

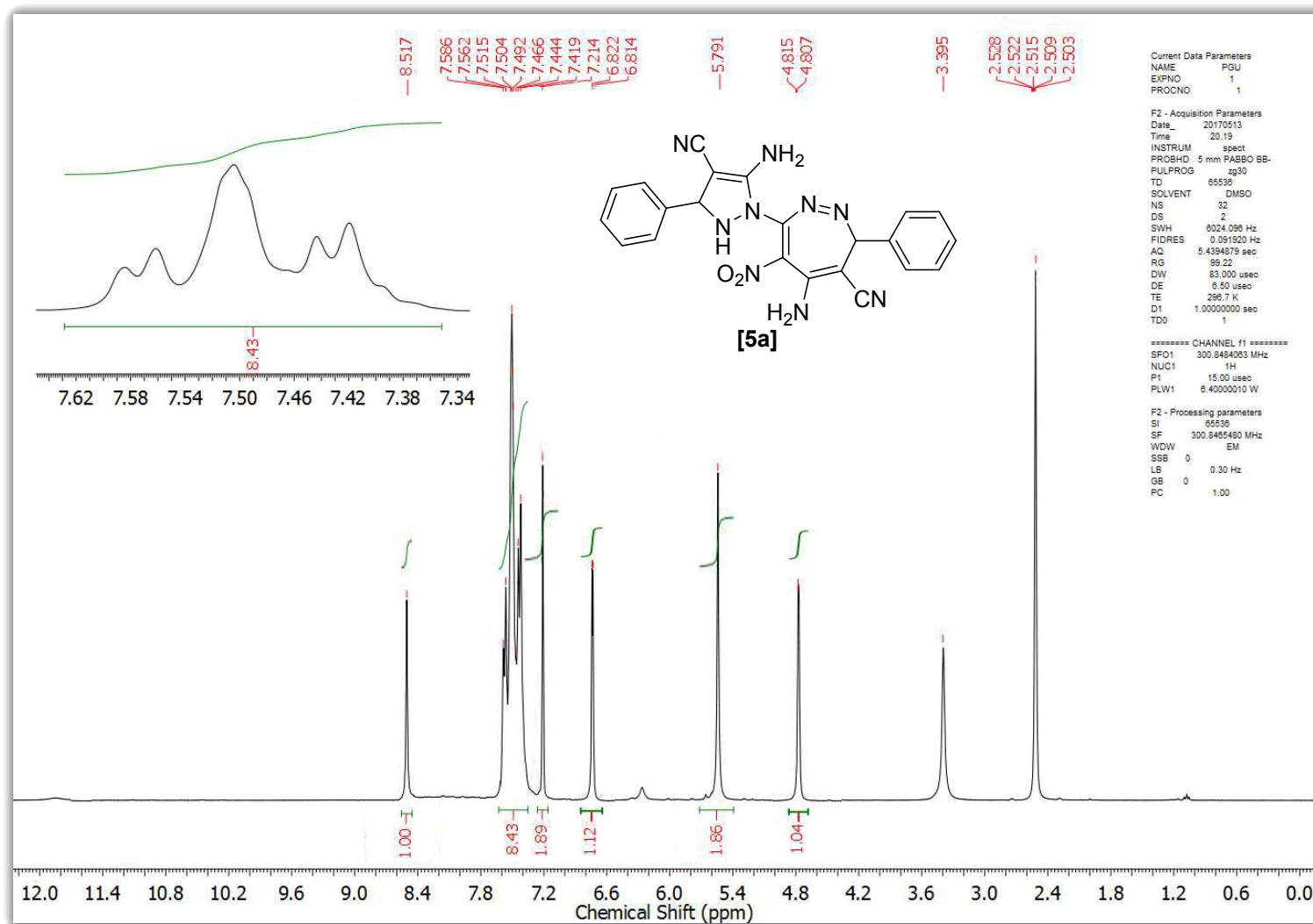
Highly Efficient, Catalyst-free, One-pot, *Pseudo* Seven-Component Synthesis of Novel Poly Substituted Pyrazolyl-1,2-Diazepine Derivatives

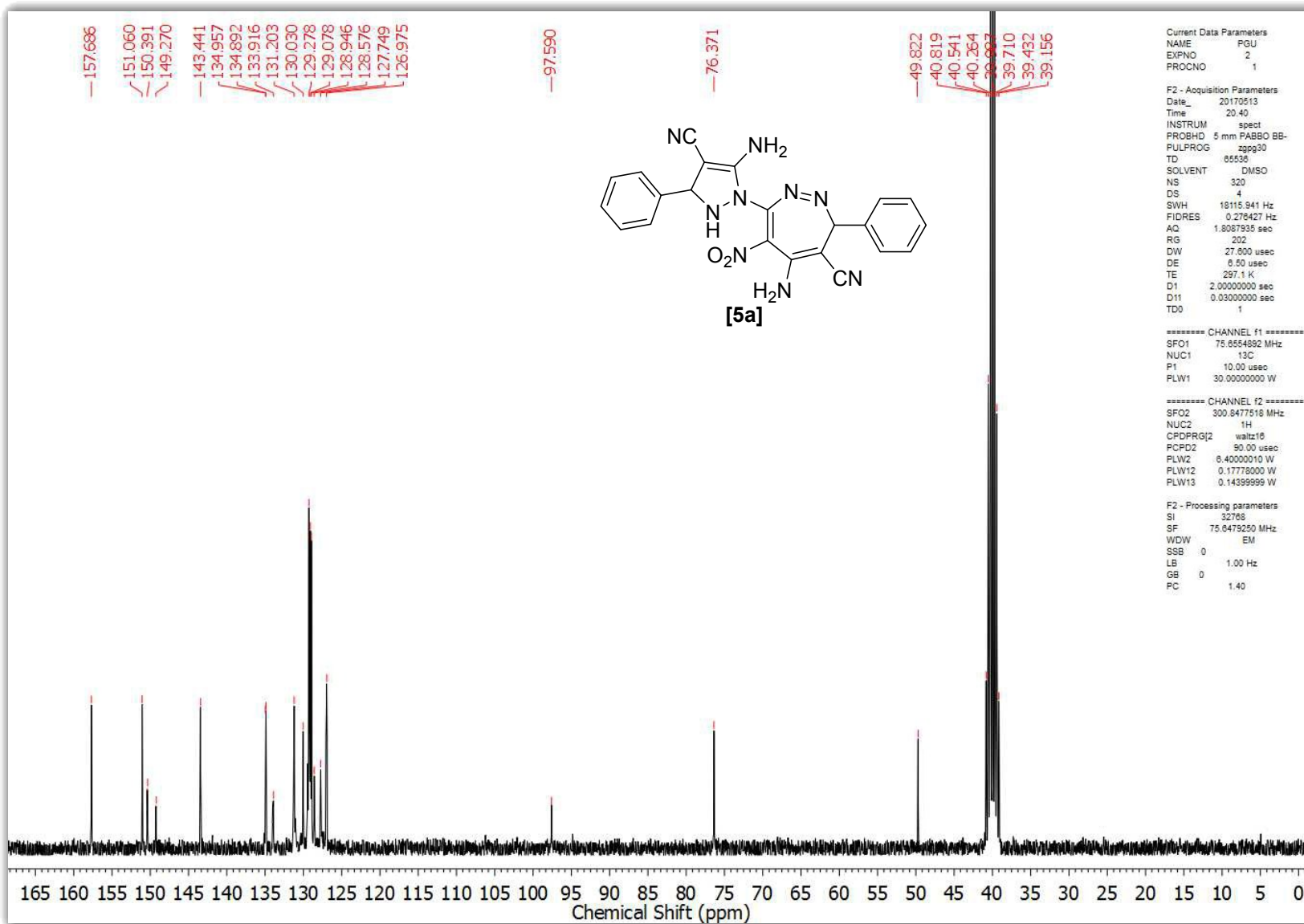
Sanaz Mojikhalifeh, Alireza Hasaninejad*

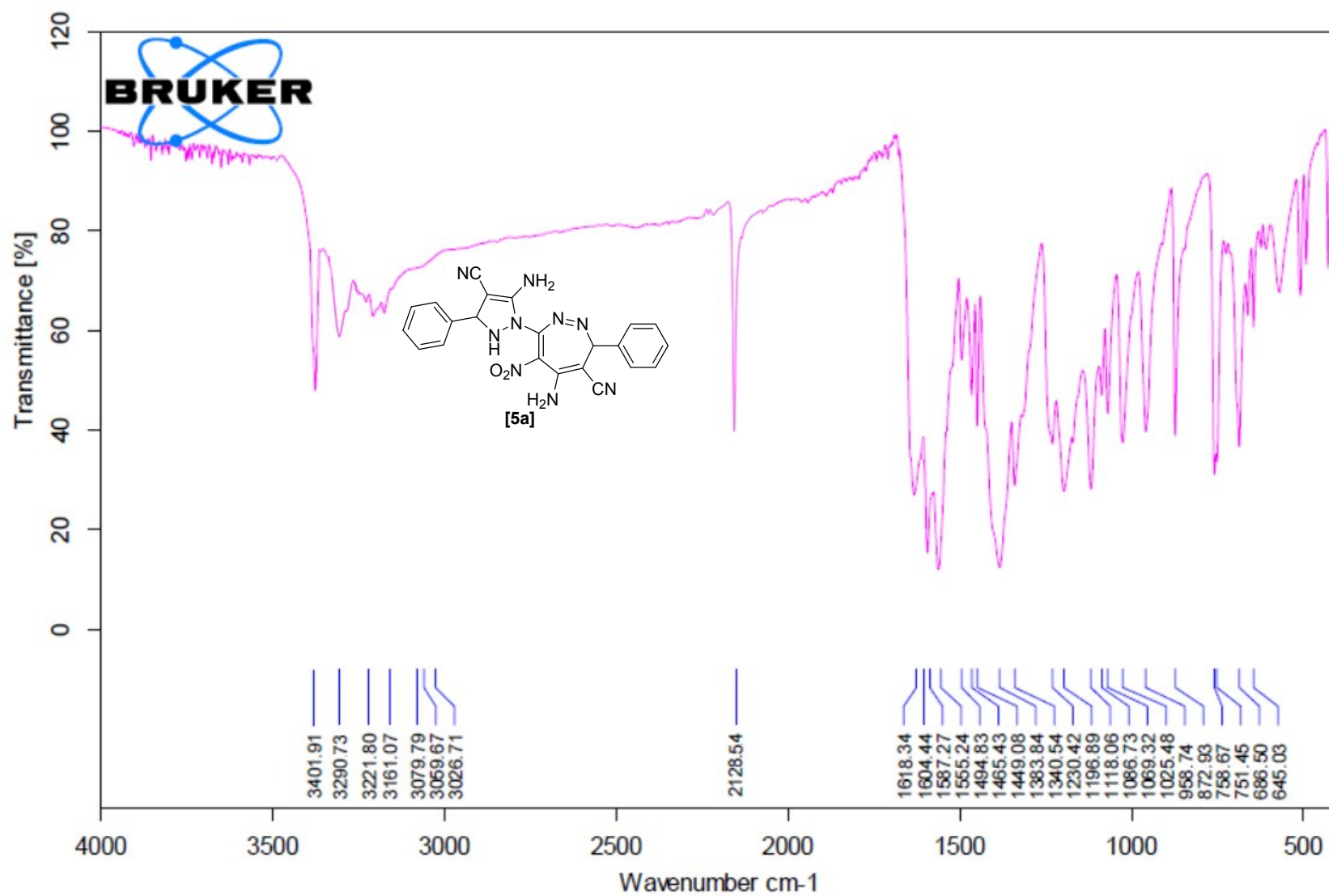
Department of Chemistry, Faculty of Sciences, Persian Gulf University, Bushehr 7516913817, Iran

Fax: +98(77)33441494; E-mail: a_hasaninejad@yahoo.com

5-Amino-7-(5-amino-4-cyano-3-phenyl-2,3-dihydro-1H-pyrazol-1-yl)-6-nitro-3-phenyl-3H-1,2-diazepine-4-carbonitrile (**5a**)

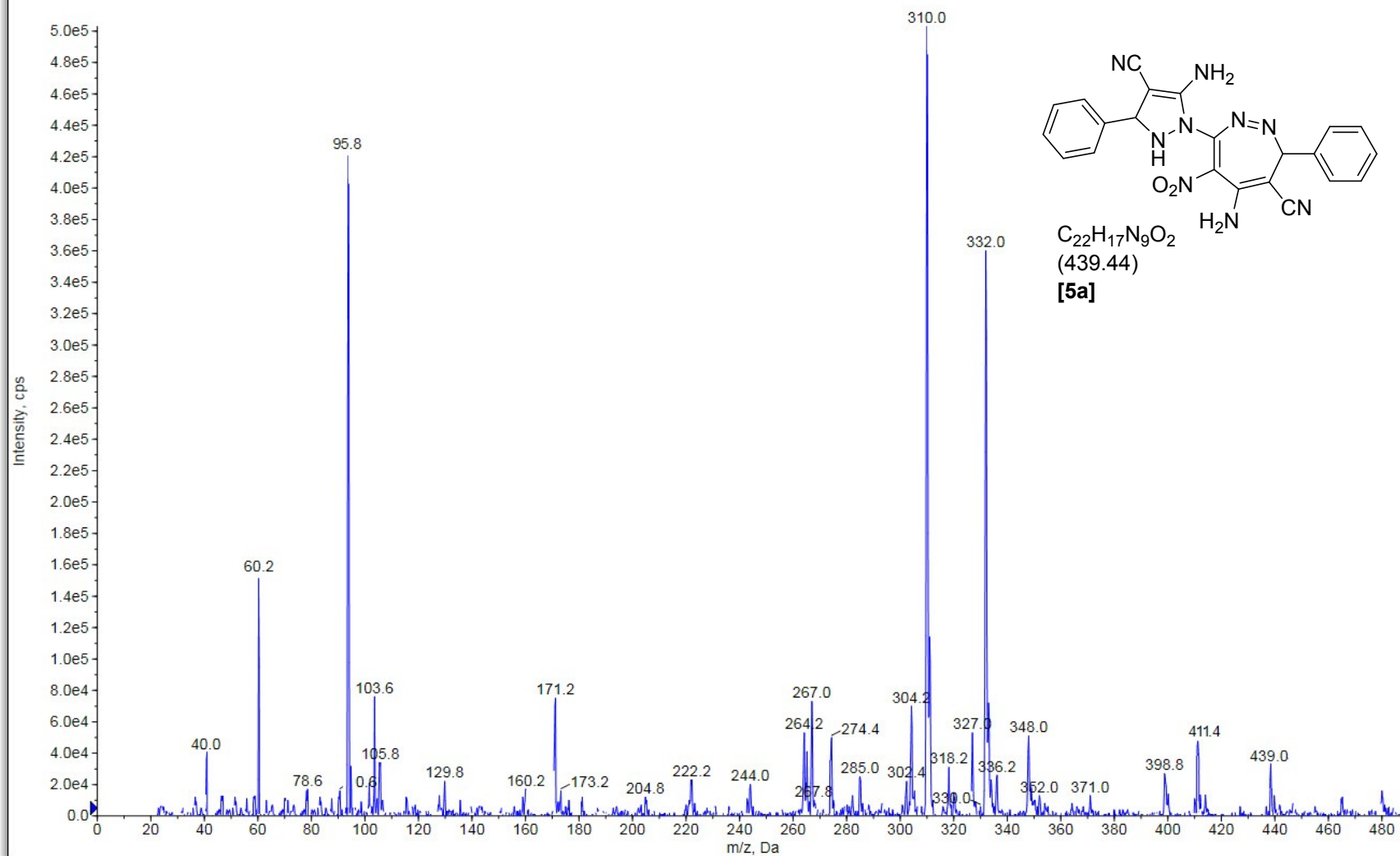




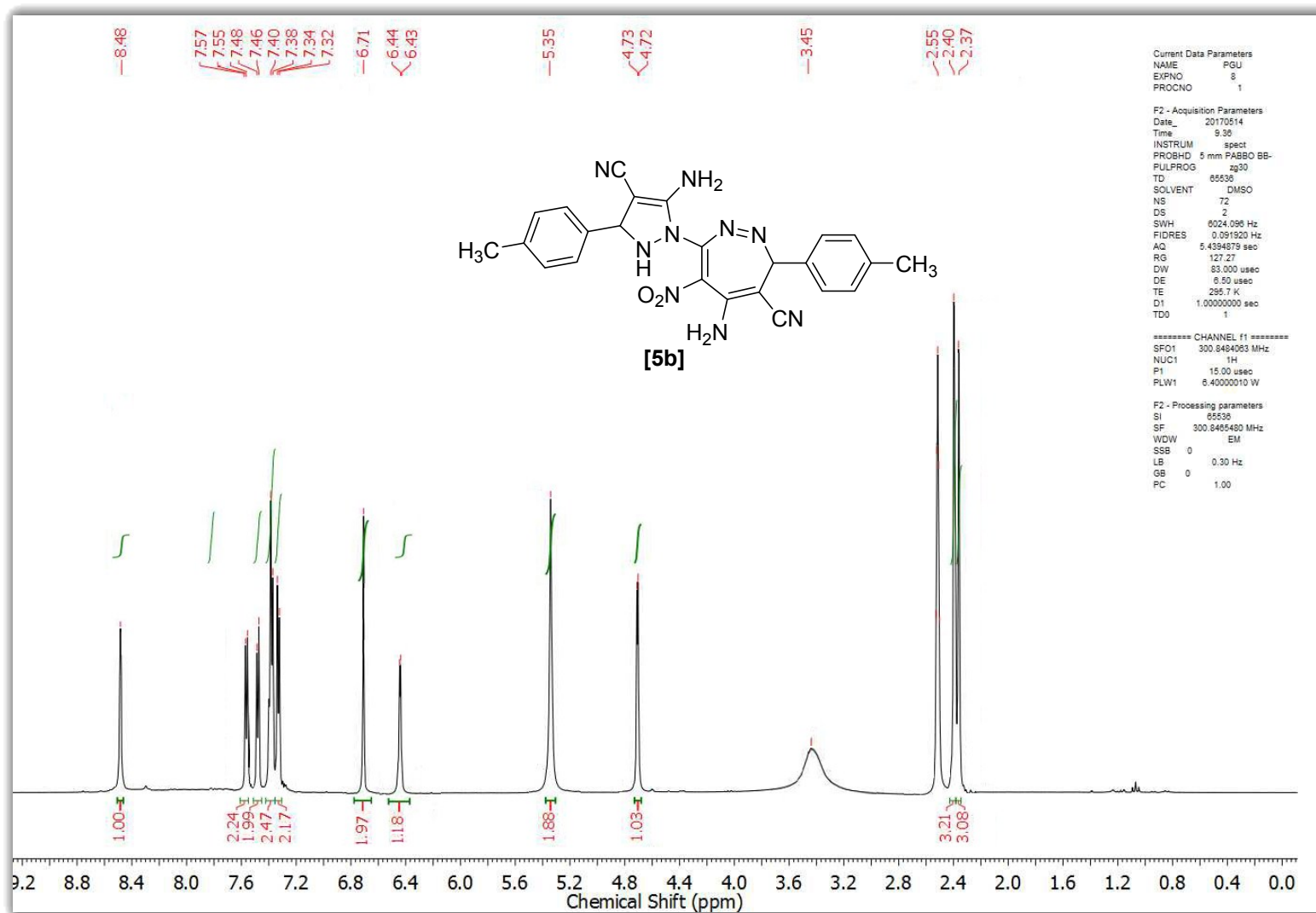


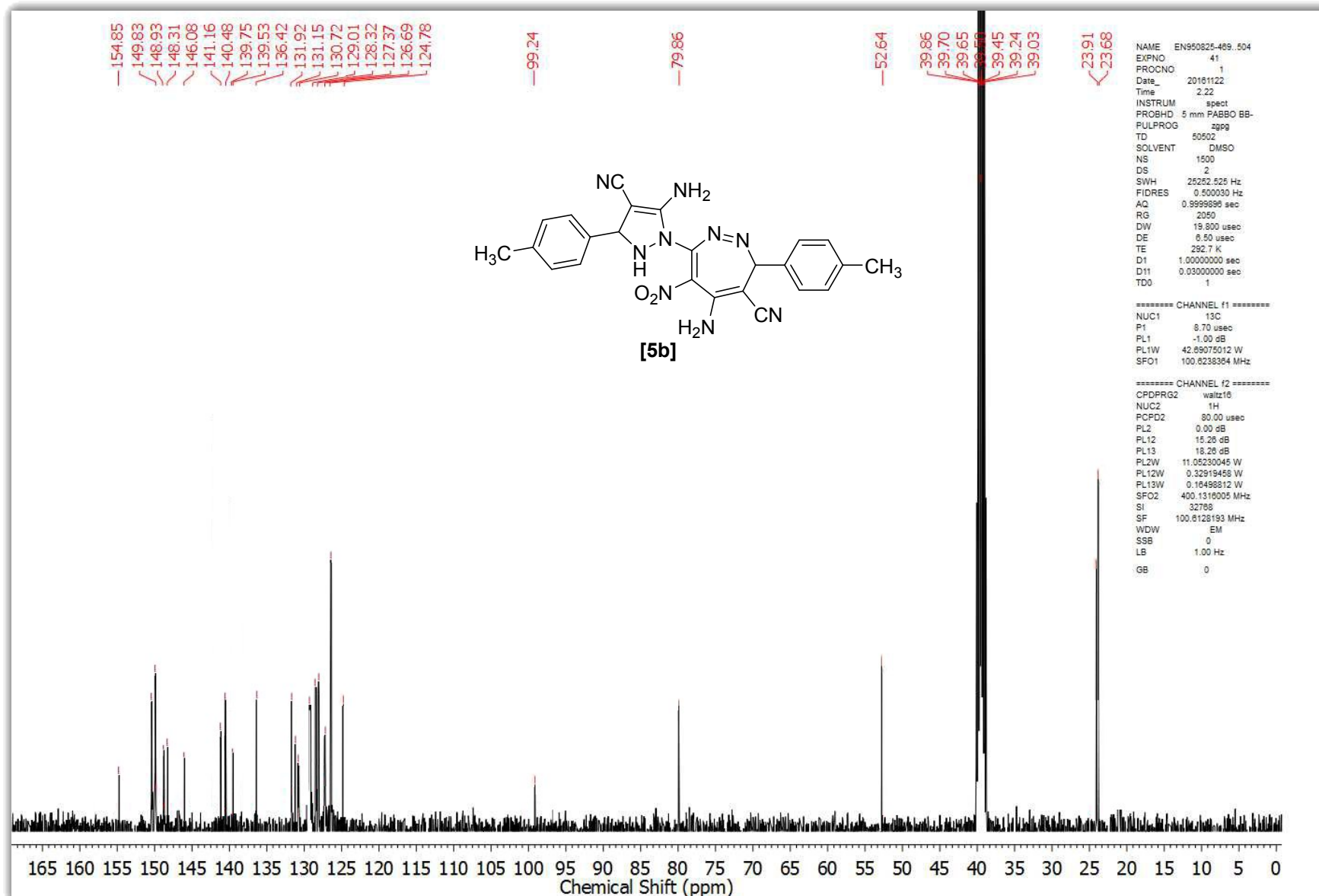
+Q1: 5 MCA scans from Sample 1 (TuneSampleName) of Mrs.moji(0-490)+ aceto_BP_Pos.wiff (Turbo Spray)

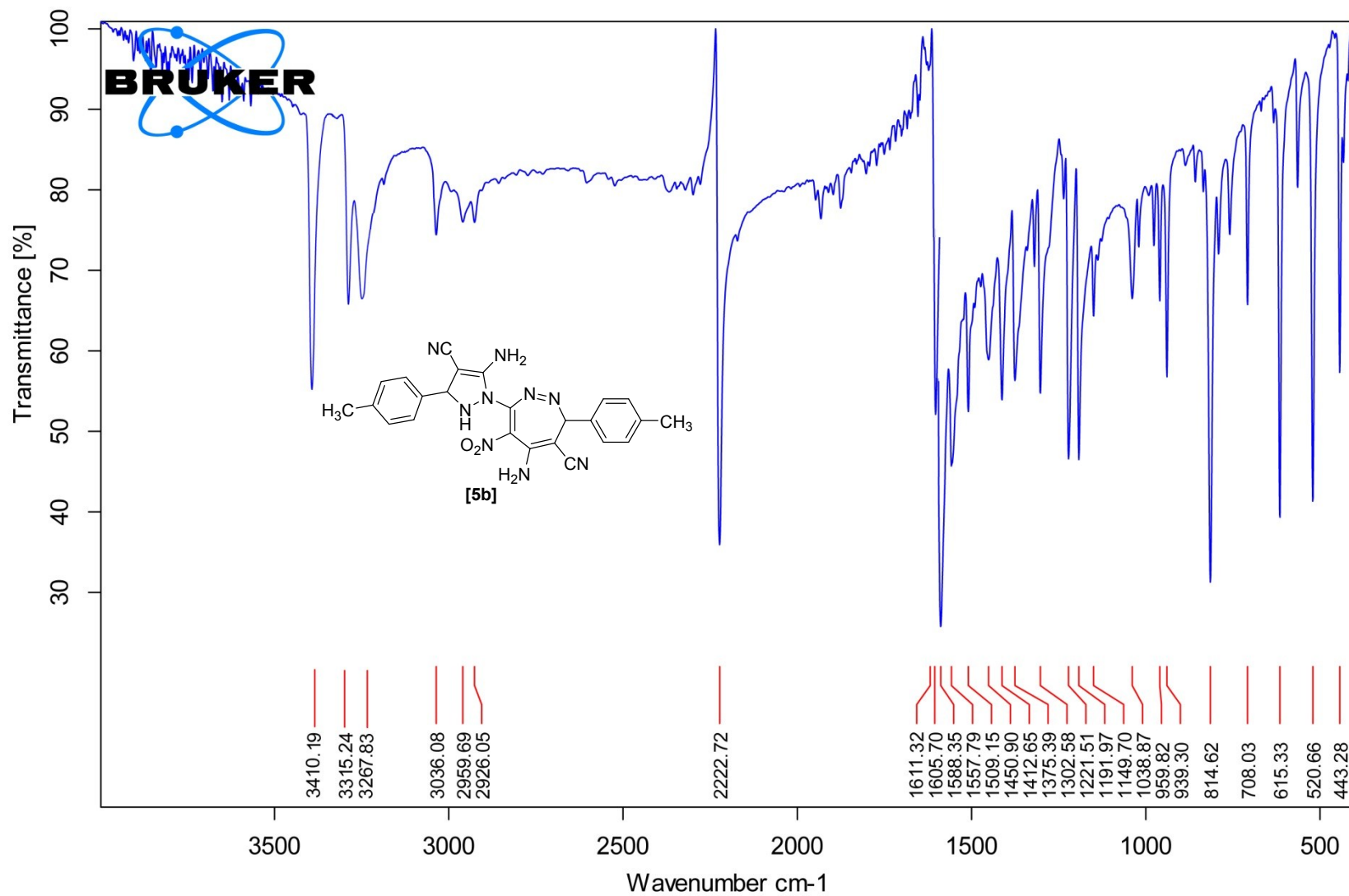
Max. 5.0e5 cps.



