

Supplementary Data

Synthesis molecular docking and DFT studies on novel indazole derivatives

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1. General methods

All the reactions were carried out in round bottom flasks. All the solvents and chemical materials were purchased from commercial sources. The 1-butyl-1H-indazole-3-carboxamide was prepared according to the reported protocols. ¹H and ¹³C NMR spectra were recorded on Bruker Avance400 spectrometer and are referred to the residual solvent signal CDCl₃: (7.26) for ¹H and (77.16) for ¹³C NMR: dimethyl sulfoxide-d₆ (2.50) for ¹H and (39.50) for ¹³C NMR: chemical shift (δ) 3s given in ppm and coupling constant (J) were measured in Hz. The following abbreviations are used: s- singlet, d-doublet, dd-doublet of doublet, t-triplet, td-triplet of doublet, dt- doublet of triplet, q-quartet, qd- quartet of doublet, qn-quintet, br-broad, m-multiplet. HRMS ESI-MS was recorded using Xeo G2 XS OT of (water) and values are given m/z. Column chromatography was carried out using silica gel (100-200 mesh) packed in a glass column. Analytical TLC was carried out on Macherey-Nagel 60 F245 aluminium-backed silica gel plates.

2. Scheme and Experimental procedure for indazole derivative

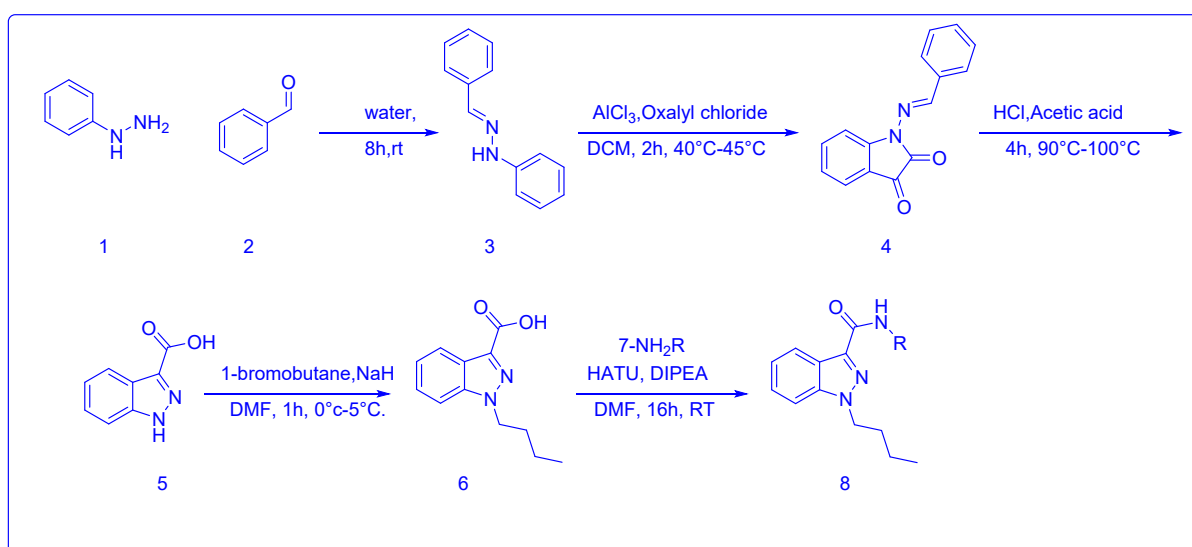


Table-1

2.1. Preparation of 2-benzylidene-1-phenylhydrazine (3):

To a stirred solution of phenyl hydrazine (50 gm) in water (500mL, 10 vol), add benzaldehyde (equivalent) very slowly at room temperature and stir for 8h. TLC showed the completion of starting material. Filter off the solid washed with water (150 mL) and chilled isopropyl alcohol (50 mL), and dry the solid under the oven at 70°C to 80°C for 8h to get 2-benzylidene-1-phenylhydrazine as a white solid

2.2. Preparation of 1H-indazole-3-carboxylic acid (5):

To a stirred solution of 2-benzylidene-1-phenylhydrazine (70 gm) in DCM (500 mL), oxalyl chloride (1.05 equivalent) was added at room temperature and stirred at 40°C to 45°C for 2h. TLC showed the completion of 2-benzylidene-1-phenylhydrazine, add aluminium trichloride (1.5 equivalent) at 40°C to 45°C and stir for 2h. TLC showed the completion of the intermediate (oxalyl chloride intermediate). Poured the reaction mixture into cooled water (350 mL), wash the combined organic layer and extract the aqueous layer with DCM (2x200 mL), wash the combined organic layer with 10% HCl and brine solution. Dry the organic layer over sodium sulphate and concentrated under reduced pressure. To the obtained crude add acetic acid (300 mL) and conc. HCl (100 mL), heated at 90°C to 100°C for 4h. Cool the reaction mixture to room temperature and stir for 2h. Filter off the solid material and washed with water. Dissolve the obtained solid into 5N sodium hydroxide solution, filter off the solid, wash with water, and discard the solid material. Take the aqueous layer into round bottom flask, and acidify the layer with conc. HCl up to pH 2, stir for 30 min and filter off the solid, wash the solid with water and dry the solid material under oven at 80°C for 4-5h to get 1H-indazole-3-carboxylic off white solid.

2.3. Preparation of 1-butyl-1H-indazole-3-carboxylic acid:

To a stirred suspension of sodium hydride (1.2 equivalent) in DMF (250 mL), add 1H-indazole-carboxylic acid (50 gm) dissolved in DMF (150 mL) at 5°C and stir for 1h. To this reaction, mass adds 1-Bromobutane (1.05 equivalent) at 10°C and stir at room temperature for 8h. TLC showed the completion of starting material and the formation of the non-polar spot. Quenched the reaction mass into ice water, wash the aqueous layer with ethyl acetate, and acidify the organic layer using con. HCl up to pH reaches 1, extract the layer with ethyl acetate (2 x 200 mL), wash the organic layer with brined solution (2 x 100 mL), dry over sodium sulphate and concentrate. The obtained crude was stirred in n-hexane at 15°C for 1h. Filter off the solid compound, wash with chilled hexane, after that washed with sodium bicarbonate and organic layer was acidify with conc. HCl up to PH 2, concerted organic layer under reduced pressure to obtained solid was dried in oven at 50°C-60°C to get 1-butyl-1H-indazole-3-carboxylic acid as off white solid.

2.4. General Procedure for the synthesis 8a-8z:

To a stirred solution of 1-butyl-1H-indazole-3-carboxylic acid (250 mg, 1.146mmol) was dissolved in DMF (10 mL), HATU (2 equivalents) and DIPEA (3 equivalents) were added to the reaction mixture, then commercial amines (2 equivalents) were added. The reaction mixture was stirred at room temperature for 8-16h. After completion of the reaction, the resultant reaction mixture was poured into water, the solution was extracted with water and ethyl acetate (4 x 20 mL). The organic layer was dried with anhydrous sodium sulphate and the solvent was removed under reduced pressure to afford crude product. The crude was purified by silica gel chromatography to obtain pure products **8a-8z**.

2.5. Plausible mechanism:

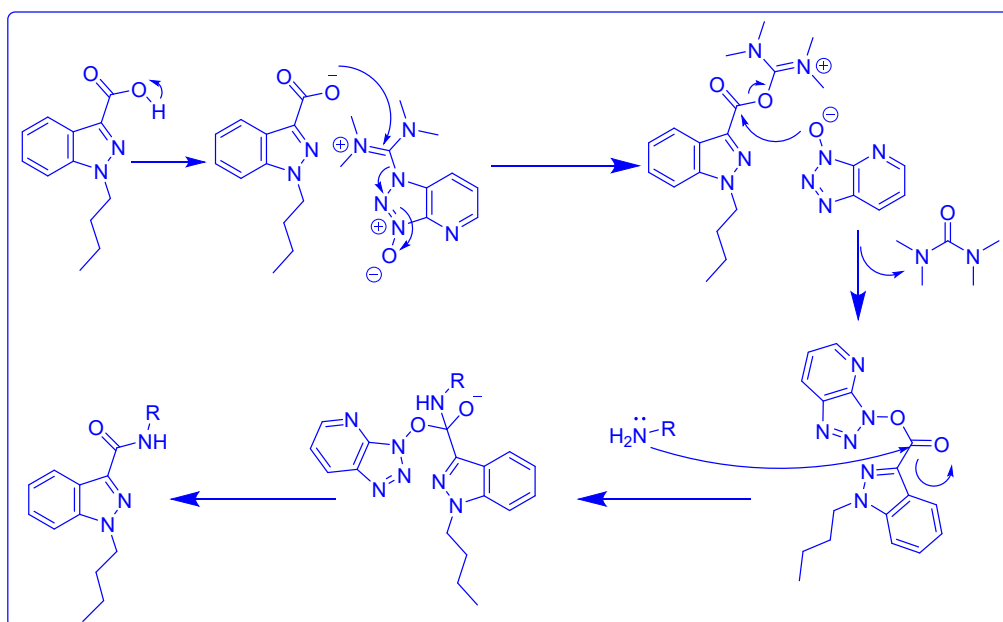


Table-2

R = 8a-8z aliphatic and aromatic amines

8a = Ammonium chloride

8b = Aniline

8c = phenylmethanamine

8d = 3-bromoaniline

8e = 2-amino-5-iodobenzoic acid

8f = 4-benzylaniline

8g = ethyl 4-aminobenzoate

8h = (4-nitrophenyl)hydrazine

8i = 4-bromoaniline

8j = 4-aminophenol

8k = 2-amino-3-methylphenol

8l = m-toluidine

8m = o-toluidine

8n = 5-methylpyridin-2-amine

8o = 4-methoxyaniline

8p = 4-fluoroaniline

8q = 2-methoxyaniline

8r = 3-aminophenol

8s = 4H-1,2,4-triazol-4-amine

8t = 4-nitrobenzene-1,2-diamine

8u = phenylhydrazine

8v = (2,4-dinitrophenyl)hydrazine

8w = 4-hydrazineylbenzonitrile

8x = 4-hydrazineylphenol

8y = (4-bromophenyl)hydrazine

8z = 4-nitroaniline

Table-3

Chemical structures of 1-ethyl-3-phenyl-1H-indazole-4-carboxamide derivatives (8a-8z) are shown. The structures are arranged in a grid, with the indazole ring system substituted with an ethyl group at position 1 and a phenyl group at position 3. The carboxamide group at position 4 is substituted with various groups, including amide, ester, and amine derivatives.

8a: 1-ethyl-3-phenyl-1H-indazole-4-carboxamide

8b: 1-ethyl-3-phenyl-1H-indazole-4-carboxamide

8c: 1-ethyl-3-phenyl-1H-indazole-4-carboxamide

8d: 1-ethyl-3-phenyl-1H-indazole-4-carboxamide

8e: 1-ethyl-3-phenyl-1H-indazole-4-carboxamide

8f: 1-ethyl-3-phenyl-1H-indazole-4-carboxamide

8g: 1-ethyl-3-phenyl-1H-indazole-4-carboxamide

8h: 1-ethyl-3-phenyl-1H-indazole-4-carboxamide

8i: 1-ethyl-3-phenyl-1H-indazole-4-carboxamide

8j: 1-ethyl-3-phenyl-1H-indazole-4-carboxamide

8k: 1-ethyl-3-phenyl-1H-indazole-4-carboxamide

8l: 1-ethyl-3-phenyl-1H-indazole-4-carboxamide

8m: 1-ethyl-3-phenyl-1H-indazole-4-carboxamide

8n: 1-ethyl-3-phenyl-1H-indazole-4-carboxamide

8o: 1-ethyl-3-phenyl-1H-indazole-4-carboxamide

8p: 1-ethyl-3-phenyl-1H-indazole-4-carboxamide

8q: 1-ethyl-3-phenyl-1H-indazole-4-carboxamide

8r: 1-ethyl-3-phenyl-1H-indazole-4-carboxamide

8s: 1-ethyl-3-phenyl-1H-indazole-4-carboxamide

8t: 1-ethyl-3-phenyl-1H-indazole-4-carboxamide

8u: 1-ethyl-3-phenyl-1H-indazole-4-carboxamide

8v: 1-ethyl-3-phenyl-1H-indazole-4-carboxamide

8w: 1-ethyl-3-phenyl-1H-indazole-4-carboxamide

8x: 1-ethyl-3-phenyl-1H-indazole-4-carboxamide

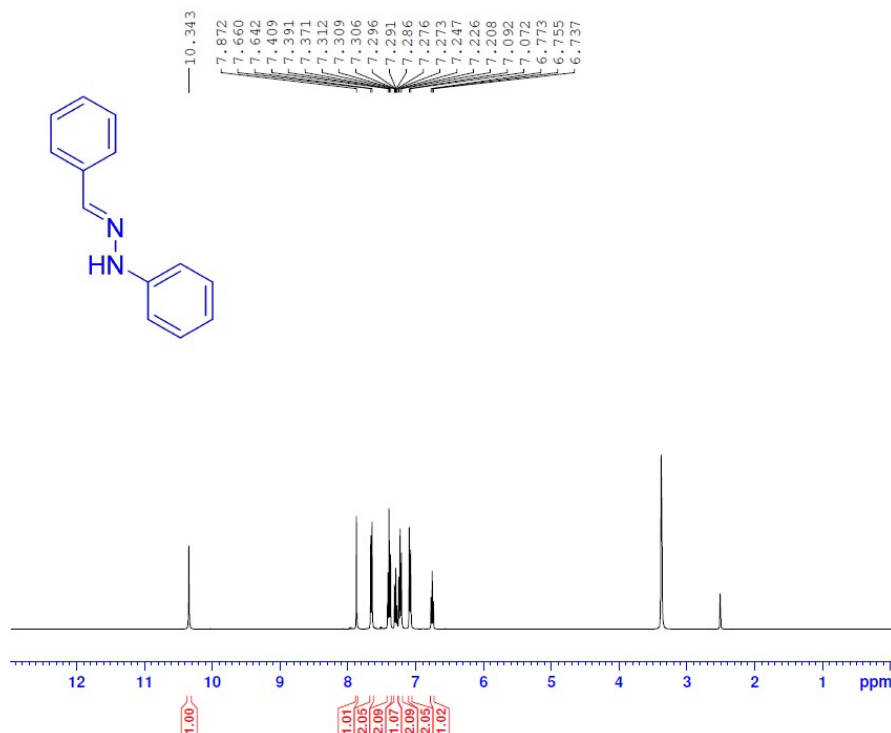
8y: 1-ethyl-3-phenyl-1H-indazole-4-carboxamide

8z: 1-ethyl-3-phenyl-1H-indazole-4-carboxamide

3. ¹H and ¹³C NMR, Dept-135, COSY, HSQC, IR and HRMS spectra of the compounds

¹H-NMR [400MHz, DMSO-d₆] spectrum of 1-benzylidene-2-phenylhydrazine(3).

Signature SIF VIT VELLORE
SM-02



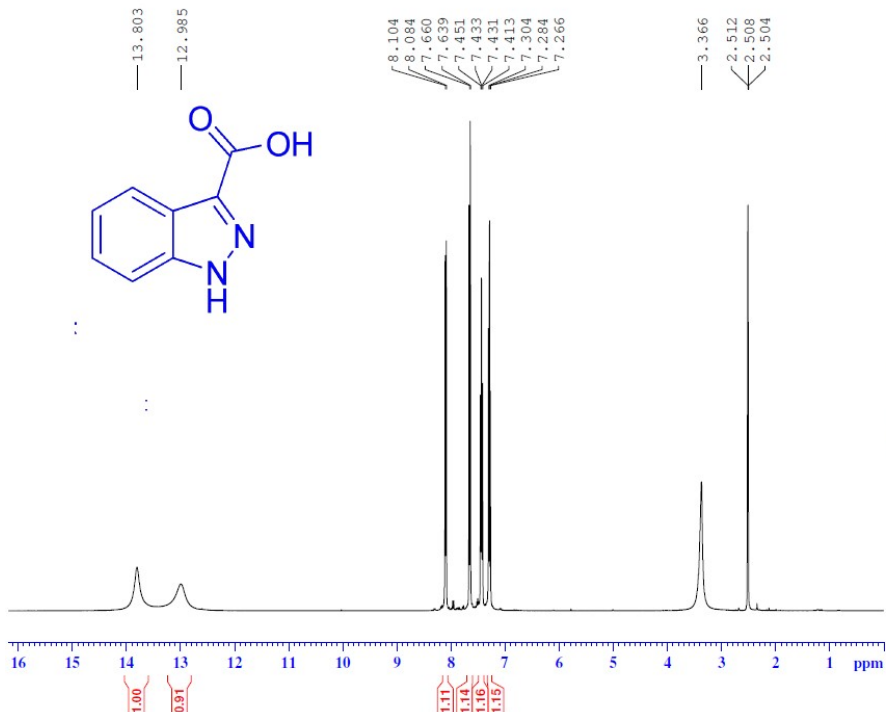
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¹H-NMR [400MHz, DMSO-d₆] spectrum of 1H-indazole-3-carboxylic acid (5).

Signature SIF VIT VELLORE
SM-03



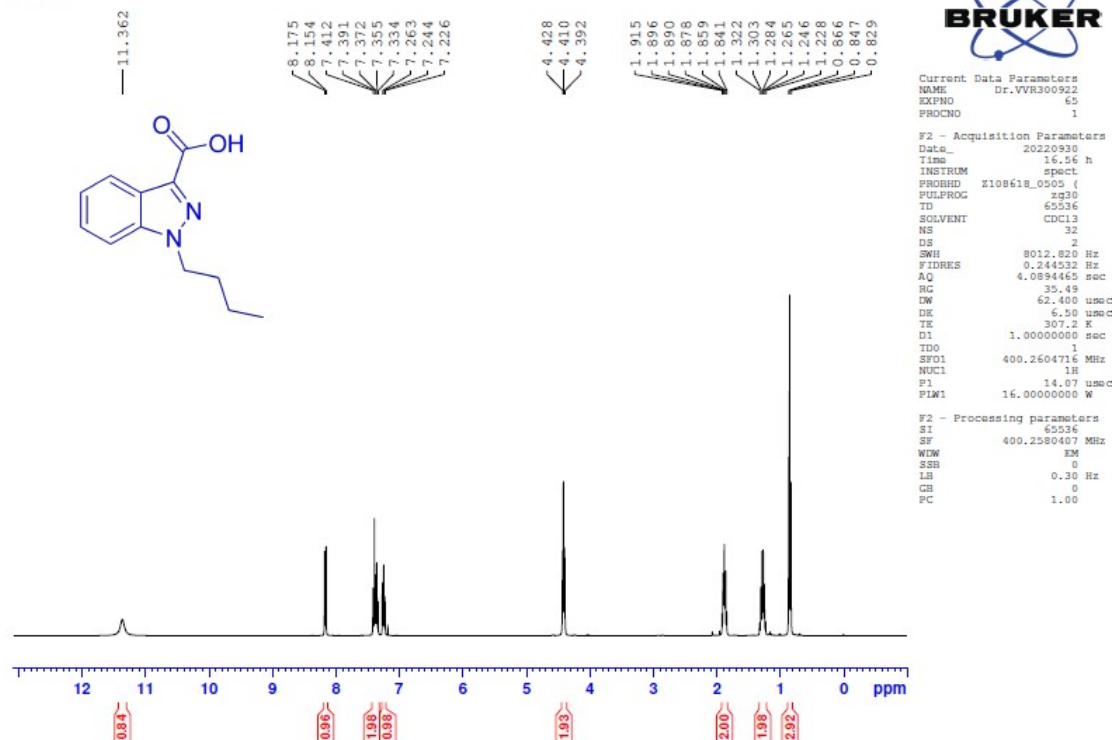
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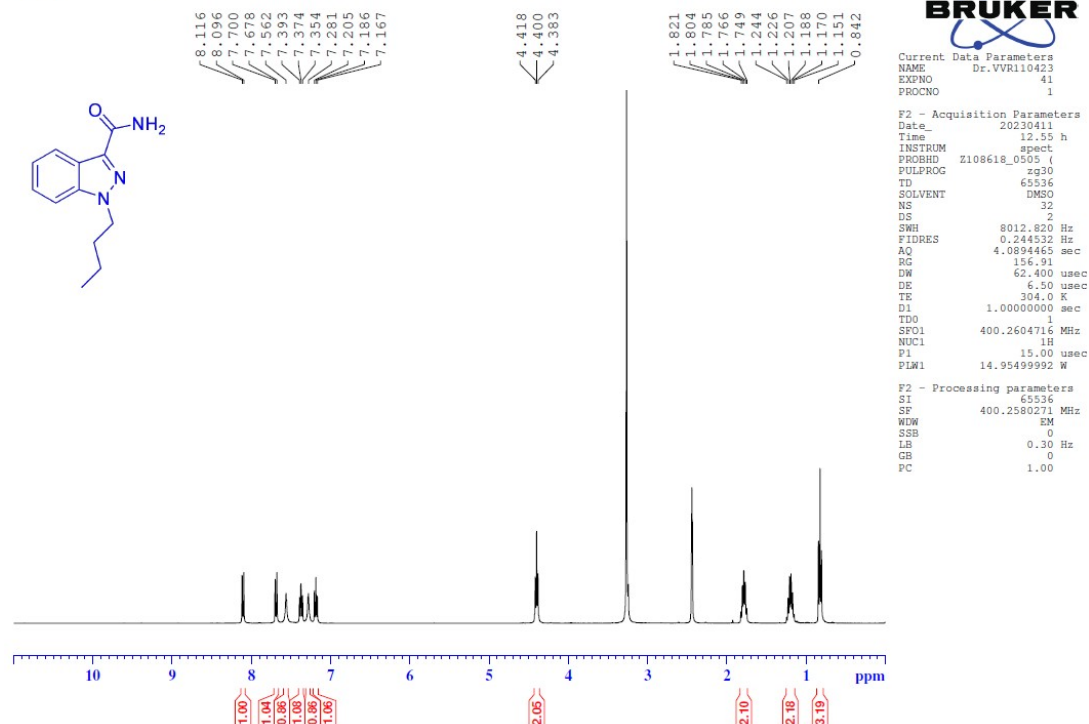
¹H-NMR [400MHz, DMSO-d₆] spectrum of 1-butyl-1H-indazole-3-carboxylic acid (6).

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SM-04a



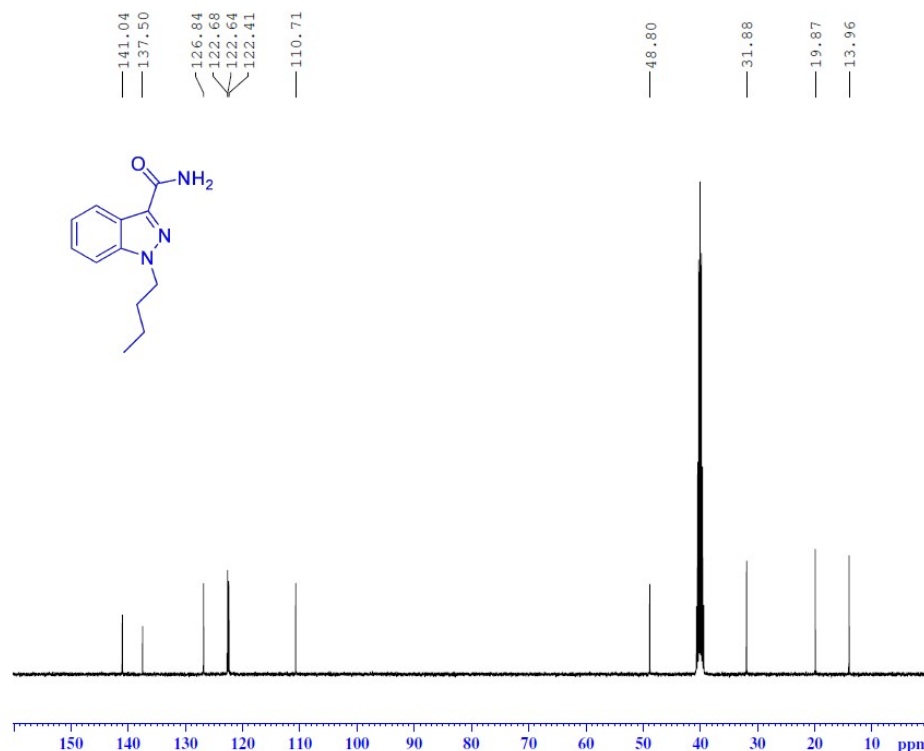
¹H-NMR [400MHz, DMSO-*d*₆] spectrum of 1-butyl-1H-indazole-3-carboxamide (8a).

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VG-001



¹³C-NMR [100MHz, DMSO-d₆] spectrum of 1-butyl-1H-indazole-3-carboxamide (8a).

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VG-001



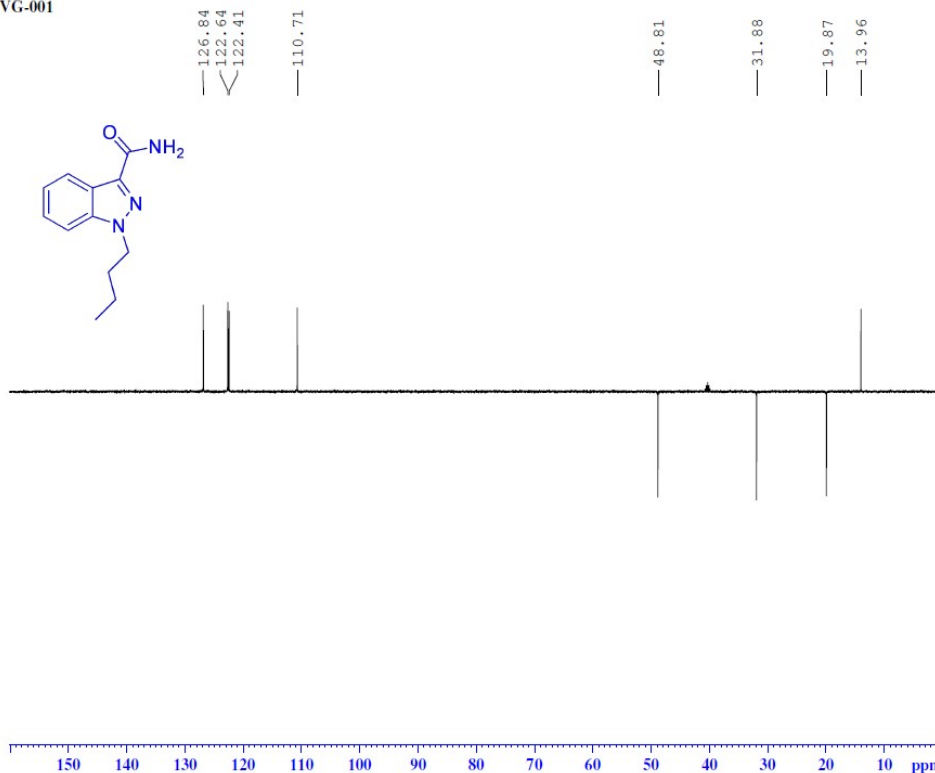
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SFO2 400.2596010 MHz
NUC2 1H
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¹³⁵DEPT-NMR [100MHz, DMSO-d₆] spectrum of 1-butyl-1H-indazole-3-carboxamide (8a).

Signature SIF VIT VELLORE
VG-001

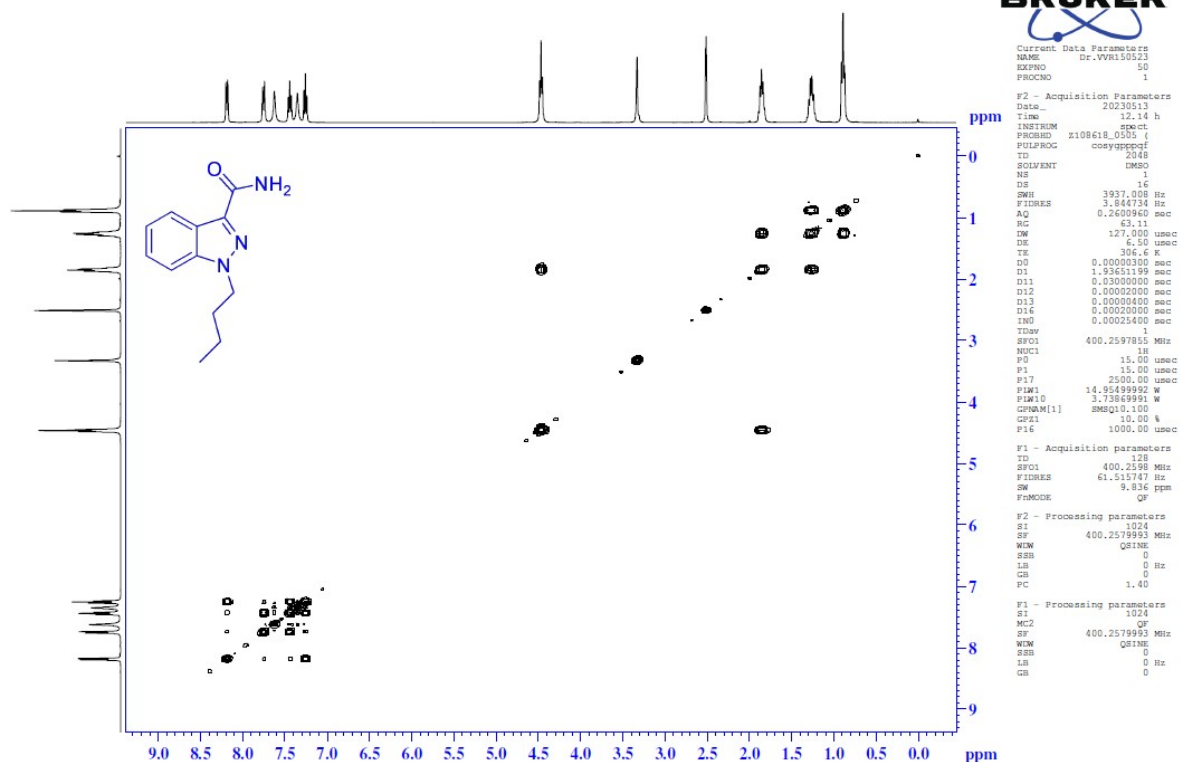


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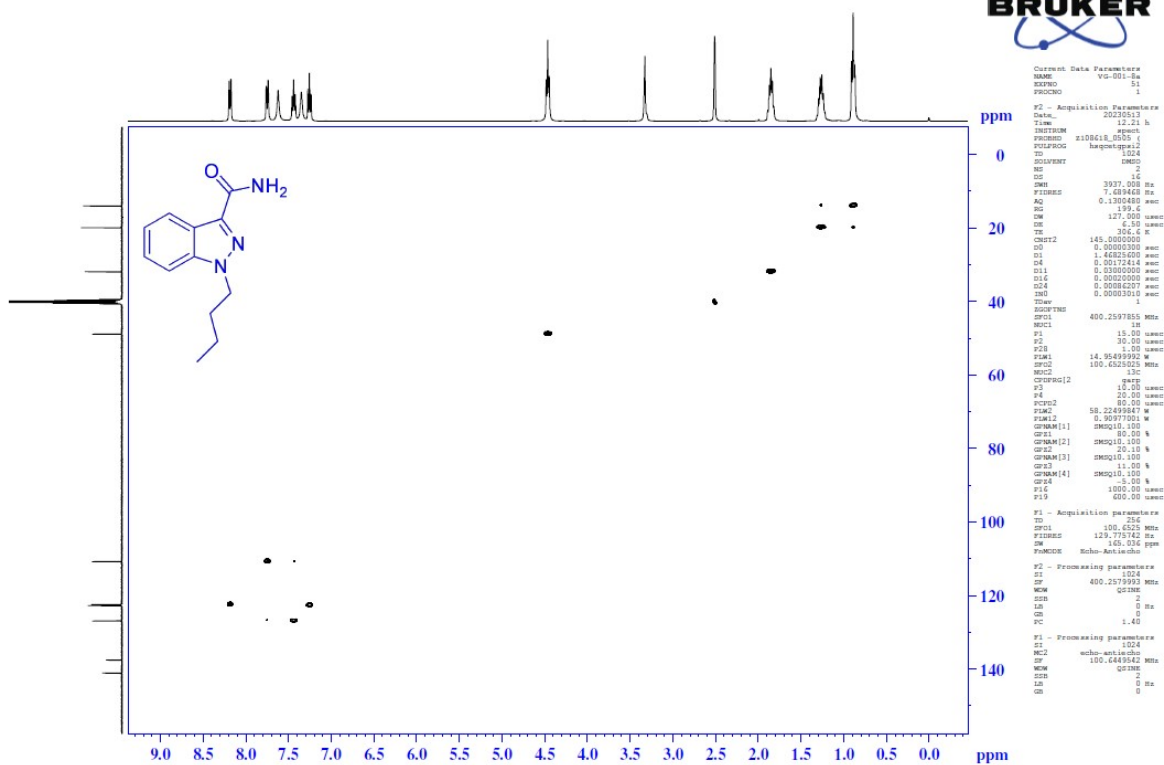
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P13 2000.00 usec
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SFOFF5 0 Hz
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SFO2 400.2596010 MHz
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PLW12 0.41542000 W

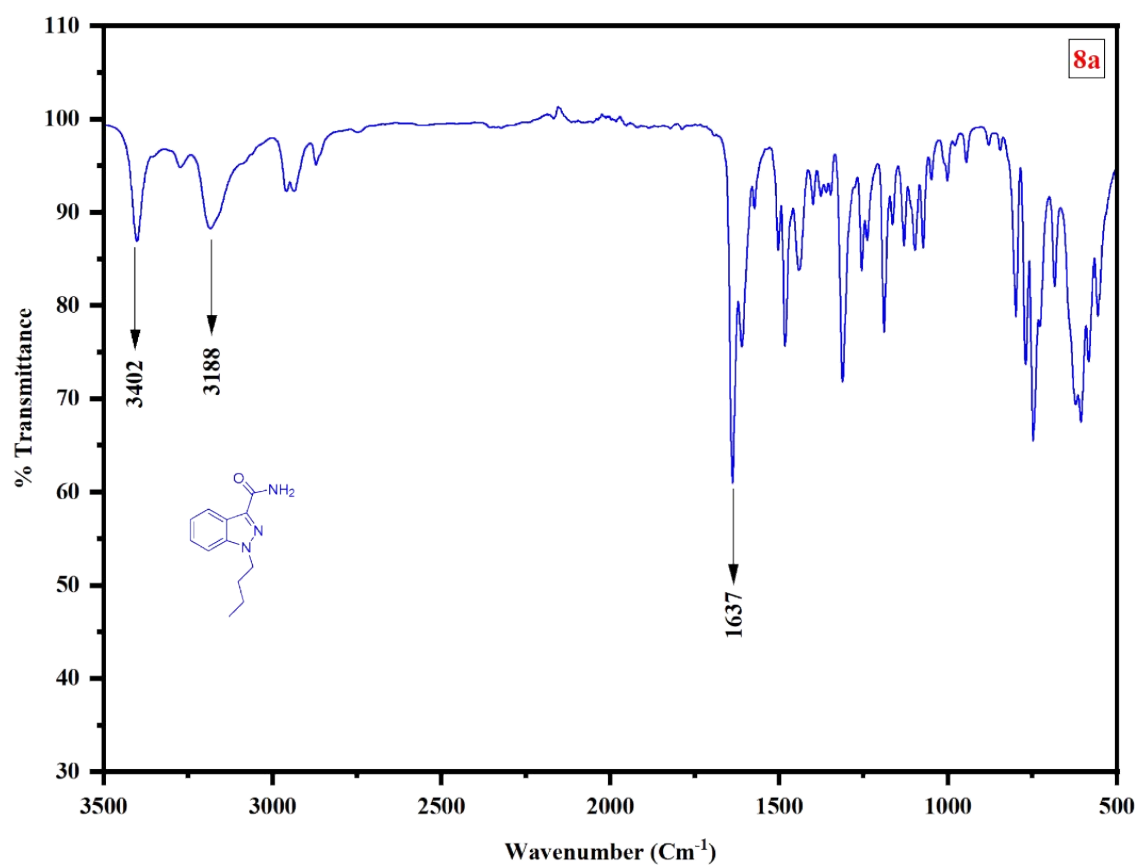
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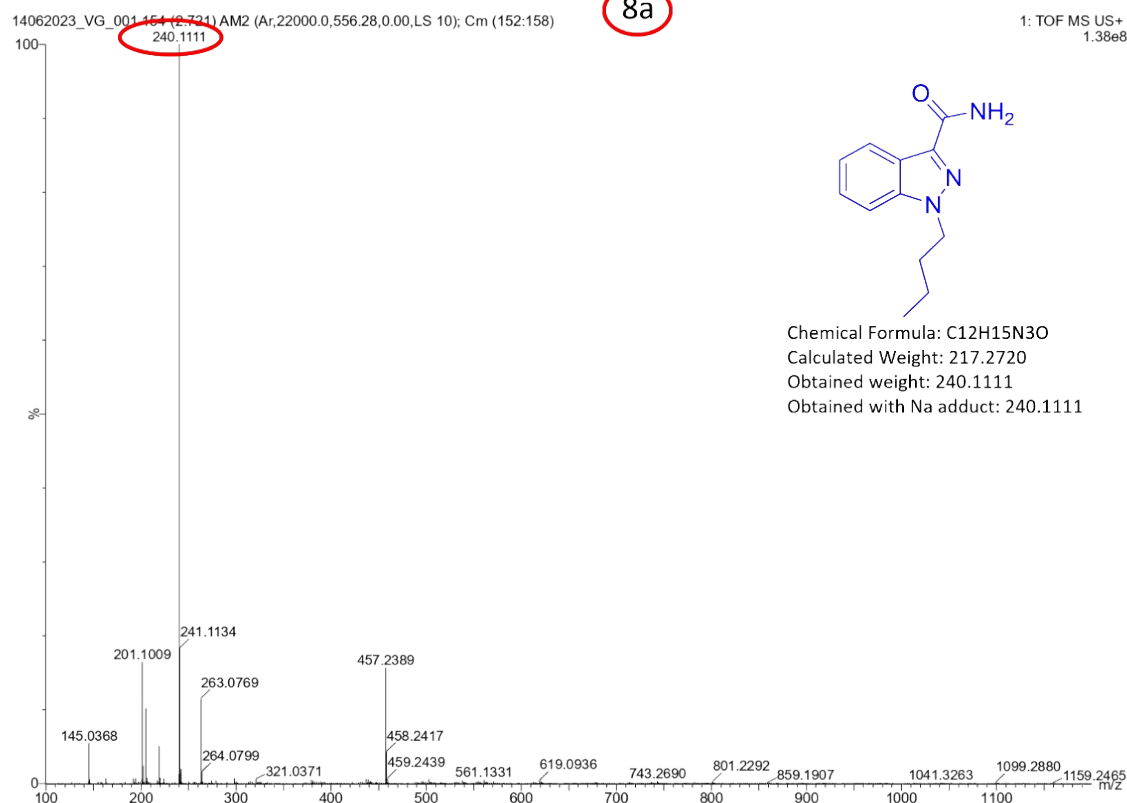
COSY-NMR [400MHz, DMSO-d₆] spectrum of 1-butyl-1H-indazole-3-carboxamide (8a).



HSQC-NMR [400MHz, DMSO-d₆] spectrum of 1-butyl-1H-indazole-3-carboxamide (8a).

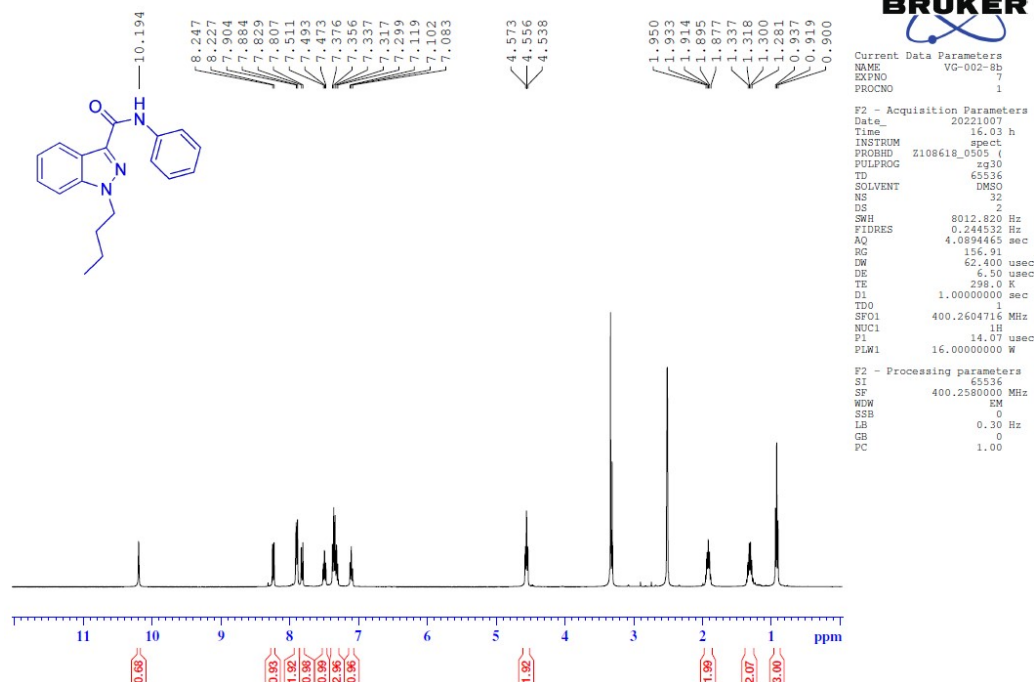






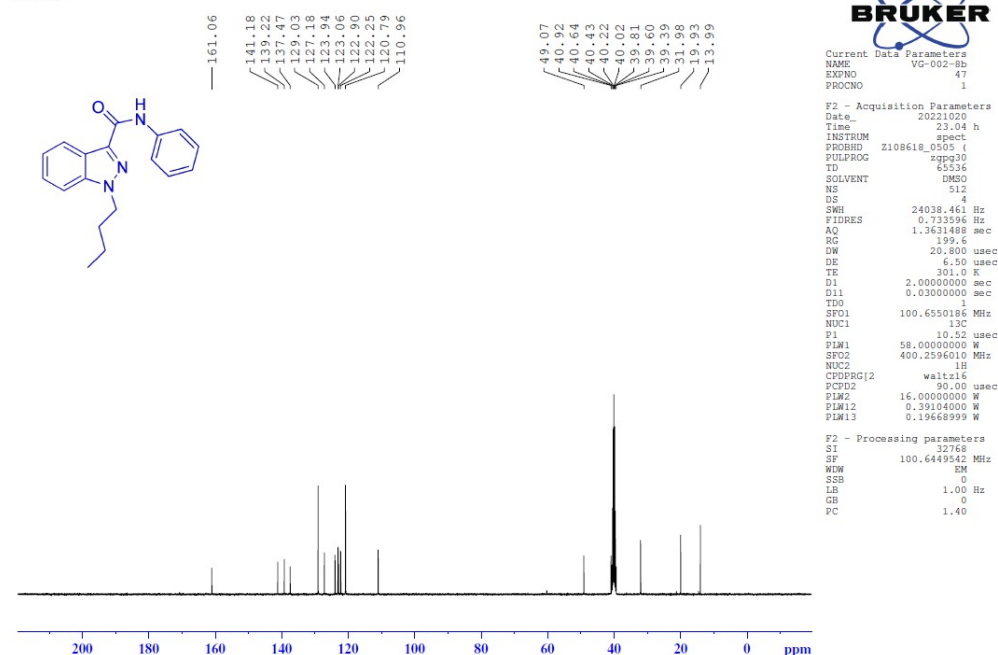
¹H-NMR [400MHz, DMSO-d₆] spectrum of 1-butyl-N-phenyl-1H-indazole-3-carboxamide (8b).

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 VG-002



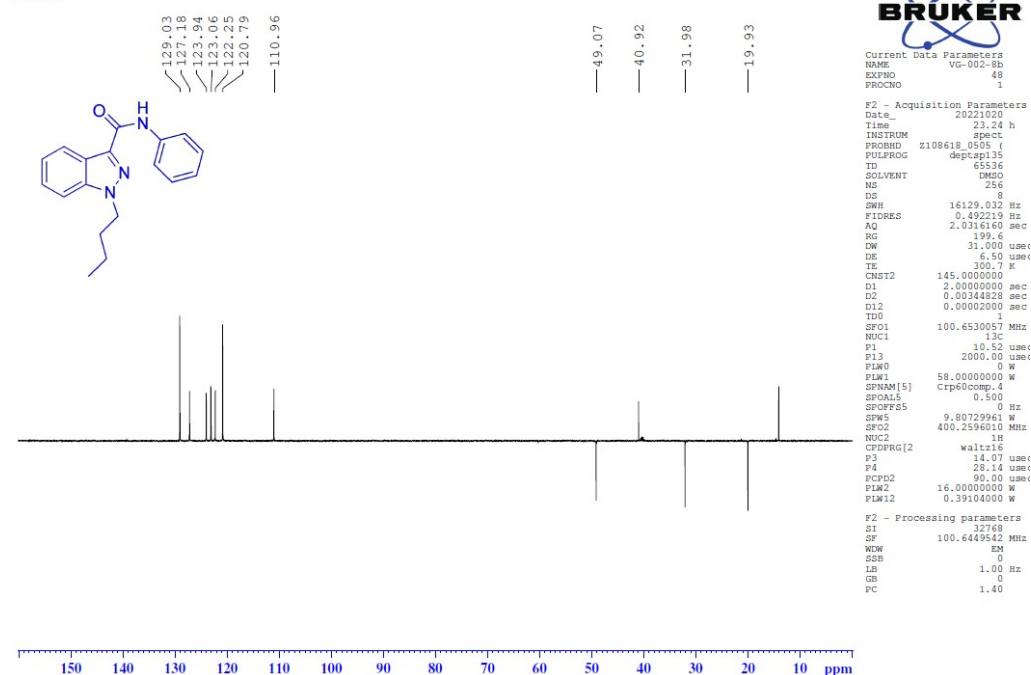
¹³C-NMR [100MHz, DMSO-d₆] spectrum of 1-butyl-N-phenyl-1H-indazole-3-carboxamide (8b).

Signature SIF VIT VELLORE
VG-002

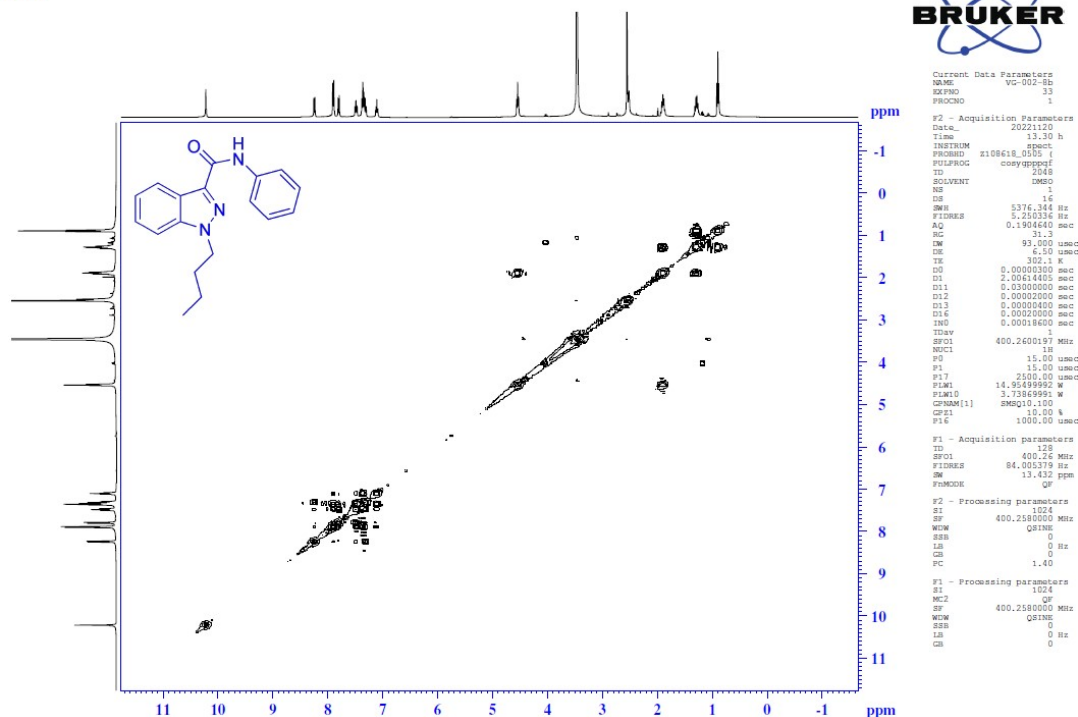


¹³⁵DEPT-NMR [100MHz, DMSO-d₆] spectrum of 1-butyl-N-phenyl-1H-indazole-3-carboxamide (8b).

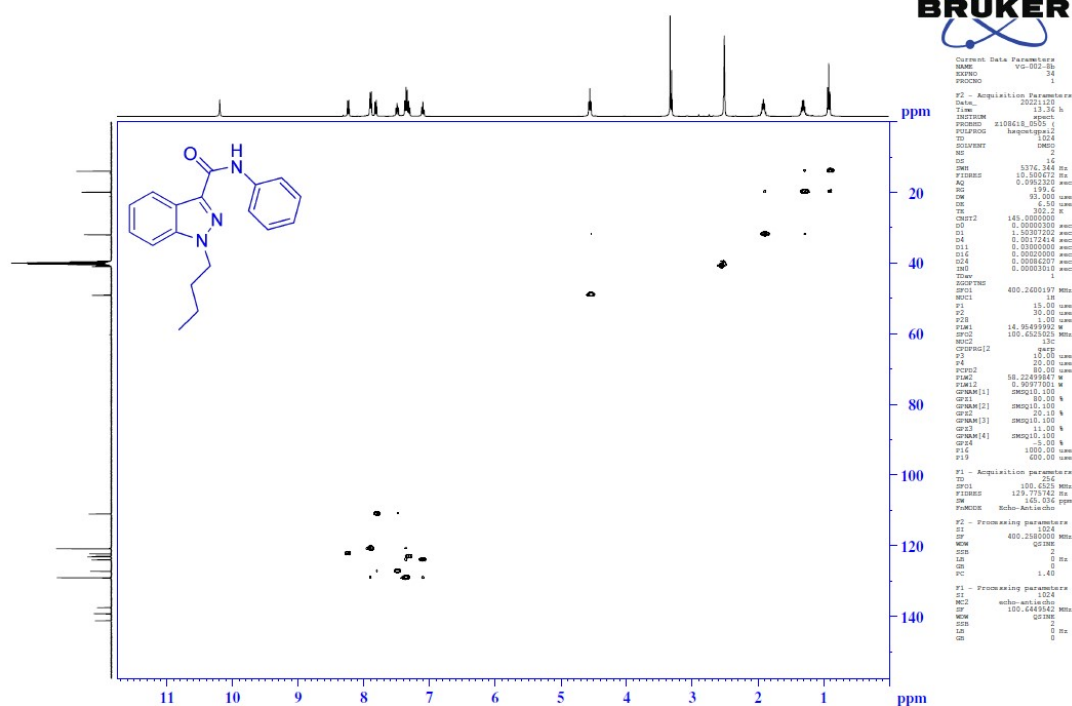
Signature SIF VIT VELLORE
VG-002

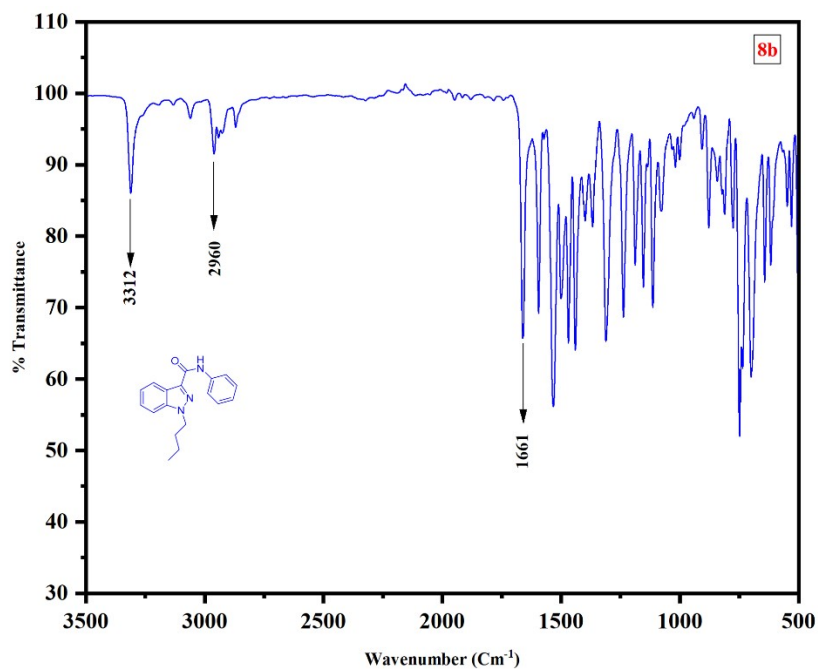


COSY-NMR [400MHz, DMSO-d₆] spectrum of 1-butyl-N-phenyl-1H-indazole-3-carboxamide (8b).

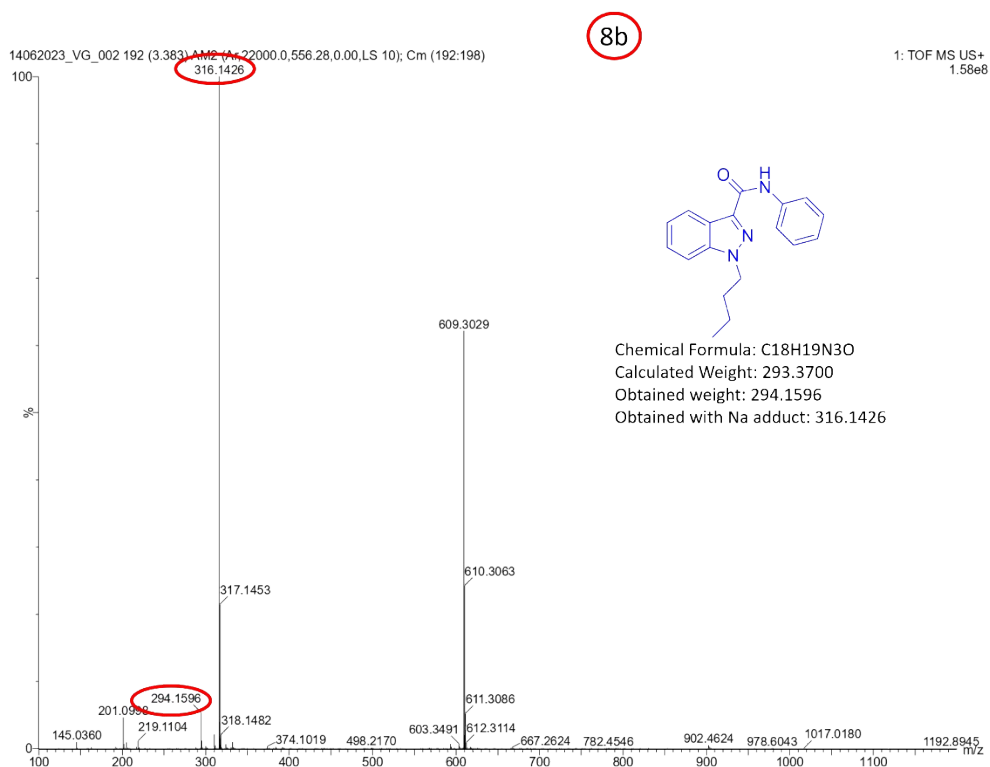


HSQC-NMR [400MHz, DMSO-d₆] spectrum of 1-butyl-N-phenyl-1H-indazole-3-carboxamide (8b).



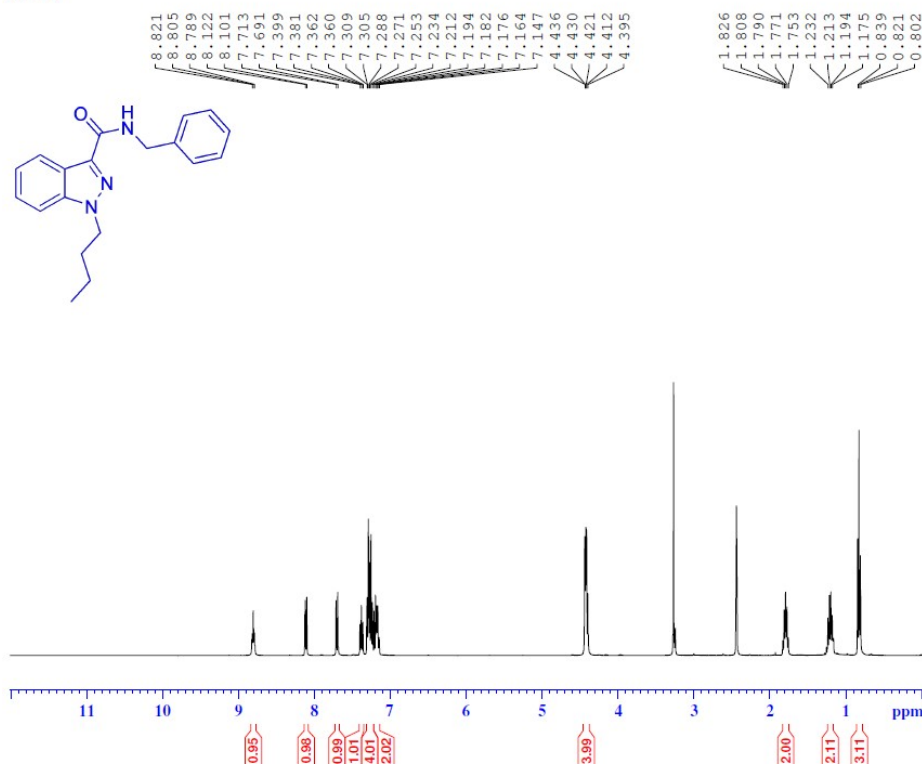


HRMS of 1-butyl-N-phenyl-1H-indazole-3-carboxamide (8b).



¹H-NMR [400MHz, DMSO-d₆] spectrum of N-benzyl-1-butyl-1H-indazole-3-carboxamide (8c).

Signature SIF VIT VELLORE
VG-003



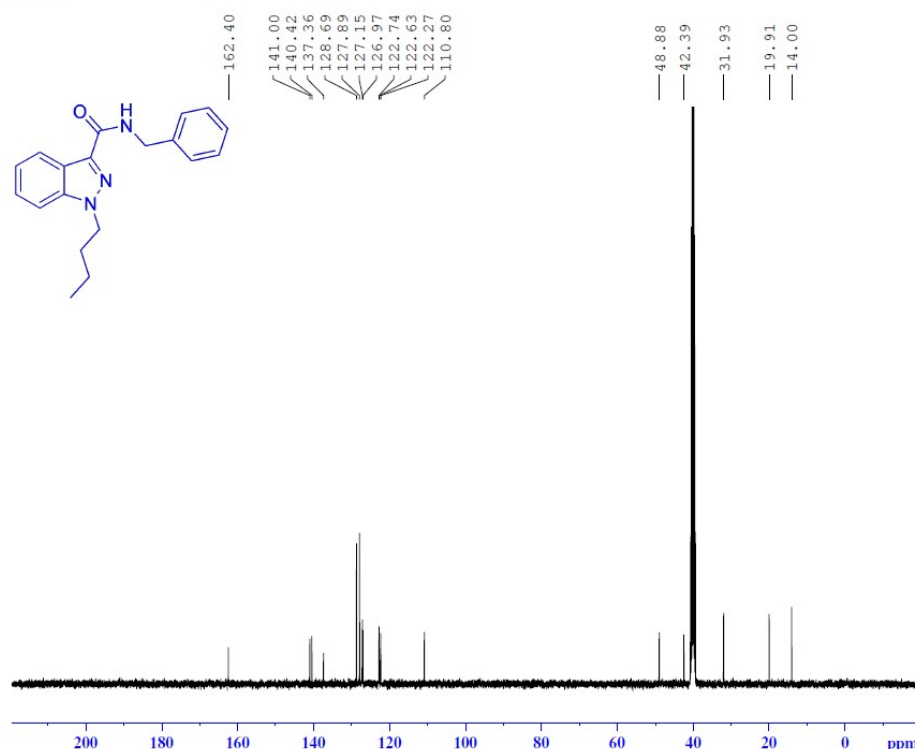
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F2 - Processing parameters
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GB 0
PC 1.00

¹³C-NMR [100MHz, DMSO-d₆] spectrum of N-benzyl-1-butyl-1H-indazole-3-carboxamide (8c).

Signature SIF VIT VELLORE
VG-003



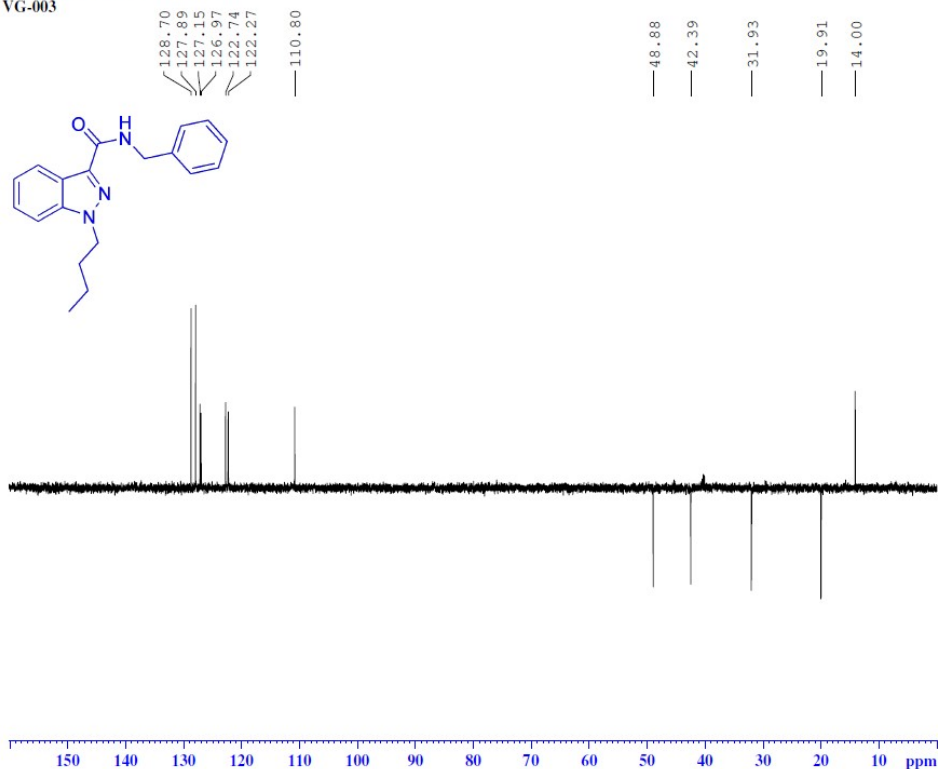
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TDO 1
SFO1 100.6550186 MHz
NUC1 13C
P1 10.00 usec
PLW1 58.22499847 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
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PLW13 0.20895000 W

F2 - Processing parameters
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¹³⁵-DEPT-NMR [100MHz, DMSO-d₆] spectrum of N-benzyl-1-butyl-1H-indazole-3-carboxamide (8c).

Signature SIF VIT VELLORE
VG-003



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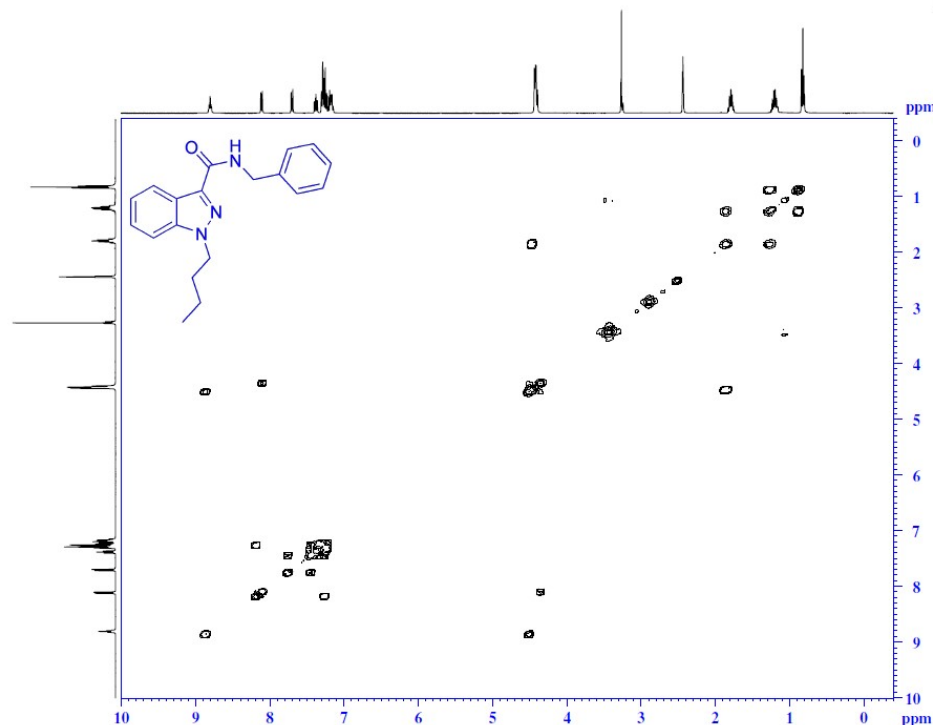
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COSY-

NMR [400MHz, DMSO- d_6] spectrum of N-benzyl-1-butyl-1H-indazole-3-carboxamide (8c).

Signature SIF VIT VELLORE
VG-003



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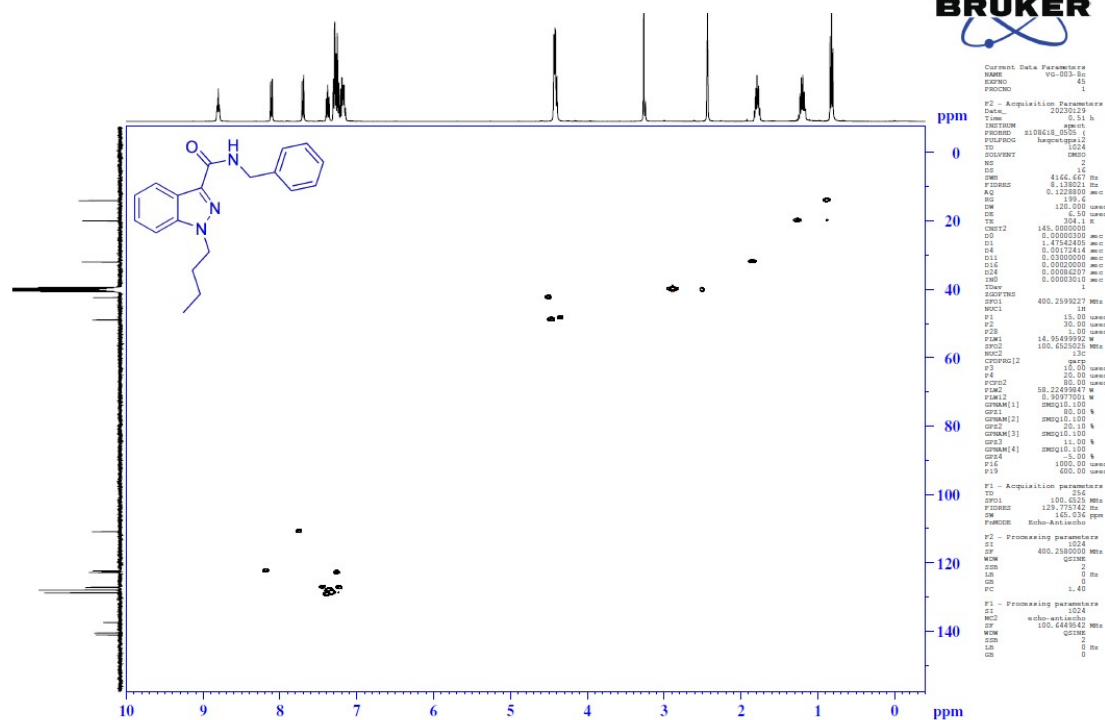
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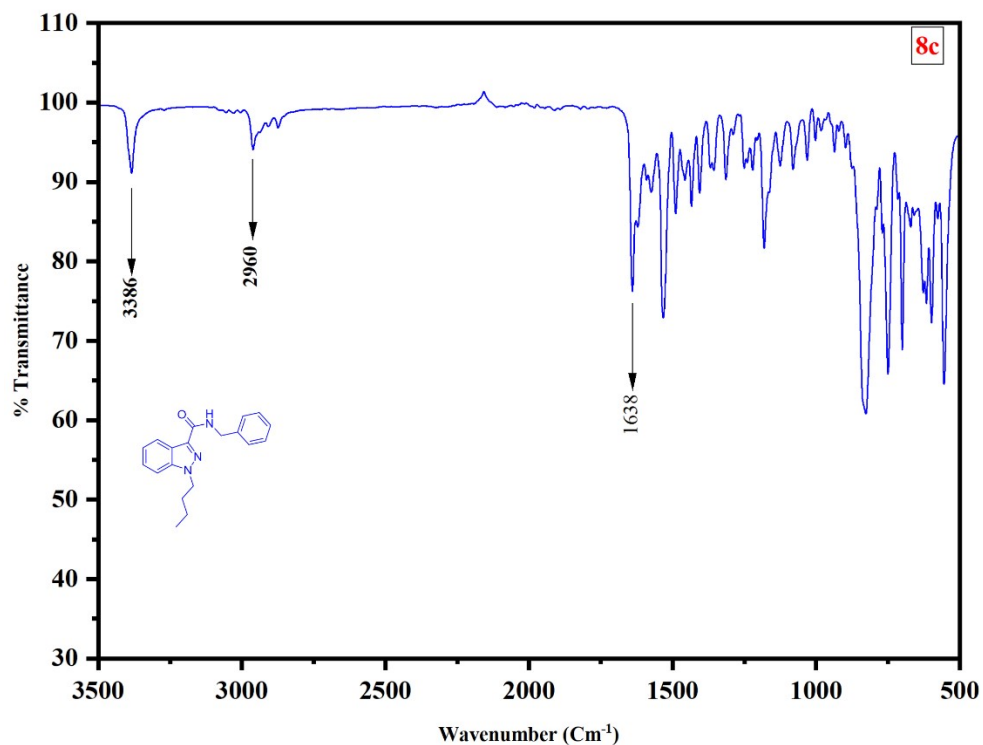
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SSB: 0
LB: 0 Hz
GB: 0
PC: 1.40

F1 - Processing parameters
SI: 1024
MC2: QF
SF: 400.2580000 MHz
WDW: Q8INE
SSB: 0
LB: 0 Hz
GB: 0

HSQC-NMR [400MHz, DMSO- d_6] spectrum of N-benzyl-1-butyl-1H-indazole-3-carboxamide (8c).

