

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) 3is 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

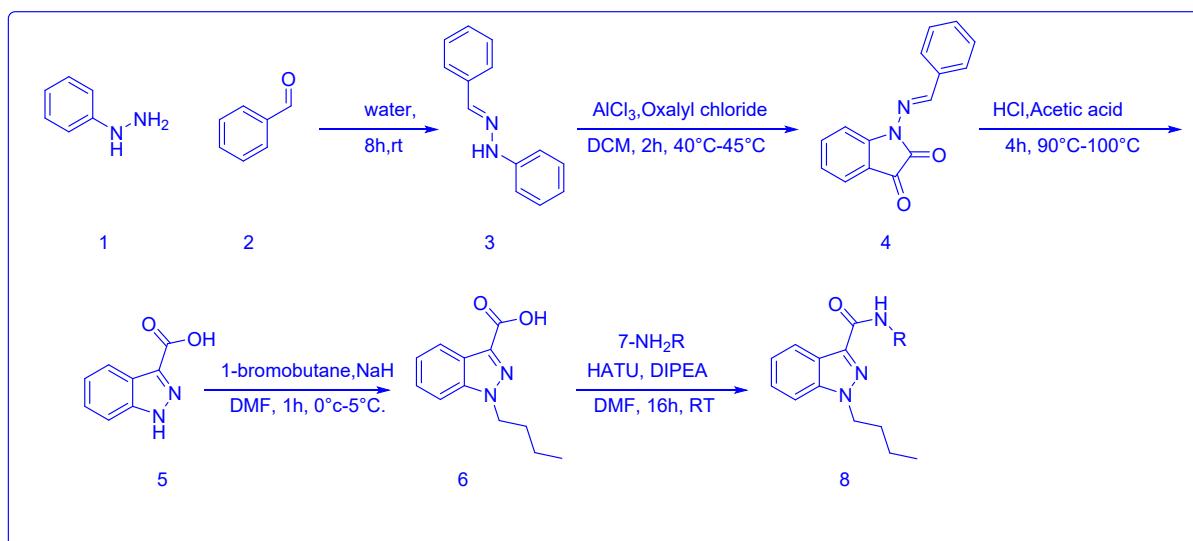


Table-1

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-carboxalic 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:

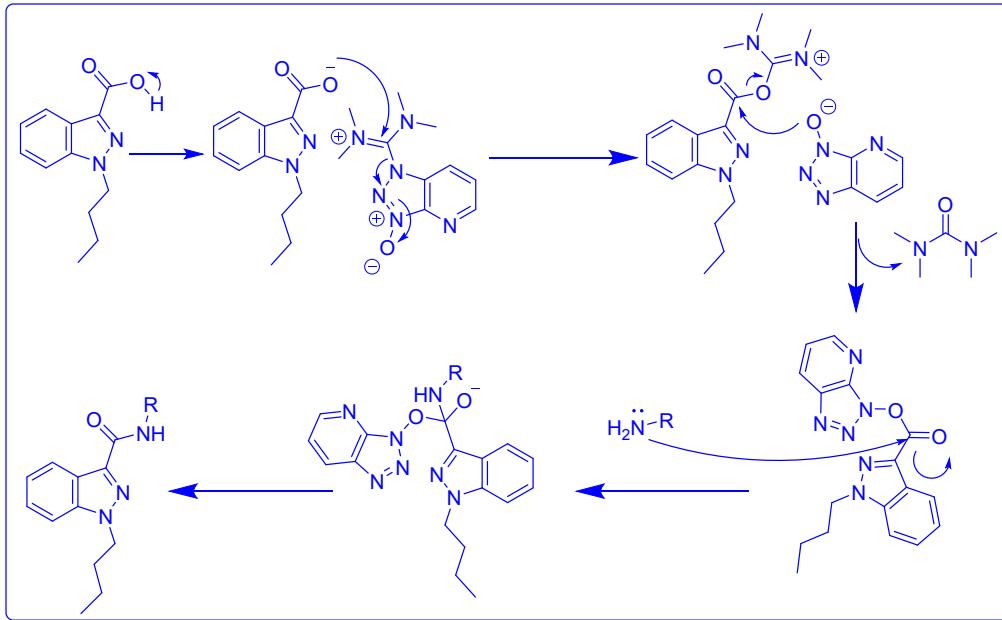


Table-2

R = 8a-8z aliphatic and aromatic amines

8a = Ammonium chloride	8g = ethyl 4-aminobenzoate	8n = 5-methylpyridin-2-amine	8u = phenylhydrazine
8b = Aniline	8h = (4-nitrophenyl)hydrazine	8o = 4-methoxyaniline	8v = (2,4-dinitrophenyl)hydrazine
8c = phenylmethanamine	8i = 4-bromoaniline	8p = 4-fluoroaniline	8w = 4-hydrazinylbenzonitrile
8d = 3-bromoaniline	8j = 4-aminophenol	8q = 2-methoxyaniline	8x = 4-hydrazinylphenol
8e = 2-amino-5-iodobenzoic acid	8k = 2-amino-3-methylphenol	8r = 3-aminophenol	8y = (4-bromophenyl)hydrazine
8f = 4-benzylaniline	8l = m-toluidine	8s = 4H-1,2,4-triazol-4-amine	8z = 4-nitroaniline
	8m = o-toluidine	8t = 4-nitrobenzene-1,2-diamine	

Table-3

2.6. Acid- Amide cross-coupling derivatives of indazole amides (8a-8z)

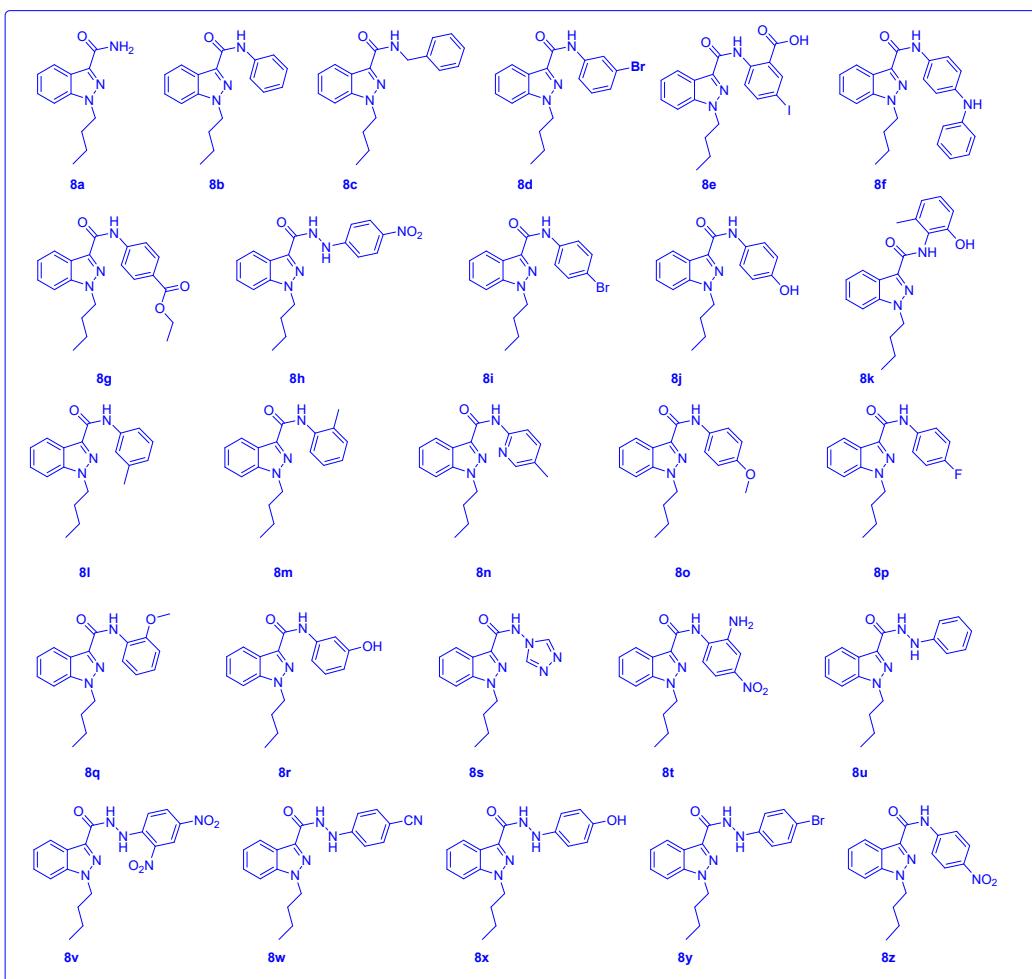
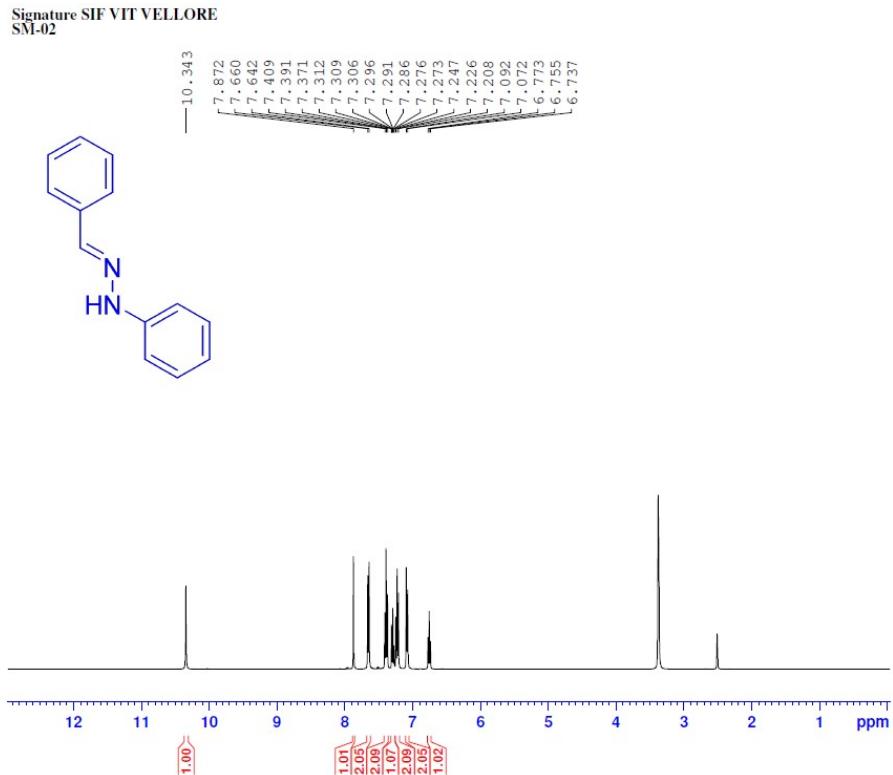


Table-4

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

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

**Signature SIF VIT VELLORE
SM-02**



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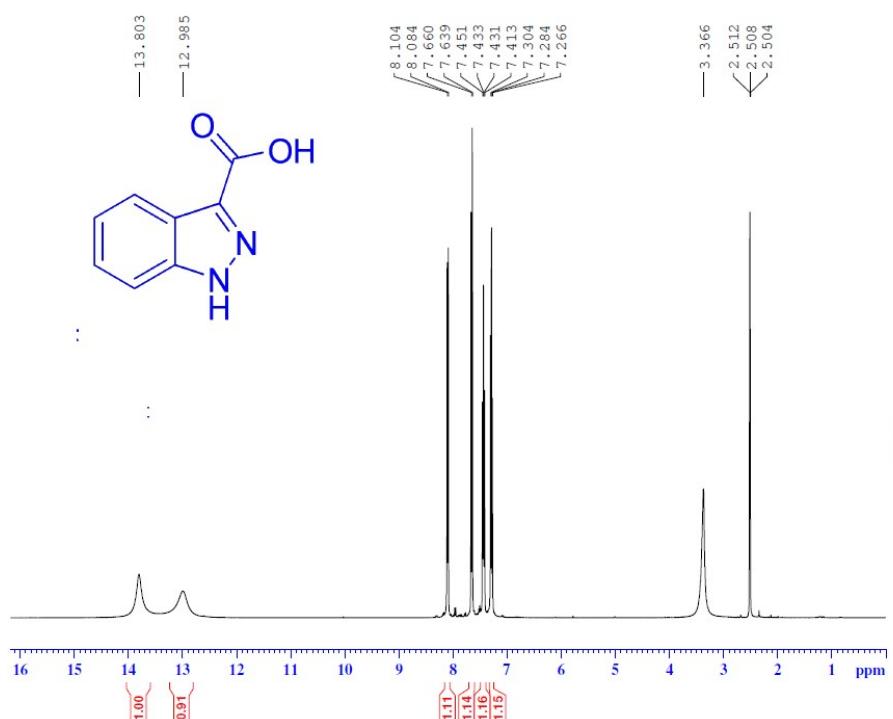
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NUC1           1H
P1              15.00 usec
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¹H-NMR [400MHz, DMSO-d₆] spectrum of 1H-indazole-3-carboxalic acid (5).