5-Amino-7-(5-amino-4-cyano-3-(p-tolyl)-2,3-dihydro-1H-pyrazol-1-yl)-6-nitro-3-(p-tolyl)-3H-1,2-diazepine-4-carbonitrile (**5b**)

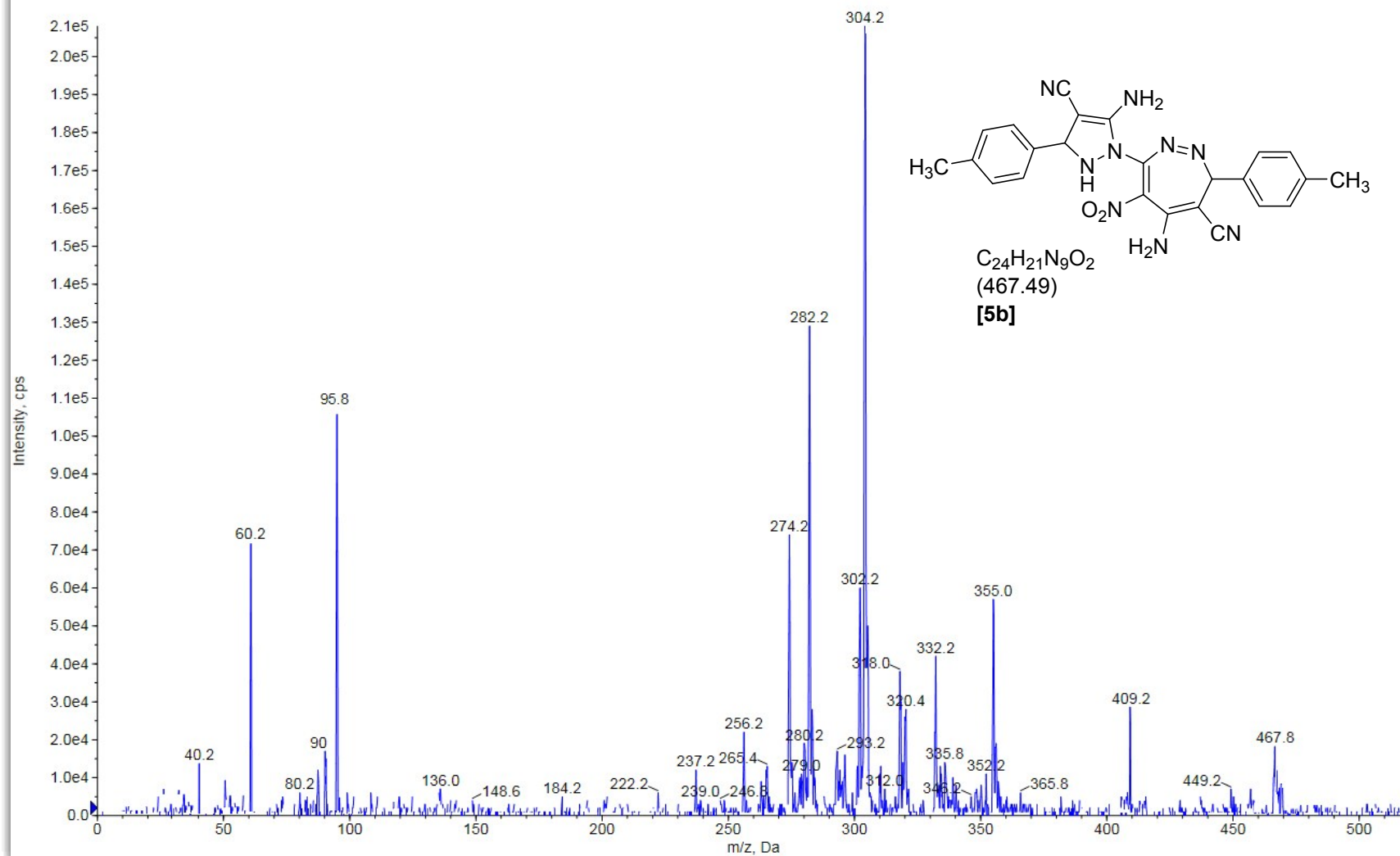




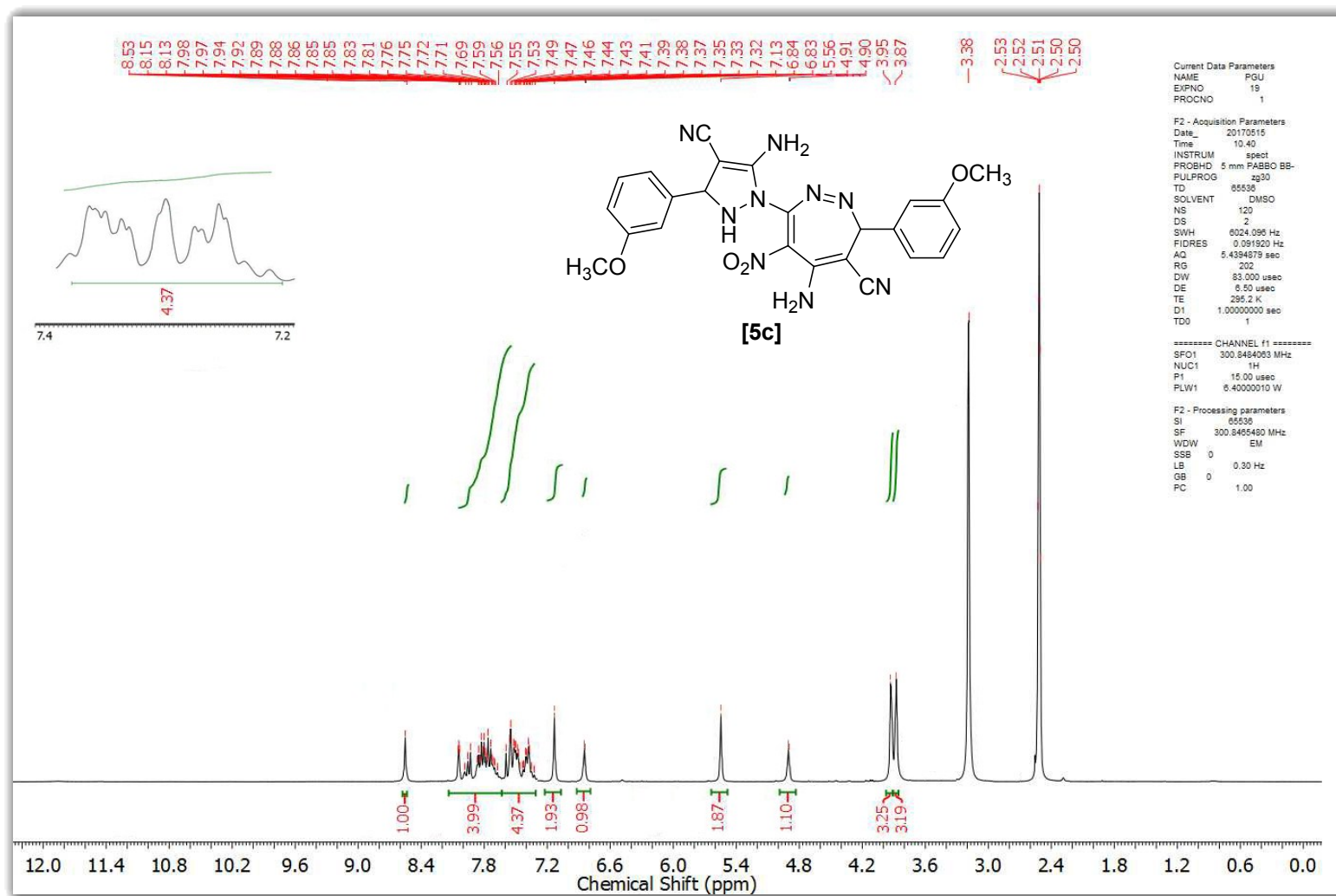


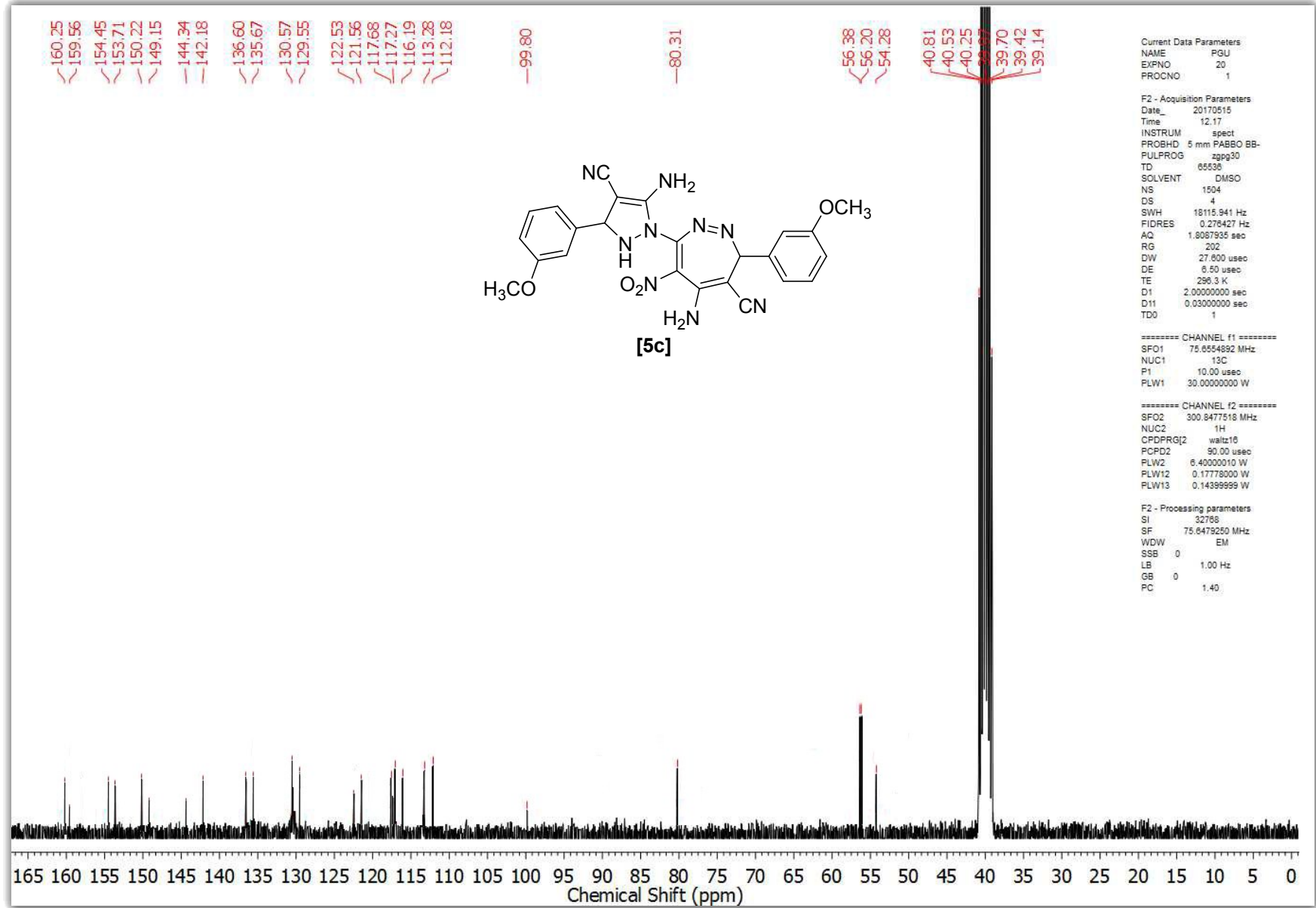
+Q1: 5 MCA scans from Sample 1 (TuneSampleName) of Mrs.moji (0-520)+ aceto_BP_Pos.wiff (Turbo Spray)

Max. 2.1e5 cps.



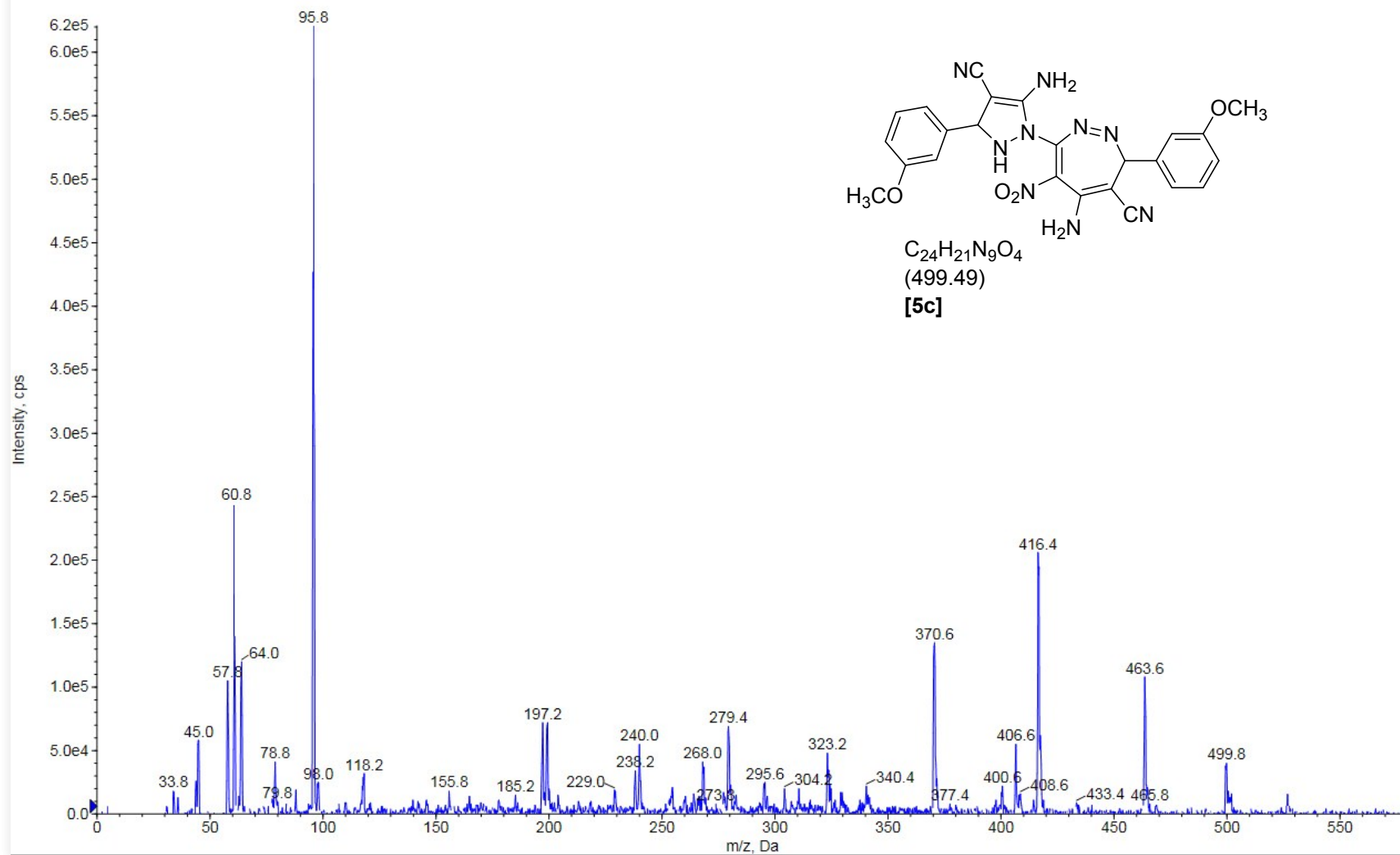
5-Amino-7-(5-amino-4-cyano-3-(3-methoxyphenyl)-2,3-dihydro-1H-pyrazol-1-yl)-3-(3-methoxyphenyl)-6-nitro-3H-1,2-diazepine-4-carbonitrile (**5c**)



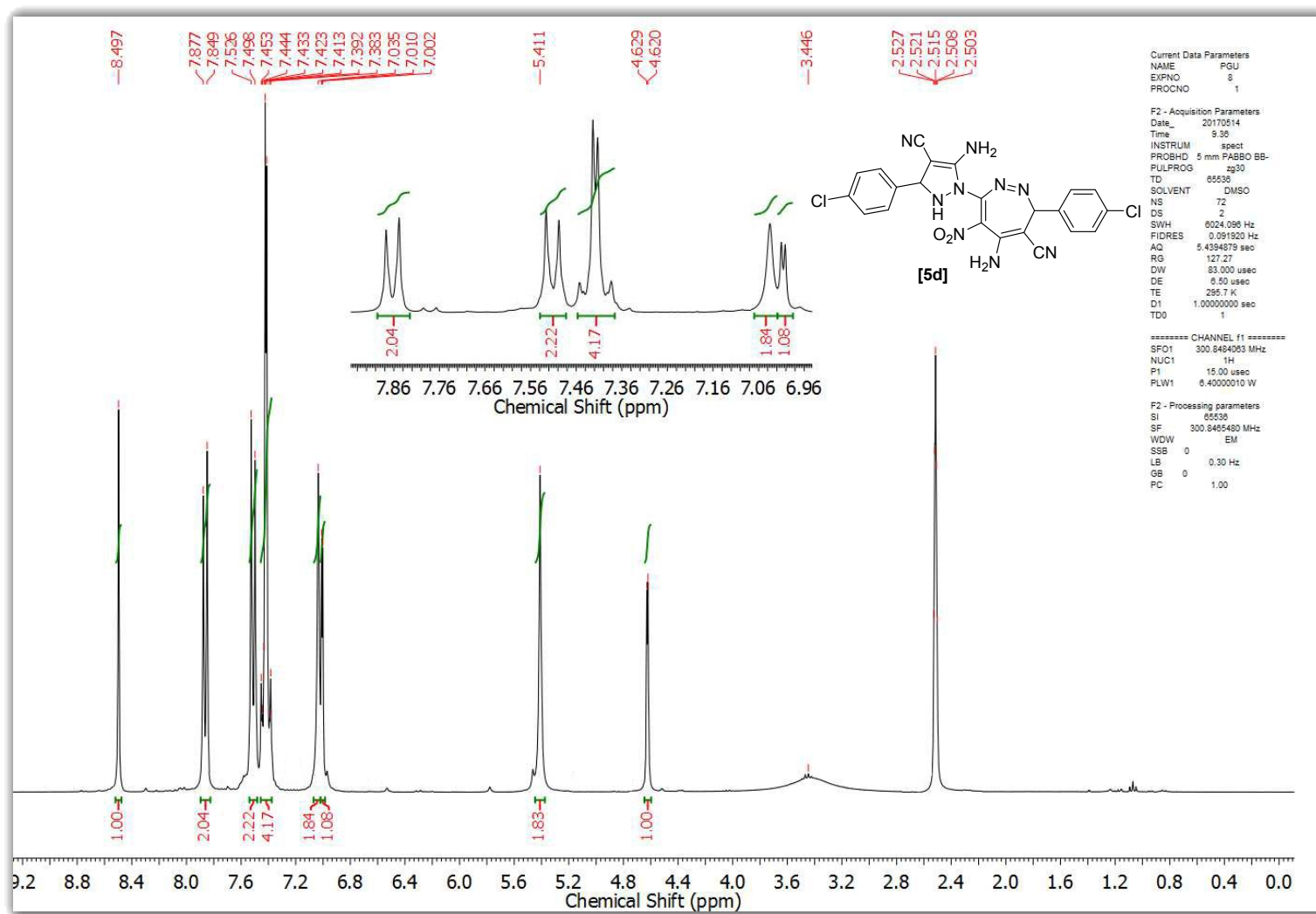


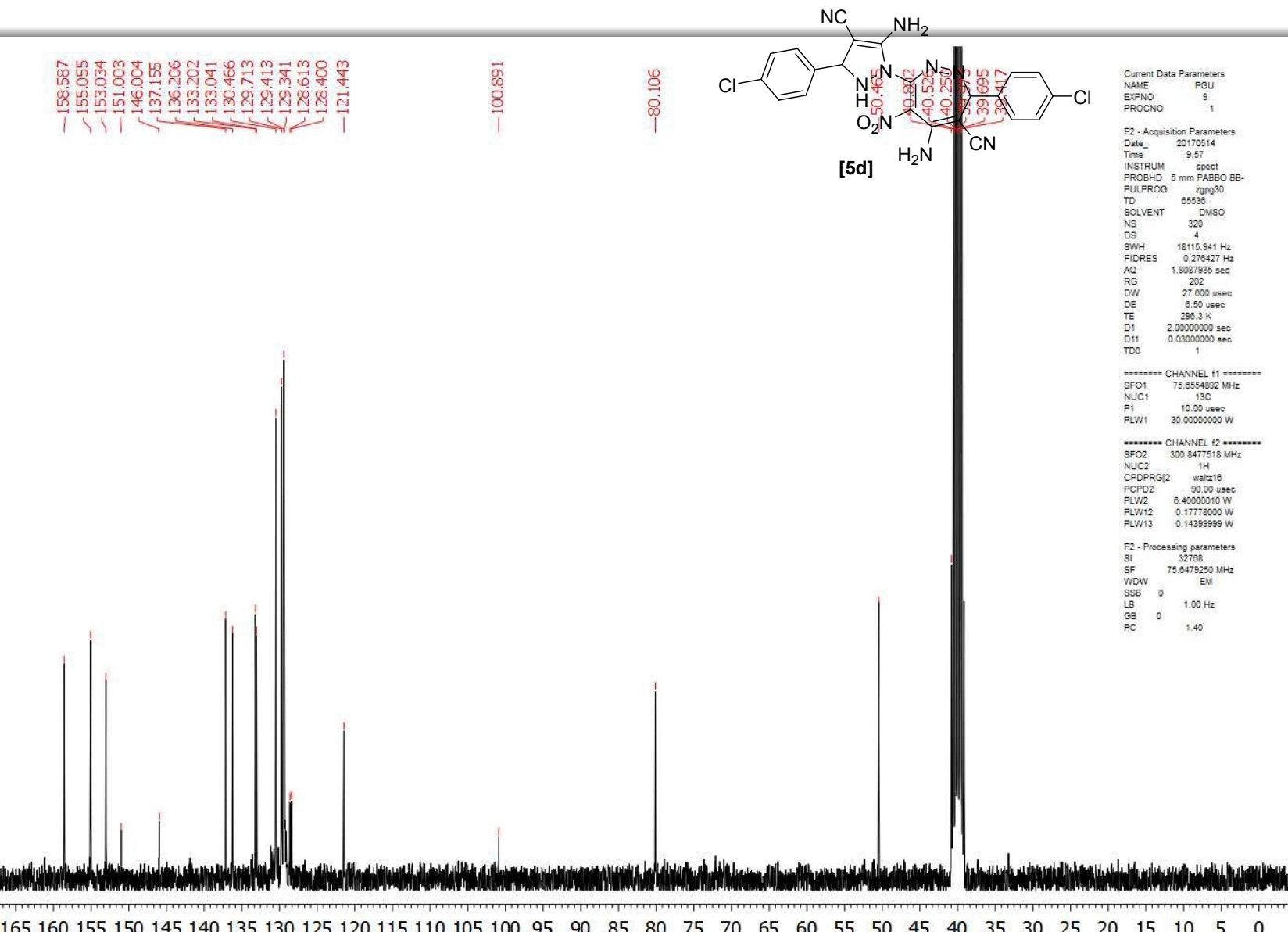
■ -Q1: 5 MCA scans from Sample 1 (TuneSampleName) of Mrs.moji (0-580)-_BP_Neg.wiff (Turbo Spray)

Max. 6.2e5 cps.