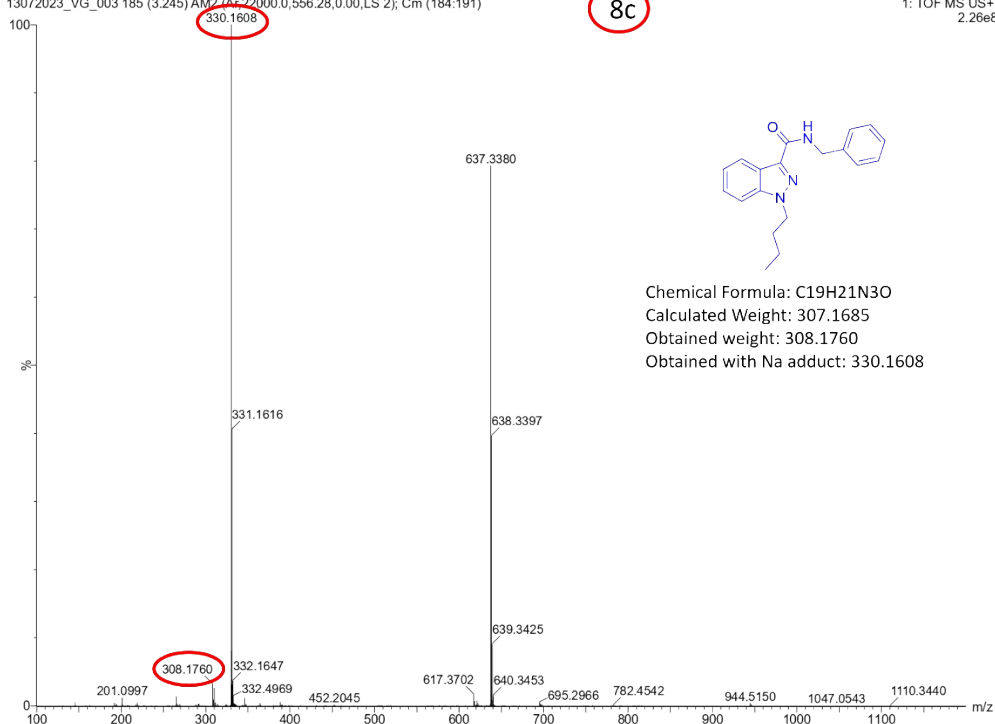


FT-IR spectrum of N-benzyl-1-butyl-1H-indazole-3-carboxamide (8c).



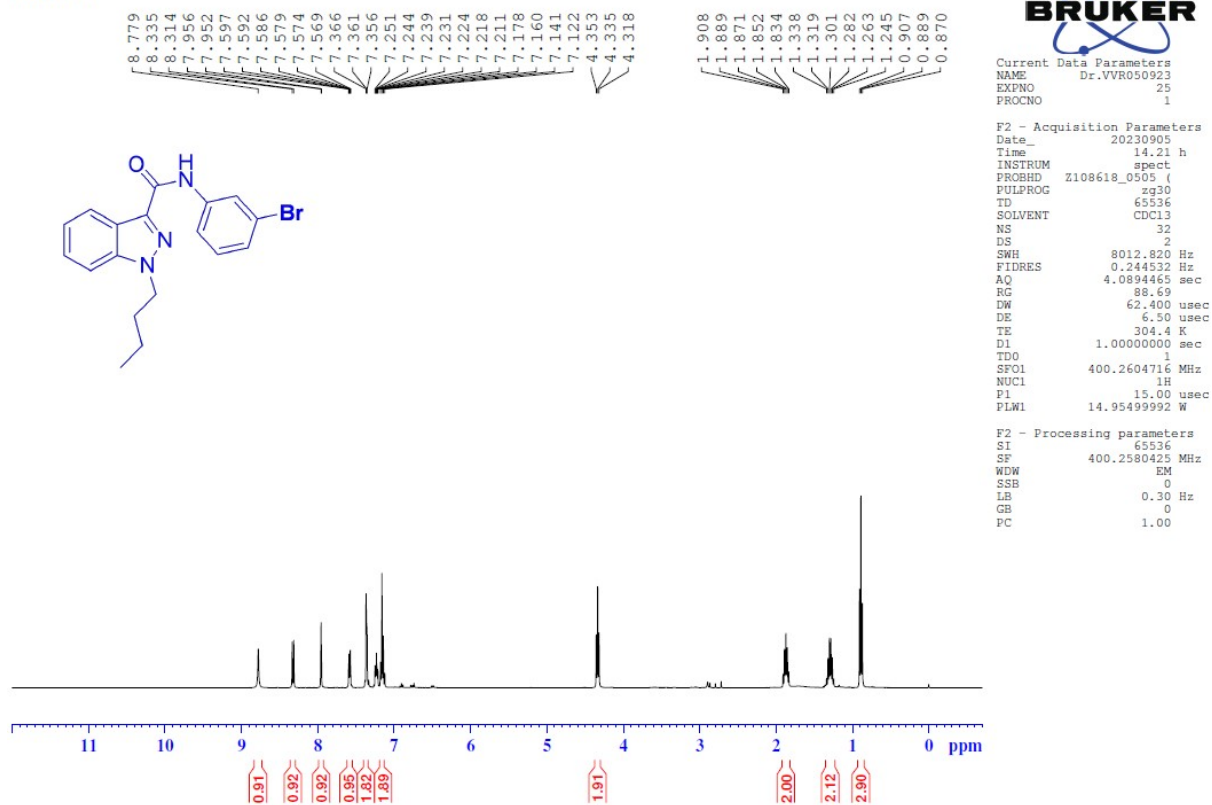
HRMS of N-benzyl-1-butyl-1H-indazole-3-carboxamide (8c).

13072023_VG_003 185 (3.245) AM2 (Ar: 22000.0, 556.28, 0.00, LS 2); Cm (184:191)



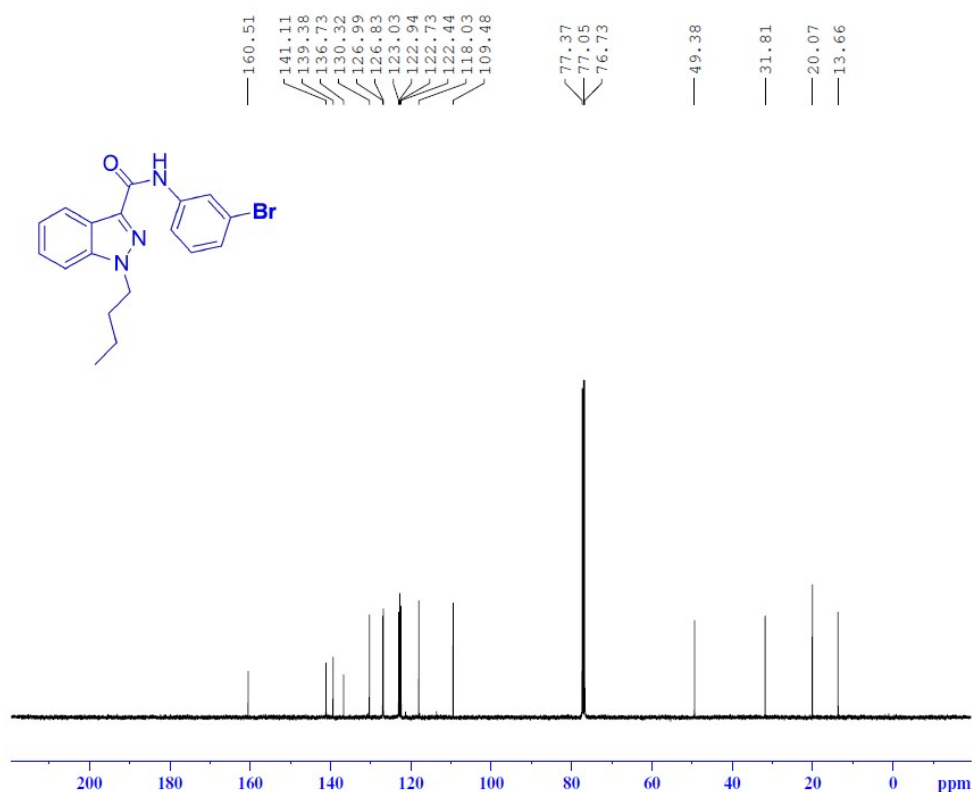
¹H-NMR [400MHz, DMSO-d₆] spectrum of 1-butyl-N-(6-methylpyridine-2yl)-1H-indazole-3-carboxamide (8d).

Signature SIF VIT VELLORE
 VG-009-B



¹³C-NMR [100MHz, DMSO-d₆] spectrum of 1-butyl-N-(6-methylpyridine-2yl)-1H-indazole-3-carboxamide (8d).

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VG-009-B



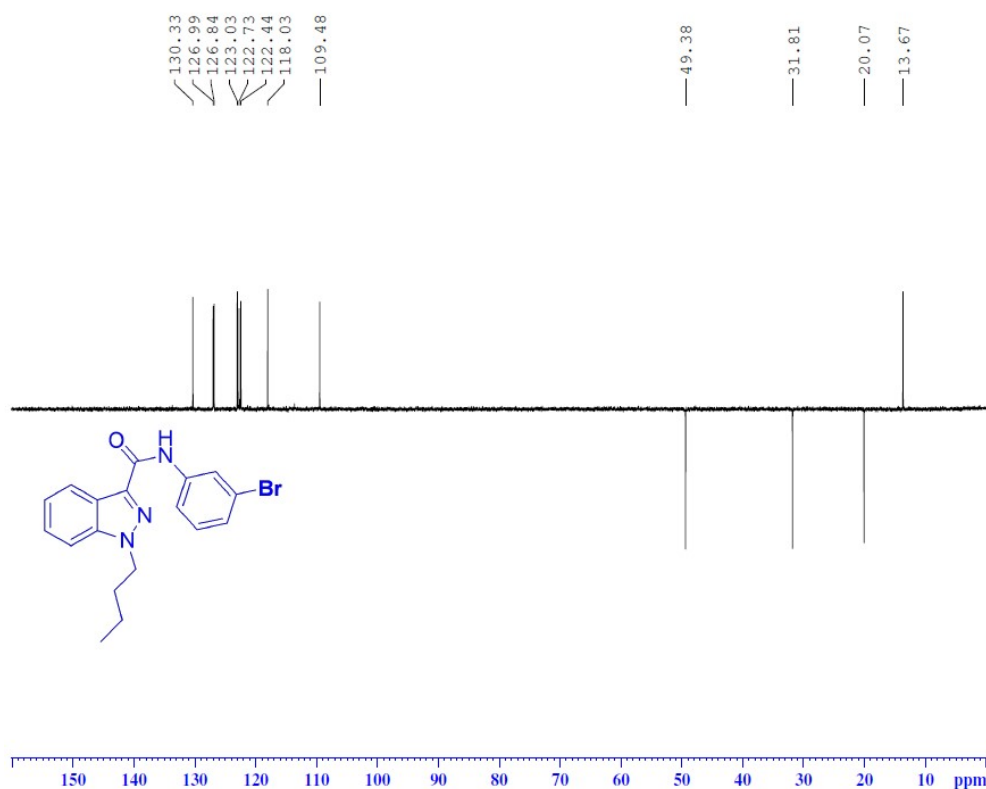
Current Data Parameters
NAME VG-009(B)
EXPNO 82
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230921
Time 3.56 h
INSTRUM spect
PROBHD Z108618_0505 ()
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.733594 Hz
AQ 1.3631488 sec
RG 199.6
DW 20.800 usec
DE 6.50 usec
TE 306.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6550186 MHz
NUC1 13C
P1 10.00 usec
PLW1 58.22499847 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 14.95499992 W
PLW12 0.41542000 W
PLW13 0.20895000 W

F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

135-DEPT-NMR [100MHz, DMSO-d₆] spectrum of 1-butyl-N-(6-methylpyridine-2-yl)-1H-indazole-3-carboxamide (8d).

Signature SIF VIT VELLORE
VG-009-B



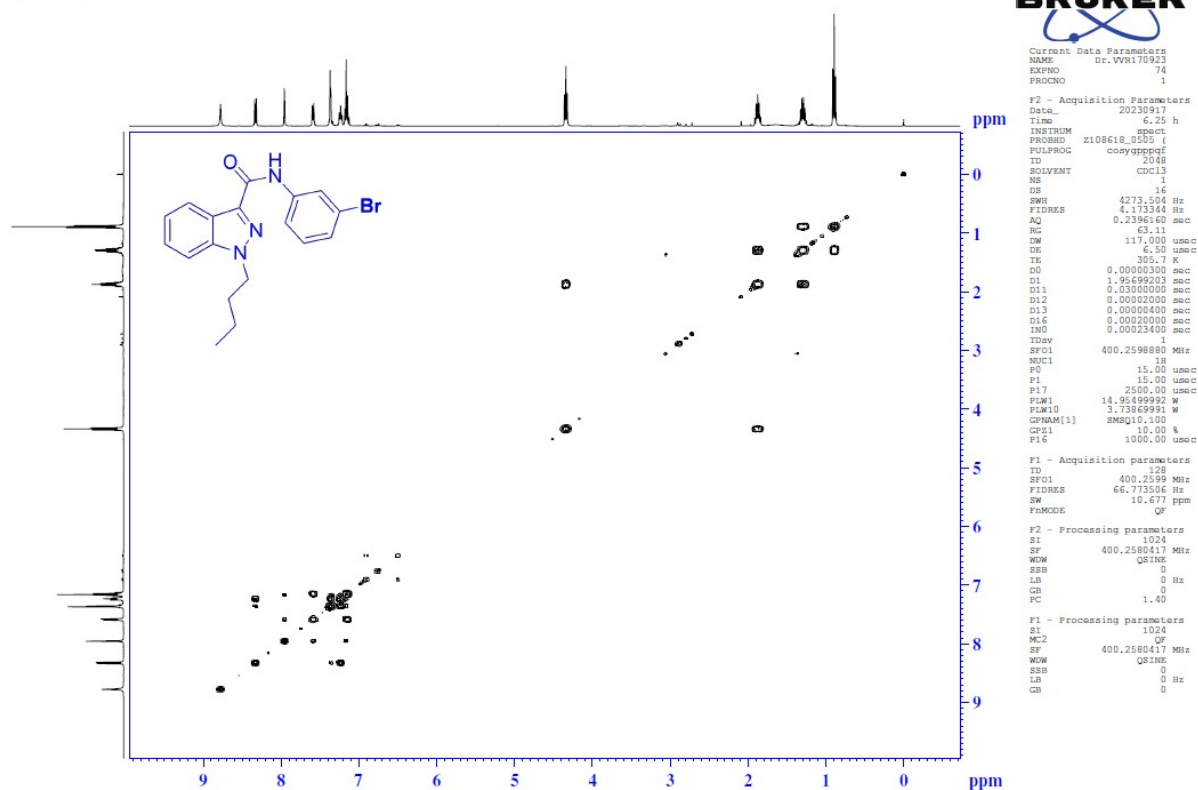
Current Data Parameters
NAME VG-009(B)
EXPNO 81
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230921
Time 3.25 h
INSTRUM spect
PROBHD z108618_0505 ()
PULPROG deptsp135
TD 65536
SOLVENT CDC13
NS 256
DS 8
SWH 16129.032 Hz
FIDRES 0.492219 Hz
AQ 2.0316160 sec
RG 199.6
DW 31.000 usec
DE 6.50 usec
TE 306.1 K
CNST2 145.0000000
D1 2.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1
SFO1 100.6530057 MHz
NUC1 13C
P1 10.00 usec
P13 2000.00 usec
PLW0 58.22499847 W
SPNAM[5] Crp60comp.4
SFOAL5 0.500
SPOFFS5 8.89610004 Hz
SPW5 8.89610004 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG2 waltz16
P3 15.00 usec
P4 30.00 usec
PCPD2 90.00 usec
PLW2 14.95499992 W
PLW12 0.41542000 W

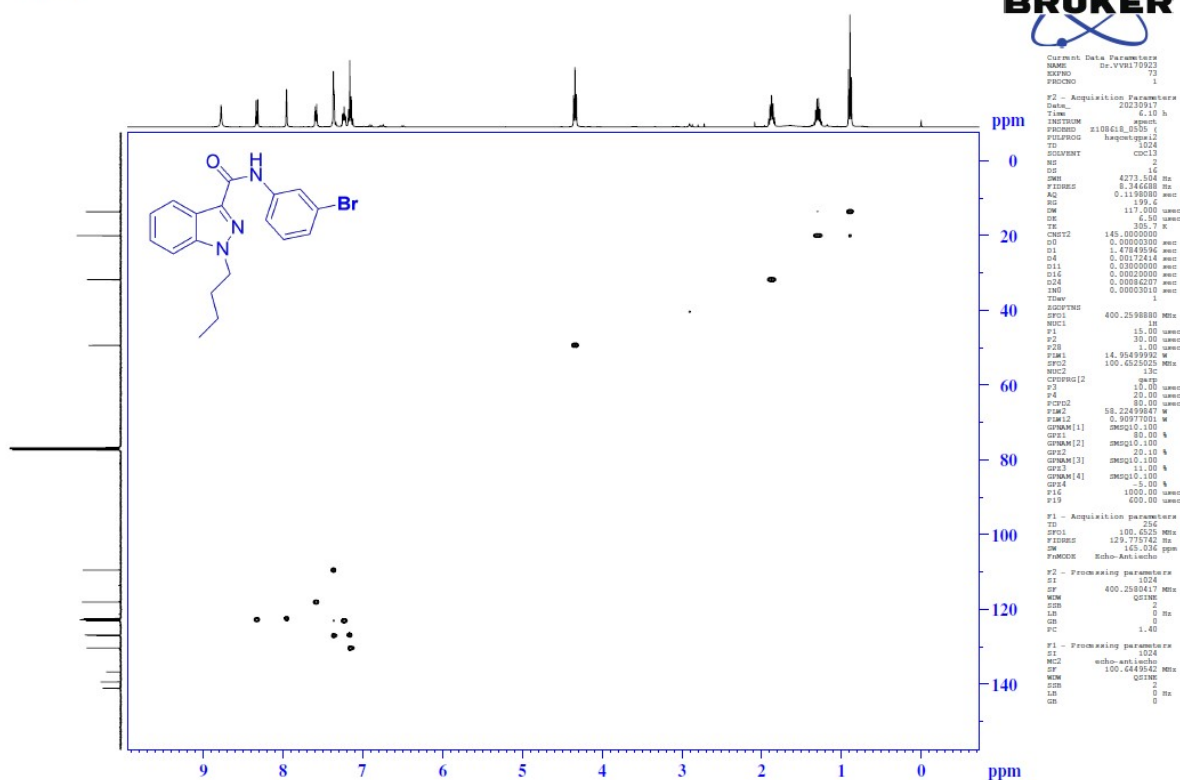
F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

COSY-NMR [400MHz, DMSO-d₆] spectrum of 1-butyl-N-(6-methylpyridine-2-yl)-1H-indazole-3-carboxamide (8d).

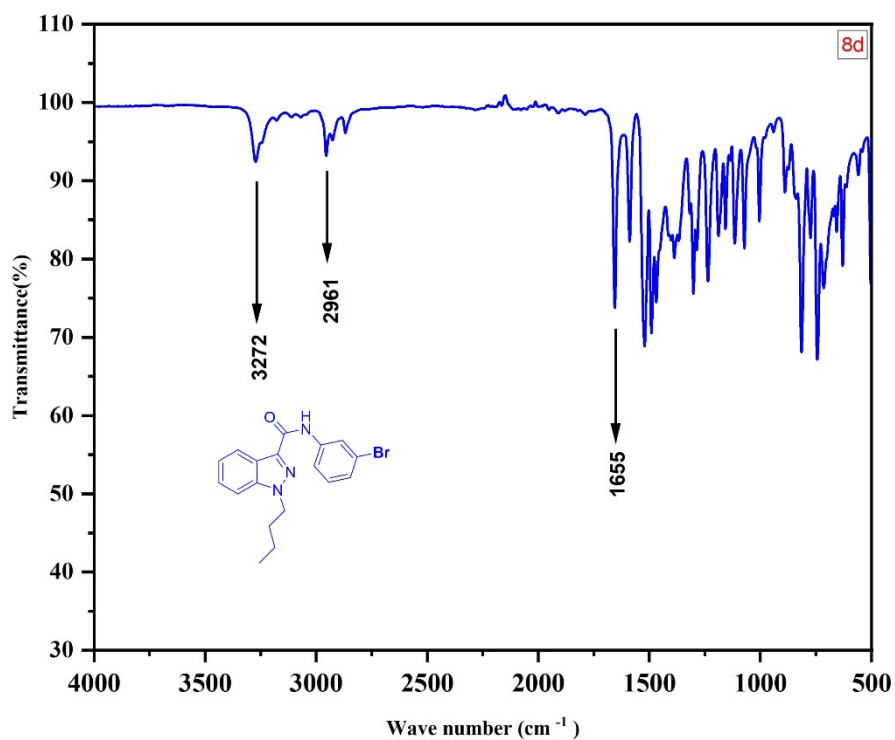
Signature SIF VIT VELLORE
VG-00-9(B)



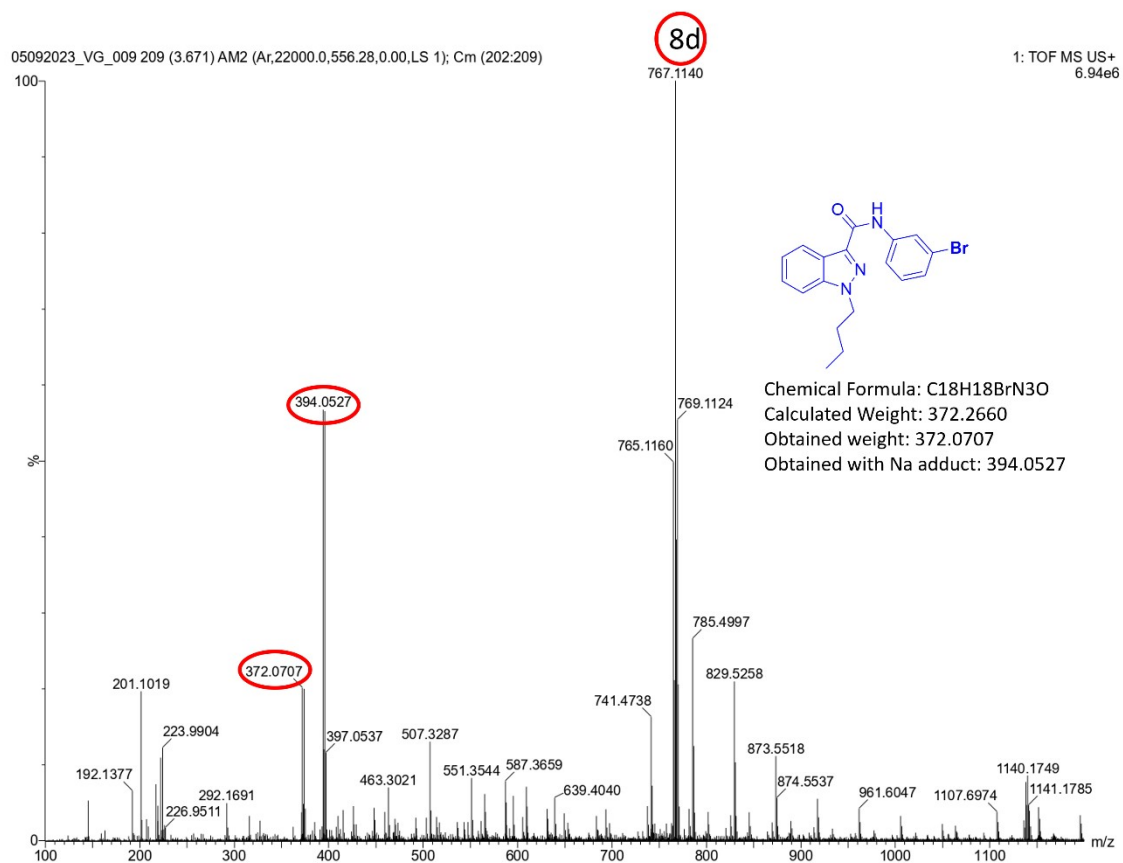
HSQC-NMR [400MHz, DMSO-d₆] spectrum of 1-butyl-N-(6-methylpyridine-2-yl)-1H-indazole-3-carboxamide (8d).



FT-IR spectrum of 1-butyl-N-(6-methylpyridine-2-yl)-1H-indazole-3-carboxamide (8d).

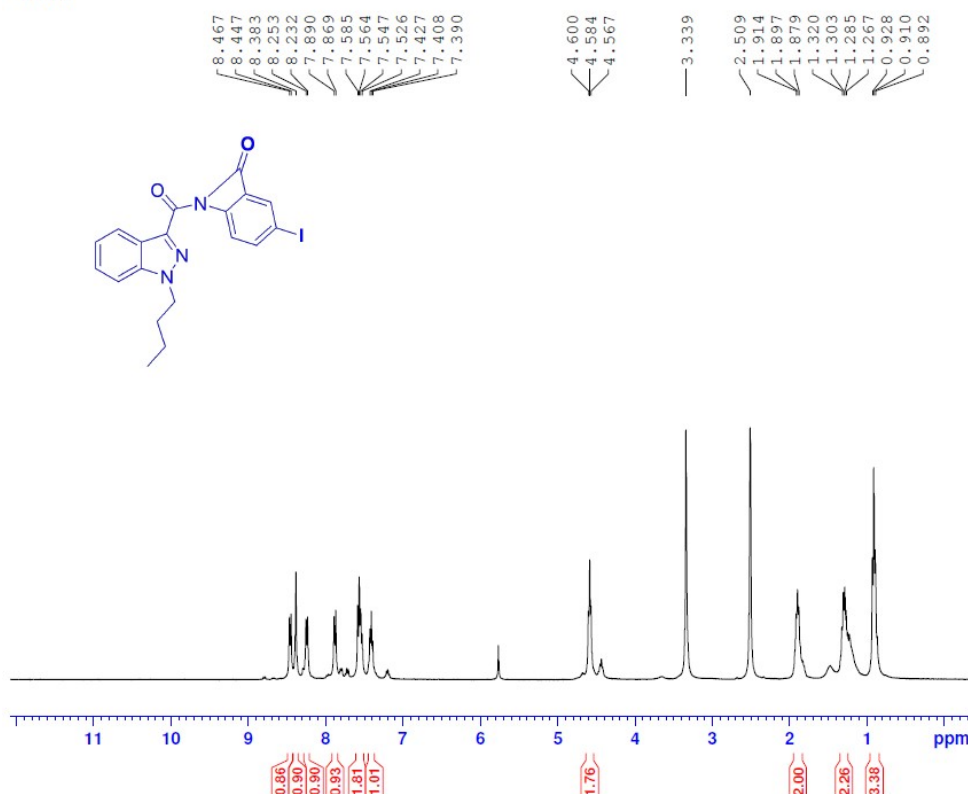


HRMS of 1-butyl-N-(6-methylpyridine-2-yl)-1H-indazole-3-carboxamide (8d).



¹H-NMR [400MHz, DMSO-d₆] spectrum of 2-(1-butyl-1H-indazole -3-carboxamido)-5-iodobenzoic acid (8e).

Signature SIF VIT VELLORE
VG-005

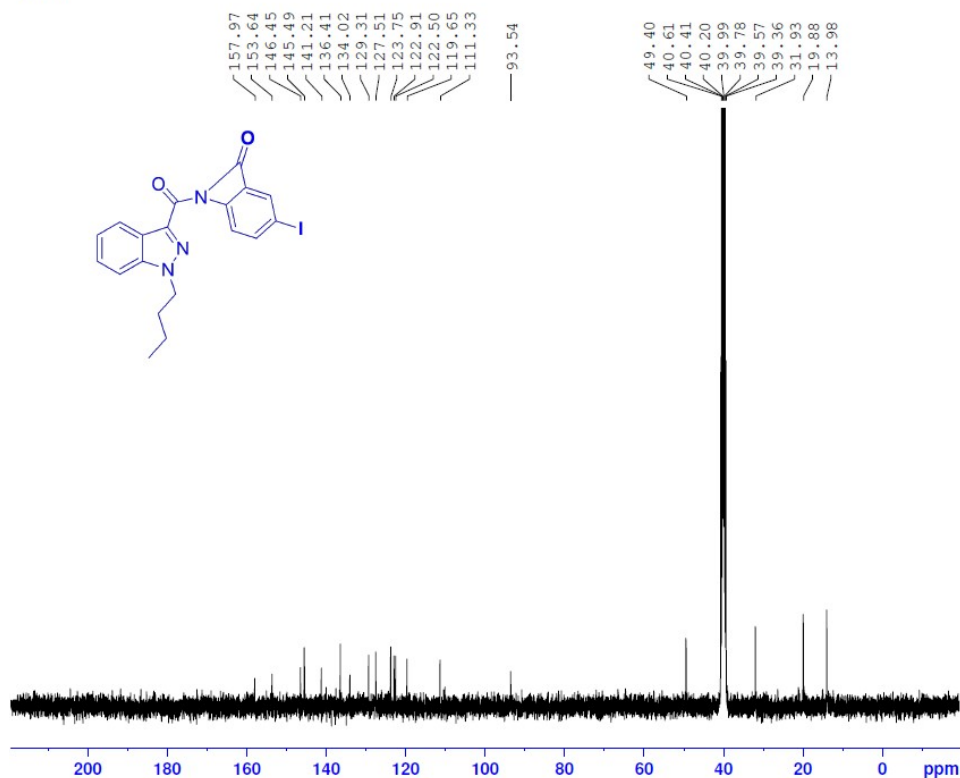


Current Data Parameters
NAME VG-005-8e
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230302
Time 8.10 h
INSTRUM spect
PROBHD Z108618_0505 (1
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 143.73
DM 62.400 usec
DE 6.50 usec
TE 301.4 K
D1 1.00000000 sec
TDO 1
SFO1 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PLW1 14.95499992 W

F2 - Processing parameters
SI 65536
SF 400.2580000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Signature SIF VIT VELLORE
VG-005



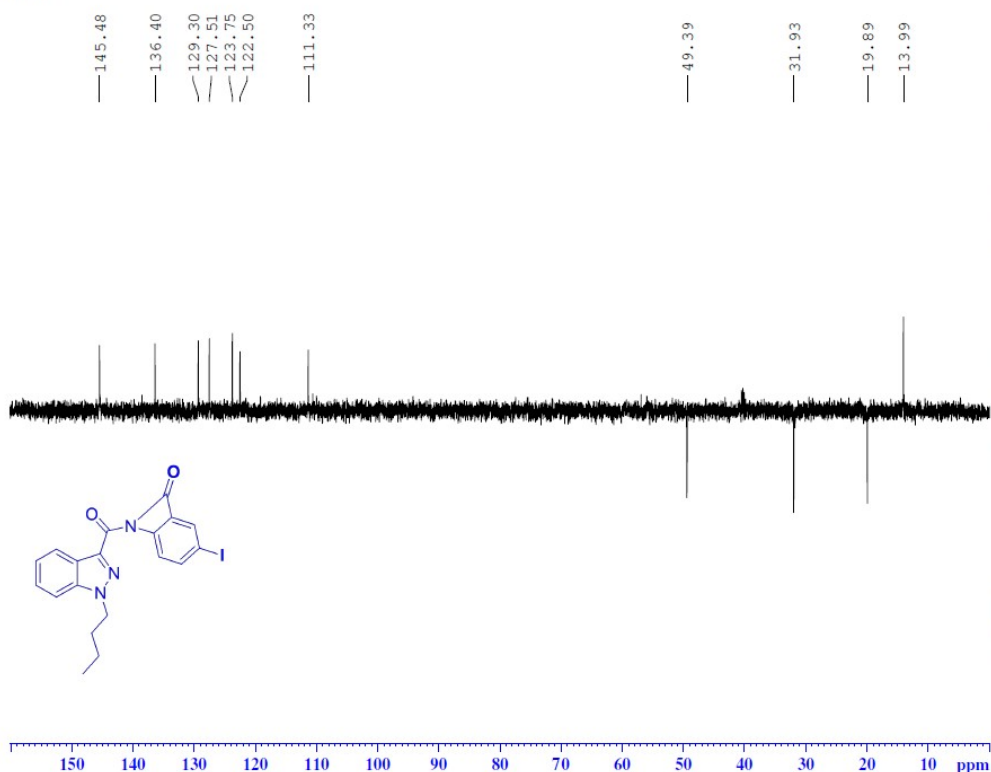
Current Data Parameters
NAME VG-005-8e
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230302
Time 8.41 h
INSTRUM spect
PROBHD Z108618_0505 (1
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 156.91
DM 20.800 usec
DE 6.50 usec
TE 302.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1
SFO1 100.6550186 MHz
NUC1 13C
P1 10.00 usec
PLW1 58.22499847 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 14.95499992 W
PLW12 0.41542000 W
PLW13 0.20895000 W

F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

¹³⁵-DEPT-NMR [100MHz, DMSO-d₆] spectrum of 2-(1-butyl-1H-indazole-3-carboxamido)-5-iodobenzoic acid (8e).

Signature SIF VIT VELLORE
VG-005



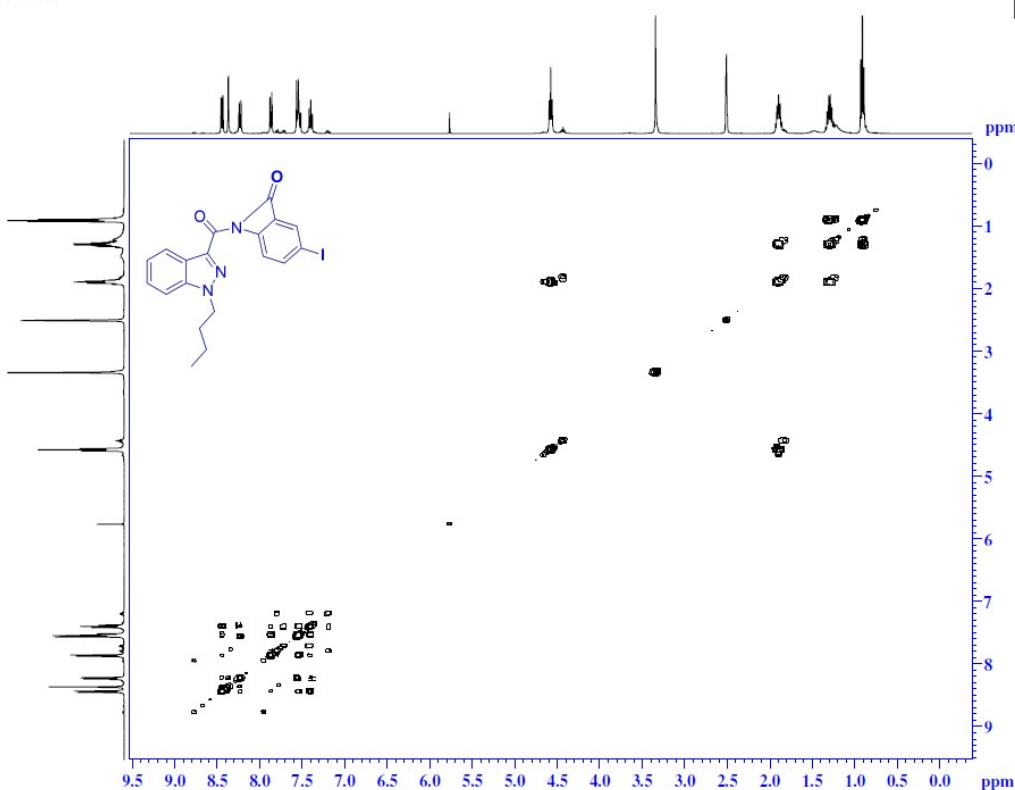
Current Data Parameters
NAME Desktop
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230302
Time 9.00 h
INSTRUM spect
PROBHD z108618_0505 ()
PULPROG deptsp135
TD 65536
SOLVENT DMSO
NS 256
DS 8
SWH 16129.032 Hz
FIDRES 0.492219 Hz
AQ 2.0316160 sec
RG 199.6
DW 31.000 usec
DE 6.50 usec
TE 302.0 K
CNS12 145.0000000
D1 2.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1
SFO1 100.6530057 MHz
NUC1 13C
P1 10.00 usec
P13 2000.00 usec
PLW0 0 W
PLW1 58.22499847 W
SPNAM[5] Crp60comp 4
SPOFF5 0.500
SPOFF55 0 Hz
SPW5 8.89610004 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG[2] waltz16
P3 15.00 usec
P4 30.00 usec
PCPD2 90.00 usec
PLW2 14.95499992 W
PLW12 0.41542000 W

F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

COSY-NMR [400MHz, DMSO-d₆] spectrum of 2-(1-butyl-1H-indazole -3-carboxamido)-5-iodobenzoic acid (8e).

Signature SIF VIT VELLORE
VG-005



Current Data Parameters
NAME Desktop
EXPNO 14
PROCNO 1

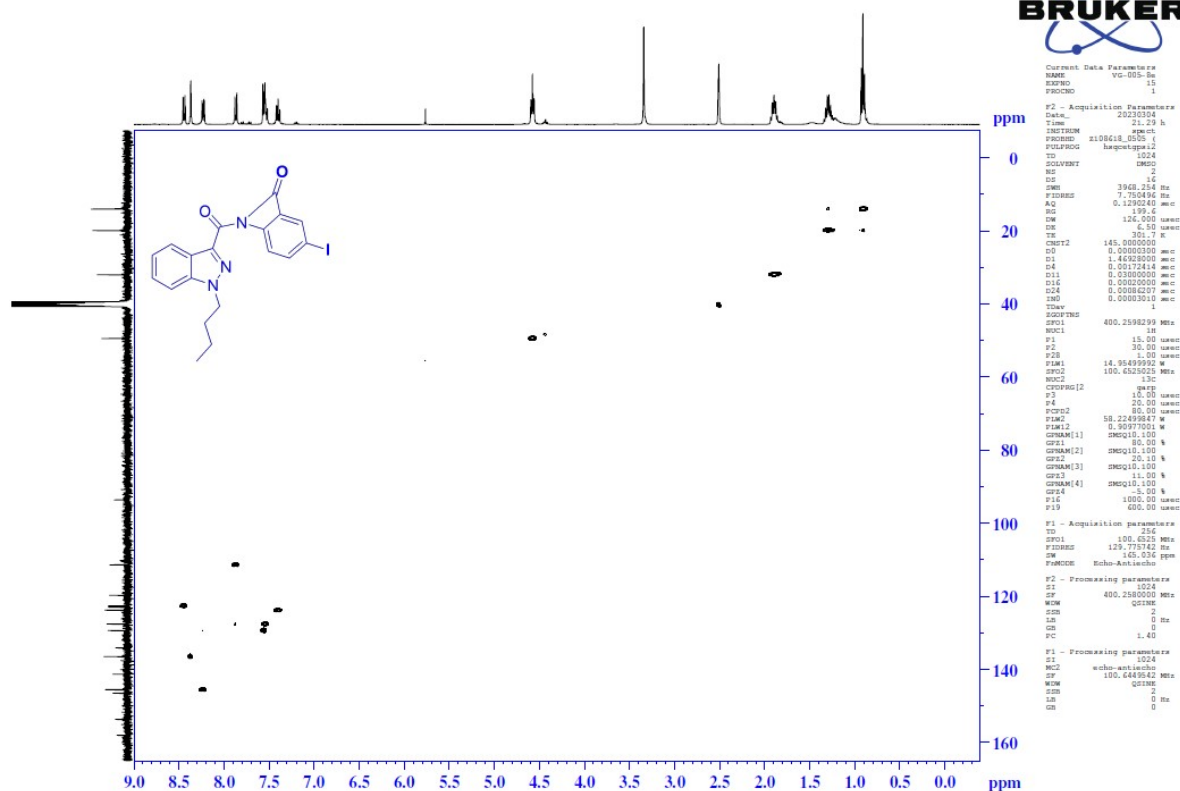
F2 - Acquisition Parameters
Date_ 20230304
Time 21.22 h
INSTRUM spect
PROBHD z108618_0505 ()
PULPROG cosygpgpgf
TD 2048
SOLVENT DMSO
NS 16
DS 16
SWH 3968.254 Hz
FIDRES 3.675248 Hz
AQ 0.2580480 sec
RG 63.11
DW 124.000 usec
DE 6.50 usec
TE 301.7 K
D0 0.00000300 sec
D1 1.93856001 sec
D11 0.00000000 sec
D12 0.00002000 sec
D13 0.00000400 sec
D16 0.00002000 sec
D10 0.00023200 sec
TDW 1
SFO1 400.2598299 MHz
NUC1 1H
P0 15.00 usec
P17 2500.00 usec
PLW1 14.95499992 W
PLW10 3.73869991 W
CPNAM[1] SMO10.100
CPZ1 10.00 %
P16 1000.00 usec

F1 - Acquisition parameters
ID 128
SFO1 400.2598 MHz
FIDRES 62.003967 Hz
SW 9.914 ppm
FNAMECOSY QF

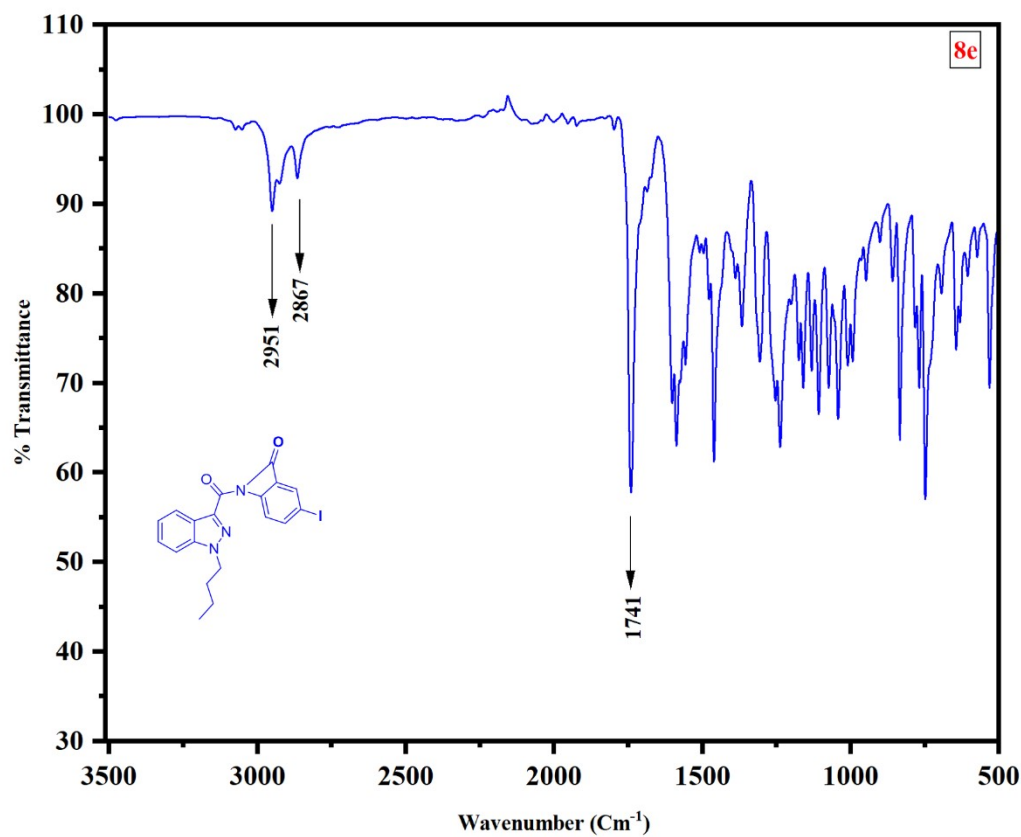
F2 - Processing parameters
SI 1024
SF 400.2580000 MHz
WDW Q8INE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 400.2580000 MHz
WDW Q8INE
SSB 0
LB 0 Hz
GB 0
PC 1.40

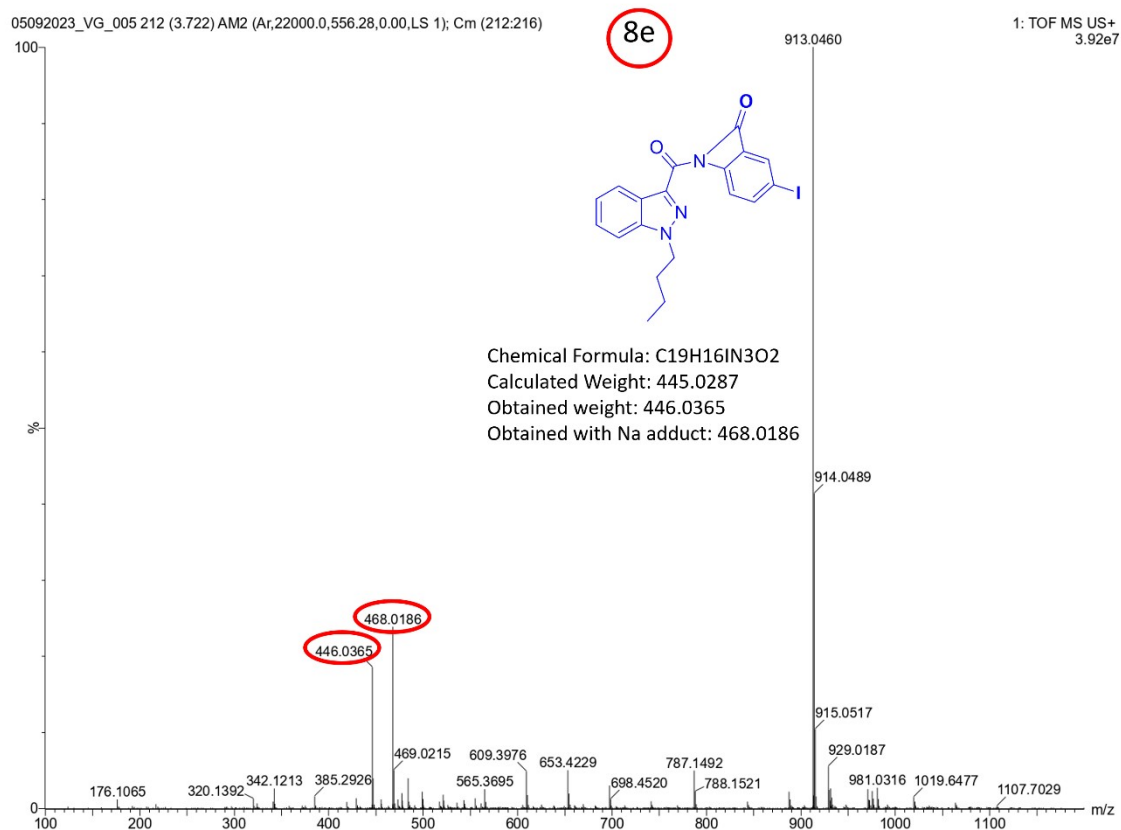
HSQC-NMR [400MHz, DMSO-d₆] spectrum of 2-(1-butyl-1H-indazole -3-carboxamido)-5-iodobenzoic acid (8e).



FT-IR spectrum of 2-(1-butyl-1H-indazole -3-carboxamido)-5-iodobenzoic acid (8e).

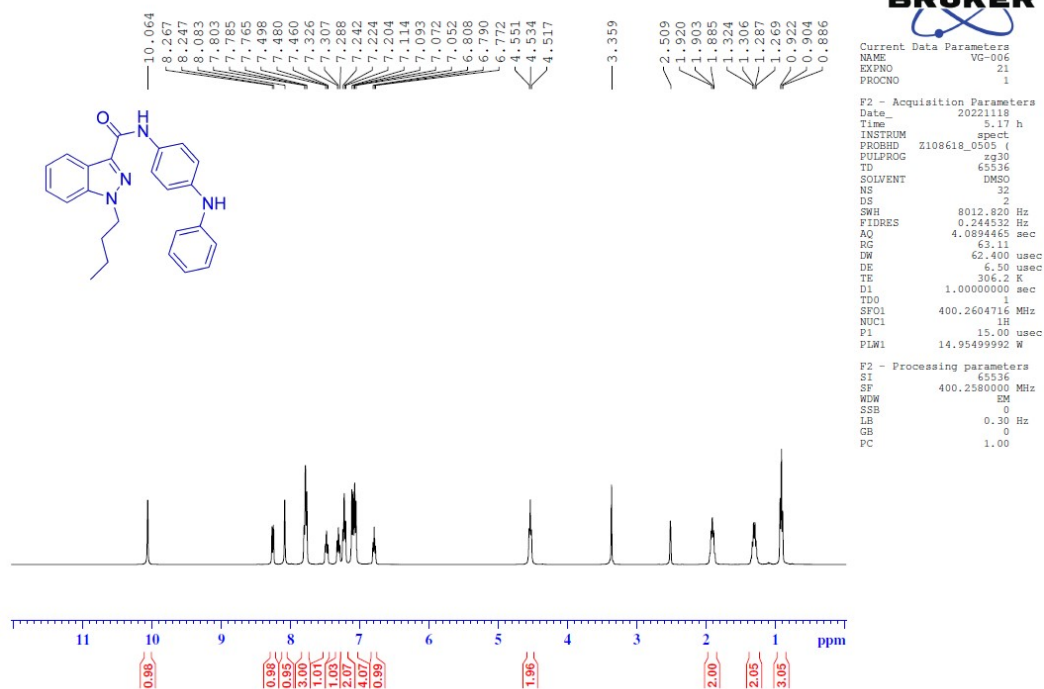


HRMS of 2-(1-butyl-1H-indazole-3-carboxamido)-5-iodobenzoic acid (8e).



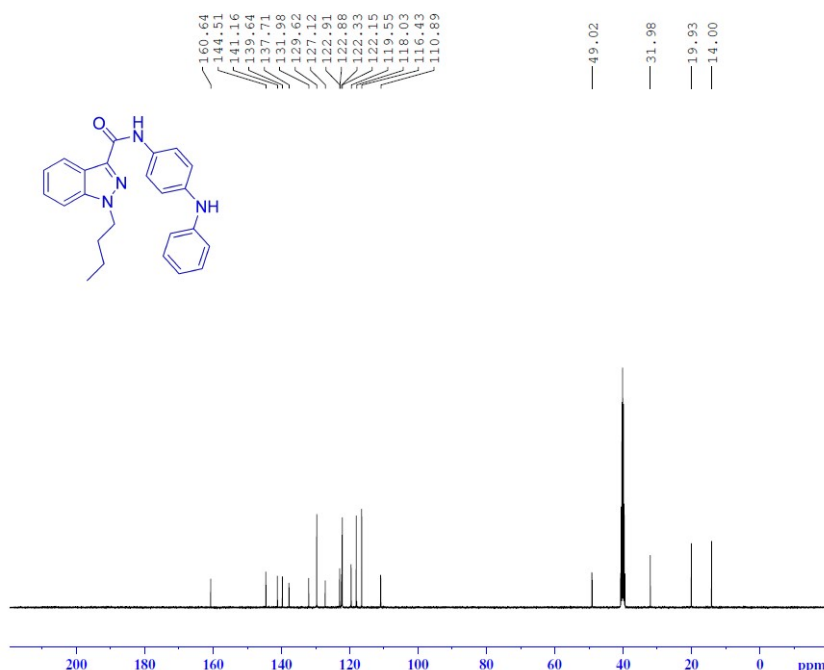
¹H-NMR [400MHz, DMSO-d₆] spectrum of 1-butyl-N-(4-(phenylamino) phenyl)-1H-indazole-3-carboxamide (8f).

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VG006



¹³C-NMR [100MHz, DMSO-d₆] spectrum of 1-butyl-N-(4-(phenylamino) phenyl)-1H-indazole-3-carboxamide (8f).

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VG006



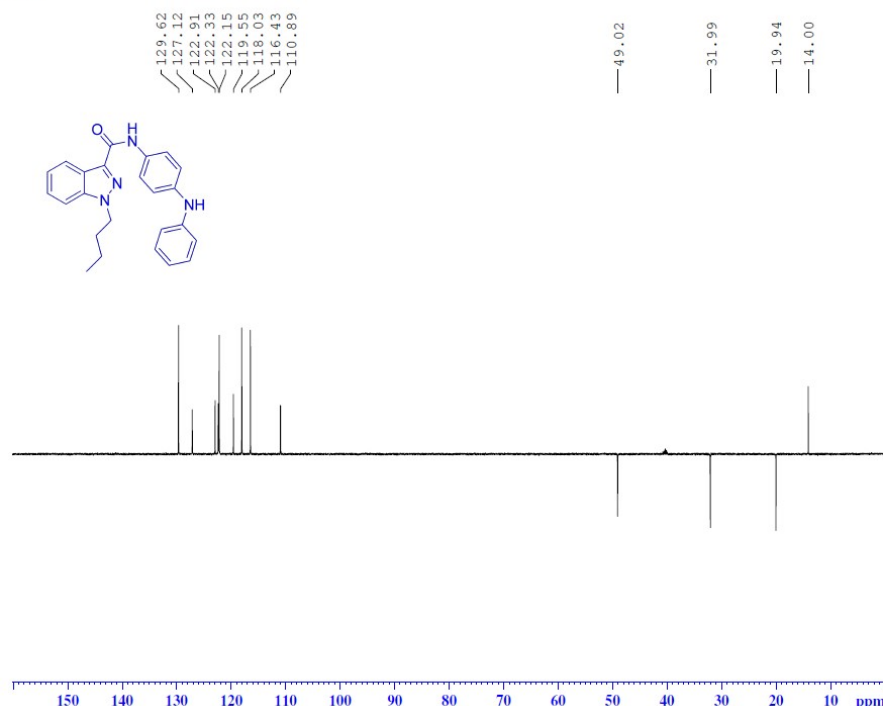
Current Data Parameters
NAME VG-006
EXPNO 22
PROCNO 1

F2 - Acquisition Parameters
Date_ 20221118
Time 5.47 h
INSTRUM spect
PROBHD Z108618_0505 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 512
DS 8
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 199.6
DW 20.800 usec
DE 6.50 usec
TE 306.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6550186 MHz
NUC1 13C
P1 10.00 usec
PLW1 58.22499847 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 14.95499992 W
PLW12 0.41542000 W
PLW13 0.20895000 W

F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

¹³⁵DEPT-NMR [100MHz, DMSO-d₆] spectrum of 1-butyl-N-(4-(phenylamino)phenyl)-1H-indazole-3-carboxamide (8f).

Signature SIF VIT VELLORE
VG006

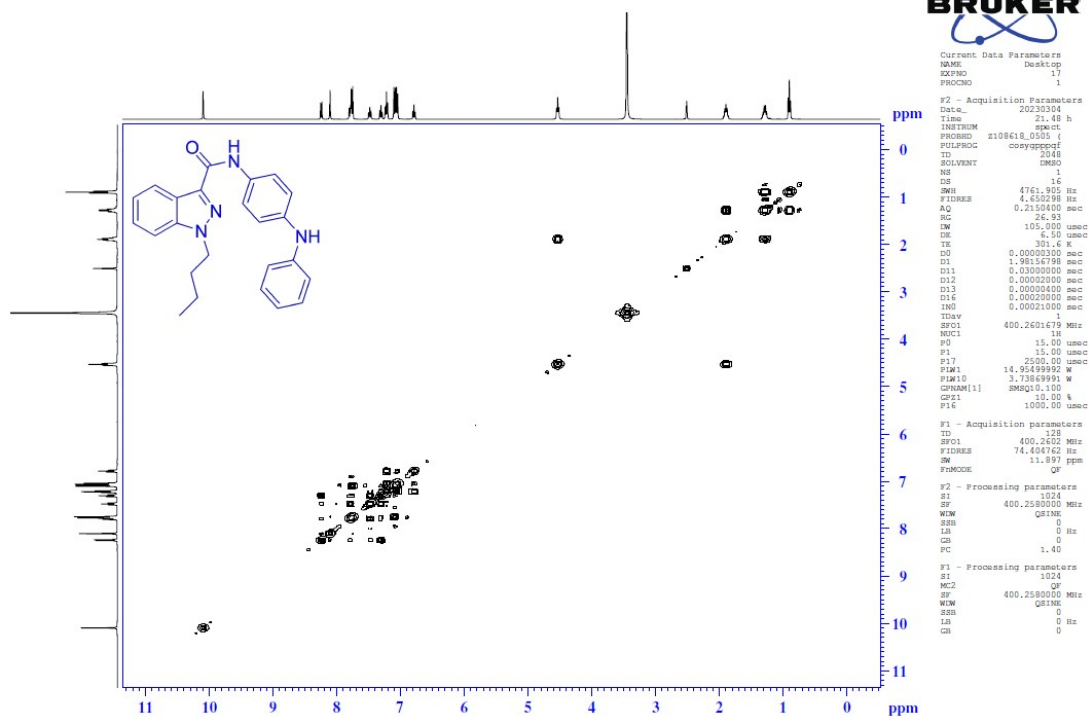


Current Data Parameters
NAME VG-006
EXPNO 23
PROCNO 1

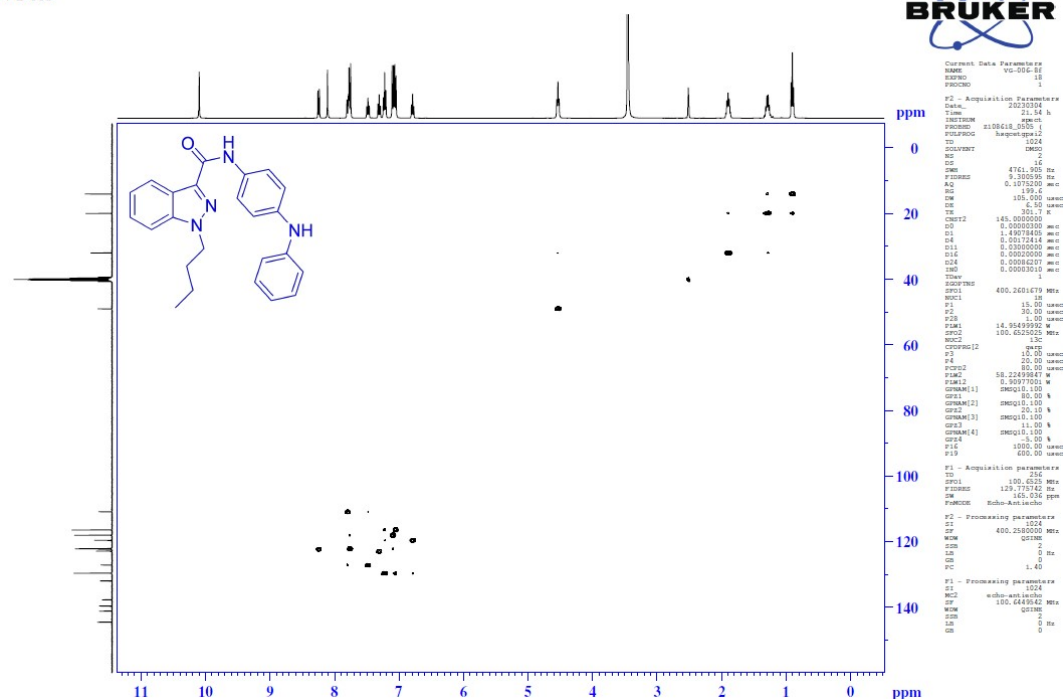
F2 - Acquisition Parameters
Date_ 20221118
Time 6.07 h
INSTRUM spect
PROBHD Z108618_0505 (
PULPROG deptap135
TD 65536
SOLVENT DMSO
NS 256
DS 8
SWH 16129.032 Hz
FIDRES 0.492219 Hz
AQ 2.0316160 sec
RG 199.6
DW 31.000 usec
DE 6.50 usec
TE 306.5 K
CONST 145.0000000
D1 2.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1
SFO1 100.6530057 MHz
NUC1 13C
P1 10.00 usec
PLW1 58.22499847 W
SPNAM[5] Crp60comp.4
SFOAL5 0.500
SPOFFS5 0 Hz
SPW5 8.89610004 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG2 waltz16
P3 15.00 usec
P4 30.00 usec
PCPD2 90.00 usec
PLW2 14.95499992 W
PLW12 0.41542000 W

F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

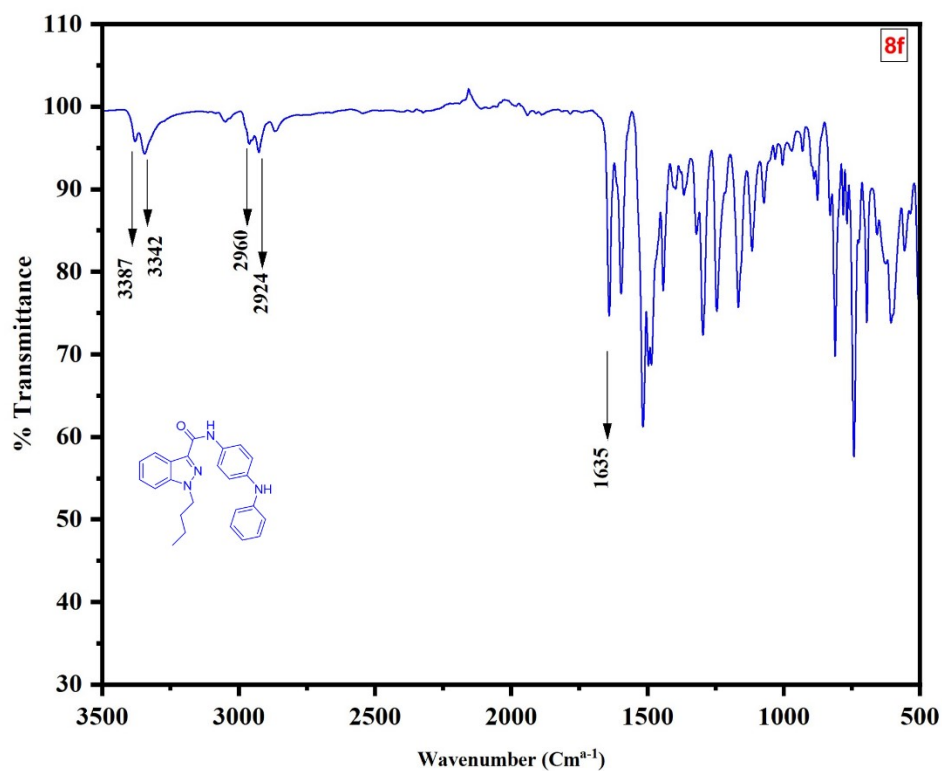
COSY-NMR [400MHz, DMSO-d₆] spectrum of 1-butyl-N-(4-(phenylamino)phenyl)-1H-indazole-3-carboxamide (8f).



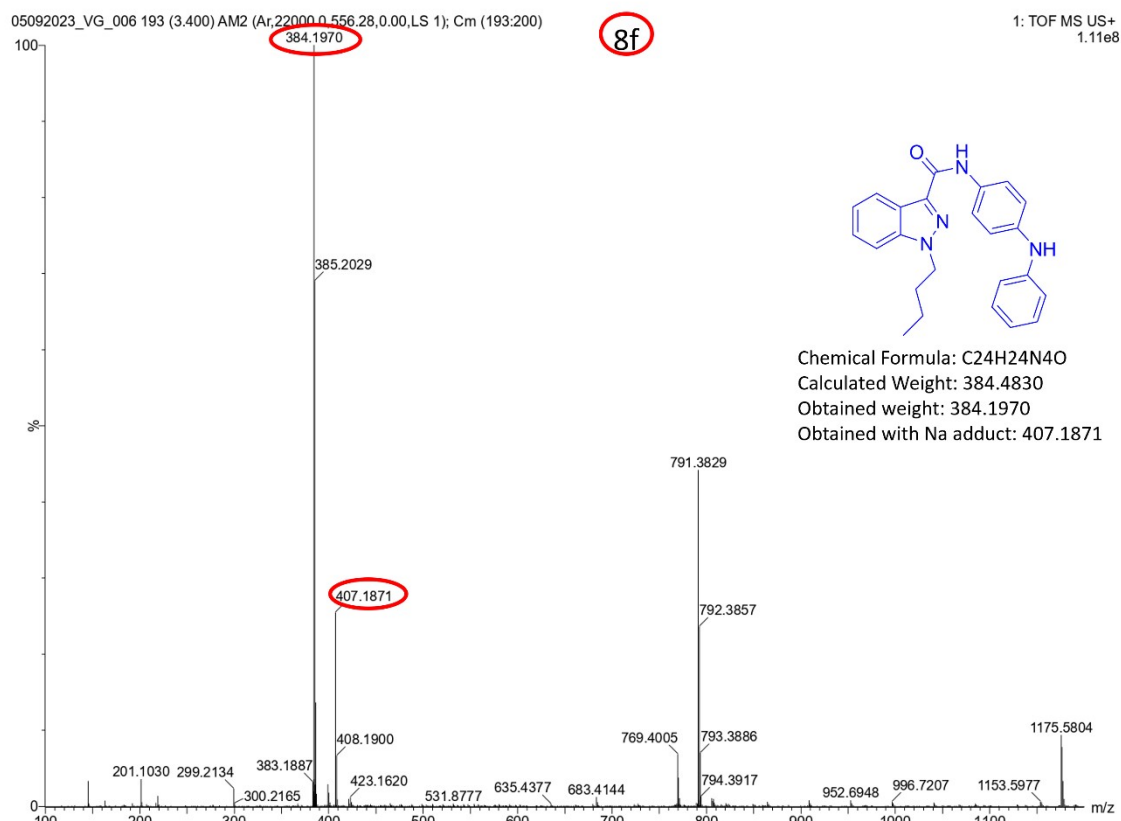
HSQC-NMR [400MHz, DMSO-d₆] spectrum of 1-butyl-N-(4-(phenylamino)phenyl)-1H-indazole-3-carboxamide (8f).



FT-IR spectrum of 1-butyl-N-(4-(phenylamino)phenyl)-1H-indazole-3-carboxamide (8f).