**Signature SIF VIT VELLORE
SM-03**





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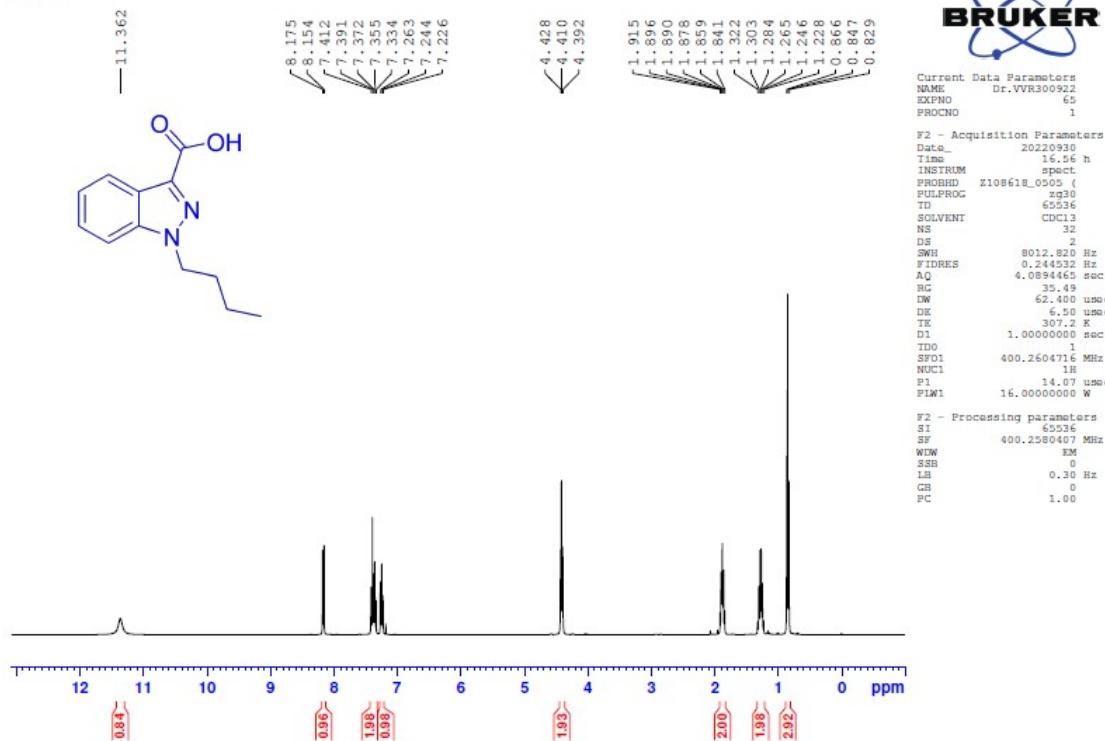
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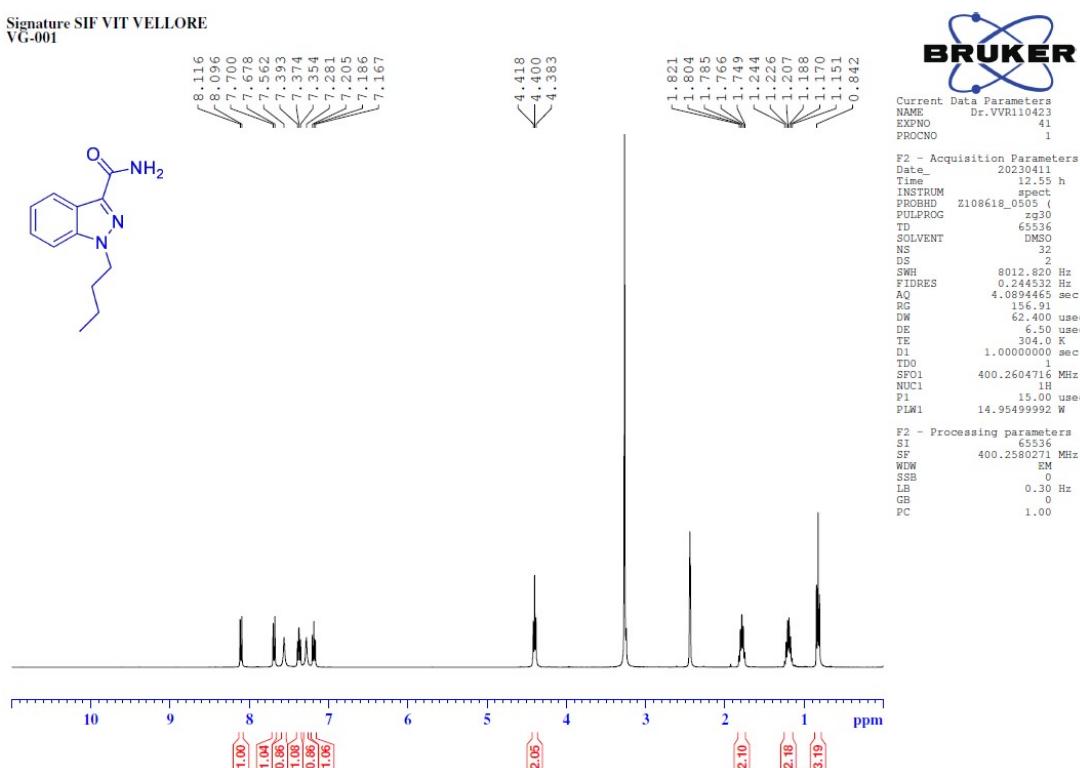
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¹H-NMR [400MHz, DMSO-d₆] spectrum of 1-butyl-1H-indazole-3-carboxylic acid (6).

Signature SIF VIT VELLORE
SM- 04a

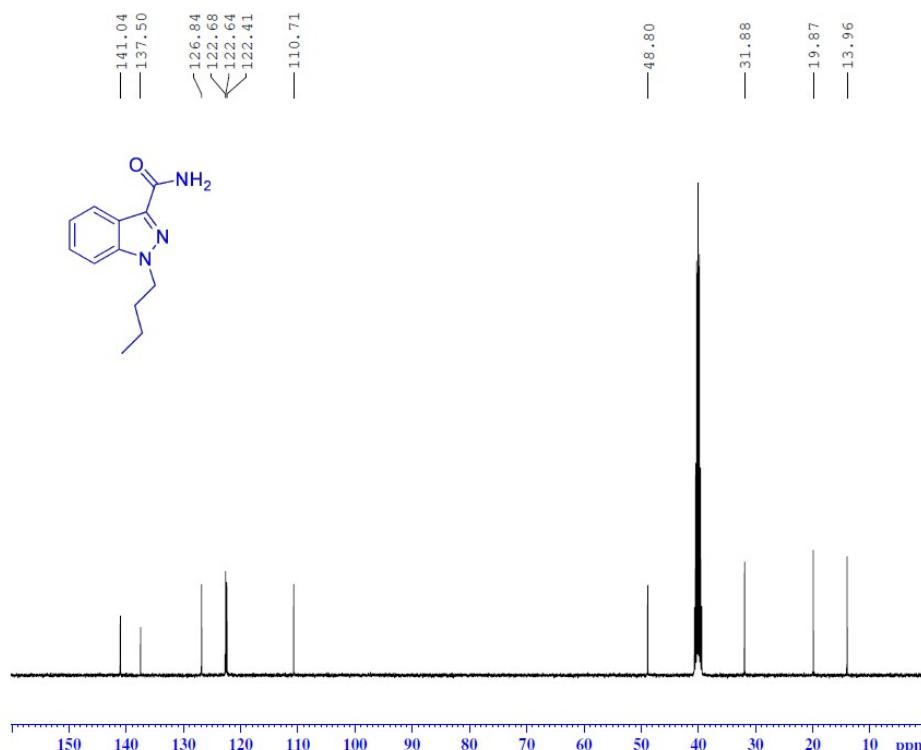


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VG-001



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

Signature SIF VIT VELLORE
VG-001



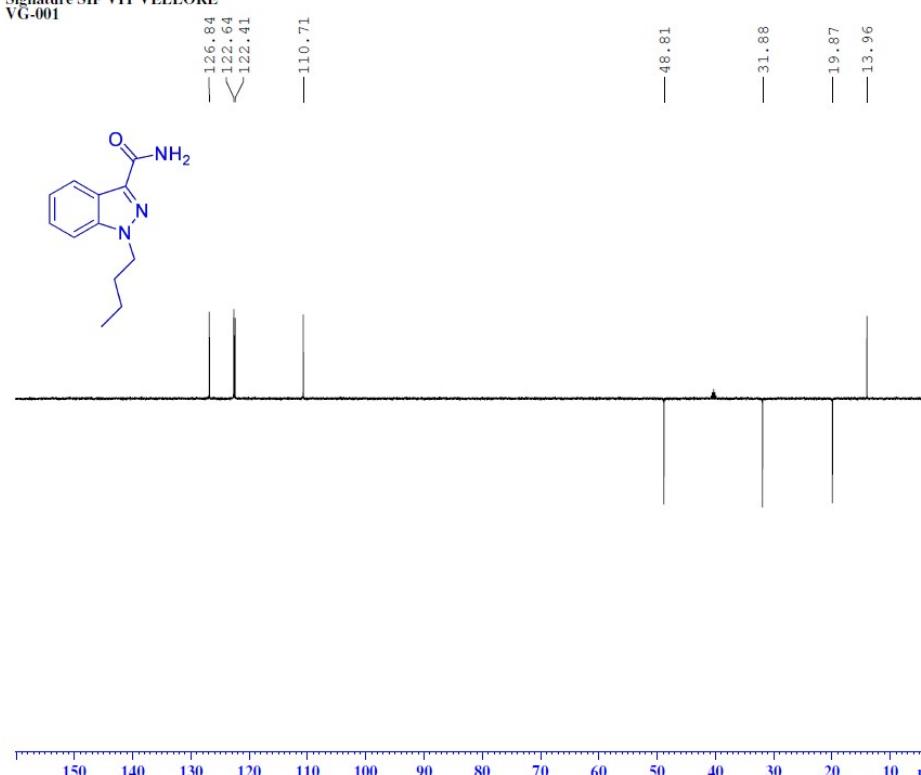
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¹³⁵-DEPT-NMR [100MHz, DMSO-d₆] spectrum of 1-butyl-1H-indazole-3-carboxamide (8a).