5-Amino-7-(5-amino-3-(4-chlorophenyl)-4-cyano-2,3-dihydro-1H-pyrazol-1-yl)-3-(4-chloro-phenyl)-6-nitro-3H-1,2-diazepine-4-carbonitrile (**5d**)





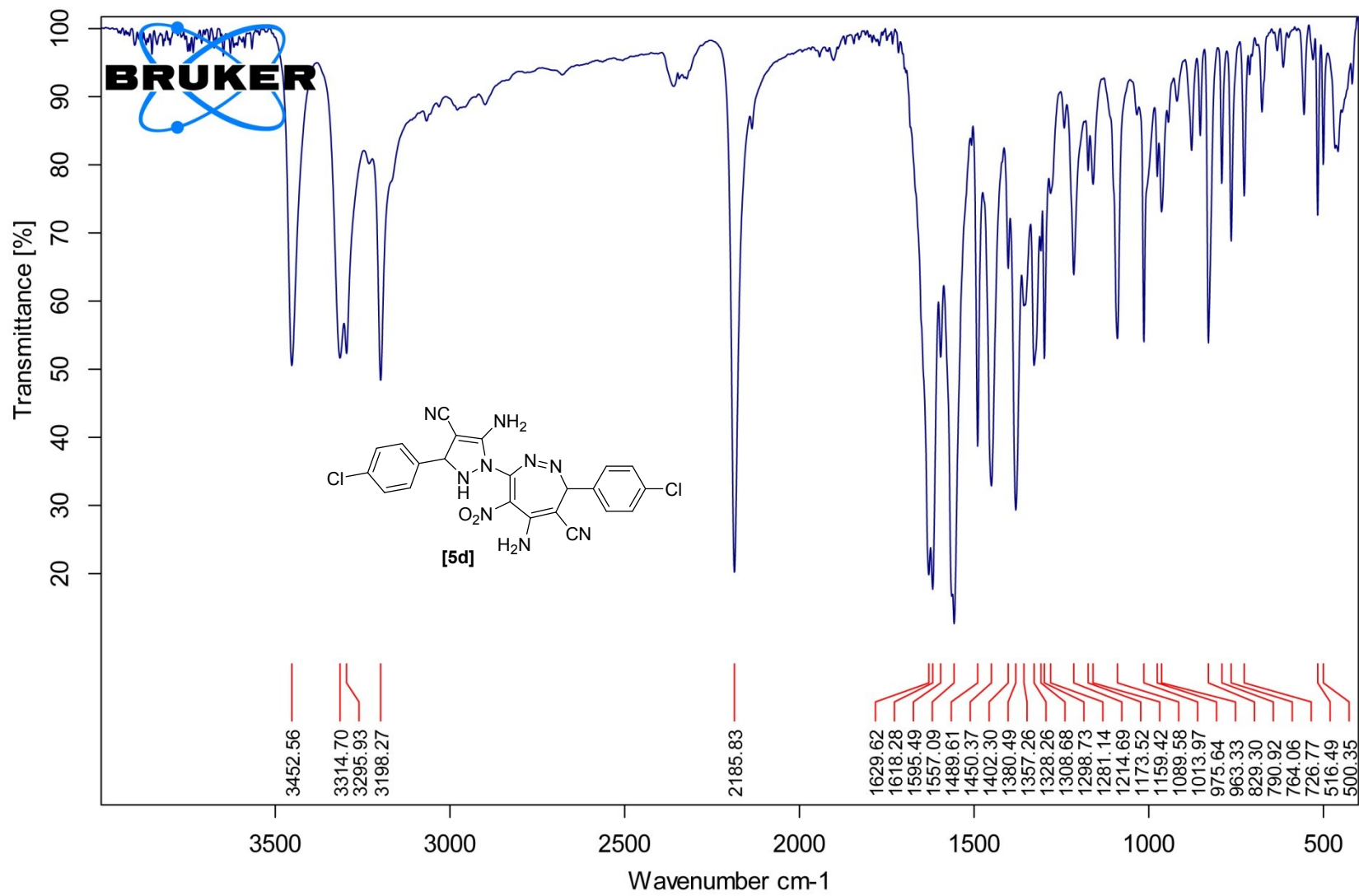
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NAME PGU
EXPNO 9
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170514
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INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 320
DS 4
SWH 18115.941 Hz
FIDRES 0.276427 Hz
AQ 1.8087935 sec
RG 202
DW 27.600 usec
DE 6.50 usec
TE 296.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

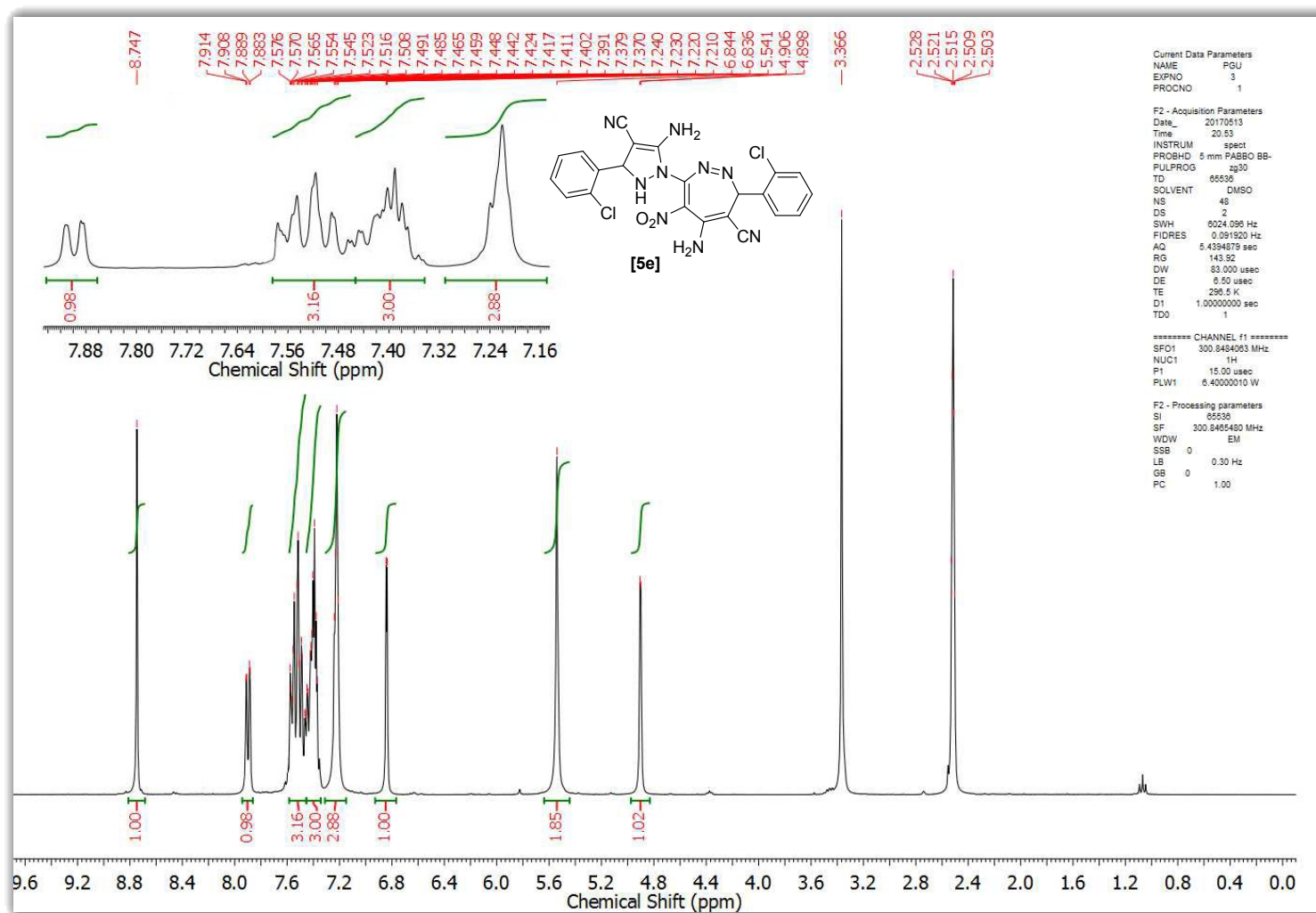
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NUC1 13C
P1 10.00 usec
PLW1 30.00000000 W

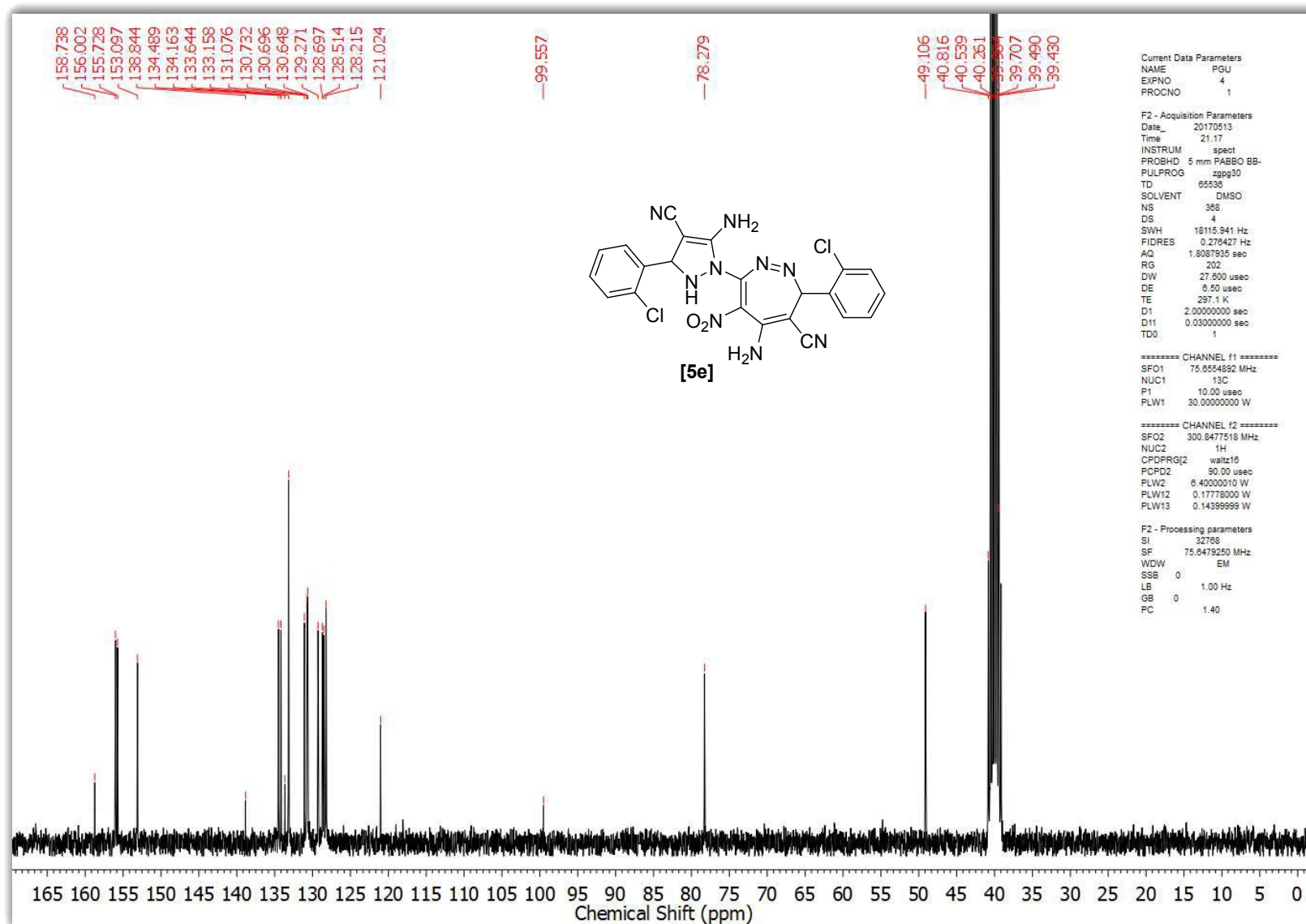
===== CHANNEL f2 =====
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NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 6.40000010 W
PLW12 0.17778000 W
PLW13 0.14399999 W

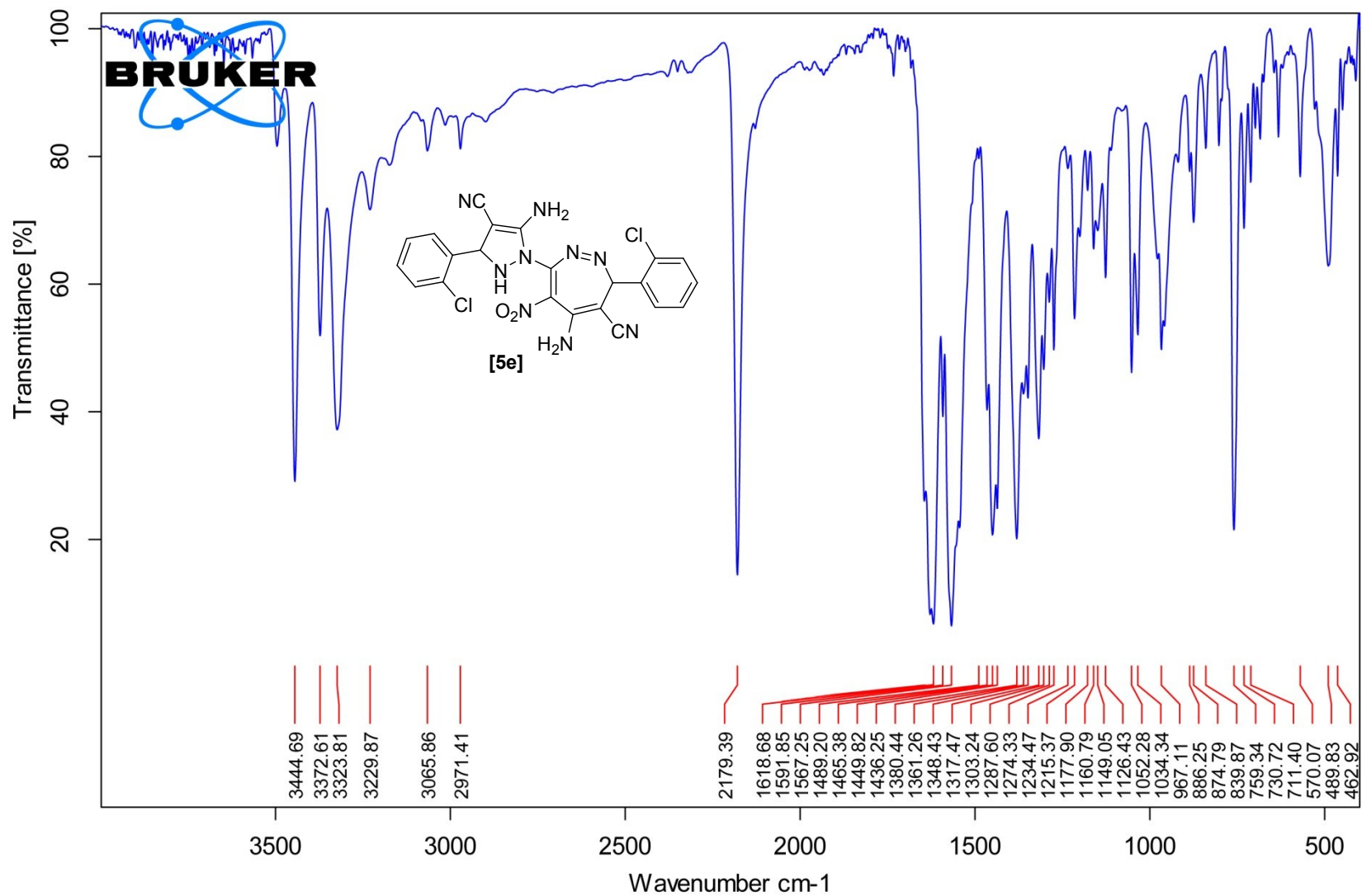
F2 - Processing parameters
SI 32768
SF 75.6479250 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
FC 1.40



5-Amino-7-(5-amino-3-(2-chlorophenyl)-4-cyano-2,3-dihydro-1H-pyrazol-1-yl)-3-(2-chlorophenyl)-6-nitro-3H-1,2-diazepine-4-carbonitrile (**5e**)

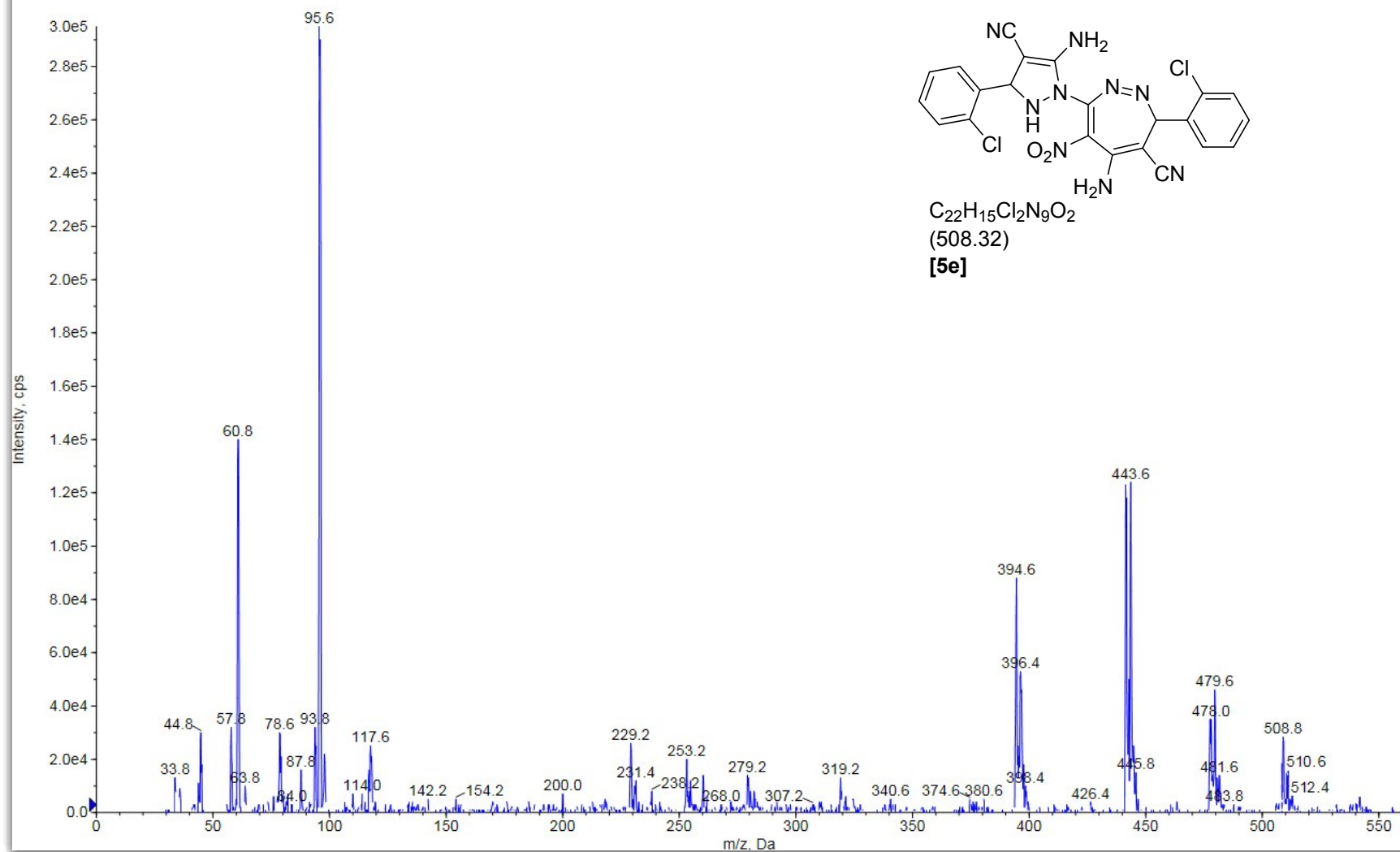




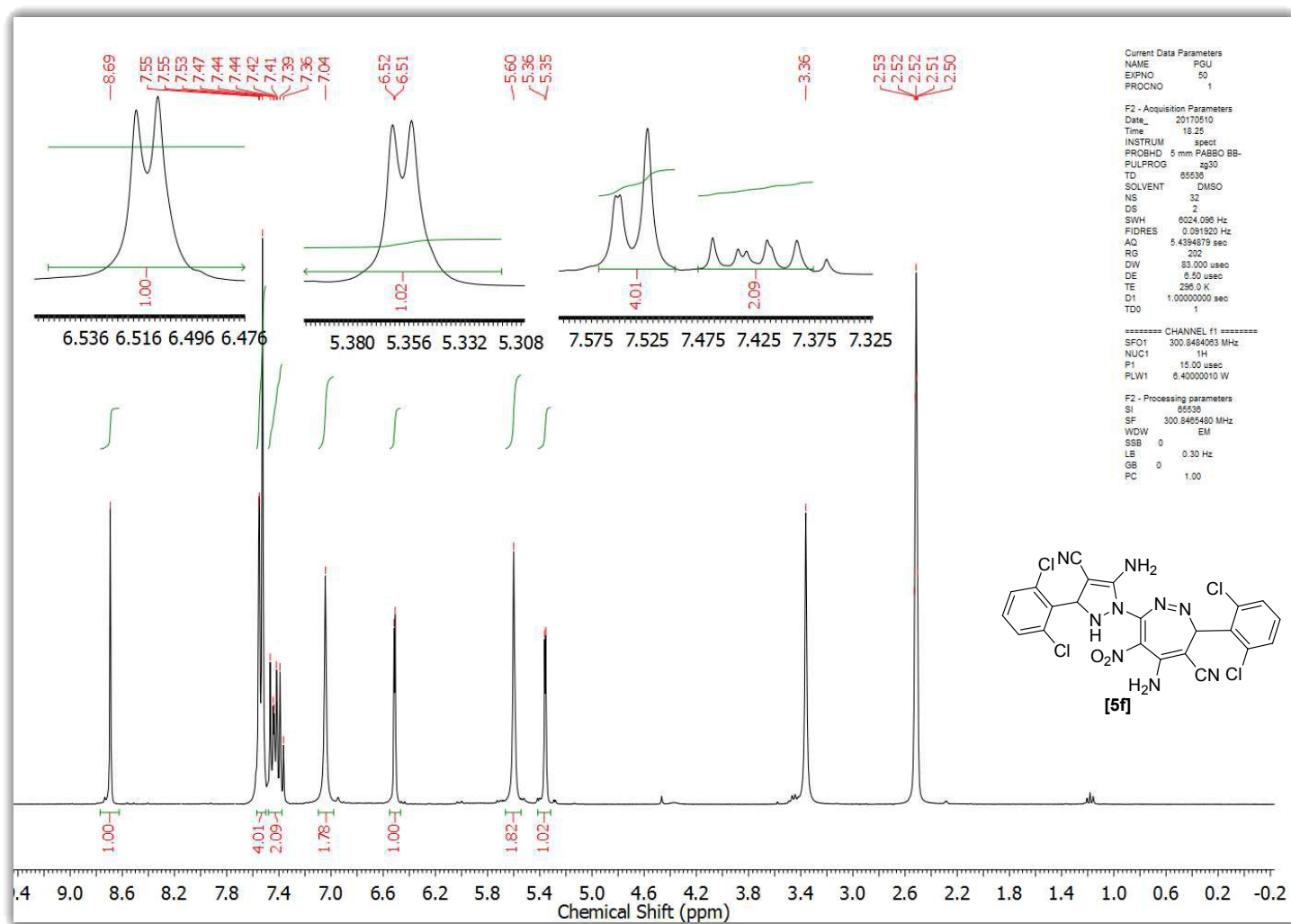


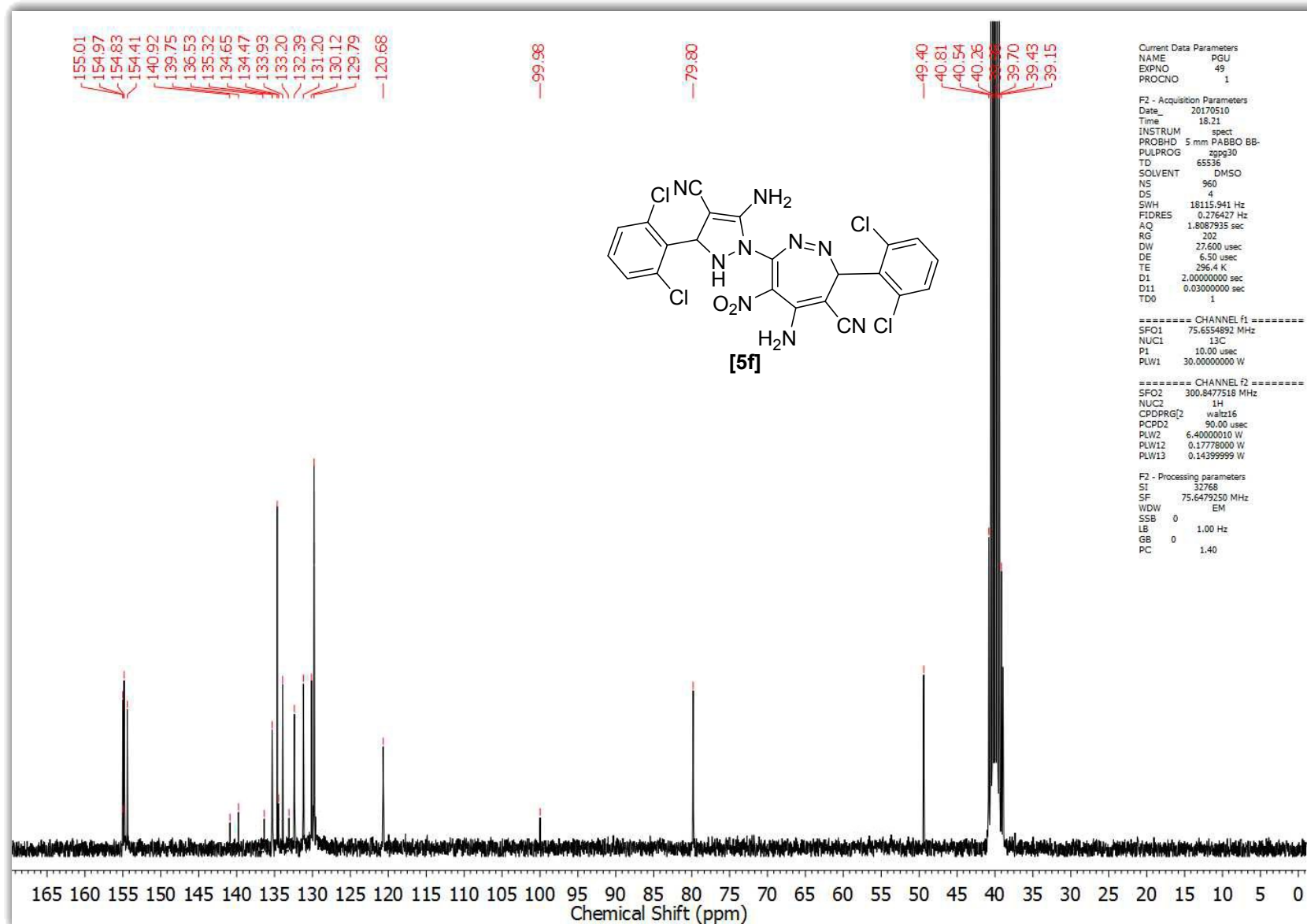
■ -Q1: 5 MCA scans from Sample 1 (TuneSampleName) of Mrs.moji (0-560)-_BP_Neg.wiff (Turbo Spray)