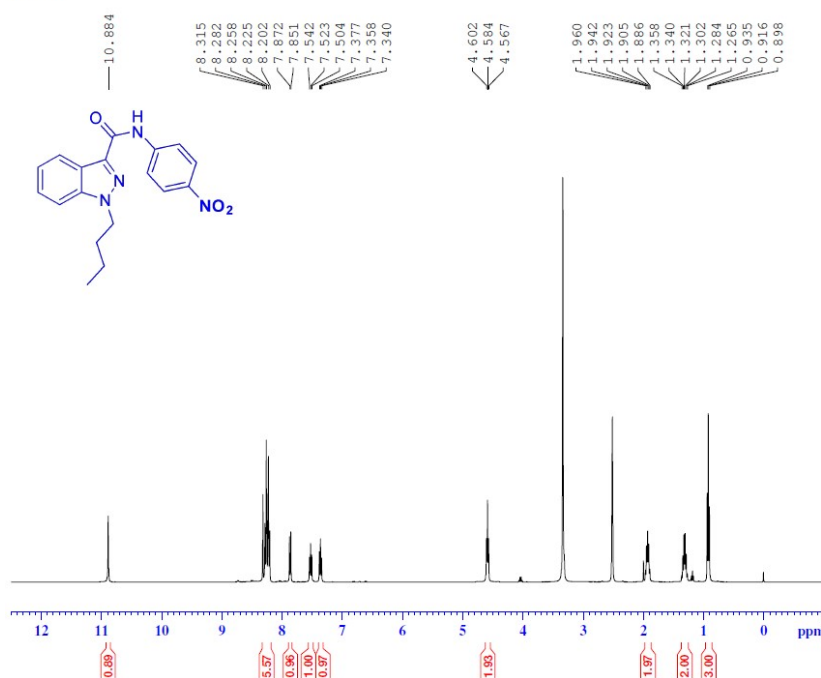


HRMS of 1-butyl-N-(4-(phenylamino)phenyl)-1H-indazole-3-carboxamide (8f).



¹H-NMR [400MHz, DMSO-d₆] spectrum of 1-butyl-N-(4-nitrophenyl)-1H-indazole-3-carboxamide (8g).

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VG-036



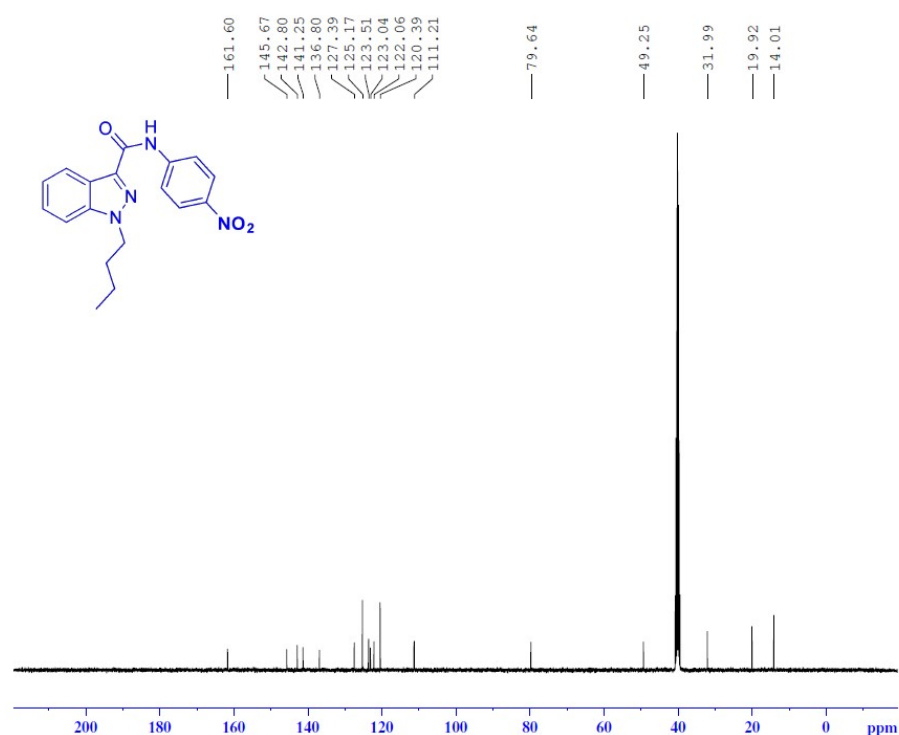
Current Data Parameters
NAME VG-036
EXPNO 70
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230518
Time 15.38 h
INSTRUM spect
PROBHD z108618_0505 (z30)
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 143.73
DW 62.400 usec
DE 6.50 usec
TE 305.9 K
D1 1.00000000 sec
TD0 1
SFO1 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PLW1 14.95499992 W

F2 - Processing parameters
SI 55536
SF 400.2579990 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹³C-NMR [100MHz, DMSO-d₆] spectrum of 1-butyl-N-(4-nitrophenyl)-1H-indazole-3-carboxamide (8g).

Signature SIF VIT VELLORE
VG-036



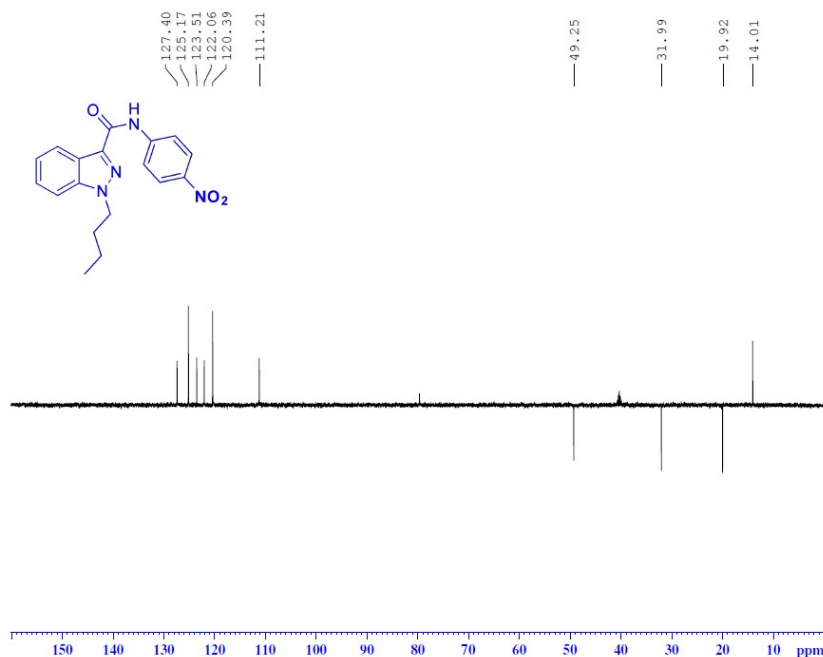
Current Data Parameters
NAME Dr.VVR160523
EXPNO 58
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230516
Time 1.18 h
INSTRUM spect
PROBHD z108618_0505 (zpg30)
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 199.6
DW 20.800 usec
DE 6.50 usec
TE 305.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6550186 MHz
NUC1 13C
P1 10.00 usec
PLW1 58.22499847 W
SFO2 400.2596010 MHz
NUC2 1H
CFDPFG[2] waltz16
PCFDD 90.00 usec
PLW2 14.95499992 W
PLW12 0.41542000 W
PLW13 0.20895000 W

F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

¹³⁵-DEPT-NMR [400MHz, DMSO-d₆] spectrum of 1-butyl-N-(4-nitrophenyl)-1H-indazole-3-carboxamide (8g).

Signature SIF VIT VELLORE
VG-036

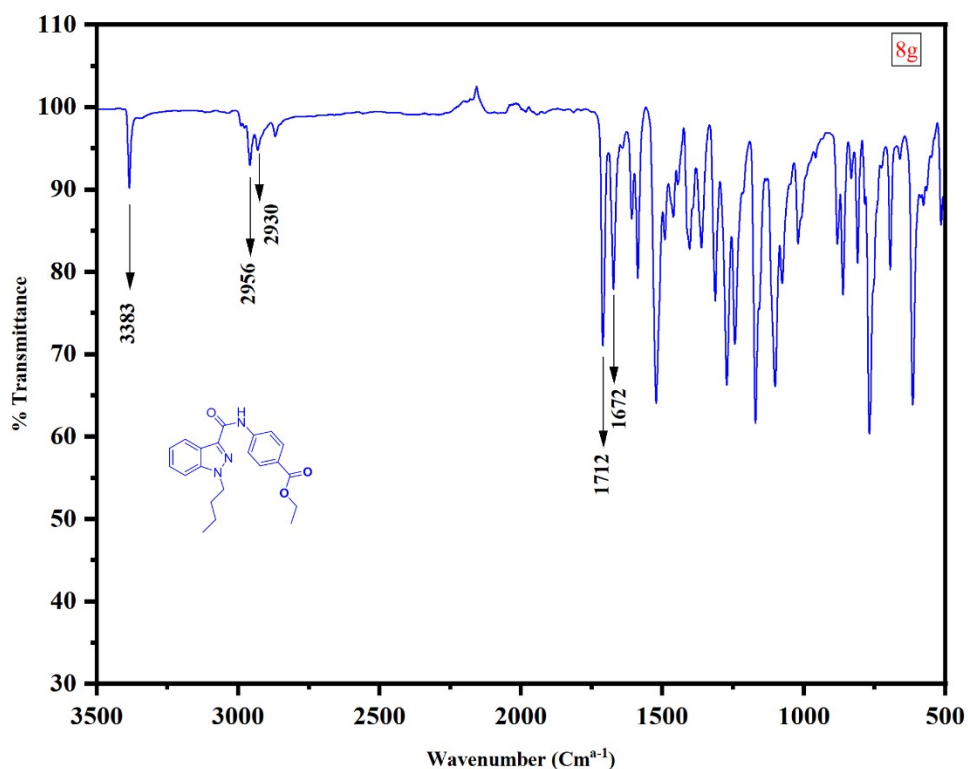


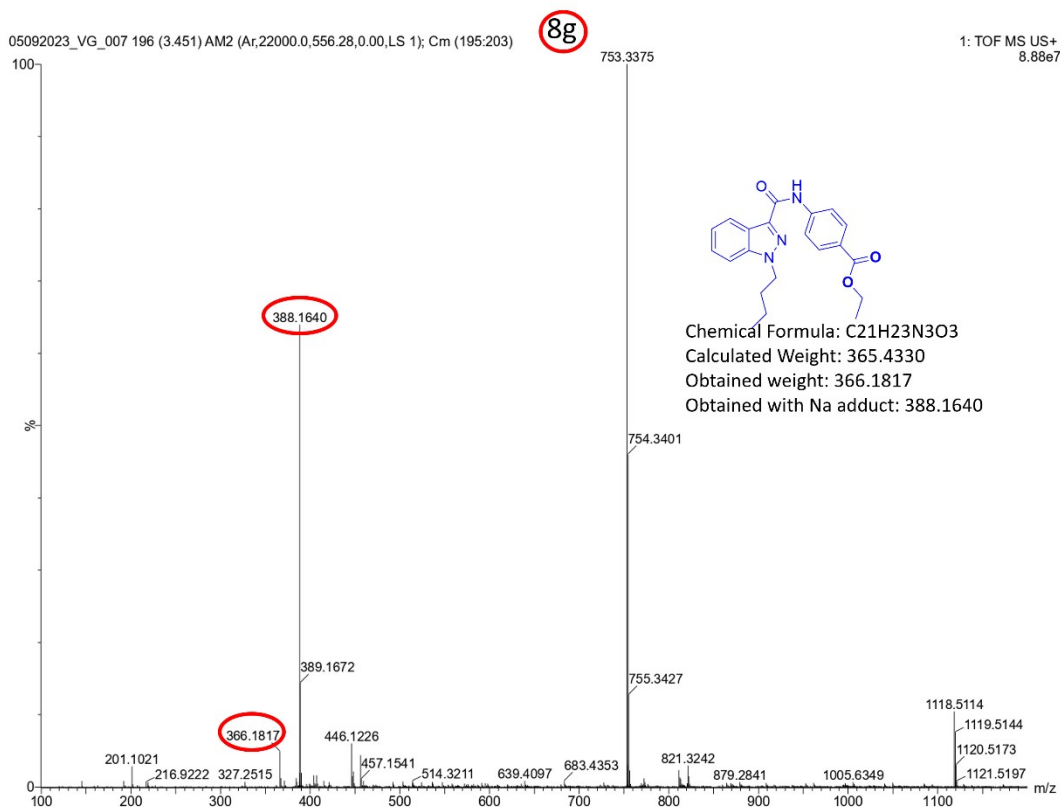
Current Data Parameters
NAME Dr.VVR160523
EXPNO 59
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230516
Time 1.38 h
INSTRUM spect
PROBHD z108618_0505 (4
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 256
DS 8
SWH 16129.032 Hz
FIDRES 0.492219 Hz
AQ 2.8316160 sec
RG 199.6
DW 31.000 usec
DE 6.50 usec
TE 304.8 K
CNS12 165.000000
D1 2.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TDO 1
SFO1 100.6530057 MHz
NUC1 13C
P1 10.00 usec
P13 2000.00 usec
PLW0 0 W
PLW1 58.22499847 W
SPNAM[5] Crp60comp.4
SFOAL5 0.500
SFOFF55 0 Hz
SPW5 8.89610004 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG2 waltz16
P3 15.00 usec
P4 30.00 usec
PCPD2 90.00 usec
PLW2 18.95499992 W
PLW12 0.41542000 W

F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

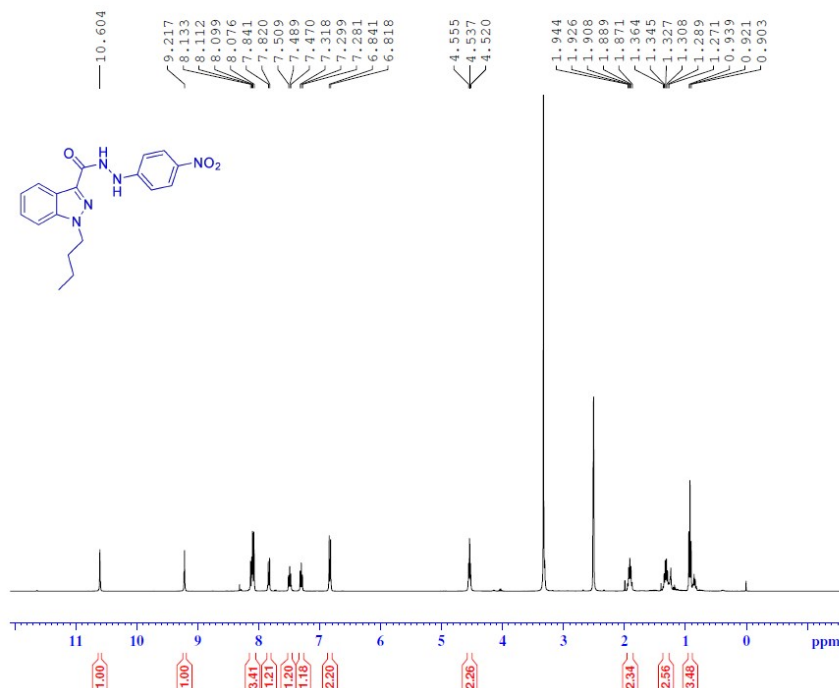
FT-IR spectrum of 1-butyl-N-(4-nitrophenyl)-1H-indazole-3-carboxamide (8g).





¹H-NMR [400MHz, DMSO-d₆] spectrum of 1-butyl-N-(4-nitrophenyl)-1H-indazole-3-carbohydrazide (8h).

Signature SIF VIT VELLORE
 VG-039



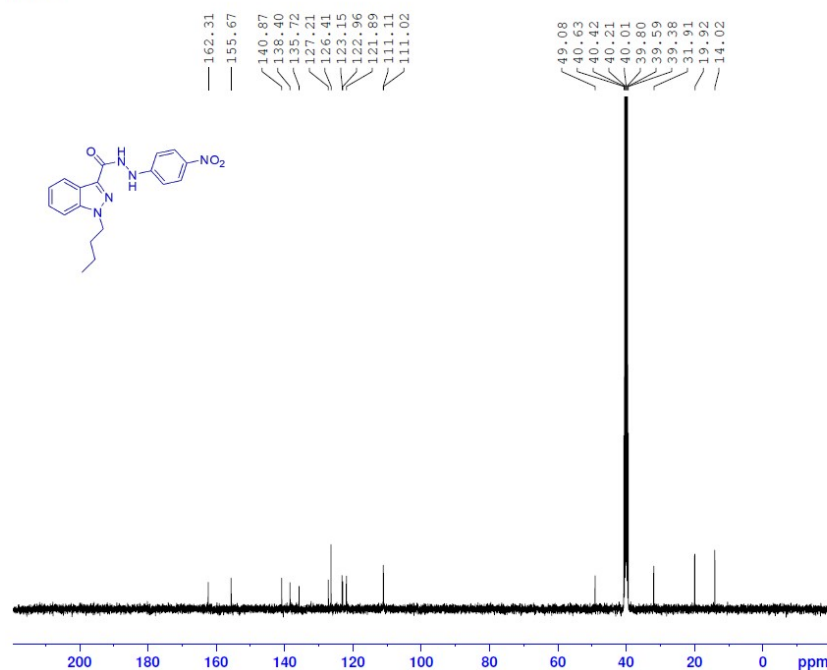
Current Data Parameters
 NAME Dr.SSW220523
 EXPNO 64
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20230522
 Time_ 14.10 h
 INSTRUM spect
 PROBRD Z108618_0505 (zg30)
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 32
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 4.0894465 sec
 RG 143.73
 DW 62.400 usec
 DE 6.50 usec
 TE 303.5 K
 D1 1.00000000 sec
 TDO 1
 SFO1 400.2604716 MHz
 NUC1 1H
 P1 15.00 usec
 PLW1 14.95499992 W

F2 - Processing parameters
 SI 65536
 SF 400.2580014 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

¹³C-NMR [100MHz, DMSO-d₆] spectrum of 1-butyl-N-(4-nitro phenyl)-1H-indazole-3-carbohydrazide (8h).

Signature SIF VIT VELLORE
VG-039



BRUKER

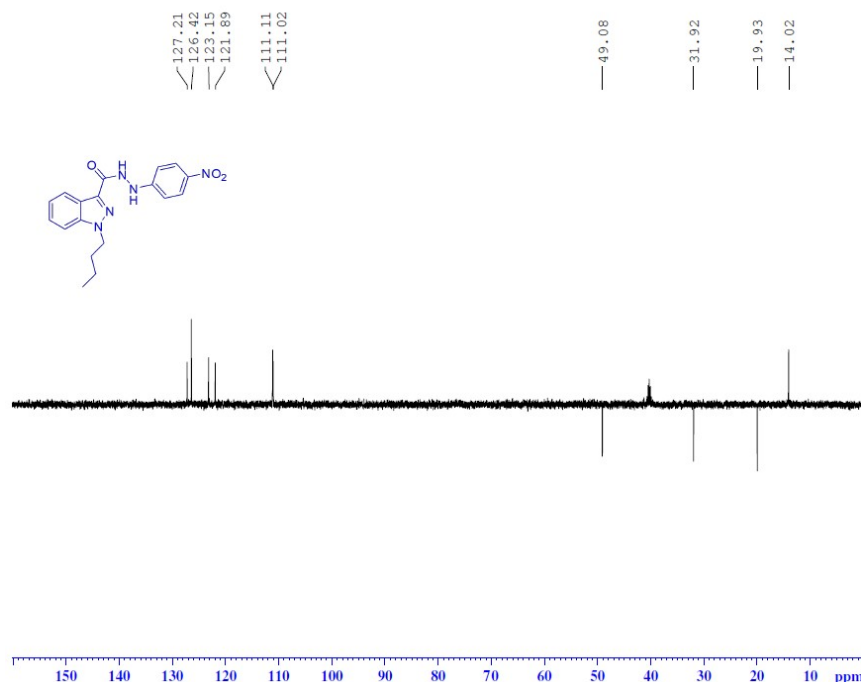
Current Data Parameters
NAME VG-039-8h
EXPNO 71
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230524
Time 9.46 h
INSTRUM spect
PROBHD Z108618_0505 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 199.6
DW 20.800 usec
DE 6.50 usec
TE 305.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1
SFO1 100.6550186 MHz
NUC1 13C
P1 10.00 usec
PLW1 58.22499847 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 14.95499992 W
PLW12 0.41542000 W
PLW13 0.20895000 W

F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

135-DEPT-NMR [100MHz, DMSO-d₆] spectrum of 1-butyl-N-(4-nitrophenyl)-1H-indazole-3-carbohydrazide (8h).

Signature SIF VIT VELLORE
VG-039



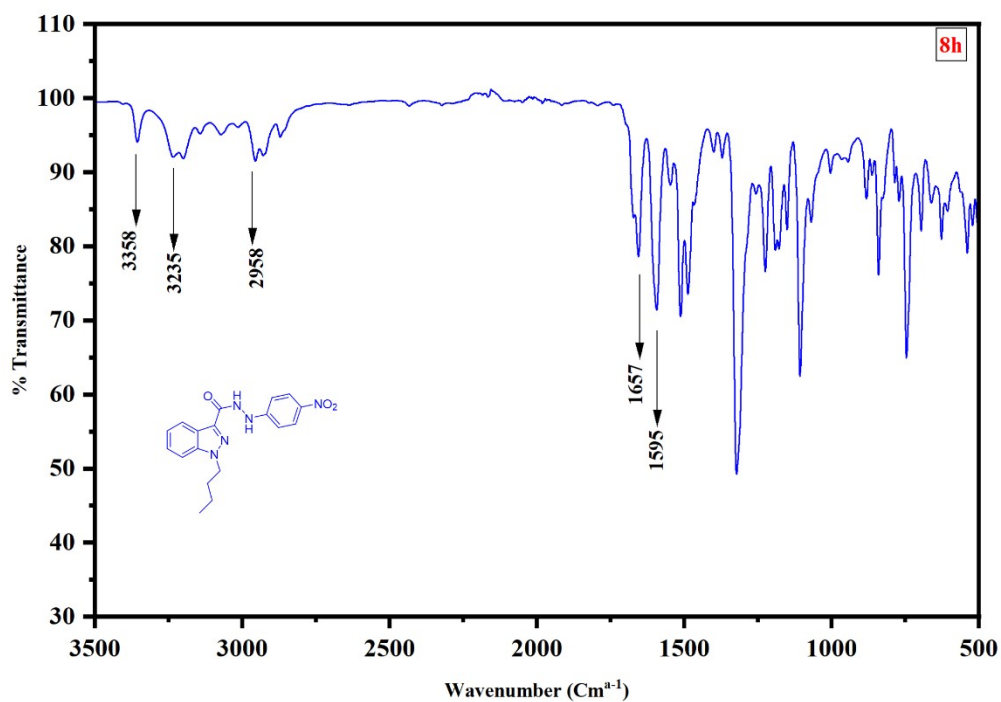
BRUKER

Current Data Parameters
NAME Dr.SSW230523
EXPNO 72
PROCNO 1

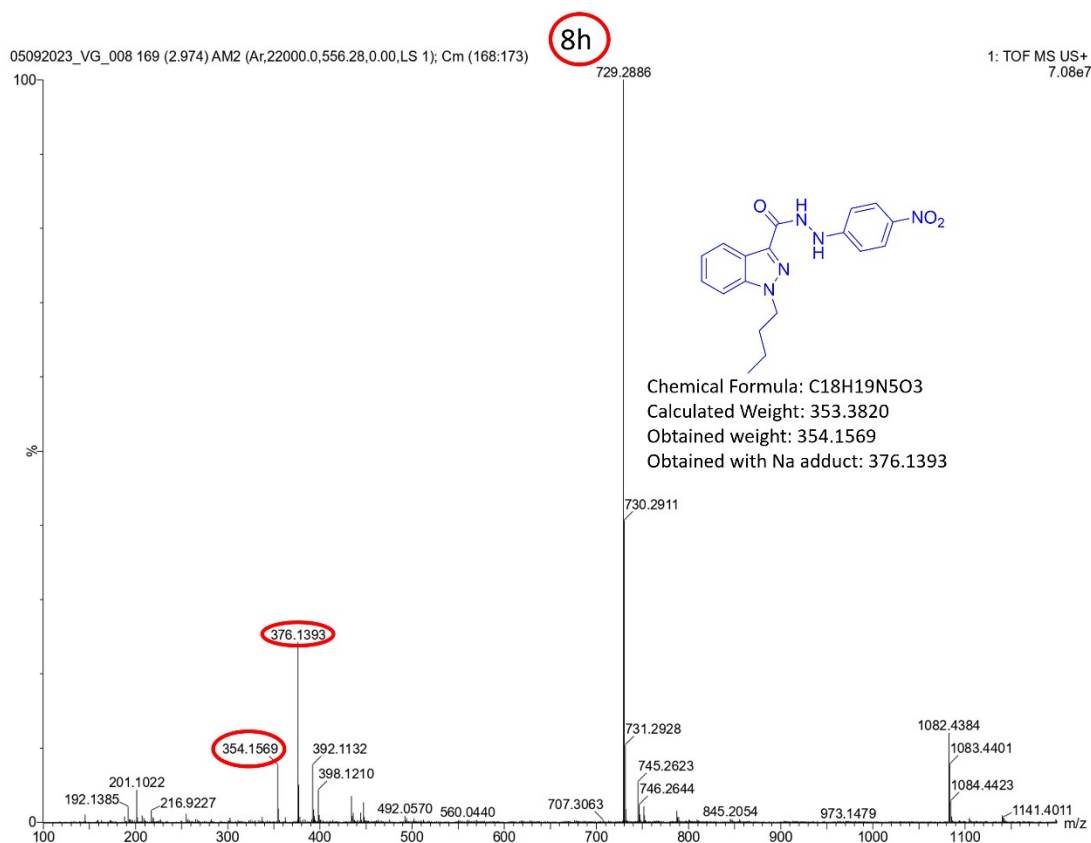
F2 - Acquisition Parameters
Date_ 20230524
Time 10.06 h
INSTRUM spect
PROBHD Z108618_0505 (
PULPROG deptsp135
TD 65536
SOLVENT DMSO
NS 256
DS 8
SWH 16129.032 Hz
FIDRES 0.492219 Hz
AQ 2.0336160 sec
RG 199.6
DW 31.000 usec
DE 6.50 usec
TE 305.3 K
CNST2 145.0000000 sec
D1 2.00000000 sec
D2 0.00344828 sec
D12 0.00020000 sec
TDO 1
SFO1 100.6530057 MHz
NUC1 13C
P1 10.00 usec
P13 2000.00 usec
PLW0 0 W
PLW1 58.22499847 W
SPNAM[5] Crp60comp.4
SFOAL5 0.500
SPOFF55 0 Hz
SFW5 8.89610000 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG2 waltz16
P3 15.00 usec
P4 30.00 usec
PCPD2 90.00 usec
PLW2 14.95499992 W
PLW12 0.41542000 W

F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

FT-IR spectrum of 1-butyl-N-(4-nitrophenyl)-1H-indazole-3-carbohydrazide (8h).

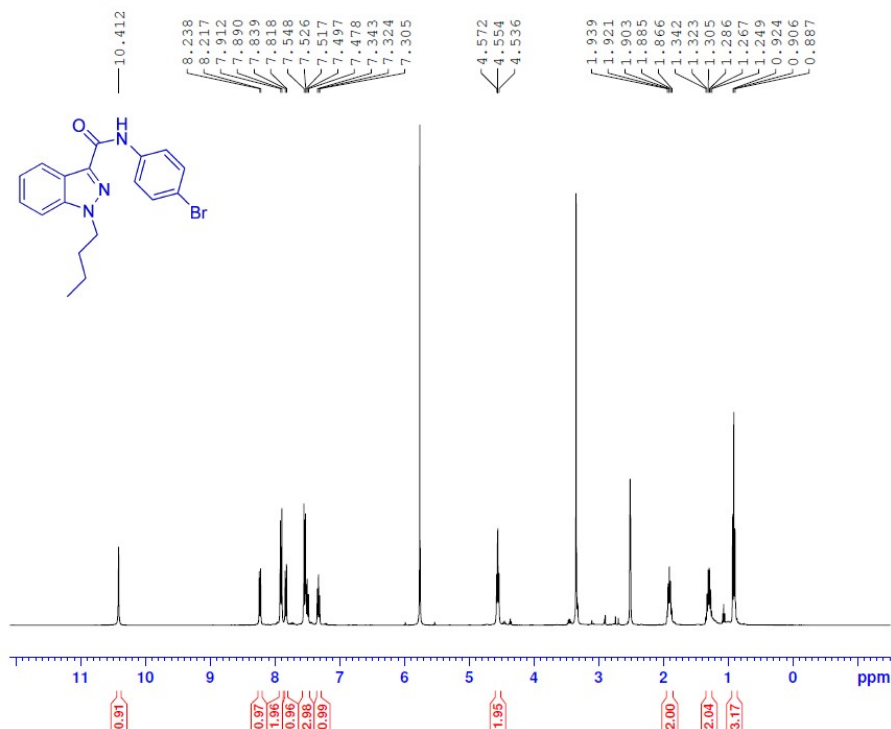


HRMS of 1-butyl-N-(4-nitrophenyl)-1H-indazole-3-carbohydrazide (8h).



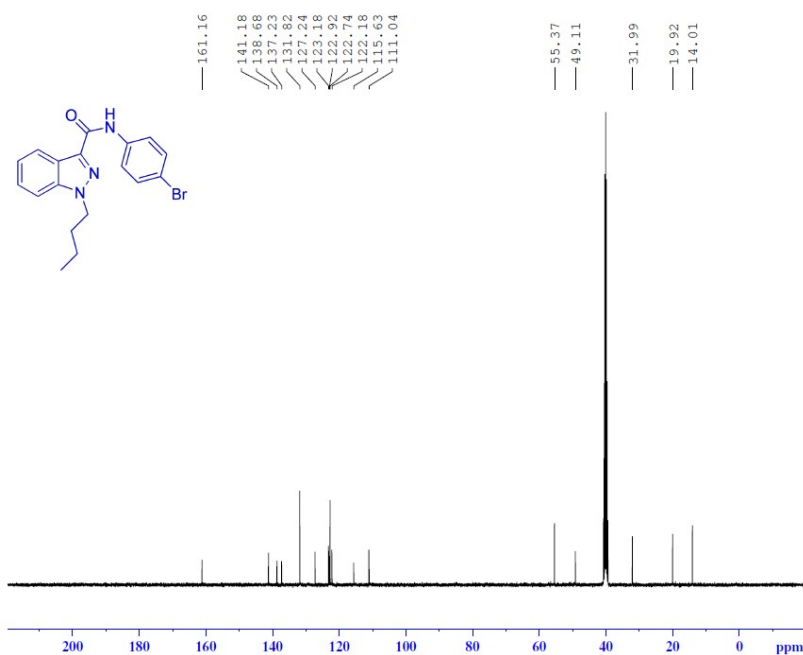
¹H-NMR [400MHz, DMSO-d₆] spectrum of N-(4-Bromophenyl)-1-butyl-1H-indazole-3-carboxamide (8i).

Signature SIF VIT VELLORE
VG-009



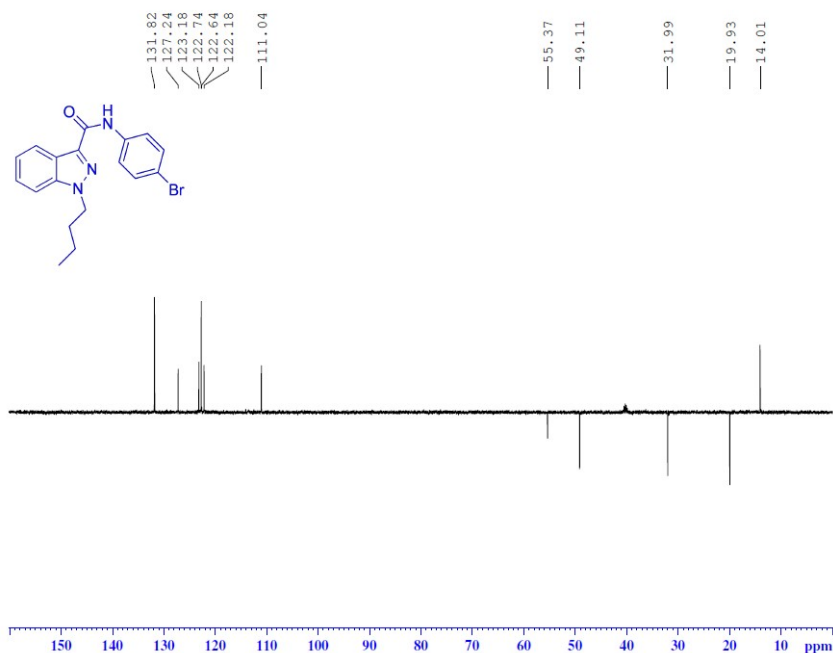
¹³C-NMR [100MHz, DMSO-d₆] spectrum of N-(4-Bromophenyl)-1-butyl-1H-indazole-3-carboxamide (8i).

Signature SIF VIT VELLORE
VG009



¹³⁵-DEPT-NMR [100MHz, DMSO-d₆] spectrum of N-(4-Bromophenyl)-1-butyl-1H-indazole-3-carboxamide (8i).

Signature SIF VIT VELLORE
VG009



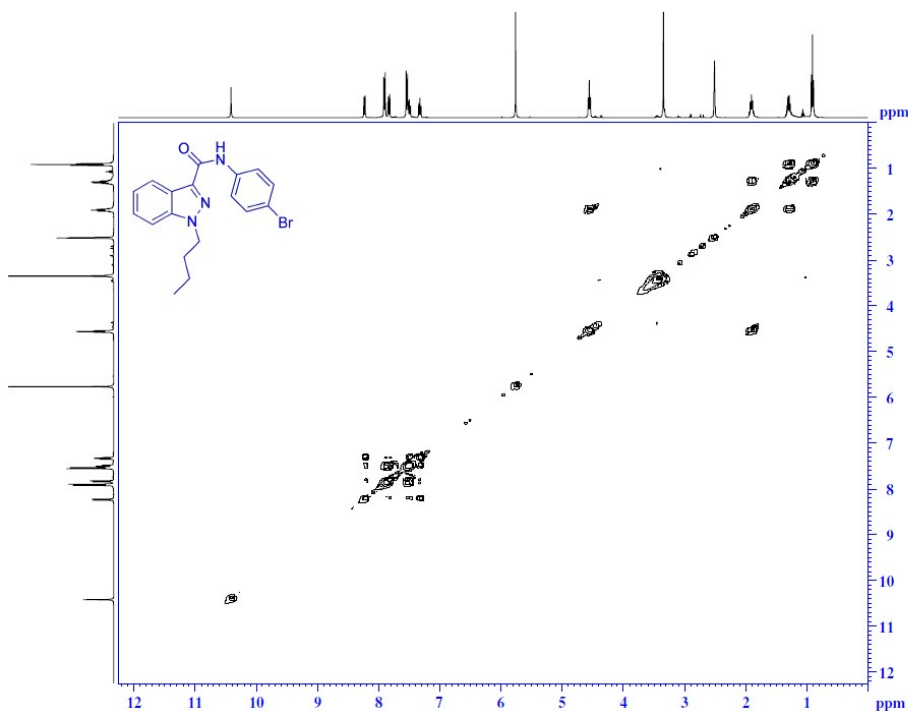
Current Data Parameters
NAME VG-009
EXPNO 41
PROCNO 1

F2 - Acquisition Parameters
Date_ 20221125
Time 19.10 h
INSTRUM spect
PROBHD z108618.0505 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 256
DS 8
SWH 16129.032 Hz
FIDRES 0.492219 Hz
AQ 2.0316160 sec
RG 199.6
DW 31.000 usec
DE 6.50 usec
TE 304.4 K
CNS2 145.000000
D1 2.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1
SFO1 100.6530057 MHz
NUC1 13C
P1 10.00 usec
P13 2000.00 usec
PLW0 0 W
PLW1 58.22499847 W
SPNAM[5] Crp60comp.4
SFOA15 0.500
SFOFF25 0 Hz
SWH 8.89610004 W
SFO2 400.2580010 MHz
NUC2 1H
CPDPRG2 waltz16
P3 15.00 usec
P4 30.00 usec
PCPD2 90.00 usec
PLW2 14.95499992 W
PLW12 0.41542000 W

F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

COSY-NMR [400MHz, DMSO-d₆] spectrum of N-(4-Bromophenyl)-1-butyl-1H-indazole-3-carboxamide (8i).

Signature SIF VIT VELLORE
VG-009



Current Data Parameters
NAME 43
EXPNO 44
PROCNO 1

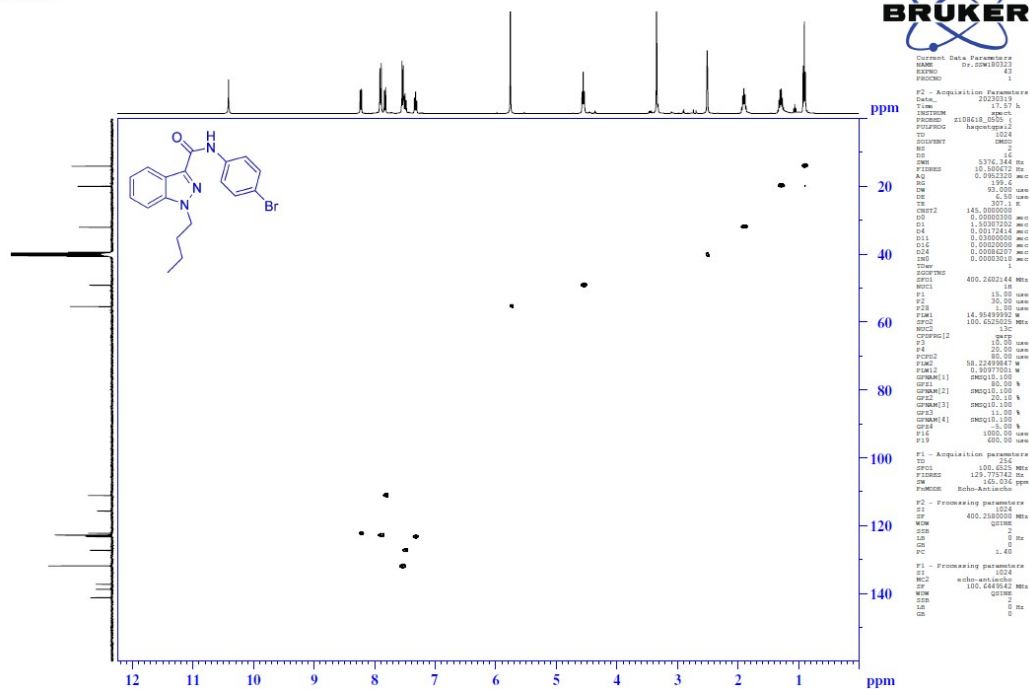
F2 - Acquisition Parameters
Date_ 20230319
Time 18.13 h
INSTRUM spect
PROBHD z108618.0505 (
PULPROG zgpg30
TD 256
SOLVENT DMSO
NS 1
DS 16
SWH 5376.344 Hz
FIDRES 5.220336 Hz
AQ 0.1904640 sec
RG 35.49
DW 93.000 usec
DE 6.50 usec
TE 304.9 K
D0 0.00000000 sec
D1 2.00614405 sec
D11 0.03000000 sec
D12 0.00002000 sec
D13 0.00000400 sec
D16 0.00020000 sec
DNO 0.00018600 sec
TD0 1
SFO1 400.2602144 MHz
NUC1 1H
P0 15.00 usec
P1 15.00 usec
P17 2500.00 usec
PLW1 14.95499992 W
PLW10 3.73668991 W
CPNAM[1] SNAQ10.100
CHP1 10.00 %
P16 1000.00 usec

F1 - Acquisition parameters
SI 1324
SF 400.2602 MHz
FIDRES 84.005379 Hz
SW 13.432 ppm
FNAME QF

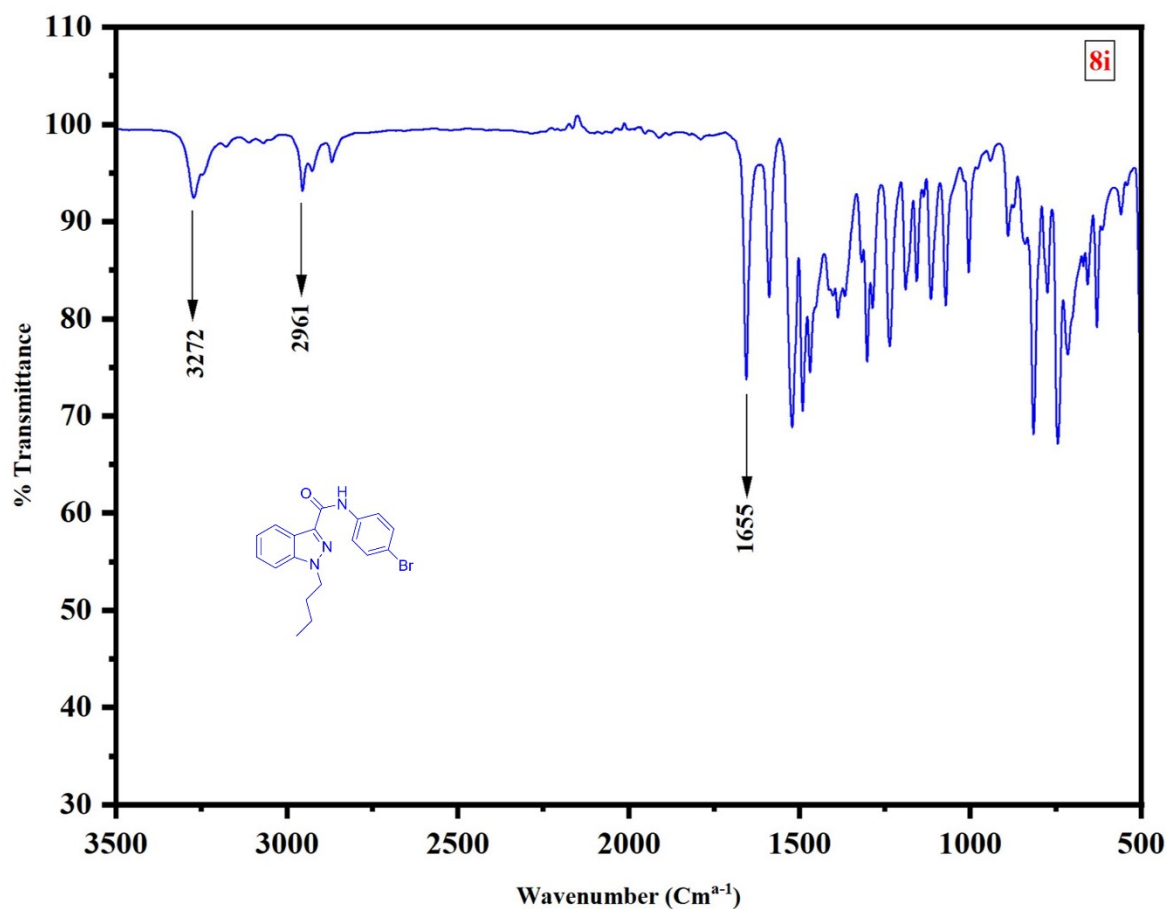
F2 - Processing parameters
SI 1324
SF 400.2580000 MHz
WDW QFINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1324
MC2 QF
SF 400.2580000 MHz
WDW QFINE
SSB 0
LB 0 Hz
GB 0

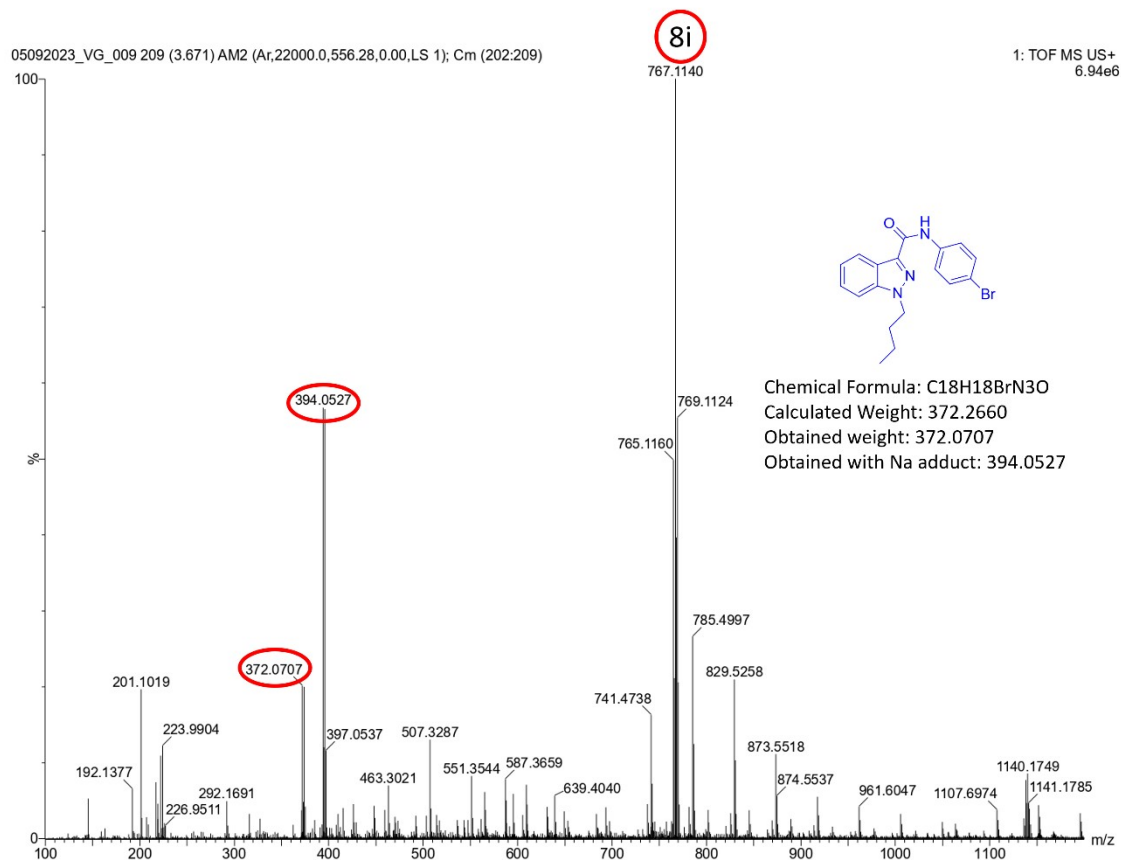
HSQC-NMR [400MHz, DMSO-d₆] spectrum of N-(4-Bromophenyl)-1-butyl-1H-indazole-3-carboxamide (8i).



FT-IR spectrum of N-(4-Bromophenyl)-1-butyl-1H-indazole-3-carboxamide (8i).

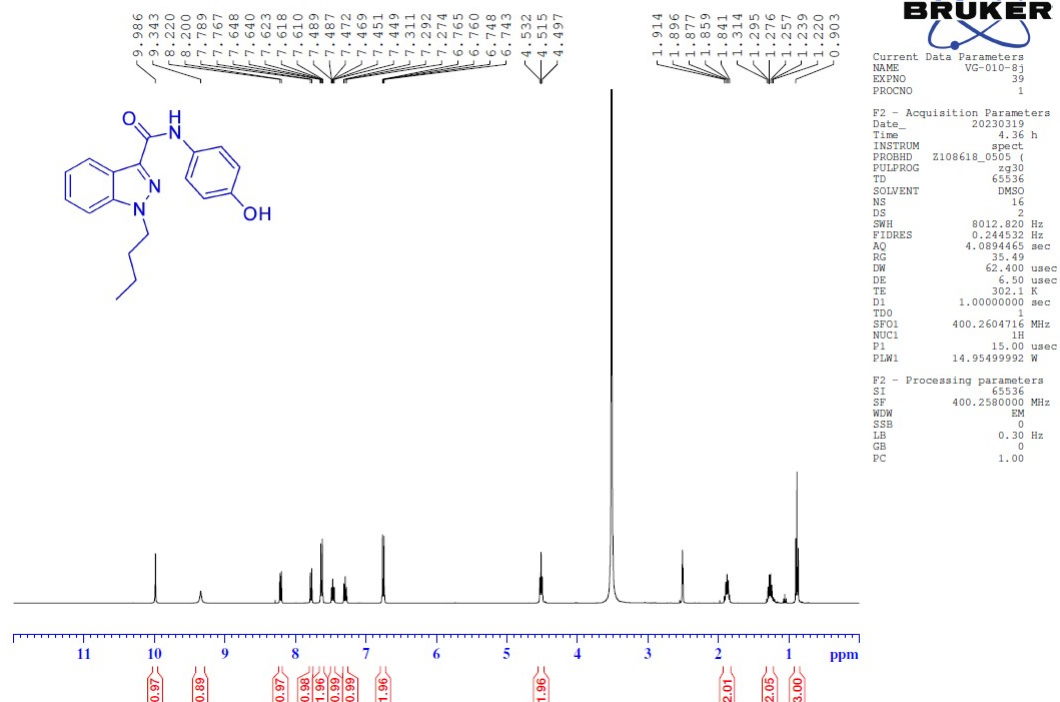


HRMS of N-(4-Bromophenyl)-1-butyl-1H-indazole-3-carboxamide (8i).



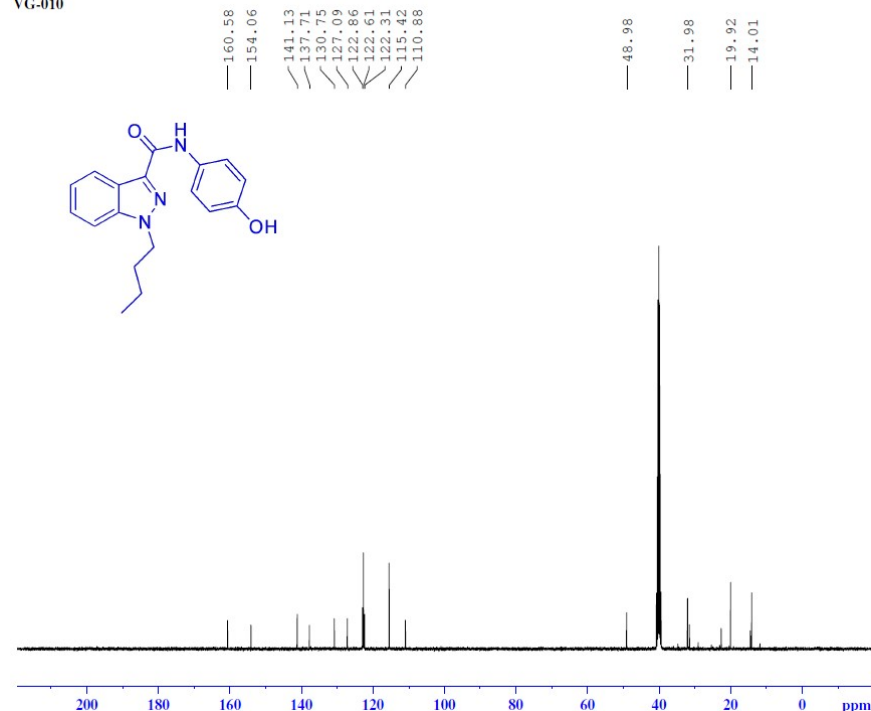
¹H-NMR [400MHz, DMSO-d₆] spectrum of 1-butyl-N-(4-hydroxyphenyl)-1H-indazole-3-carboxamide (8j).

Signature SIF VIT VELLORE
VG-010



¹³C-NMR [100MHz, DMSO-d₆] spectrum of 1-butyl-N-(4-hydroxyphenyl)-1H-indazole-3-carboxamide (8j).

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VG-010



BRUKER

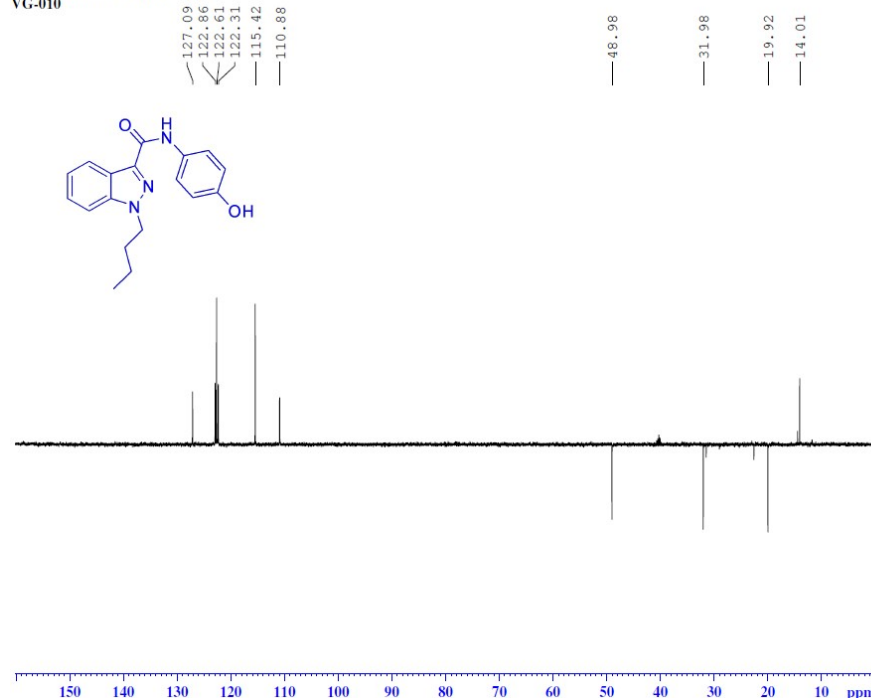
Current Data Parameters
NAME VG-010-8j
EXPNO 44
PROCNO 1

F2 - Acquisition Parameters
Date_ 20221127
Time 0.27 h
INSTRUM spect
PROBHD Z108618_0505 (Z
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 199.6
DW 20.800 usec
DE 6.50 usec
TE 304.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6550186 MHz
NUC1 13C
P1 10.00 usec
PLW1 58.22499847 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 14.95499992 W
PLW12 0.41542000 W
PLW13 0.20895000 W

F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

¹³⁵-DEPT-NMR [100MHz, DMSO-d₆] spectrum of 1-butyl-N-(4-hydroxyphenyl)-1H-indazole-3-carboxamide (8j).

Signature SIF VIT VELLORE
VG-010



BRUKER

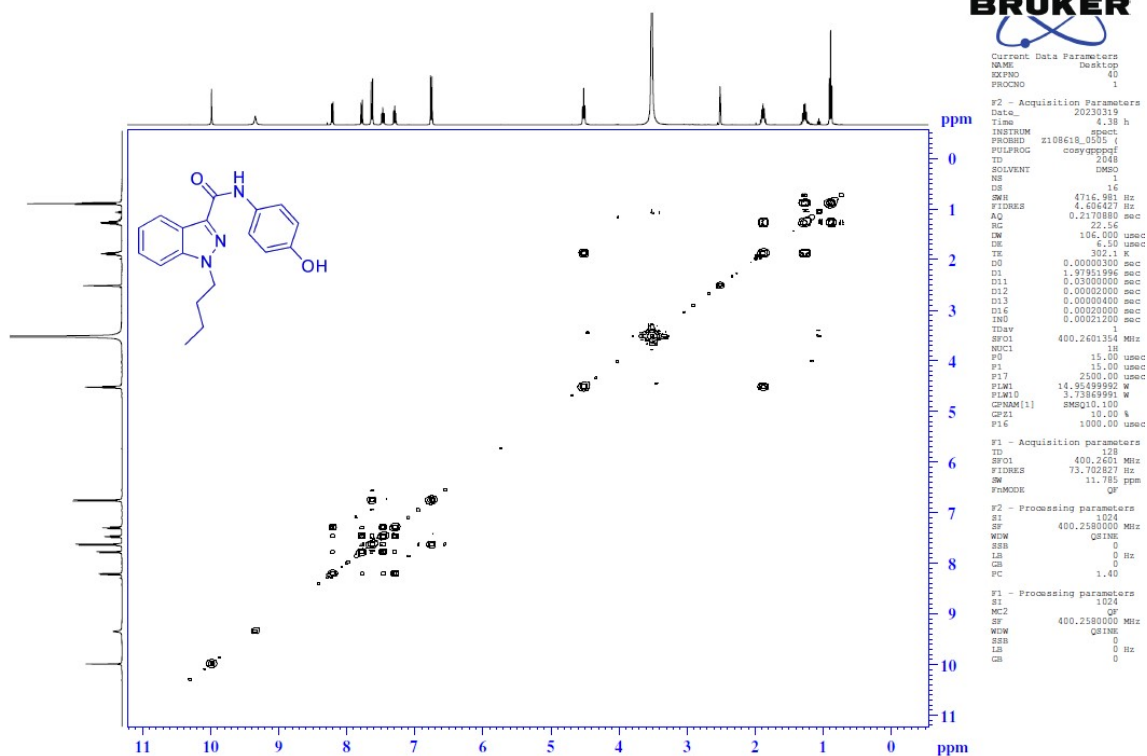
Current Data Parameters
NAME VG-010-8j
EXPNO 45
PROCNO 1

F2 - Acquisition Parameters
Date_ 20221127
Time 0.47 h
INSTRUM spect
PROBHD Z108618_0505 (Z
PULPROG deptap135
TD 65536
SOLVENT DMSO
NS 256
DS 8
SWH 16129.032 Hz
FIDRES 0.492219 Hz
AQ 2.0316160 sec
RG 199.6
DW 31.000 usec
DE 6.50 usec
TE 304.8 K
CNST2 145.0000000
D1 2.00000000 sec
D2 0.0034828 sec
D12 0.00002000 sec
TD0 1
SFO1 100.6530057 MHz
NUC1 13C
P1 10.00 usec
PLW1 58.22499847 W
SPNAM[5] Crp60comp.4
SFOAL5 0.500
SFOAL5 0 Hz
SPW5 8.89610004 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG2 waltz16
P3 15.00 usec
P4 30.00 usec
PCPD2 90.00 usec
PLW2 14.95499992 W
PLW12 0.41542000 W

F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

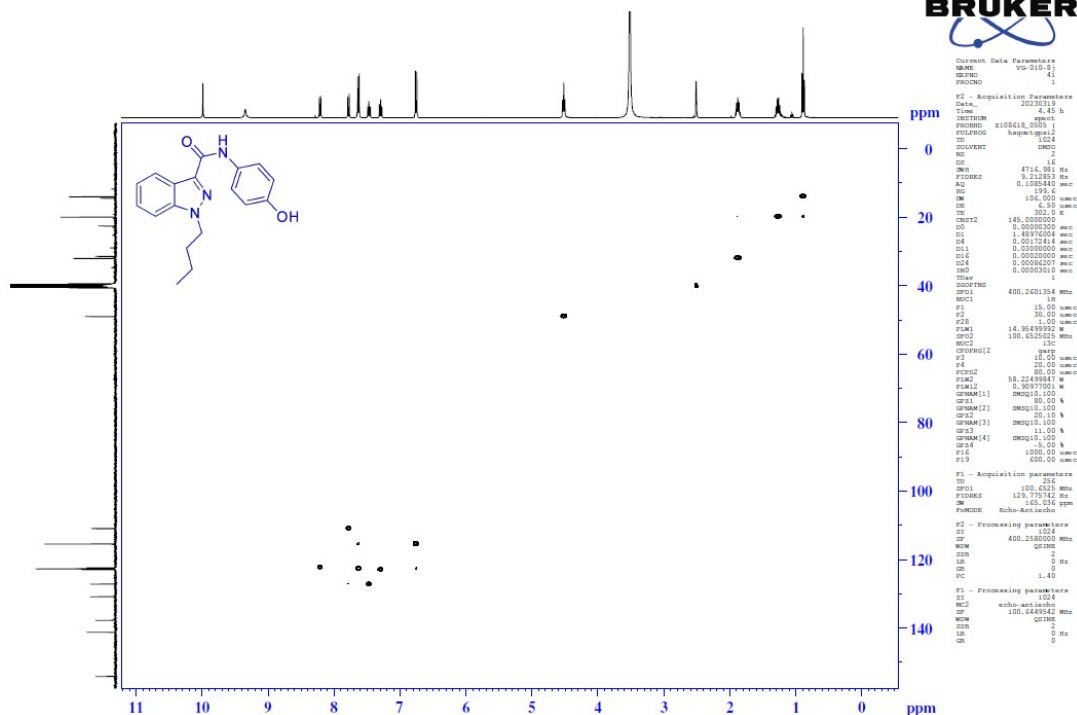
COSY-NMR [400MHz, DMSO-d₆] spectrum of 1-butyl-N-(4-hydroxyphenyl)-1H-indazole-3-carboxamide (8j).

Signature SIF VIT VELLORE
VG-010

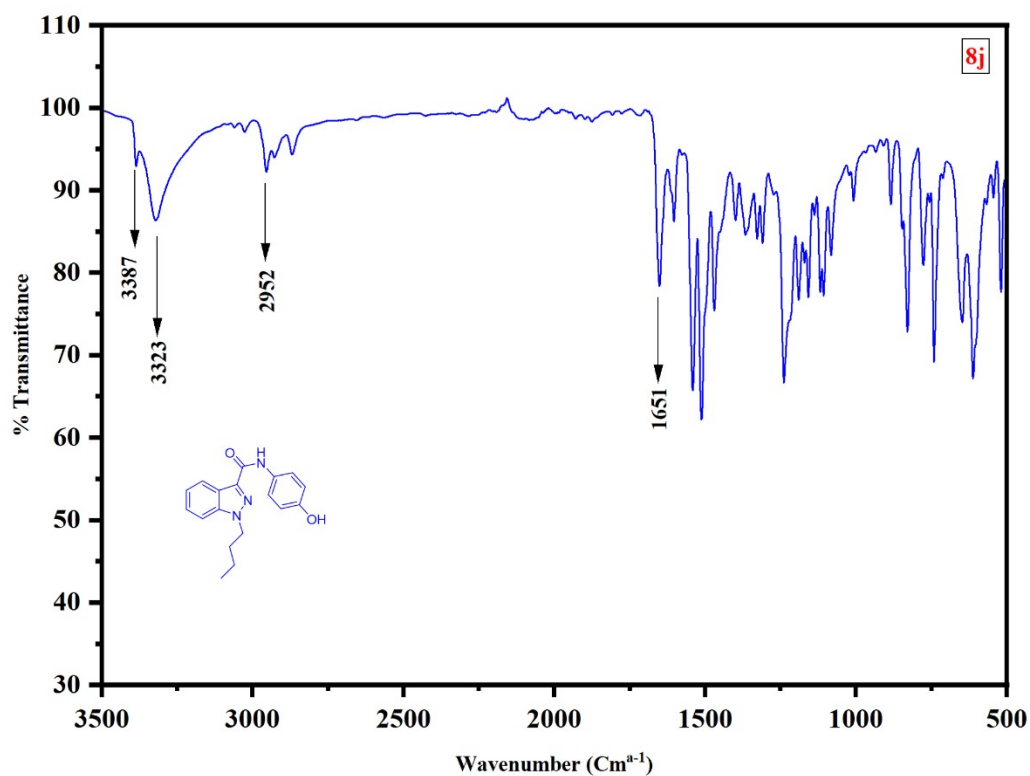


HSQC-NMR [400MHz, DMSO- d_6] spectrum of 1-butyl-N-(4-hydroxyphenyl)-1H-indazole-3-carboxamide (8j).

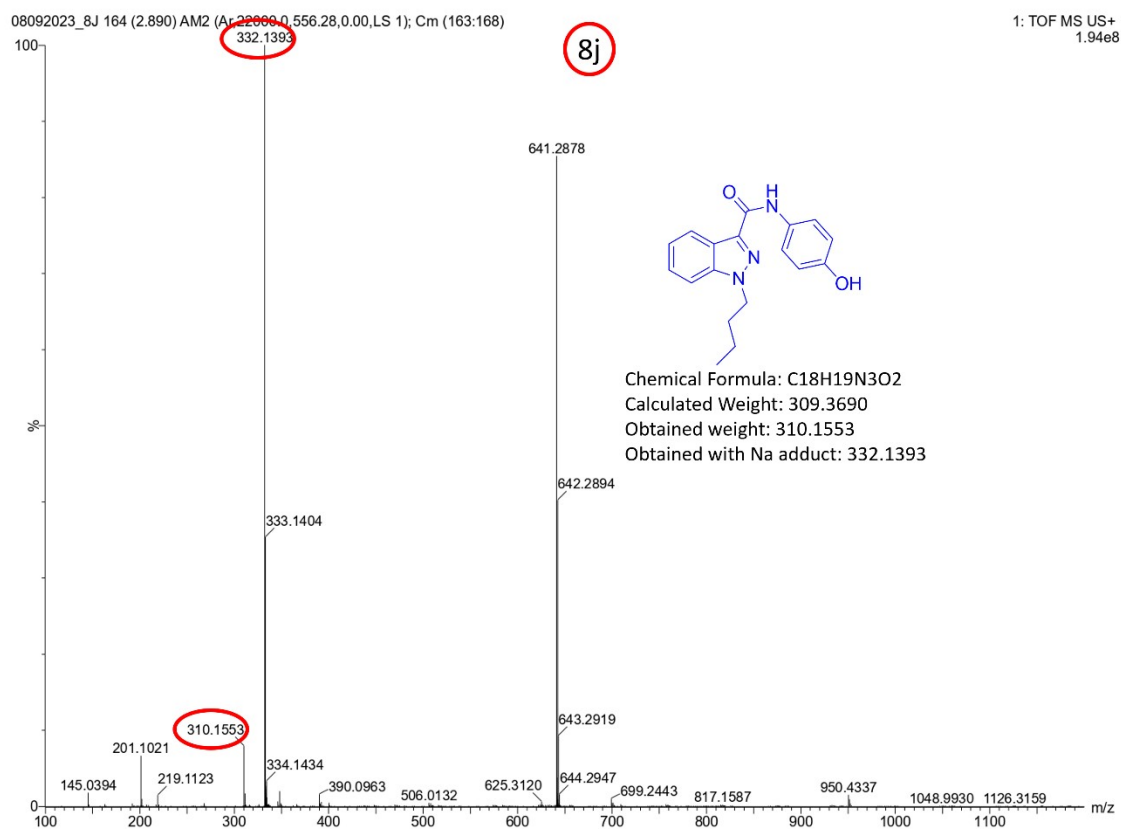
Signature SIF VIT VELLORE
VG-010



FT-IR spectrum of 1-butyl-N-(4-hydroxyphenyl)-1H-indazole-3-carboxamide (8j).

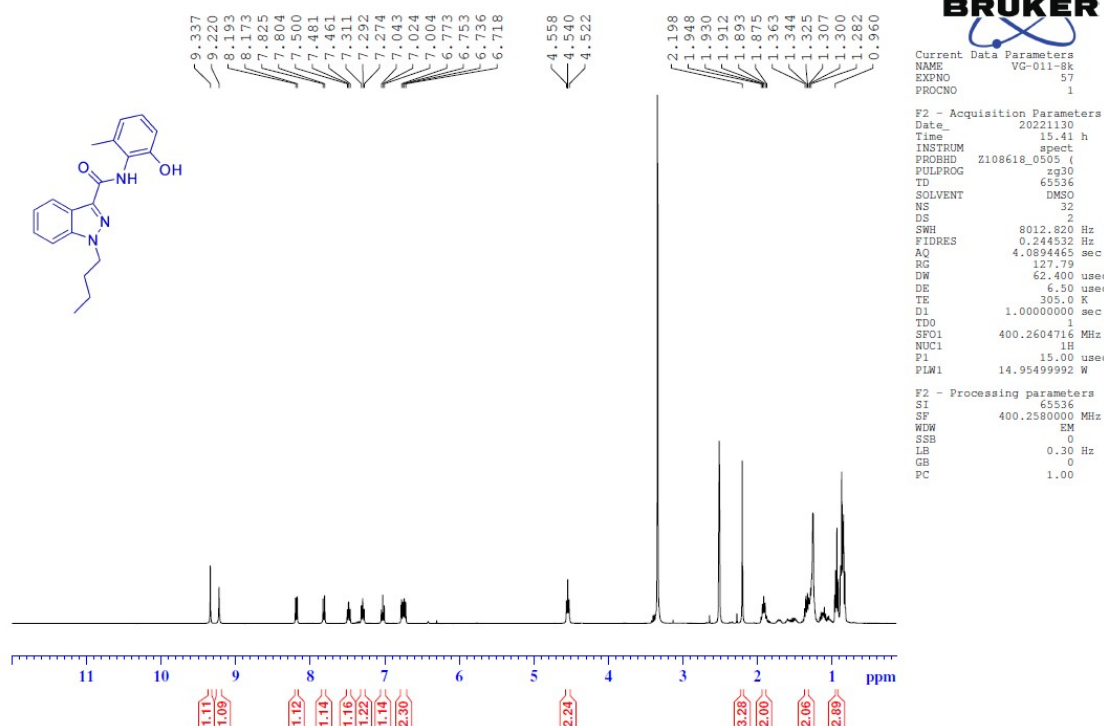


HRMS of 1-butyl-N-(4-hydroxyphenyl)-1H-indazole-3-carboxamide (8j).