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VG-001



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

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VG-001



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FIDRES 3.844734 Hz

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RG 63.17

DW 127.000 usec

DE 4.000 usec

TE 306.477

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D11 1.93551198 sec

D13 0.03000000 sec

D12 0.00002000 sec

D13 0.00000000 sec

D14 0.00000000 sec

INDU 0.000025400 sec

TDwv 400.2597851 MHz

SWC1 18

P0 15.00 usec

P1 15.00 usec

P17 250.00 usec

P1W1 14.9549992 w

P1W10 3.7386993 w

GR1W1 [1] SWFOUR 1

GPZ1 10.00 %

P1E 1000.00 usec

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FIDRES 61.515747 Hz

SW 9.838 ppm

FnMode QF

P2 - Processing parameters

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SW 400.2597851 MHz

QSWINE

SSB 0

LB 0

RR 1

PC 1.40

P1 - Processing parameters

SI 1024

SW 400.2597851 MHz

QSWINE

SSB 0

LB 0

RR 0

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

Signature SIF VIT VELLORE
VG-001



Current Data Parameters

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EXPNO 51

PROCNO 1

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TE 306.477

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TDwv 400.2597851 MHz

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P1 15.00 usec

P2 1.00 usec

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GR1W1 [3] SWFOUR 20.10 %

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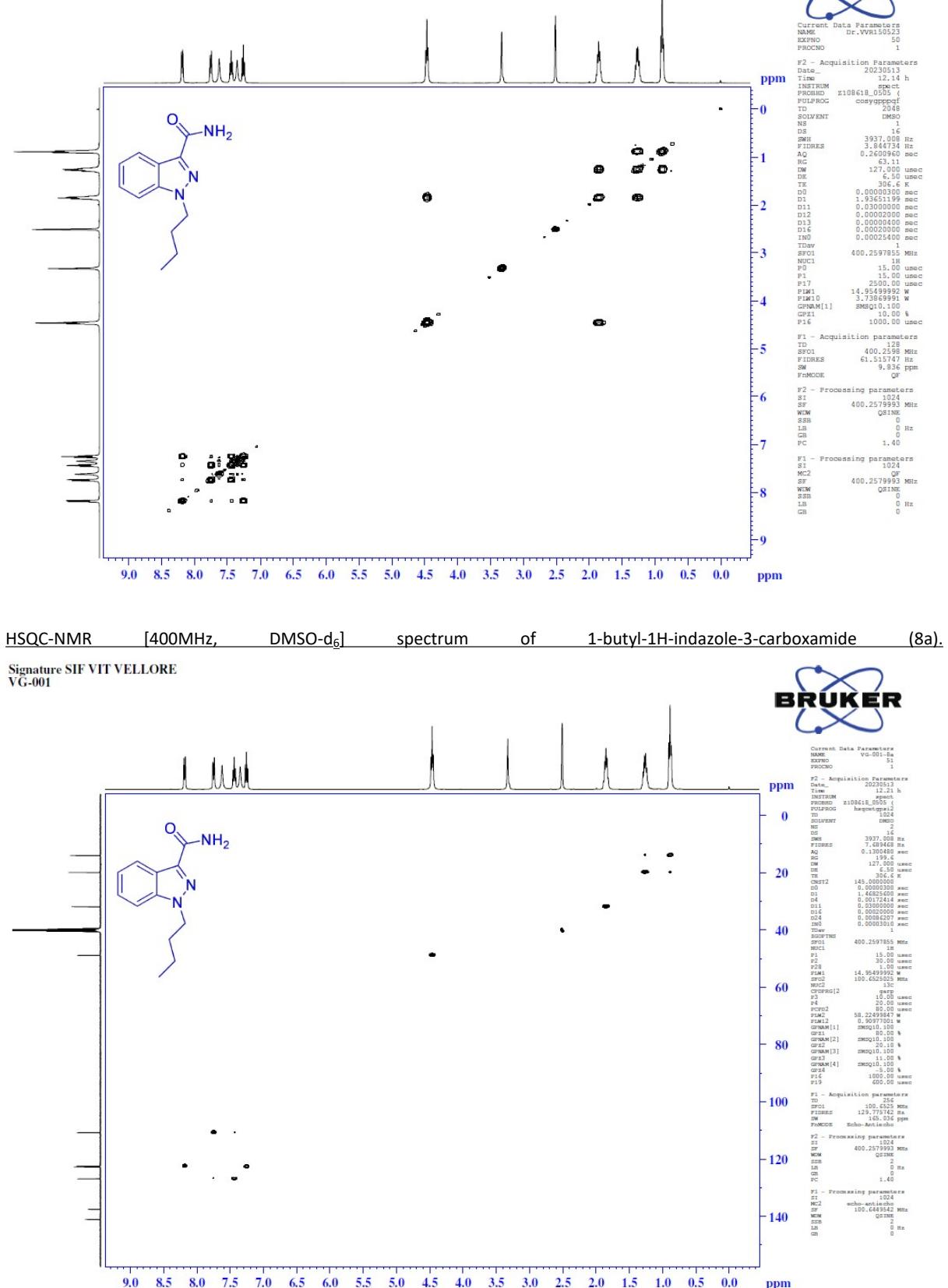
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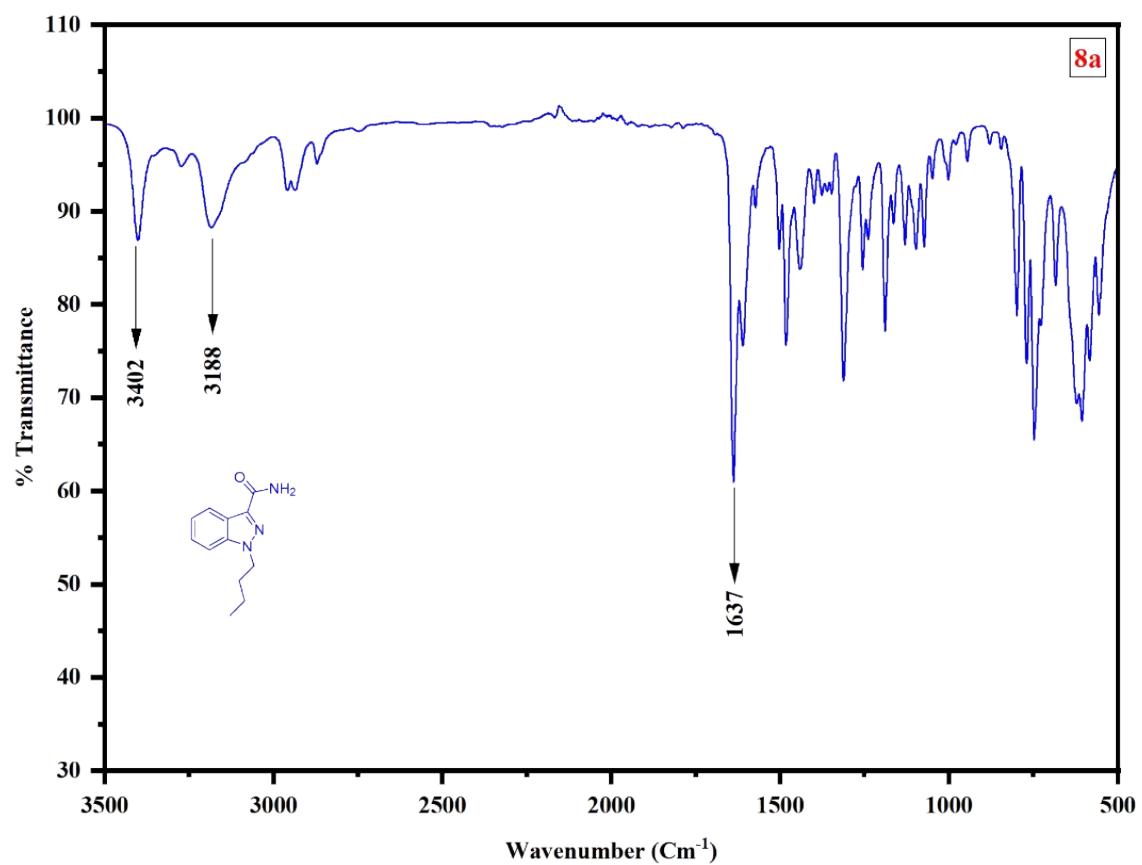
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FT-IR spectrum of 1-butyl-1H-indazole-3-carboxamide (8a).

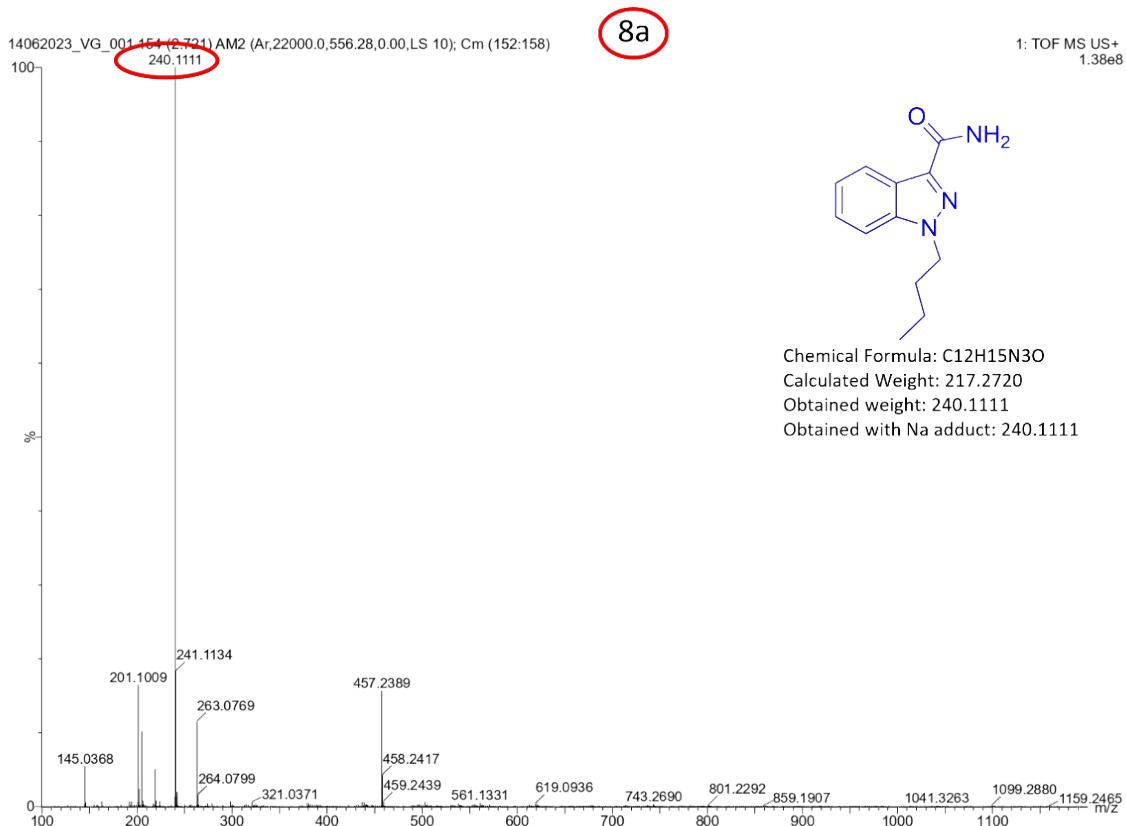
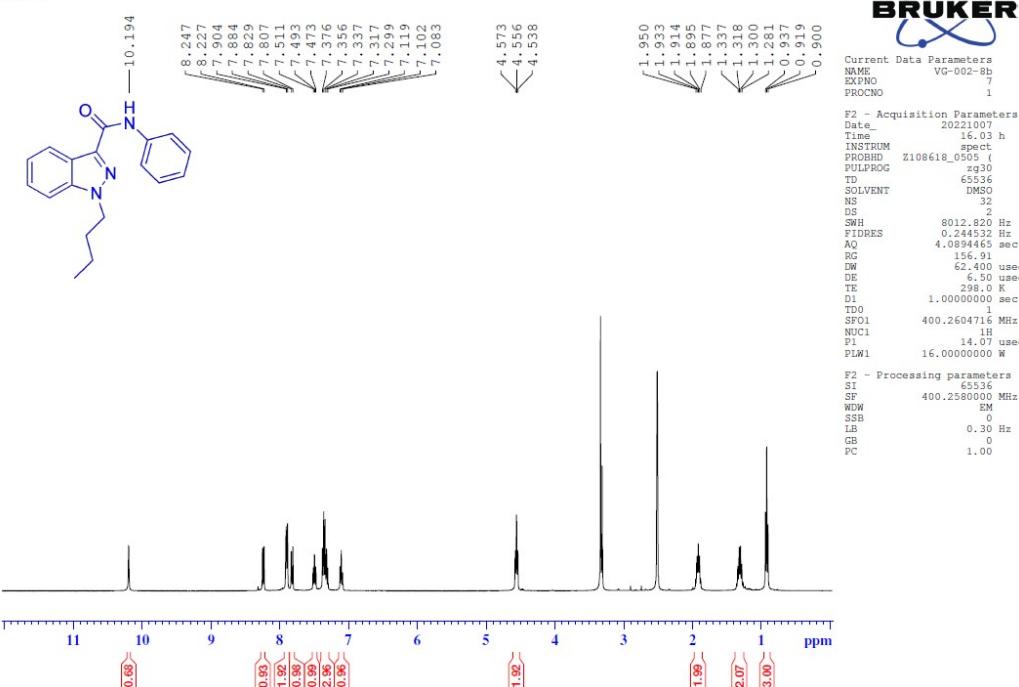