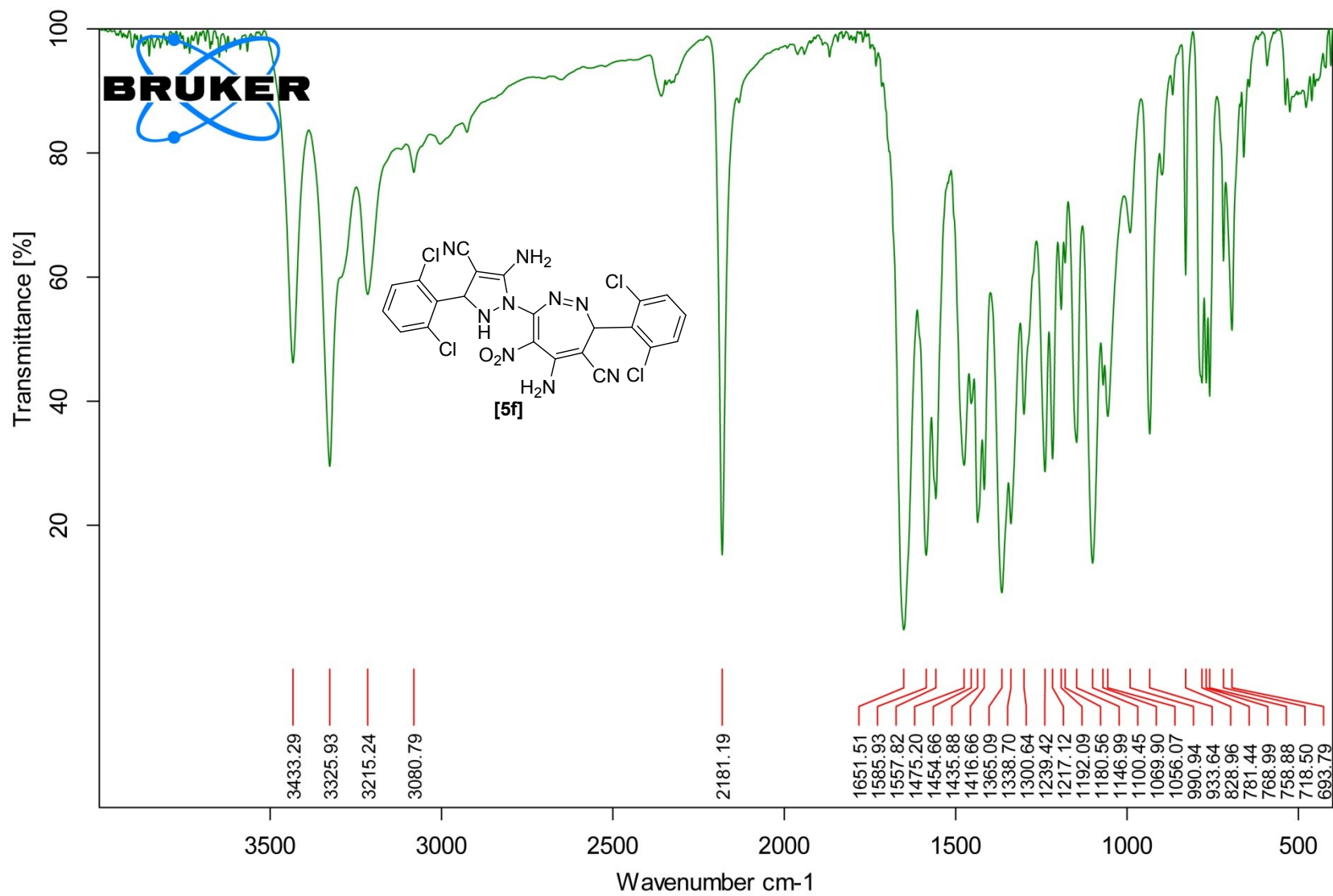
Max. 3.0e5 cps.



5-Amino-7-(5-amino-4-cyano-3-(2,6-dichlorophenyl)-2,3-dihydro-1H-pyrazol-1-yl)-3-(2,6-dichlorophenyl)-6-nitro-3H-1,2-diazepine-4-carbonitrile (**5f**)

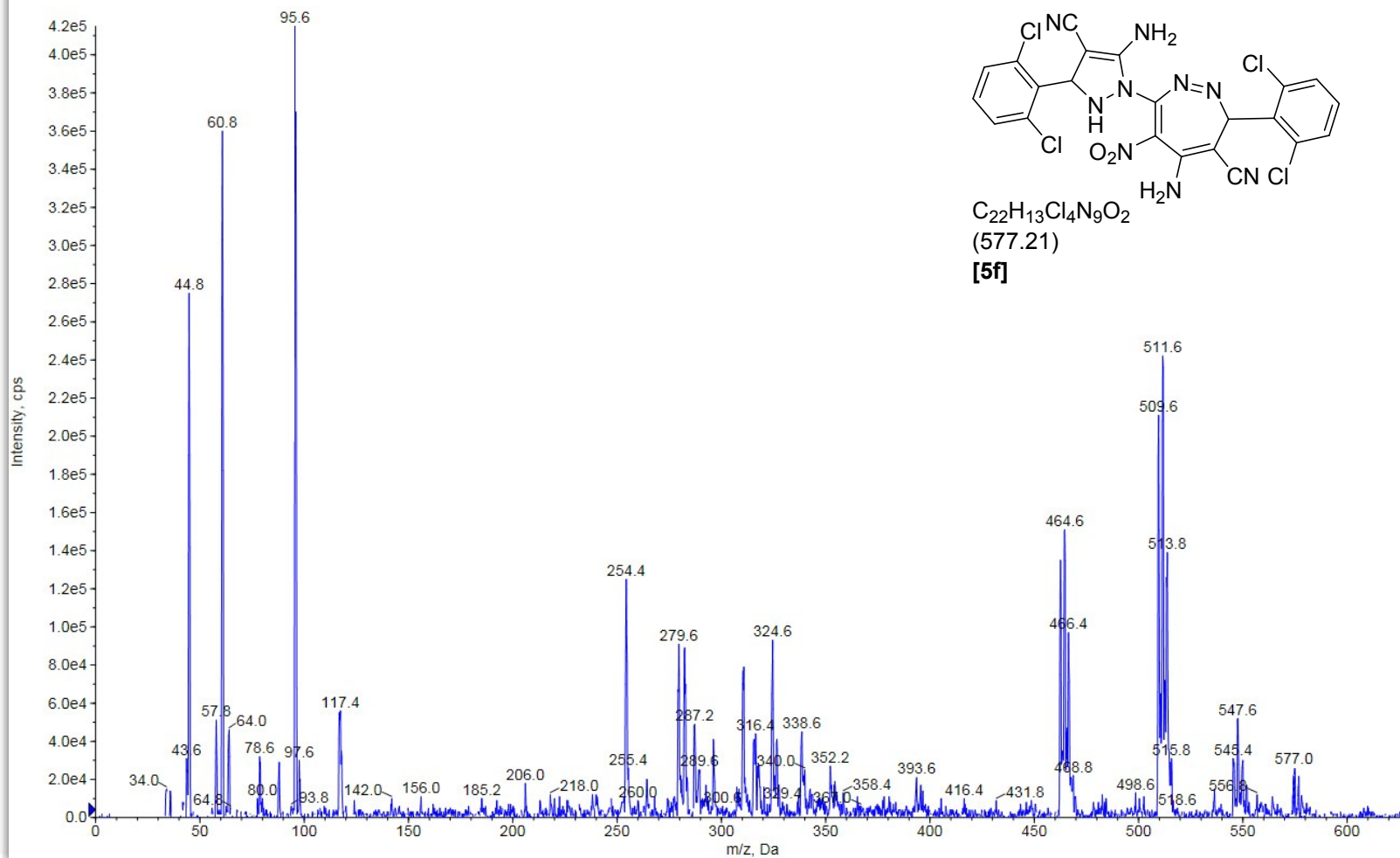






-Q1: 5 MCA scans from Sample 1 (TuneSampleName) of Mrs.moji (0-630)- me_BP_Neg.wiff (Turbo Spray)

Max. 4.2e5 cps.



Chemical Structure [5g]:

Nc1nc(C2=CC=CC=C2C3=CC(=CC=C3)N=C4C(=N2)C(=C(C(=N4)C#N)N)C#N)C5=CC=C(C=C5)Br

1H NMR Spectrum (DMSO-d₆):

Chemical Shift (ppm)	Integration
7.803, 7.879, 7.872, 7.854, 7.847, 7.737, 7.733, 7.711, 7.707, 7.687, 7.682, 7.486, 7.464, 7.459, 7.442, 7.439, 7.431, 7.424, 7.417, 7.413, 7.405, 7.399, 7.381, 7.374, 7.374, 7.318, 7.313, 7.293, 7.287, 7.267, 7.262, 7.230, 7.230, 7.224, 7.204, 7.198, 6.869, 6.861, 5.554, 4.868, 4.860, 3.371	1.09, 2.14, 3.07, 3.96, 1.01, 1.92, 1.01

Current Data Parameters:

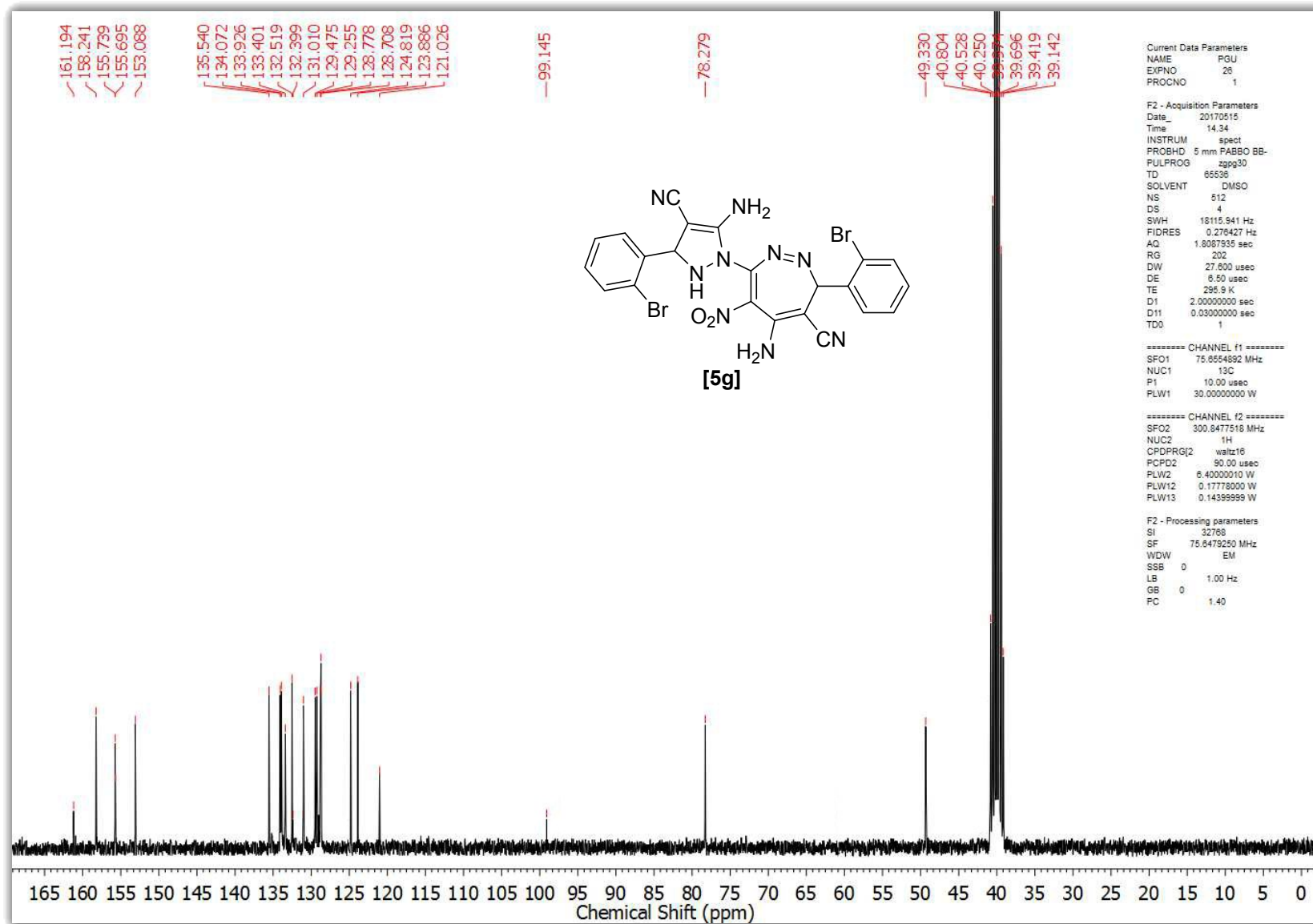
NAME	PGU
EXPNO	25
PROCNO	1

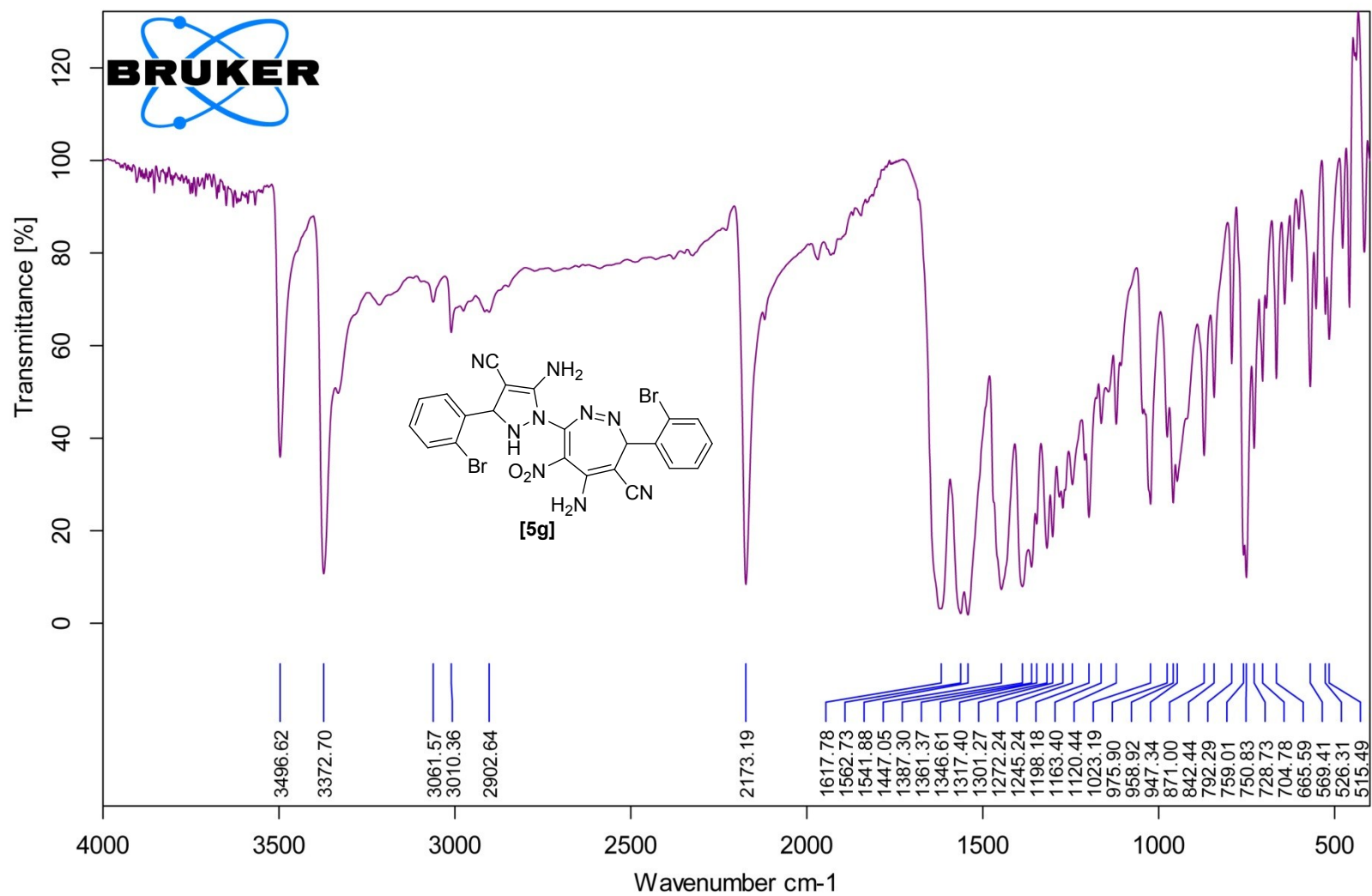
F2 - Acquisition Parameters:

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Time	14.00
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PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	64
DS	2
SWH	6024.096 Hz
FIDRES	0.091920 Hz
AQ	5.4384879 sec
RG	143.92
DW	83.000 usec
DE	6.50 usec
TE	295.4 K
D1	1.00000000 sec
TD0	1

F2 - Processing parameters:

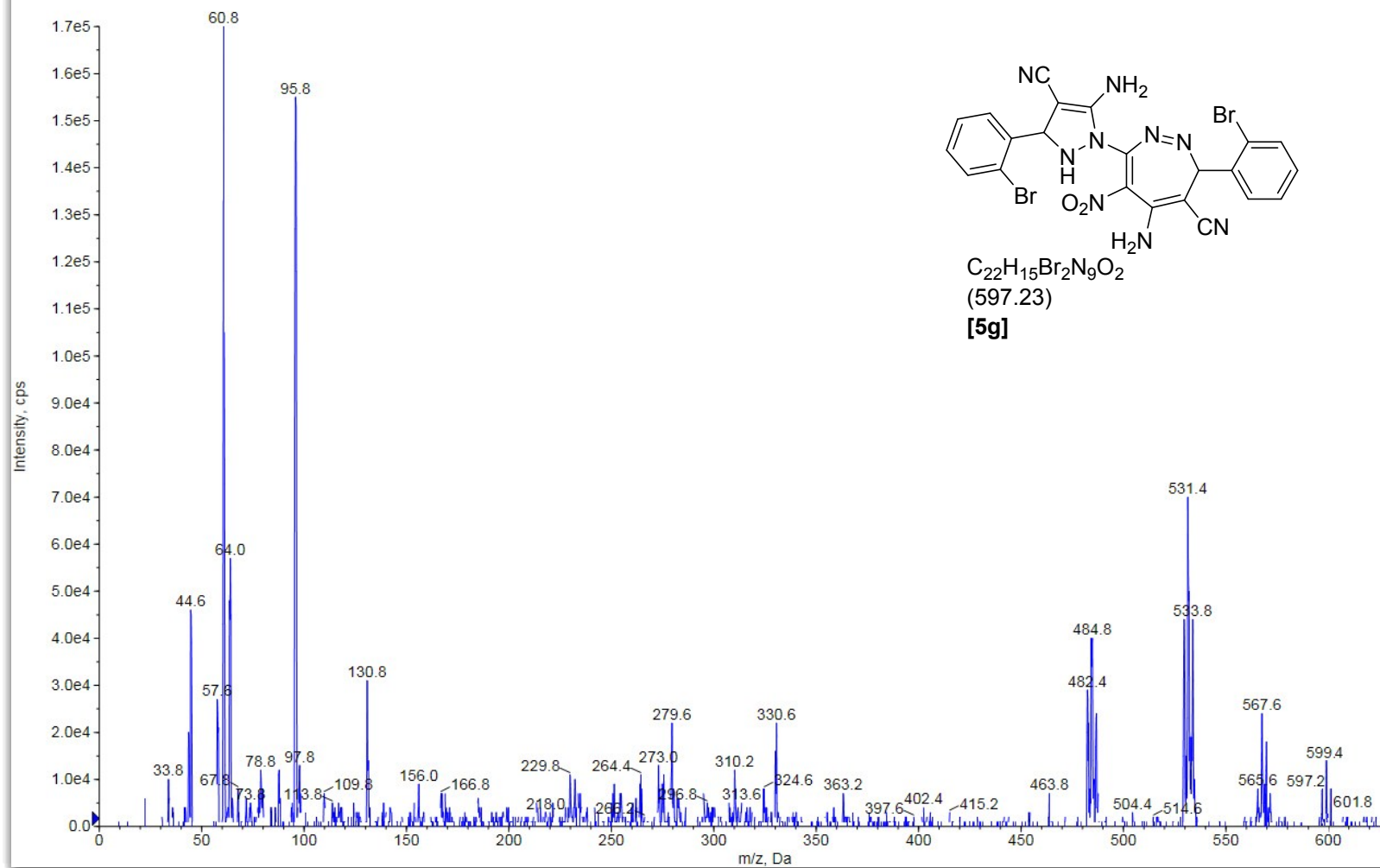
SI	65536
SF	300.645460 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