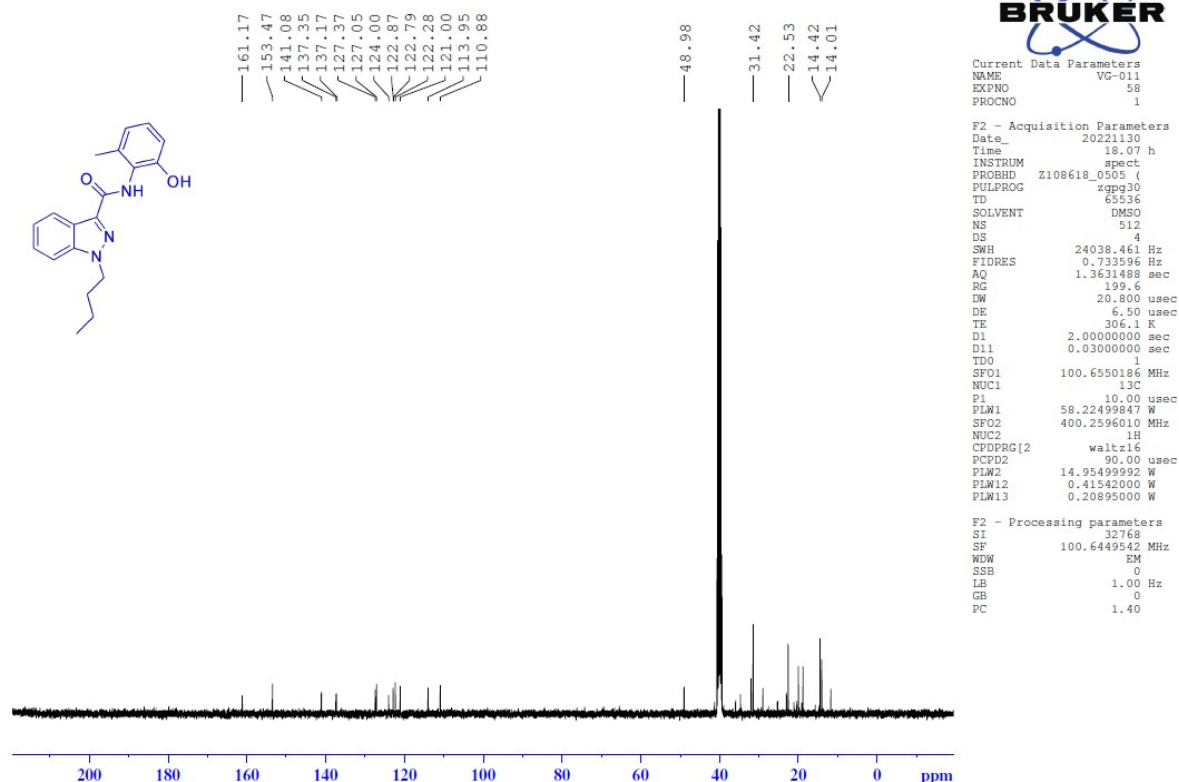
¹H-NMR [400MHz, DMSO-d₆] spectrum of 1-butyl-N-(2-hydroxy-6-methylphenyl)-1H-indazole-3-carboxamide (8k).

Signature SIF VIT VELLORE
VG011



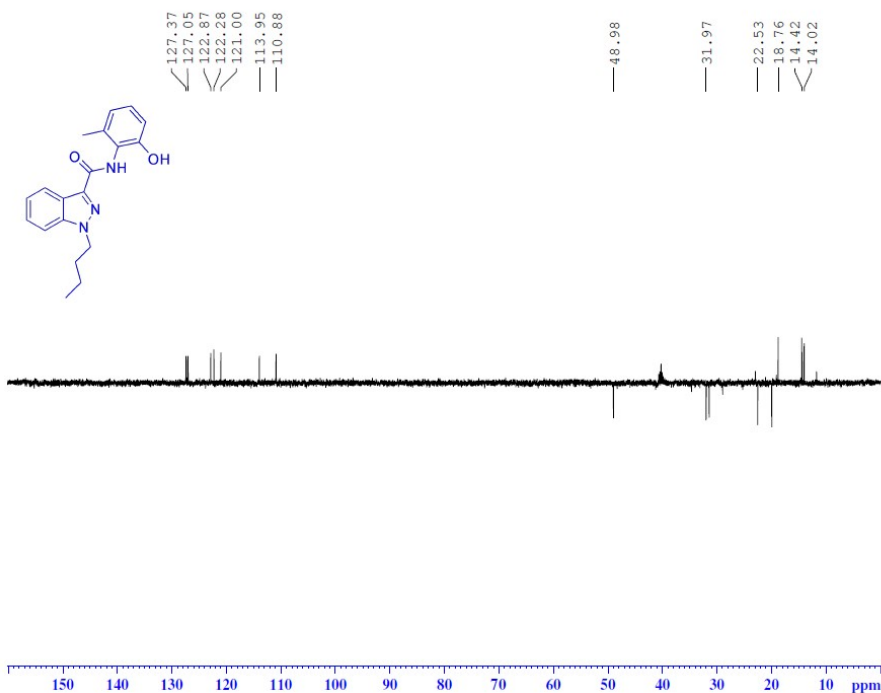
¹³C-NMR [100MHz, DMSO-d₆] spectrum of 1-butyl-N-(2-hydroxy-6-methylphenyl)-1H-indazole-3-carboxamide (8k).

Signature SIF VIT VELLORE
VG011

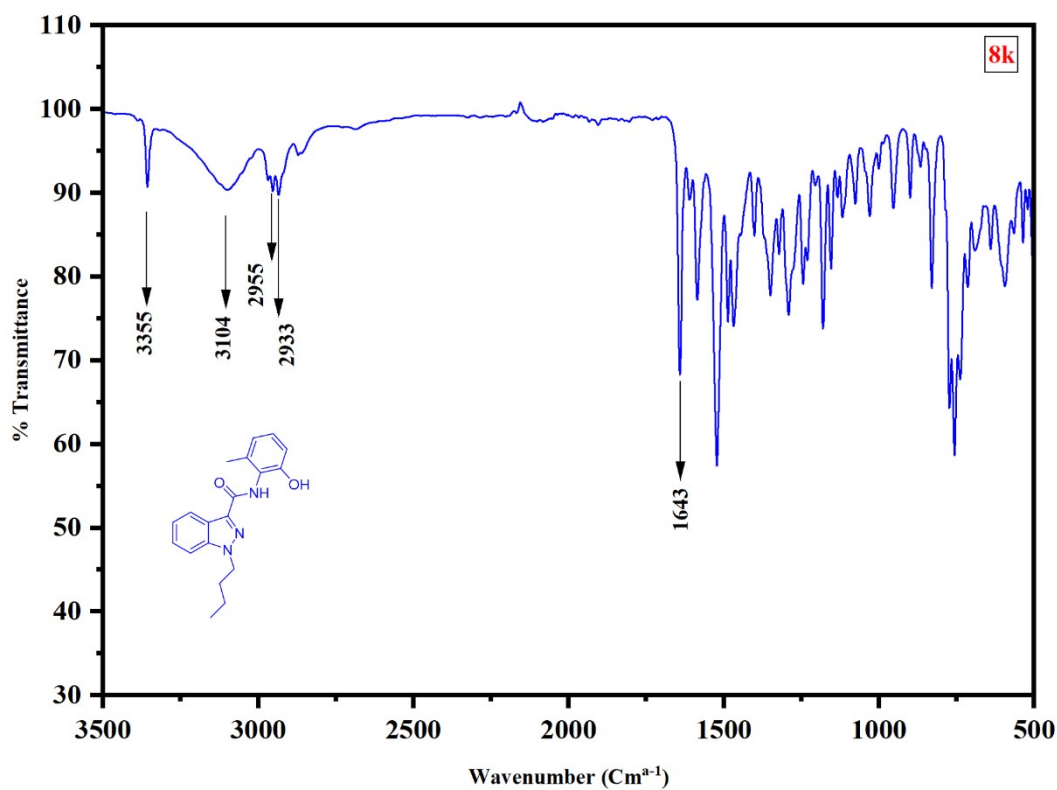


5-DEPT-NMR [100MHz, DMSO-d₆] spectrum of 1-butyl-N-(2-hydroxy-6-methylphenyl)-1H-indazole-3-carboxamide (8k).

Signature SIF VIT VELLORE
VG011



FT-IR spectrum of 1-butyl-N-(2-hydroxy-6-methylphenyl)-1H-indazole-3-carboxamide (8k).

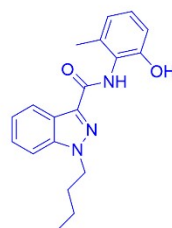
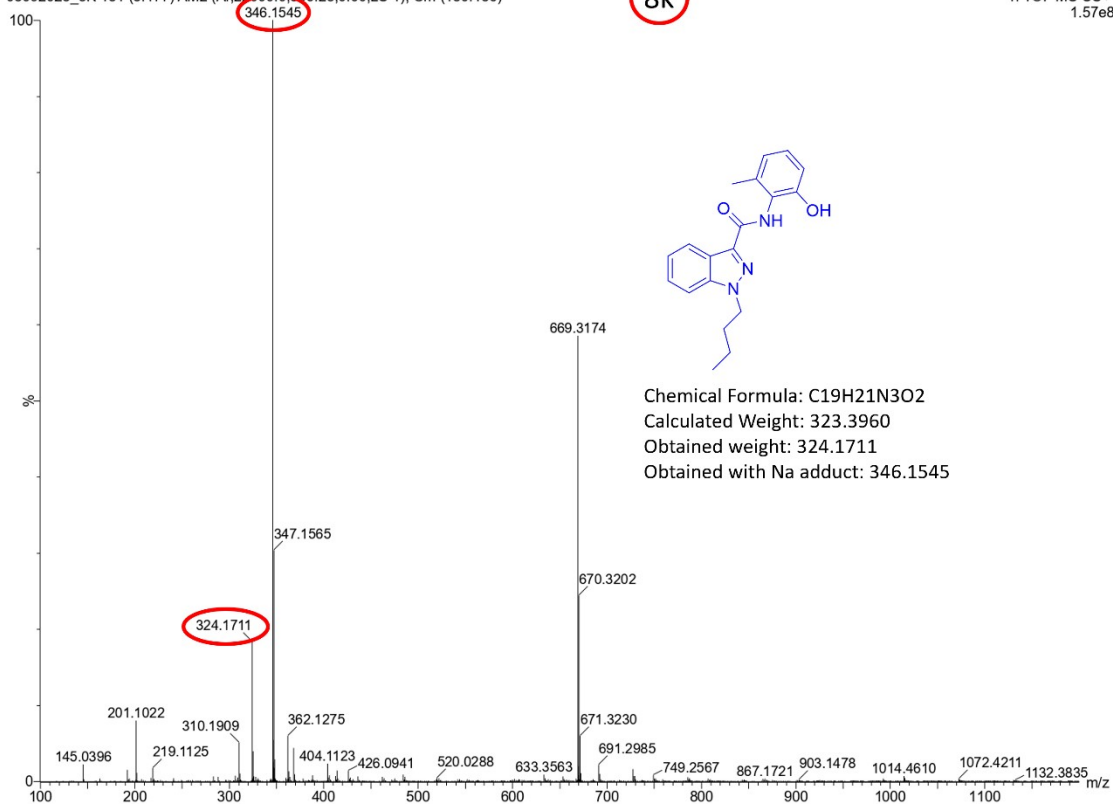


HRMS of 1-butyl-N-(2-hydroxy-6-methylphenyl)-1H-indazole-3-carboxamide (8k).

08092023_8K 181 (3.177) AM2 (Ar.220.66, 0.556.28, 0.00, LS 1); Cm (180:186)

8k

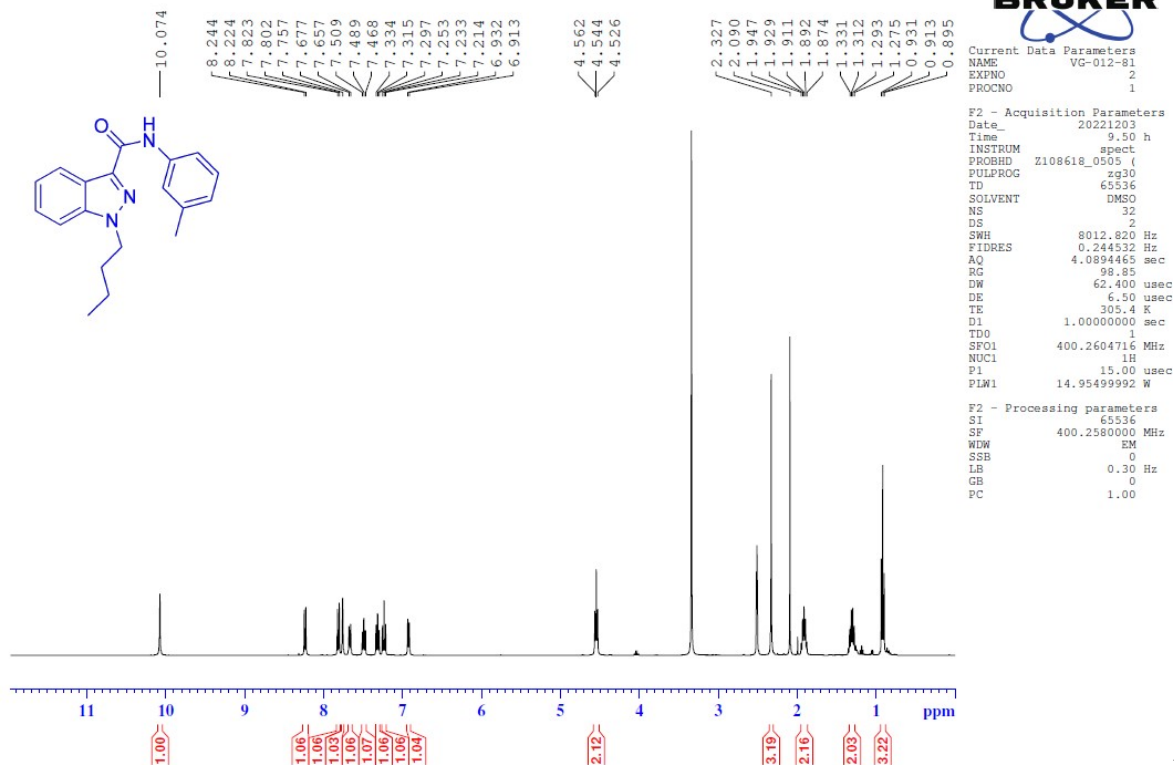
1: TOF MS US+
1.57e8



Chemical Formula: C₁₉H₂₁N₃O₂
Calculated Weight: 323.3960
Obtained weight: 324.1711
Obtained with Na adduct: 346.1545

¹H-NMR [400MHz, DMSO-d₆] spectrum of 1-butyl-N-(m-tolyl)-1H-indazole-3-carboxamide (8l).

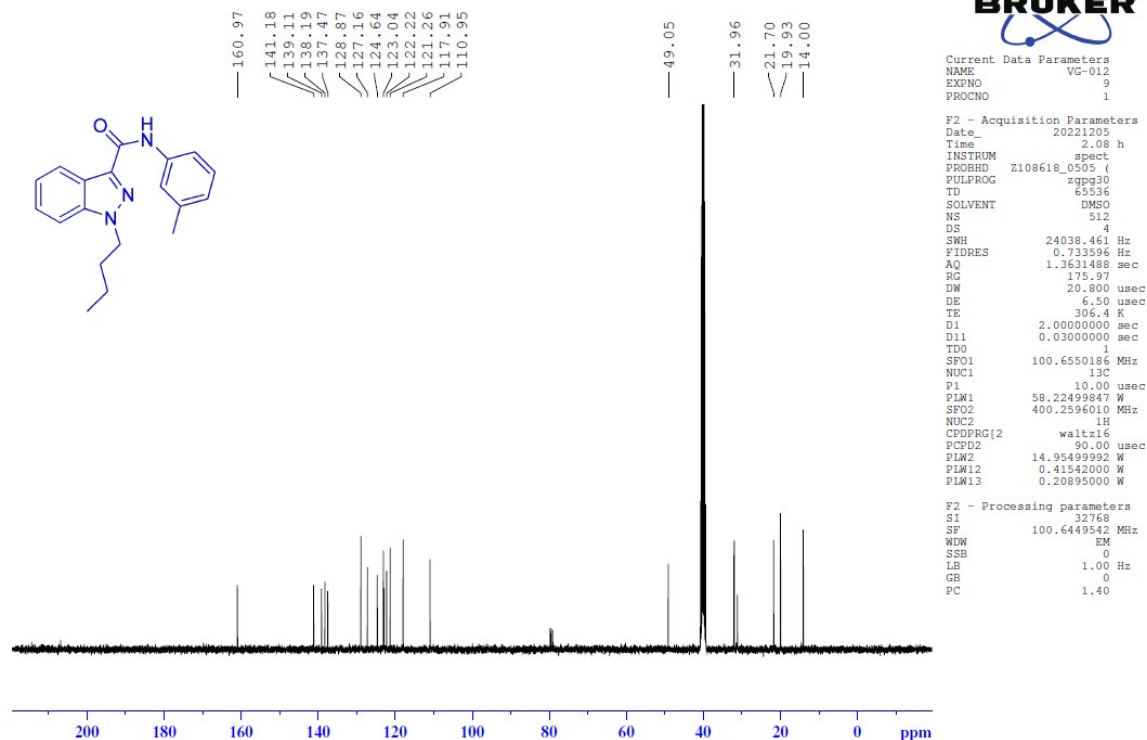
Signature SIF VIT VELLORE
VG012



¹³C

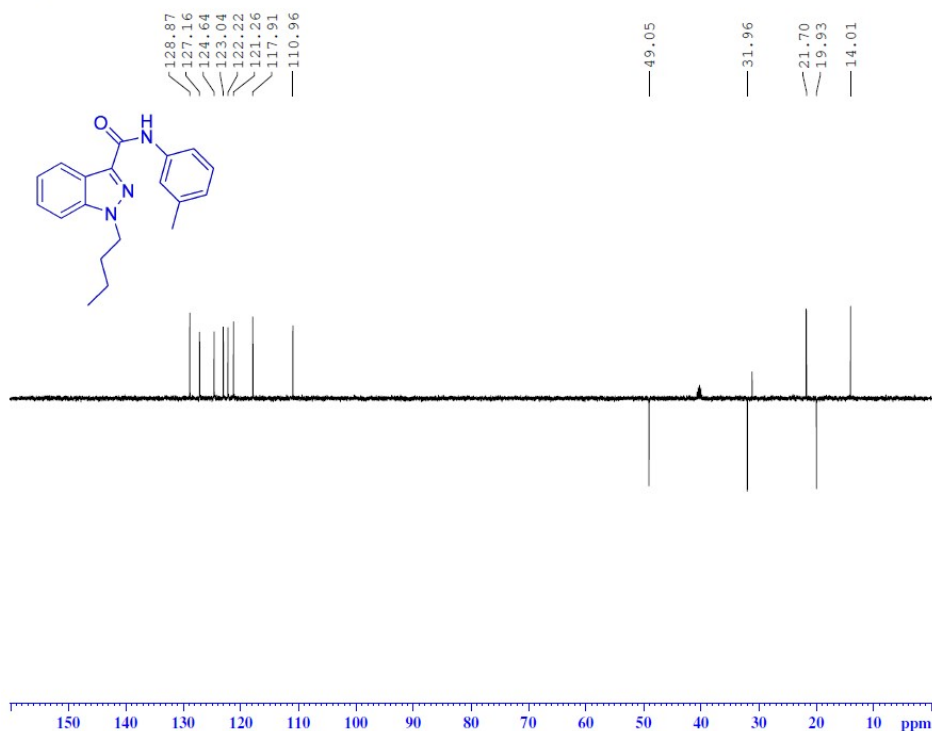
¹³C-NMR [100MHz, DMSO-d₆] spectrum of 1-butyl-N-(m-tolyl)-1H-indazole-3-carboxamide (8l).

Signature SIF VIT VELLORE
VG012



¹³⁵-DEPT-NMR [100MHz, DMSO-d₆] spectrum of 1-butyl-N-(m-tolyl)-1H-indazole-3-carboxamide (8l).

Signature SIF VIT VELLORE
VG-012



Current Data Parameters
NAME VG-012
EXPNO 10
PROCNO 1

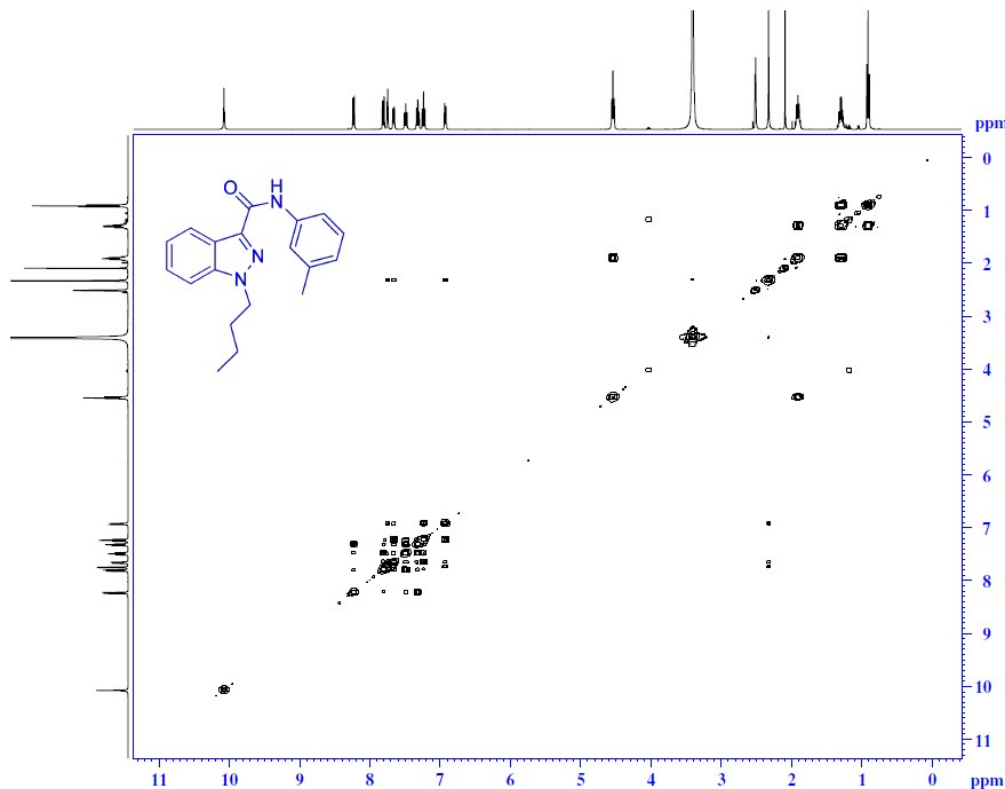
F2 - Acquisition Parameters
Date_ 20221205
Time 2.27 h
INSTRUM spect
PROBHD z108618_0505 (deptapl35
PULPROG deptapl35
TD 65536
SOLVENT DMSO
NS 256
DS 8
SWH 16129.032 Hz
FIDRES 0.492219 Hz
AQ 2.0316160 sec
RG 199.6
DW 31.000 usec
DE 6.50 usec
TE 306.1 K
CNS12 145.0000000
D1 2.000000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1
SFO1 100.6530057 MHz
NUC1 13C
P1 10.00 usec
P13 2000.00 usec
PLW0 0 W
PLW1 58.22499847 W
SPNAM[5] Crp60comp.4
SFOAL5 0.500
SPOFFS5 0 Hz
SPW5 8.89610004 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG[2] waltz16
P3 15.00 usec
P4 30.00 usec
PCPD2 90.00 usec
PLW2 14.95499992 W
PLW12 0.41542000 W

F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

COSY-

NMR [400MHz, DMSO-d₆] spectrum of 1-butyl-N-(m-tolyl)-1H-indazole-3-carboxamide (8l).

Signature SIF VIT VELLORE
VG-012



Current Data Parameters
NAME VG-012-81
EXPNO 5
PROCNO 1

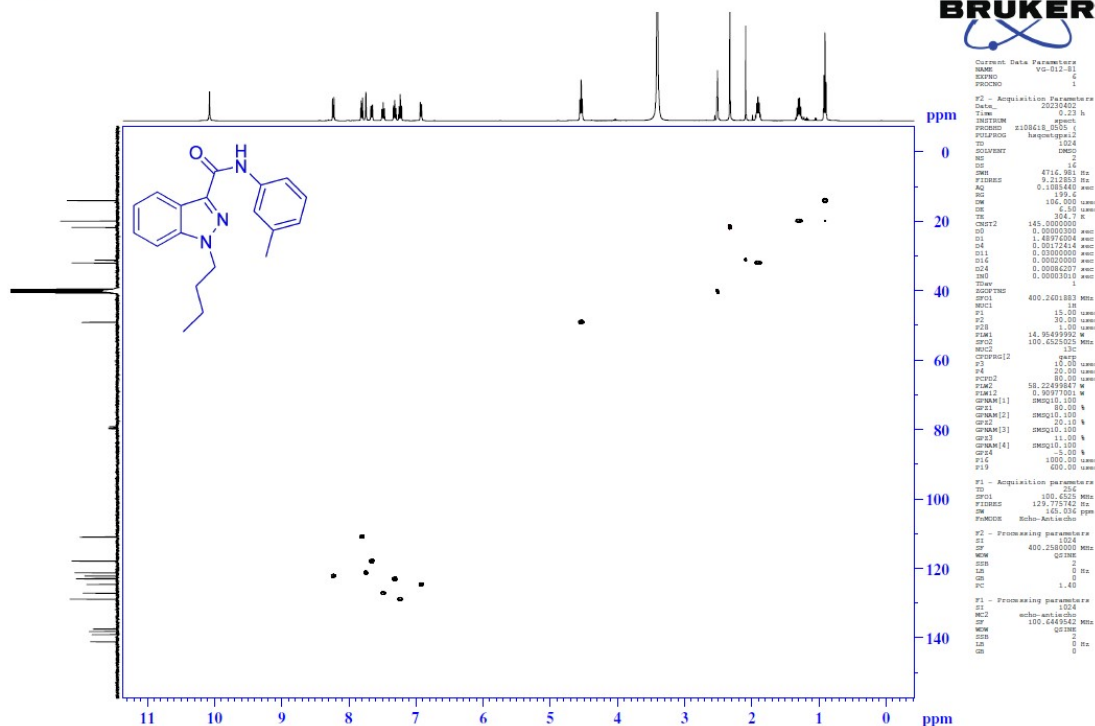
F2 - Acquisition Parameters
Date_ 20230402
Time 0.17 h
INSTRUM spect
PROBHD z108618_0505 (cosypppqr
PULPROG cosypppqr
TD 2148
SOLVENT DMSO
NS 16
DS 16
SWH 4716.981 Hz
FIDRES 4.606427 Hz
AQ 0.2170880 sec
RG 48.98
DW 106.300 usec
DE 6.50 usec
TE 304.6 K
D0 0.00000300 sec
D1 1.97951996 sec
D11 0.03000000 sec
D12 0.00002000 sec
D13 0.00000400 sec
D16 0.00020000 sec
TDW 1
SFO1 400.2601883 MHz
NUC1 1H
P0 15.00 usec
P1 15.00 usec
P17 2000.00 usec
PLW1 14.95499992 W
PLW10 3.73869991 W
CPHAM[1] SMOG10.100
GP1 10.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SFO1 400.2602 MHz
FIDRES 73.702827 Hz
SW 11.785 ppm
FNM000 QF

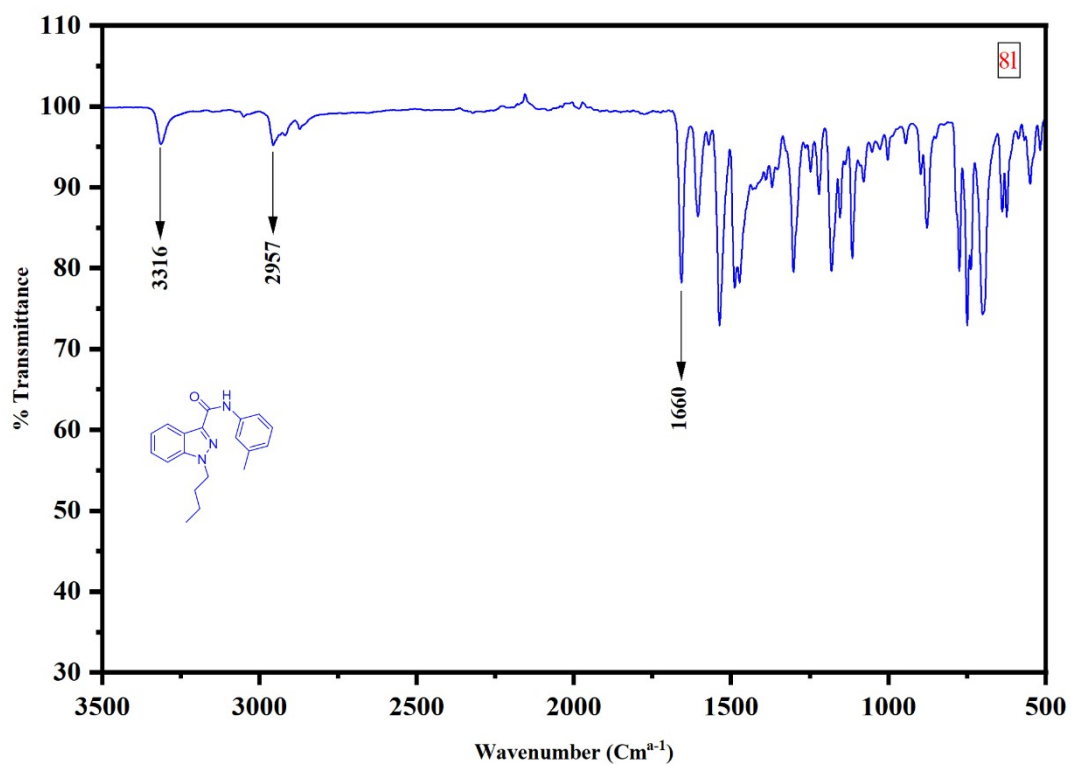
F2 - Processing parameters
SI 1024
SF 400.2580000 MHz
WDW QF16
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 400.2580000 MHz
WDW QF16
SSB 0
LB 0 Hz
GB 0

HSQC-NMR [400MHz, DMSO-d₆] spectrum of 1-butyl-N-(m-tolyl)-1H-indazole-3-carboxamide (8l).



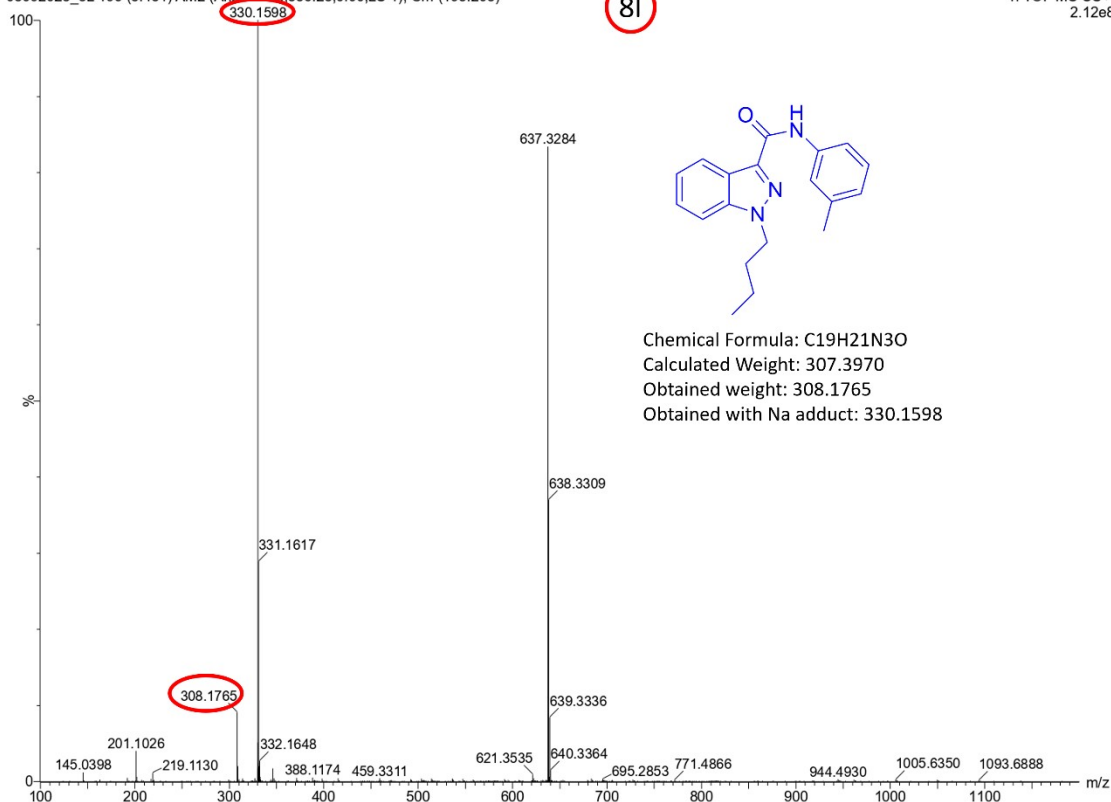
FT-IR spectrum of 1-butyl-N-(m-tolyl)-1H-indazole-3-carboxamide (8l).



HRMS of 1-butyl-N-(m-tolyl)-1H-indazole-3-carboxamide (8l).

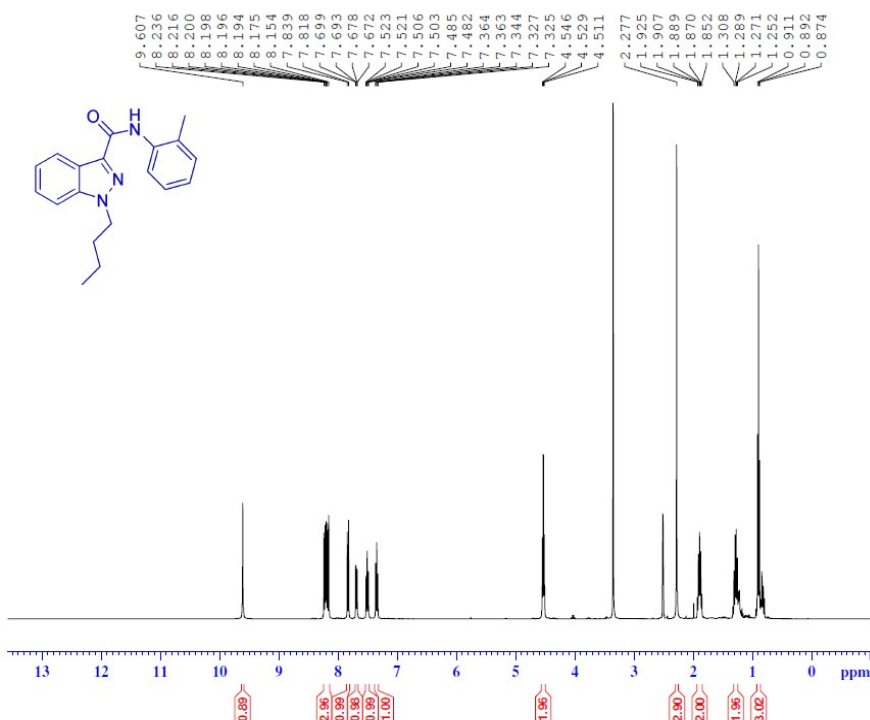
08092023_8L 196 (3.451) AM2 (Ar 22000,0.556.28,0.00,LS 1); Cm (195:203)

1: TOF MS US+
2.12e8



¹H-NMR [400MHz, DMSO-d₆] spectrum of 1-butyl-N-(4-tolyl)-1H-indazole-3-carboxamide (8m).

Signature SIF VIT VELLORE
VG-013



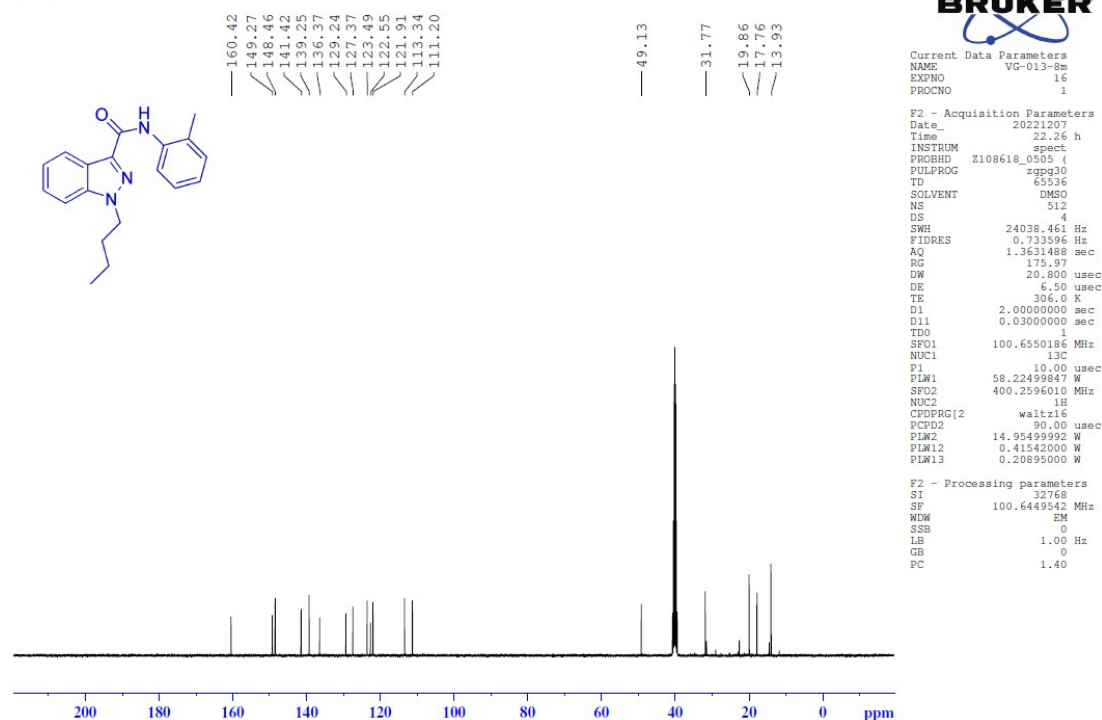
Current Data Parameters
NAME VG-013-8m
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20221205
Time 11.39 h
INSTRUM spect
PROBHD Z108618_0505 (zg30)
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 77.73
DW 62.400 usec
DE 6.50 usec
TE 305.2 K
D1 1.00000000 sec
TDO 1
SFO1 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PLW1 14.95499992 W

F2 - Processing parameters
SI 65536
SF 400.2580000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

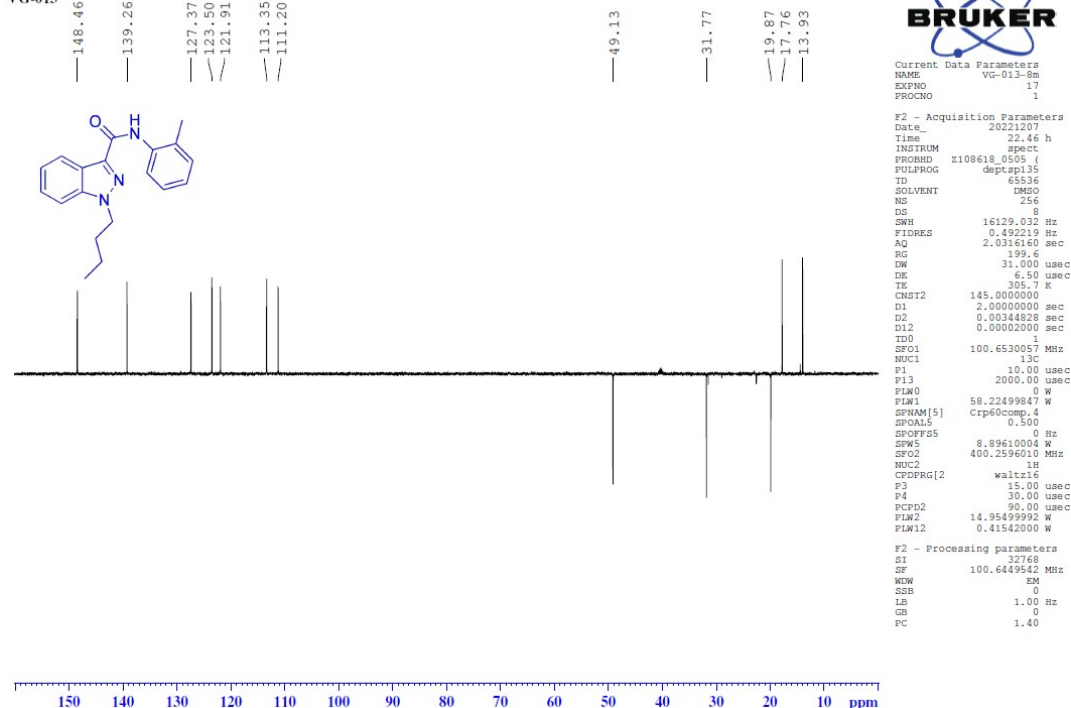
¹³C-NMR [100MHz, DMSO-d₆] spectrum of 1-butyl-N-(o-tolyl)-1H-indazole-3-carboxamide (8m).

Signature SIF VIT VELLORE
VG-013

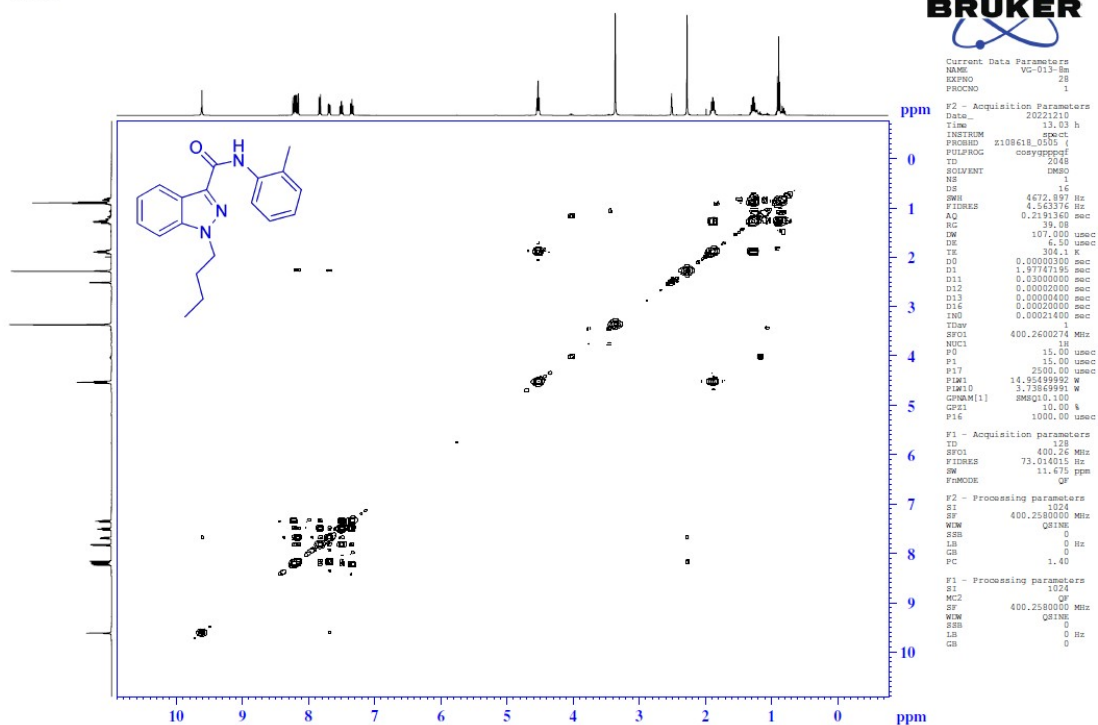


¹³⁵-DEPT-NMR [100MHz, DMSO-d₆] spectrum of 1-butyl-N-(o-tolyl)-1H-indazole-3-carboxamide (8m).

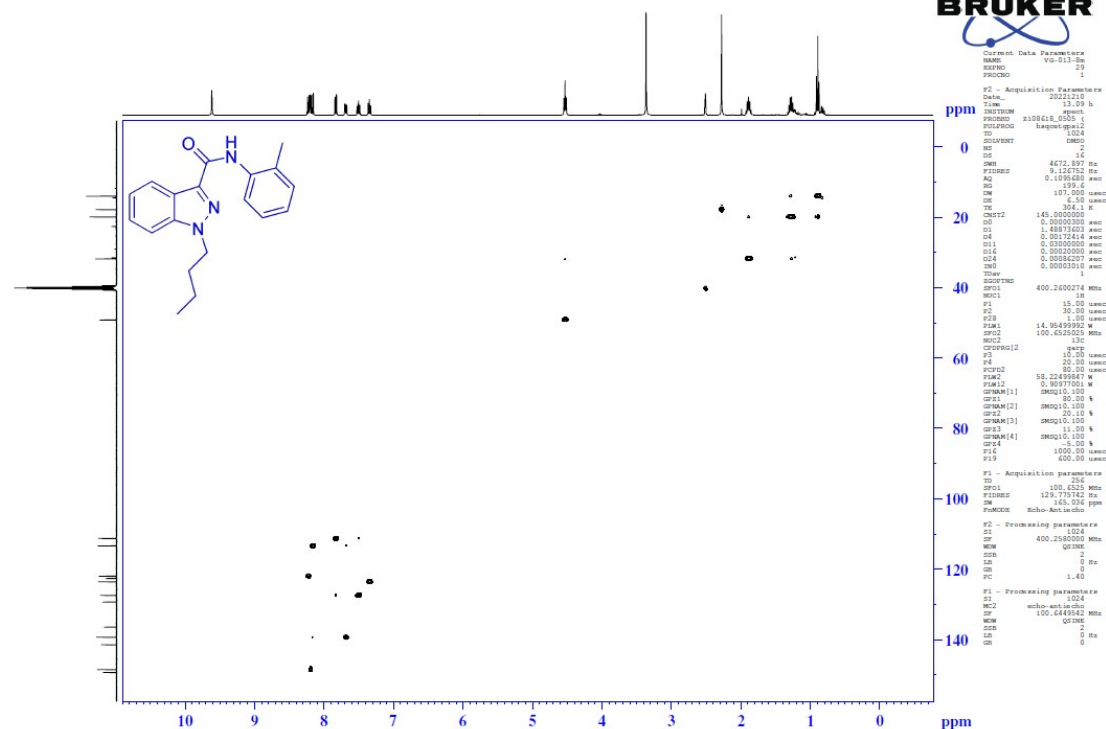
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VG-013



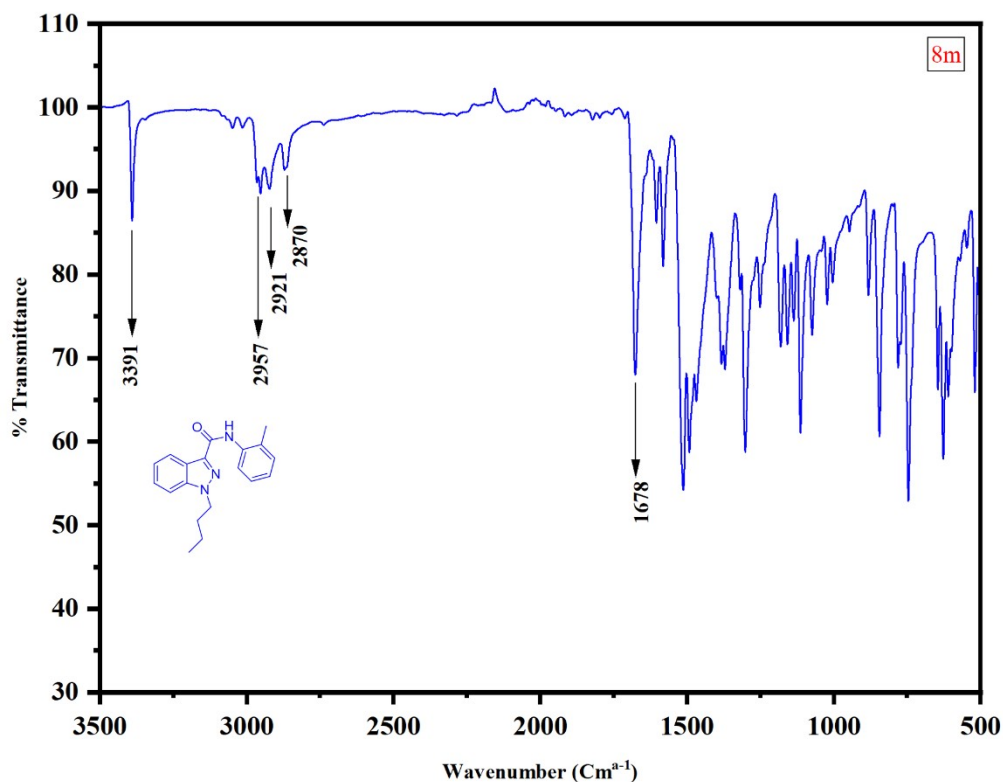
COSY-NMR [400MHz, DMSO-d₆] spectrum of 1-butyl-N-(o-tolyl)-1H-indazole-3-carboxamide (8m).



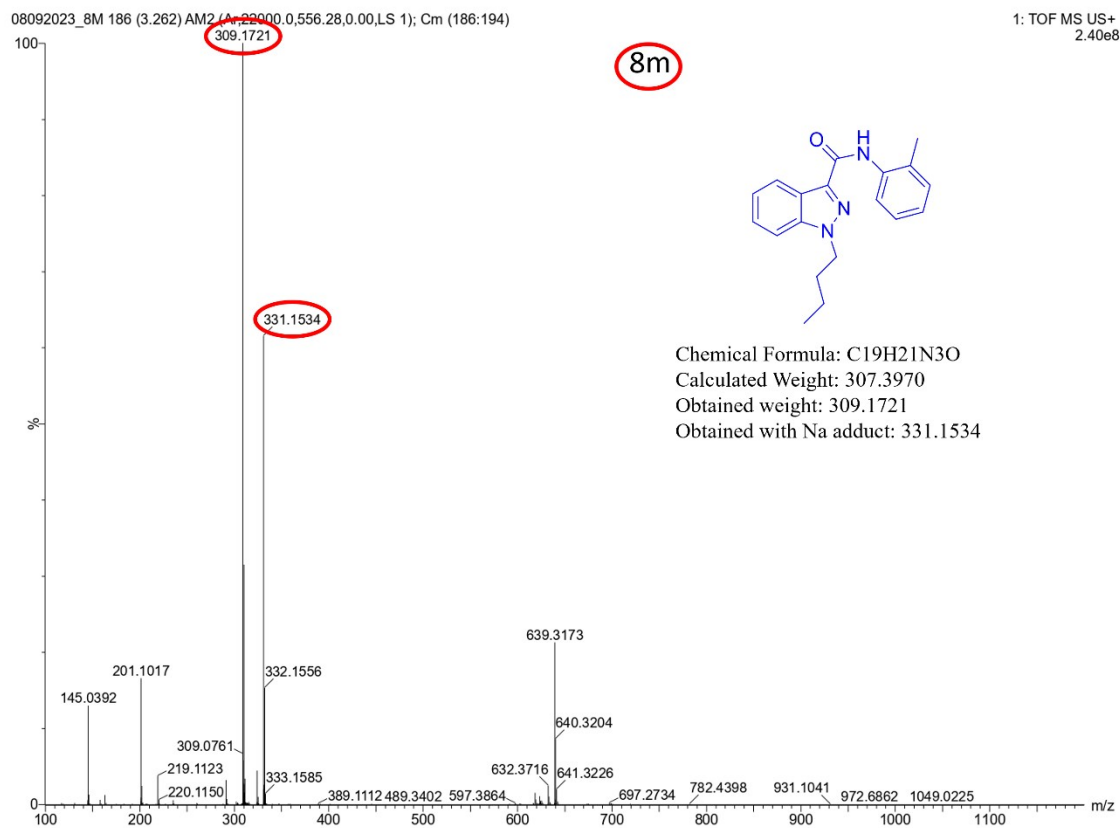
HSQC-NMR [400MHz, DMSO-d₆] spectrum of 1-butyl-N-(o-tolyl)-1H-indazole-3-carboxamide (8m).



FT-IR spectrum of 1-butyl-N-(o-tolyl)-1H-indazole-3-carboxamide (8m).

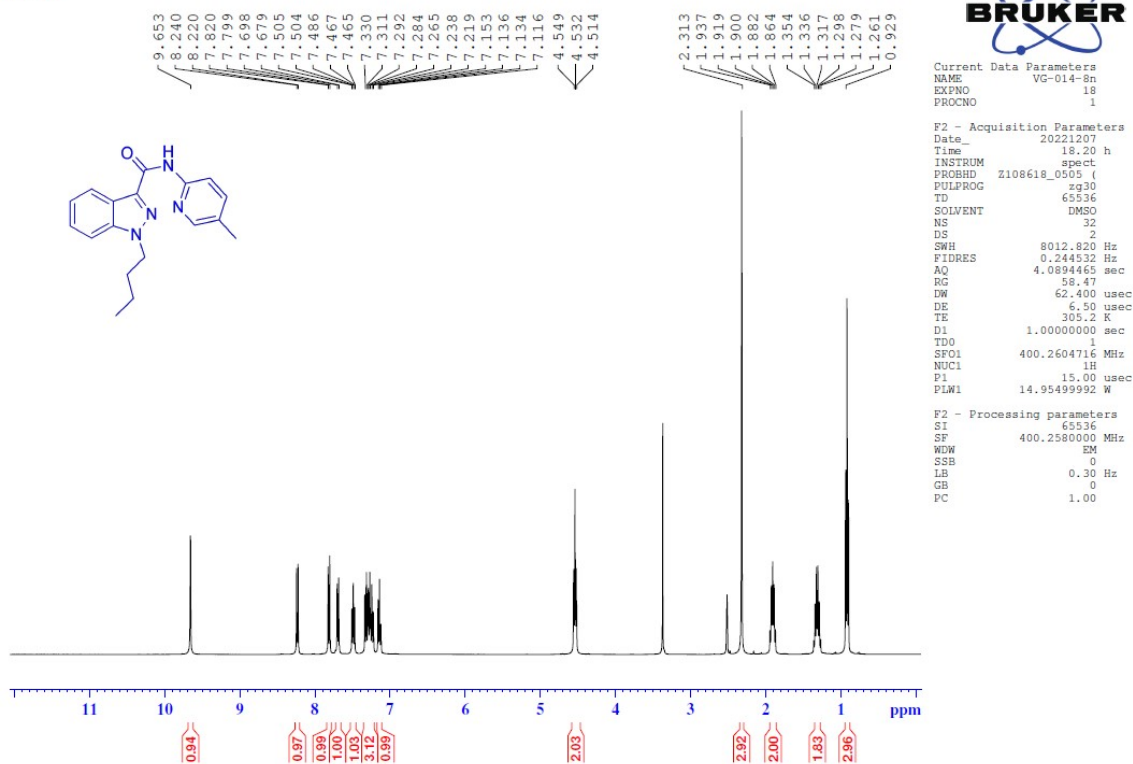


HRMS of 1-butyl-N-(o-tolyl)-1H-indazole-3-carboxamide (8m).



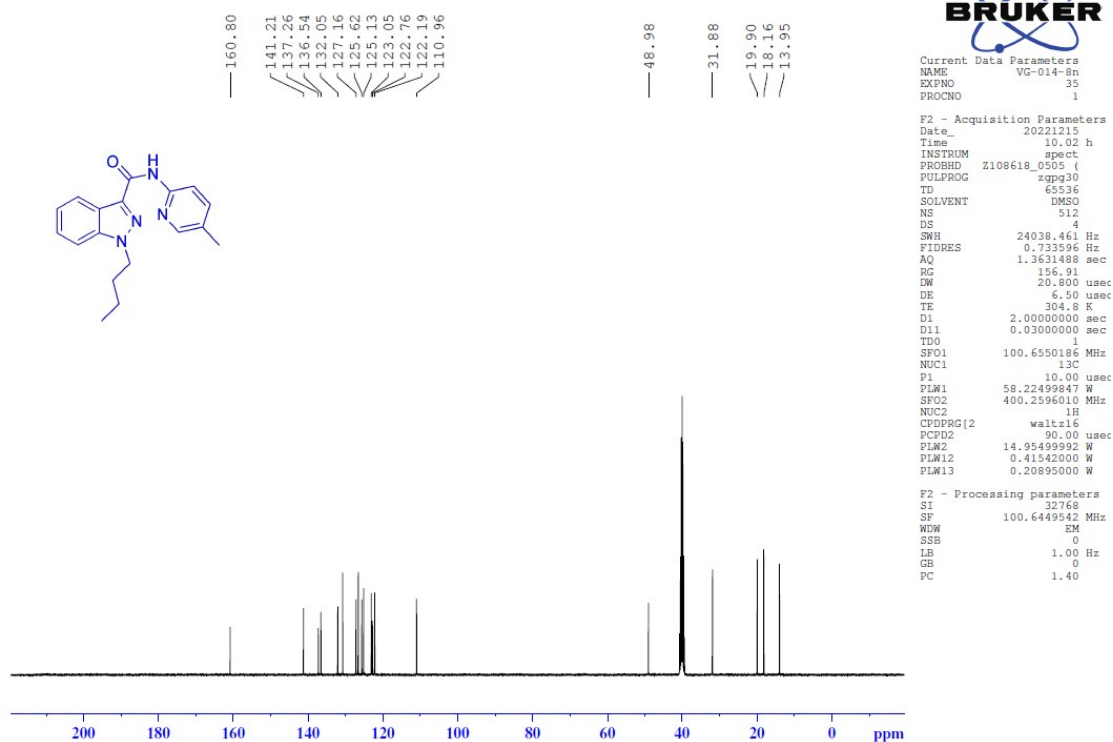
¹H-NMR [400MHz, DMSO-d₆] spectrum of 1-butyl-N-(5-methylpyridin-2-yl)-1H-indazole-3-carboxamide (8n).

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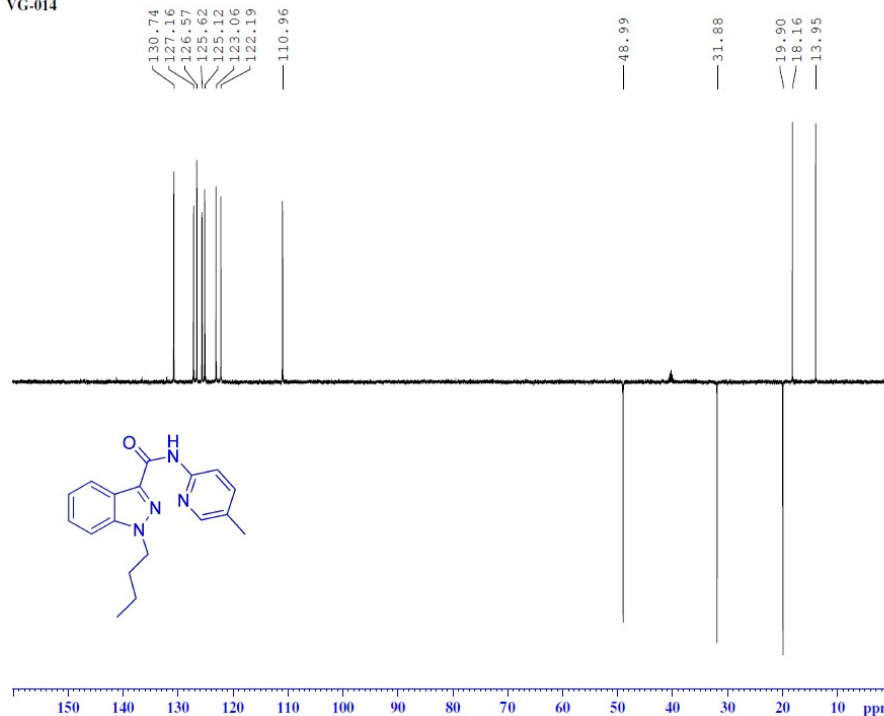
¹³C-NMR [100MHz, DMSO-d₆] spectrum of 1-butyl-N-(5-methylpyridin-2-yl)-1H-indazole-3-carboxamide (8n).

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¹³⁵DEPT-NMR [100MHz, DMSO-d₆] spectrum of 1-butyl-N-(5-methylpyridin-2-yl)-1H-indazole-3-carboxamide (8n).

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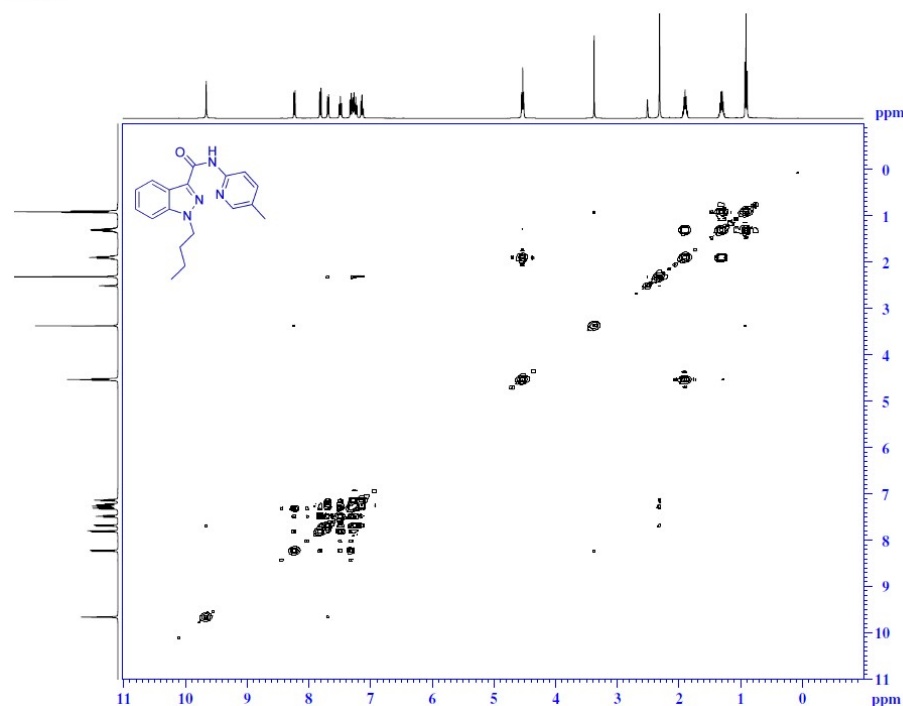
Current Data Parameters
NAME VG-014-8n
EXPNO 34
PROCNO 1

F2 - Acquisition Parameters
Date_ 20221214
Time 18.51 h
INSTRUM spect
PROBHD Z108618.0505 (f
PULPROG deptapi35
TD 65536
SOLVENT DMSO
NS 256
DS 8
SWH 16129.032 Hz
FIDRES 0.492219 Hz
AQ 2.0316160 sec
RG 199.6
DW 31.000 usec
DE 6.50 usec
TE 305.0 K
CNS12 145.000000
D1 2.0000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1
SFO1 100.630057 MHz
NUC1 13C
P1 10.00 usec
P13 2000.00 usec
PLW0 58.22499847 W
SPINAM[5] Crp60comp.4
SPCAL5 0.500
SPOFFAS 0 Hz
SPW5 8.89610004 W
SFO2 400.259610 MHz
NUC2 1H
CPDPRG[2] waltz16
P3 15.00 usec
P4 30.00 usec
PCPD2 90.00 usec
PLW2 14.95499992 W
PLW12 0.41542000 W

F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

COSY-NMR [400MHz, DMSO-d₆] spectrum of 1-butyl-N-(5-methylpyridin-2-yl)-1H-indazole-3-carboxamide (8n).

