**).

Figure S7: The GC-MS spectrum of 4-[(2,4-dichlorophenyl)carbamoyl]butanoic acid (**1**).

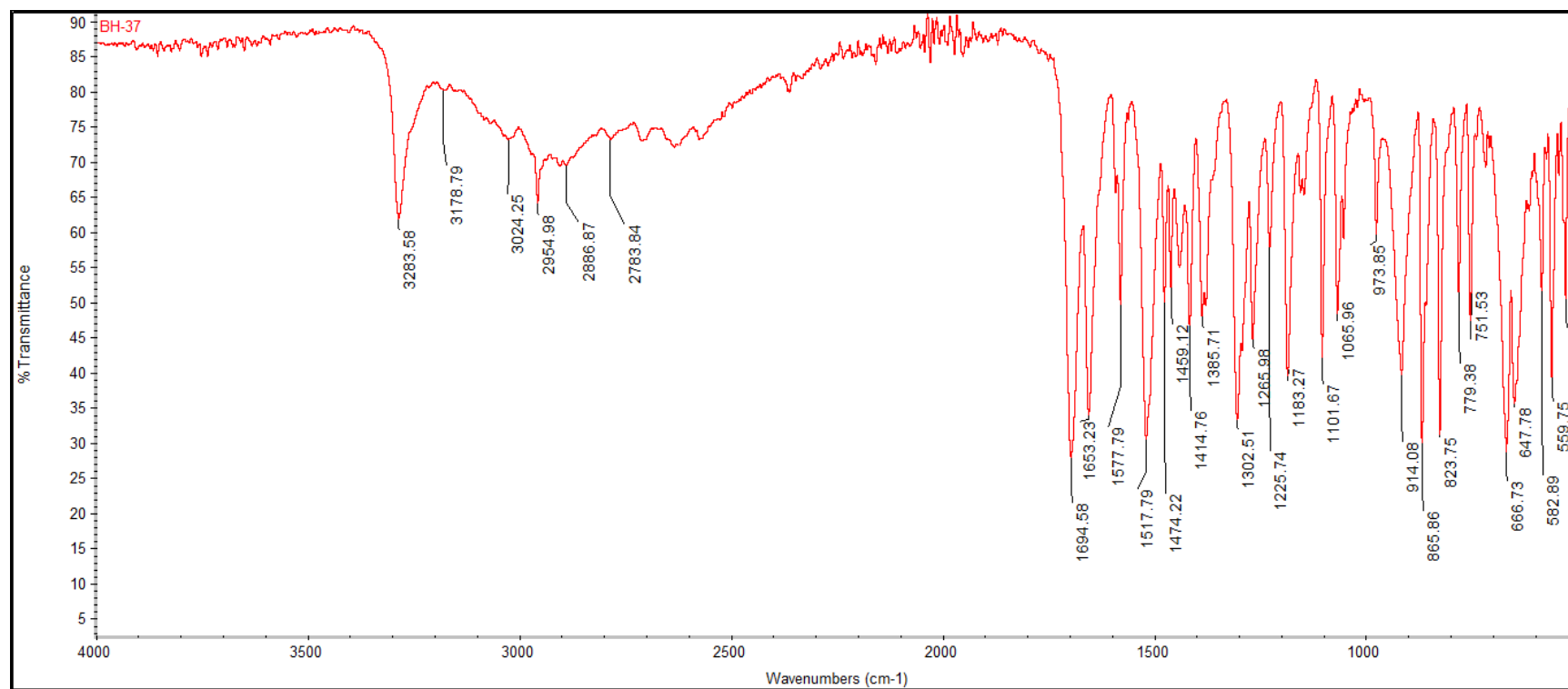
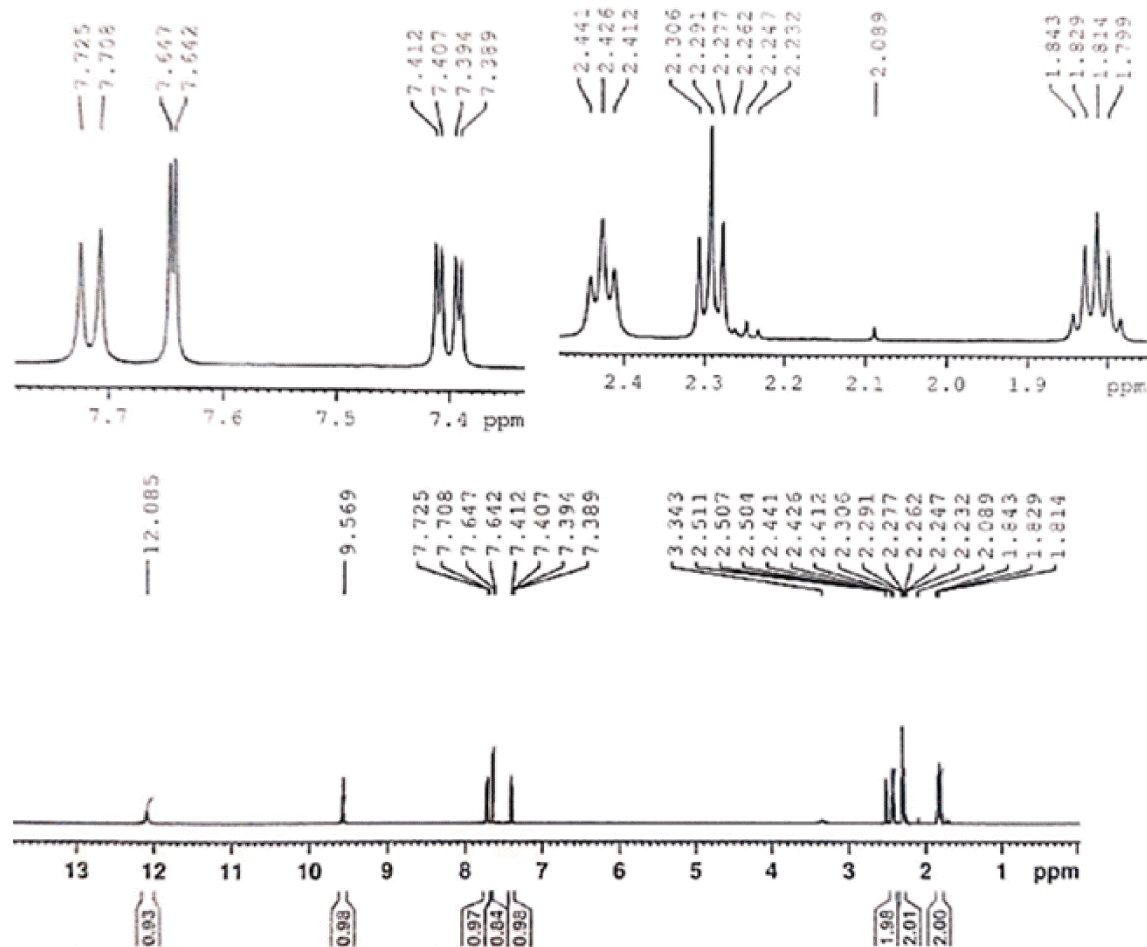