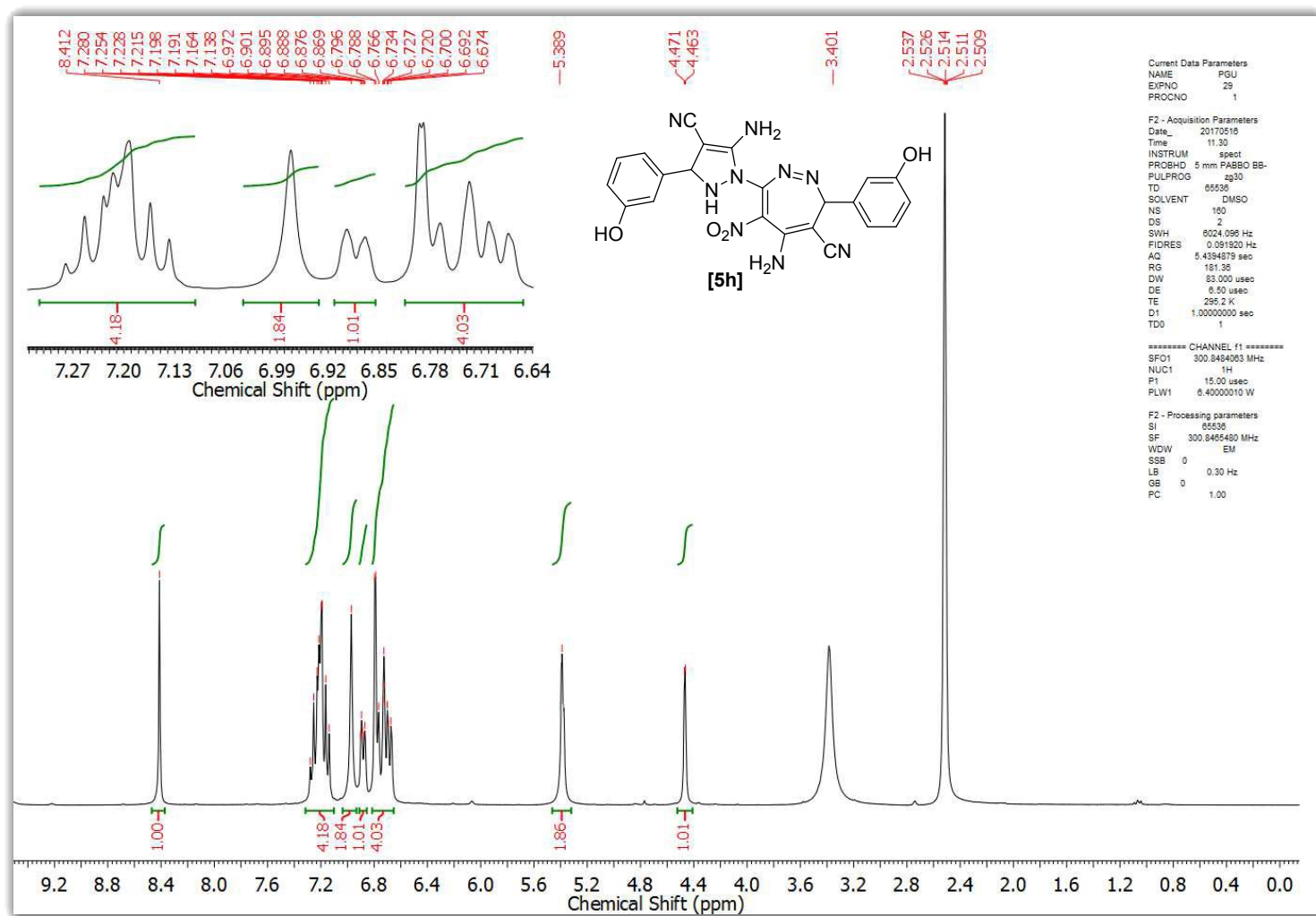


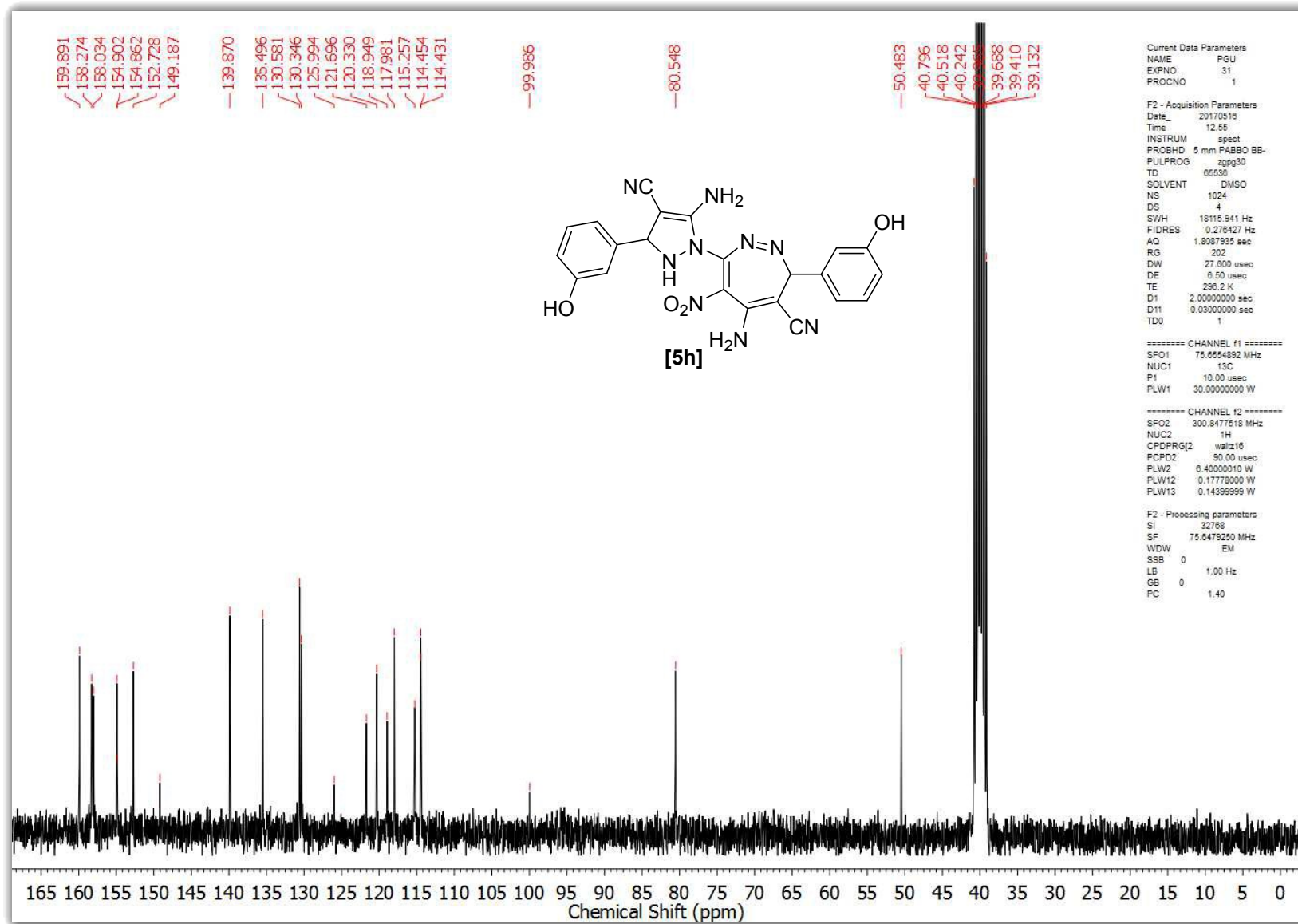
■ -Q1: 5 MCA scans from Sample 1 (TuneSampleName) of Mrs.moji (0-650)-_BP_Neg.wiff (Turbo Spray)

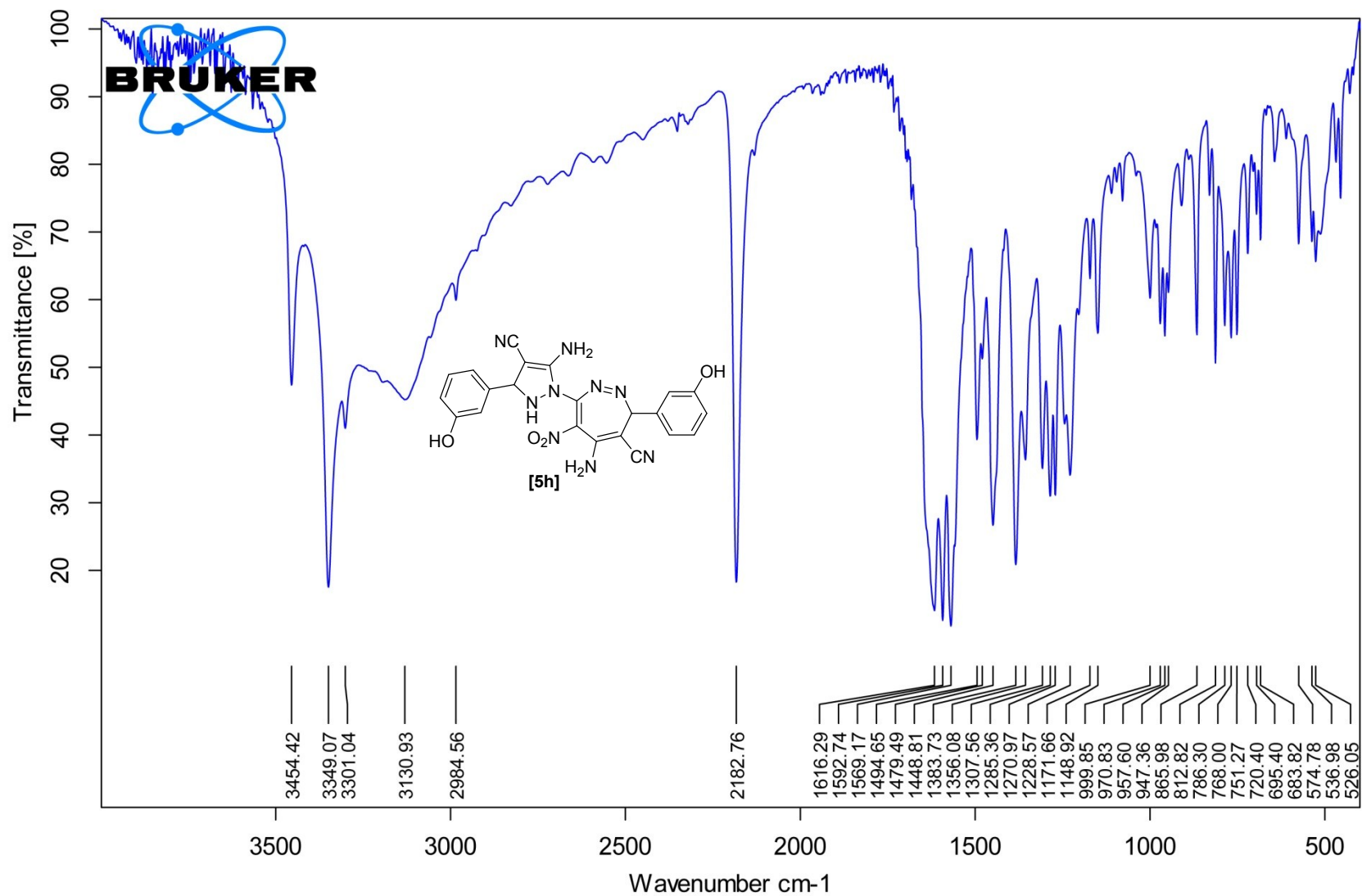
Max. 1.7e5 cps.



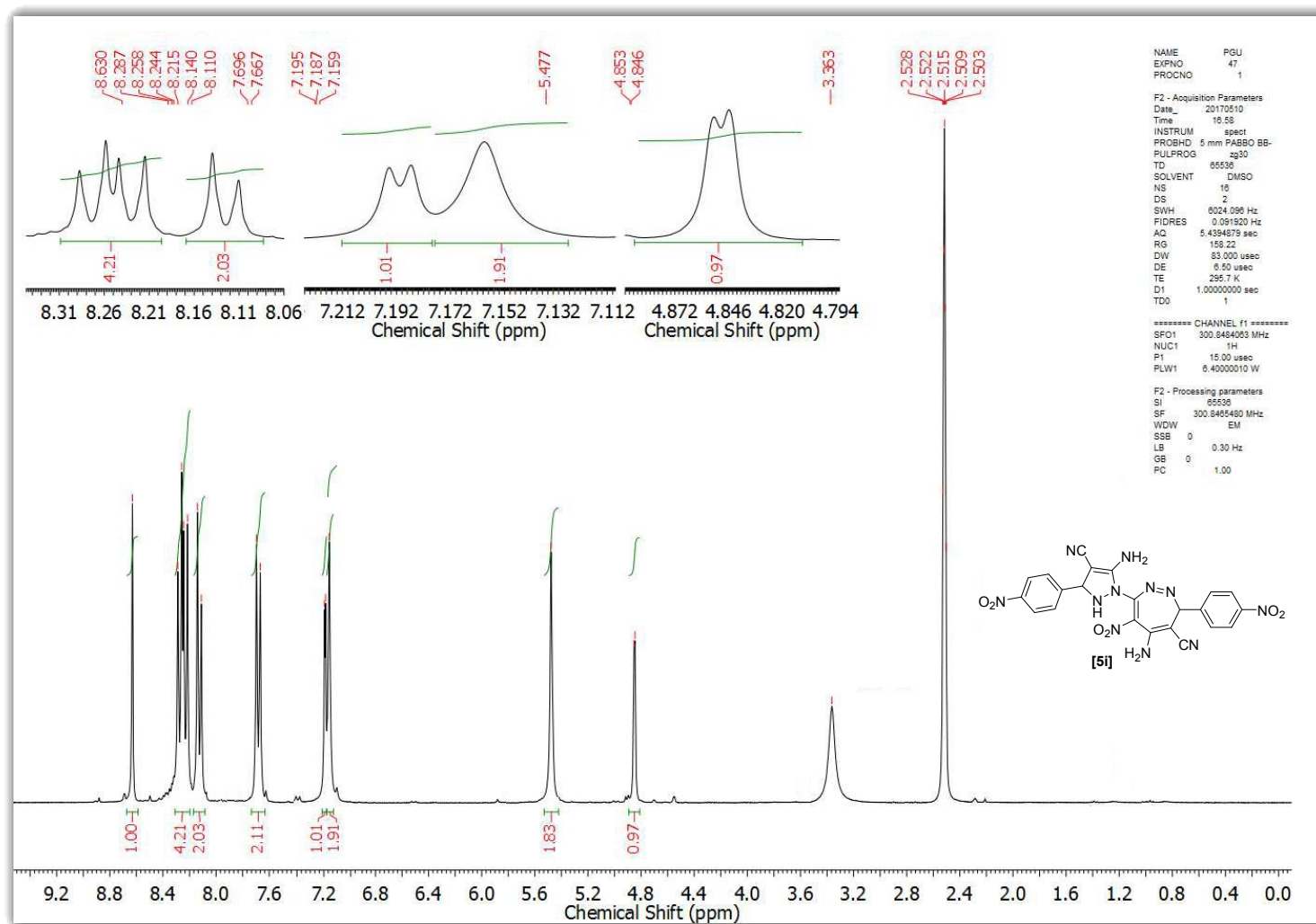
5-Amino-7-(5-amino-4-cyano-3-(3-hydroxyphenyl)-2,3-dihydro-1H-pyrazol-1-yl)-3-(3-hydroxyphenyl)-6-nitro-3H-1,2-diazepine-4-carbonitrile (**5h**)



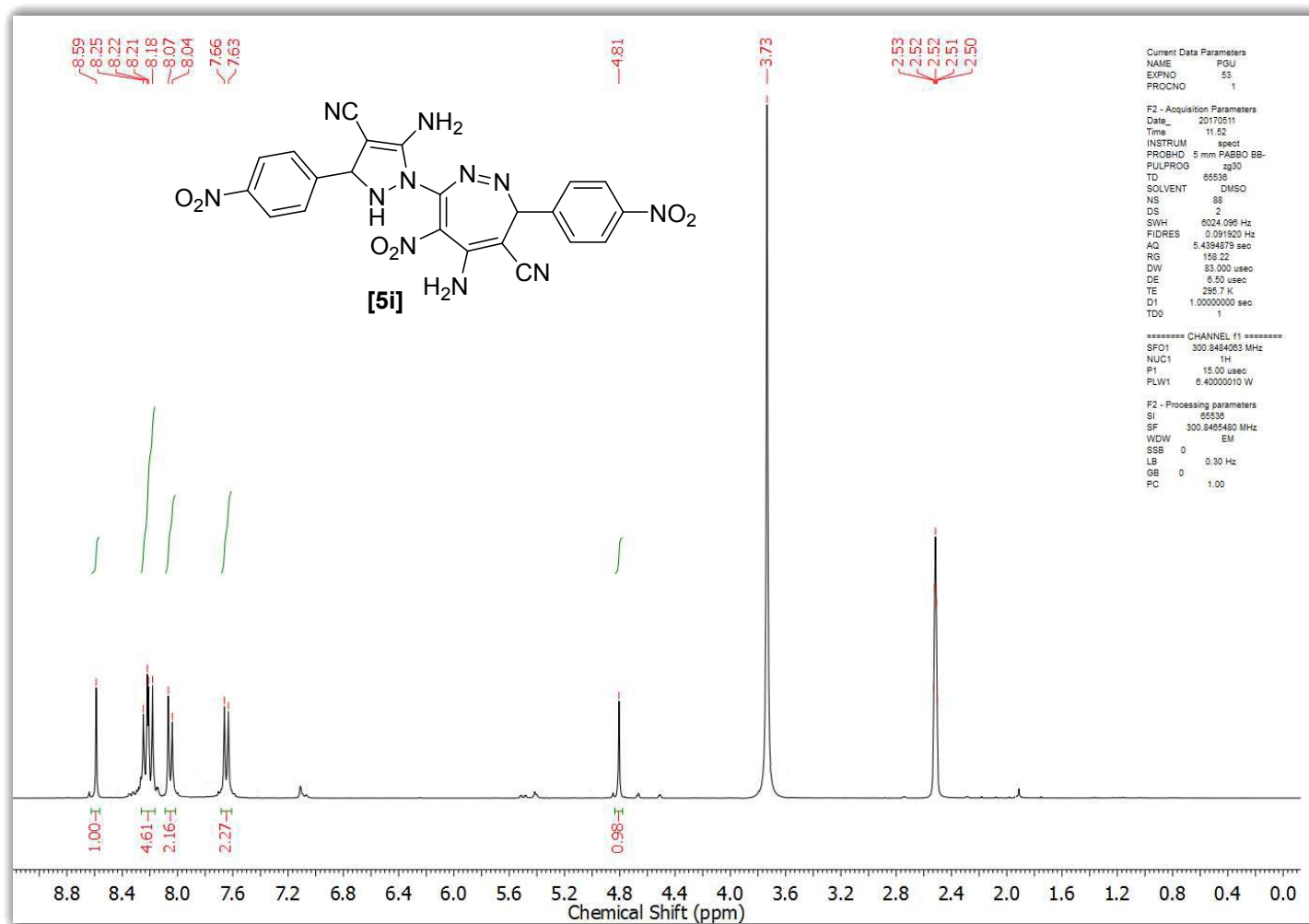


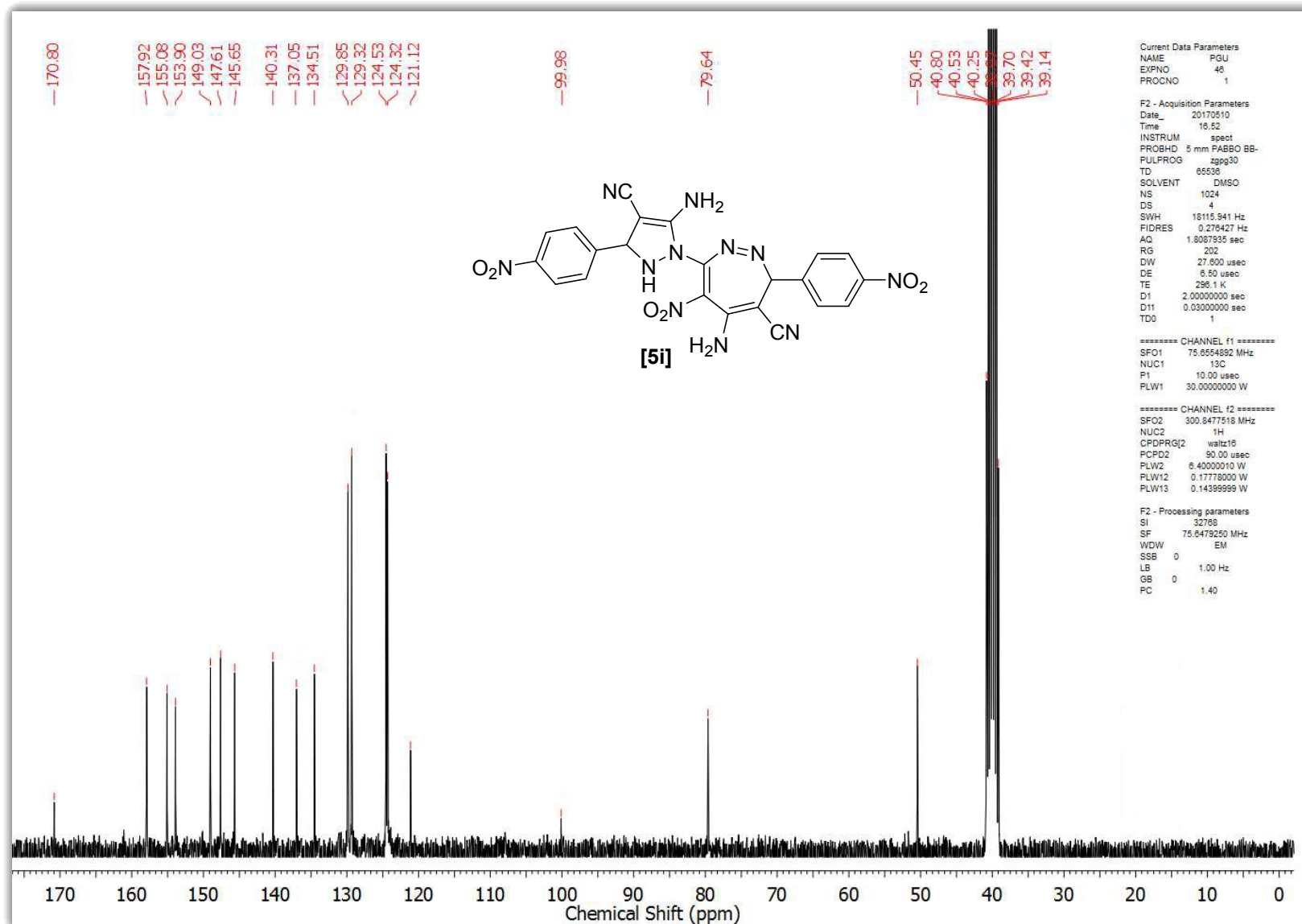


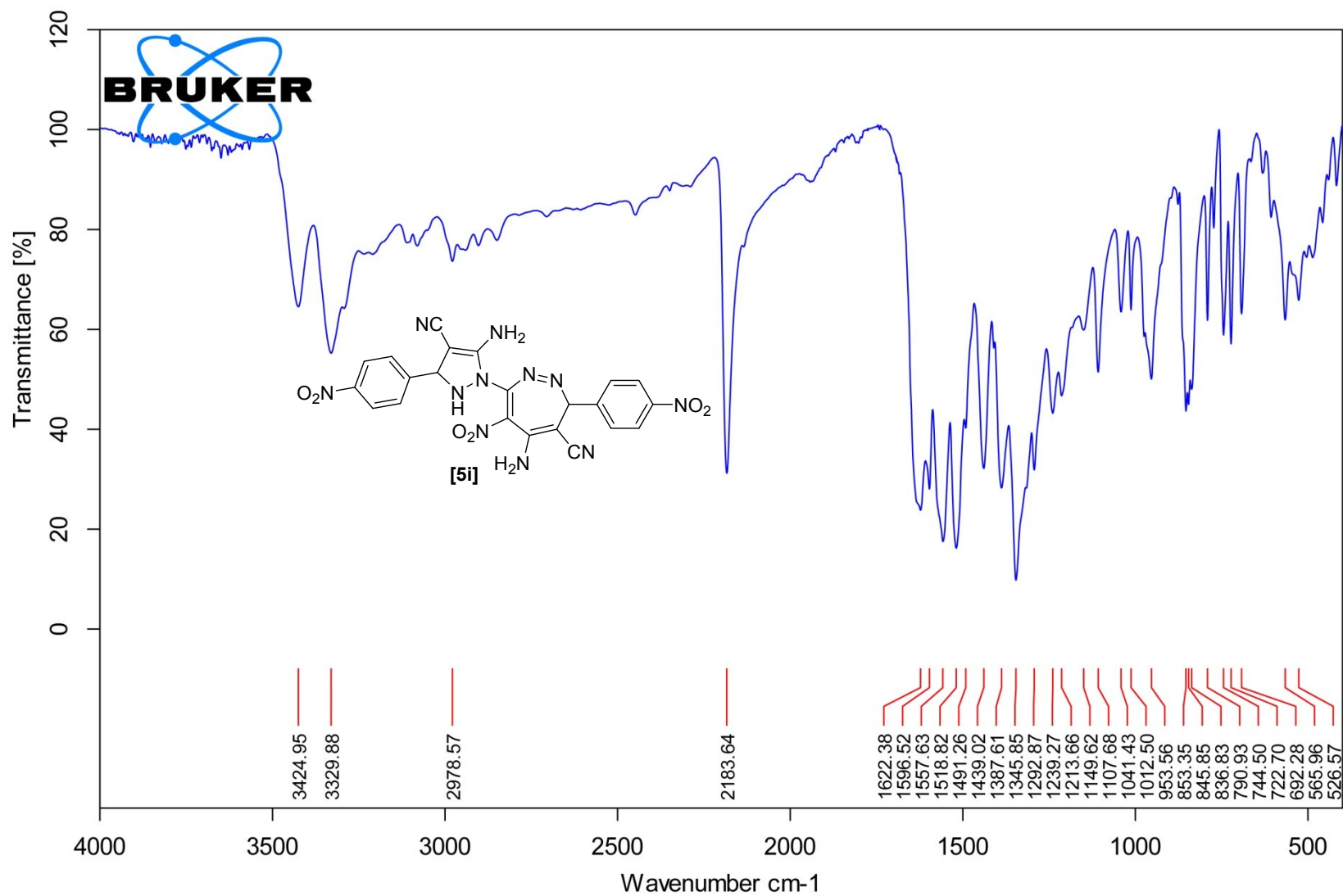
5-Amino-7-(5-amino-4-cyano-3-(4-nitrophenyl)-2,3-dihydro-1H-pyrazol-1-yl)-6-nitro-3-(4-nitrophenyl)-3H-1,2-diazepine-4-carbonitrile (**5i**)



D₂O-exchange spectrum of compound [5i]