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VG-014



Current Data Parameters
NAME VG-014-8n
EXPNO 25
PROCNO 1

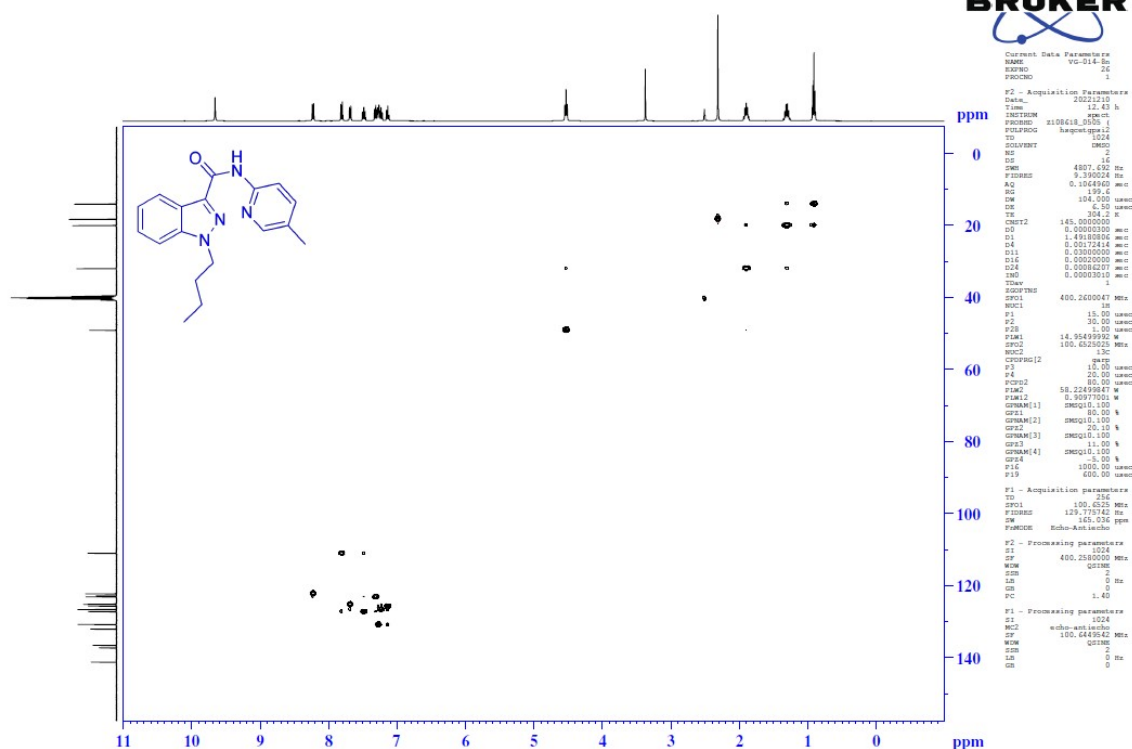
F2 - Acquisition Parameters
Date_ 20221210
Time 12.36 h
INSTRUM spect
PROBHD z108618.0105 (f
PULPROG cosyppgpgf
TD 3248
SOLVENT DMSO
NS 1
DS 16
SWH 4807.492 Hz
FIDRES 4.65013 Hz
AQ 0.2129920 sec
RG 25.67
DW 104.000 usec
DE 6.50 usec
TE 304.2 K
CNS12 0.0000300 sec
D1 1.98361599 sec
D11 0.03000000 sec
D12 0.00002000 sec
D13 0.00000400 sec
D16 0.00020000 sec
D18 0.00020800 sec
TD0 1
SFO1 400.2600047 MHz
NUC1 13C
P0 15.00 usec
P1 15.00 usec
P17 2500.00 usec
PLW1 14.95499992 W
PLW10 3.73849991 W
CPHAM[1] SMOG10.100
CPH1 10.00 W
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SFO1 400.26 MHz
FIDRES 75.120193 Hz
SW 12.011 ppm
F2MODE QF

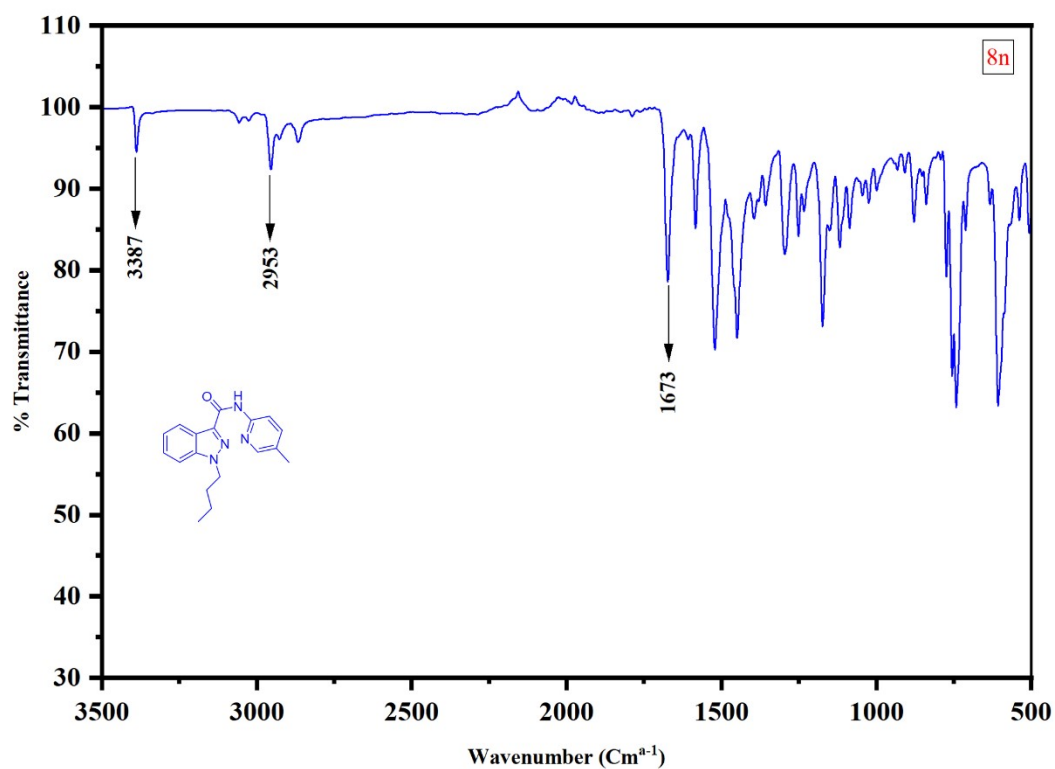
F2 - Processing parameters
SI 1024
SF 400.2580000 MHz
WDW Q8136
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 400.2580000 MHz
WDW Q8136
SSB 0
LB 0 Hz
GB 0

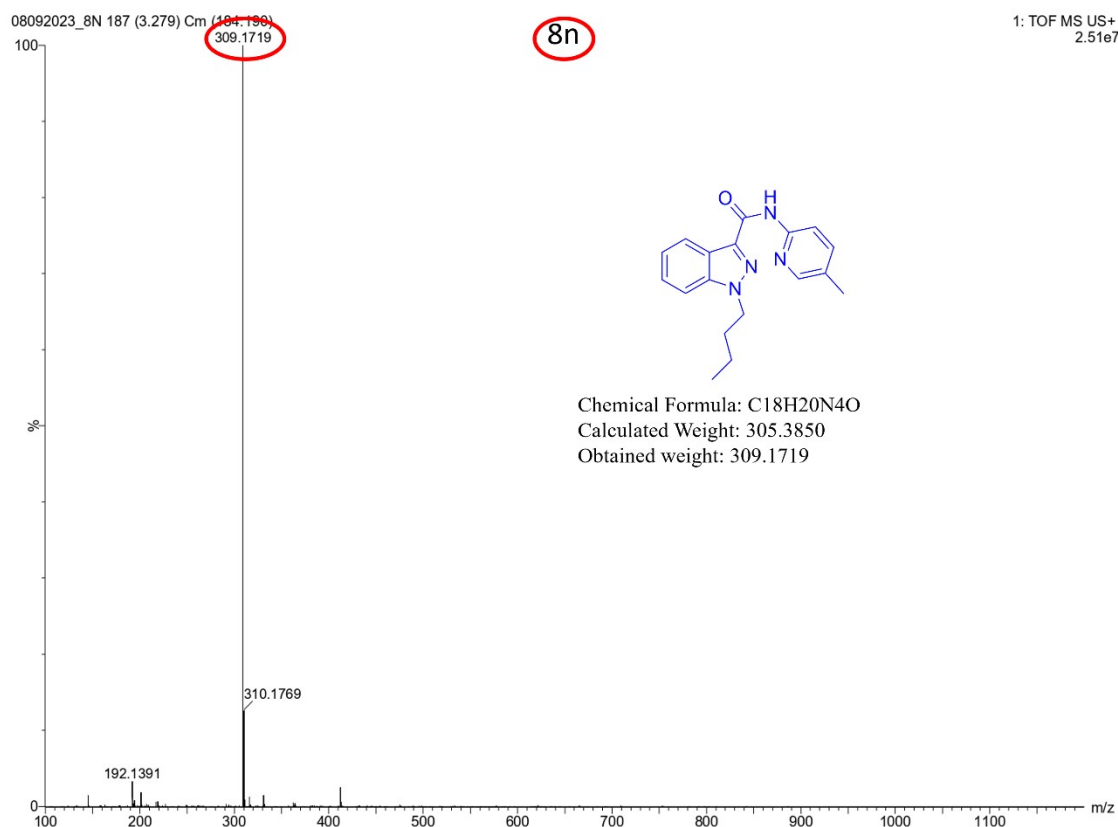
HSQC-NMR [400MHz, DMSO-d₆] spectrum of 1-butyl-N-(5-methylpyridin-2-yl)-1H-indazole-3-carboxamide (8n).



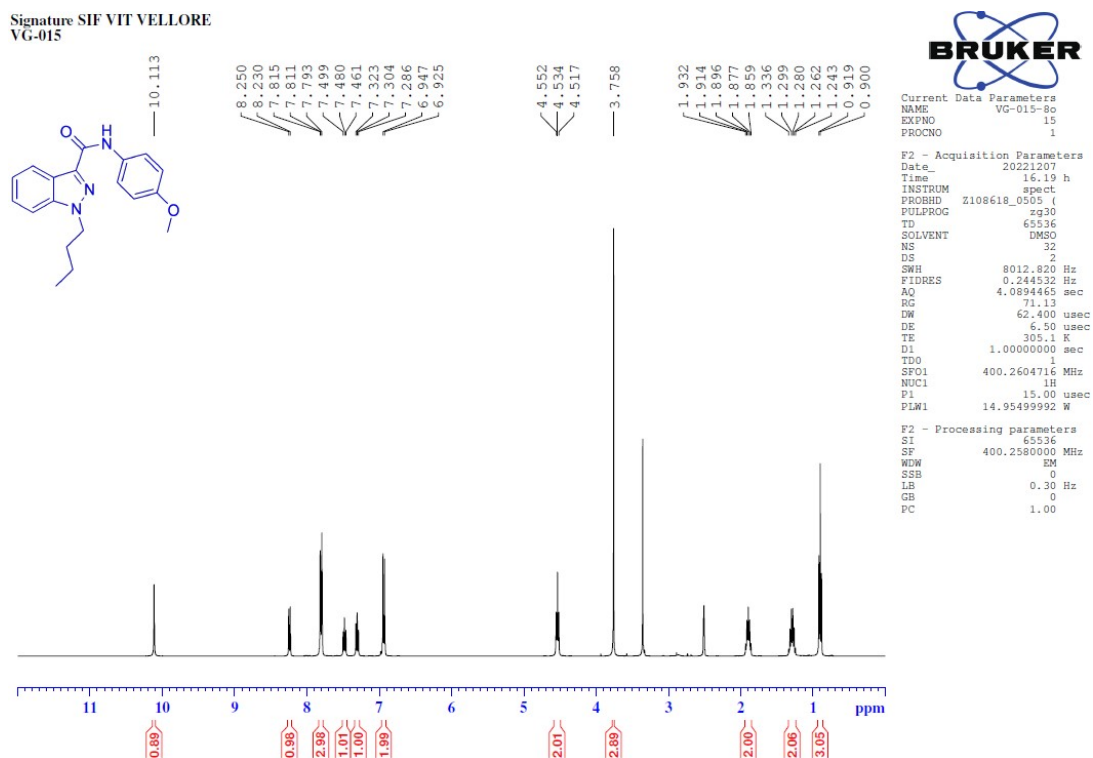
FT-IR spectrum of 1-butyl-N-(5-methylpyridin-2-yl)-1H-indazole-3-carboxamide (8n).



HRMS of 1-butyl-N-(5-methylpyridin-2-yl)-1H-indazole-3-carboxamide (8n).

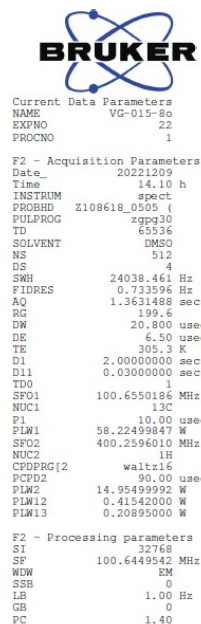
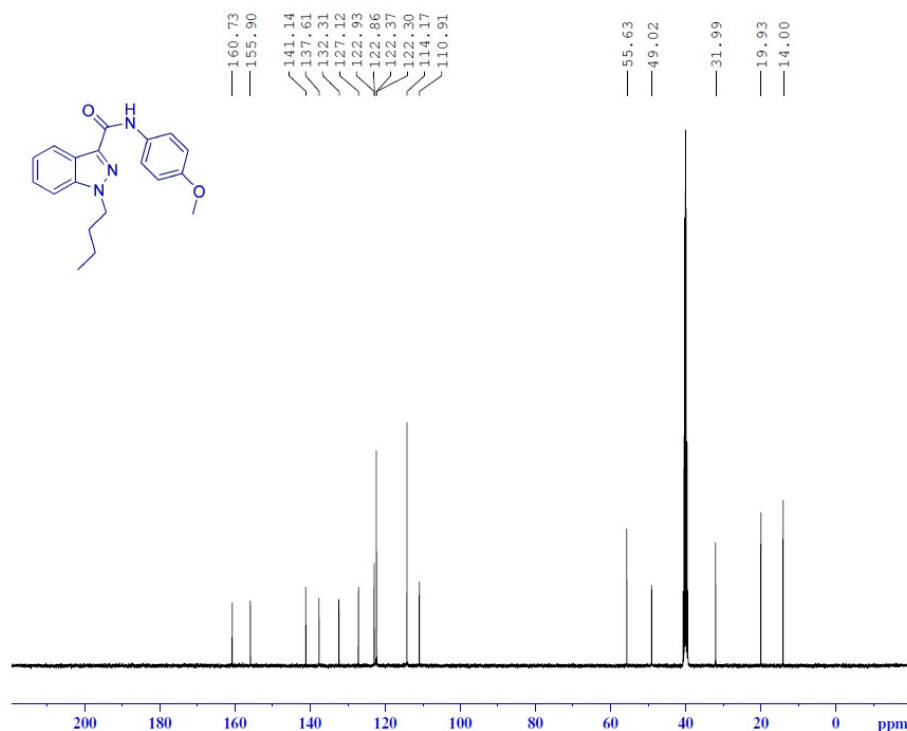


¹H-NMR [400MHz, DMSO-d₆] spectrum of 1-butyl-N-(4-methoxyphenyl)-1H-indazole-3-carboxamide (8o).



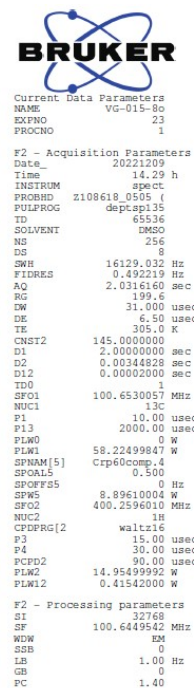
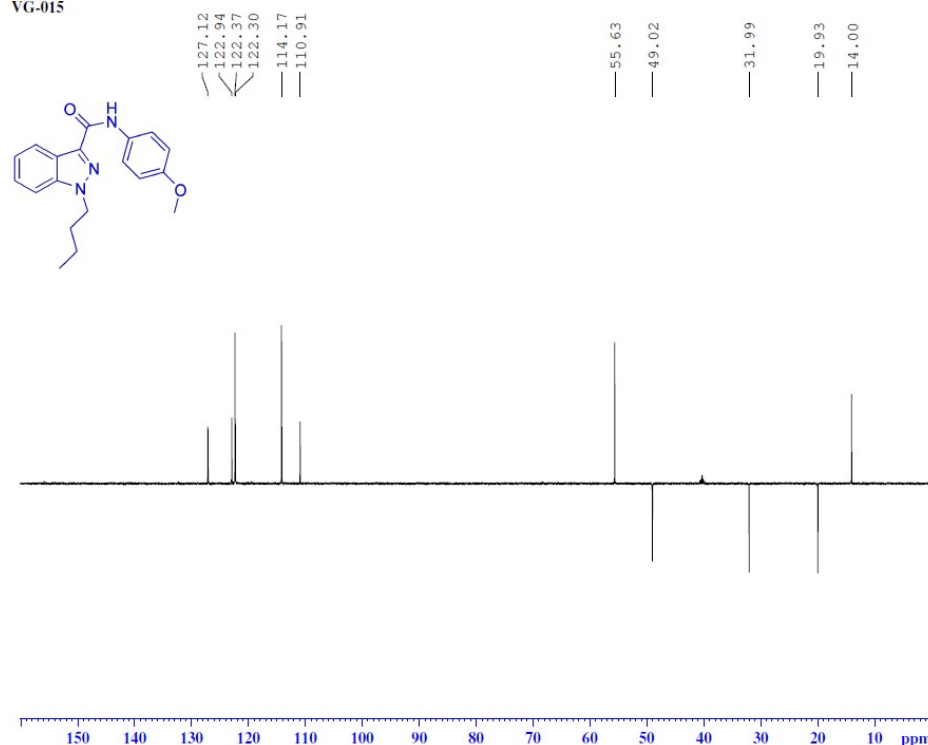
¹³C-NMR [400MHz, DMSO-d₆] spectrum of 1-butyl-N-(4-methoxyphenyl)-1H-indazole-3-carboxamide (8o).

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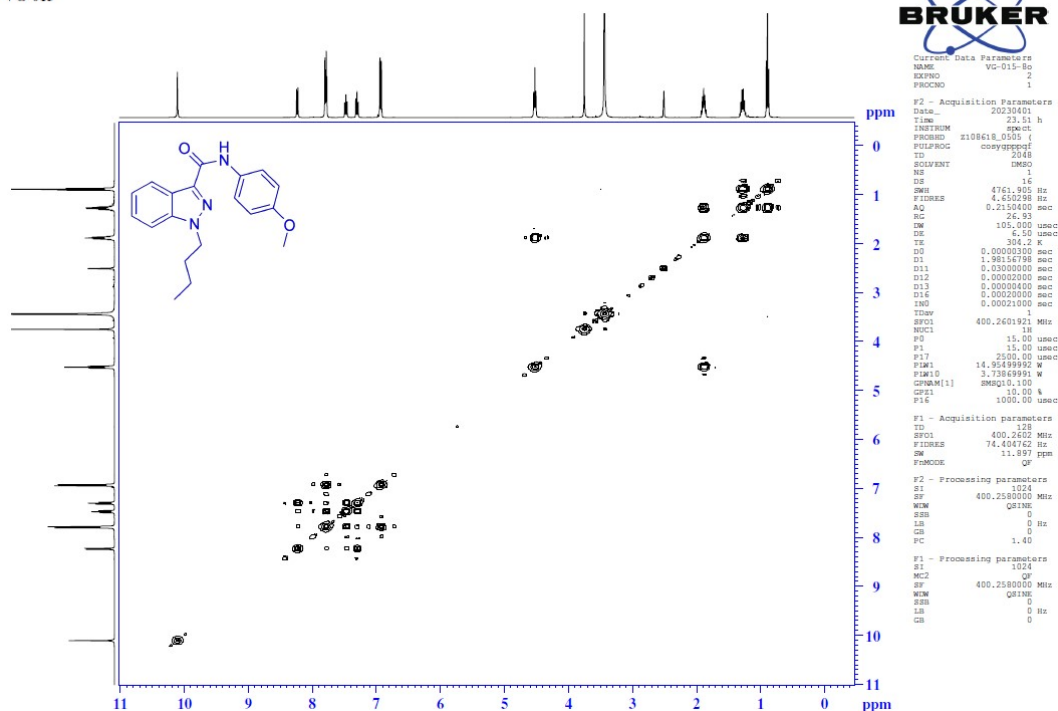


135-DEPT-NMR [400MHz, DMSO-d₆] spectrum of 1-butyl-N-(4-methoxyphenyl)-1H-indazole-3-carboxamide (8o).

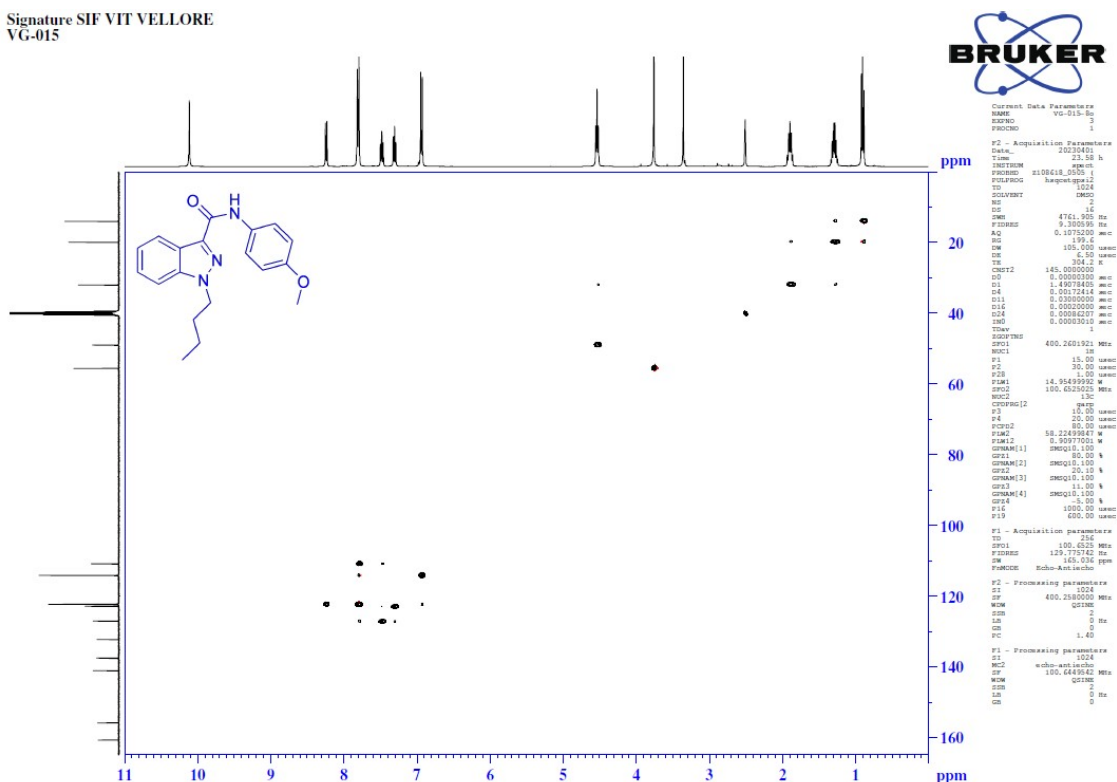
Signature SIF VIT VELLORE
VG-015



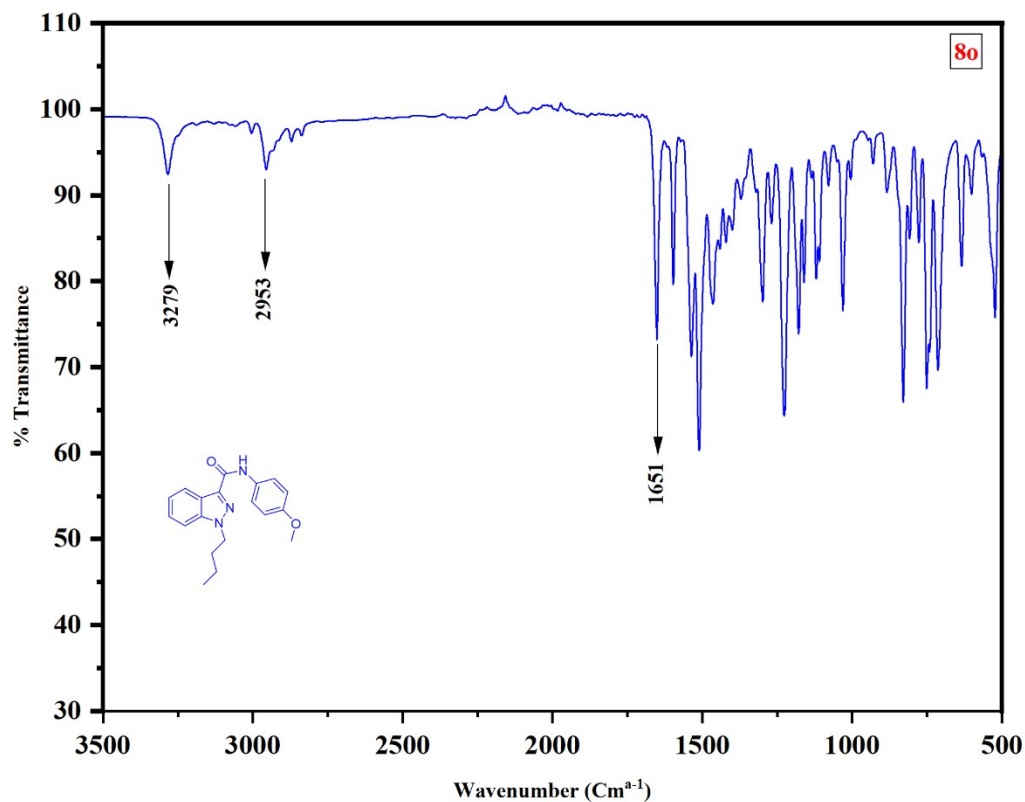
COSY-NMR [400MHz, DMSO-d₆] spectrum of 1-butyl-N-(4-methoxyphenyl)-1H-indazole-3-carboxamide (8o).



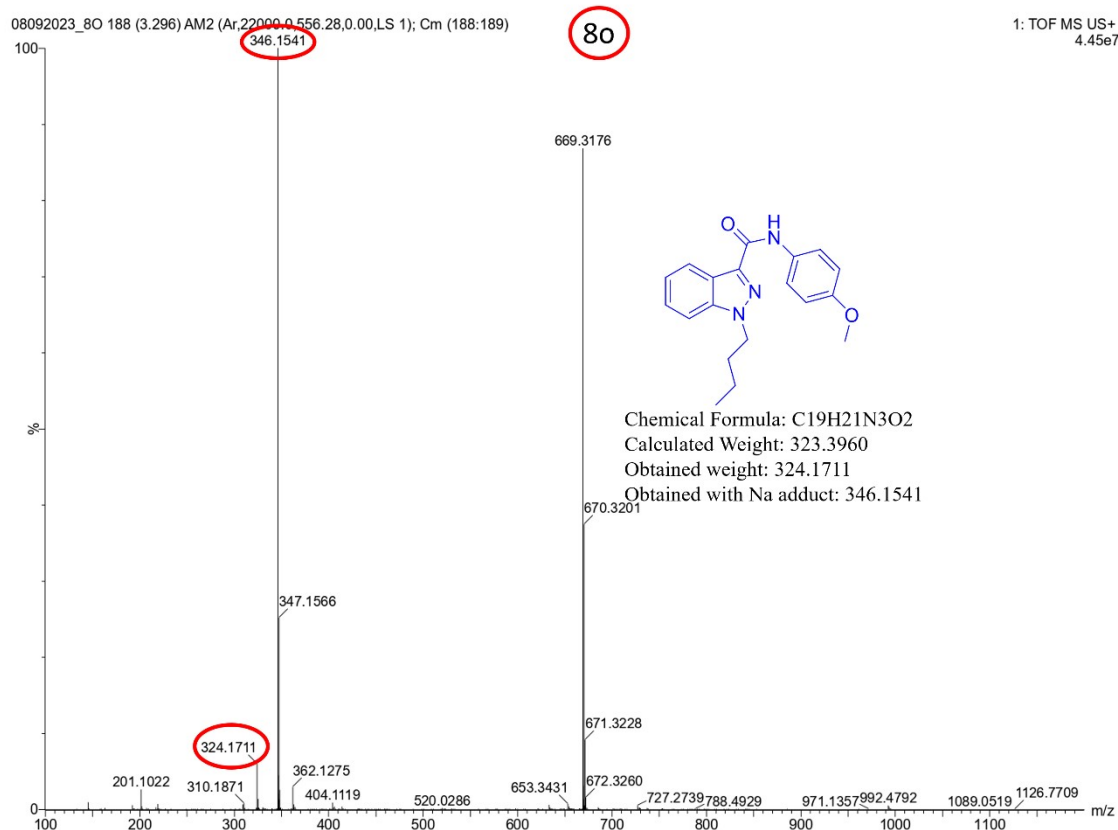
HSQC-NMR [400MHz, DMSO- d_6] spectrum of 1-butyl-N-(4-methoxyphenyl)-1H-indazole-3-carboxamide (80).



FT-IR spectrum of 1-butyl-N-(4-methoxyphenyl)-1H-indazole-3-carboxamide (80).

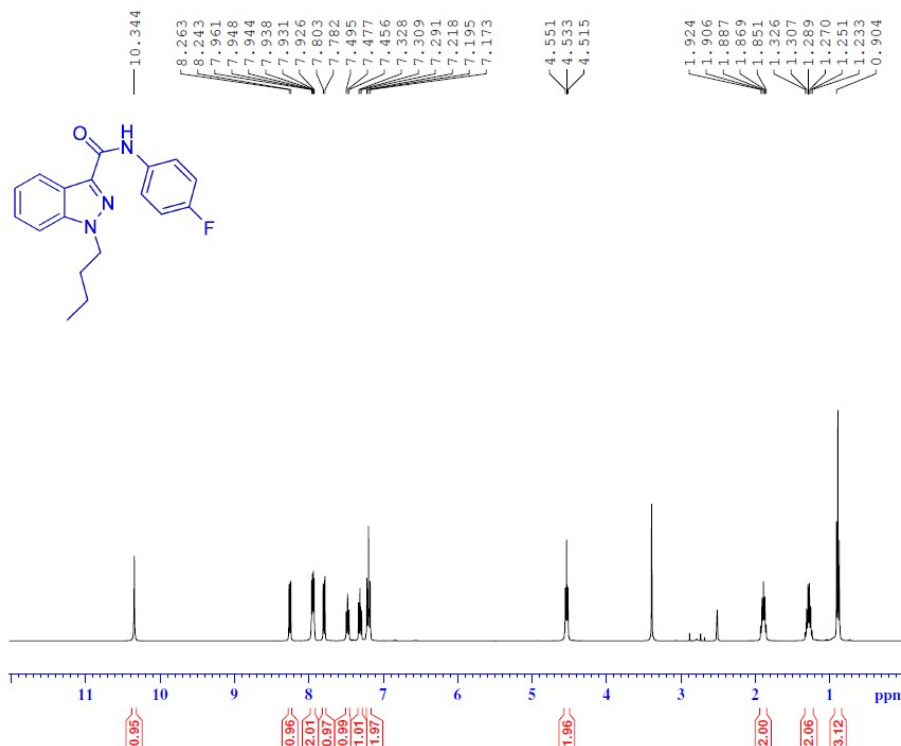


HRMS of 1-butyl-N-(4-methoxyphenyl)-1H-indazole-3-carboxamide (80).



¹H-NMR [400MHz, DMSO-d₆] spectrum of 1-butyl-N-(4-fluorophenyl)-1H-indazole-3-carboxamide (8p).

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VG-016



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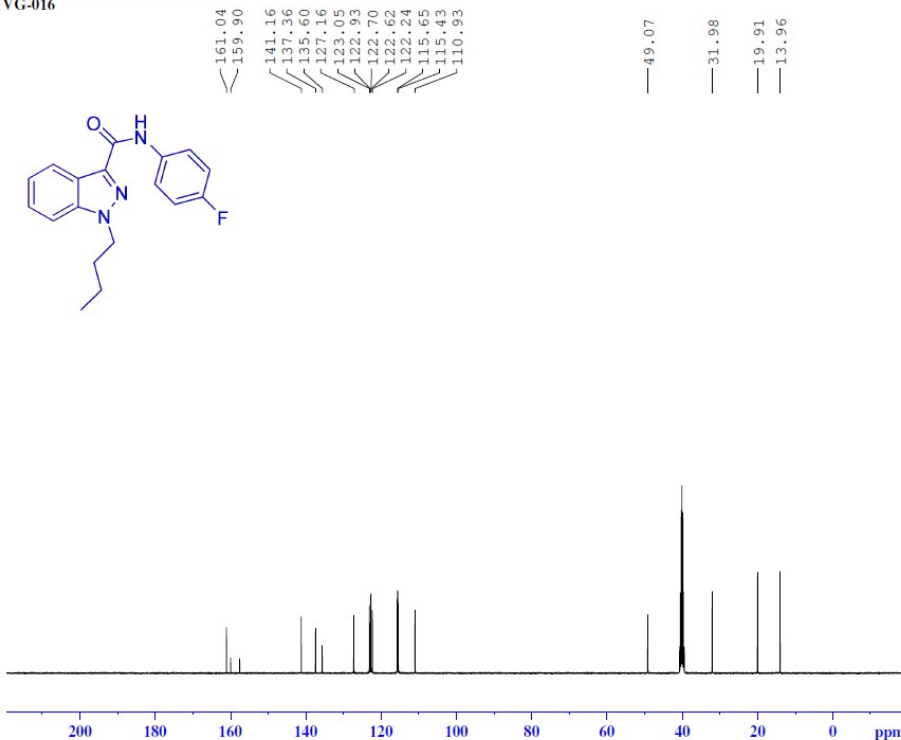
Current Data Parameters
NAME VG-016-8p
EXPNO 33
PROCNO 1

F2 - Acquisition Parameters
Date_ 20221214
Time 16.26 h
INSTRUM spect
PROBHD Z108618_0505 ()
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 35.49
DW 62.400 usec
DE 6.50 usec
TE 303.3 K
D1 1.00000000 sec
TD0 1
SFO1 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PLW1 14.95499992 W

F2 - Processing parameters
SI 65536
SF 400.2580000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹³C-NMR [100MHz, DMSO-d₆] spectrum of 1-butyl-N-(4-fluorophenyl)-1H-indazole-3-carboxamide (8p).

Signature SIF VIT VELLORE
VG-016



BRUKER

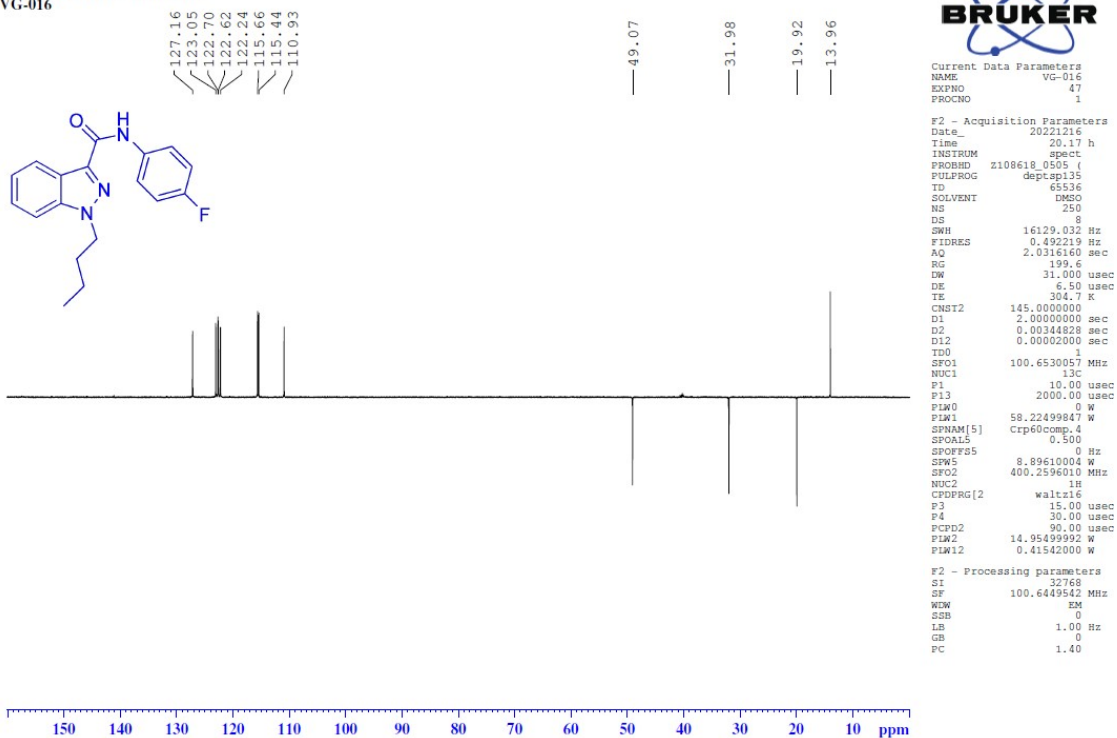
Current Data Parameters
NAME VG-016-8p
EXPNO 46
PROCNO 1

F2 - Acquisition Parameters
Date_ 20221216
Time 19.58 h
INSTRUM spect
PROBHD Z108618_0505 ()
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 510
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 175.97
DW 20.800 usec
DE 6.50 usec
TE 304.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6550186 MHz
NUC1 13C
P1 10.00 usec
PLW1 58.22499847 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 14.95499992 W
PLW12 0.41542000 W
PLW13 0.20895000 W

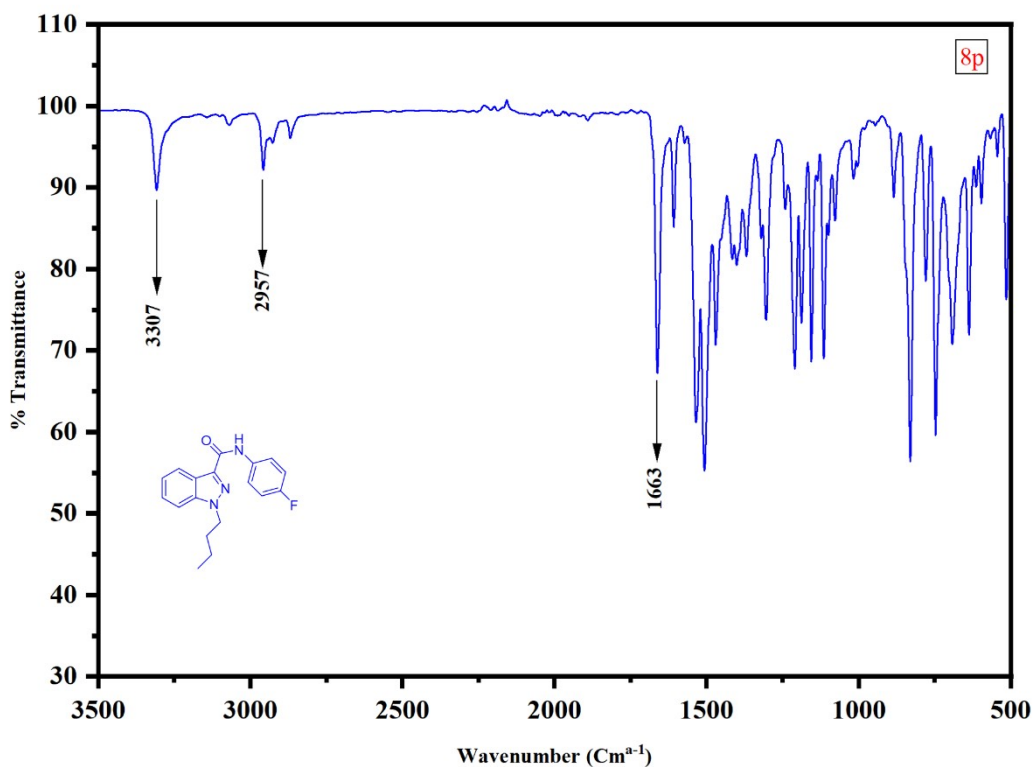
F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

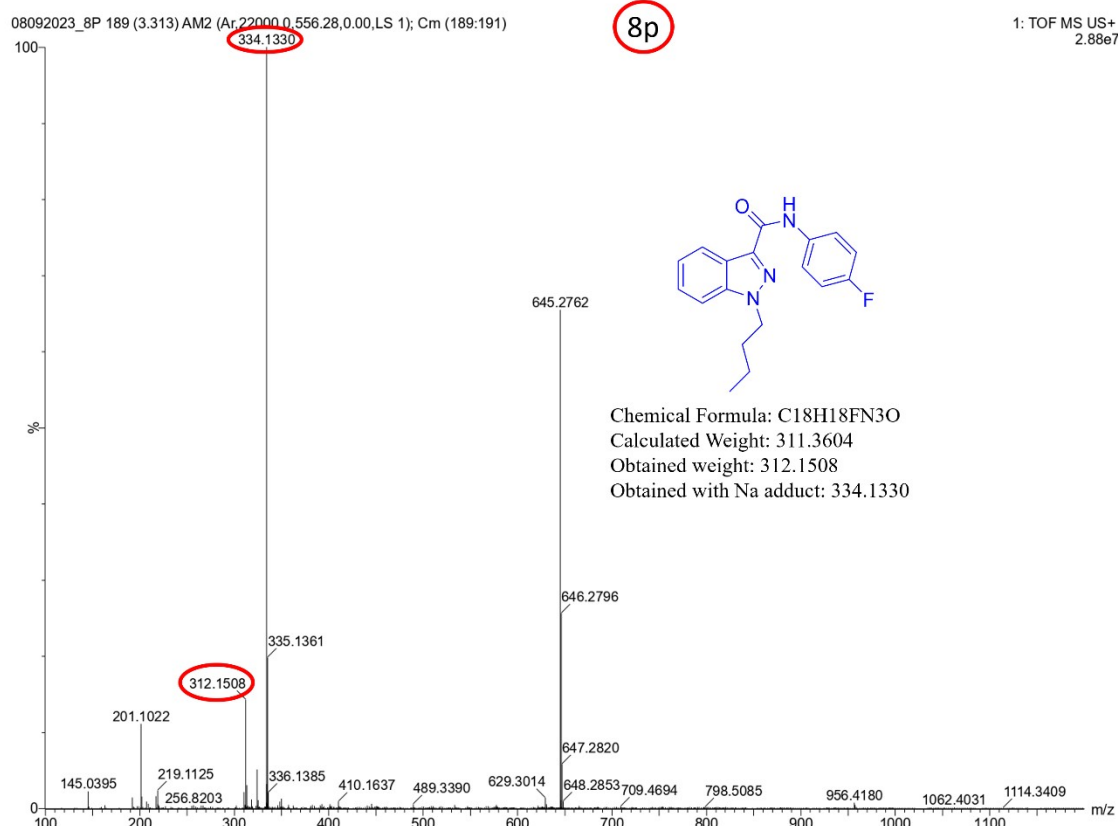
¹³⁵-DEPT-NMR [100MHz, DMSO-d₆] spectrum of 1-butyl-N-(4-fluorophenyl)-1H-indazole-3-carboxamide (8p).

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VG-016



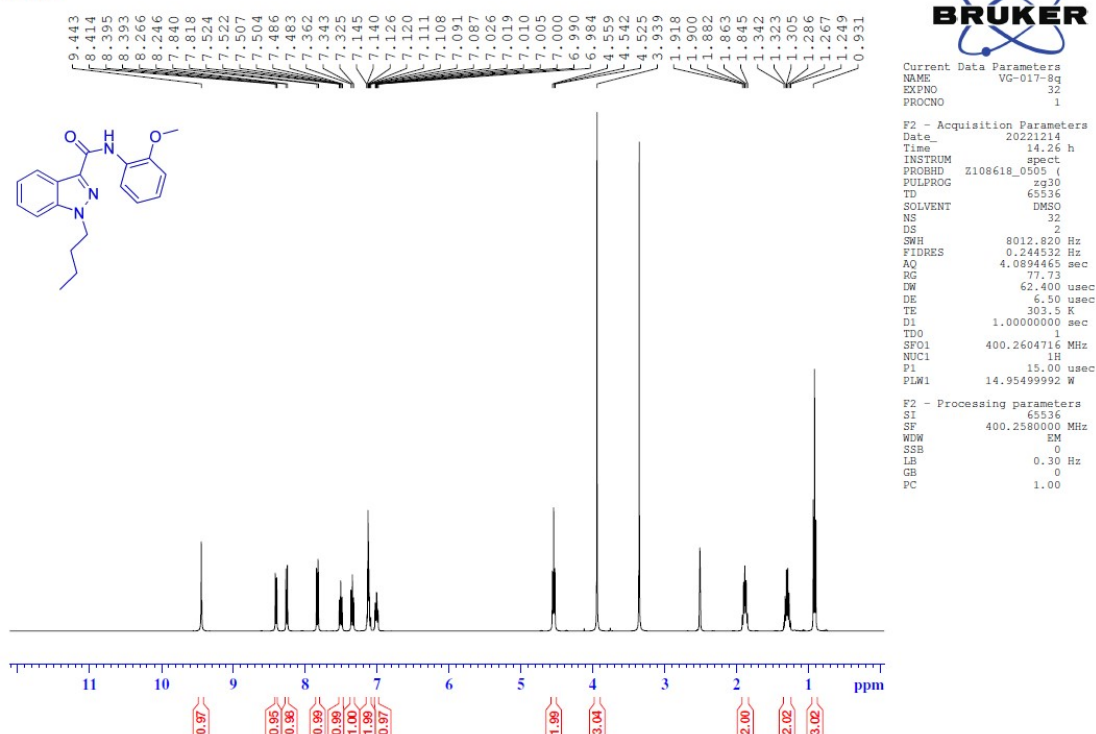
FT-IR spectrum of 1-butyl-N-(4-fluorophenyl)-1H-indazole-3-carboxamide (8p).





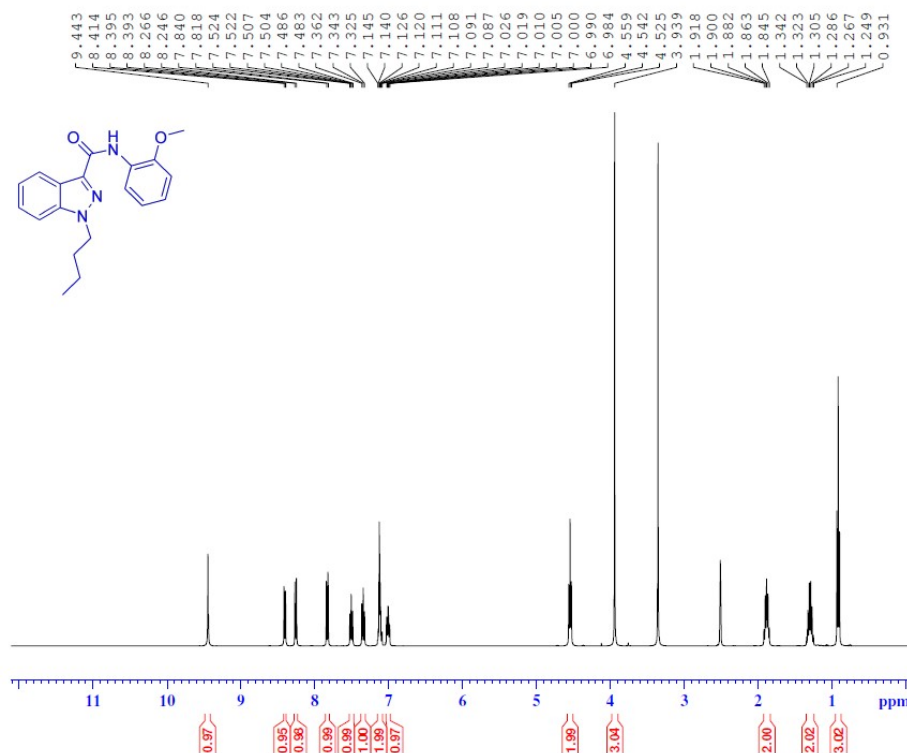
¹H-NMR [100MHz, DMSO-d₆] spectrum of 1-butyl-N-(2-methoxyphenyl)-1H-indazole-3-carboxamide (8q).

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VG-017



¹H-NMR [400MHz, DMSO-d₆] spectrum of 1-butyl-N-(2-methoxyphenyl)-1H-indazole-3-carboxamide (8q).

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VG-017



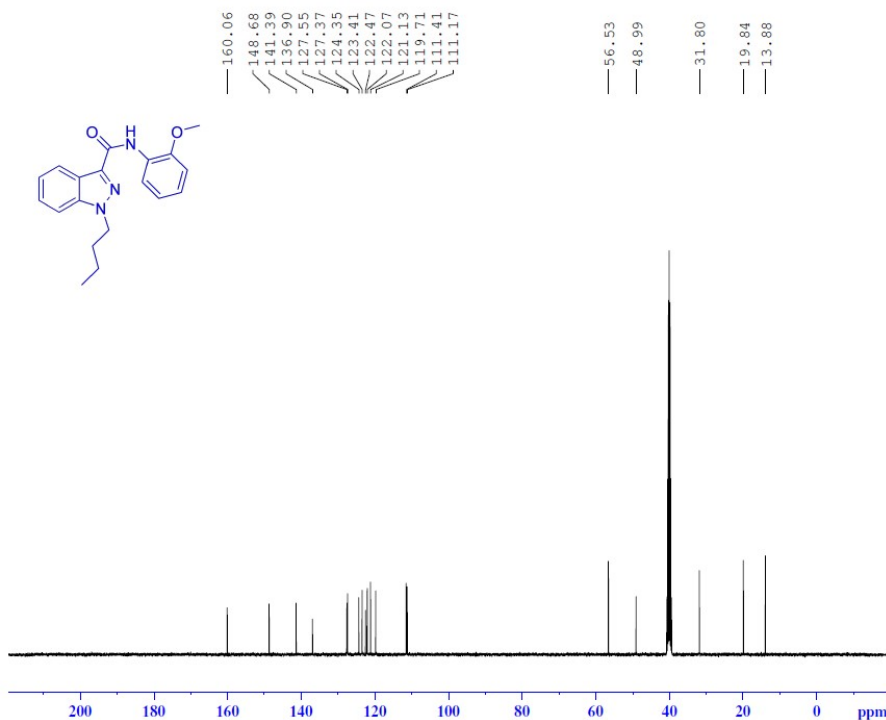
Current Data Parameters
NAME VG-017-8q
EXPNO 32
PROCNO 1

F2 - Acquisition Parameters
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PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 77.73
DW 62.400 usec
DE 6.50 usec
TE 303.5 K
D1 1.00000000 sec
TDO 1
SFO1 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PLW1 14.95499992 W

F2 - Processing parameters
SI 65536
SF 400.2580000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹³C-NMR [100MHz, DMSO-d₆] spectrum of 1-butyl-N-(2-methoxyphenyl)-1H-indazole-3-carboxamide (8q).

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VG-017



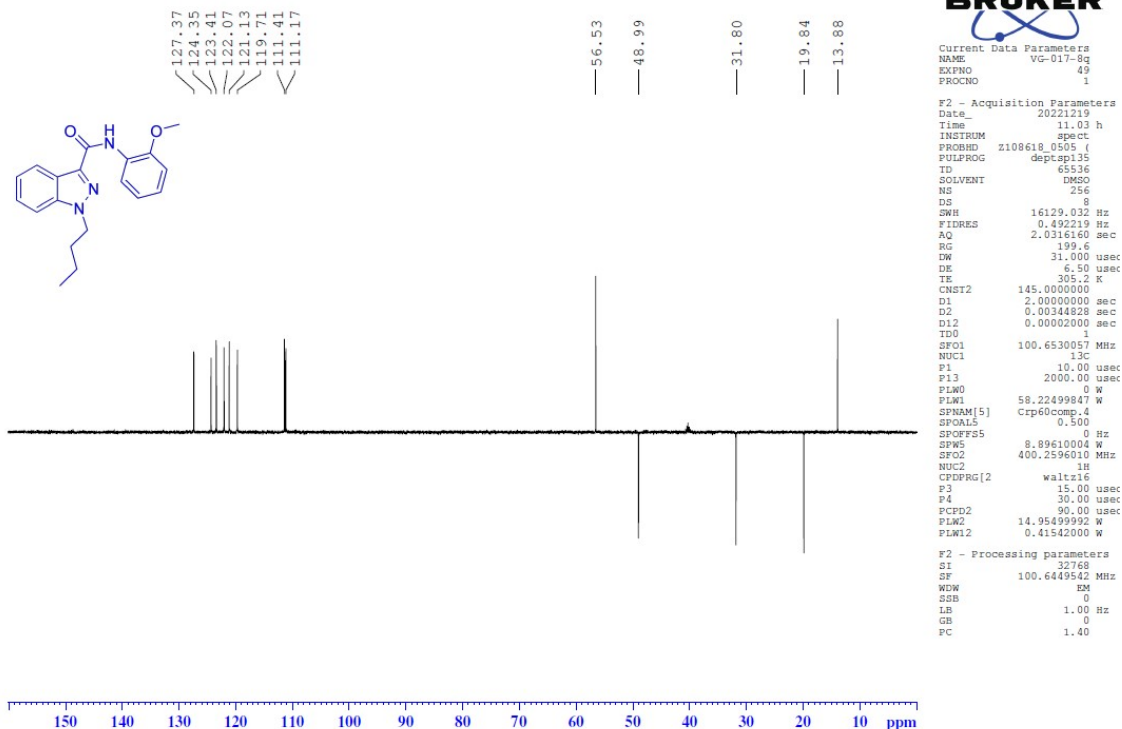
Current Data Parameters
NAME VG-017-8q
EXPNO 48
PROCNO 1

F2 - Acquisition Parameters
Date_ 20221219
Time 10.43 h
INSTRUM spect
PROBHD Z108618_0505 (4
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 812
DS 4
SWH 24038.461 Hz
FIDRES 0.733996 Hz
AQ 1.3631488 sec
RG 156.91
DW 20.800 usec
DE 6.50 usec
TE 305.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1
SFO1 100.6550186 MHz
NUC1 13C
P1 10.00 usec
PLW1 58.22499847 W
SFO2 400.2596010 MHz
NUC2 1H
PCPDPRG(2) waltz16
PCPD2 90.00 usec
PLW2 14.95499992 W
PLW12 0.41542000 W
PLW13 0.20895000 W

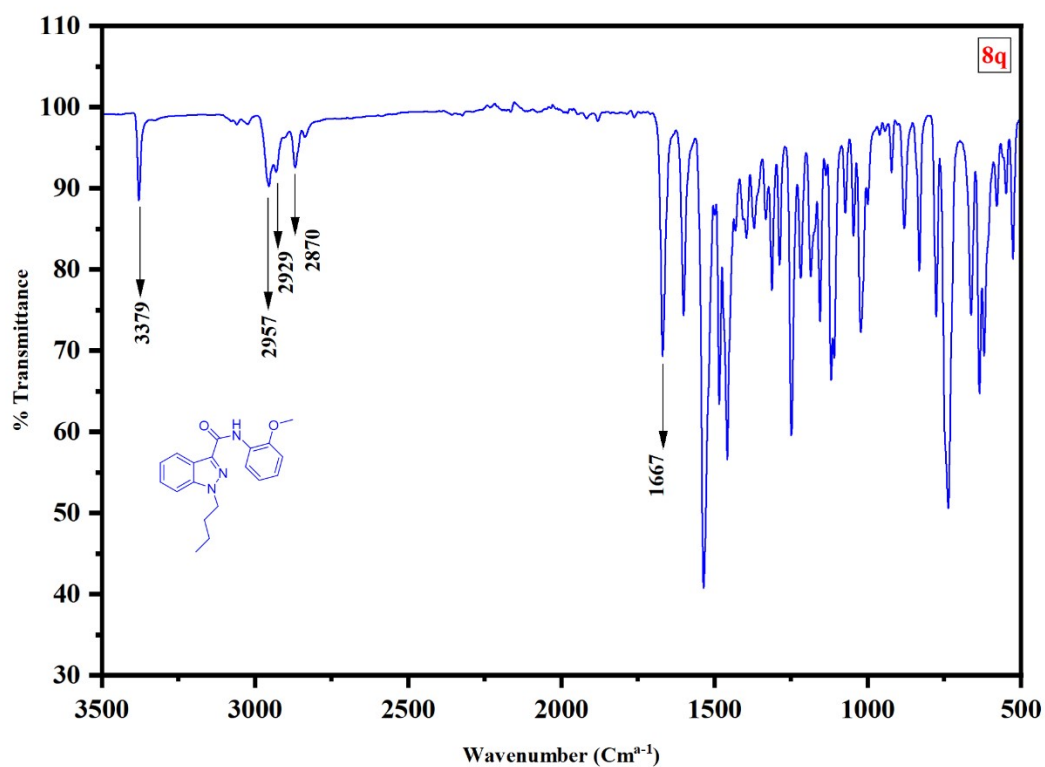
F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

¹³⁵-DEPT-NMR [100MHz, DMSO-d₆] spectrum of 1-butyl-N-(2-methoxyphenyl)-1H-indazole-3-carboxamide (8q).

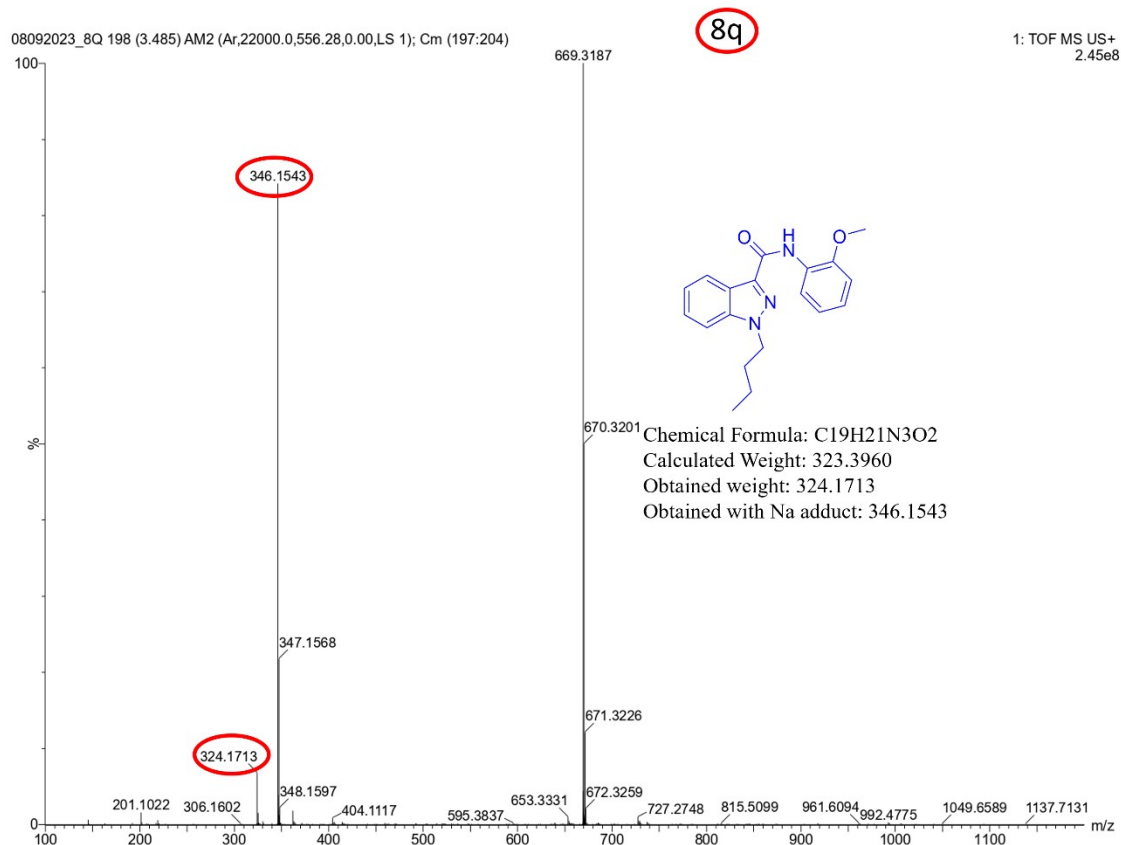
Signature SIF VIT VELLORE
VG-017



FT-IR spectrum of 1-butyl-N-(2-methoxyphenyl)-1H-indazole-3-carboxamide (8q).

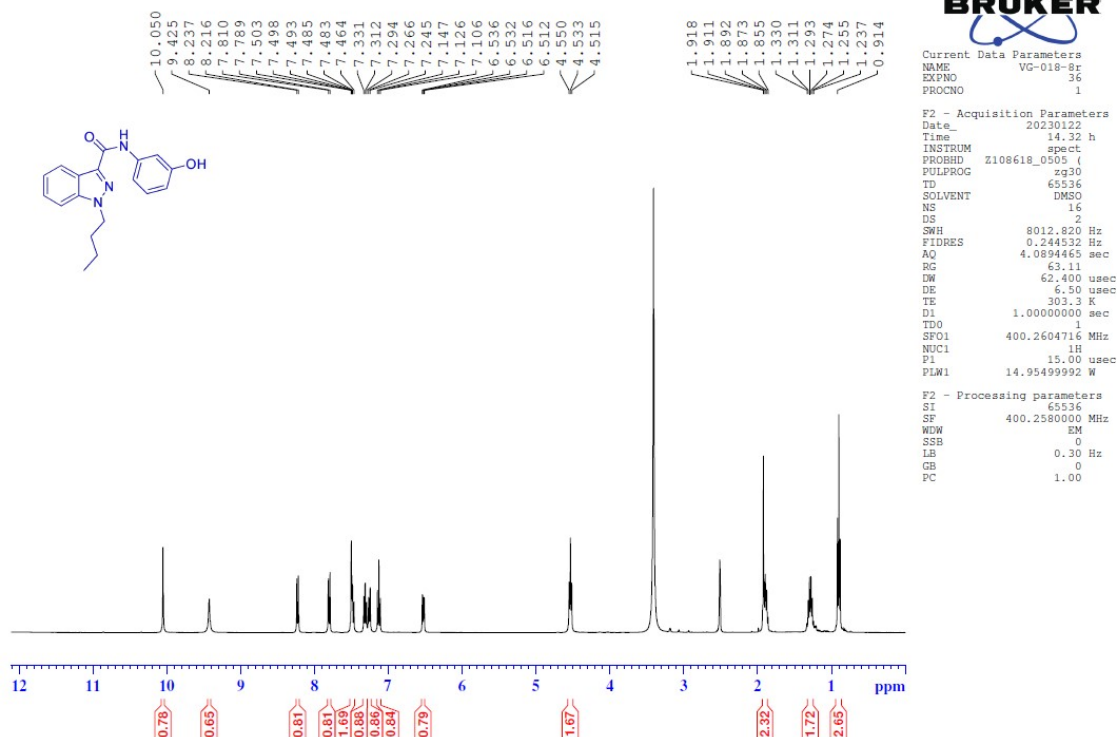


HRMS of 1-butyl-N-(2-methoxyphenyl)-1H-indazole-3-carboxamide (8q).



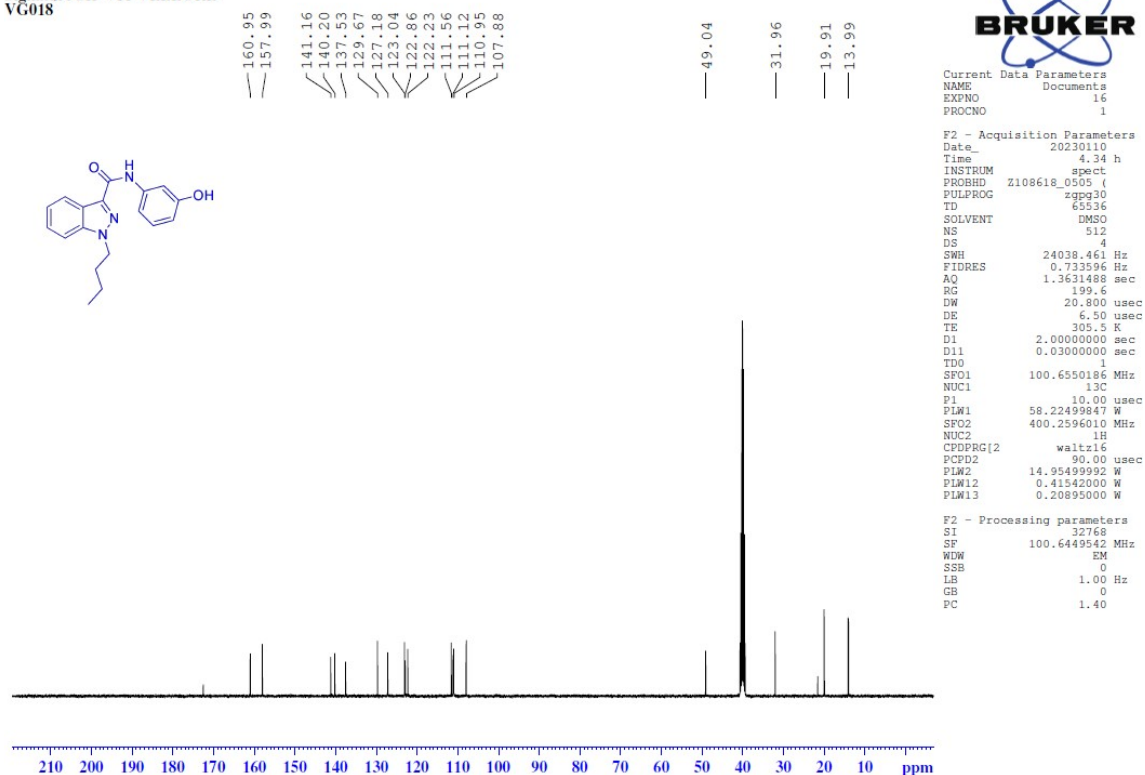
¹H-NMR [400MHz, DMSO-d₆] spectrum of 1-butyl-N-(3-hydroxyphenyl)-1H-indazole-3-carboxamide (8r).

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VG-018



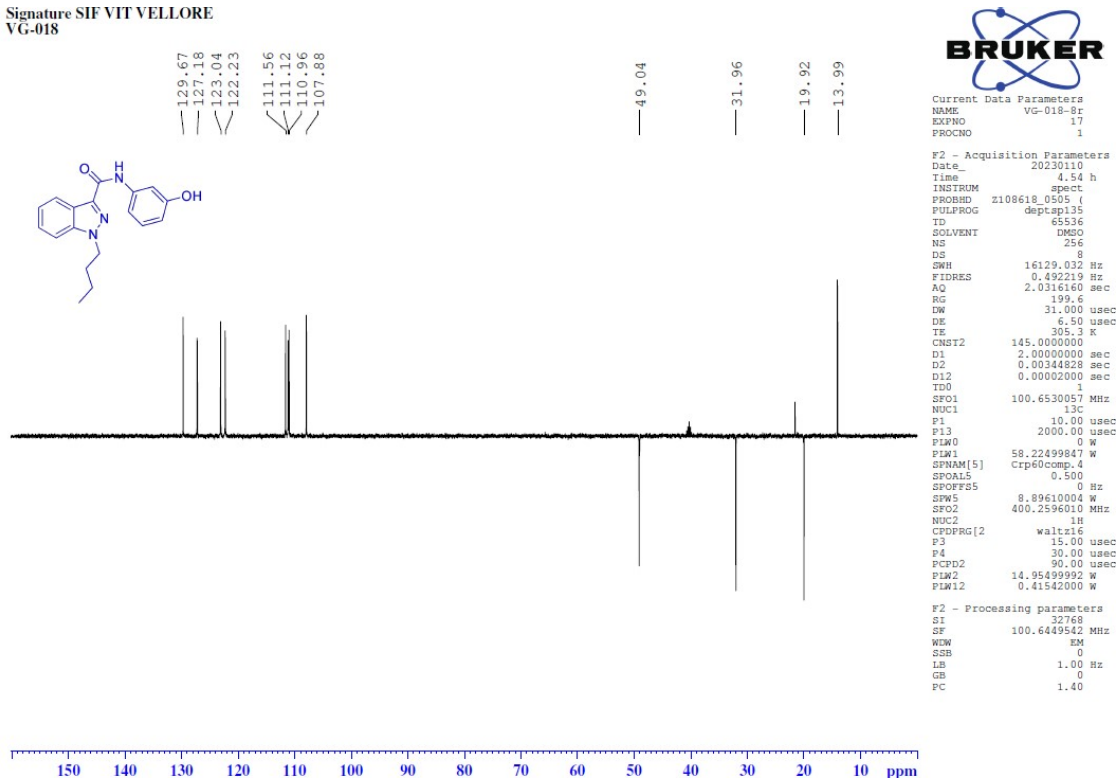
¹³C-NMR [100MHz, DMSO-d₆] spectrum of 1-butyl-N-(3-hydroxyphenyl)-1H-indazole-3-carboxamide (8r).

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VG018

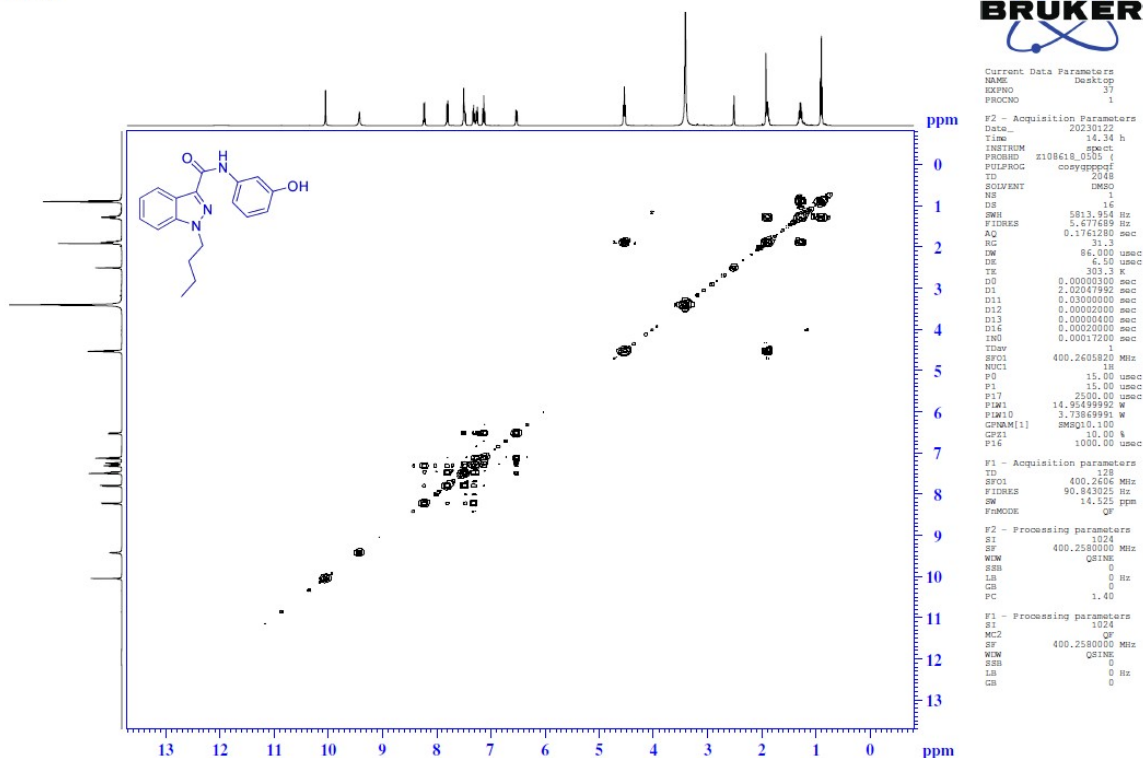


¹³⁵-DEPT-NMR [100MHz, DMSO-d₆] spectrum of 1-butyl-N-(3-hydroxyphenyl)-1H-indazole-3-carboxamide (8r).