HRMS

of

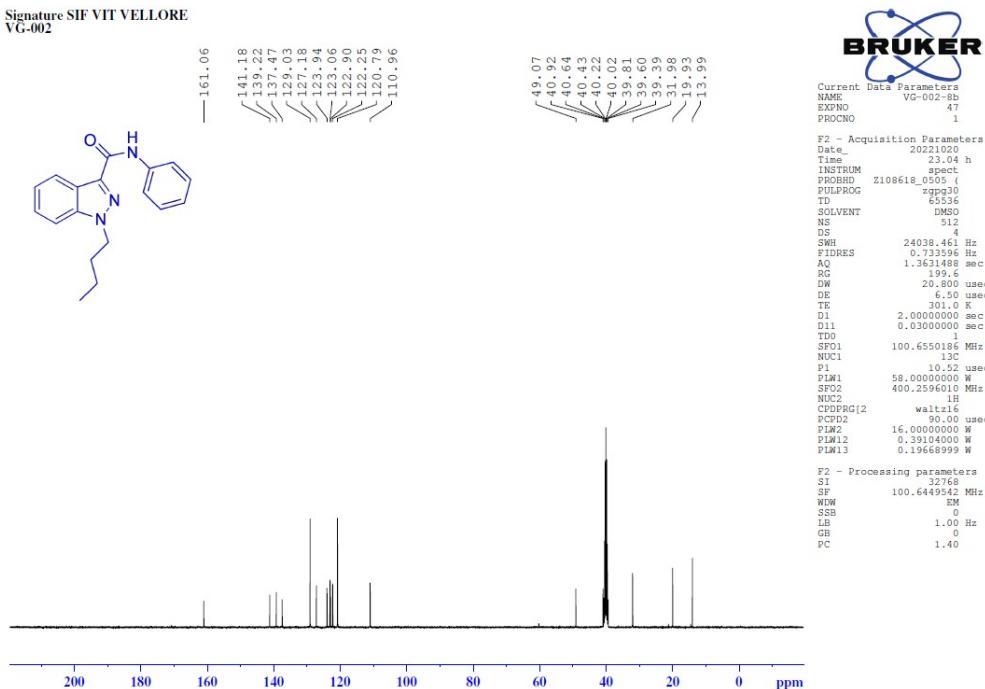
1-butyl-1H-indazole-3-carboxamide

(8a)

¹H-NMR [400MHz, DMSO-d₆] spectrum of 1-butyl-N-phenyl-1H-indazole-3-carboxamide (8b).Signature SIF VIT VELLORE
VG-002

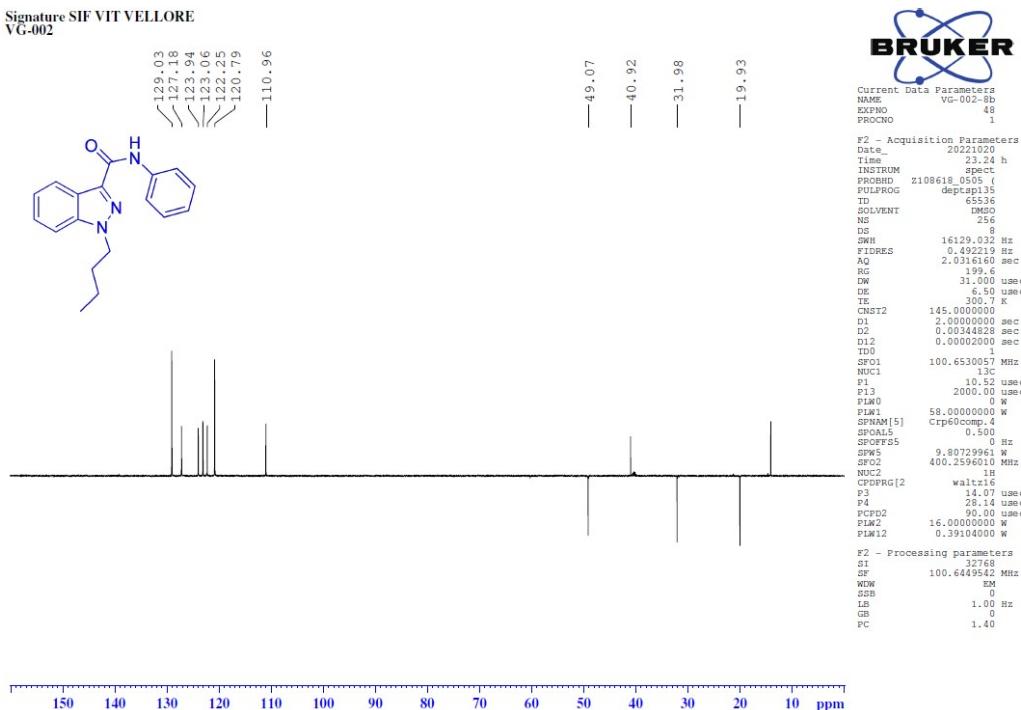
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**Signature SIF VIT VELLORE
VG-002**



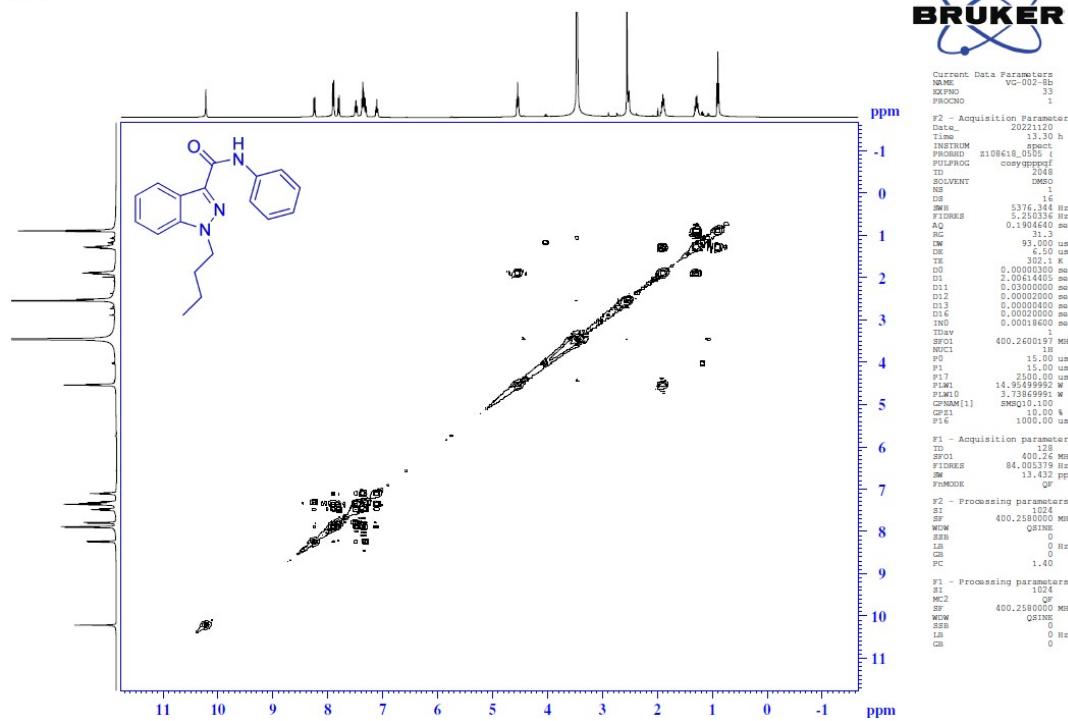
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Signature SIF VIT VELLORE
VG-002



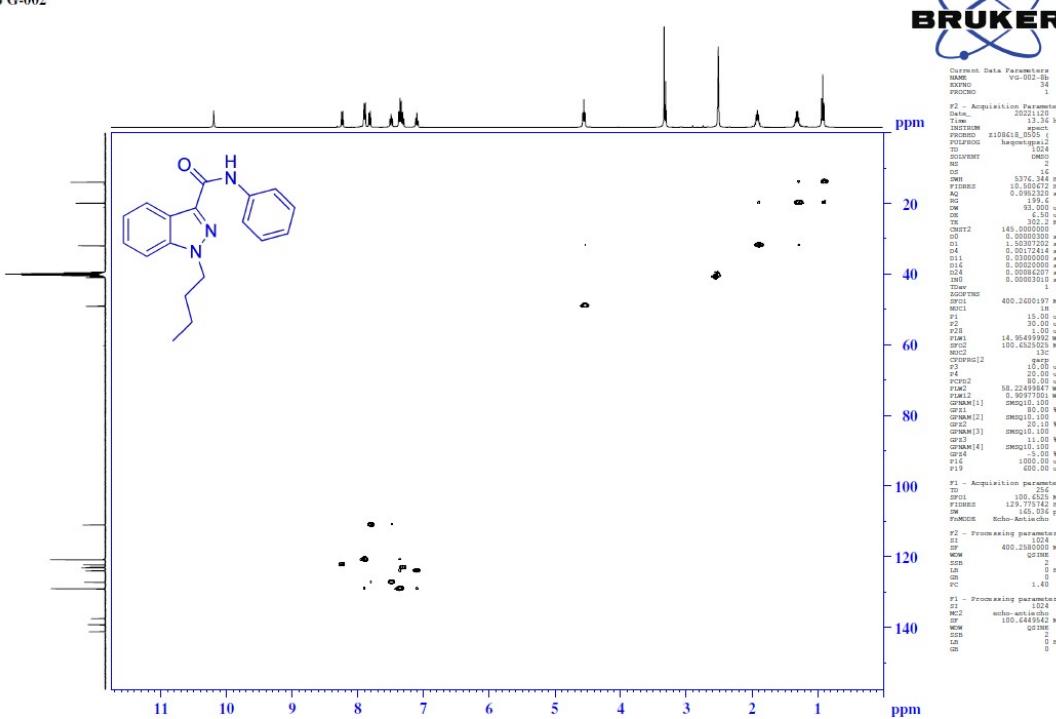
COSY-NMR [400MHz, DMSO-d₆] spectrum of 1-butyl-N-phenyl-1H-indazole-3-carboxamide (8b).

Signature SIF VIT VELLORE
VG002

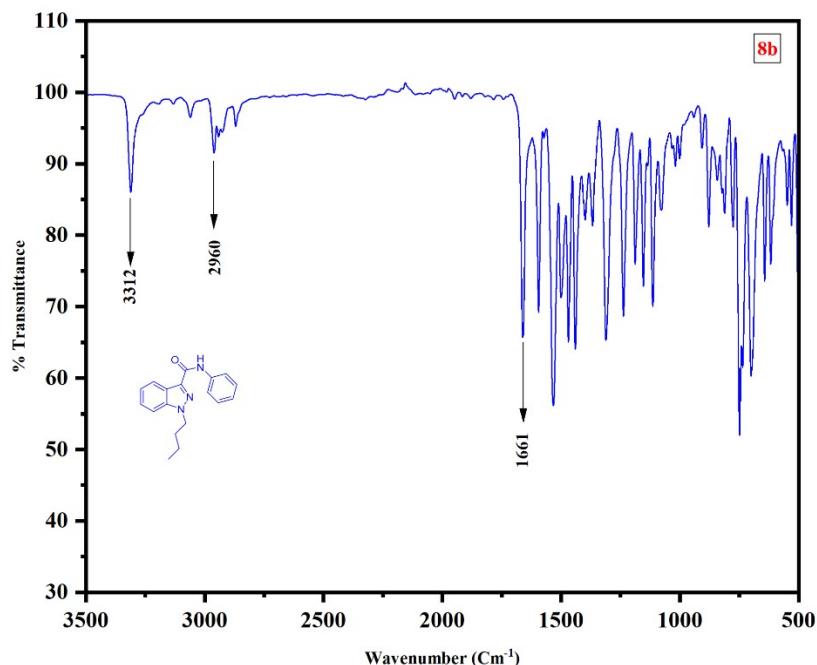


HSQC-NMR [400MHz, DMSO-d₆] spectrum of 1-butyl-N-phenyl-1H-indazole-3-carboxamide (8b).