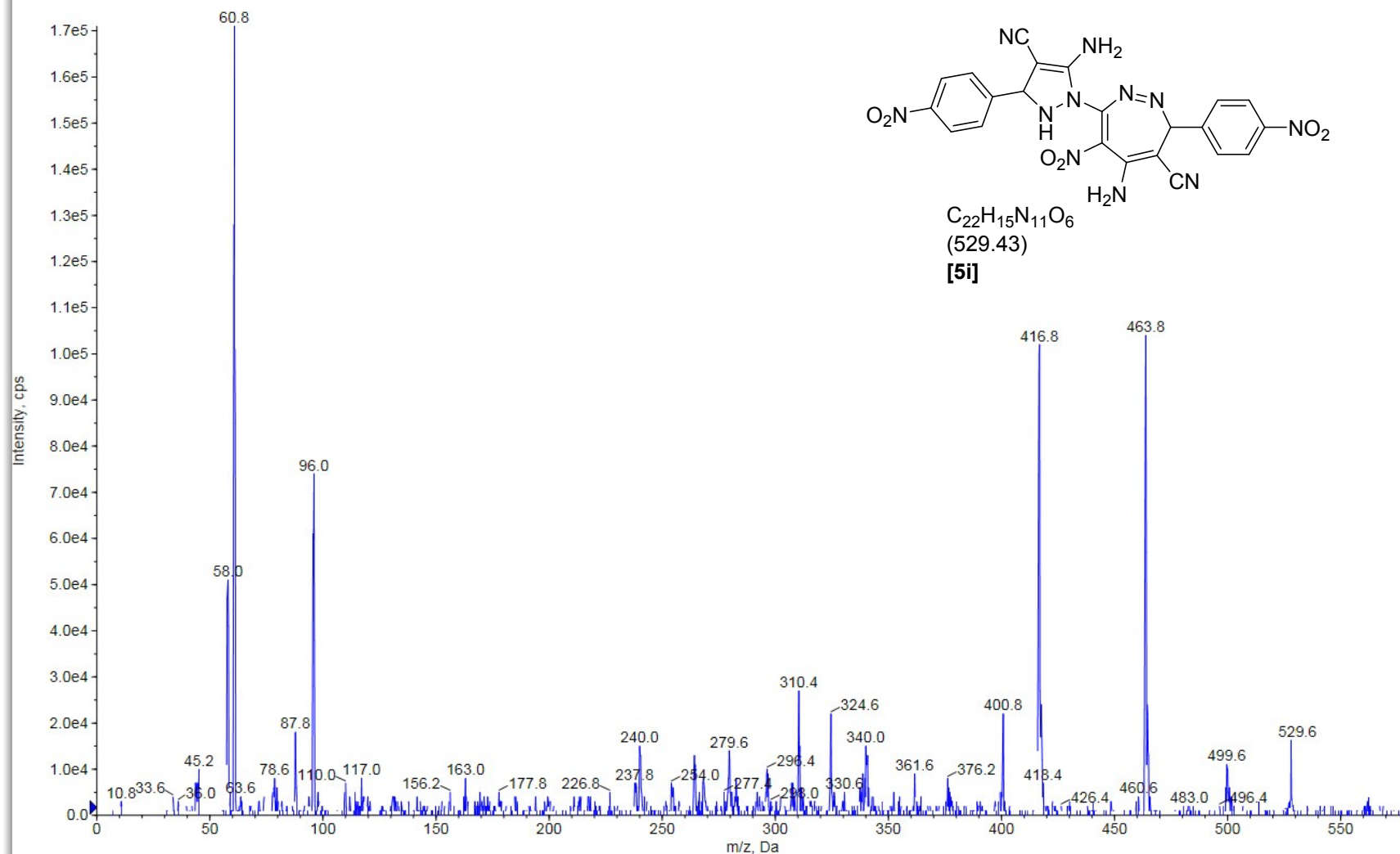




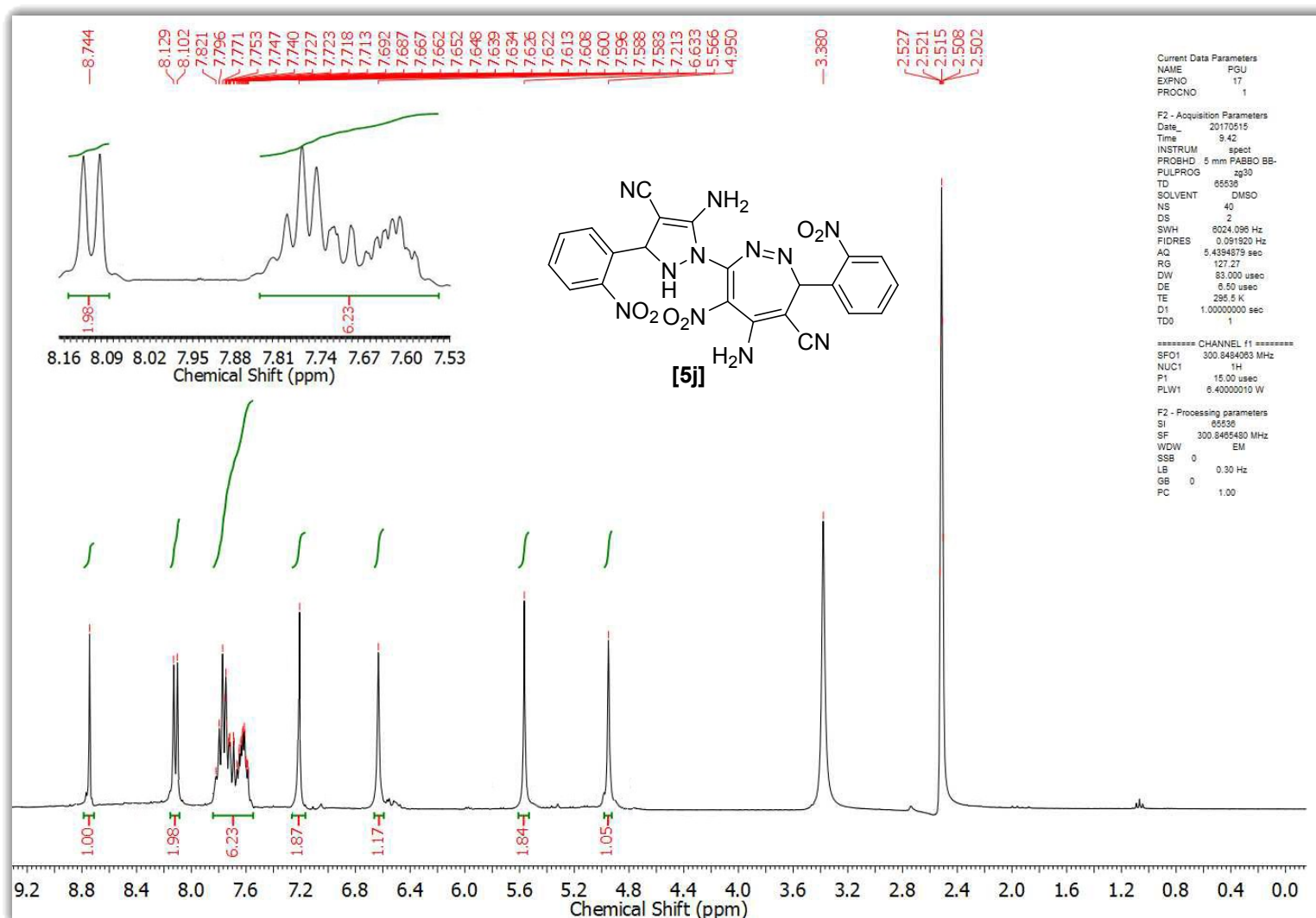


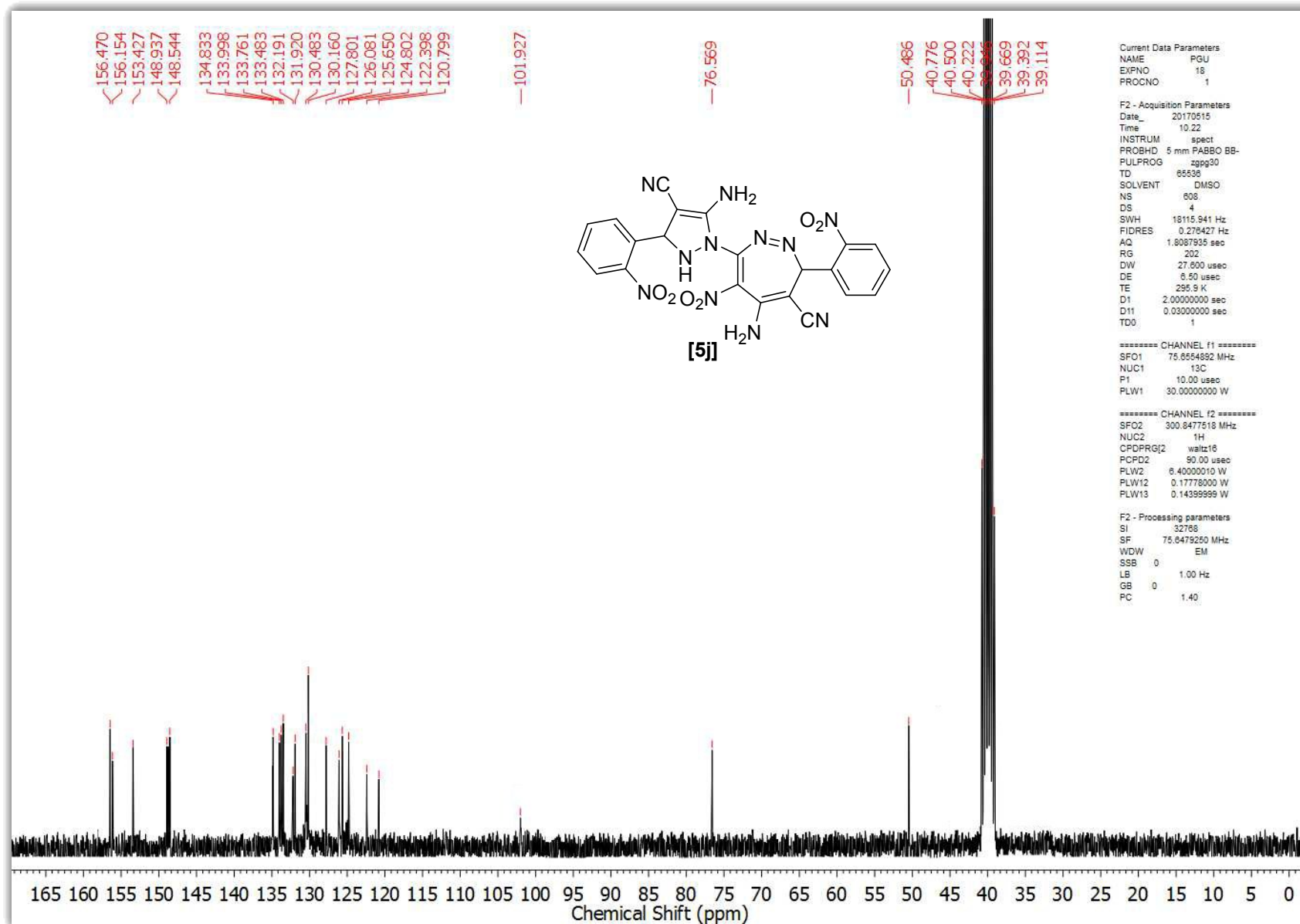
■ -Q1: 5 MCA scans from Sample 1 (TuneSampleName) of Mrs.moji (0-580)-_BP_Neg.wiff (Turbo Spray)

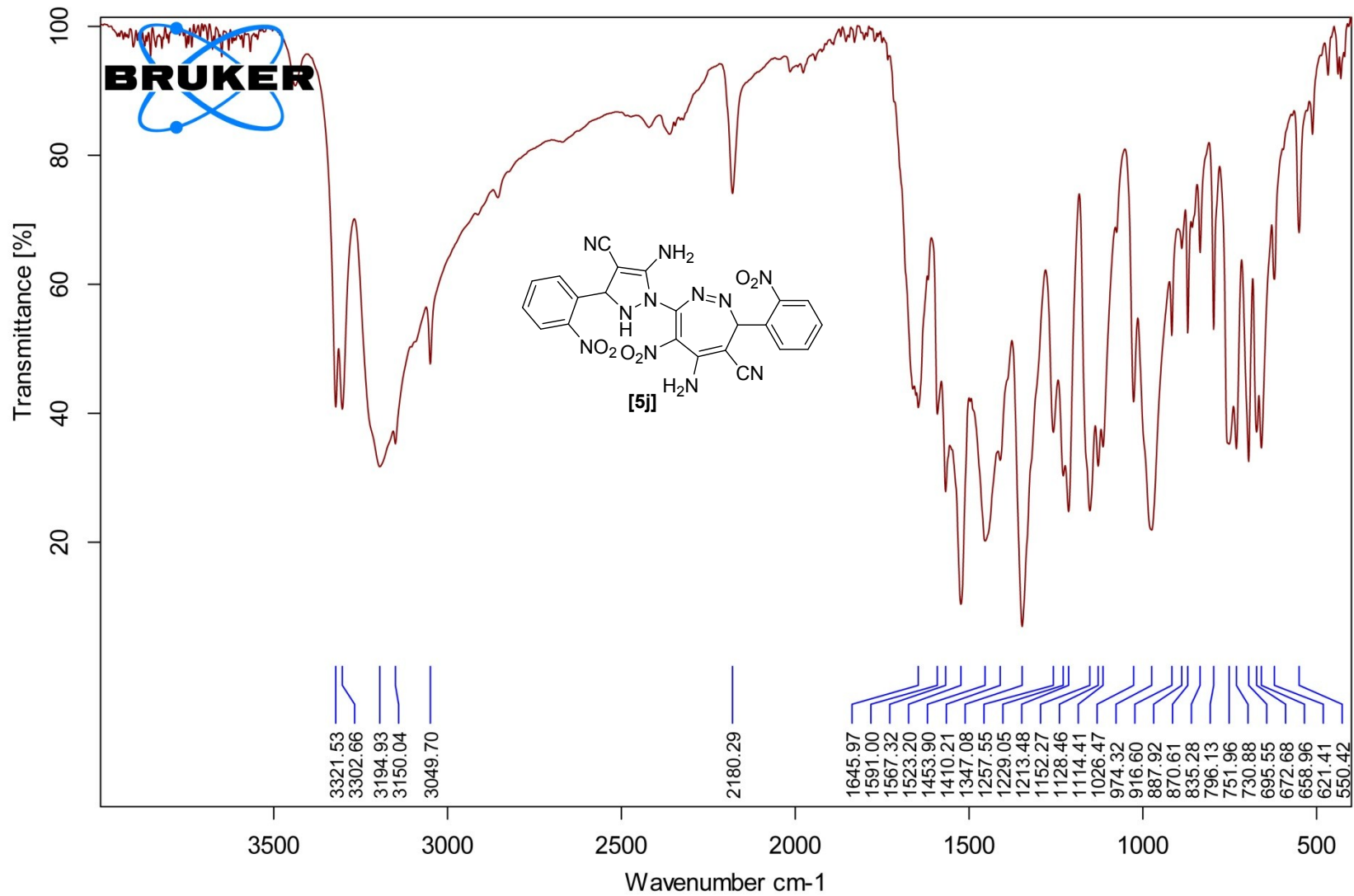
Max. 1.7e5 cps.



5-Amino-7-(5-amino-4-cyano-3-(2-nitrophenyl)-2,3-dihydro-1H-pyrazol-1-yl)-6-nitro-3-(2-nitrophenyl)-3H-1,2-diazepine-4-carbonitrile (**5j**)

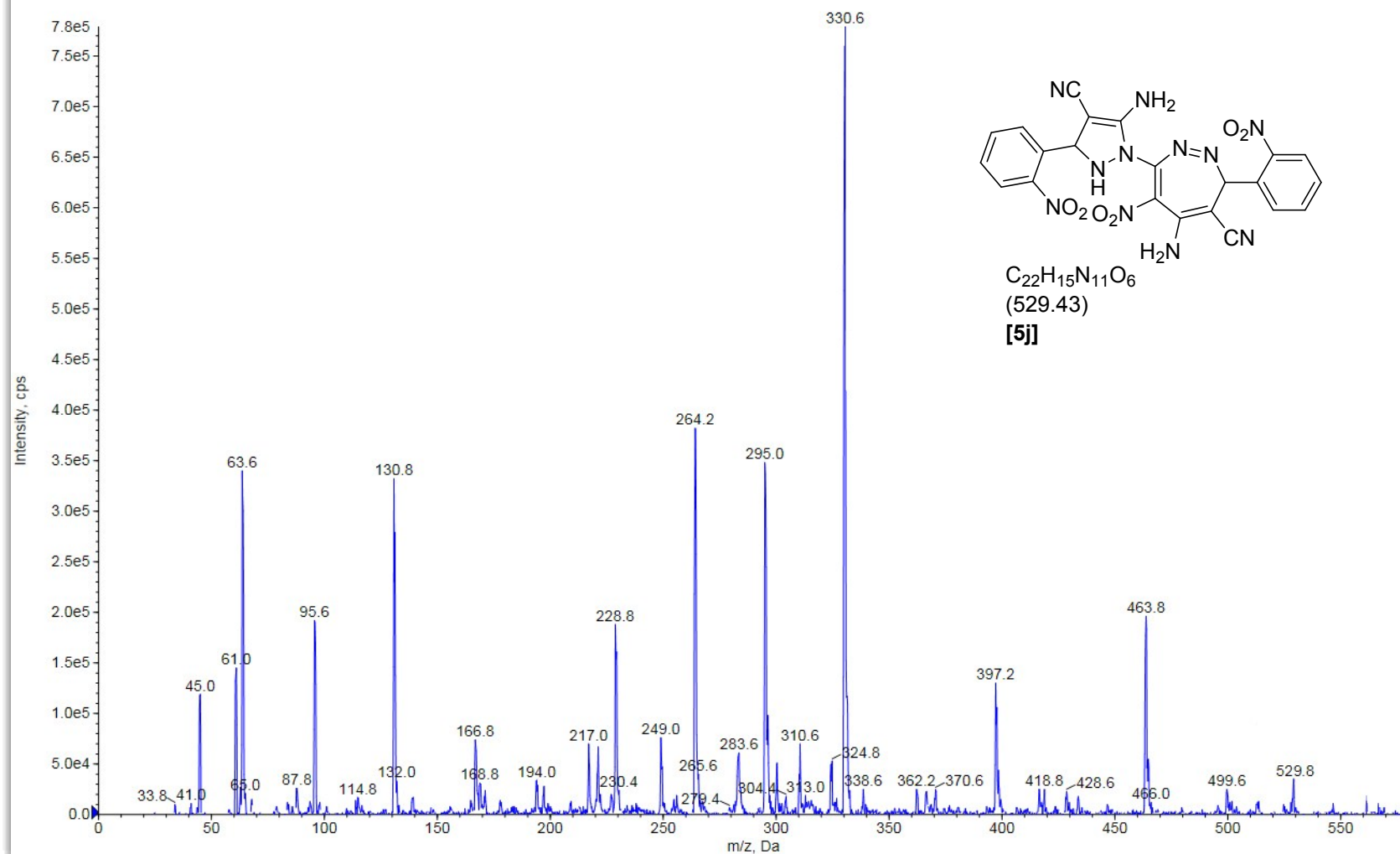




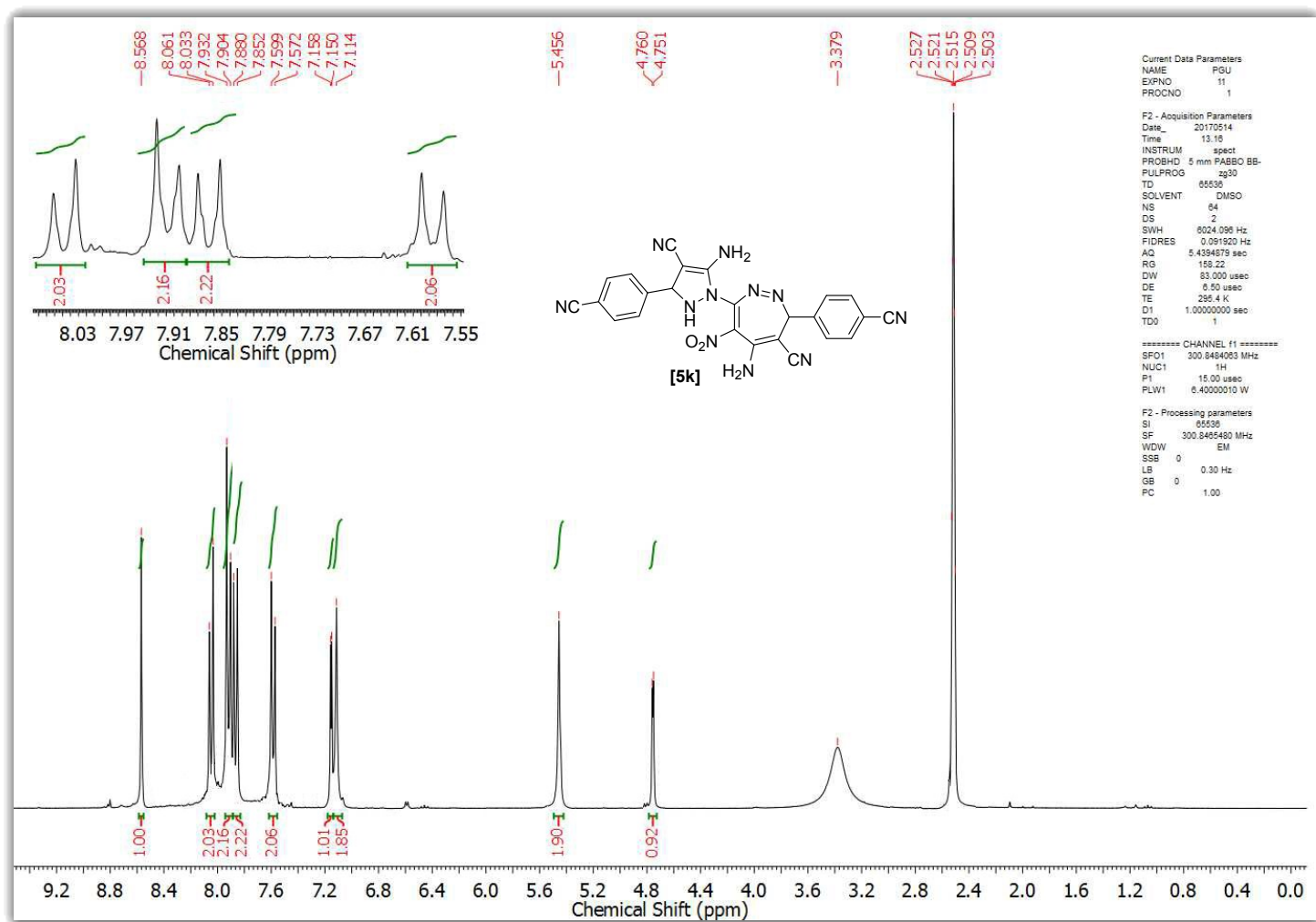


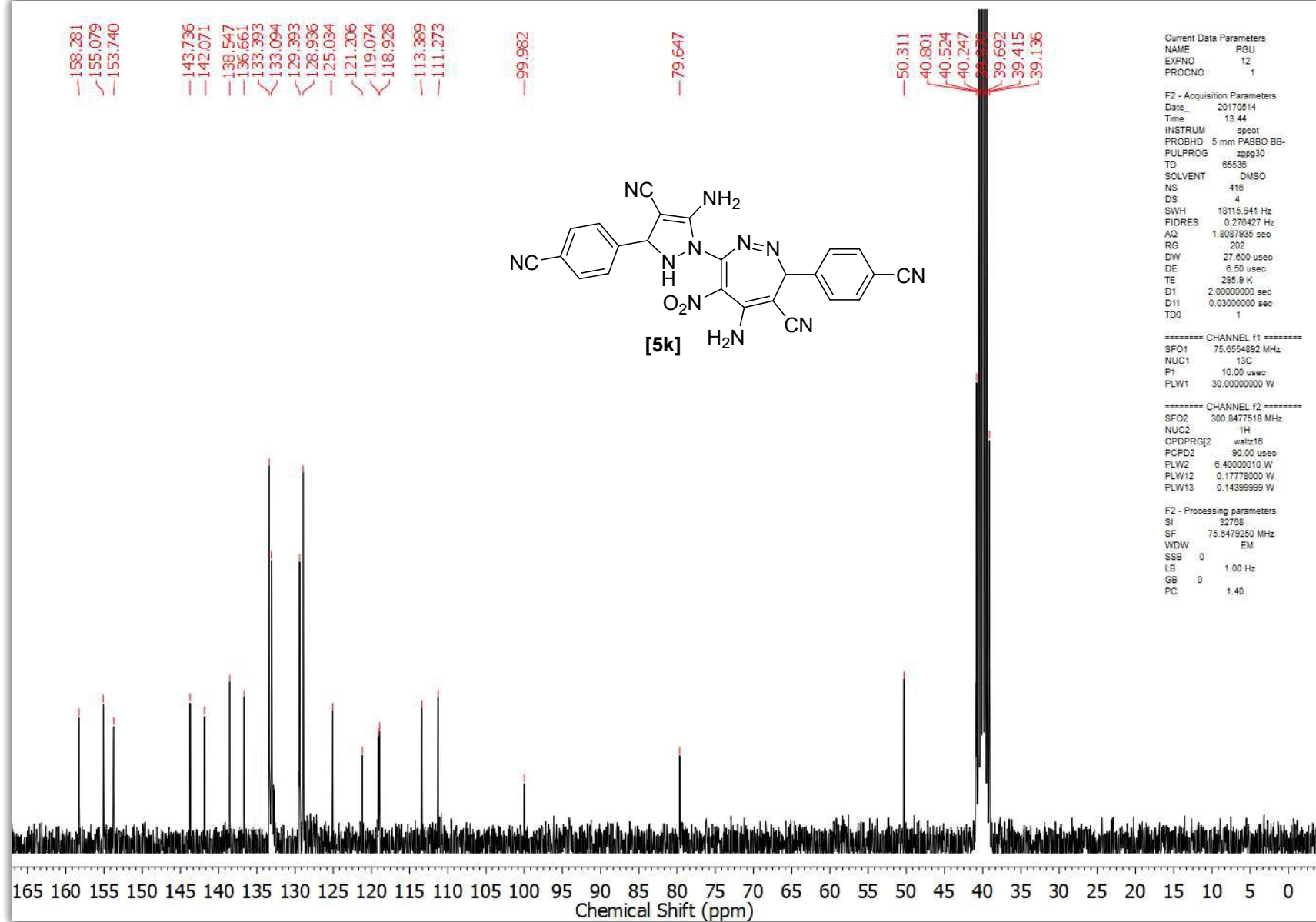
■ -Q1: 5 MCA scans from Sample 1 (TuneSampleName) of Mrs.moji (0-580)-_BP_Neg.wiff (Turbo Spray)