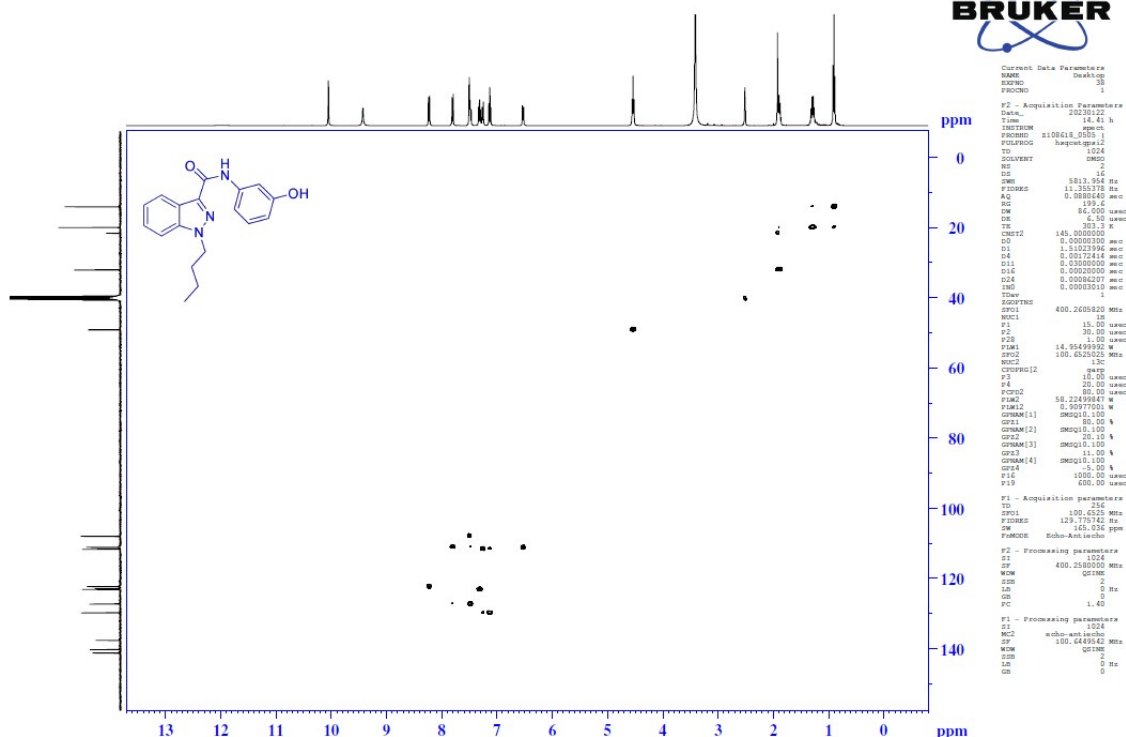
Signature SIF VIT VELLORE
VG-018



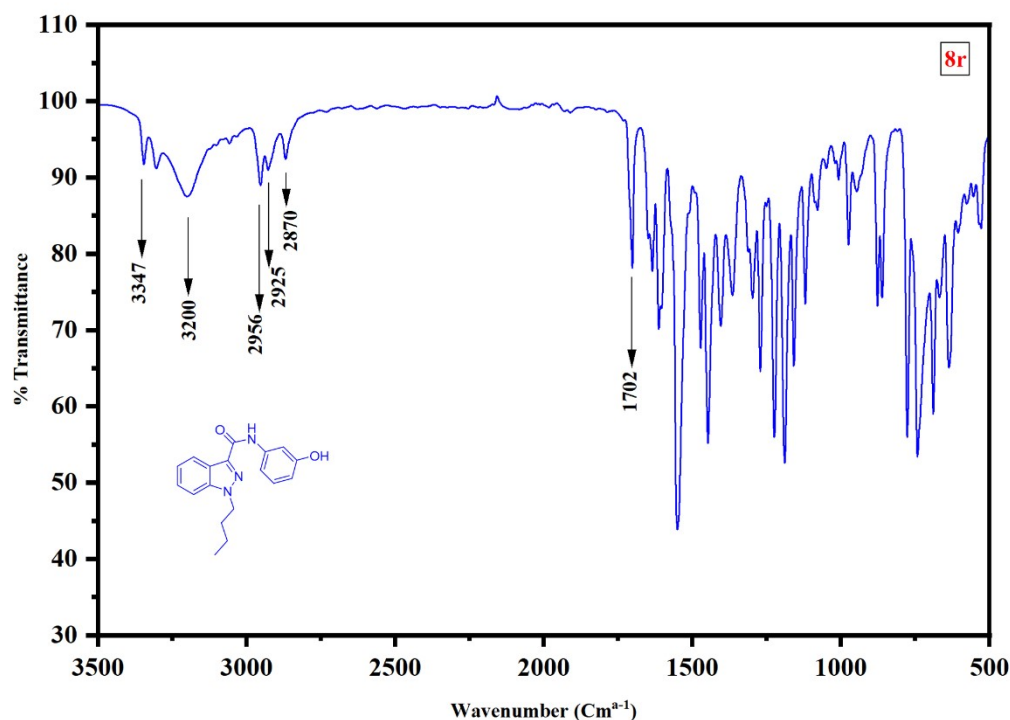
COSY-NMR [400MHz, DMSO-d₆] spectrum of 1-butyl-N-(3-hydroxyphenyl)-1H-indazole-3-carboxamide (8r).



HSQC-NMR [400MHz, DMSO-d₆] spectrum of 1-butyl-N-(3-hydroxyphenyl)-1H-indazole-3-carboxamide (8r).

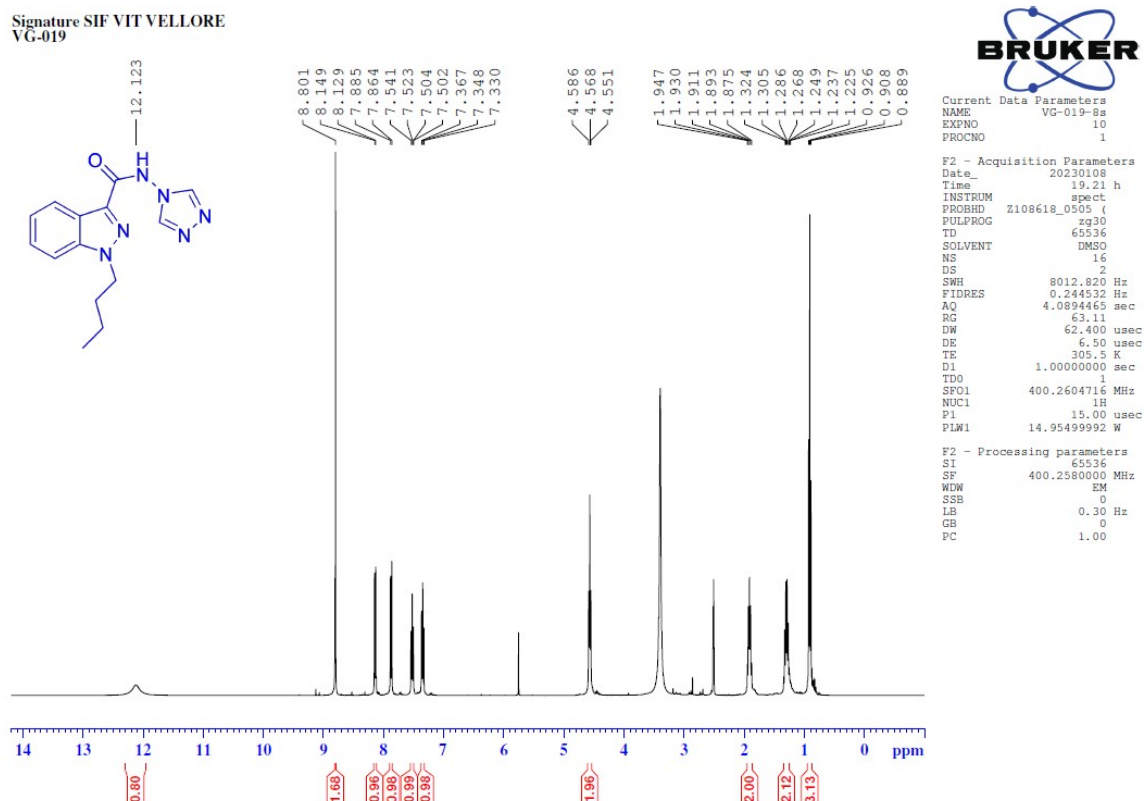


FT-IR spectrum of 1-butyl-N-(3-hydroxyphenyl)-1H-indazole-3-carboxamide (8r).



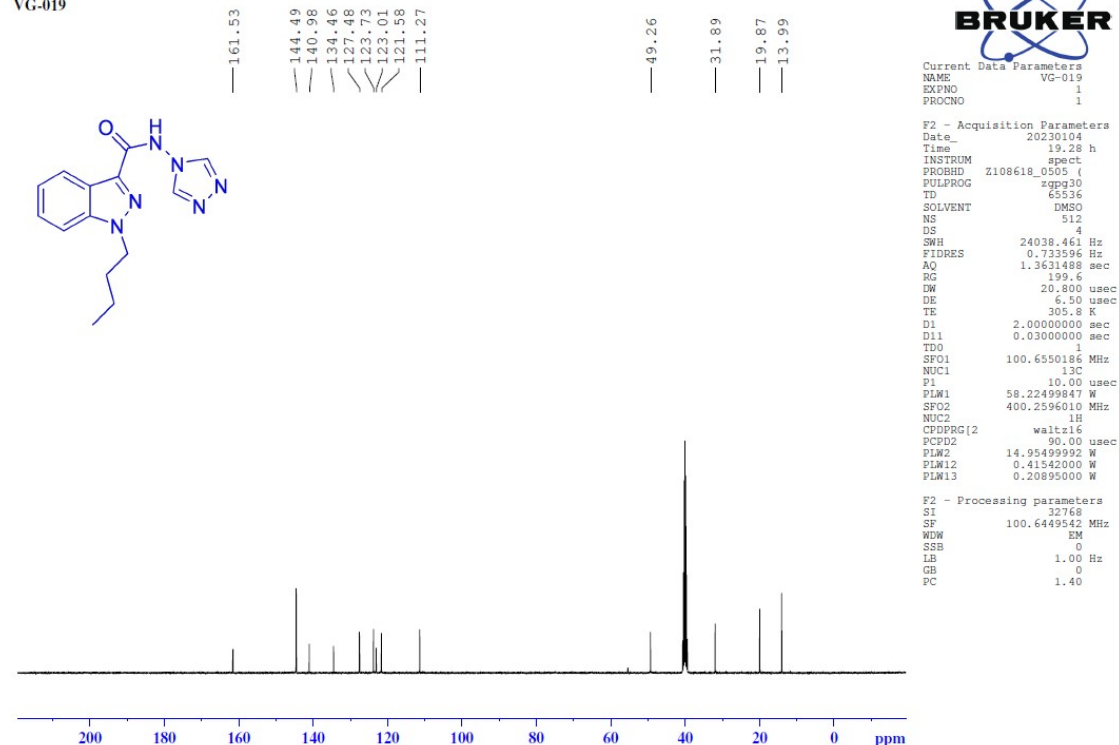
HRMS of 1-butyl-N-(3-hydroxyphenyl)-1H-indazole-3-carboxamide (8r).

¹H-NMR [400MHz, DMSO-d₆] spectrum of 1-butyl-N-(4H-1,2,4-triazol-4-yl)-1H-indazole-3-carboxamide (8s).



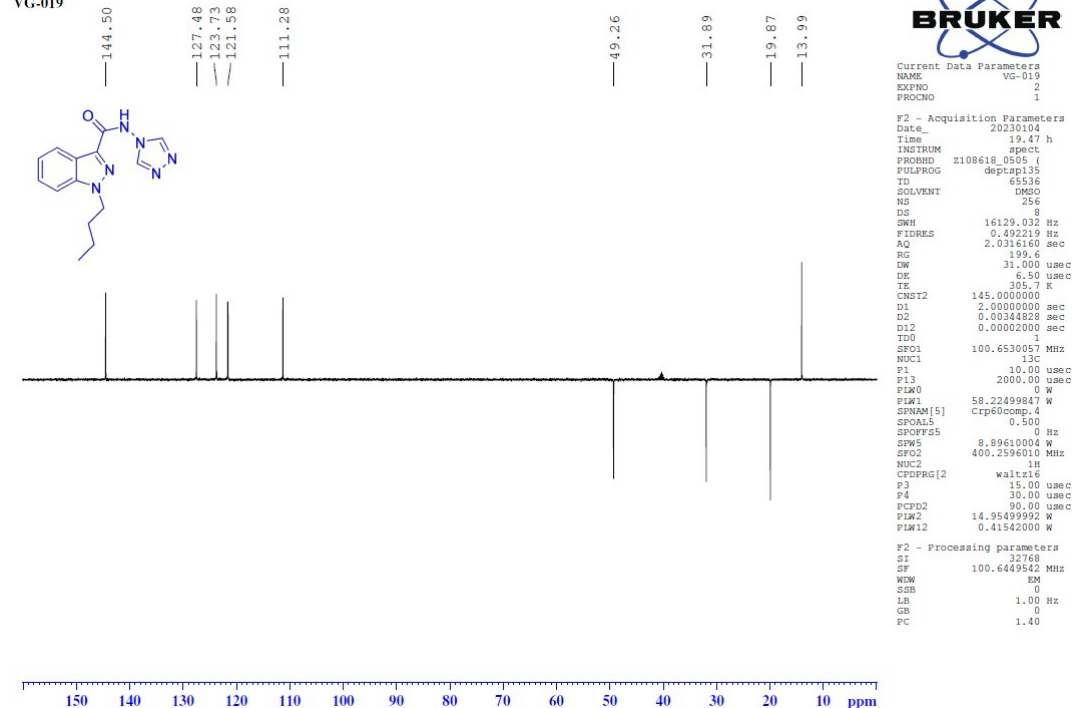
¹³C-NMR [100MHz, DMSO-d₆] spectrum of 1-butyl-N-(4H-1,2,4-triazol-4-yl)-1H-indazole-3-carboxamide (8s).

Signature SIF VIT VELLORE
VG-019



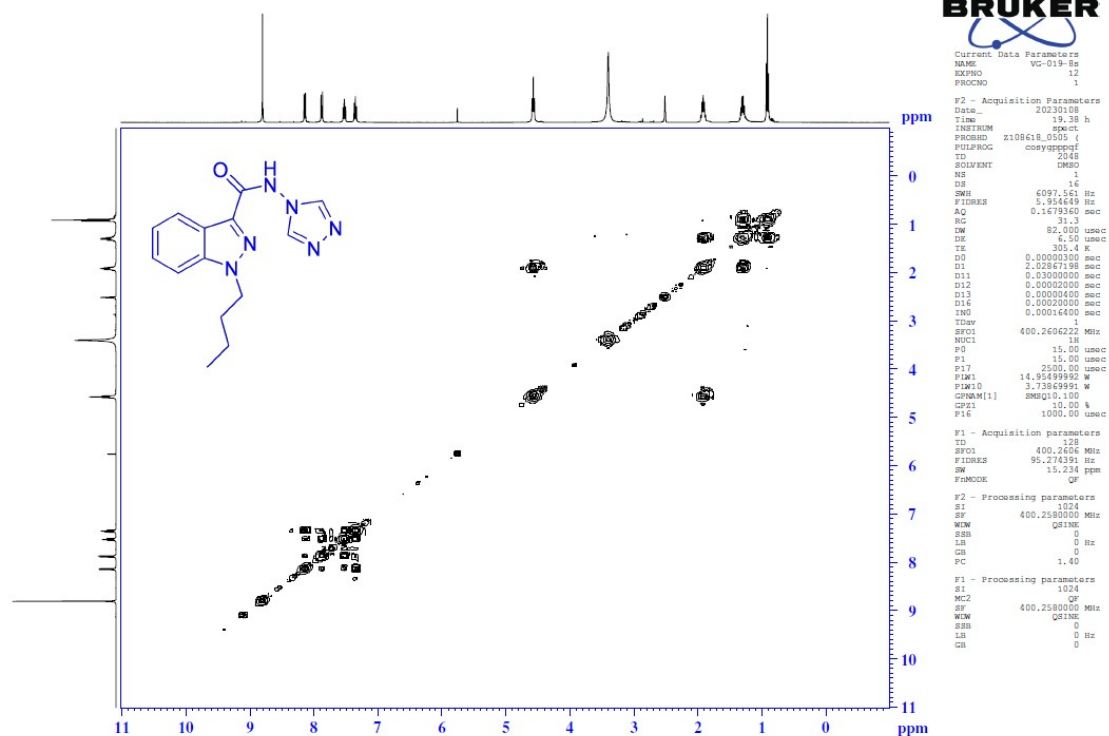
¹³S-DEPT-NMR [100MHz, DMSO-d₆] spectrum of 1-butyl-N-(4H-1,2,4-triazol-4-yl)-1H-indazole-3-carboxamide (8s).

Signature SIF VIT VELLORE
VG-019



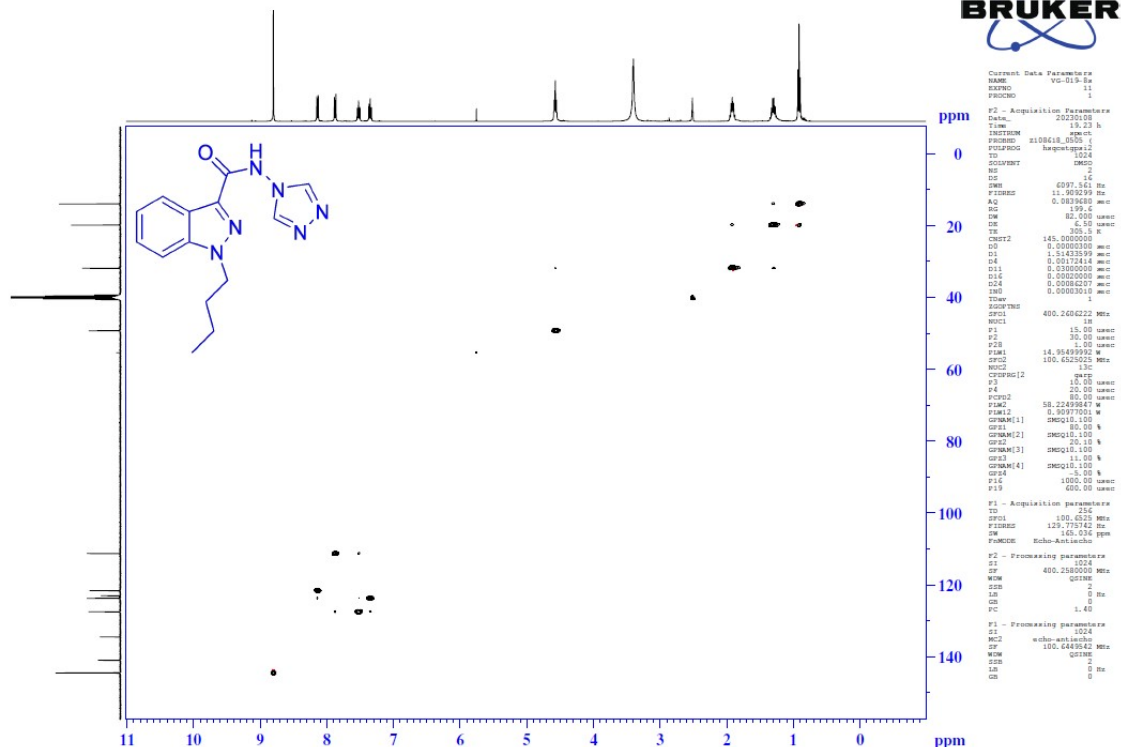
COSY-NMR [400MHz, DMSO-d₆] spectrum of 1-butyl-N-(4H-1,2,4-triazol-4-yl)-1H-indazole-3-carboxamide (8s).

Signature SIF VIT VELLORE
VG-019

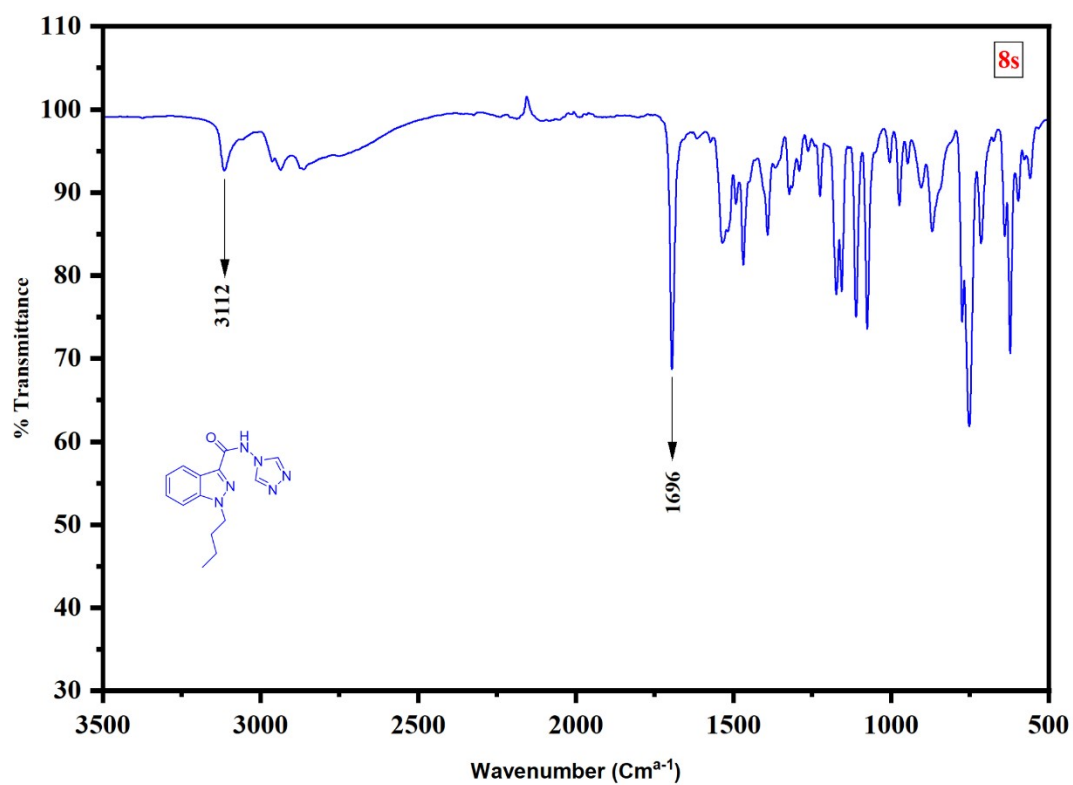


HSQC-NMR [400MHz, DMSO-d₆] spectrum of 1-butyl-N-(4H-1,2,4-triazol-4-yl)-1H-indazole-3-carboxamide (8s).

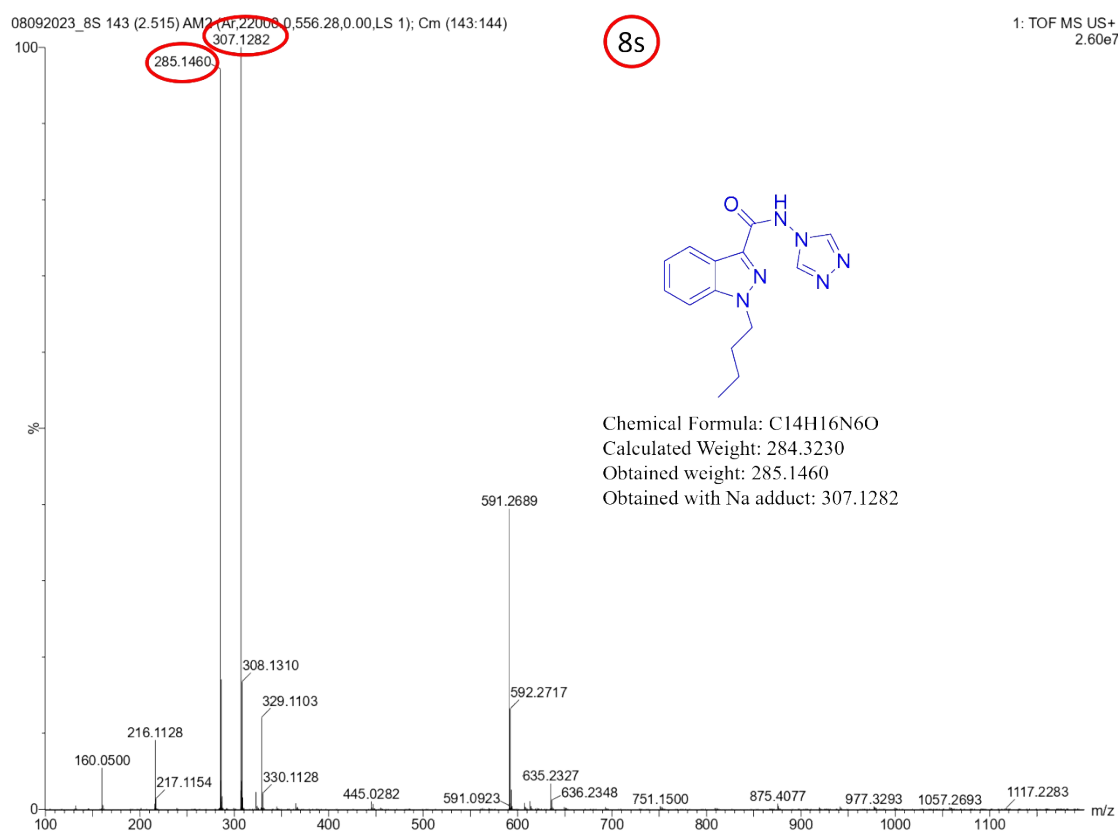
Signature SIF VIT VELLORE
VG-019



FT-IR spectrum of 1-butyl-N-(4H-1,2,4-triazol-4-yl)-1H-indazole-3-carboxamide (8s).

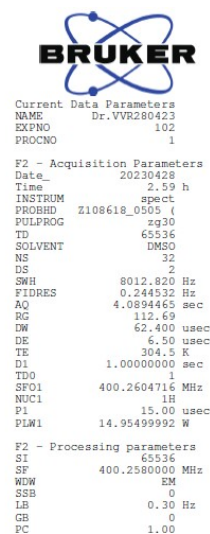
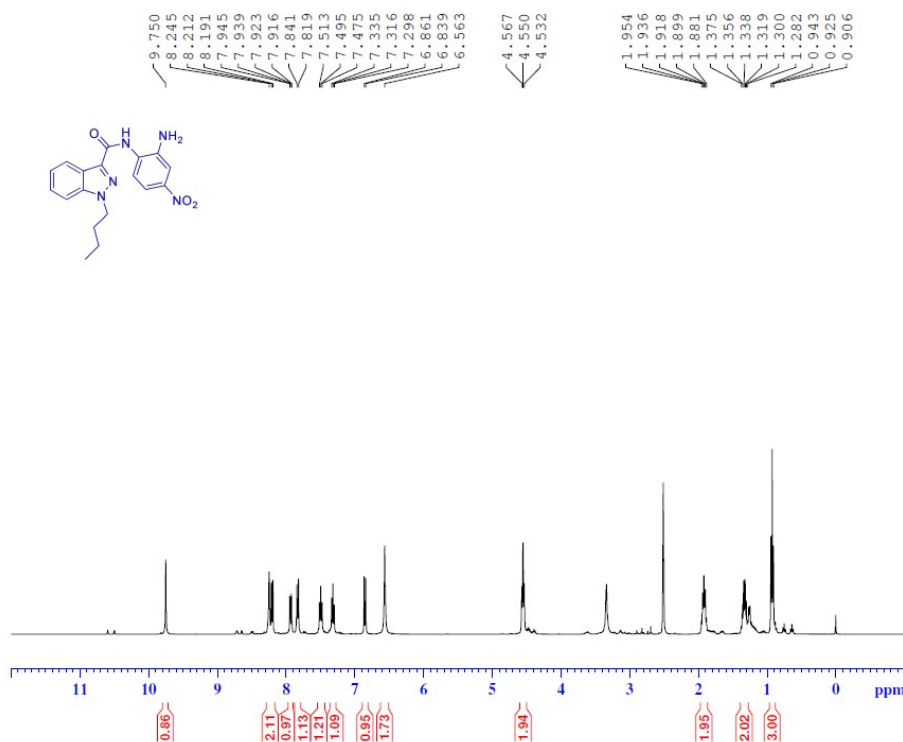


HRMS of 1-butyl-N-(4H-1,2,4-triazol-4-yl)-1H-indazole-3-carboxamide (8s).



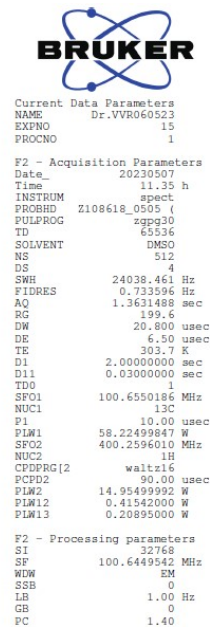
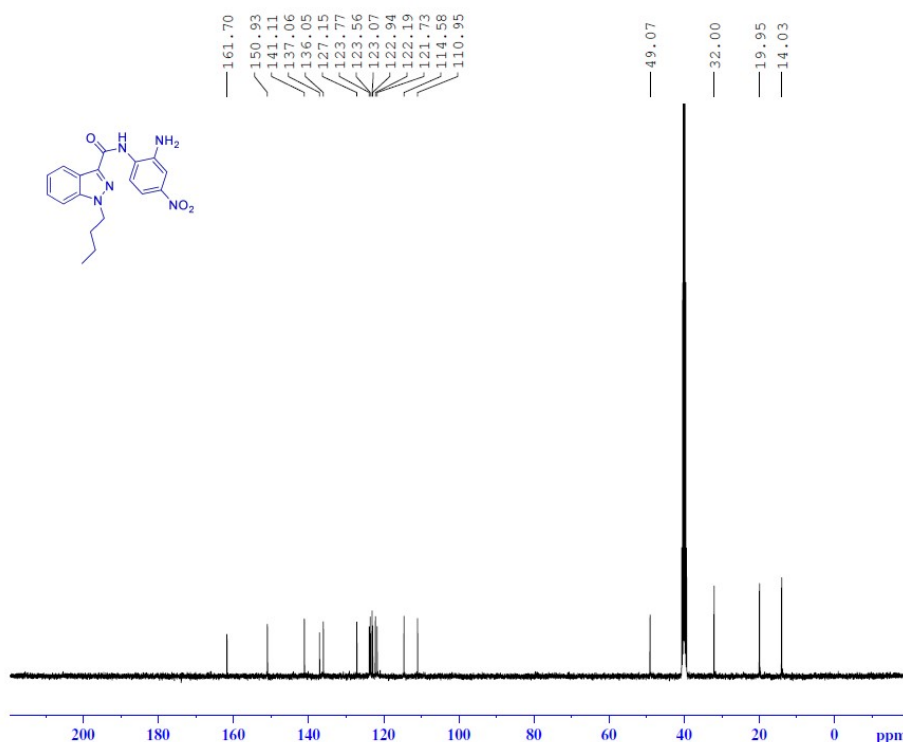
¹H-NMR [400MHz, DMSO-d₆] spectrum of N-(2-amino-4-nitrophenyl)-1-butyl-1H-indazole-3-carboxamide (8t).

Signature SIF VIT VELLORE
VG-034

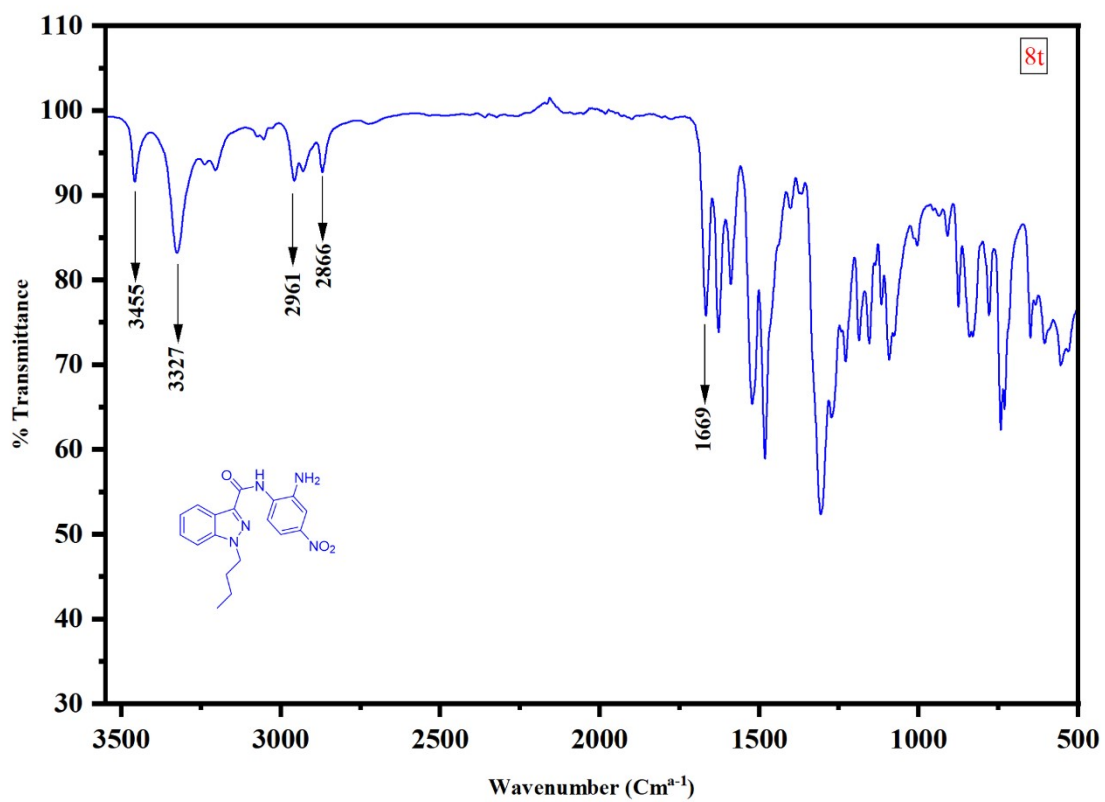


¹³C-NMR [400MHz, DMSO-d₆] spectrum of N-(2-amino-4-nitrophenyl)-1-butyl-1H-indazole-3-carboxamide (8t).

Signature SIF VIT VELLORE
VG-034



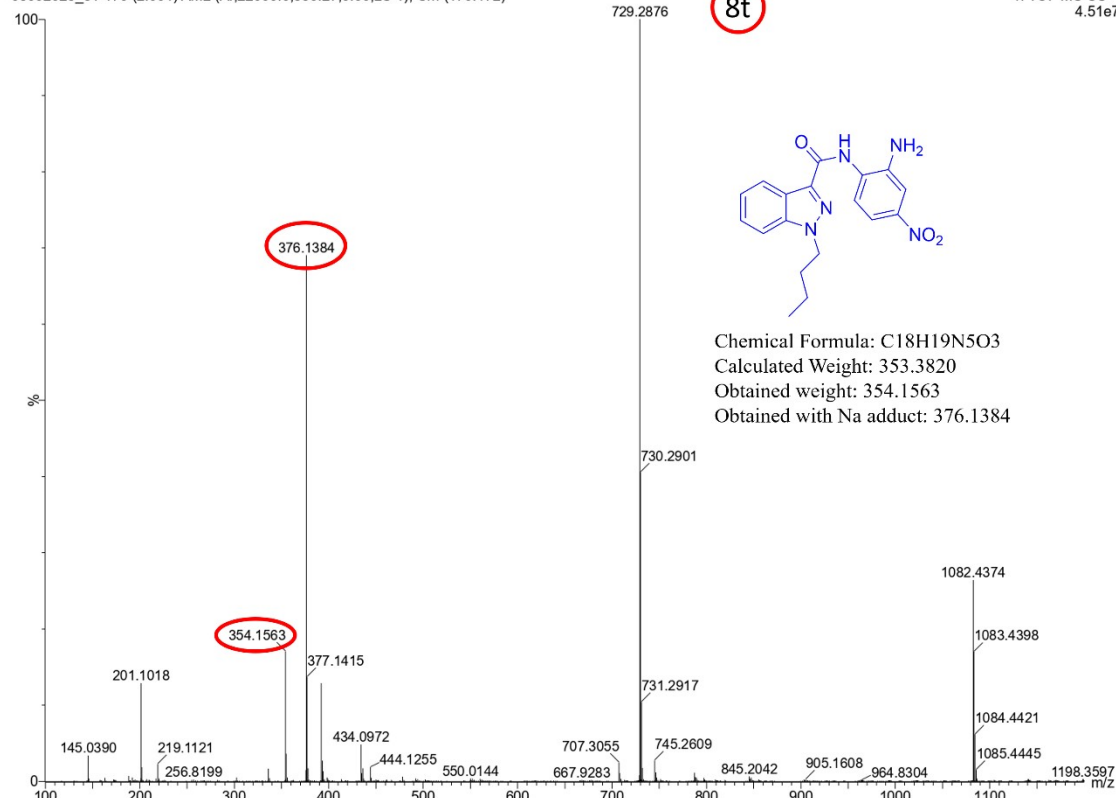
FT-IR spectrum of N-(2-amino-4-nitrophenyl)-1-butyl-1H-indazole-3-carboxamide (8t).



HRMS of N-(2-amino-4-nitrophenyl)-1-butyl-1H-indazole-3-carboxamide (8t).

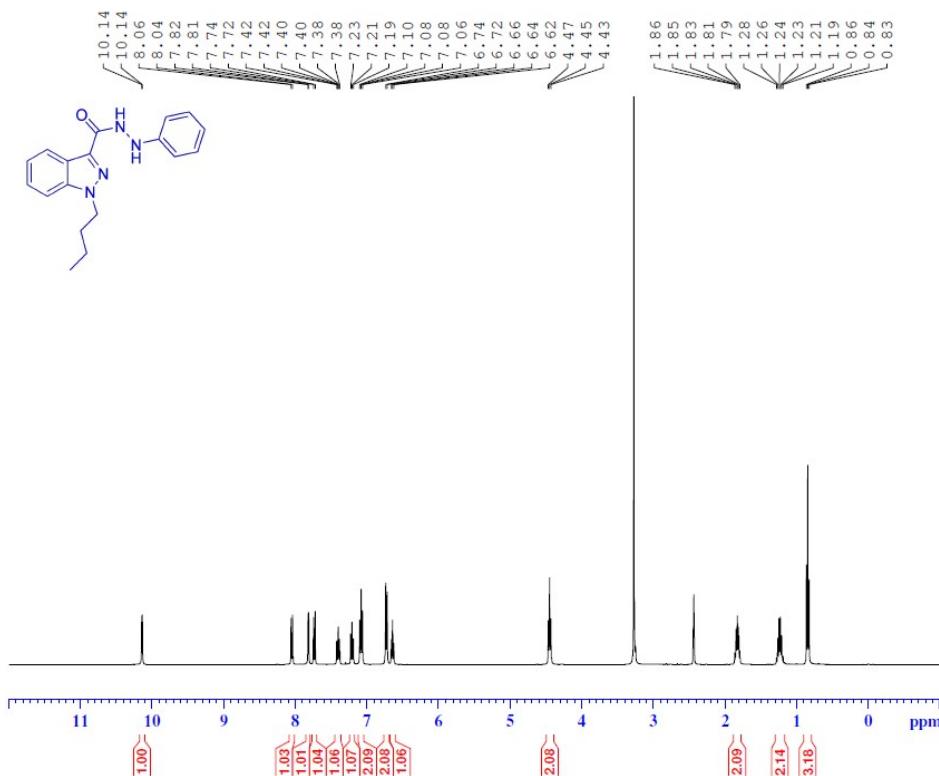
08092023_8T 170 (2.991) AM2 (Ar,22000.0,556.27,0.00,LS 1); Cm (170:172)

1: TOF MS US+
4.51e7



¹H-NMR [400MHz, DMSO-d₆] spectrum of 1-butyl-N-phenyl-1H-indazole-3-carbohydrazide (8u).

Signature SIF VIT VELLORE
VG-027



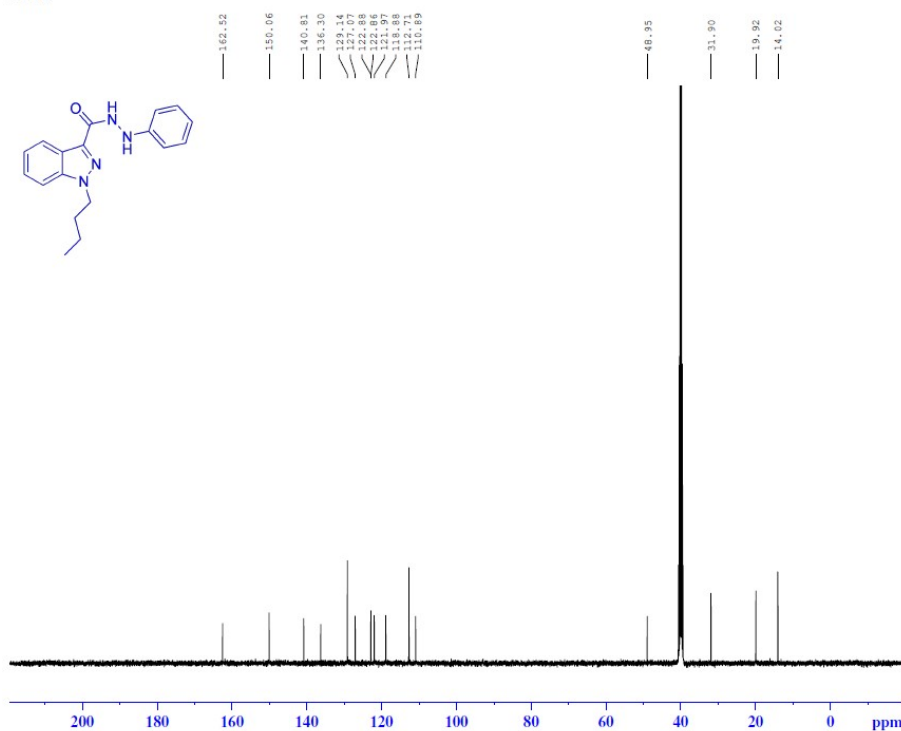
Current Data Parameters
NAME VG-027-8u
EXPNO 39
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230411
Time 11.42 h
INSTRUM spect
PROBHD Z108618_0505 (4
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 127.79
DW 62.400 usec
DE 6.50 usec
TE 303.8 K
D1 1.00000000 sec
TD0 1
SFO1 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PLW1 14.95499992 W

F2 - Processing parameters
SI 65536
SF 400.2580288 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹³C-NMR [100MHz, DMSO-d₆] spectrum of 1-butyl-N-phenyl-1H-indazole-3-carbohydrazide (8u).

Signature SIF VIT VELLORE
VG-027



BRUKER

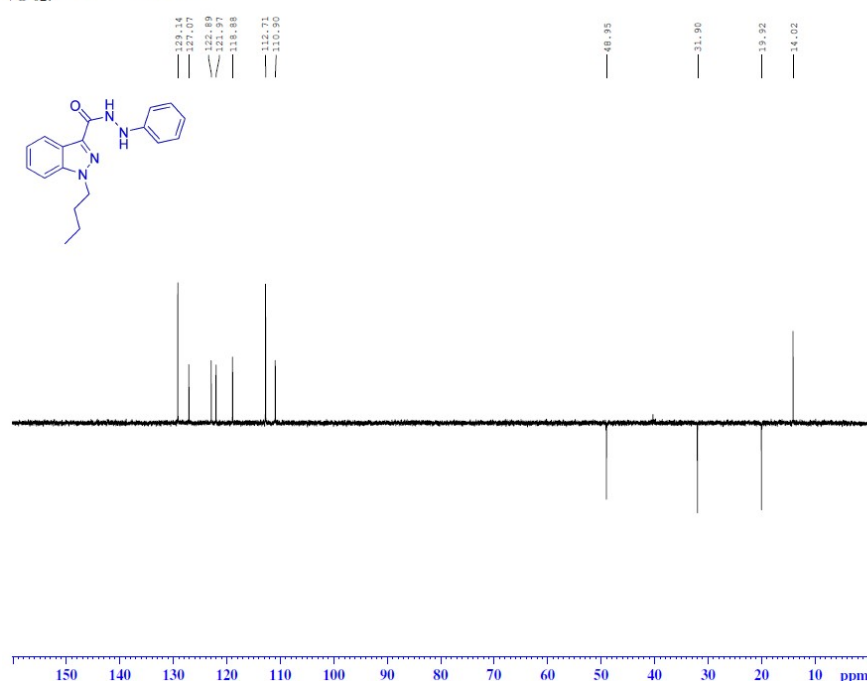
Current Data Parameters
NAME Dr.VVR130423
EXPNO 49
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230414
Time 1.19 h
INSTRUM spect
PROBHD Z108618_0505 (4
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 112.69
DW 20.800 usec
DE 6.50 usec
TE 303.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6550186 MHz
NUC1 13C
P1 10.00 usec
PLW1 58.22499847 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 14.95499992 W
PLW12 0.41542000 W
PLW13 0.20895000 W

F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

¹³⁵DEPT-NMR [100MHz, DMSO-d₆] spectrum of 1-butyl-N-phenyl-1H-indazole-3-carbohydrazide (8u).

Signature SIF VIT VELLORE
VG-027



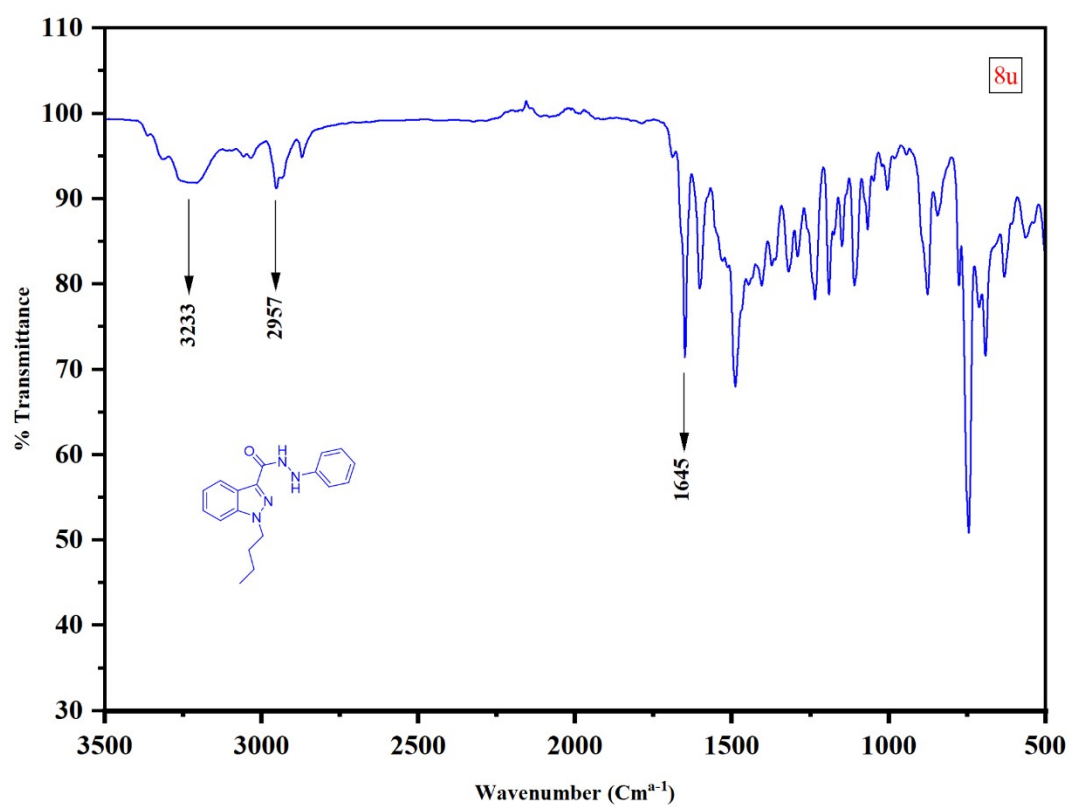
BRUKER

Current Data Parameters
NAME Dr.VVR130423
EXPNO 50
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230414
Time 1.39 h
INSTRUM spect
PROBHD Z108618_0505 (4
PULPROG deptsp135
TD 65536
SOLVENT DMSO
NS 256
DS 8
SWH 16129.032 Hz
FIDRES 0.492219 Hz
AQ 2.0316160 sec
RG 199.6
DW 31.000 usec
DE 6.50 usec
TE 302.9 K
CNST2 145.0000000
D1 2.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1
SFO1 100.6530057 MHz
NUC1 13C
P1 10.00 usec
P13 2000.00 usec
PLW0 0 W
PLW1 58.22499847 W
SPNAM[5] Crp60comp.4
SPCAL5 0.500
SCOFF5 0 Hz
SPW5 8.89610004 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG2 waltz16
P3 15.00 usec
F4 30.00 usec
PCPD2 90.00 usec
PLW2 14.95499992 W
PLW12 0.41542000 W

F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

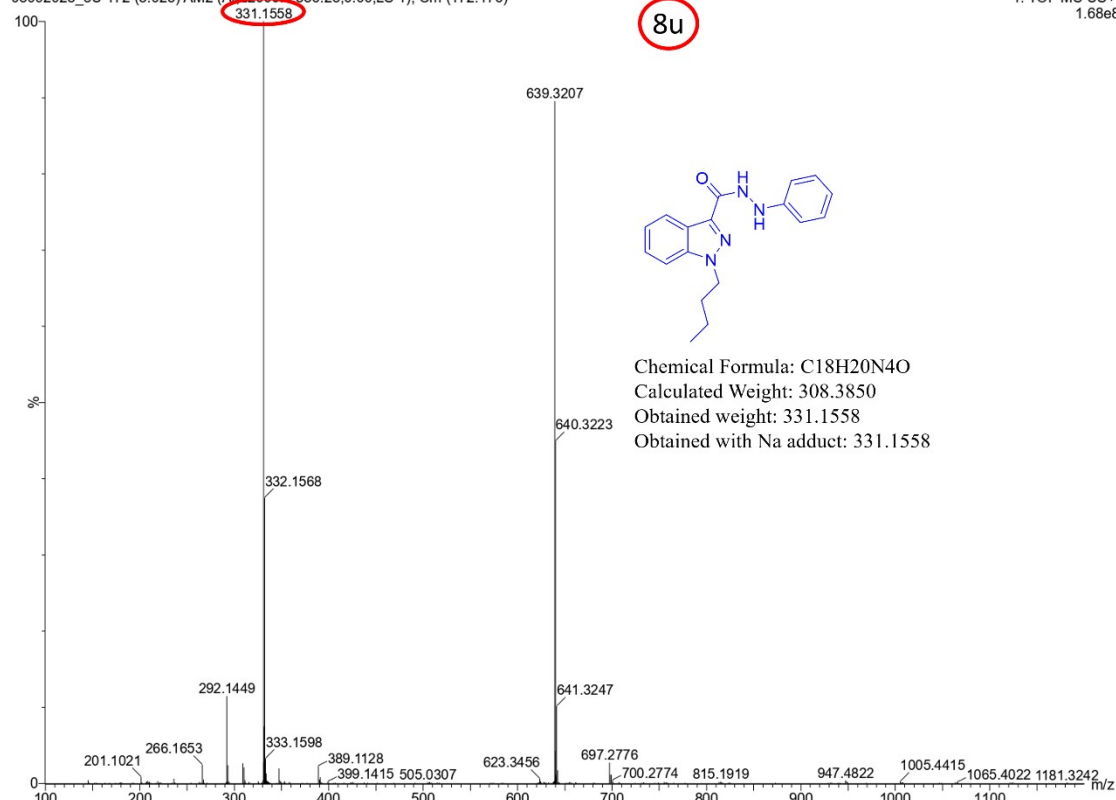
FT-IR spectrum of 1-butyl-N-phenyl-1H-indazole-3-carbohydrazide (8u).



HRMS of 1-butyl-N-phenyl-1H-indazole-3-carbohydrazide (8u).

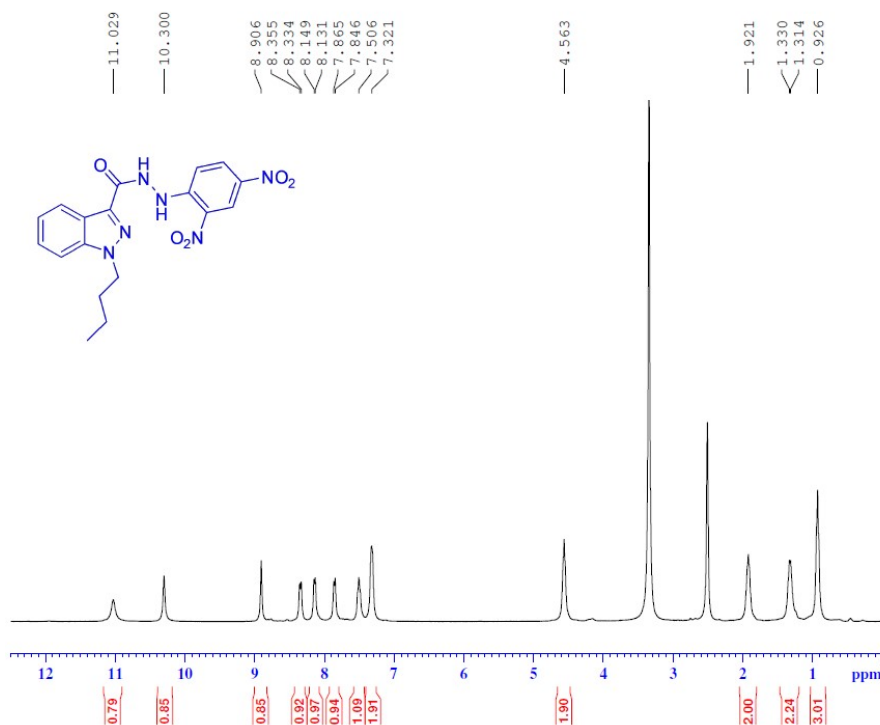
08092023_8U 172 (3.025) AM2 (Ar 22000.0 556.28,0.00,LS 1); Cm (172:176)

1: TOF MS US+
1.68e8



¹H-NMR [400MHz, DMSO-d₆] spectrum of 1-butyl-N-(2,4-dinitrophenyl)-1H-indazole-3-carbohydrazide (8v).

Signature SIF VIT VELLORE
VG-028



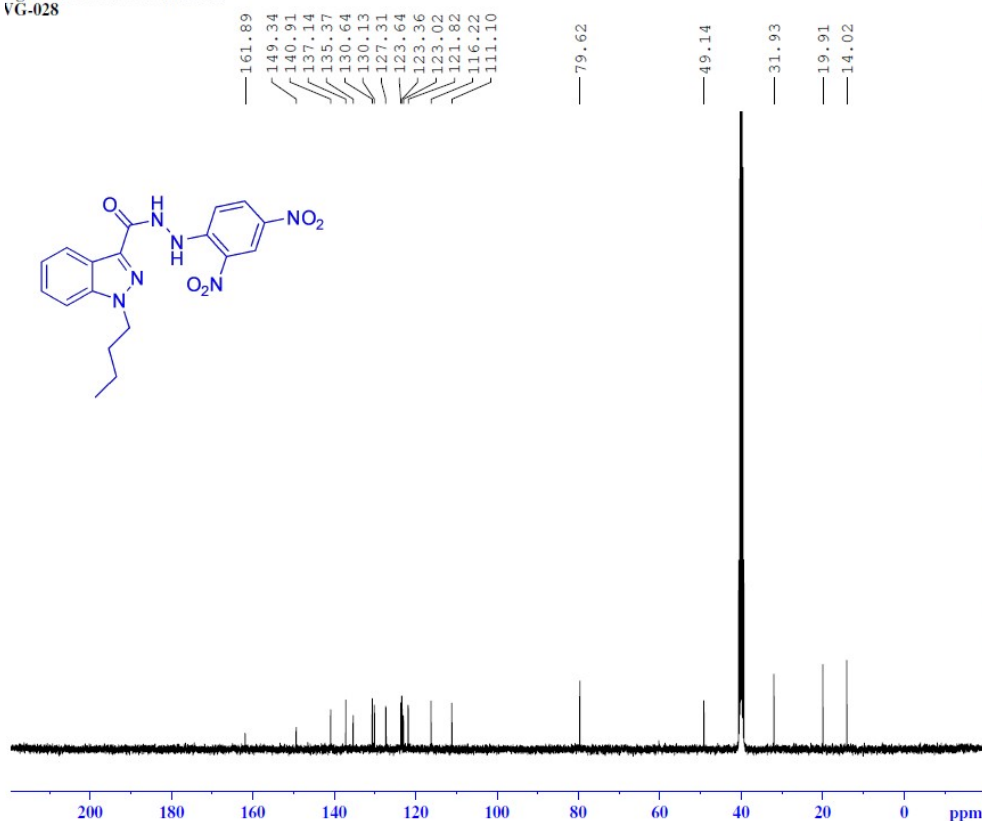
Current Data Parameters
NAME VG-028-8v
EXPNO 41
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230413
Time 13.33 h
INSTRUM spect
PROBHD Z108618_0505 ()
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 127.79
DW 62.400 usec
DE 6.50 usec
TE 303.7 K
D1 1.00000000 sec
TD0 1
SFO1 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PLW1 14.95499992 W

F2 - Processing parameters
SI 65536
SF 400.2580000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹³C-NMR [100MHz, DMSO-d₆] spectrum of 1-butyl-N-(2,4-dinitrophenyl)-1H-indazole-3-carbohydrazide (8v).

Signature SIF VIT VELLORE
VG-028



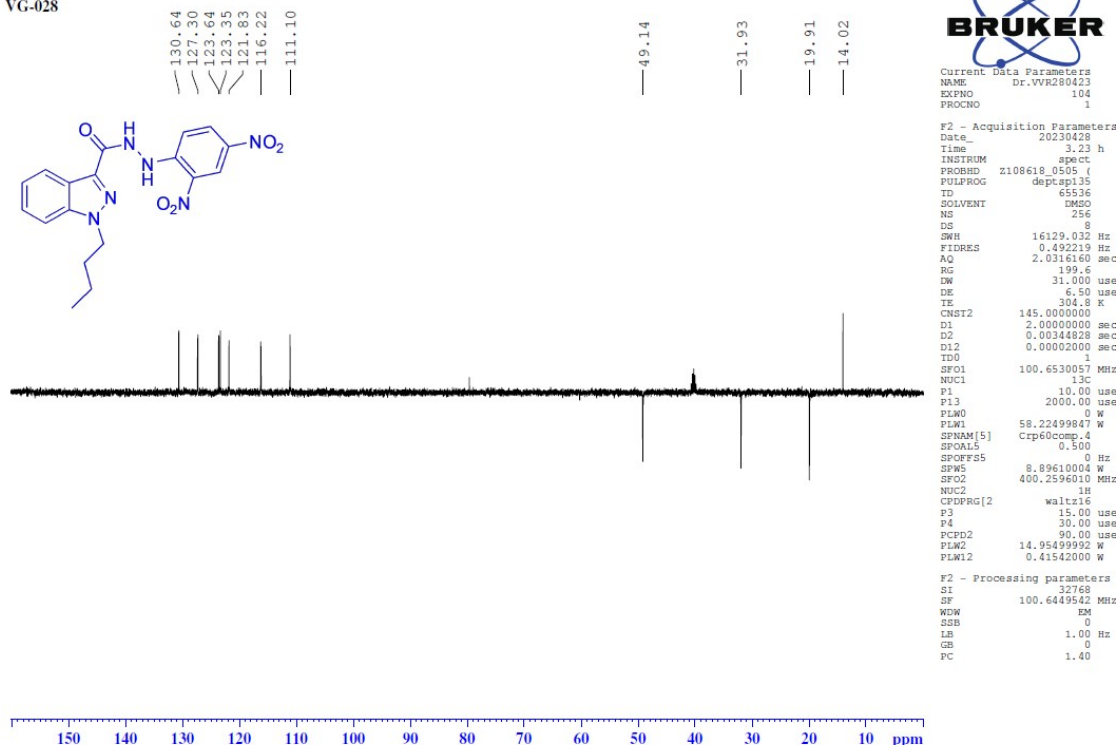
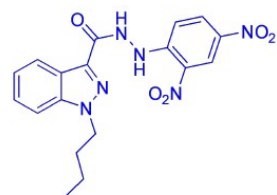
Current Data Parameters
NAME Dr.VVR060523
EXPNO 13
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230506
Time 6.55 h
INSTRUM spect
PROBHD Z108618_0505 ()
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 199.6
DW 20.800 usec
DE 6.50 usec
TE 303.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6550186 MHz
NUC1 13C
P1 10.00 usec
PLW1 58.22499847 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 14.95499992 W
PLW12 0.41542000 W
PLW13 0.20895000 W

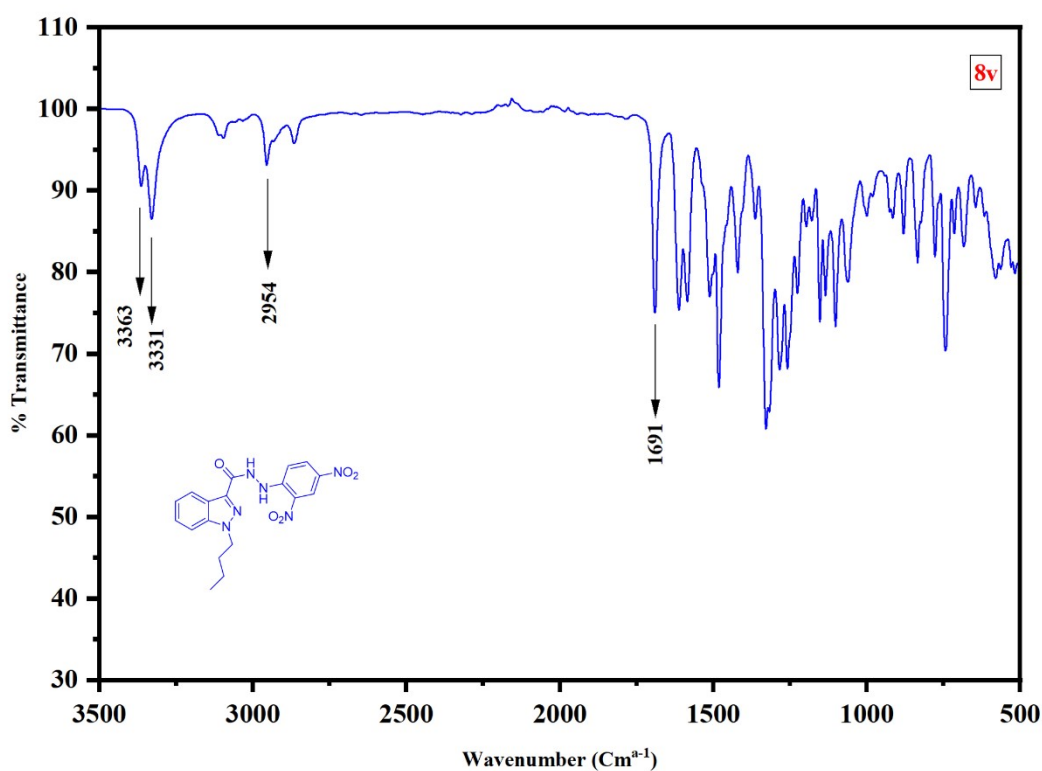
F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

¹³⁵-DEPT-NMR [100MHz, DMSO-d₆] spectrum of 1-butyl-N-(2,4-dinitrophenyl)-1H-indazole-3-carbohydrazide (8v).

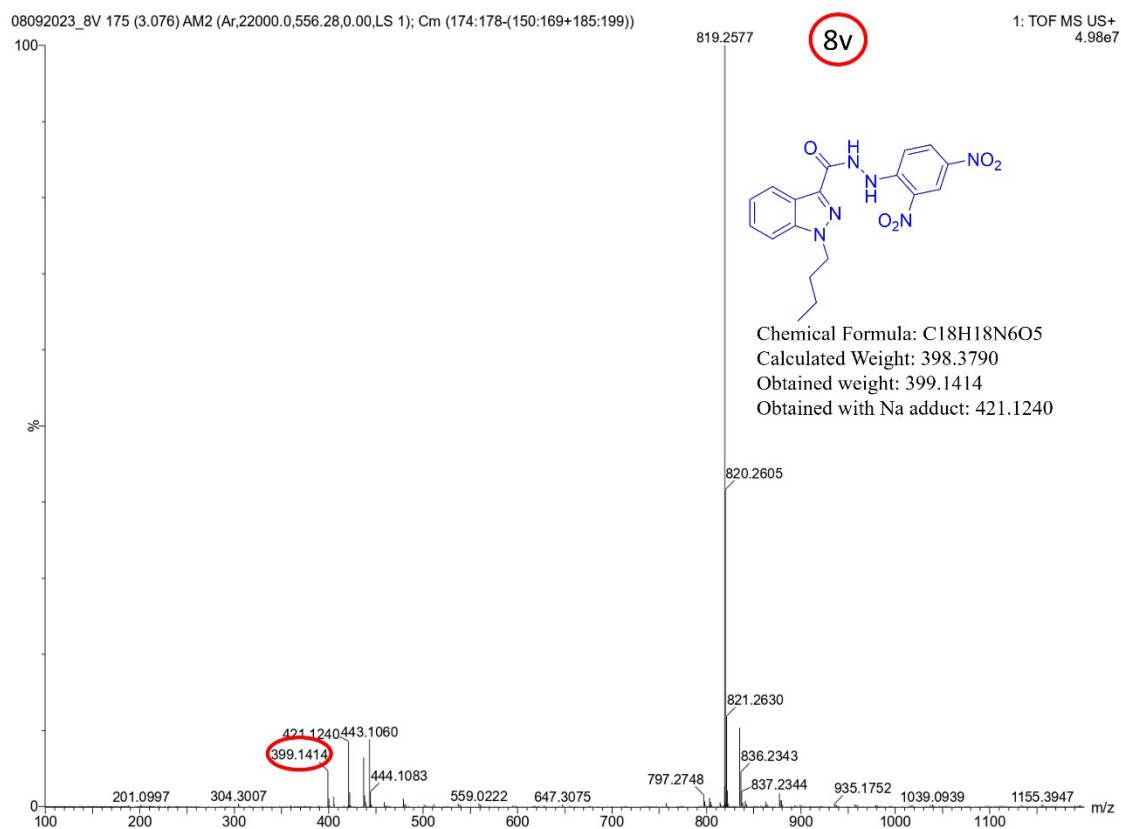
Signature SIF VIT VELLORE
VG-028



FT-IR spectrum of 1-butyl-N-(2,4-dinitrophenyl)-1H-indazole-3-carbohydrazide (8v).

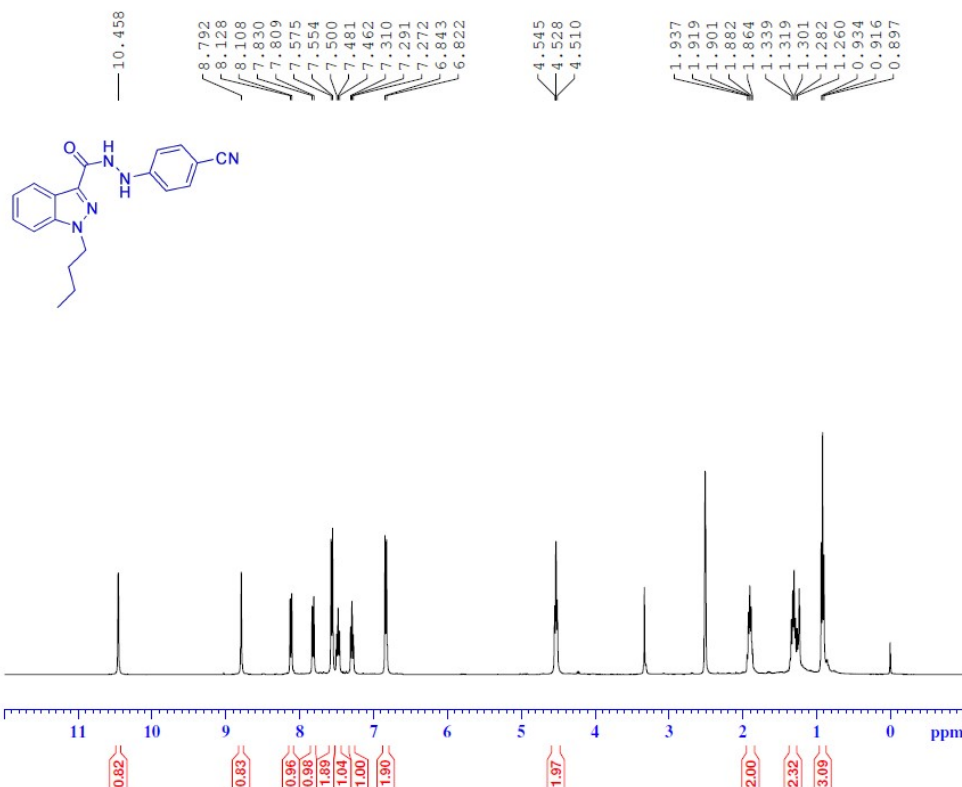


HRMS of 1-butyl-N-(2,4-dinitrophenyl)-1H-indazole-3-carbohydrazide (8v).