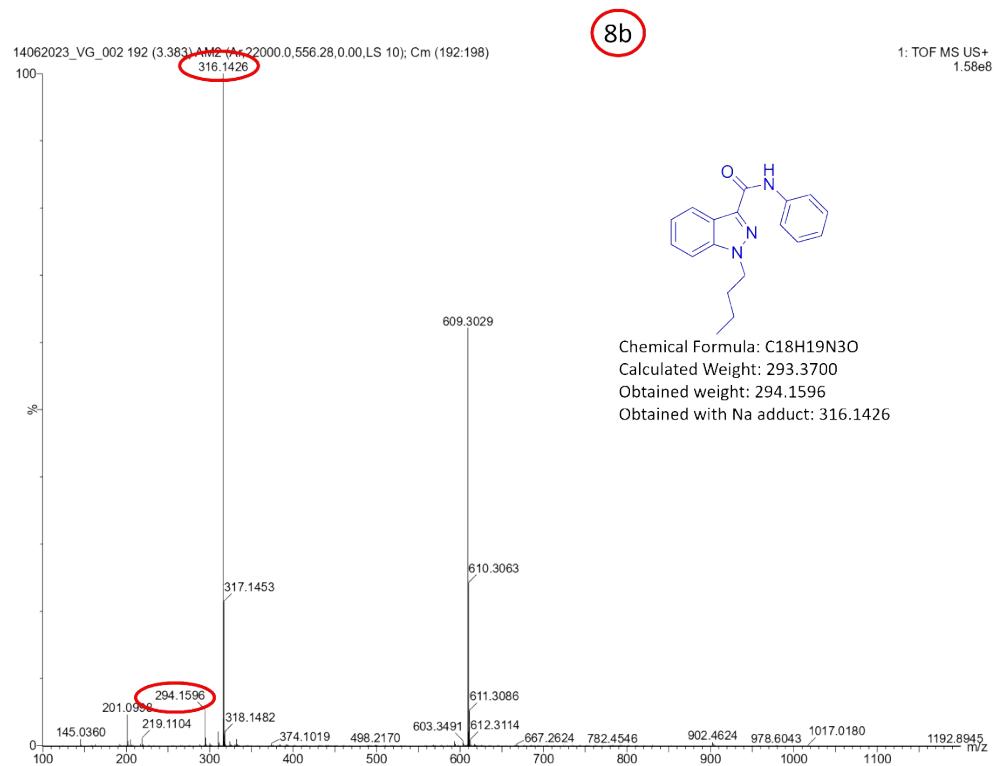
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VG-002



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

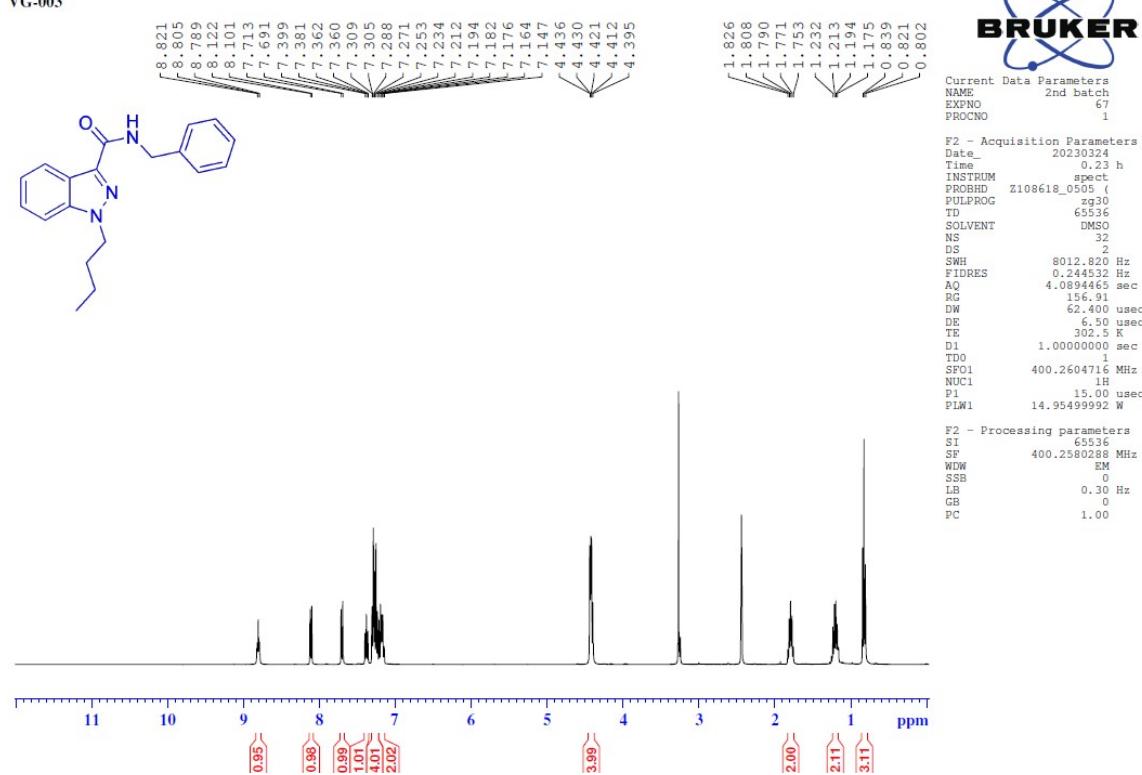


HRMS of 1-butyl-N-phenyl-1H-indazole-3-carboxamide (8b).



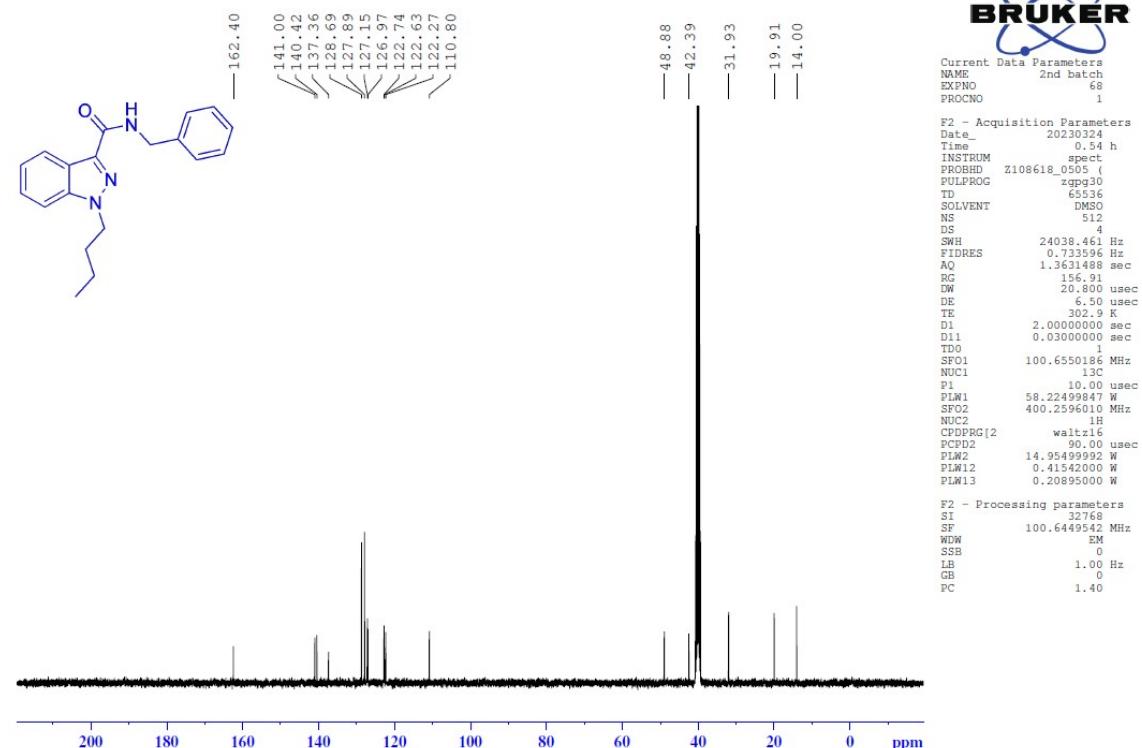
$^1\text{H-NMR}$ [400MHz, DMSO-d_6] spectrum of N-benzyl-1-butyl-1H-indazole-3-carboxamide (8c).

Signature SIF VIT VELLORE
VG-003



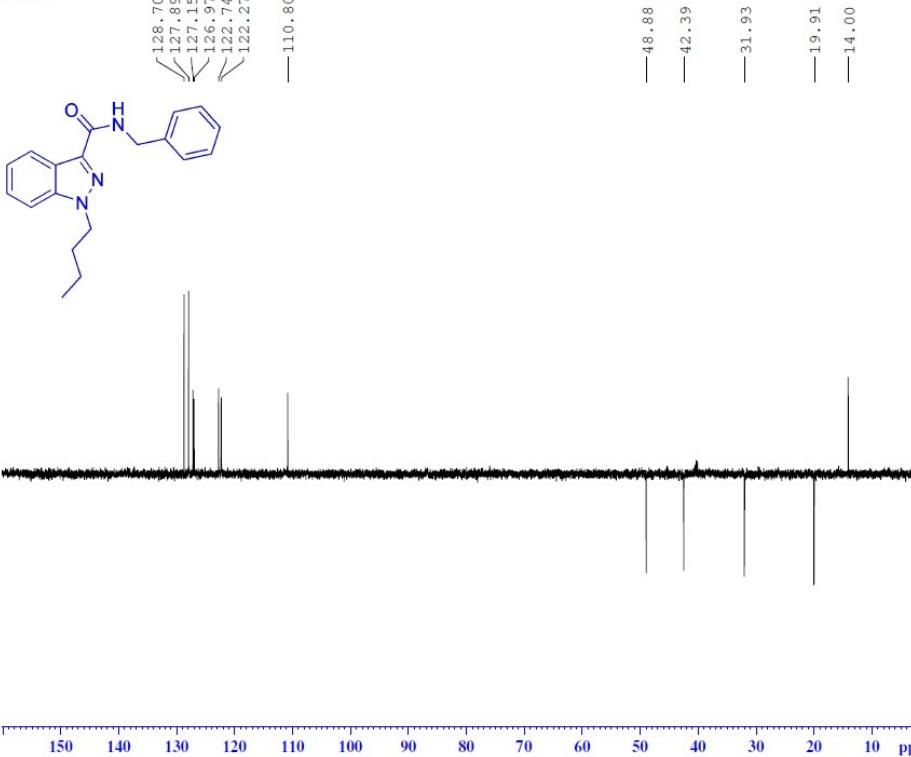
¹³C-NMR [100MHz, DMSO-d₆] spectrum of N-benzyl-1-butyl-1H-indazole-3-carboxamide (8c).