Figure S1: FTIR spectrum of 4-[(2,4-dichlorophenyl)carbamoyl]butanoic acid (**1**). The FTIR spectrum was measured on a Thermo Nicolet-6700 spectrophotometer (Vienna, Austria) from 4000 to 450 cm⁻¹.

BH-37-HNMR



Current Data Parameters
NAME 20210527-03
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210527
Time 11.53 h
INSTRUM spect
PROBHD z119470_0240 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 85.76
DW 50.000 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 500.2930893 MHz
NUC1 1H
P1 10.00 usec
PLW1 20.81399918 W

F2 - Processing parameters
SI 65536
SF 500.2900000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Figure S2: ^1H NMR spectrum of 4-[(2,4-dichlorophenyl)carbamoyl]butanoic acid (**1**). The ^1H NMR spectrum were recorded in DMSO- d_6 solution on a Bruker Avance 500 MHz NMR (Billerica, MA, USA) spectrometer with chemical shifts relative to DMSO (2.09 ppm).

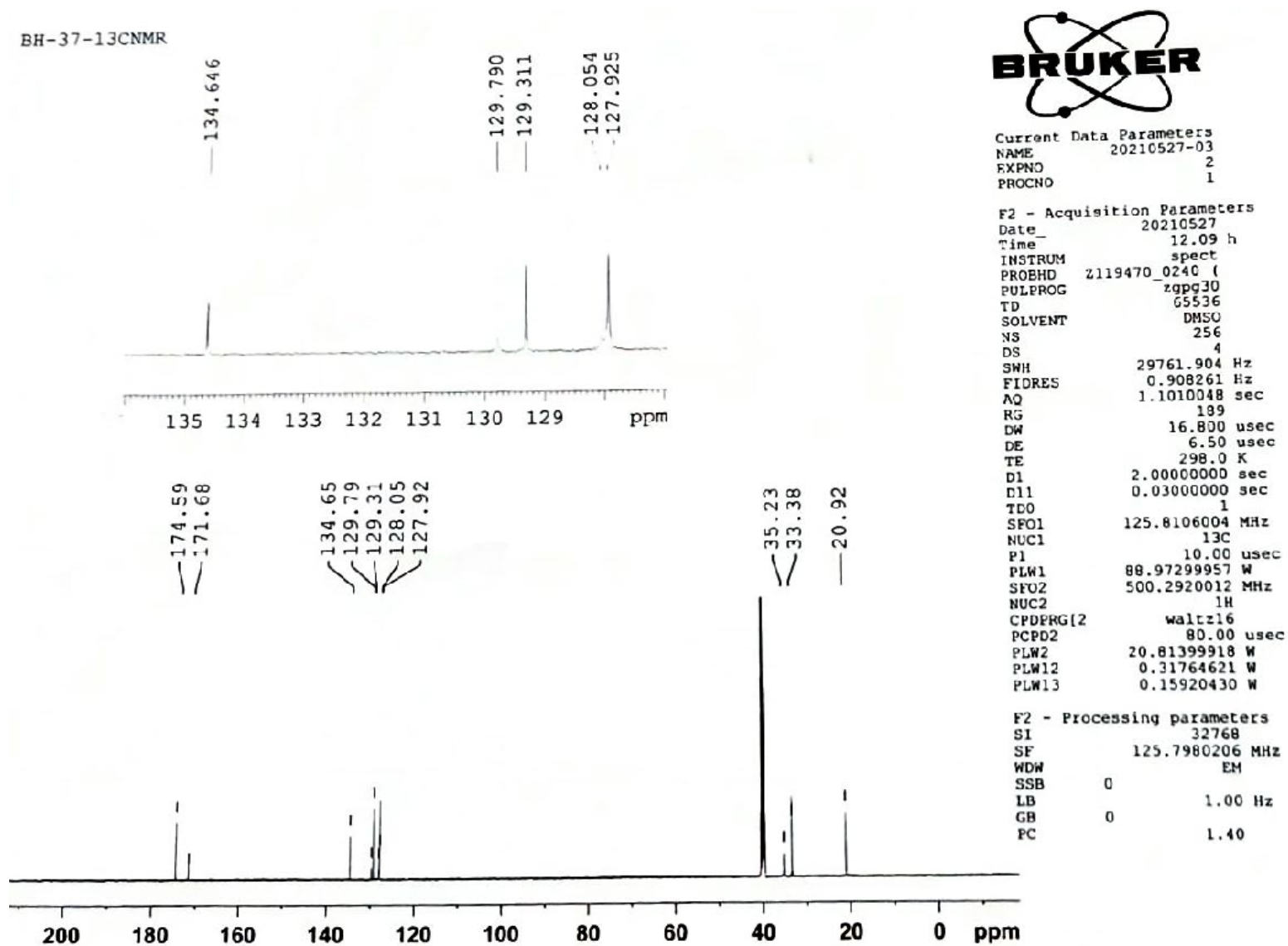
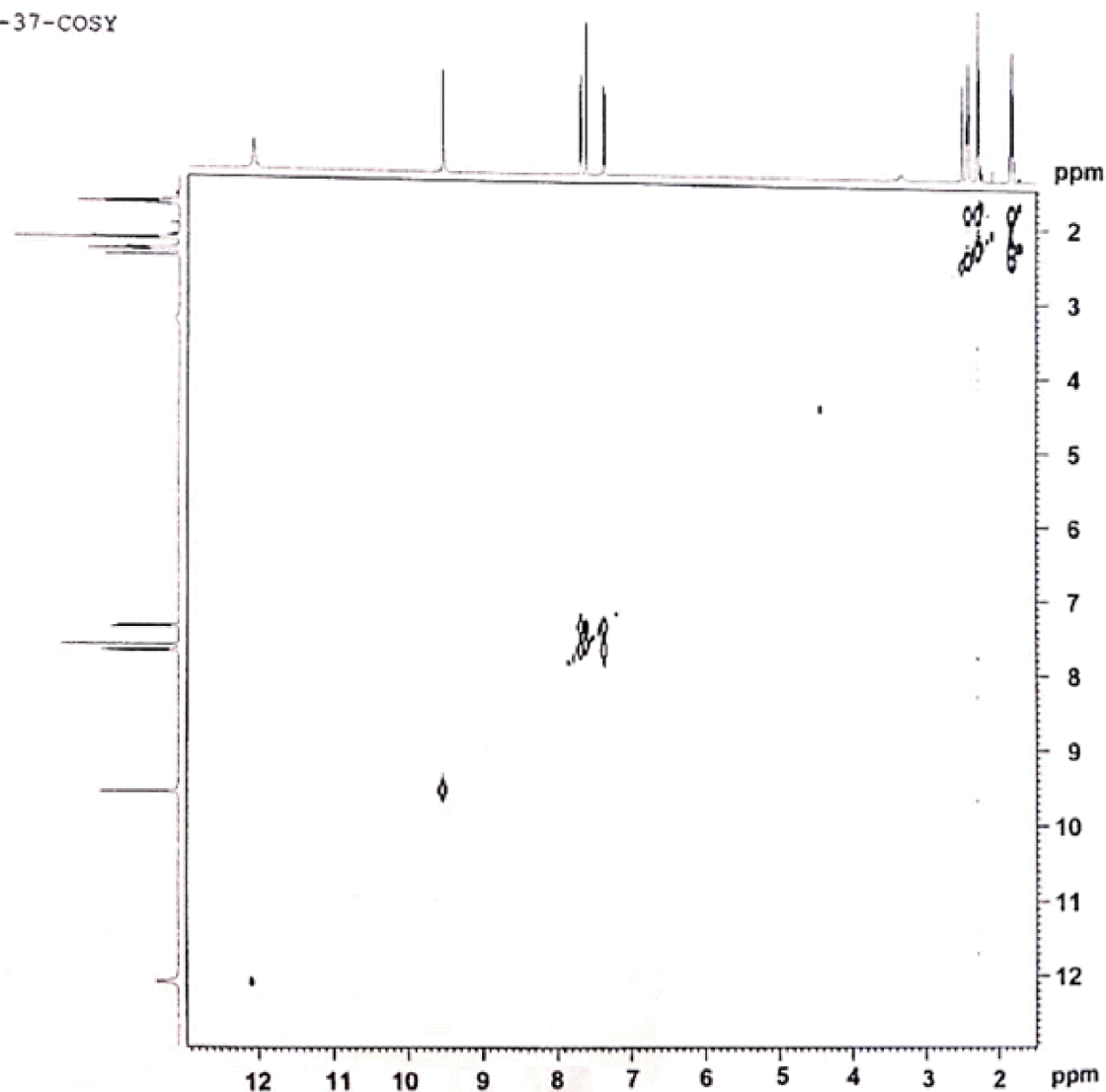