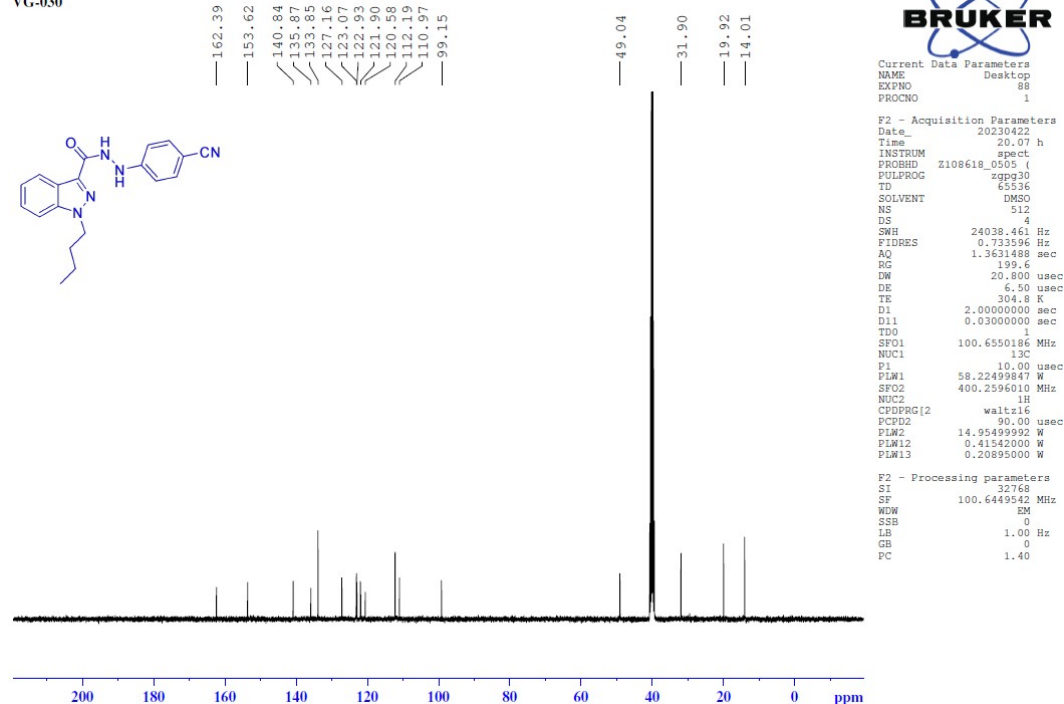
¹H-NMR [100MHz, DMSO-d₆] spectrum of 1-butyl-N-(4-cyanophenyl)-1H-indazole-3-carbohydrazide (8W).

Signature SIF VIT VELLORE
VG-030



¹³C-NMR [100MHz, DMSO-d₆] spectrum of 1-butyl-N-(4-cyanophenyl)-1H-indazole-3-carbohydrazide (8W).

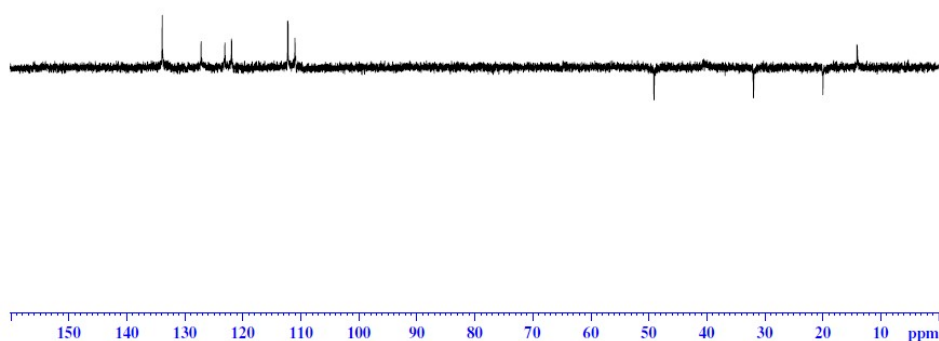
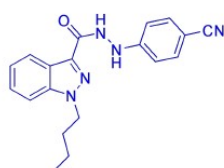
Signature SIF VIT VELLORE
VG-030



¹³⁵-DEPT-NMR [100MHz, DMSO-d₆] spectrum of 1-butyl-N-(4-cyanophenyl)-1H-indazole-3-carbohydrazide (8W).

Signature SIF VIT VELLORE
VG-030

133.85
127.16
123.07
121.91
112.20
110.98

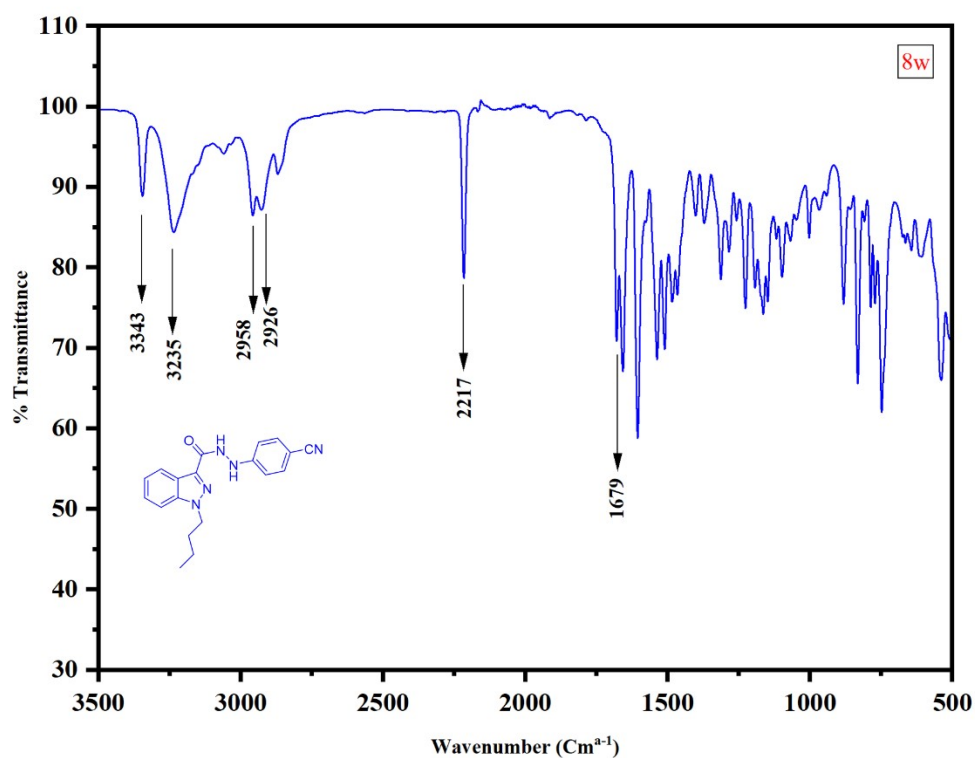


Current Data Parameters
NAME Dr.VVR260423
EXPNO 95
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230426
Time 2.33 h
INSTRUM spect
PROBHD Z108618_0505 ()
PULPROG deptapi35
TD 65536
SOLVENT DMSO
NS 256
DS 8
SWH 16129.032 Hz
FIDRES 0.492219 Hz
AQ 2.0316160 sec
RG 199.6
DW 31.000 usec
DE 6.50 usec
TE 305.5 K
CNS12 145.0000000
D1 2.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1
SFO1 100.6530057 MHz
NUC1 13C
P1 10.00 usec
P13 2000.00 usec
PLW0 0 W
PLW1 58.22499847 W
SPNAM[5] Crp60comp.4
SFOA5 0.500
SPOFFS5 0 Hz
SPW5 8.89610004 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG[2] waltz16
P2 15.00 usec
P4 30.00 usec
PCPD2 90.00 usec
PLW2 14.95499992 W
PLW12 0.41542000 W

F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

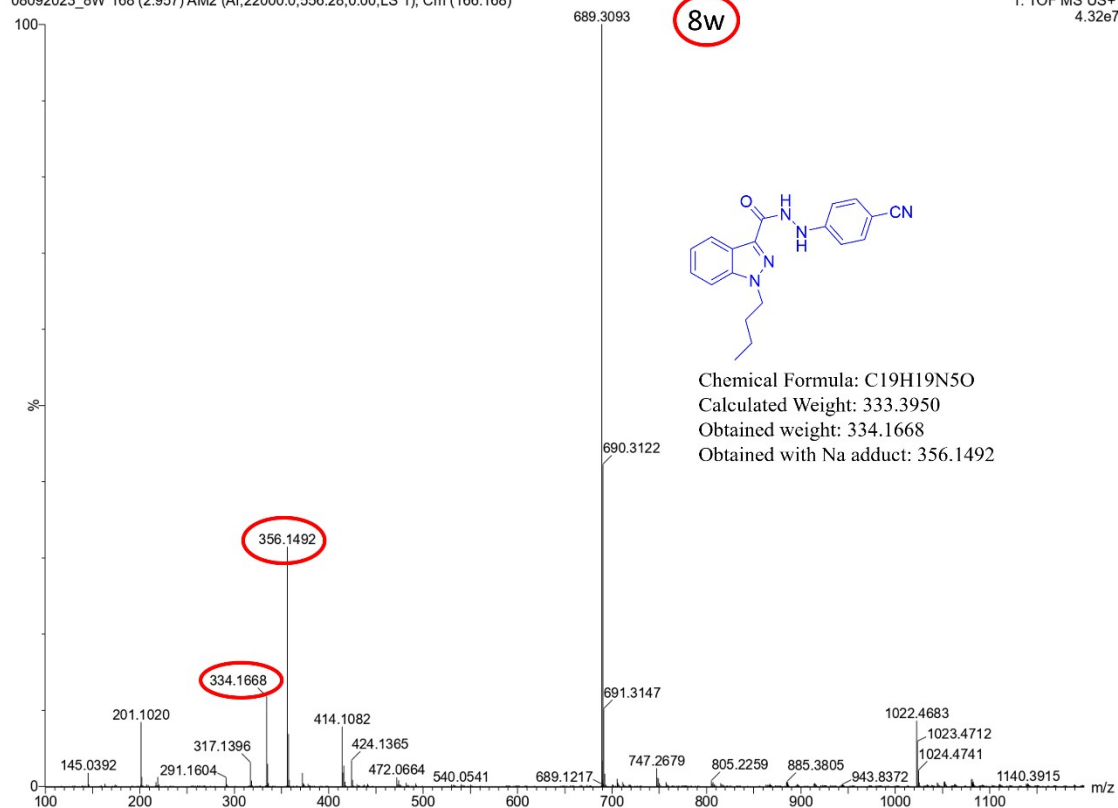
FT-IR spectrum of 1-butyl-N-(4-cyanophenyl)-1H-indazole-3-carbohydrazide (8W).



HRMS of 1-butyl-N-(4-cyanophenyl)-1H-indazole-3-carbohydrazide (8W).

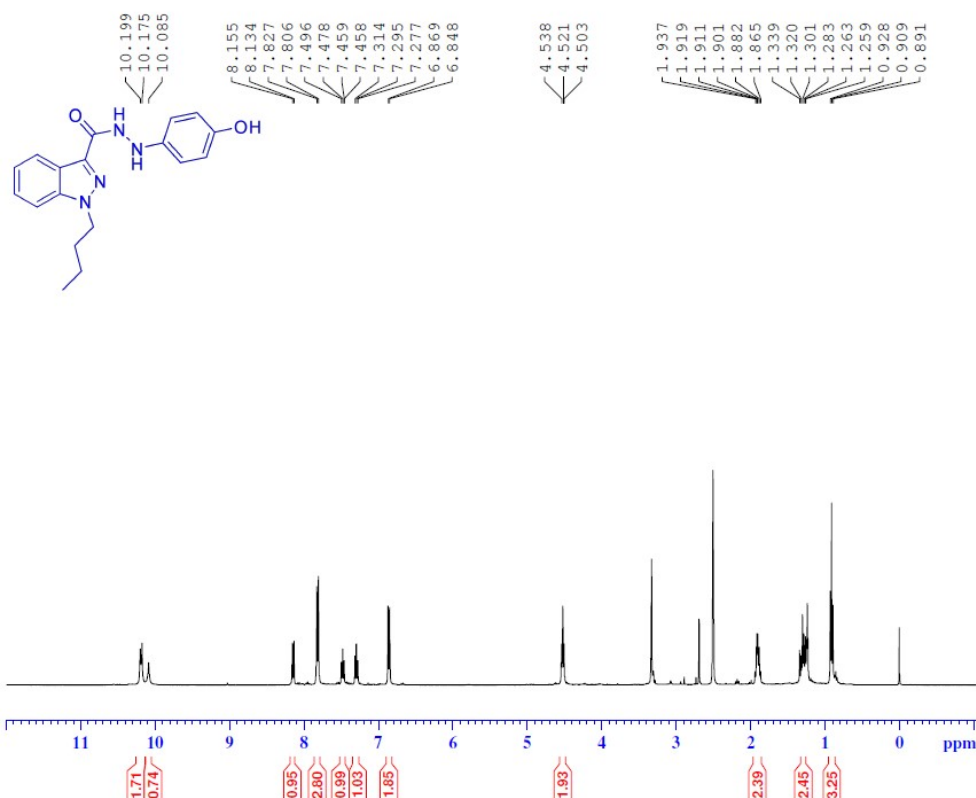
08092023_8W 168 (2.957) AM2 (Ar,22000.0,556.28,0.00,LS 1); Cm (166:168)

1: TOF MS US+
4.32e7



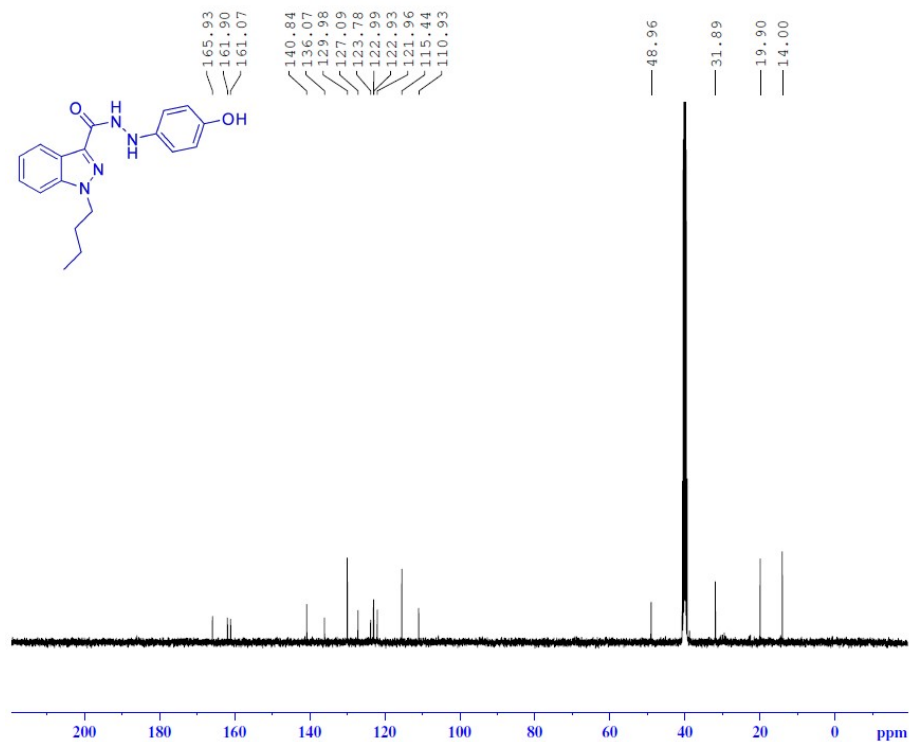
¹H-NMR [400MHz, DMSO-d₆] spectrum of 1-butyl-N-(4-hydroxyphenyl)-1H-indazole-3-carbohydrazide (8x).

Signature SIF VIT VELLORE
VG-031



¹³C-NMR [100MHz, DMSO-d₆] spectrum of 1-butyl-N-(4-hydroxyphenyl)-1H-indazole-3-carbohydrazide (8x).

Signature SIF VIT VELLORE
VG-031



¹³⁵-DEPT-NMR [100MHz, DMSO-d₆] spectrum of 1-butyl-N-(4-hydroxyphenyl)-1H-indazole-3-carbohydrazide (8x).



Current Data Parameters
NAME VG-031-8x
EXPNO 78
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230419
Time 10.36 h
INSTRUM spect
PROBHD Z108618_0505 ()
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 143.73
DW 62.400 usec
DE 6.50 usec
TE 304.3 K
D1 1.00000000 sec
TD0 1
SFO1 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PLW1 14.95499992 W

F2 - Processing parameters
SI 65536
SF 400.2580022 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

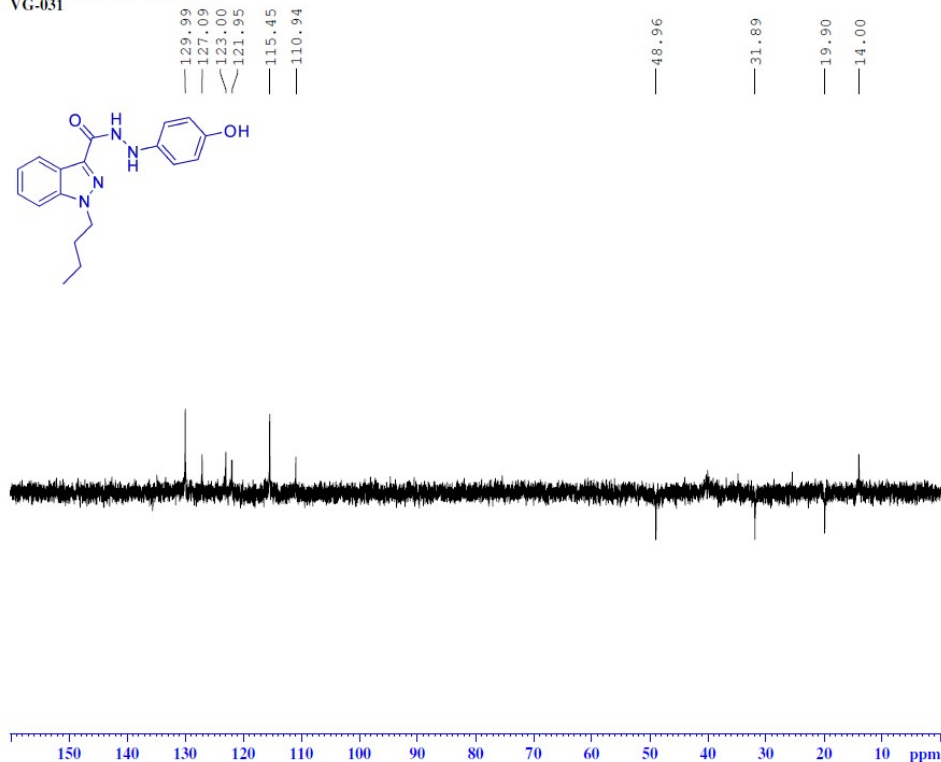
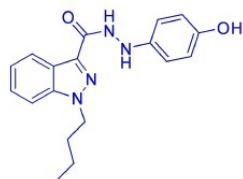


Current Data Parameters
NAME Desktop
EXPNO 87
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230422
Time 19.36 h
INSTRUM spect
PROBHD Z108618_0505 ()
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 199.6
DW 20.800 usec
DE 6.50 usec
TE 304.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6550186 MHz
NUC1 13C
P1 10.00 usec
PLW1 58.22499847 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 14.95499992 W
PLW12 0.41542000 W
PLW13 0.20895000 W

F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Signature SIF VIT VELLORE
VG-031

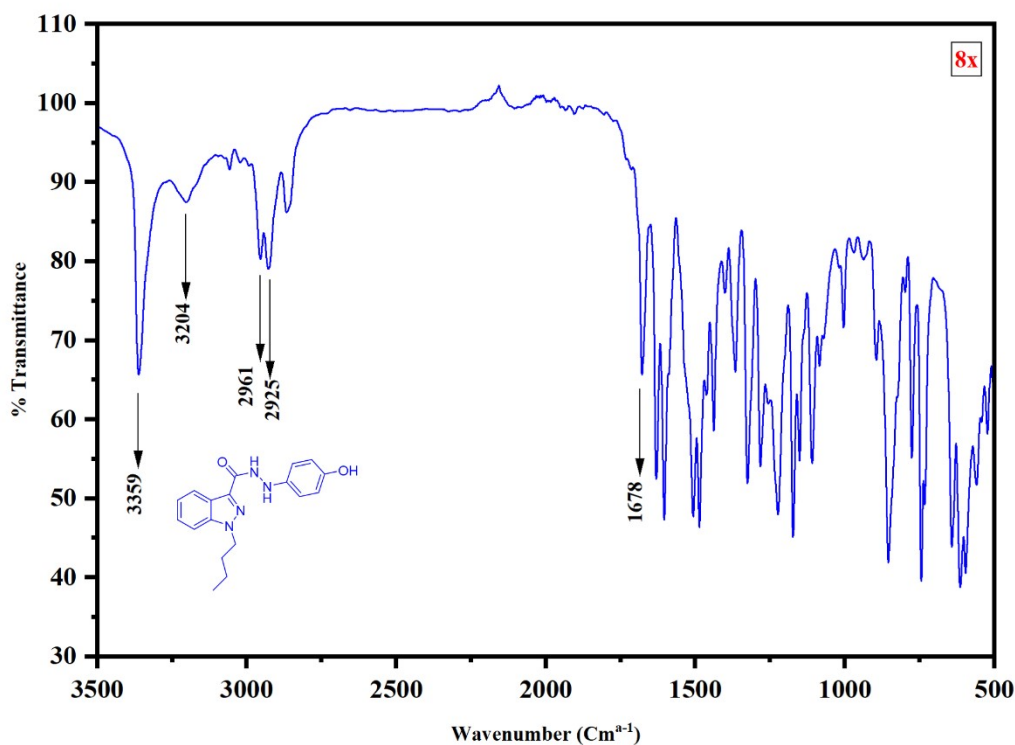


Current Data Parameters
NAME Dr.VVR260423
EXPNO 94
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230426
Time 2.13 h
INSTRUM spect
PROBHD Z108618_0505 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 256
DS 8
SWH 16129.032 Hz
FIDRES 0.492219 Hz
AQ 2.0316160 sec
RG 199.6
DW 31.000 usec
DE 6.50 usec
TE 305.6 K
CNST2 145.000000
D1 2.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1
SFO1 100.6530057 MHz
NUC1 13C
P1 10.00 usec
PL1 2000.00 usec
PLW0 0 W
PLW1 58.22499847 W
SFOAL5 0.500
SFOFF5 0 Hz
SPW5 8.89610004 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG2 waltz16
P3 15.00 usec
P4 30.00 usec
PCPD2 90.00 usec
PLW2 14.95499992 W
PLW12 0.41542000 W

F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WDW EM
GB 0
LB 1.00 Hz
GB 0
PC 1.40

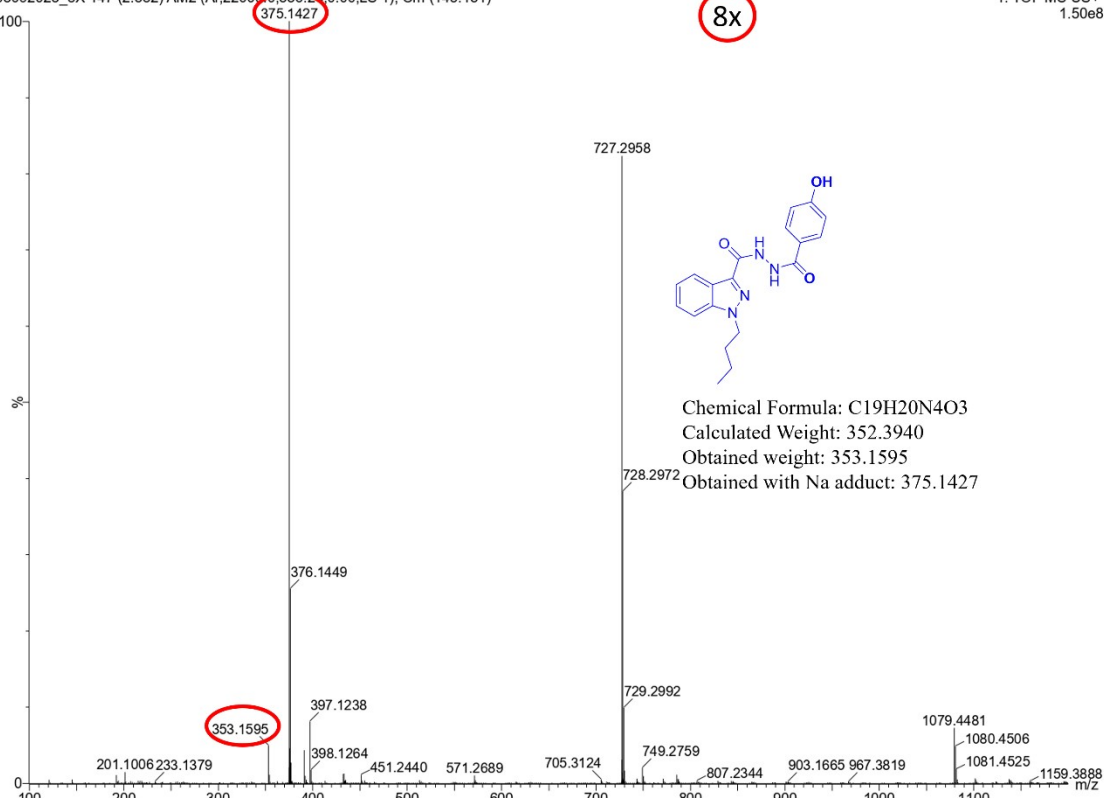
FT-IR spectrum of 1-butyl-N-(4-hydroxyphenyl)-1H-indazole-3-carbohydrazide (8x).



HRMS of 1-butyl-N-(4-hydroxyphenyl)-1H-indazole-3-carbohydrazide (8x).

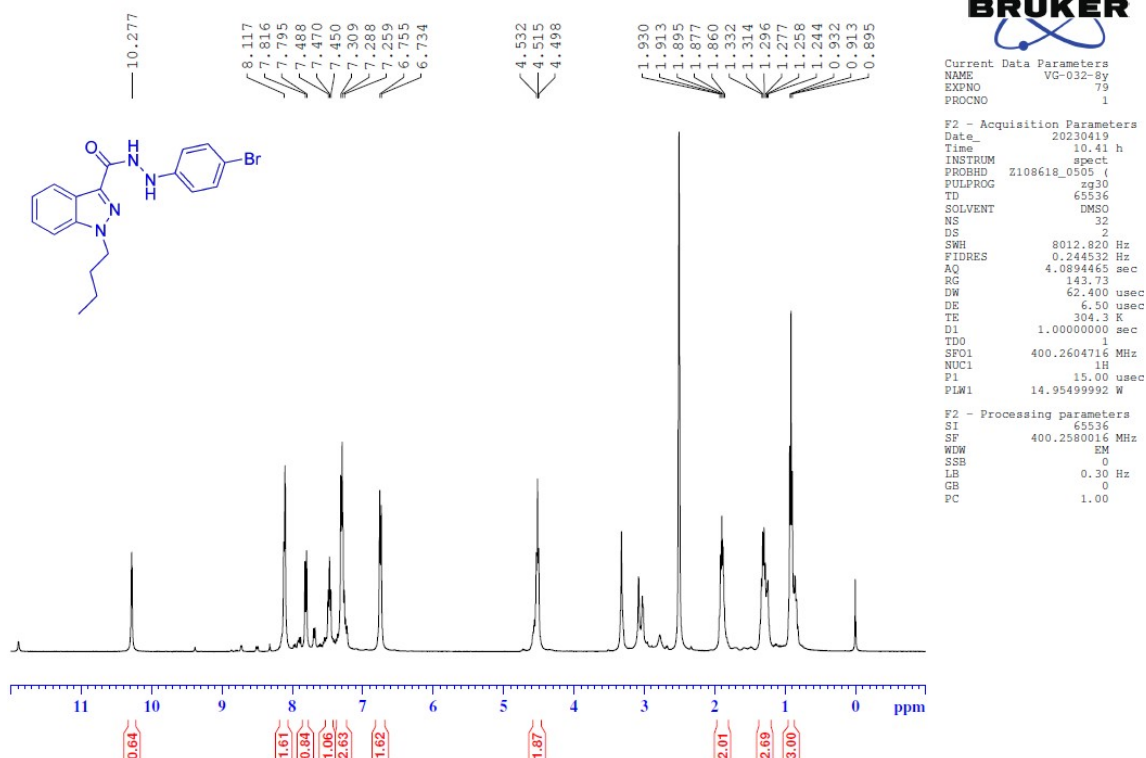
08092023_8X 147 (2.582) AM2 (Ar,22000.8,536.28,0.00,LS 1); Cm (145:151)

1: TOF MS US+
1.50e8



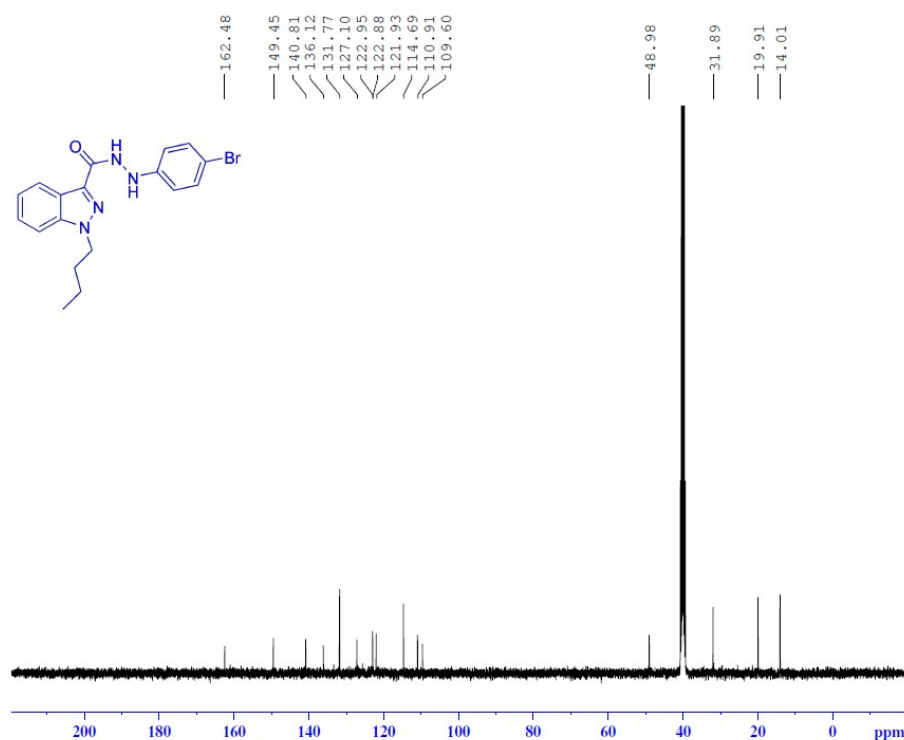
¹H-NMR [400MHz, DMSO-d₆] spectrum of N-(4-bromophenyl)1butyl-1H-indazole-3-carbohydrazide (8y).

Signature SIF VIT VELLORE
VG-032



¹³C-NMR [100MHz, DMSO-d₆] spectrum of N-(4-bromophenyl)1butyl-1H-indazole-3-carbohydrazide (8y).

Signature SIF VIT VELLORE
VG-032



BRUKER

Current Data Parameters

NAME	VG-032-8y
EXPNO	37
PROCNO	1

F2 - Acquisition Parameters

Parameter	Value
Date_	20230512
Time	11.21 h
INSTRUM	spect
PROBHD	Z108618_0505 (
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	512
DS	4
SWH	24038.461 Hz
FIDRES	0.733596 Hz
AQ	1.3611488 sec
RG	199.6
DW	20.800 usec
DE	6.50 usec
TE	305.1 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
SFO1	100.6550186 MHz
NUC1	13C
P1	10.00 usec
PLW1	58.22499847 W
SFO2	400.2596010 MHz
NUC2	1H
CPDPRG[2]	waltz16
PCPD2	90.00 usec
PLW2	14.25499992 W
PLW12	0.41542000 W
PLW13	0.20895000 W

F2 - Processing parameters

Parameter	Value
SI	32768
SF	100.6449542 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

¹³⁵-DEPT-NMR [100MHz, DMSO-d₆] spectrum of N-(4-bromophenyl)1butyl-1H-indazole-3-carbohydrazide (8y).

Signature SIF VIT VELLORE
VG-032

133.31
131.77
127.10
122.95
121.93
114.69
111.06
110.92

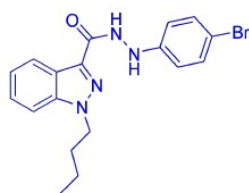
48.99
31.89
19.91
14.01



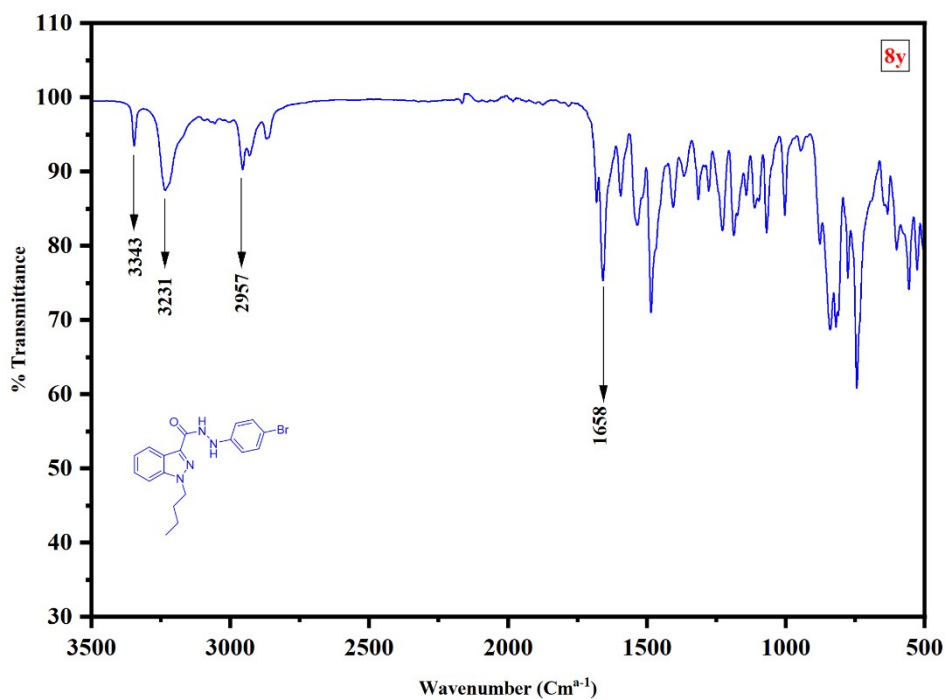
Current Data Parameters
NAME Dr.SW120523
EXPNO 38
PROCNO 1

F2 - Acquisition Parameters
Date 20230512
Time 11.41 h
INSTRUM spect
PROBHD z108618_0505 (deptspl35)
TD 65536
SOLVENT DMSO
NS 256
DS 8
SWH 16129.032 Hz
FIDRES 0.492219 Hz
AQ 2.0316160 sec
RG 199.6
DW 31.000 usec
DE 6.50 usec
TE 305.0 K
CNST2 145.0000000
D1 2.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1
SFO1 100.6530057 MHz
NUC1 13C
P1 10.00 usec
P13 2000.00 usec
PLW0 0 W
PLW1 58.22499847 W
SPNAM[5] Crp60comp.4
SFOAL5 0.500
SFOFFS5 0 Hz
SPW5 8.89610004 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG[2] waltz16
P3 15.00 usec
P4 30.00 usec
PCPD2 90.00 usec
PLW2 14.95499992 W
PLW12 0.41542000 W

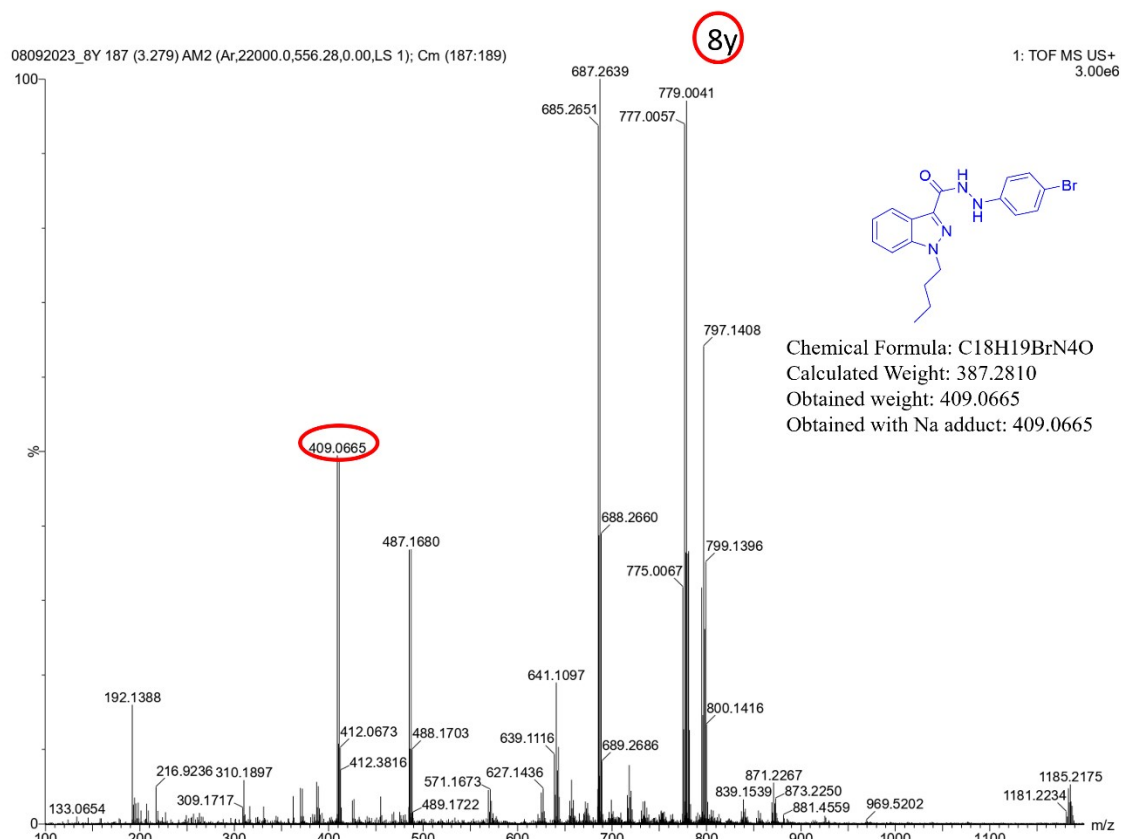
F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



FT-IR spectrum of N-(4-bromophenyl)-1-butyl-1H-indazole-3-carbohydrazide (8y).

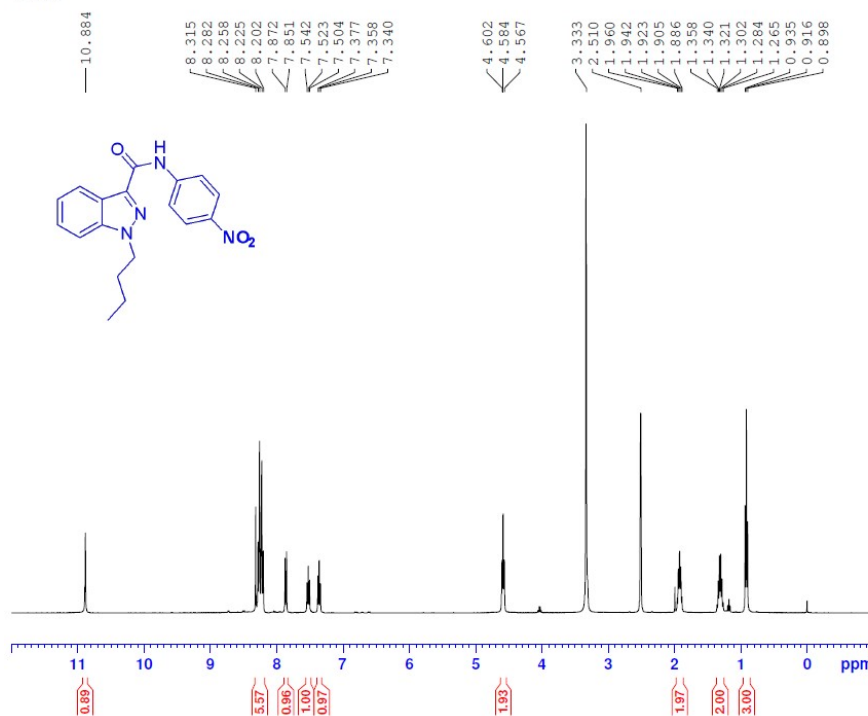


HRMS of N-(4-bromophenyl)-1-butyl-1H-indazole-3-carbohydrazide (8y).



¹H-NMR [400MHz, DMSO-d₆] 1-Butyl-1H-indazole-3-carboxylic acid to 1-butyl-N-(4-nitrophenyl)-1H-indazole-3-carboxamide (8z).

Signature SIF VIT VELLORE
 VG-036



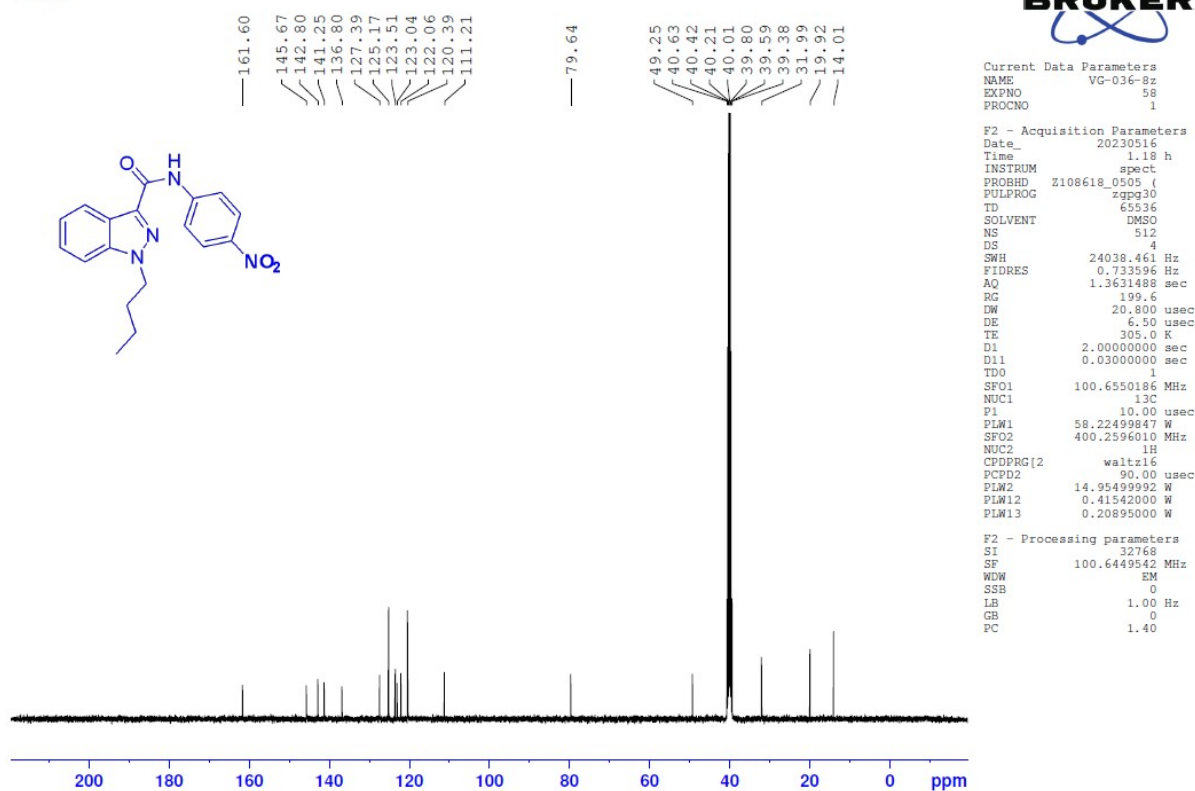
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 EXPNO 70
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 SOLVENT DMSO
 NS 32
 DS 2
 SWH 8012.820 Hz
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 NUC1 1H
 P1 15.00 usec
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F2 - Processing parameters
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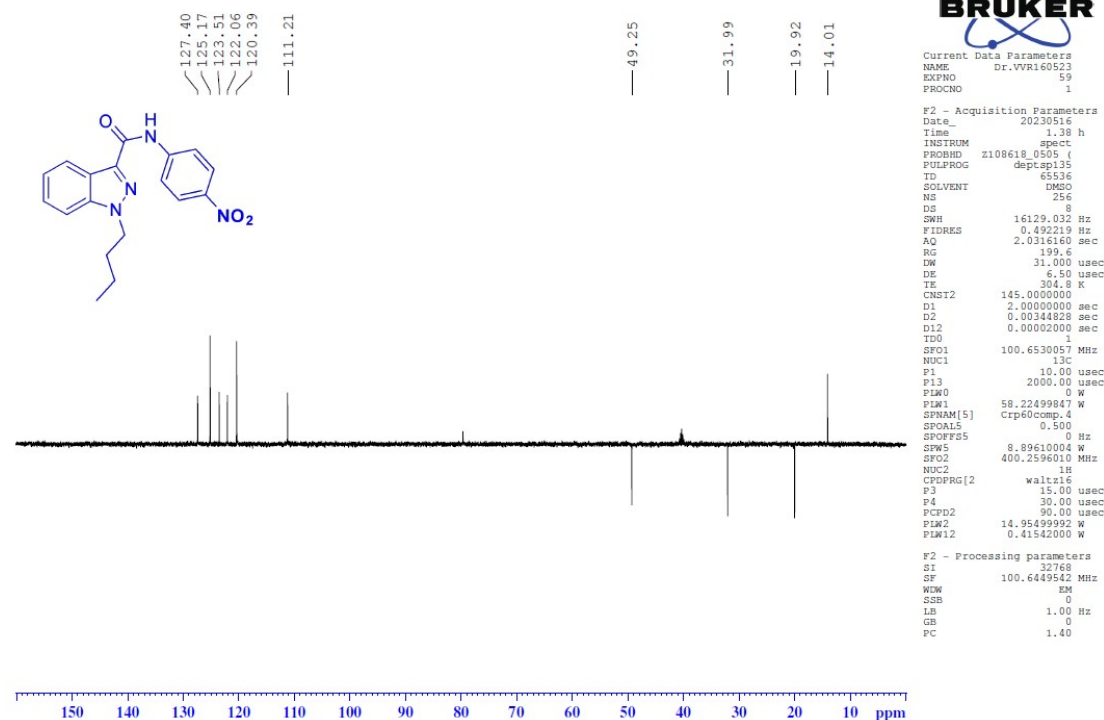
¹³C-NMR [100MHz, DMSO-d₆] 1-Butyl-1H-indazole-3-carboxylic acid to 1-butyl-N-(4-nitrophenyl)-1H-indazole-3-carboxamide (8z).

Signature SIF VIT VELLORE
VG-036

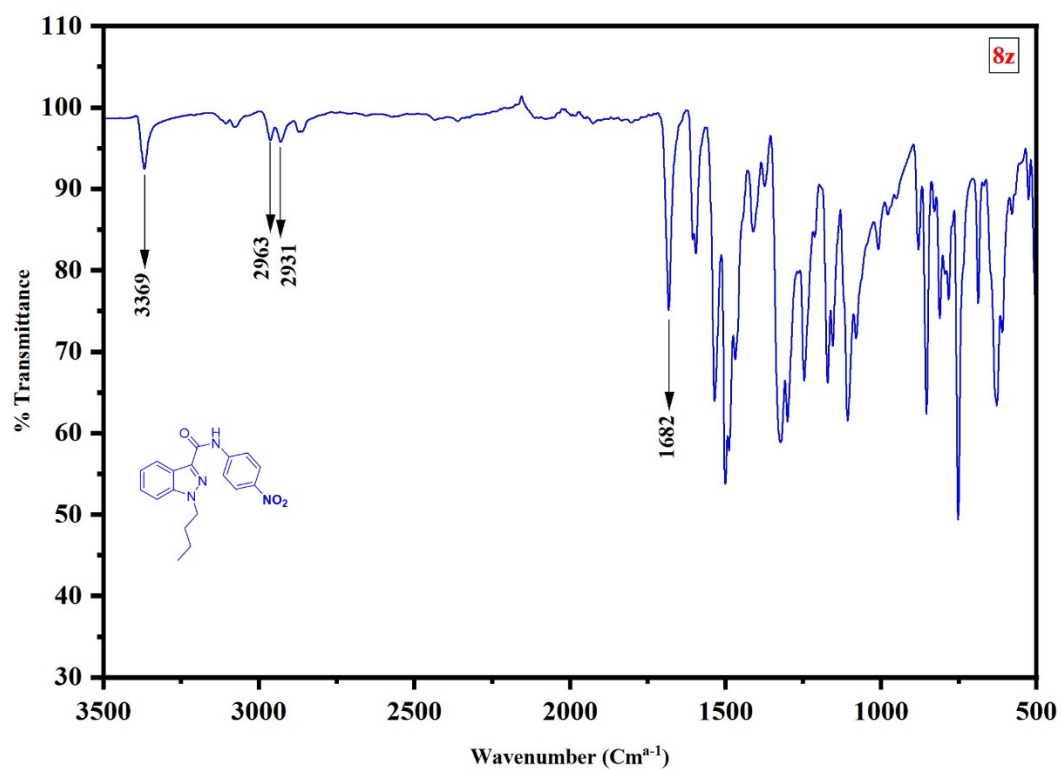


¹³⁵C-NMR [100MHz, DMSO-d₆] 1-Butyl-1H-indazole-3-carboxylic acid to 1-butyl-N-(4-nitrophenyl)-1H-indazole-3-carboxamide (8z).

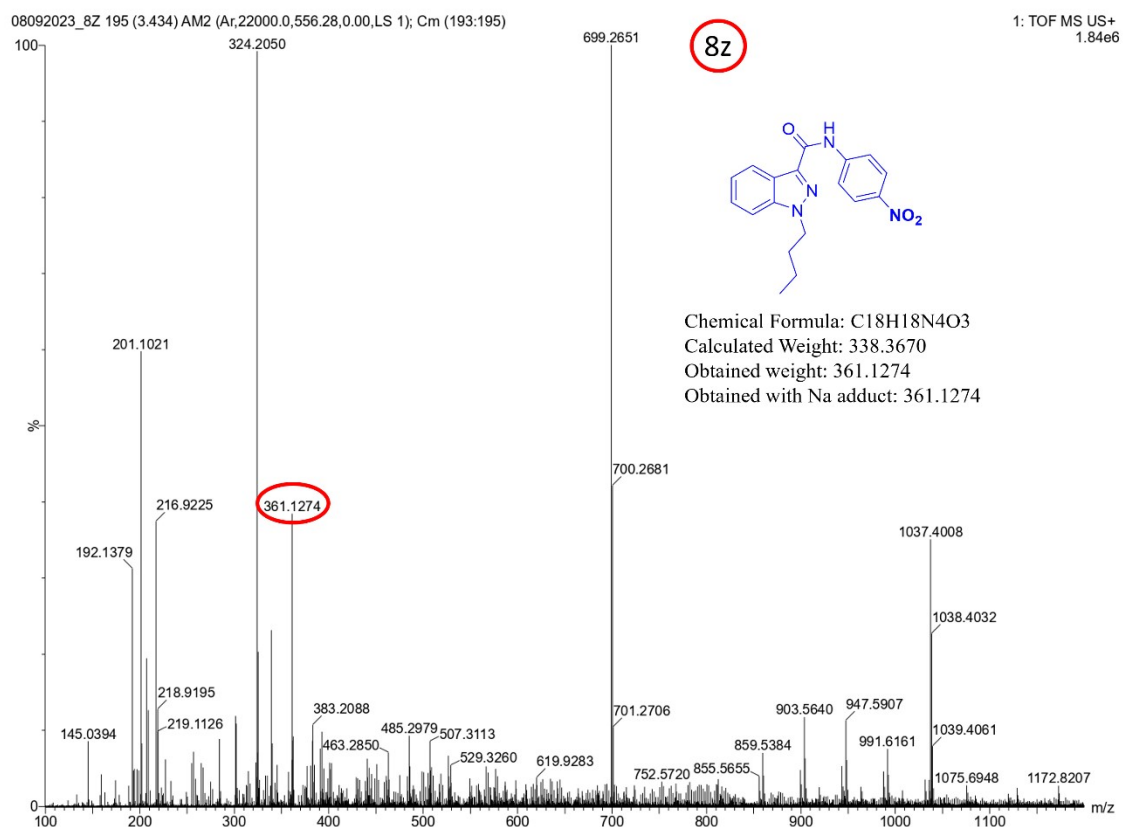
Signature SIF VIT VELLORE
VG-036



FT-IR spectrum of 1-Butyl-1H-indazole-3-carboxylic acid to 1-butyl-N-(4-nitrophenyl)-1H-indazole-3-carboxamide (**8z**).



HRMS of 1-butyl-N-(4-nitrophenyl)-1H-indazole-3-carboxamide (**8z**).



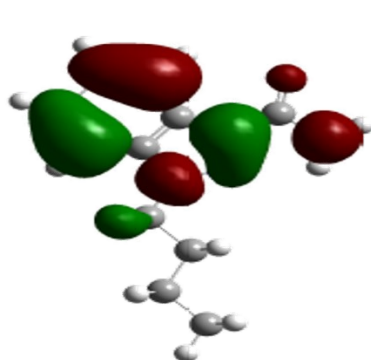
5.DFT studies indazole derivatives with HOMO and LUMO values

S. No:	COMPOUND	HOMO	LUMO	$\Delta E = E_{\text{LUMO}} - E_{\text{HOMO}}$
1	8a	-6.0453	-0.86238	5.18292
2	8b	-5.51394	-1.07163	4.44231
3	8c	-5.88654	-0.81999	5.06655
4	8d	-6.12522	-2.65032	3.4749
5	8e	-5.7888	-1.17666	4.61214
6	8f	-4.44879	-0.98955	3.45924
7	8g	-5.89761	-1.40211	4.4955
8	8h	-5.65434	-2.31201	3.34233
9	8i	-5.62275	-1.21878	4.40397
10	8j	-5.14566	-1.04112	4.10454

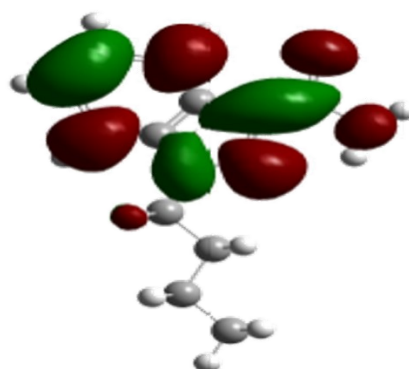
11	8k	-5.23692	-0.92853	4.30839
12	8l	-5.44563	-1.05111	4.39452
13	8m	-5.41485	-1.07244	4.34241
14	8n	-5.67216	-1.00143	4.67073
15	8o	-5.11137	-1.0287	4.08267
16	8p	-5.5039	-1.15128	4.35262
17	8q	-5.21937	-0.92529	4.29408
18	8r	-5.47317	-1.14426	4.32891
19	8s	-6.34878	-1.4283	4.92048
20	8t	-5.27715	-2.60523	2.67192
21	8u	-6.8823	-2.45457	4.42773
22	8v	-6.36687	-3.59964	2.76723
23	8w	-5.08923	-1.32435	3.76488
24	8x	-6.67332	-2.42568	4.24764
25	8y	-4.24305	-1.00143	3.24162
26	8z	-6.4638	-2.77776	6.68604

DFT studies indazole derivatives HOMO & LUMO (8a-8z)

8a

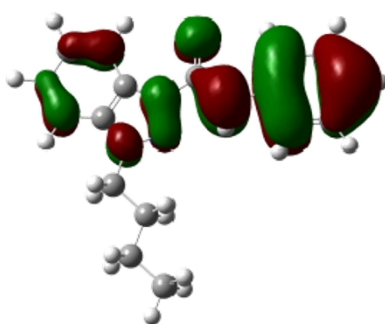


HOMO

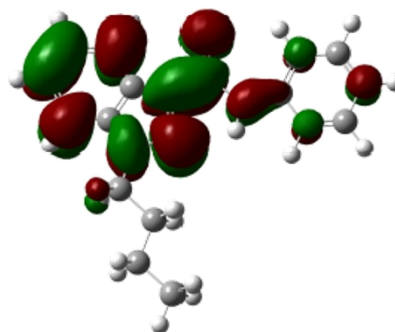


LUMO

8b

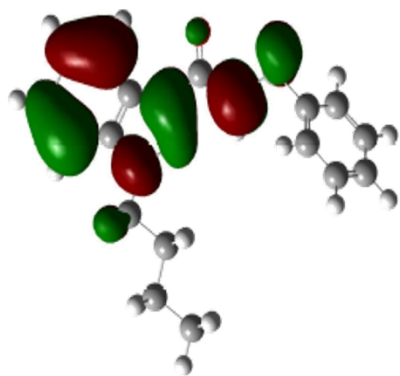


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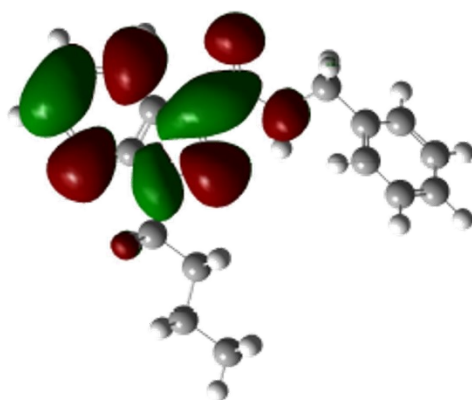


LUMO

8c

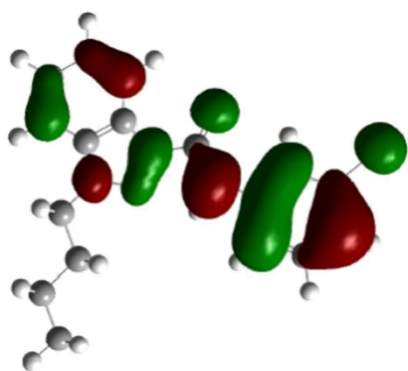


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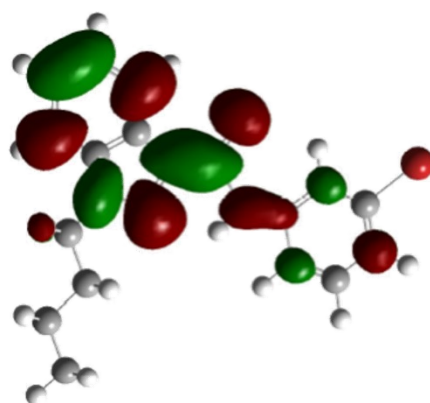


LUMO

8d

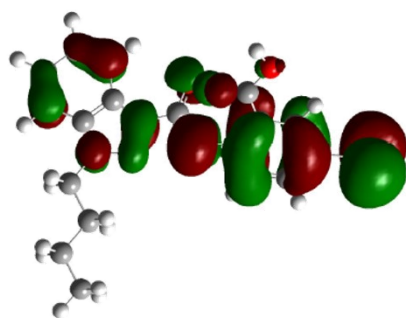


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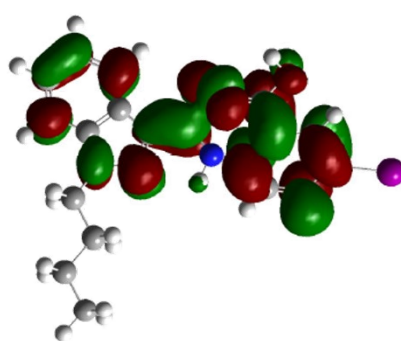


LUMO

8e

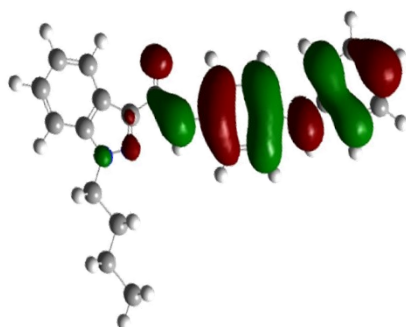


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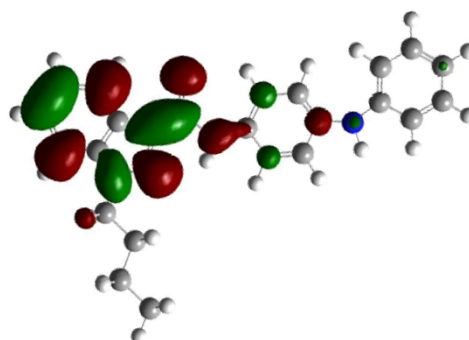


LUMO

8f

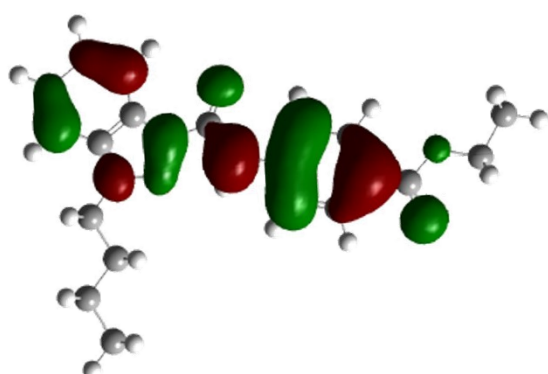


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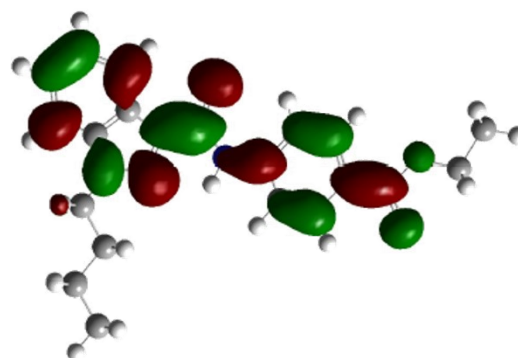


LUMO

8g

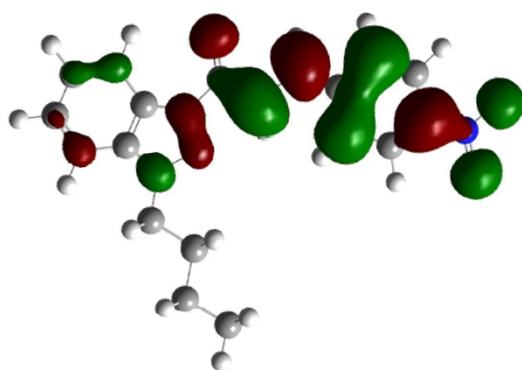


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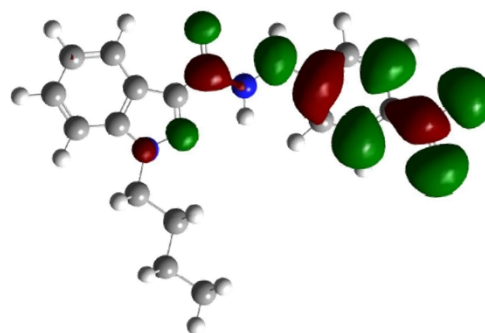


LUMO

8h

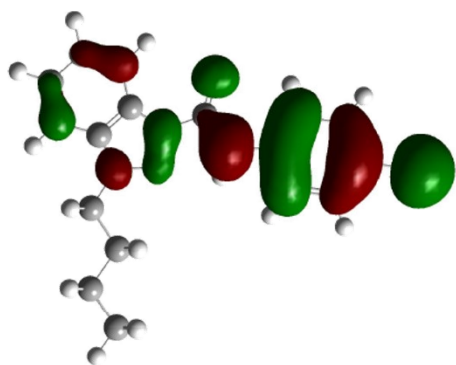


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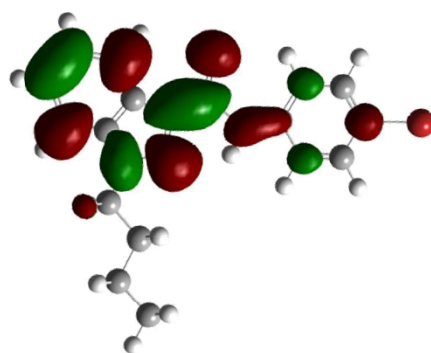


LUMO

8i

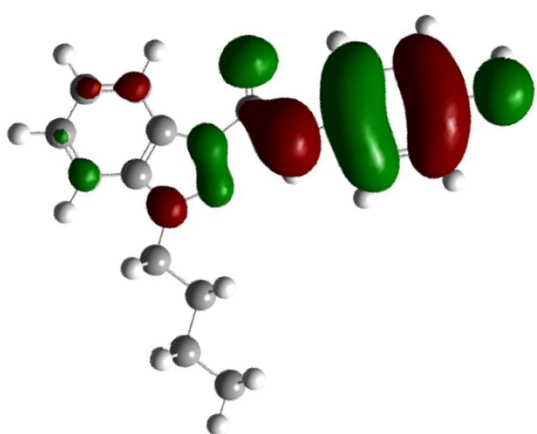


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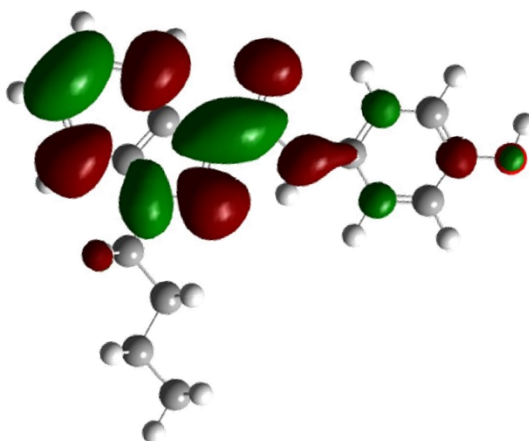


LUMO

8j

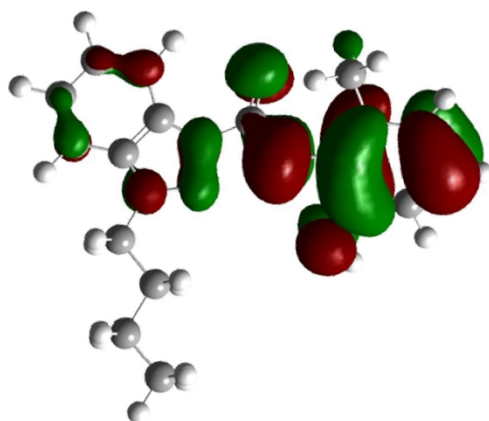


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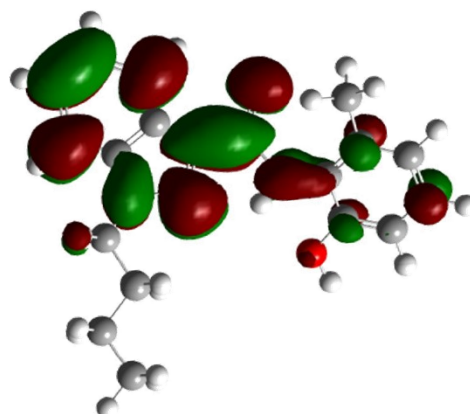


LUMO

8k

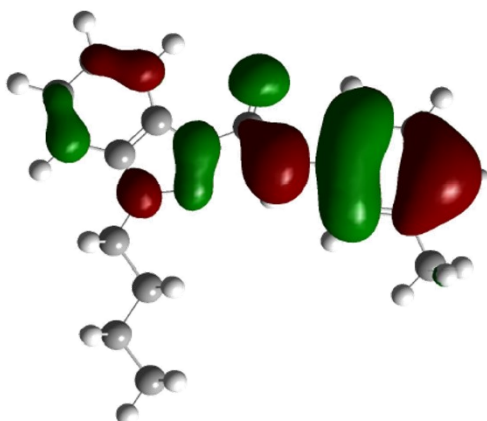


HOMO

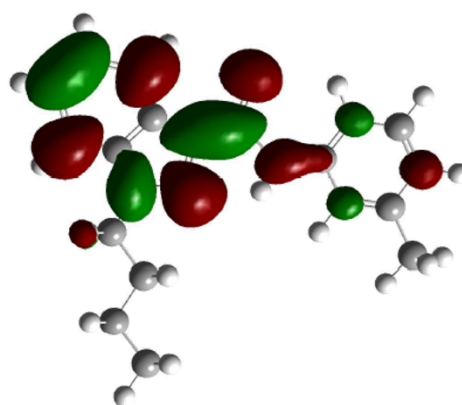


LUMO

8l

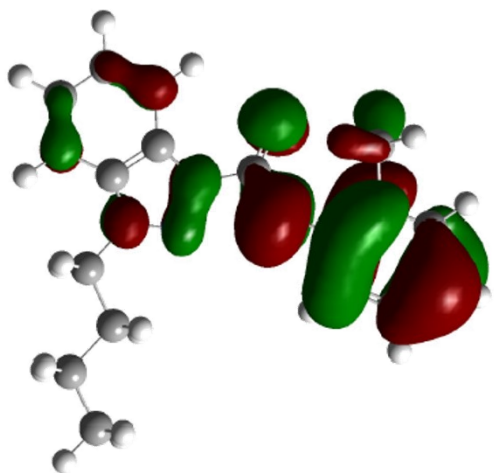


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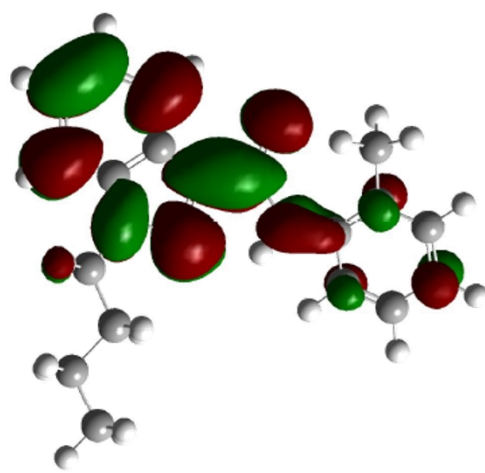