Signature SIF VIT VELLORE
VG-003



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

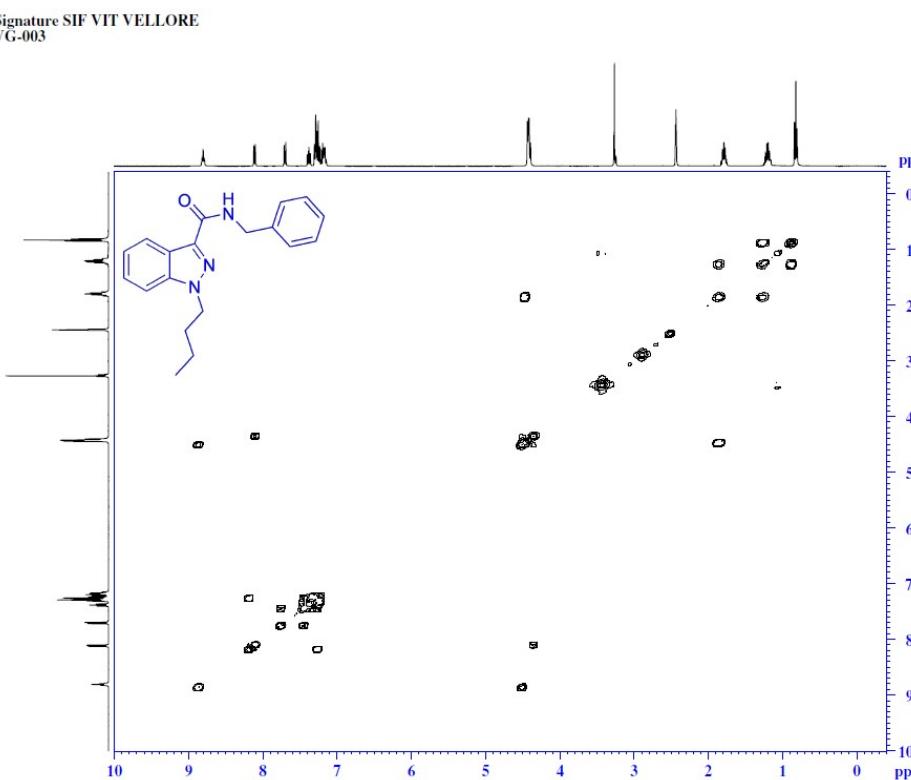
Signature SIF VIT VELLORE
VG-003



COSY-

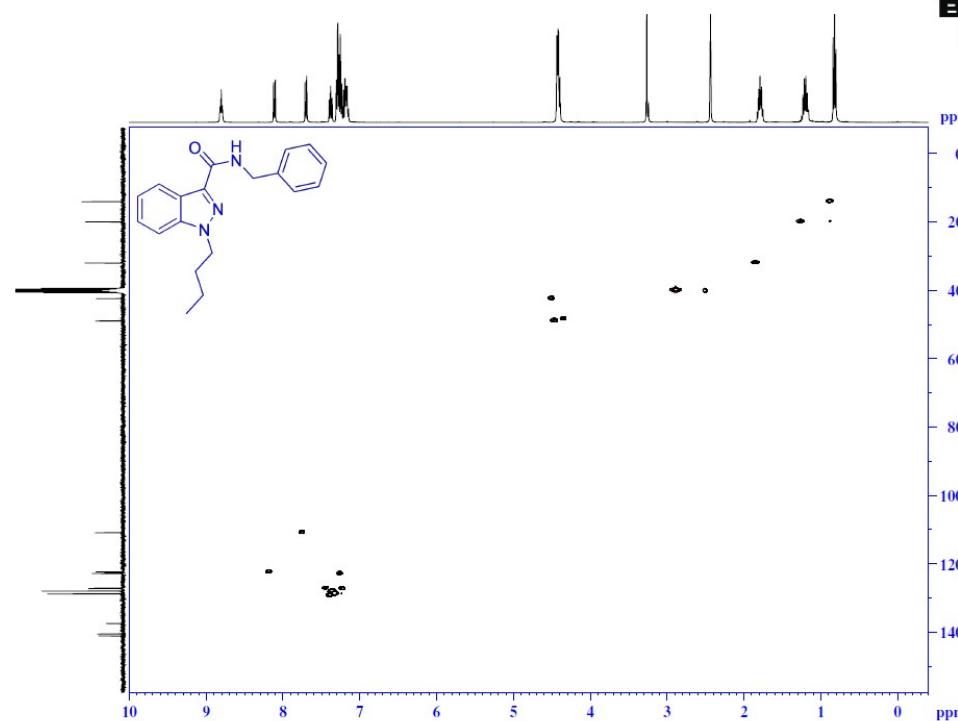
NMR [400MHz, DMSO-d₆] spectrum of N-benzyl-1-butyl-1H-indazole-3-carboxamide (8c).

Signature SIF VIT VELLORE
VG-003

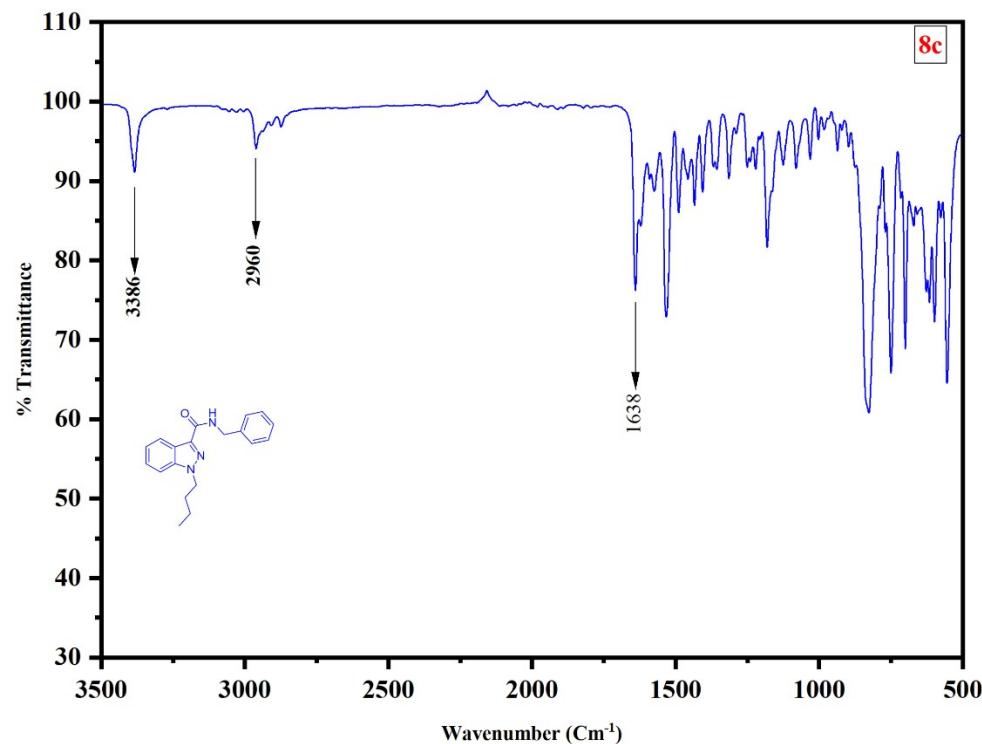


HSQC-NMR [400MHz, DMSO-d₆] spectrum of N-benzyl-1-butyl-1H-indazole-3-carboxamide (8c).

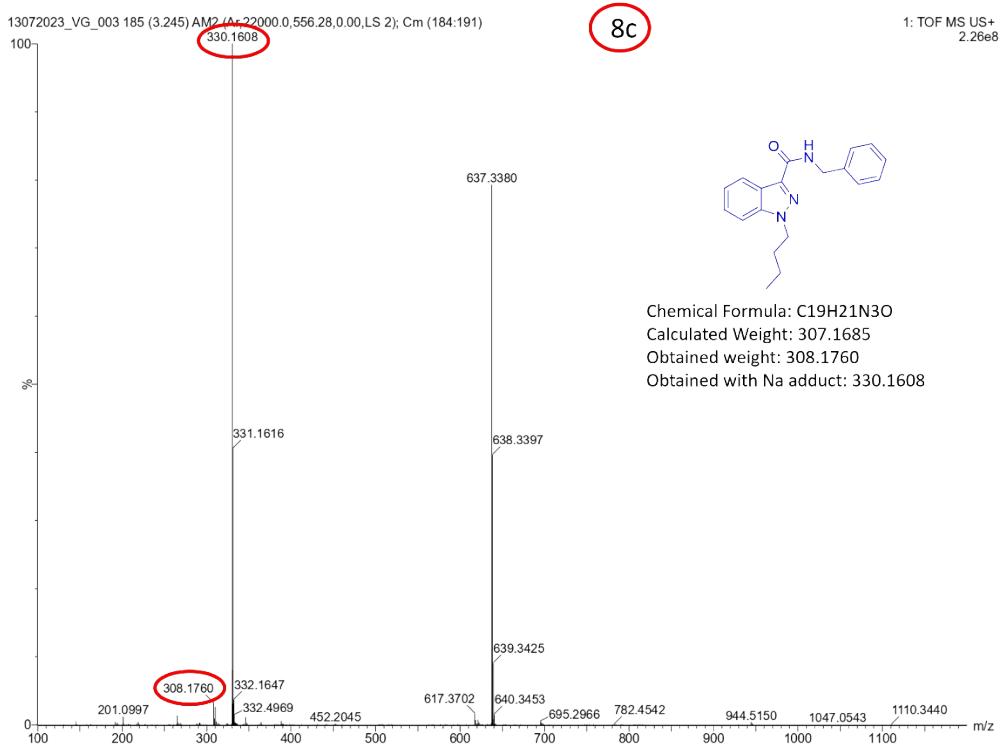
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FT-IR spectrum of N-benzyl-1-butyl-1H-indazole-3-carboxamide (8c).

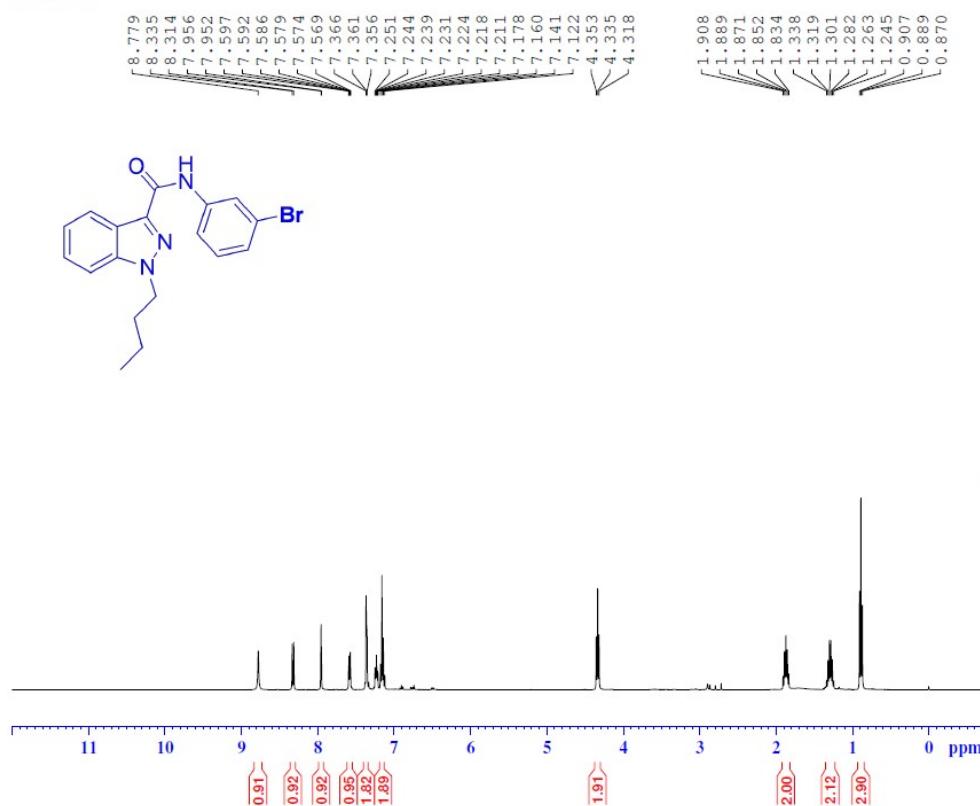


HRMS of N-benzyl-1-butyl-1H-indazole-3-carboxamide (8c).