Figure S3: The ^{13}C NMR spectrum of 4-[(2,4-dichlorophenyl)carbamoyl]butanoic acid (**1**). The ^{13}C NMR spectrum was recorded in DMSO-d_6 solution on a Bruker Avance 500 MHz NMR (Billerica, MA, USA) spectrometer with chemical shifts relative to DMSO-d_6 (40.0 ppm).

BH-37-COSY



```

Current Data Parameters
NAME      20210527-03
EXPNO     5
PROCNO    1

F2 - Acquisition Parameters
Date_     20210527
Time      13.33 h
INSTRUM   spect
PROBHD    ZH19810_0340 1
PULPROG   zgpg30ppqf
TD         2048
SOLVENT   DMSO
NS         1
DS         16
SWH        5747.226 Hz
FIDRES     5.612428 Hz
AQ          0.1781760 sec
RG          389
CW          97.000 usec
DE          6.50 usec
TE          298.0 K
D0          0.00000100 sec
D1          2.00000000 sec
D11         0.03000000 sec
D12         0.00000000 sec
D13         0.00000400 sec
D14         0.00000000 sec
IN0         0.00017400 sec
TD0         1
SFO1       500.2936115 MHz
NUC1        1H
P0          10.00 usec
P1          10.00 usec
P17         2500.00 usec
PLW1        20.81399518 W
PLW10       2.71259990 W
GPMAN[1]    RMSQ10.100
GP11        10.00 s
P16         1000.00 usec

F1 - Acquisition parameters
TD          128
SFO1       500.2936 MHz
FIDRES      89.798851 Hz
SW          11.488 ppm
PRMODE      QF

F2 - Processing parameters
SI          1024
SF          500.2900000 MHz
WDW         QSINE
SSB          0
LB           0 Hz
GB           0
PC           1.40

F1 - Processing parameters
SI          1024
MC2         QF
SF          500.2900000 MHz
WDW         QSINE
SSB          0
LB           0 Hz
PC           1
  