LUMO

8m

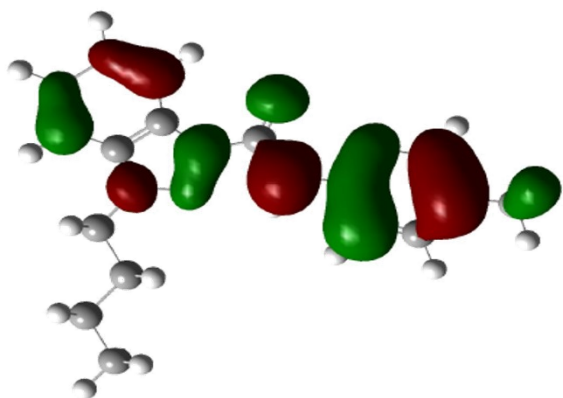


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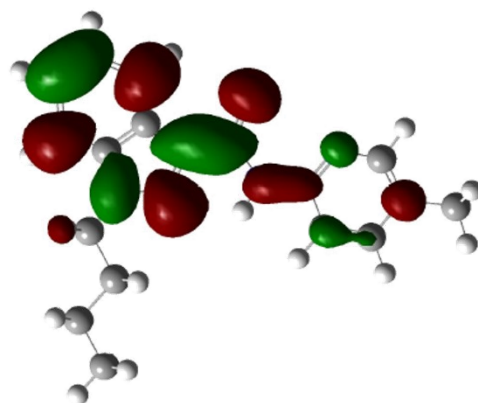


LUMO

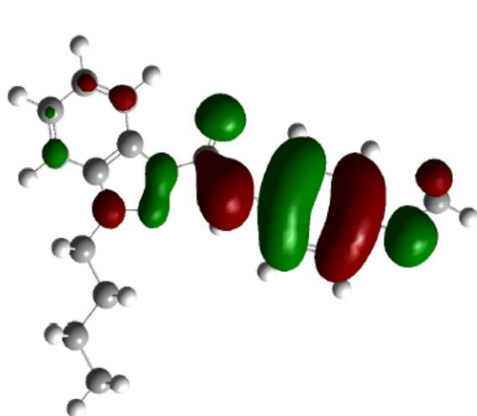
8n



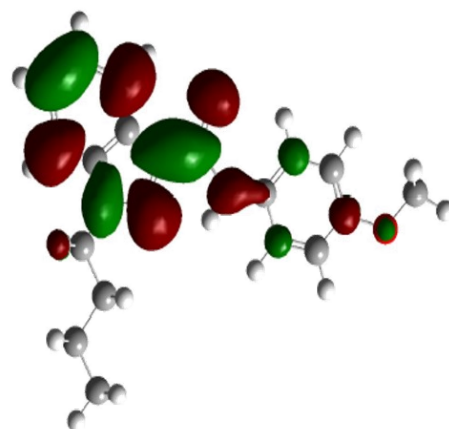
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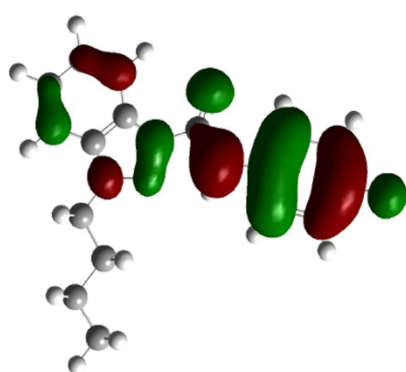


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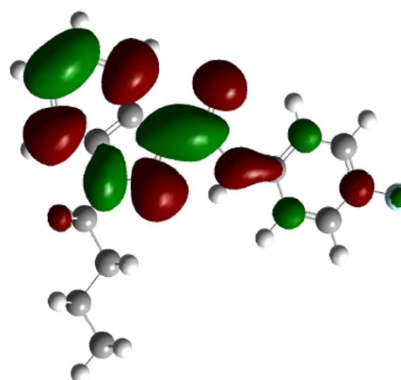


LUMO

8p

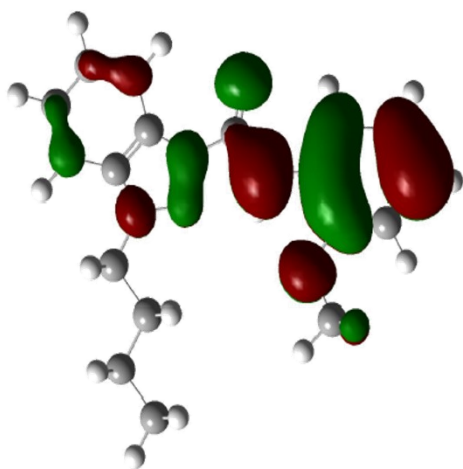


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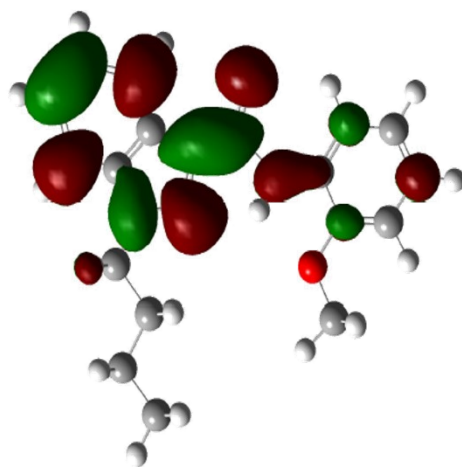


LUMO

8q

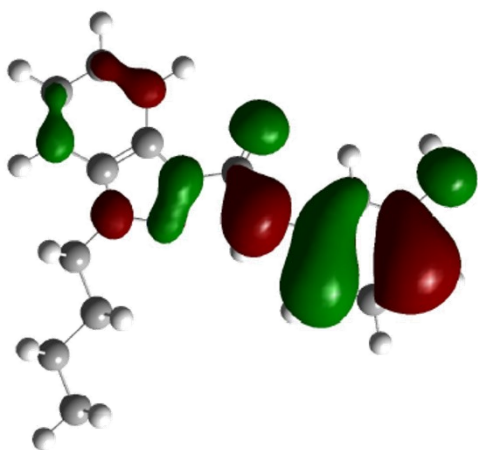


HOMO

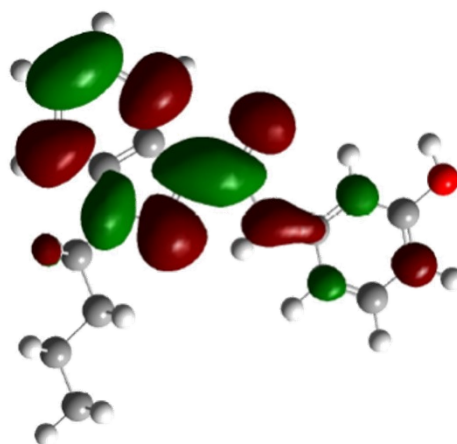


LUMO

8r

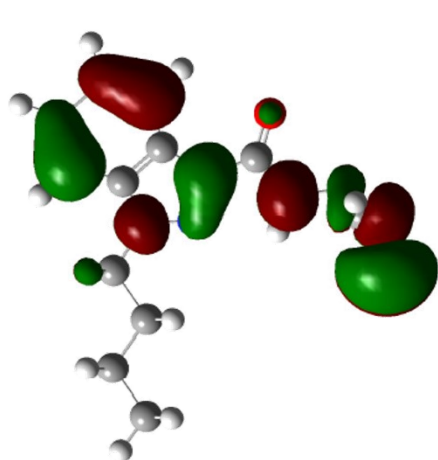


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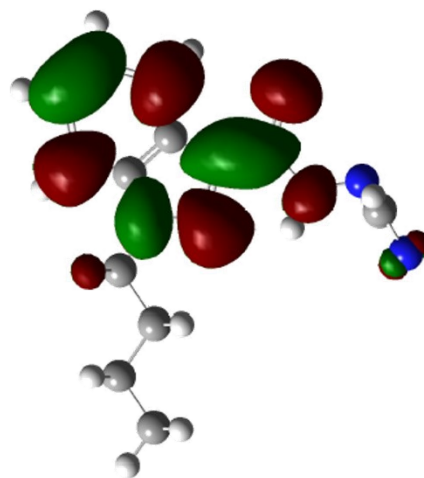


LUMO

8s

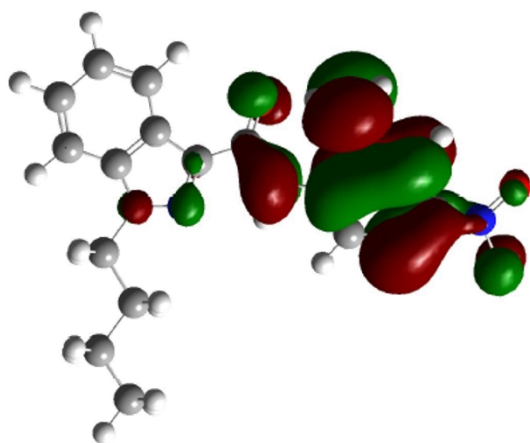


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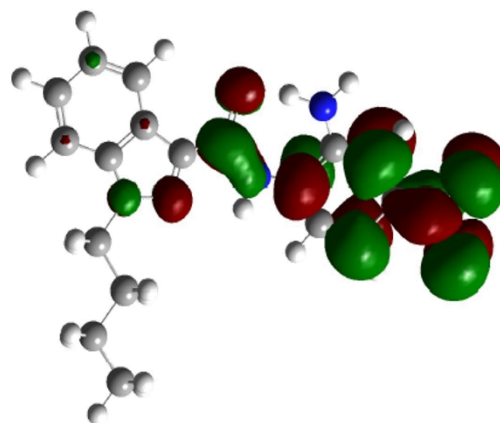


LUMO

8t

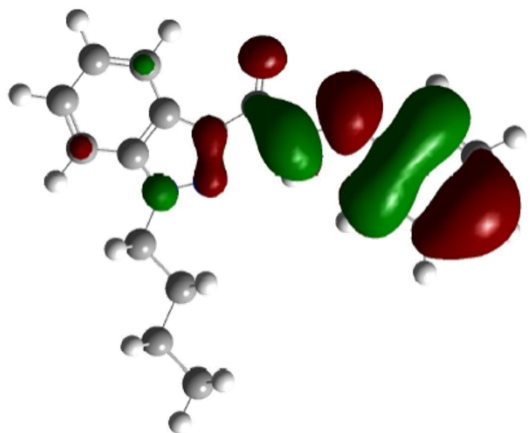


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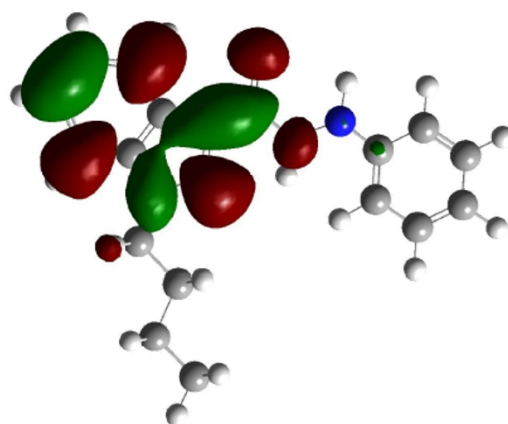


LUMO

8u

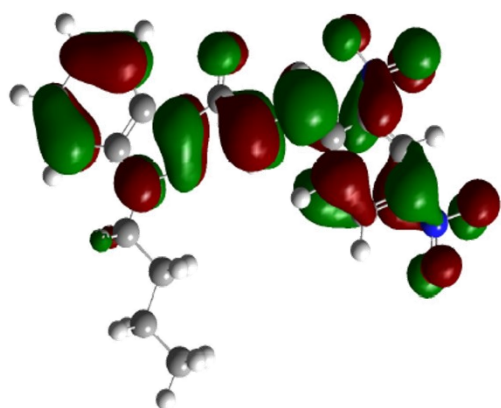


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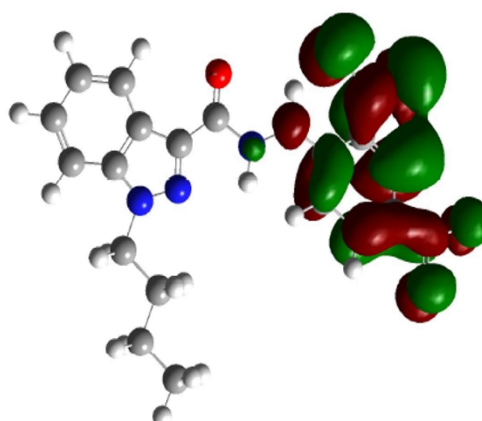


LUMO

8v

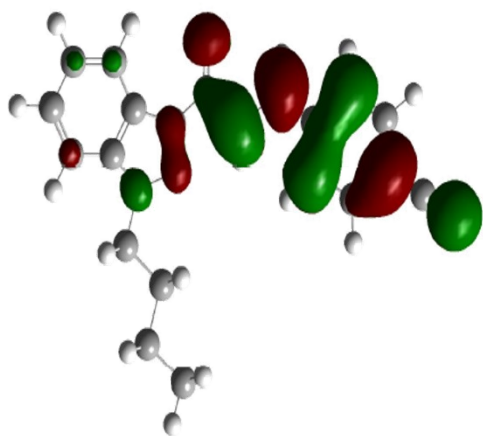


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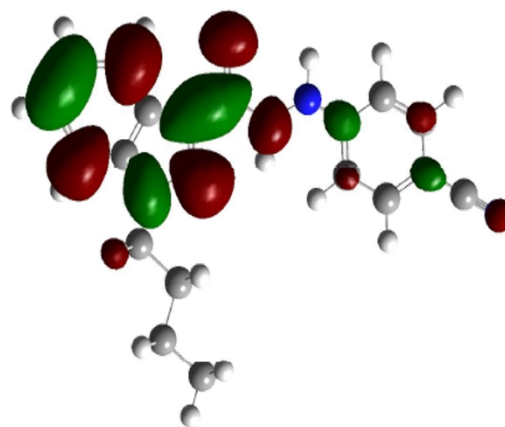


LUMO

8w

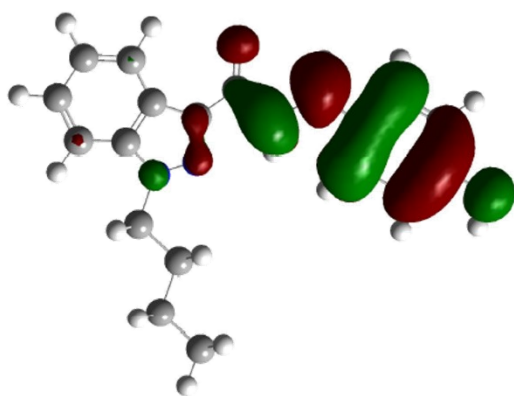


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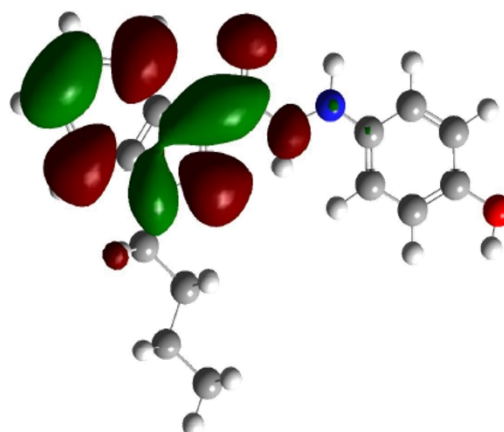


LUMO

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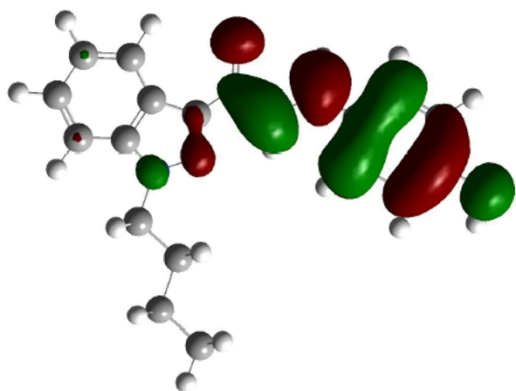


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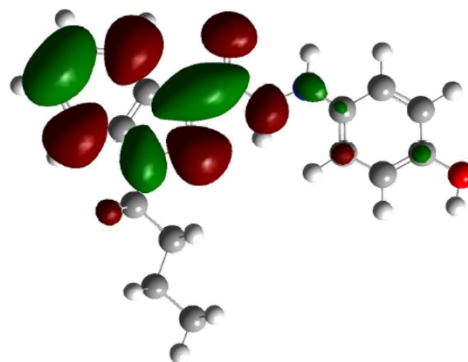


LUMO

8y

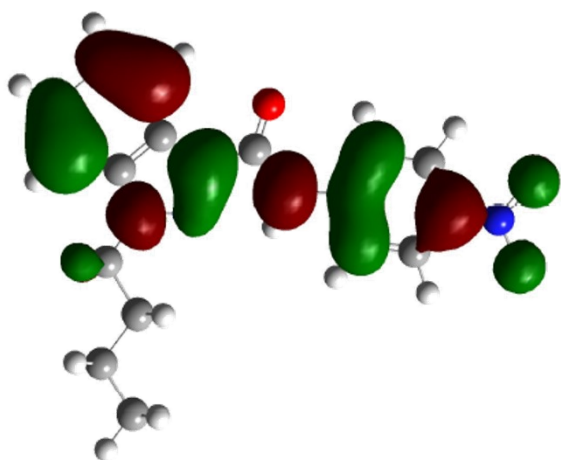


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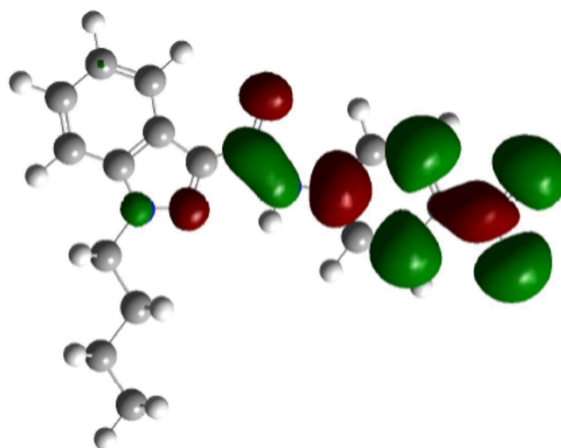


LUMO

8z

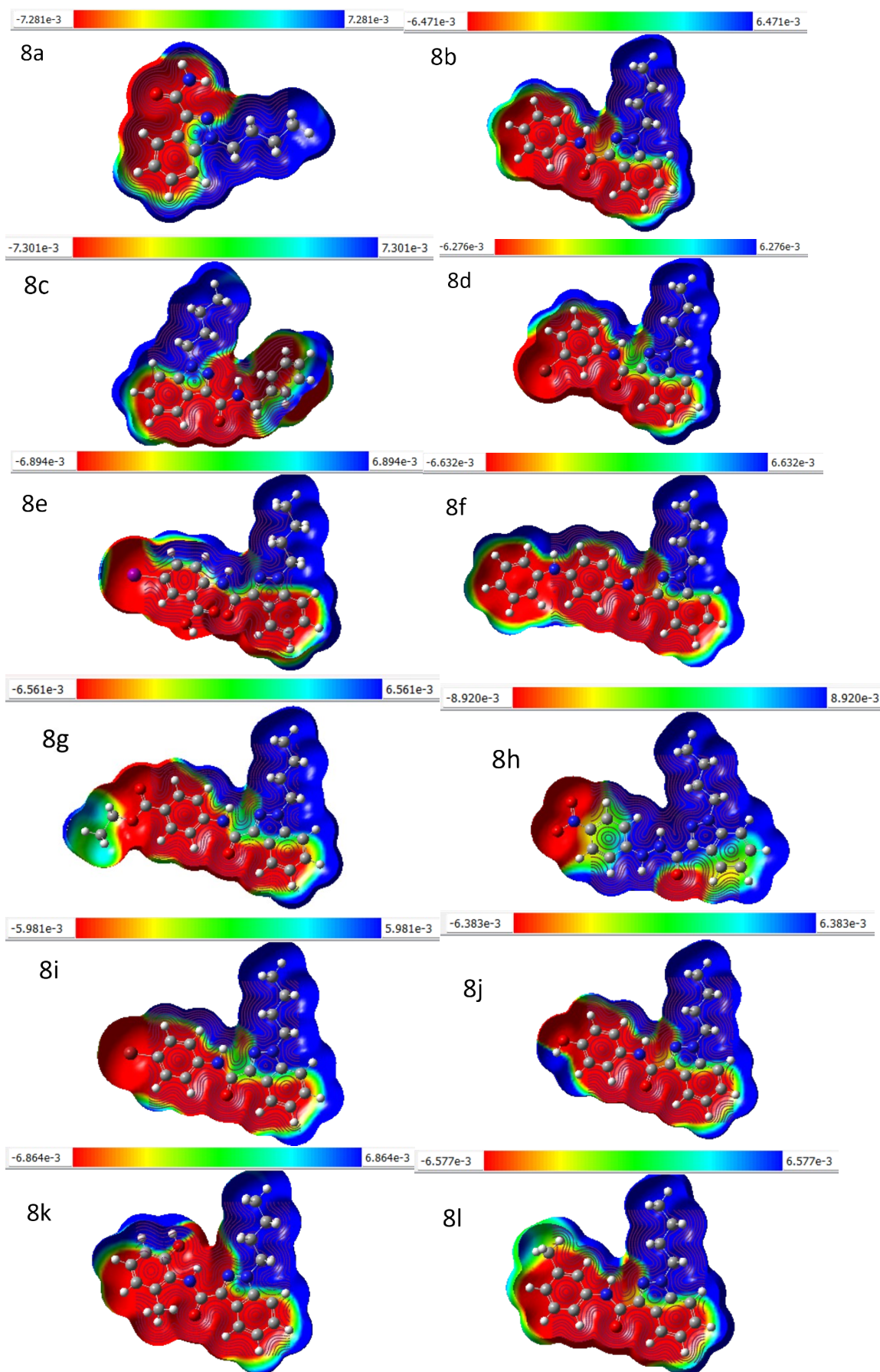


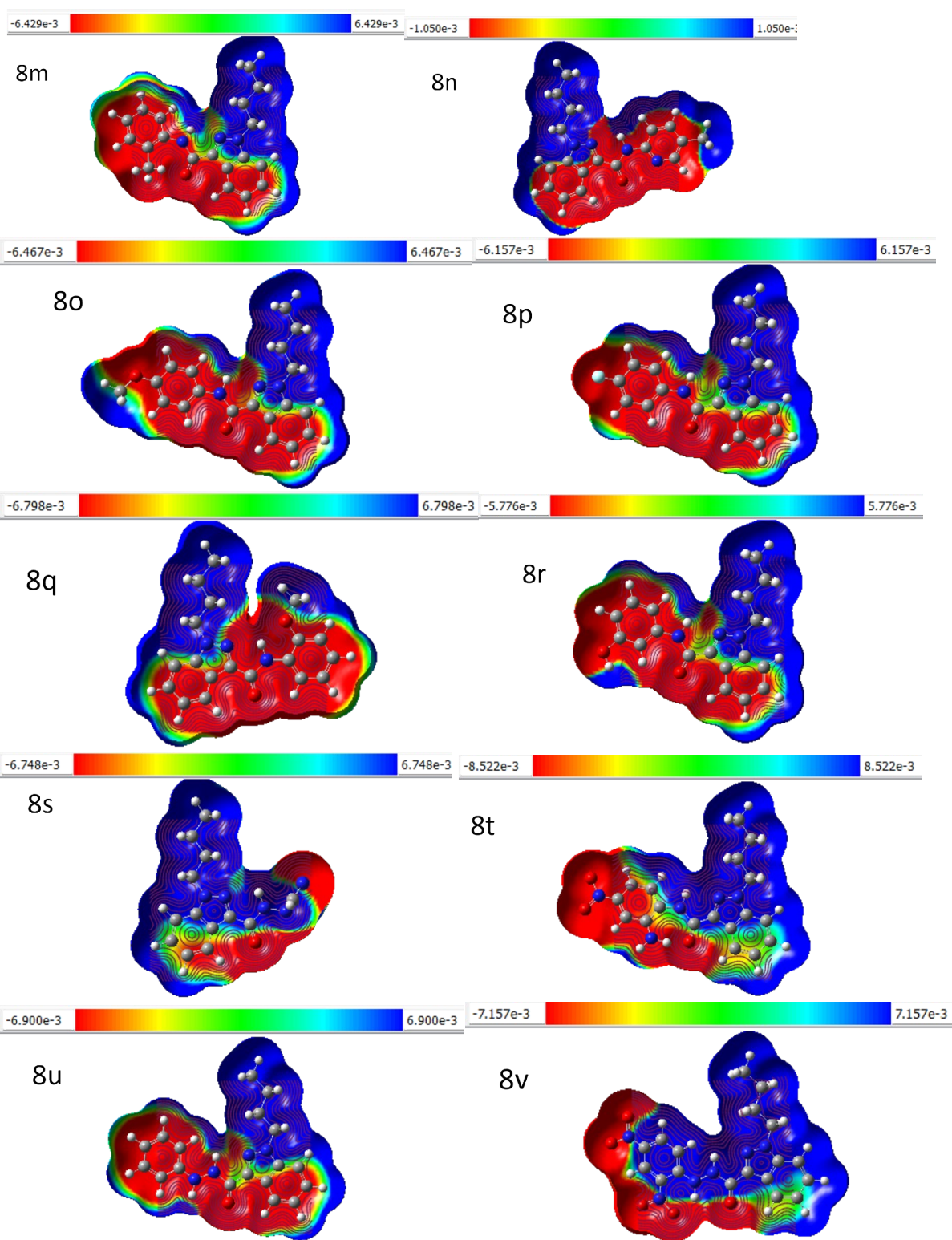
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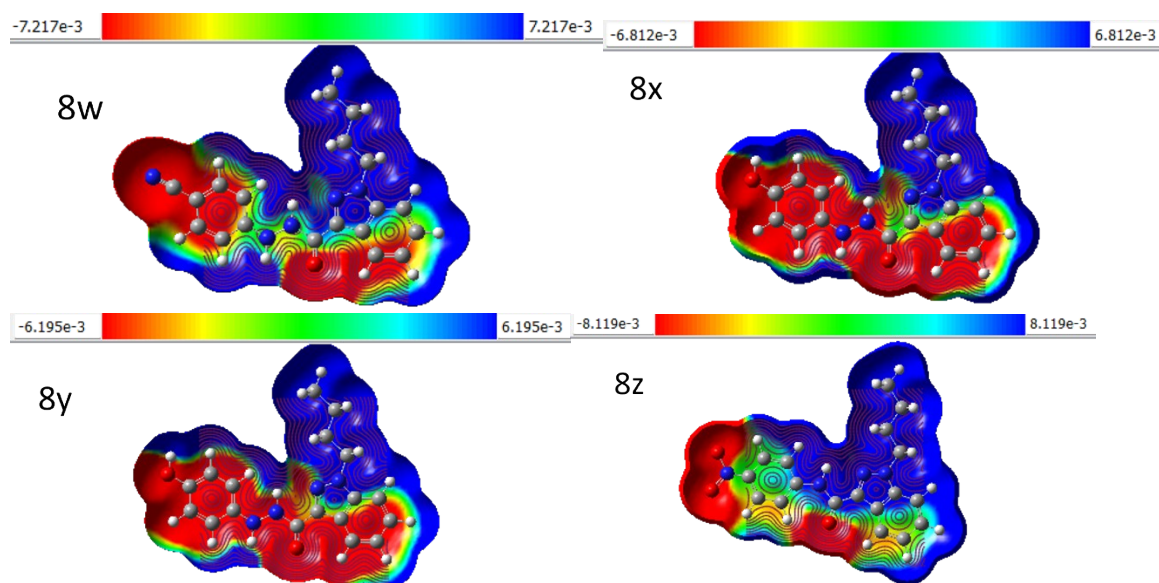


LUMO

Molecular Electrostatic Potential surface of synthesized indazole derivatives







Docking results from (8a-8z) 3-carboxamide indazole derivatives

S.no/Compound	$\Delta G_{\text{binding}}$ energy (Kcal/mol)	Ki (micromolar) [Temperature = 298.15 k] need to change nanomolar to micro molar	H bond energy (Kcal/mol)
8a	-7.03	7.00	-8.24
8b	-9.38	133.69	-10.84
8c	-10.51	19.74	-12.19
8d	-9.51	106.73	-10.67
8e	-10.23	31.66	-11.48
8f	-10.59	17.28	-12.66
8g	-10.21	32.61	-12.50
8h	-10.56	18.24	-12.48
8i	-10.47	21.07	-11.93
8j	-9.12	207.41	-10.84
8k	-9.94	51.93	-11.70
8l	-9.77	69.21	-11.24
8m	-10.18	34.63	-11.59
8n	-9.55	100.18	-11.00
8o	-9.94	51.34	-11.62
8p	-9.71	76.64	-11.15
8q	-10.22	32.11	-11.92
8r	-9.83	61.84	-11.56
8s	-8.36	729.01	-9.81
8t	-10.72	13.89	-12.63
8u	-10.38	24.47	-12.09
8v	-11.77	2.35	-13.47

8w	-11.64	2.94	-13.33
8x	-10.32	27.09	-12.31
8y	-11.52	3.61	-13.21
8z	-10.81	11.9	-12.40

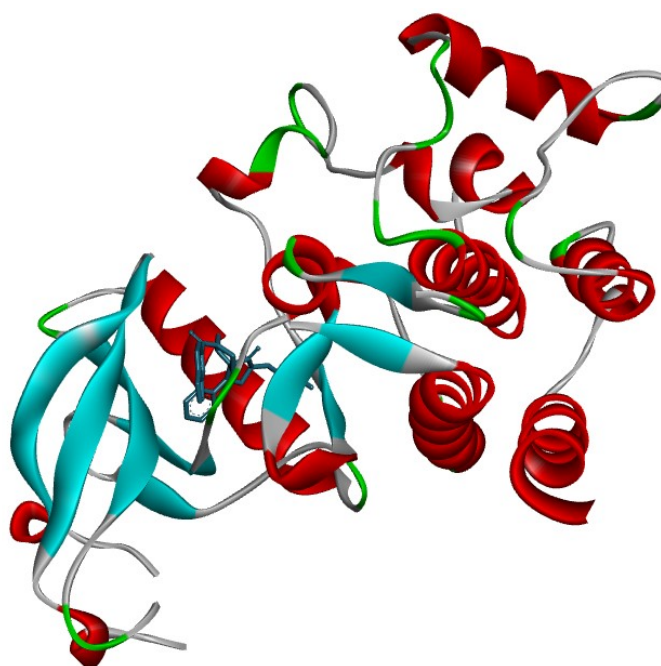
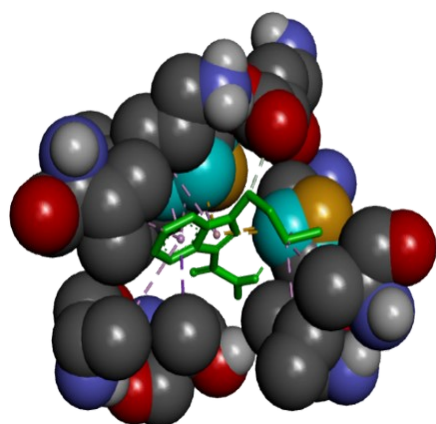


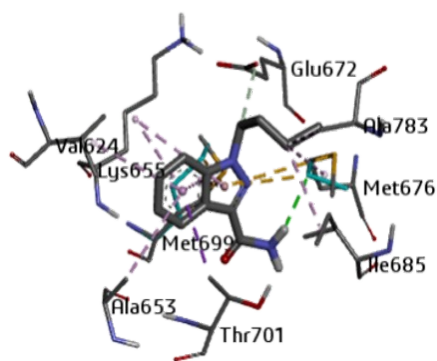
Fig 5. The crystal structure of DDR1, 2-[8-(1H-indazole-5-carbonyl)-4-oxo-1-phenyl-1,3,8-triazaspiro [4.5] decan-3-yl] -N-methyl acetamide (6FEW). 3D graphics were generated using Discovery Studio Visualizer 2021.

The binding pattern of indazole derivatives with PBD-6FEW. A) represents 3D surface representation, B) represents active ligand catalytic centre of the protein target, C) 2D-schematic LigPlot interactions shown for the docked pose of indazole derivatives shown by the spokes

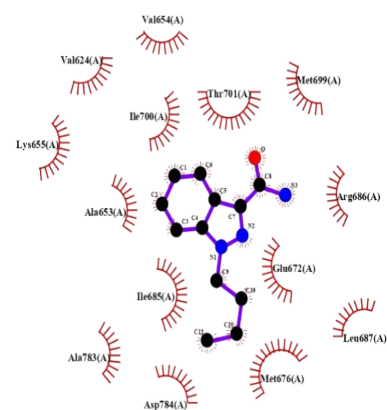
8a



A

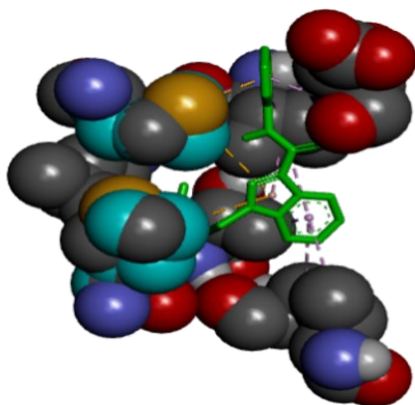


B

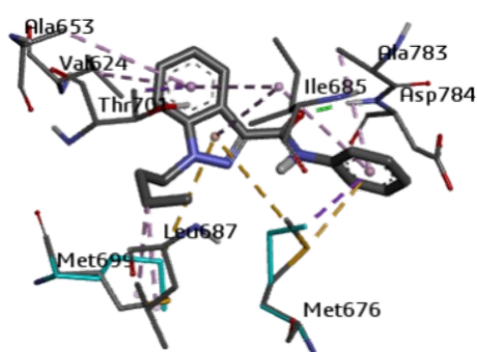


C

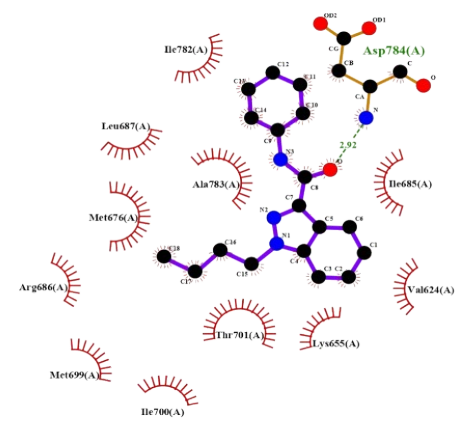
8b



A

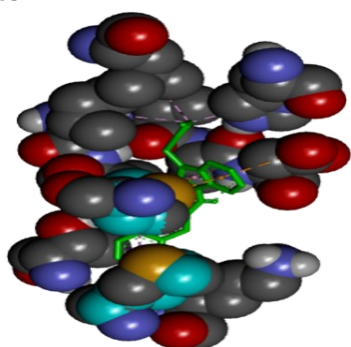


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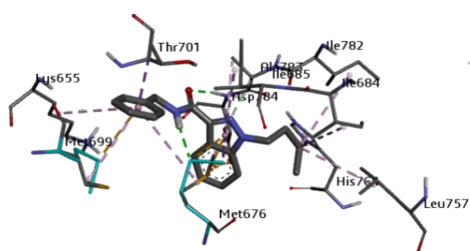


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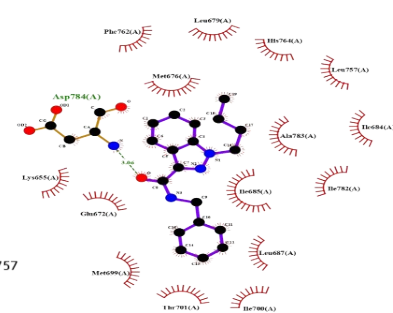
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A

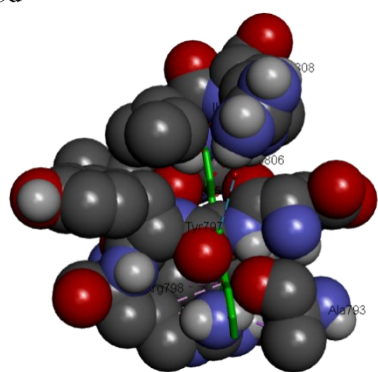


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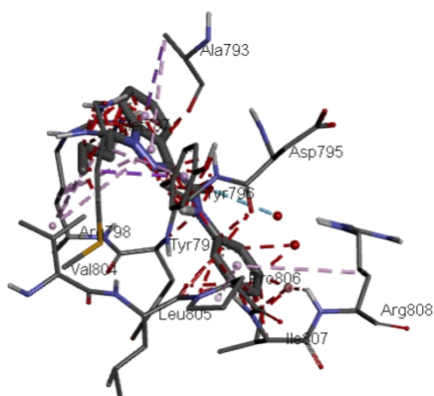


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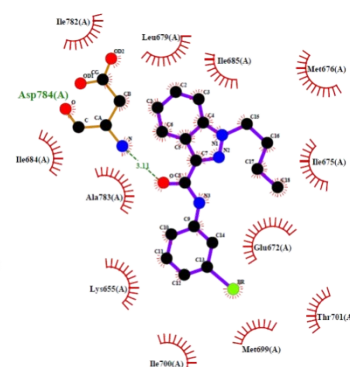
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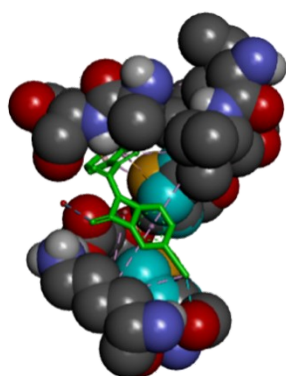


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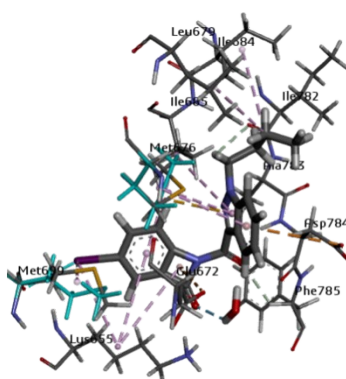


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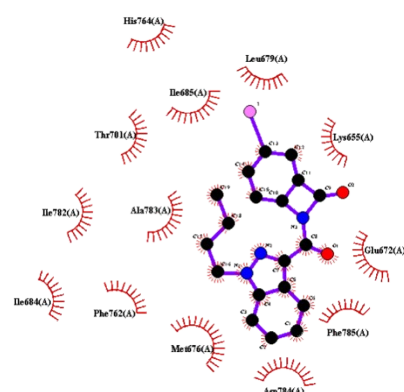
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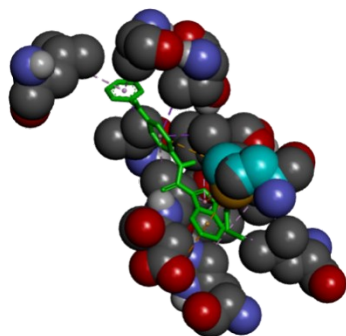


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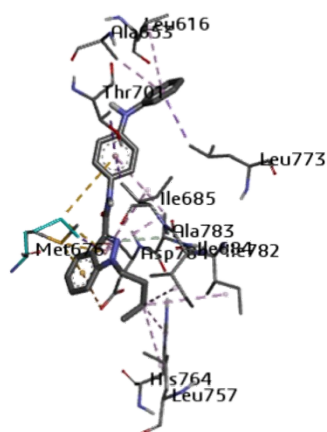


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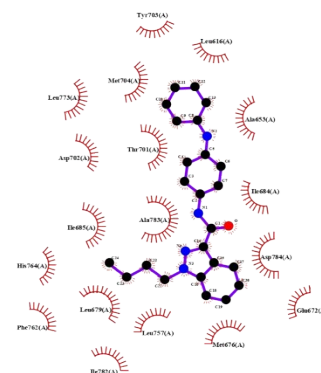
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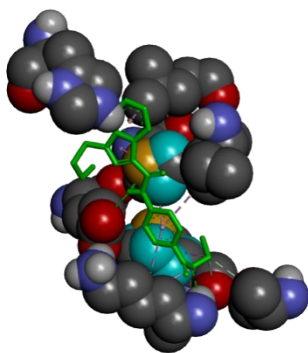


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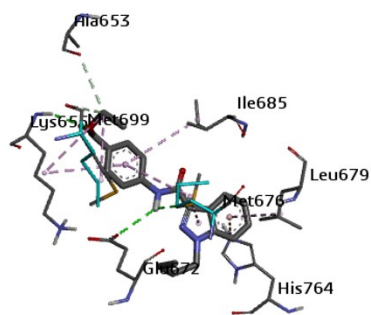


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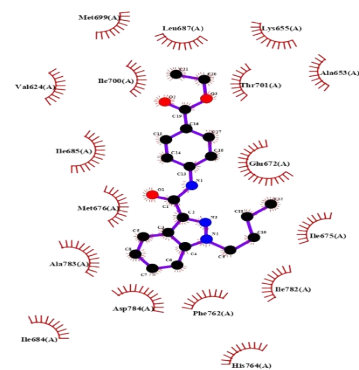
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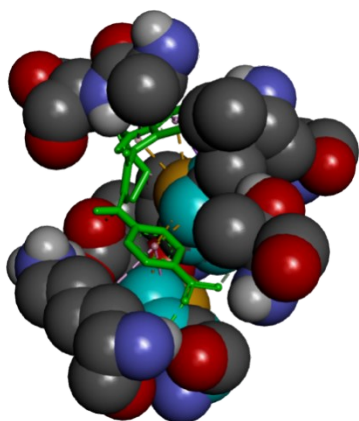


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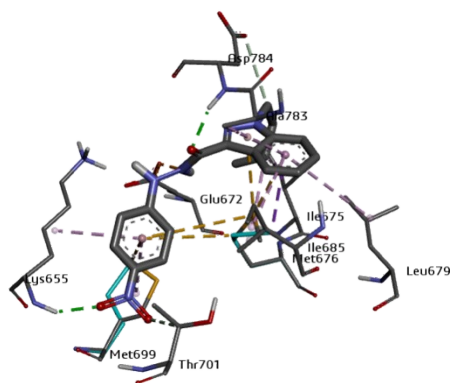


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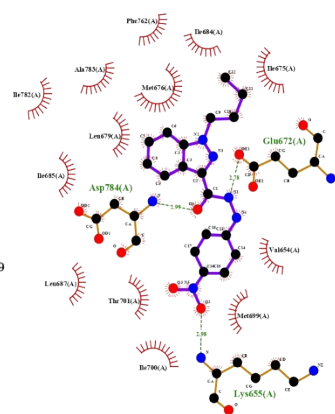
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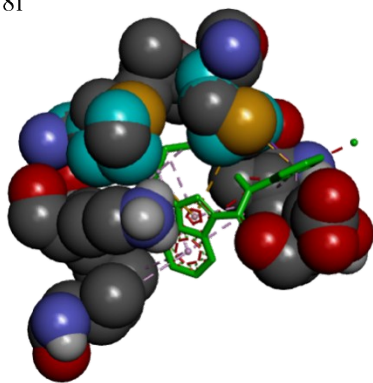


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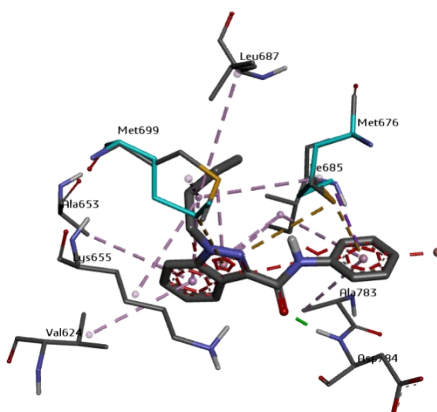


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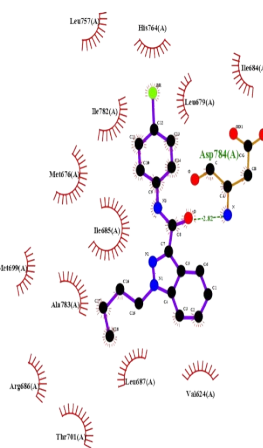
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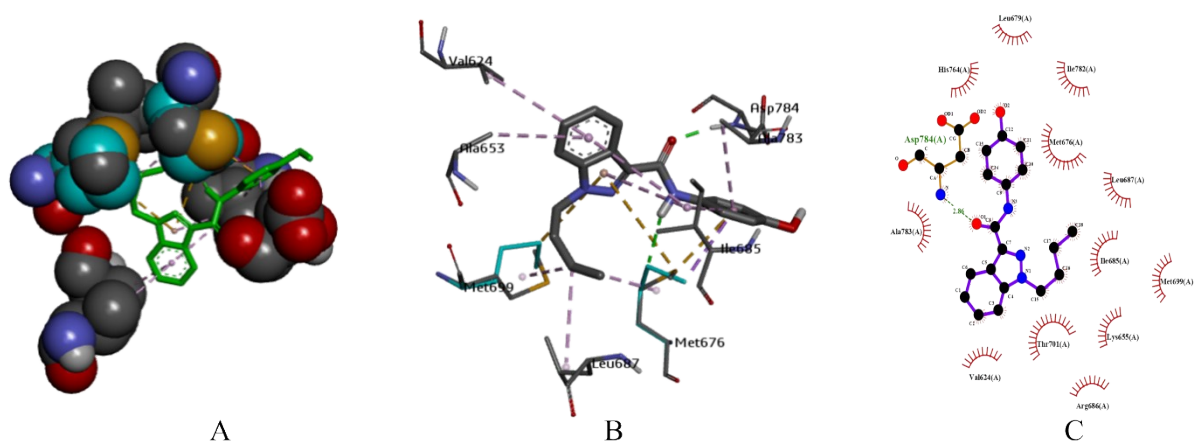


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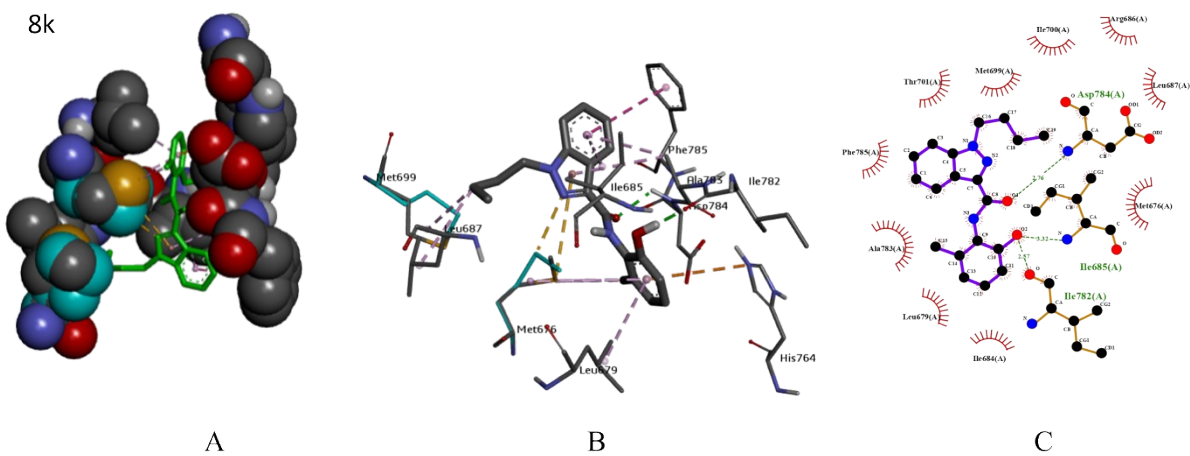


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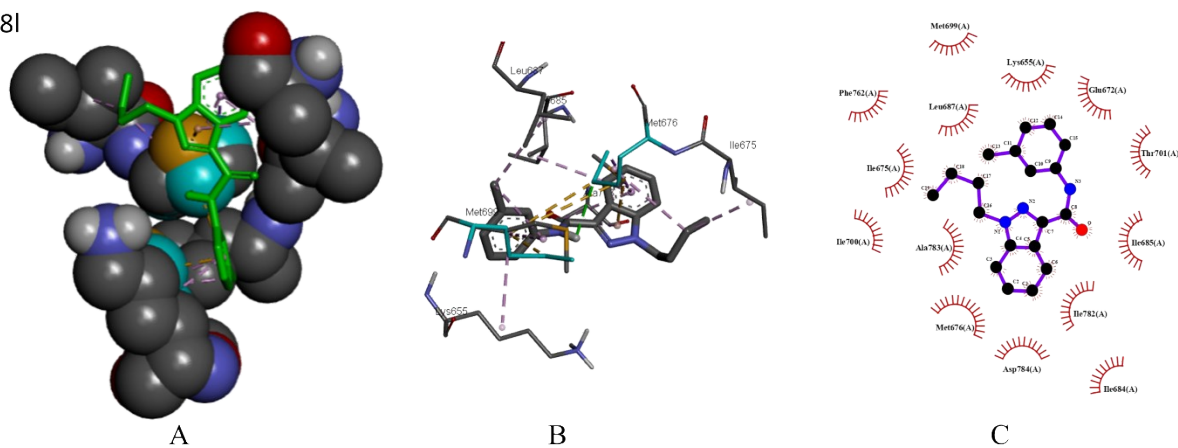
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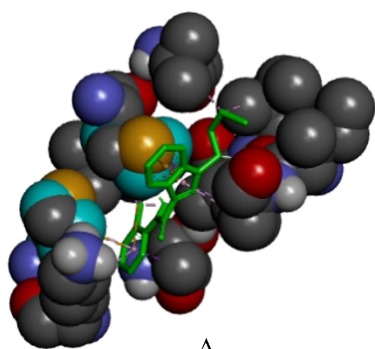
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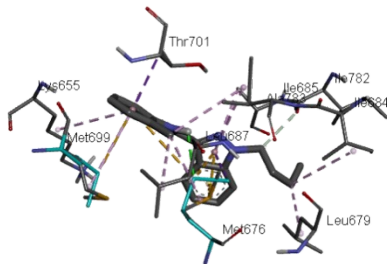
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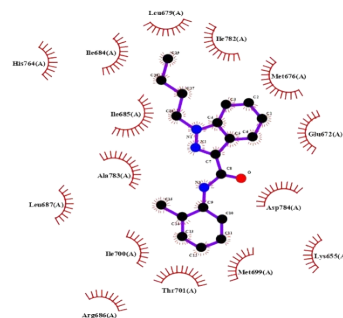
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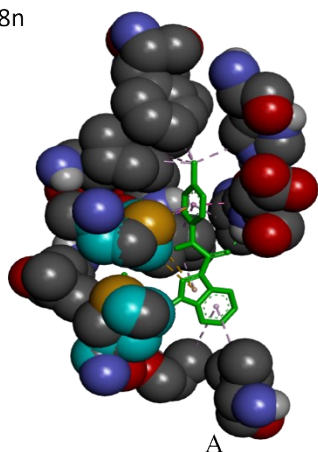


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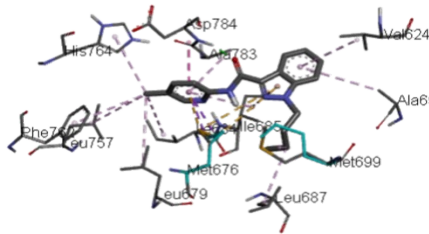


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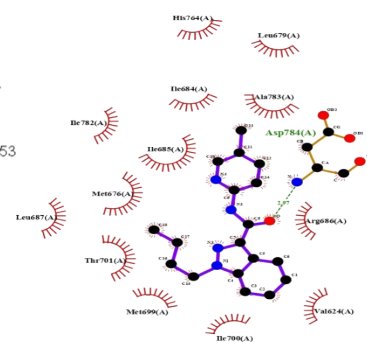
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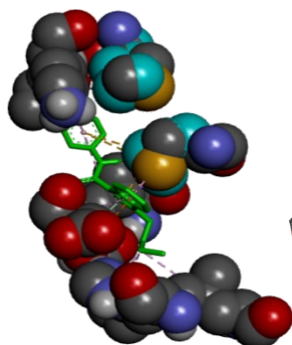


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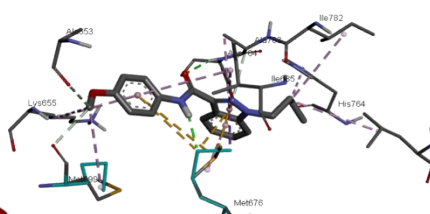


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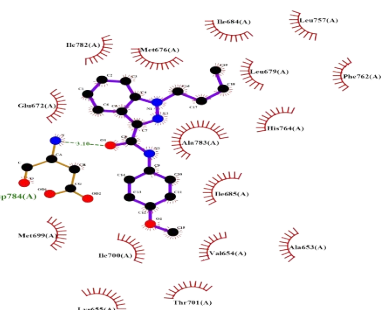
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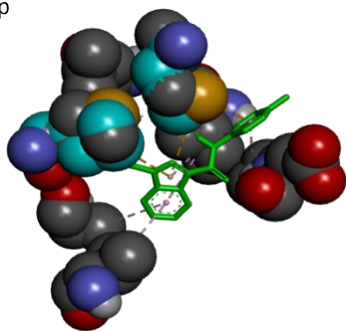


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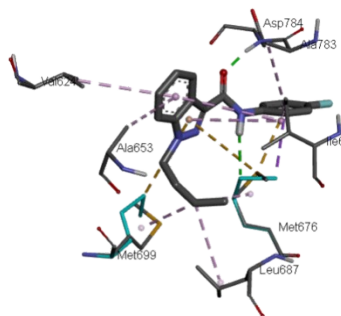


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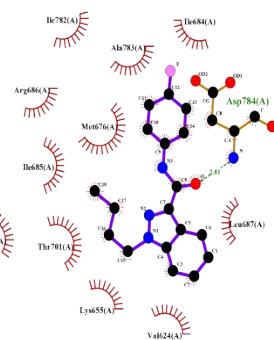
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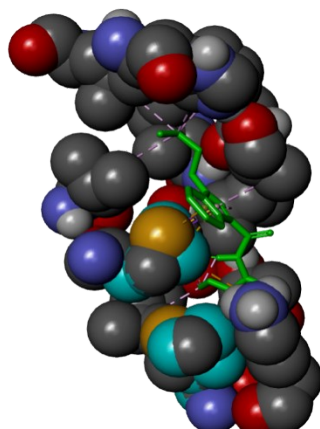


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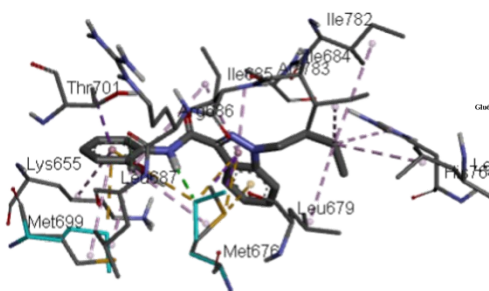


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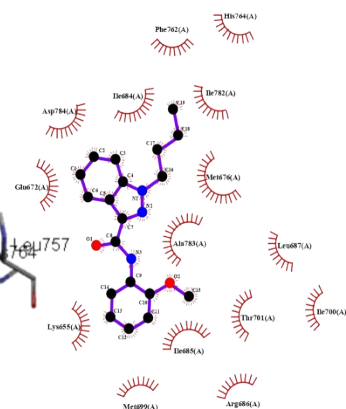
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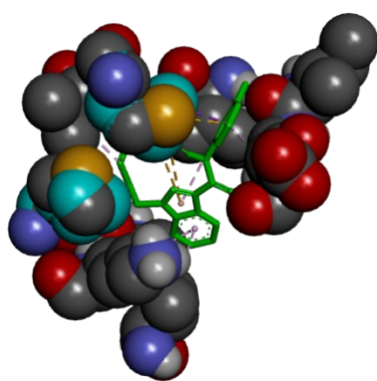


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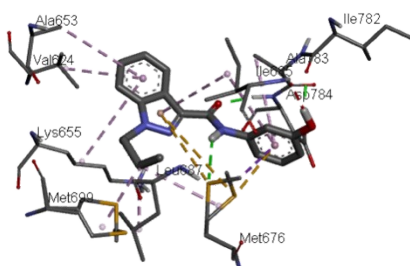


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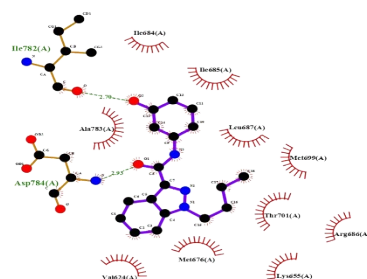
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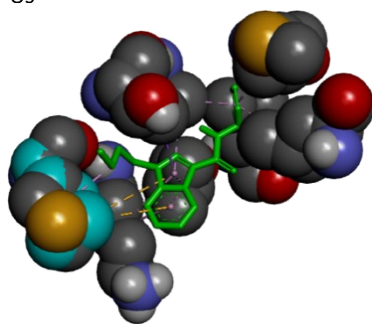


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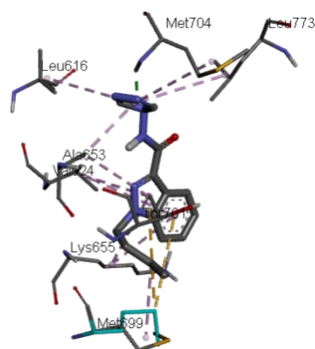


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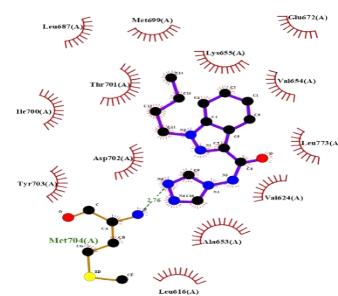
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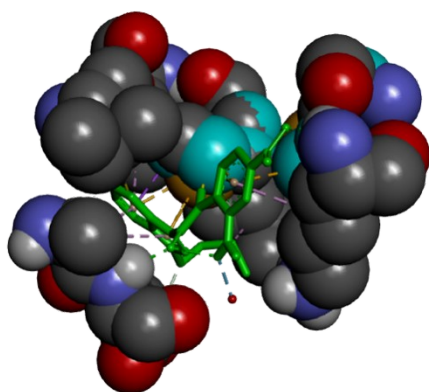


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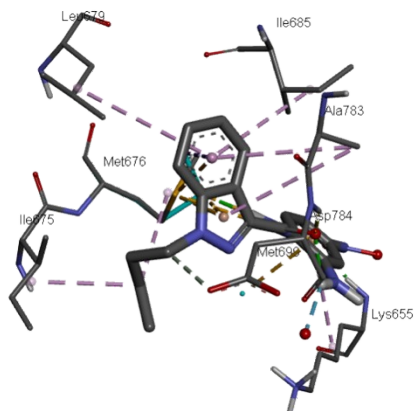


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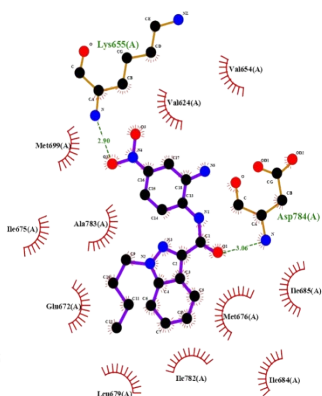
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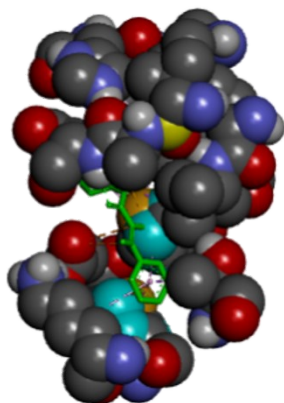


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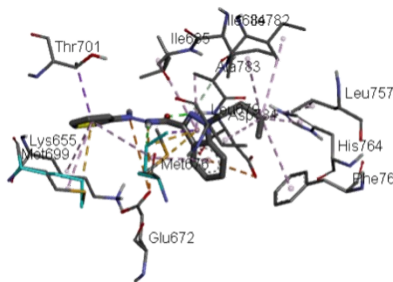


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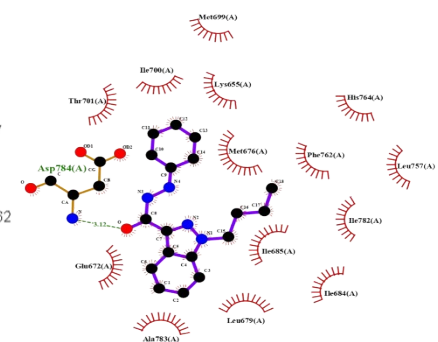
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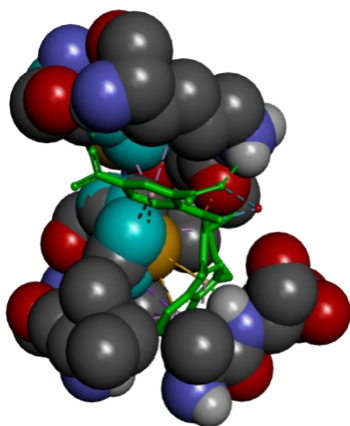


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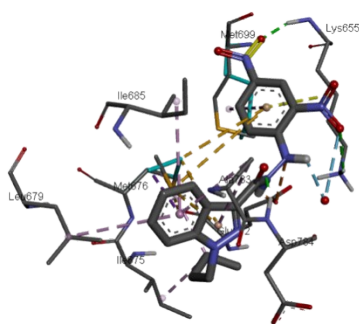


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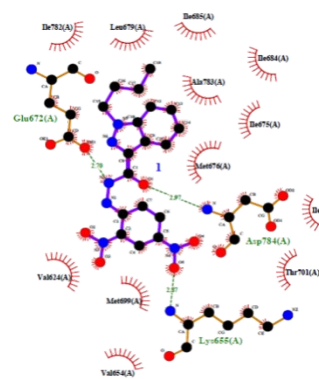
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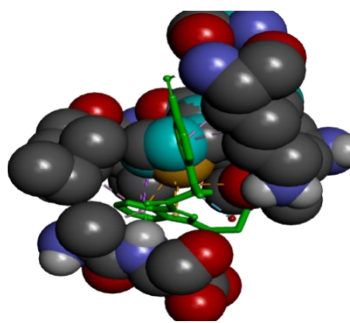


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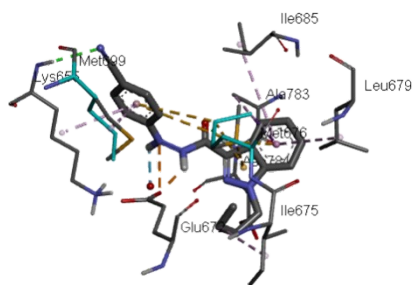


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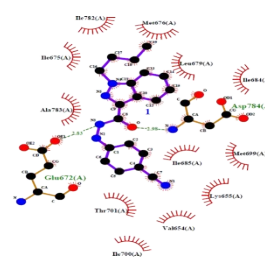
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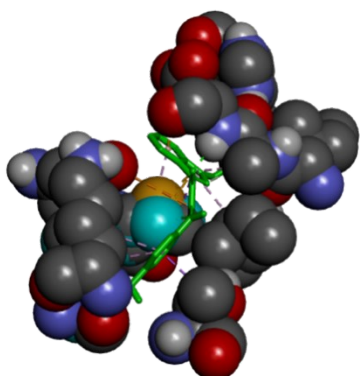


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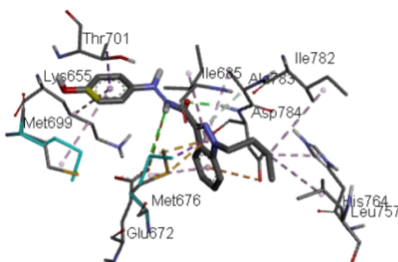


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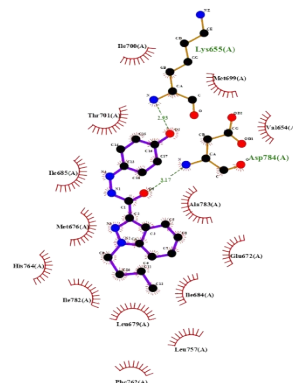
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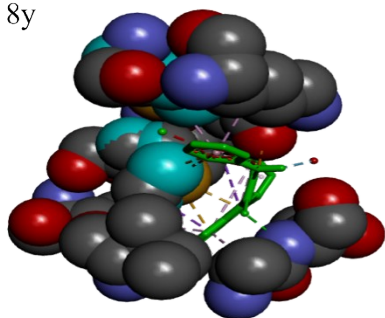


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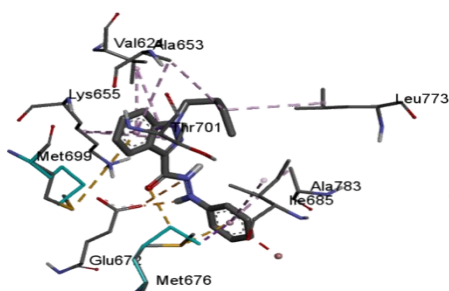


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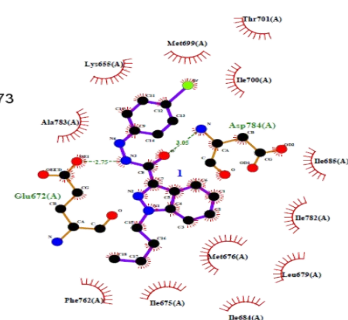
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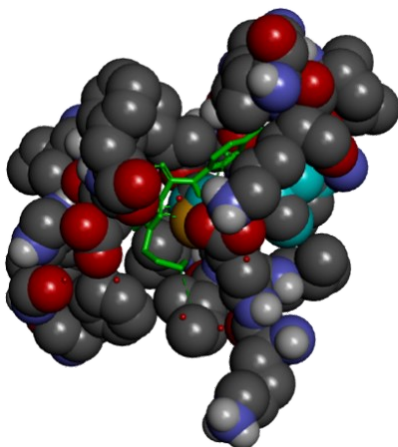


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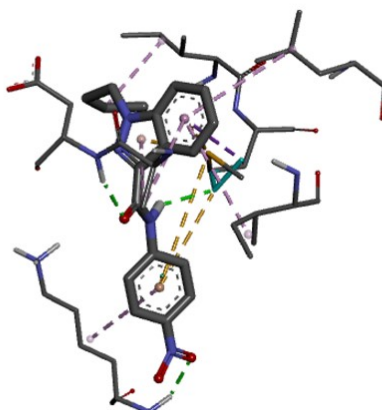


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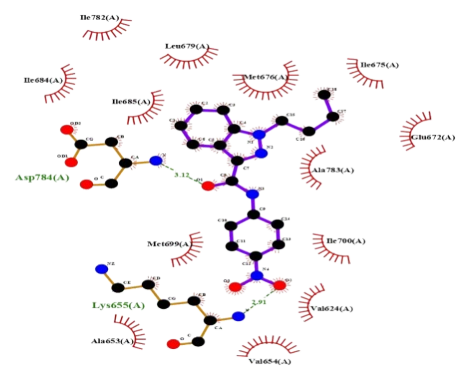
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A



B



C

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