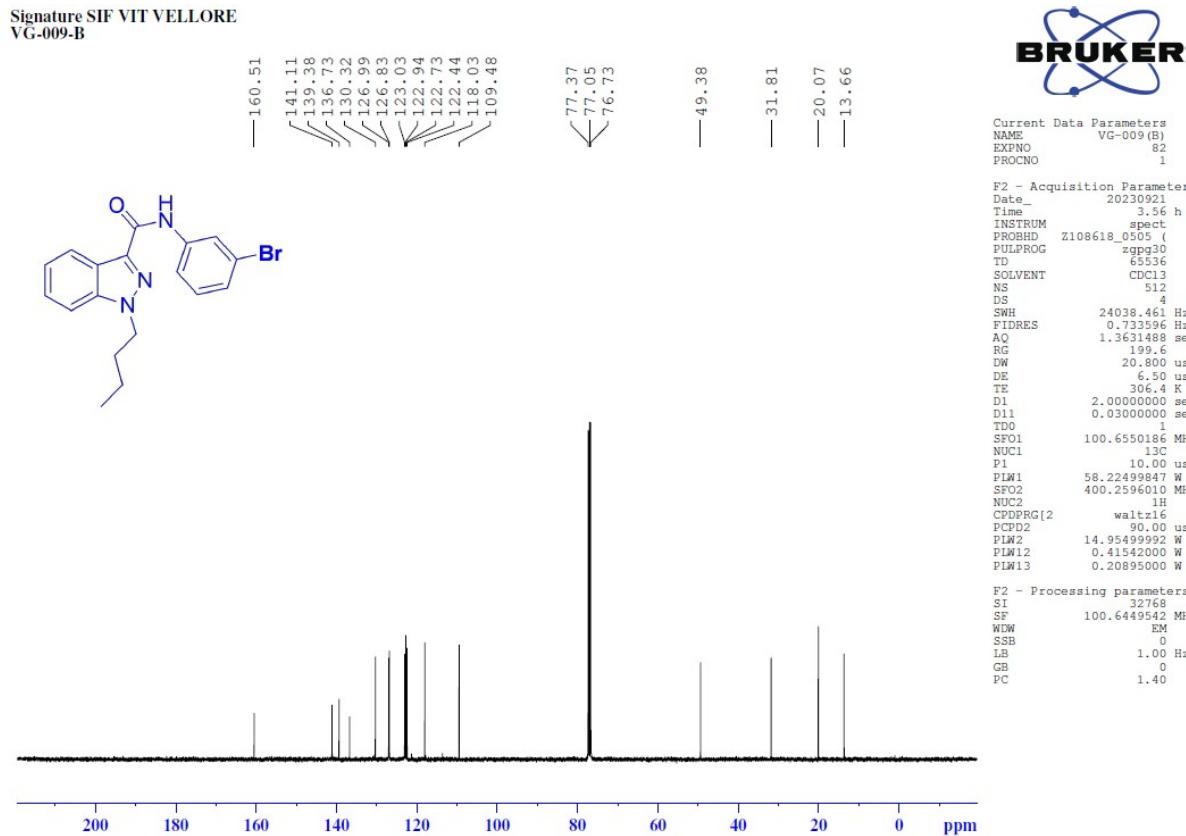
¹H-NMR [400MHz, DMSO-d₆] spectrum of 1-butyl-N-(6-methylpyridine-2yl)-1H-indazole-3-carboxamide (8d).

Signature SIF VIT VELLORE
VG-009-B



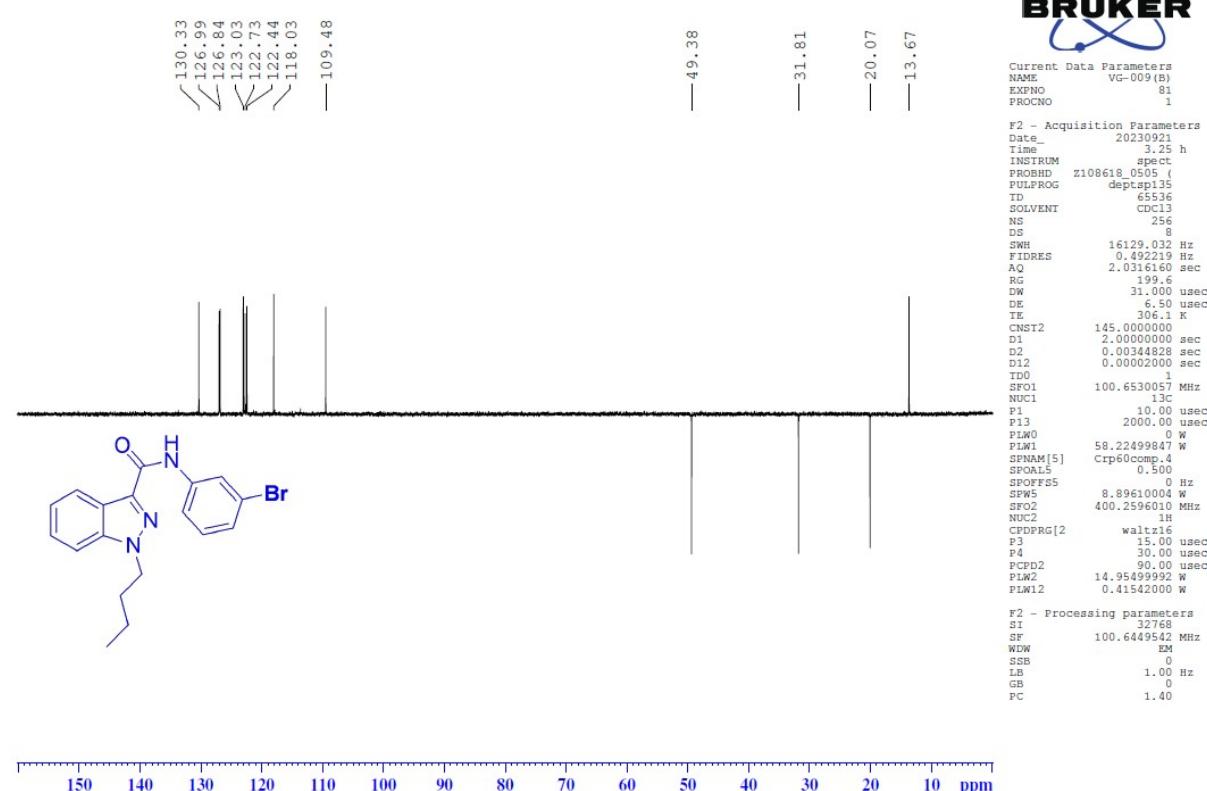
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Signature SIF VIT VELLORE
VG-009-B



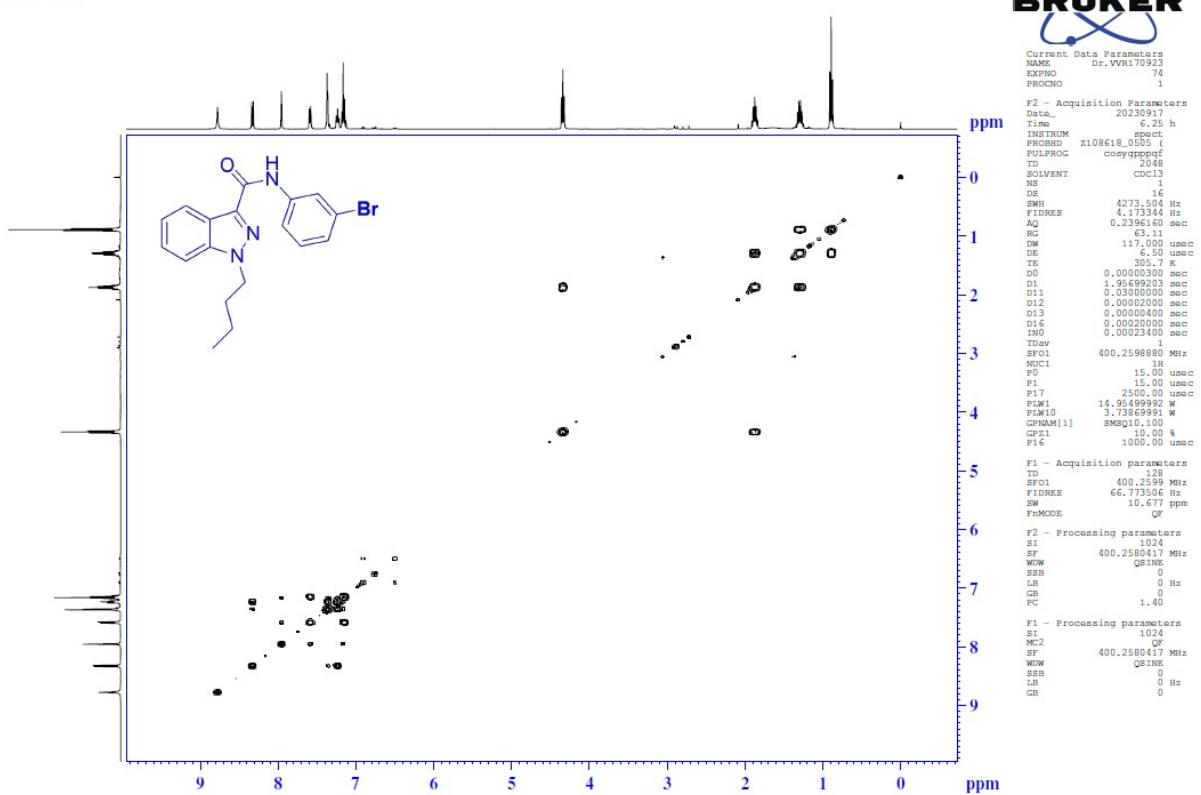
135-DEPT-NMR [100MHz, DMSO-d₆] spectrum of 1-butyl-N-(6-methylpyridine-2yl)-1H-indazole-3-carboxamide (8d).

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VG-009-B

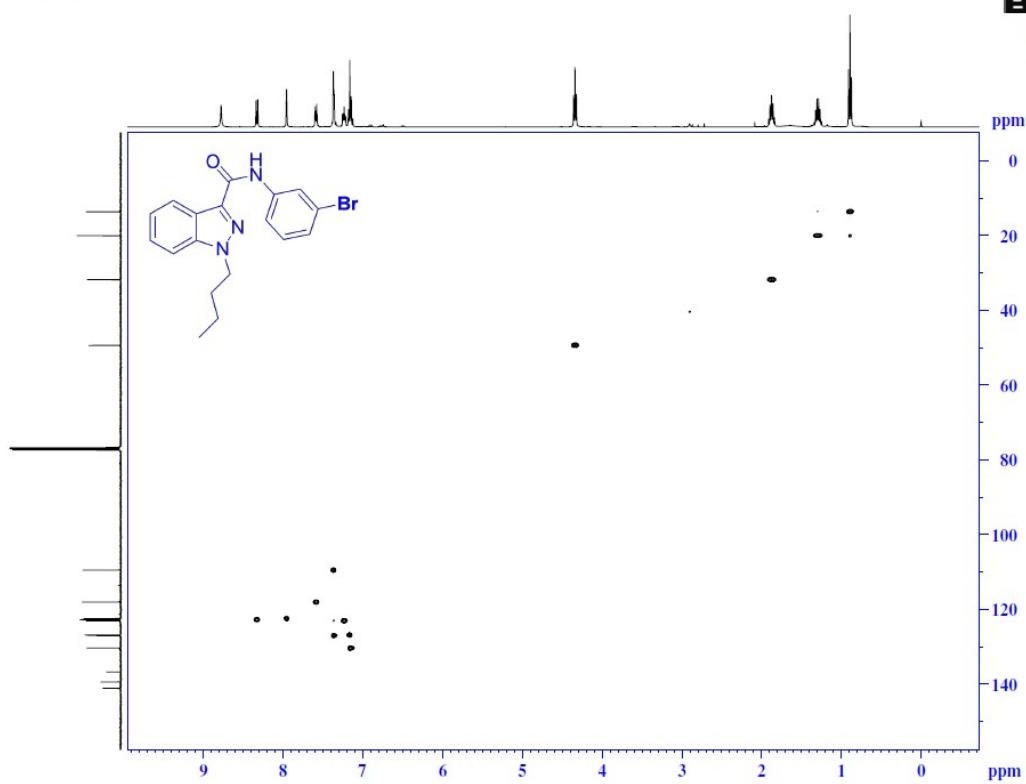


COSY-NMR [400MHz, DMSO-d₆] spectrum of 1-butyl-N-(6-methylpyridine-2yl)-1H-indazole-3-carboxamide (8d).