```

Figure S4: The COSY spectrum of 4-[(2,4-dichlorophenyl)carbamoyl]butanoic acid (**1**). The COSY spectrum was recorded in DMSO- d_6 solution on a Bruker Avance 500 MHz NMR (Billerica, MA, USA) spectrometer.

BH37-HMBC 13C

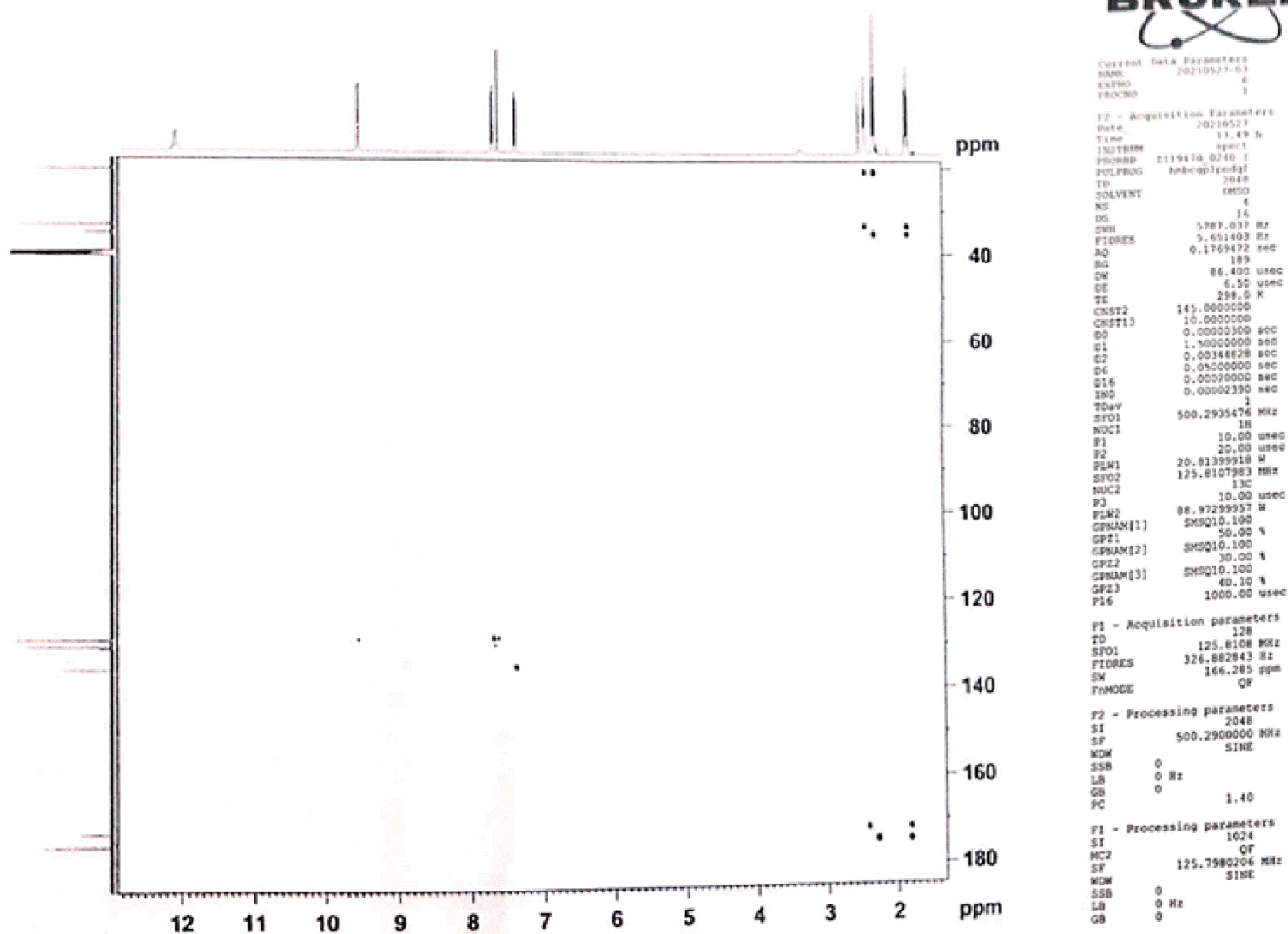


Figure S5: The HMBC spectrum of 4-[(2,4-dichlorophenyl)carbamoyl]butanoic acid (1). The HMBC spectrum was recorded in DMSO- d_6 solution on a Bruker Avance 500 MHz NMR (Billerica, MA, USA) spectrometer.