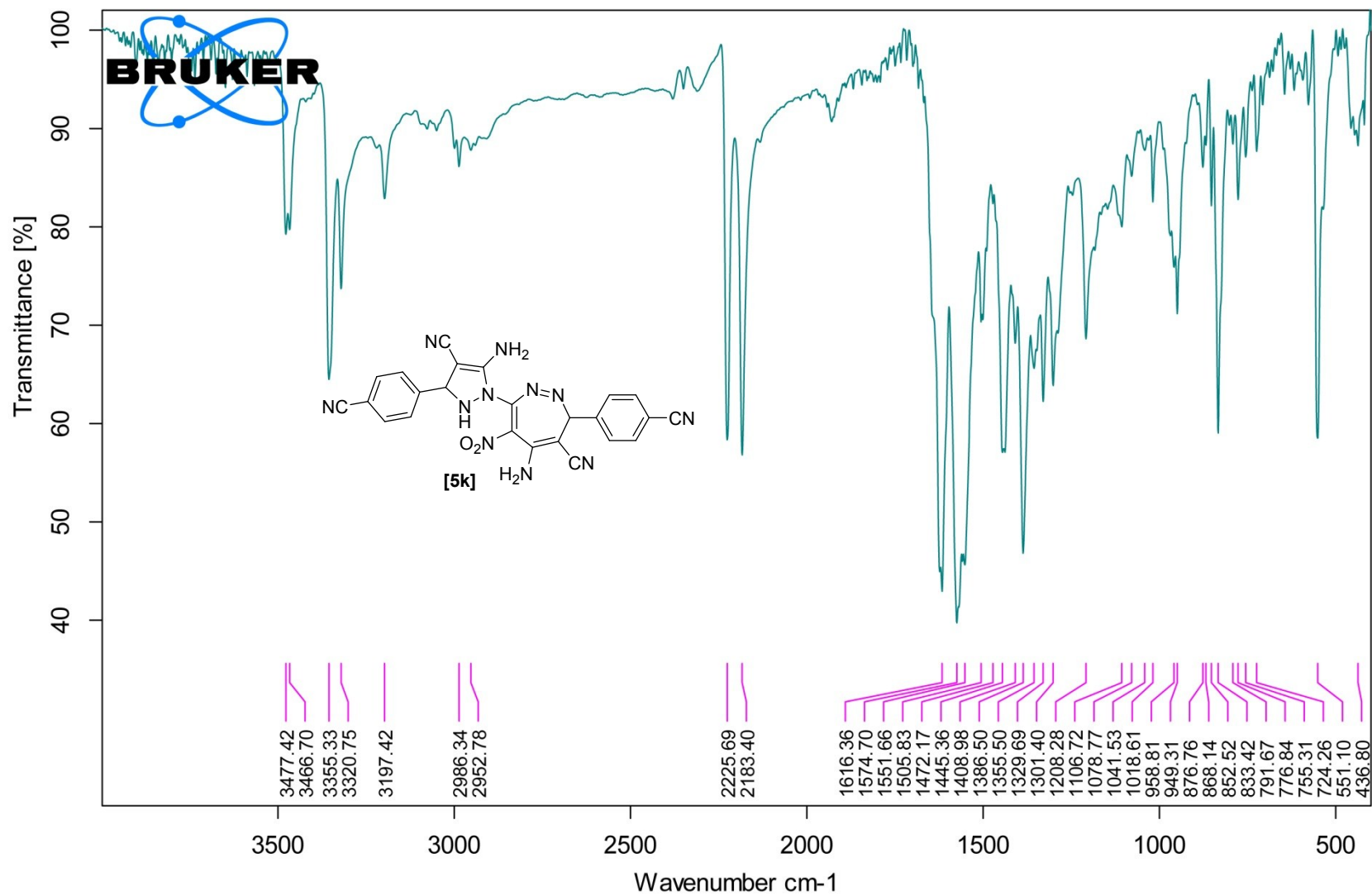
Max. 7.8e5 cps



5-Amino-7-(5-amino-4-cyano-3-(4-cyanophenyl)-2,3-dihydro-1H-pyrazol-1-yl)-3-(4-cyanophenyl)-6-nitro-3H-1,2-diazepine-4-carbonitrile (**5k**)

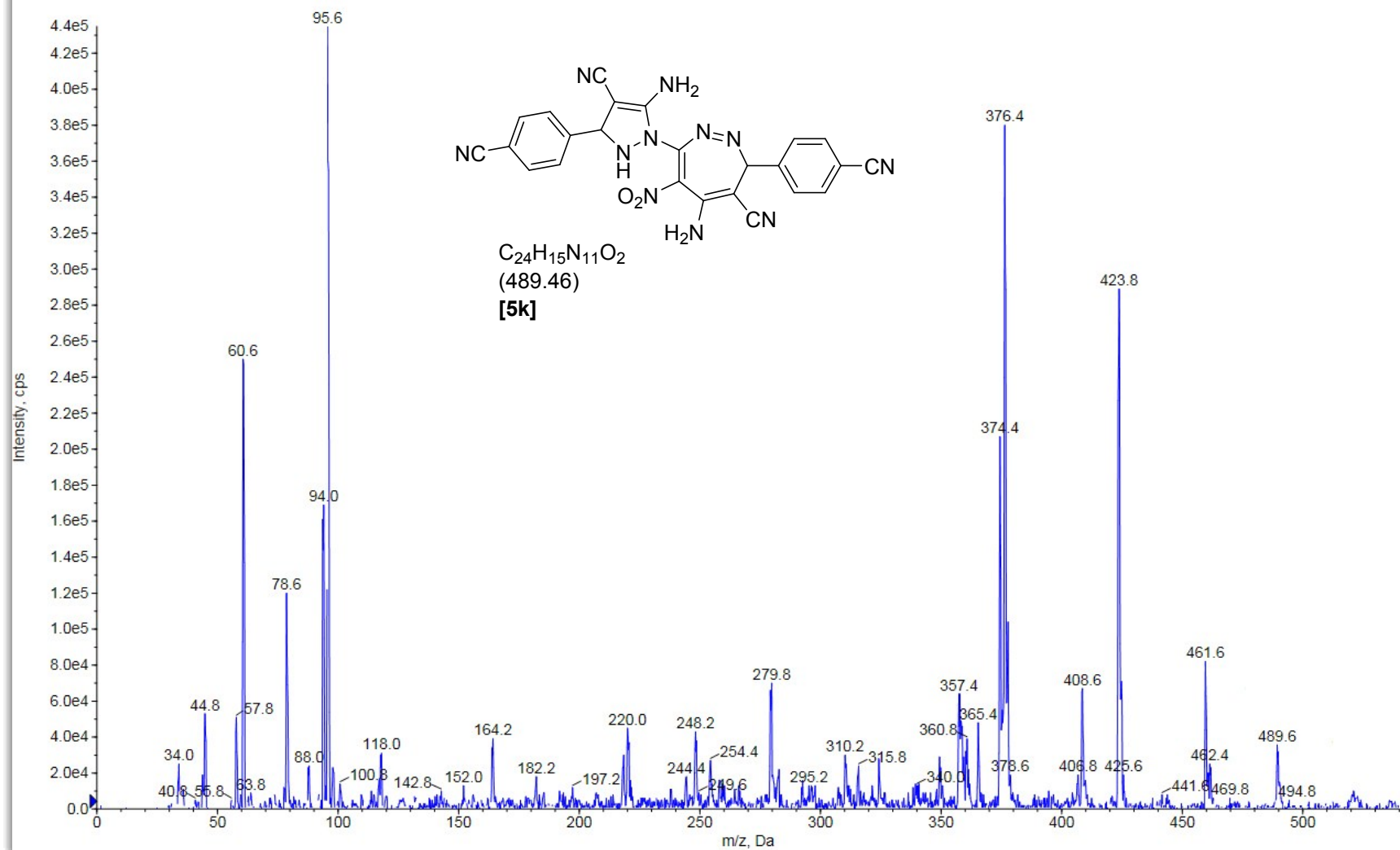




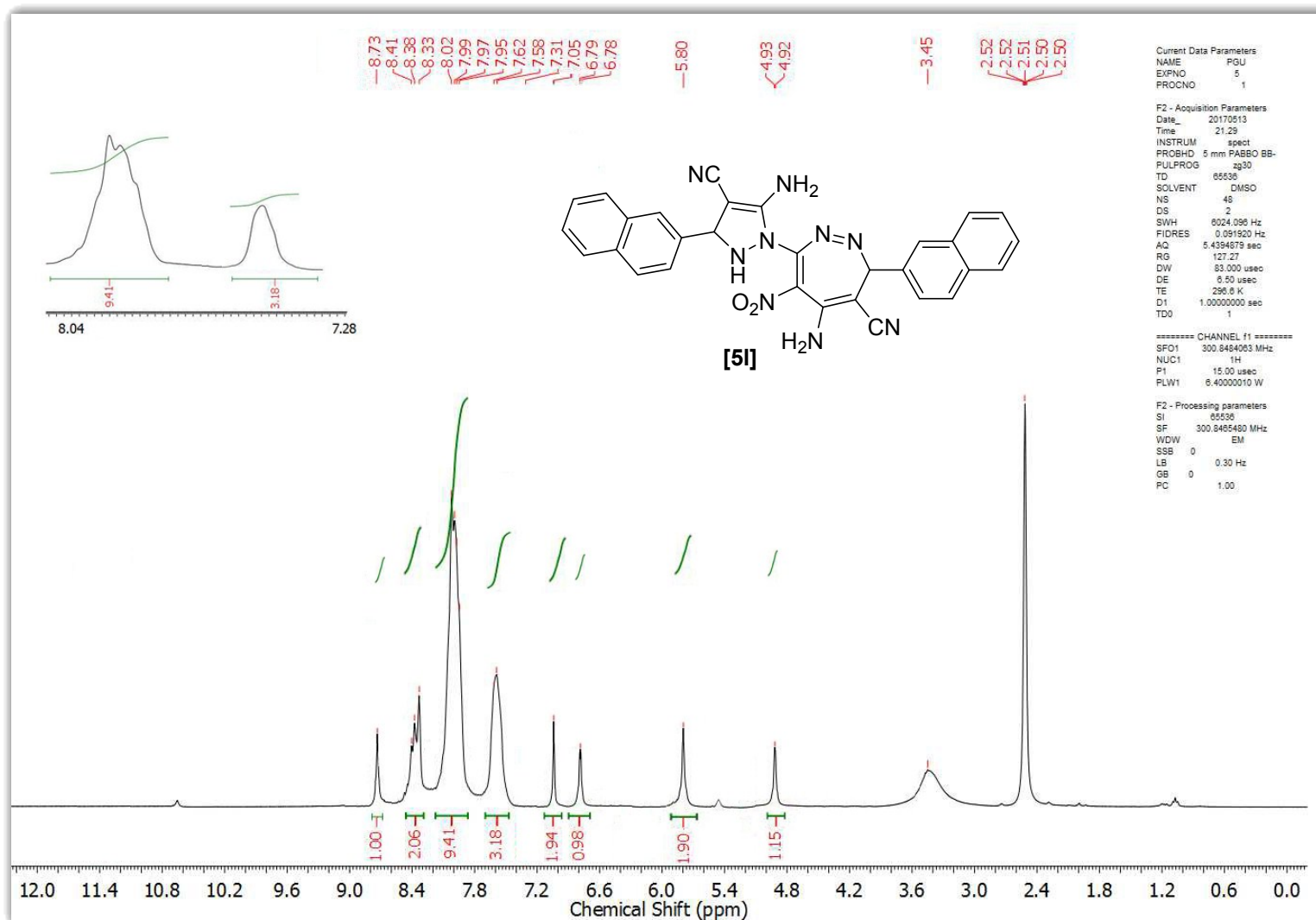


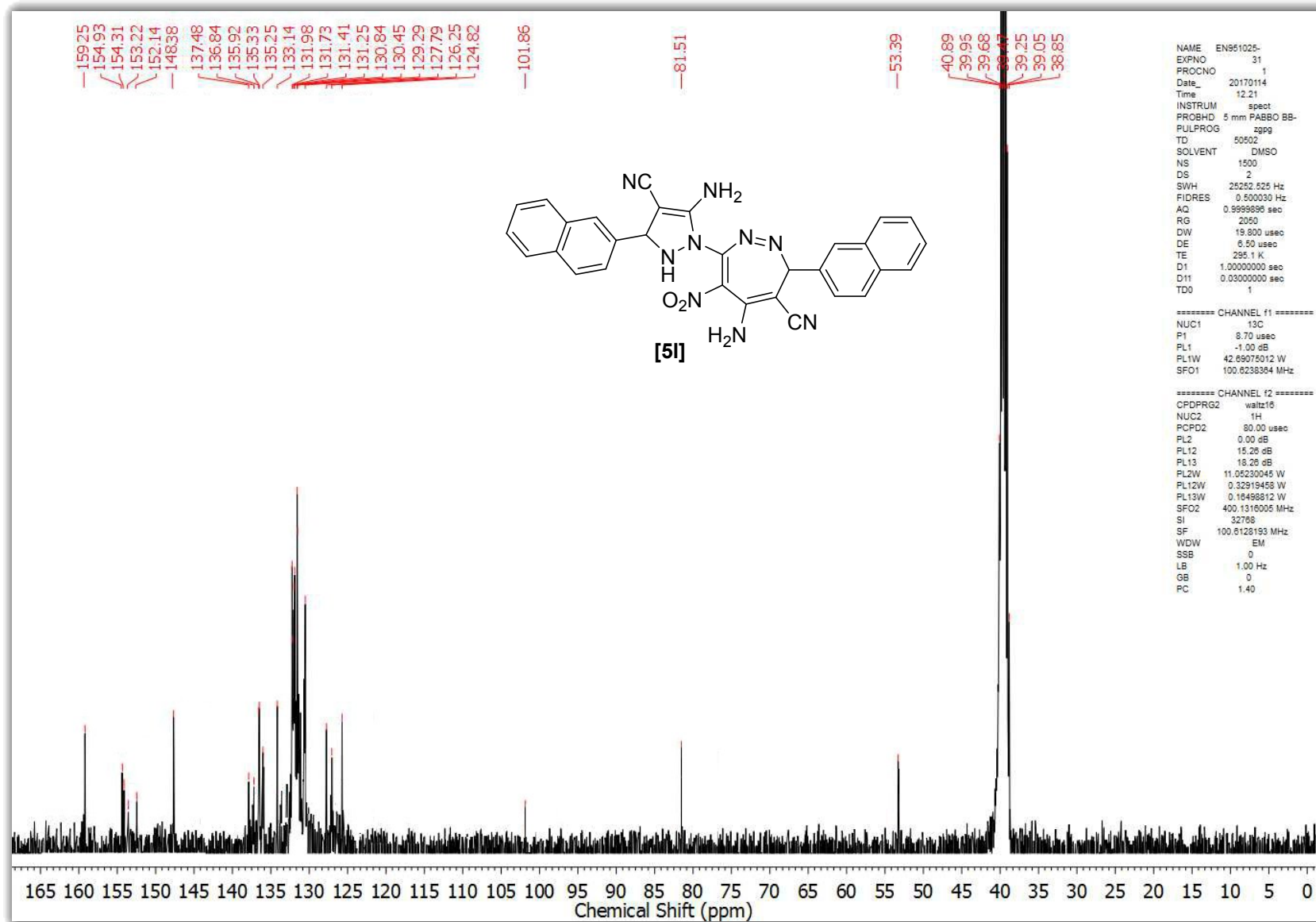
■ -Q1: 5 MCA scans from Sample 1 (TuneSampleName) of Mrs.moji (0-540)--_BP_Neg.wiff (Turbo Spray)

Max. 4.4e5 cps.



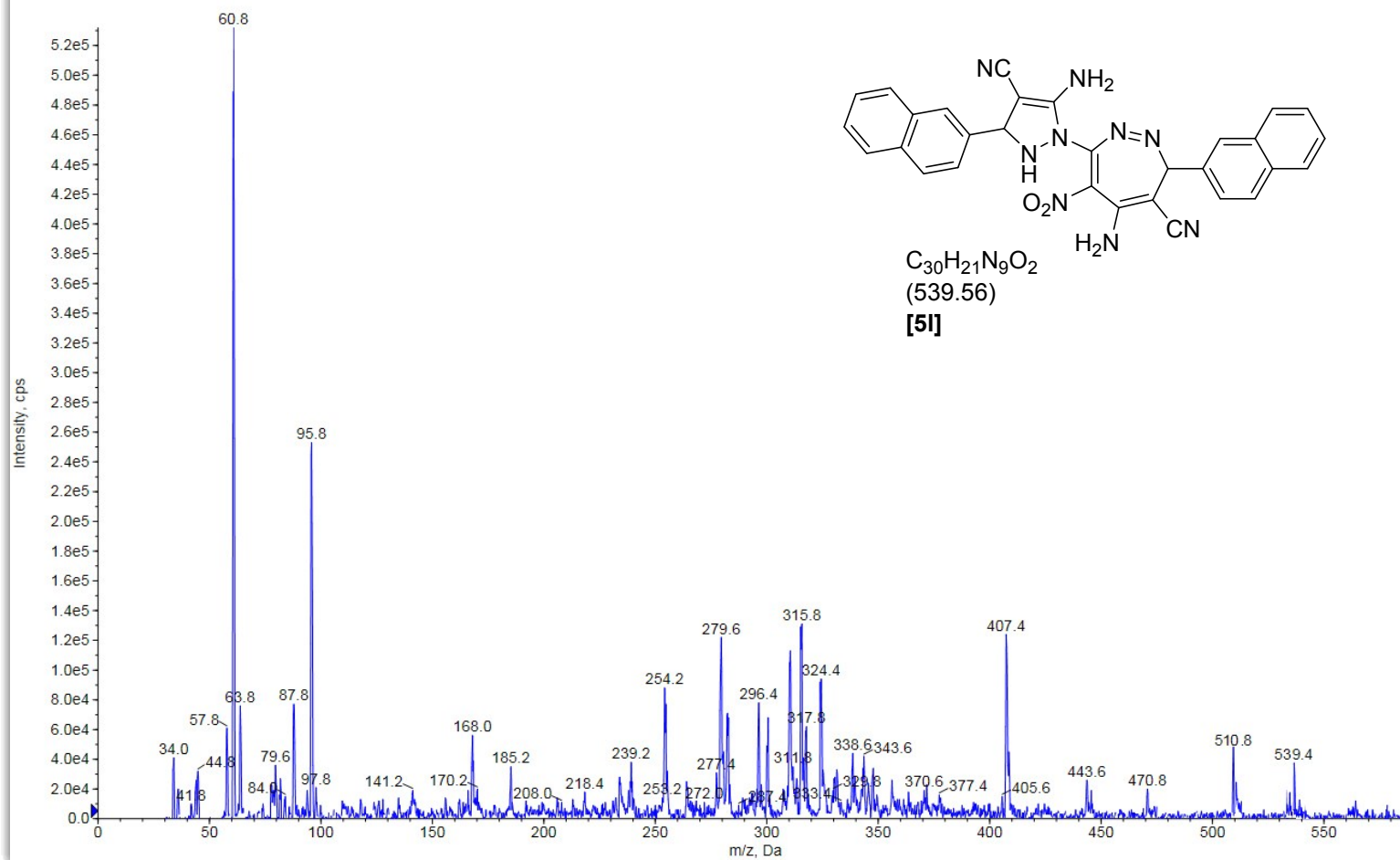
5-Amino-7-(5-amino-4-cyano-3-(naphthalen-2-yl)-2,3-dihydro-1H-pyrazol-1-yl)-3-(naphthalen-2-yl)-6-nitro-3H-1,2-diazepine-4-carbonitrile (**5I**)



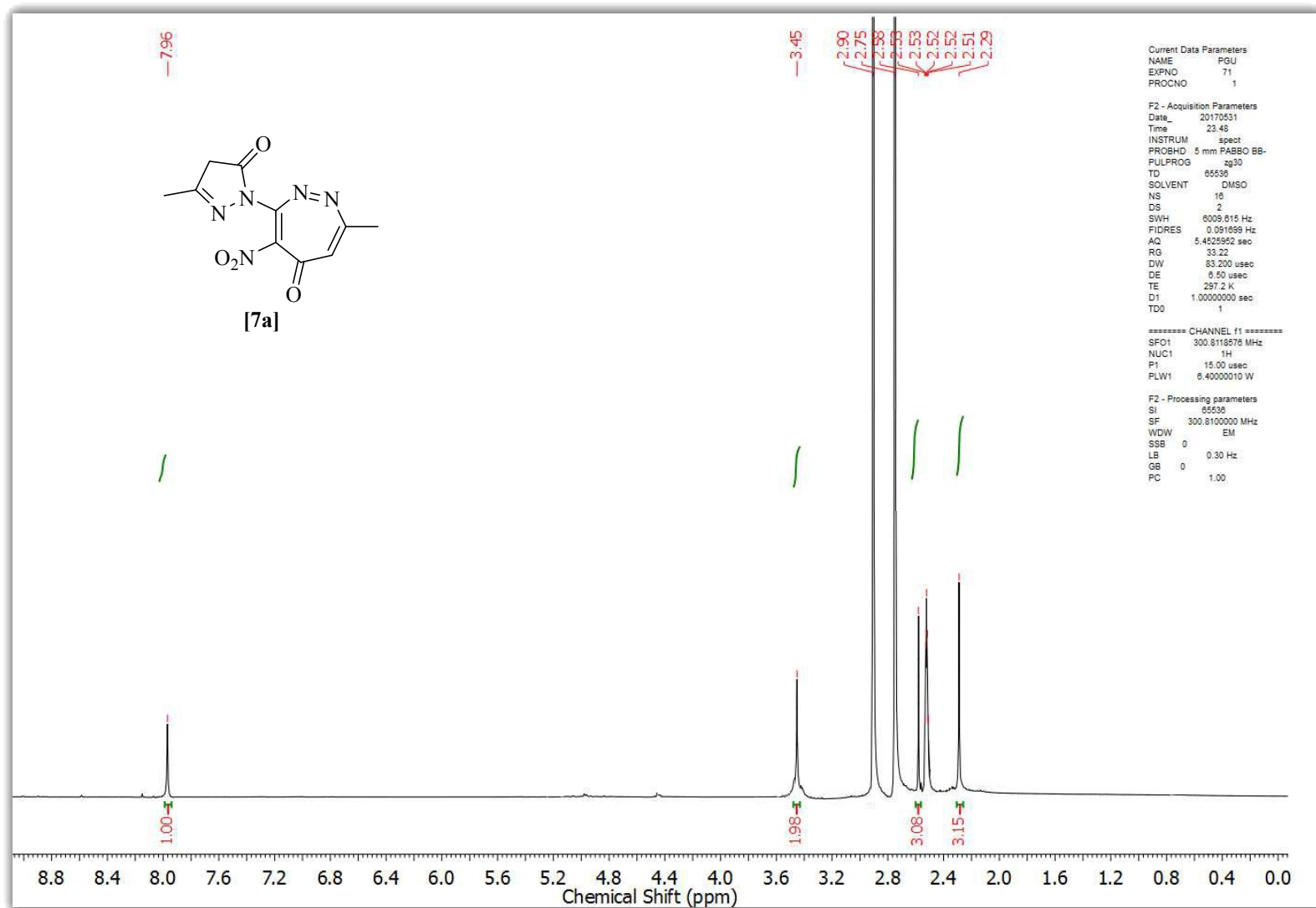


■ -Q1: 5 MCA scans from Sample 1 (TuneSampleName) of Mrs.moji (0-590)- me_BP_Neg.wiff (Turbo Spray)

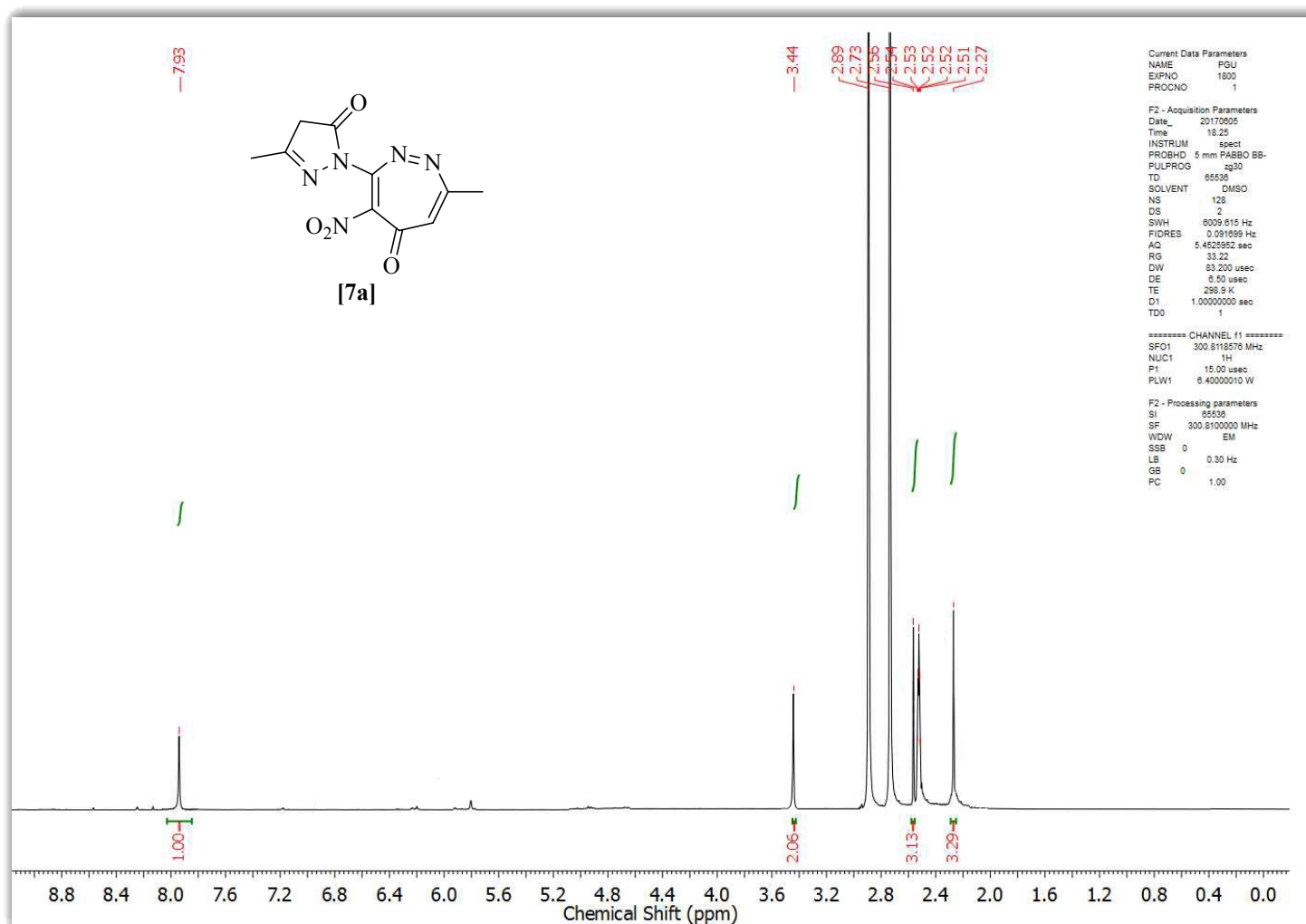
Max. 5.3e5 cps.