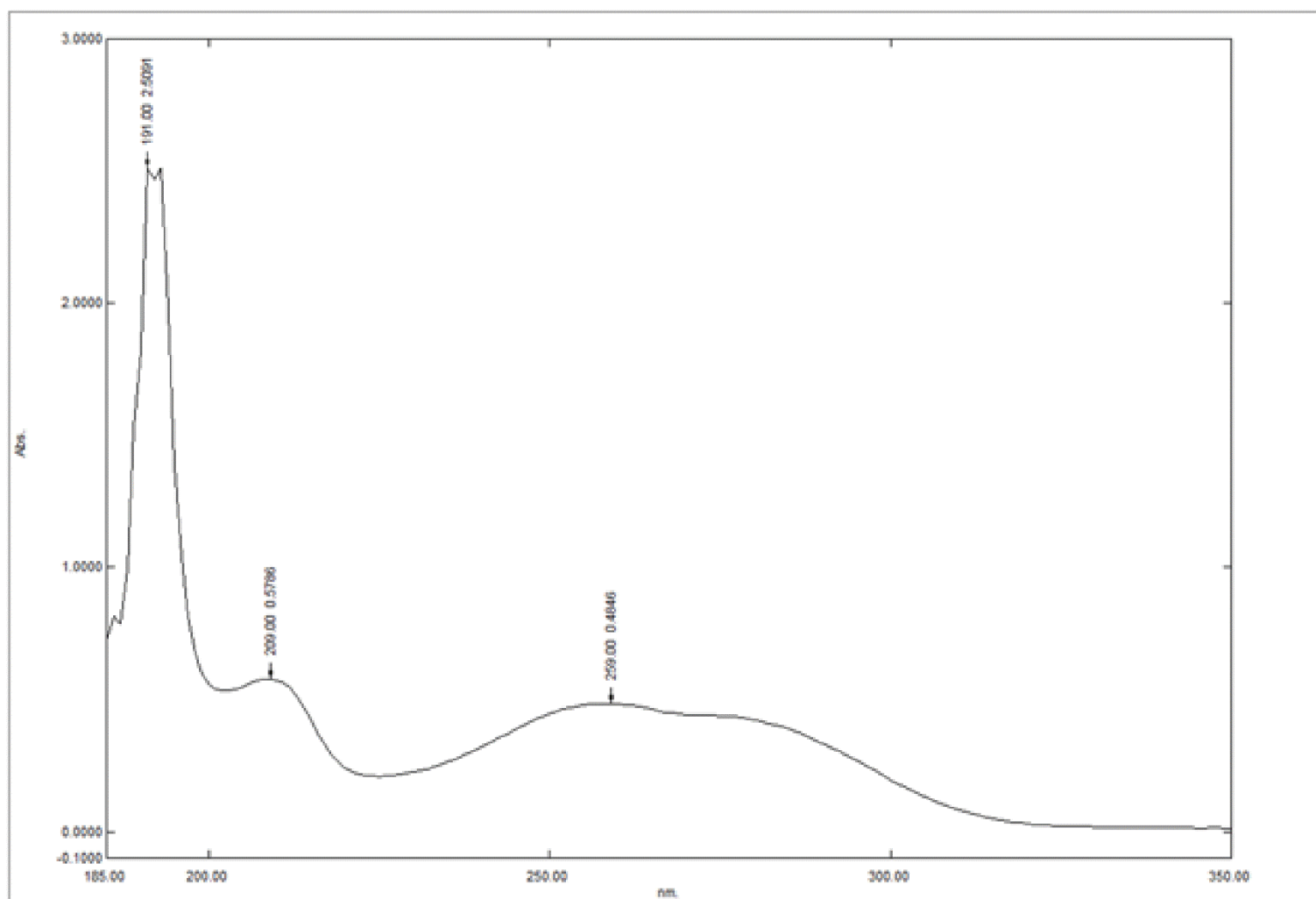


Figure S6: The UV spectrum of 4-[(2,4-dichlorophenyl)carbamoyl]butanoic acid (**1**). The optical absorption spectrum was obtained from a 1.268×10^{-5} M acetonitrile solution of (**1**) in the range 185–350 nm on a Shimadzu UV-3600 plus UV/VIS/NIR (Shimadzu Corporation, Kyoto Prefecture, Japan) spectrophotometer.

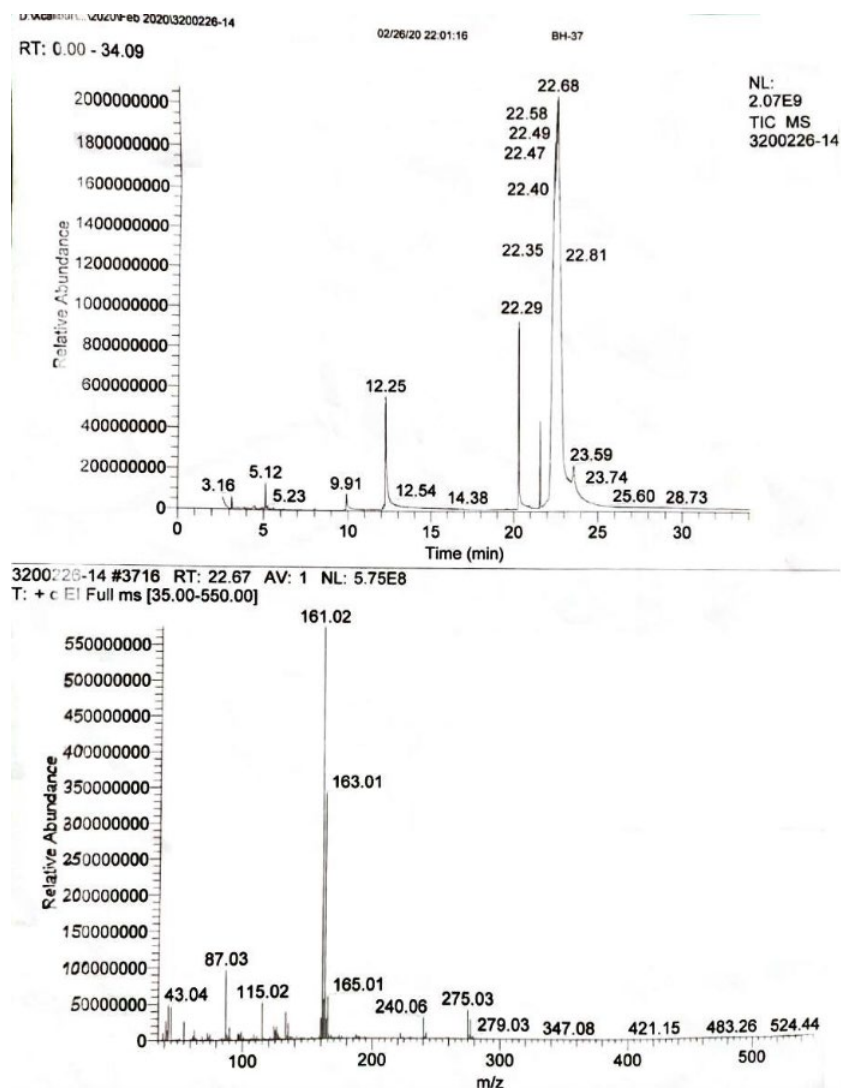


Figure S7: The GC-MS spectrum of 4-[(2,4-dichlorophenyl)carbamoyl]butanoic acid (**1**). The spectrum was obtained on a Thermo Scientific™ TRACE™ 1310 Gas Chromatograph and Thermo Scientific™ ISQ™ Series Quadrupole GC-MS (Waltham, MA, USA).