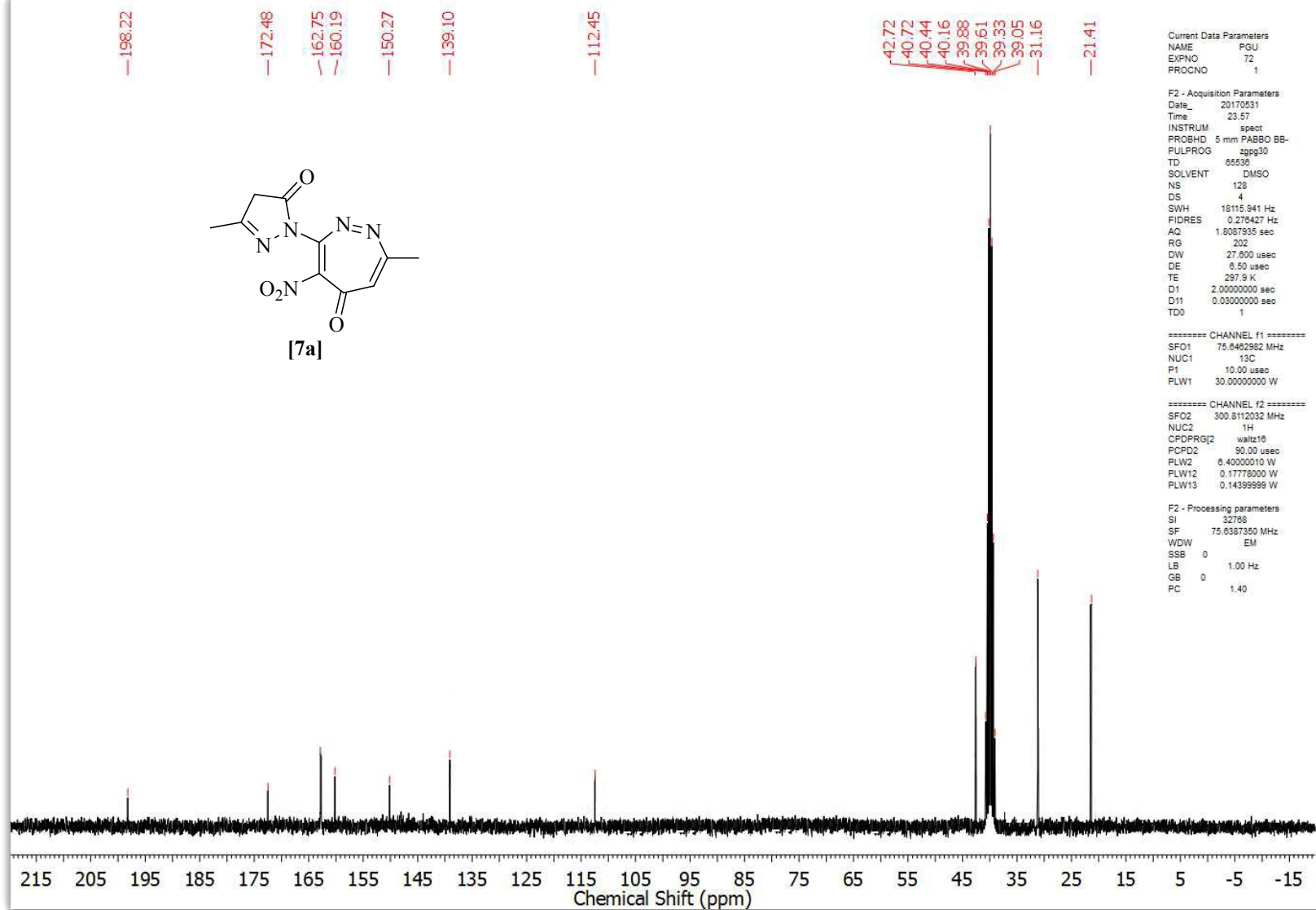
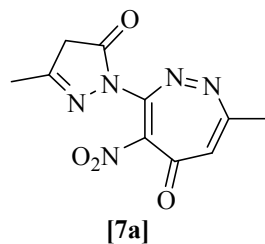


7-Methyl-3-(3-methyl-5-oxo-4,5-dihydro-1H-pyrazol-1-yl)-4-nitro-5H-1,2-diazepin-5-one] (**7a**)



D₂O-exchange spectrum of compound [7a]





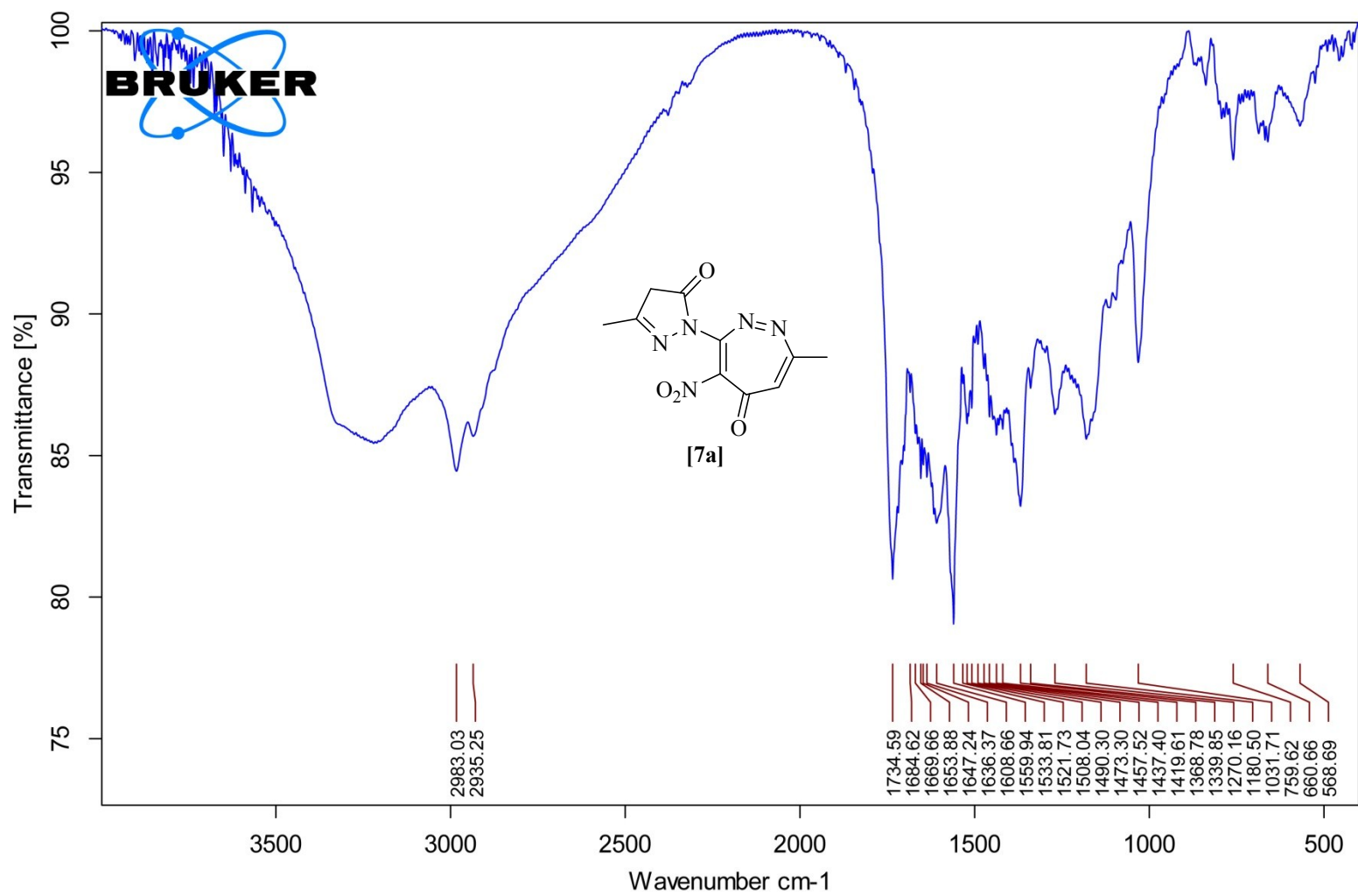
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 PROCNO 1

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 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 128
 DS 4
 SWH 18115.941 Hz
 FIDRES 0.276427 Hz
 AQ 1.8087935 sec
 RG 202
 DW 27.800 usec
 DE 6.50 usec
 TE 297.5 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

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 NUC1 13C
 P1 10.00 usec
 PLW1 30.00000000 W

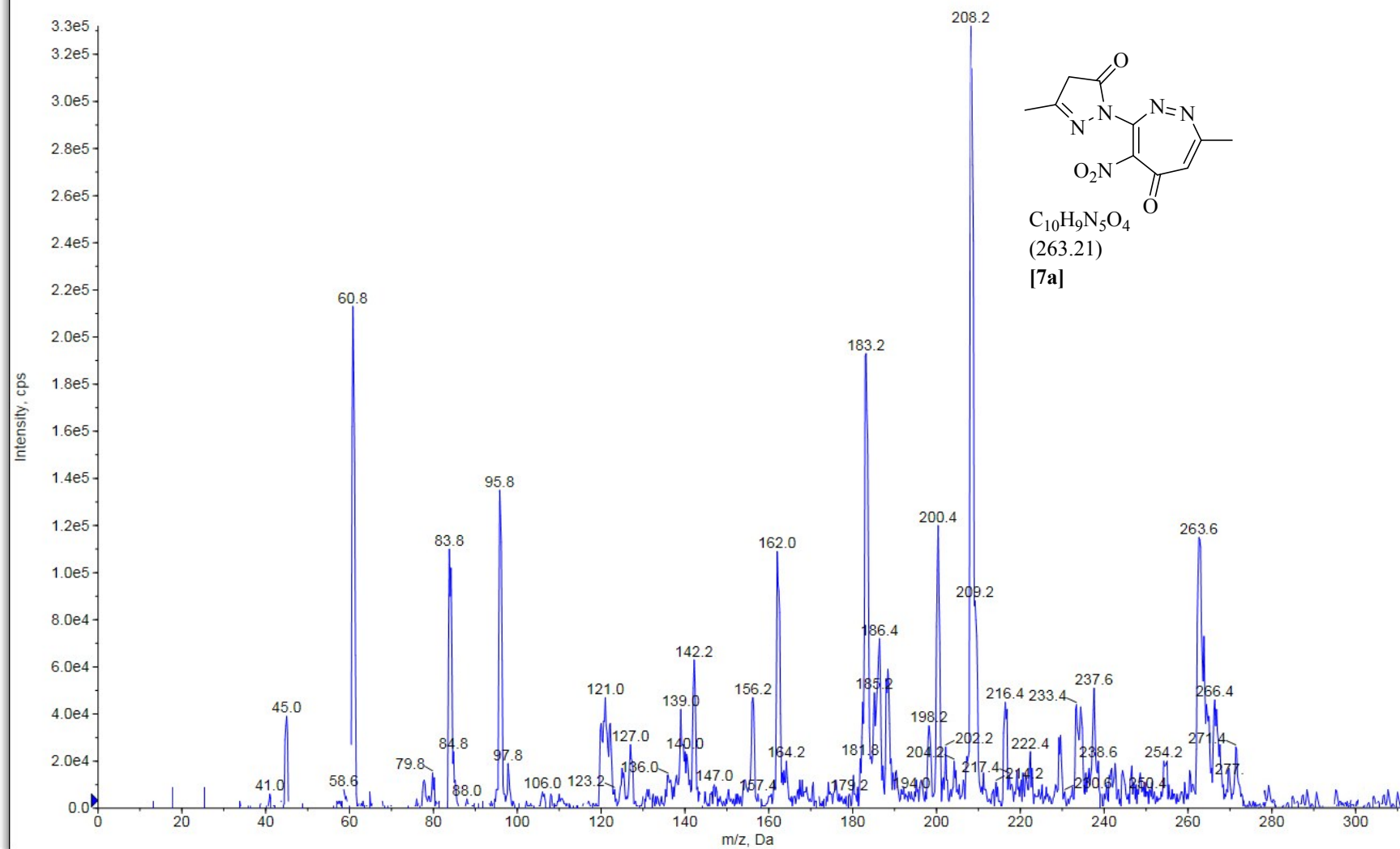
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 CPDPRG2 waltz16
 PCPD2 90.00 usec
 PLW2 6.40000010 W
 PLW12 0.17778000 W
 PLW13 0.14398999 W

F2 - Processing parameters
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 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

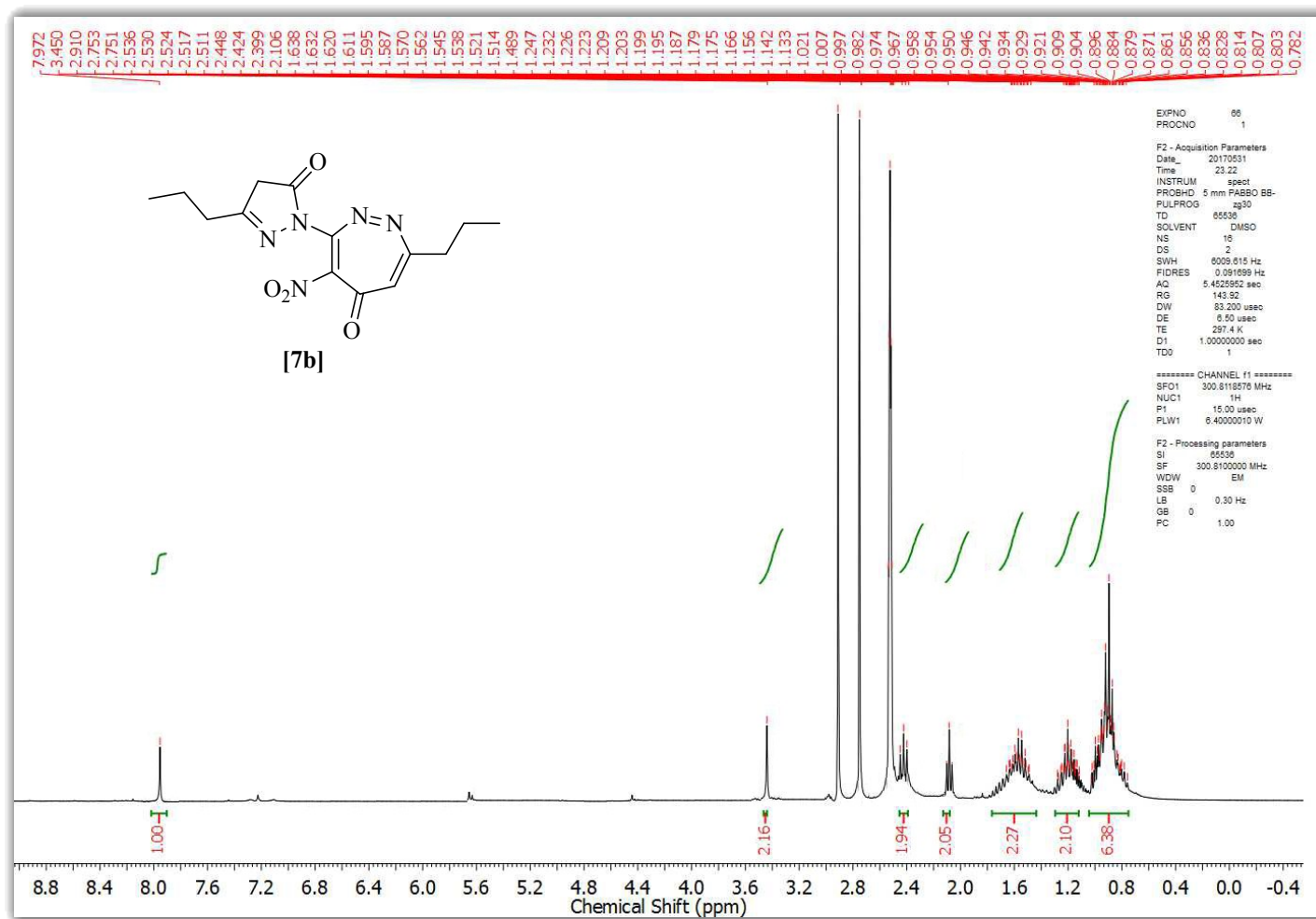


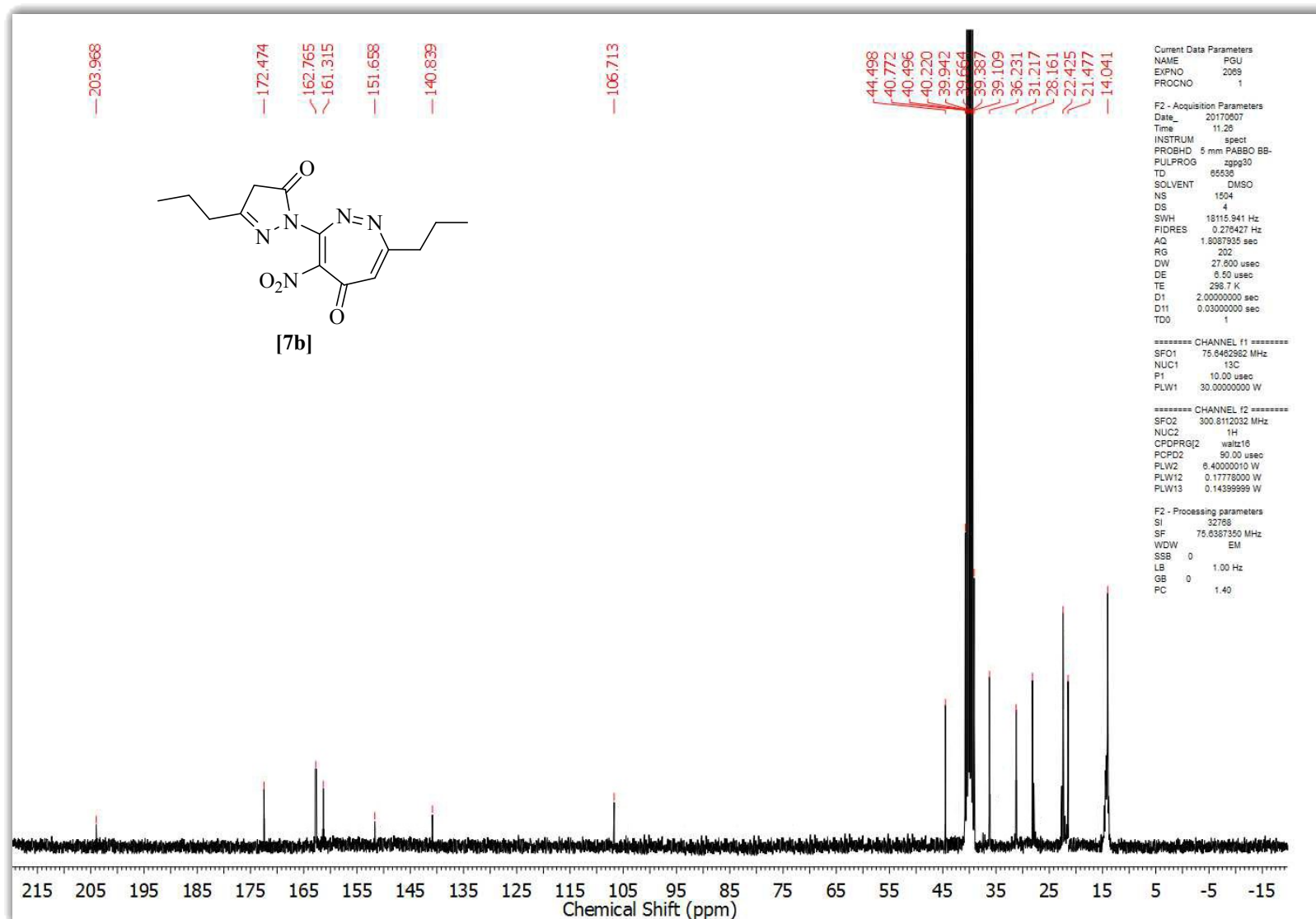
-Q1: 5 MCA scans from Sample 1 (TuneSampleName) of Mrs. moji (0-310)-BP_Neg.wiff (Turbo Spray)

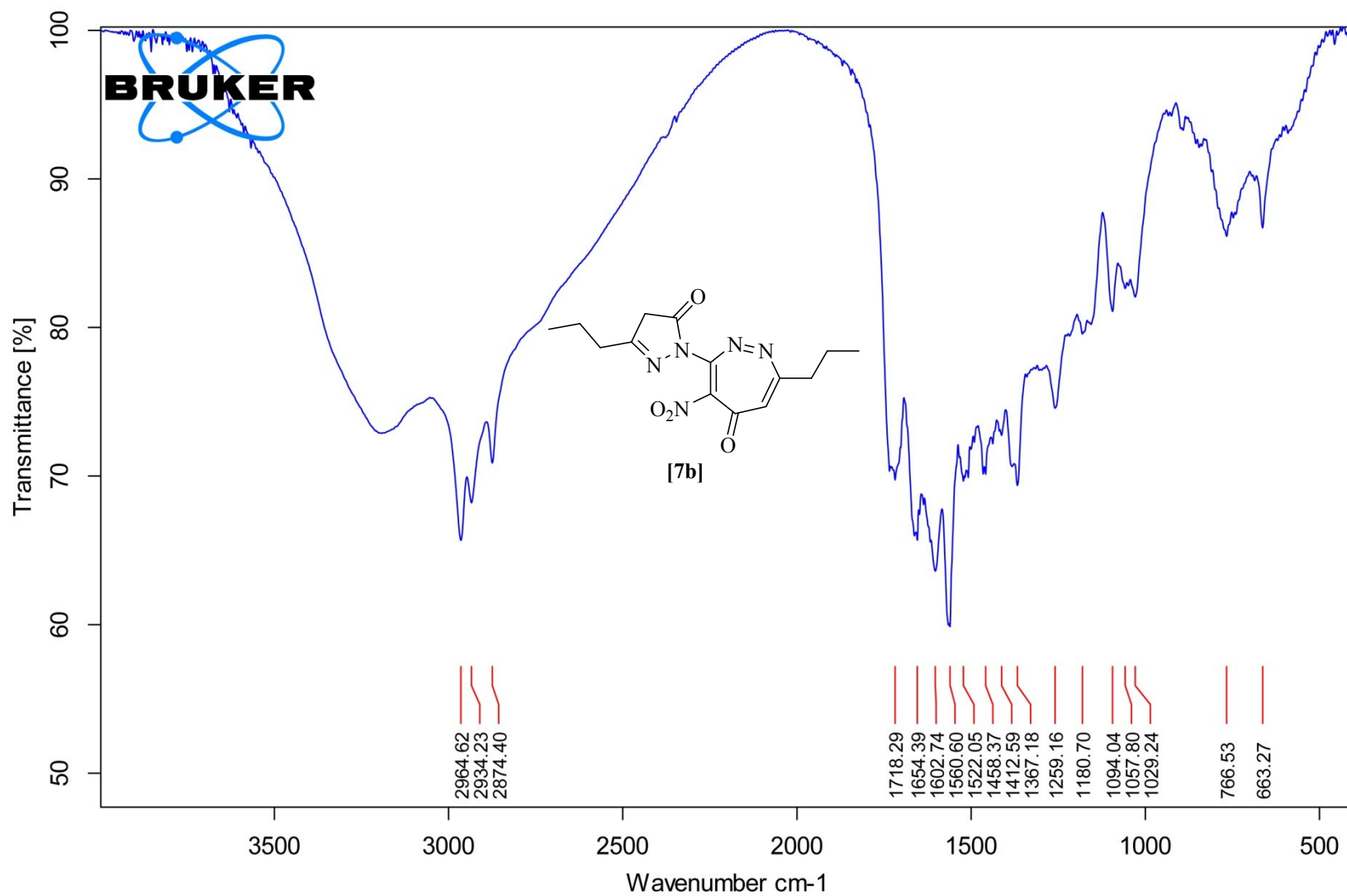
Max. 3.3e5 cps



4-Nitro-3-(5-oxo-3-propyl-4,5-dihydro-1H-pyrazol-1-yl)-7-propyl-5H-1,2-diazepin-5-one (**7b**)







■ -Q1: 5 MCA scans from Sample 1 (TuneSampleName) of Mrs. moji (0-370)-_BP_Neg.wiff (Turbo Spray)

Max. 4.5e5 cps