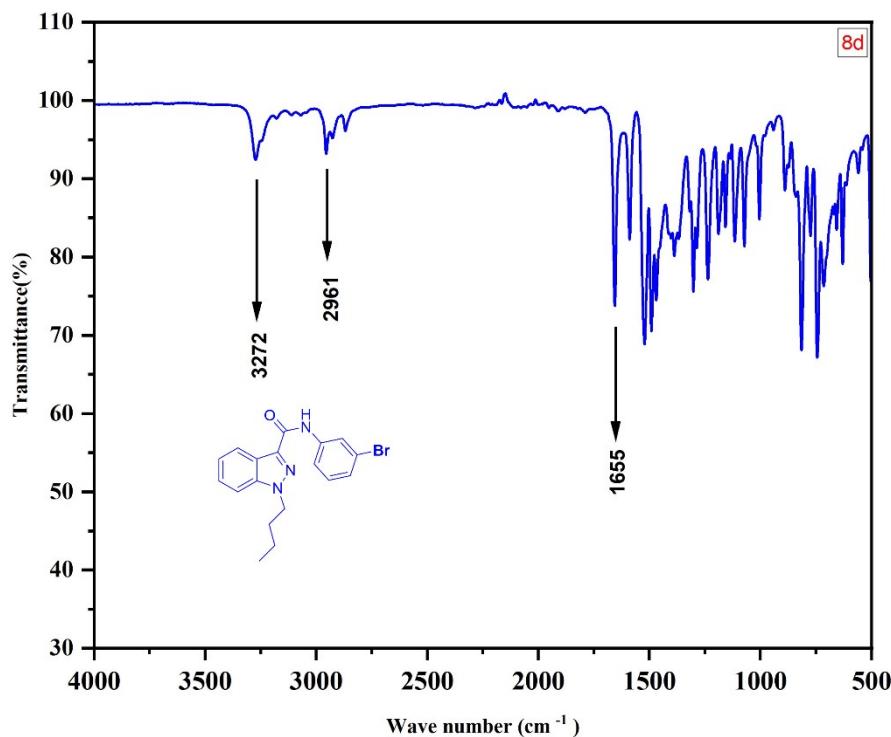
Signature SIF VIT VELLORE
VG-00-9(B)



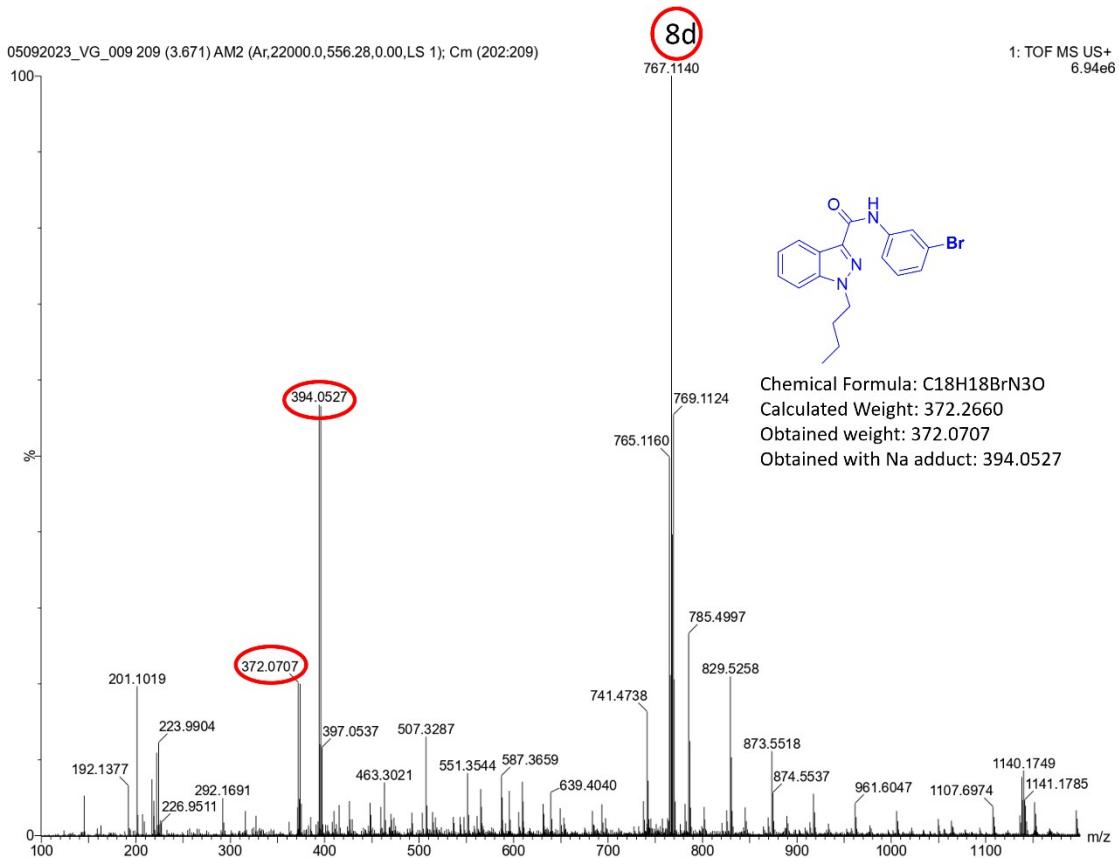
HSQC-NMR [400MHz, DMSO-d₆] spectrum of 1-butyl-N-(6-methylpyridine-2yl)-1H-indazole-3-carboxamide (8d).



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

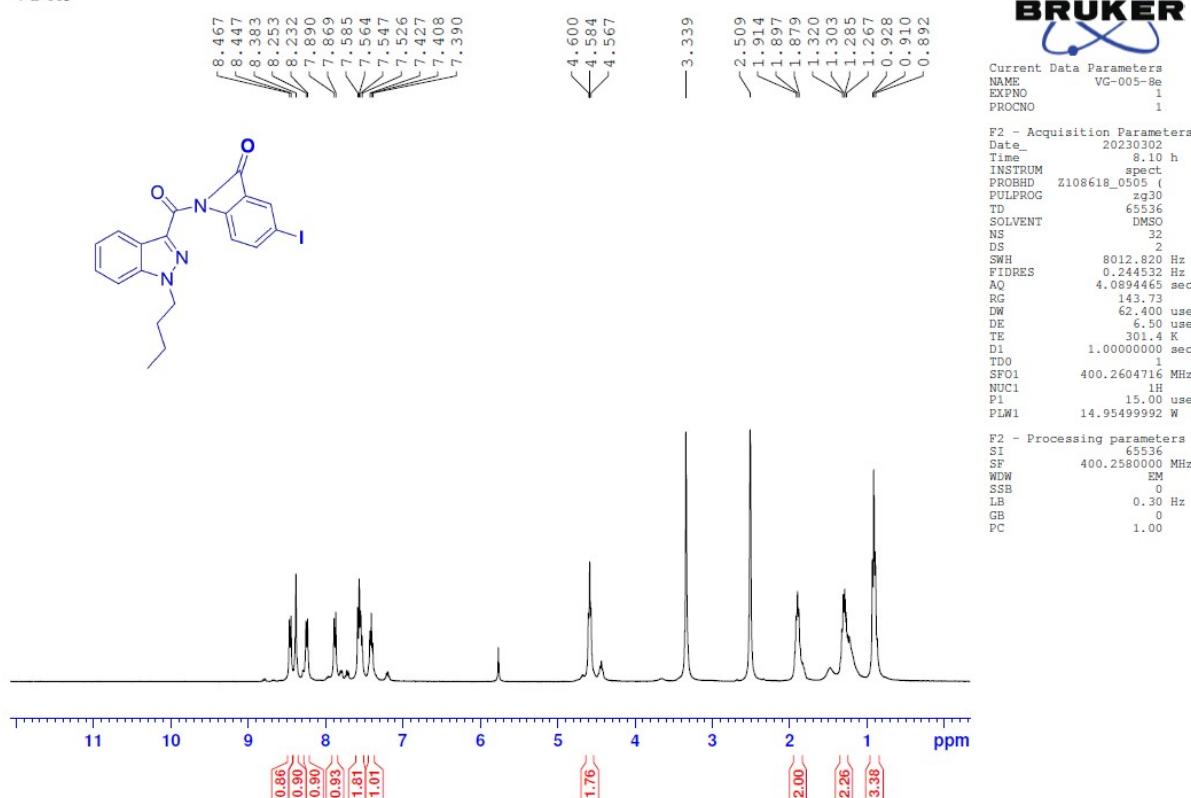


HRMS of 1-butyl-N-(6-methylpyridine-2yl)-1H-indazole-3-carboxamide (8d).



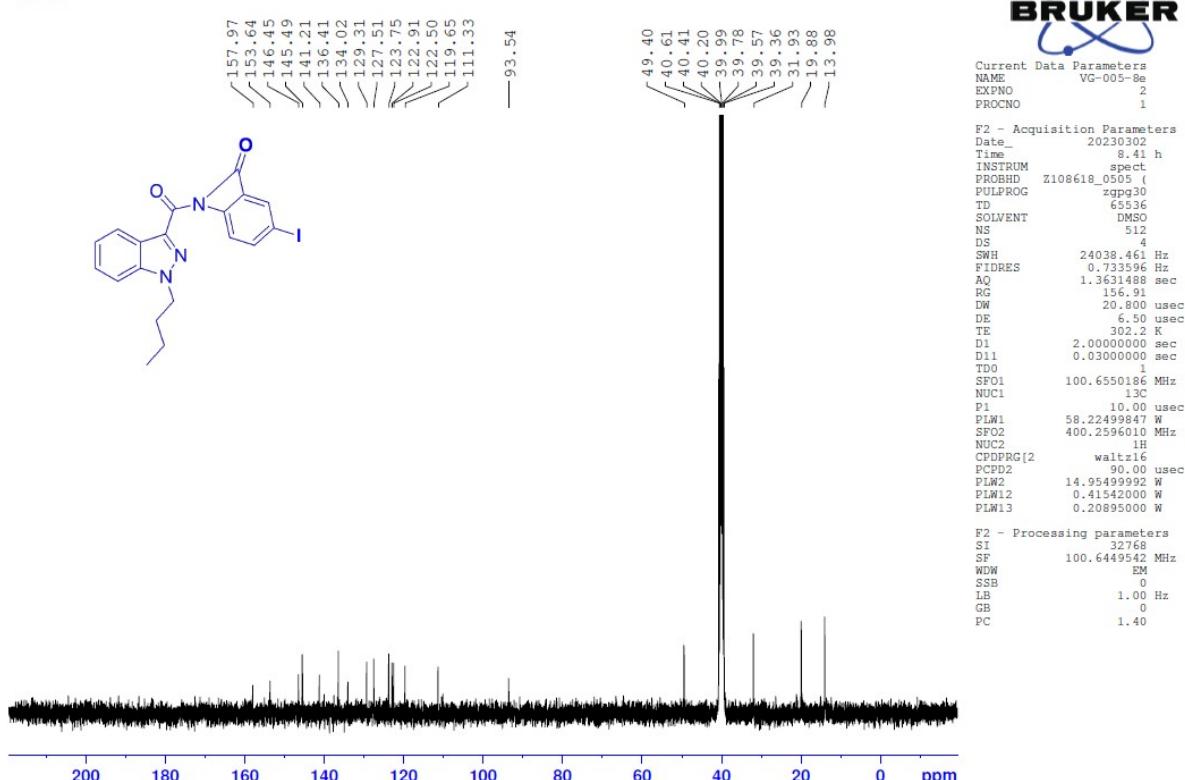
¹H-NMR [400MHz, DMSO-d₆] spectrum of 2-(1-butyl-1H-indazole -3-carboxamido)-5-iodobenzoic acid (8e).

Signature SIF VIT VELLORE
VG-005



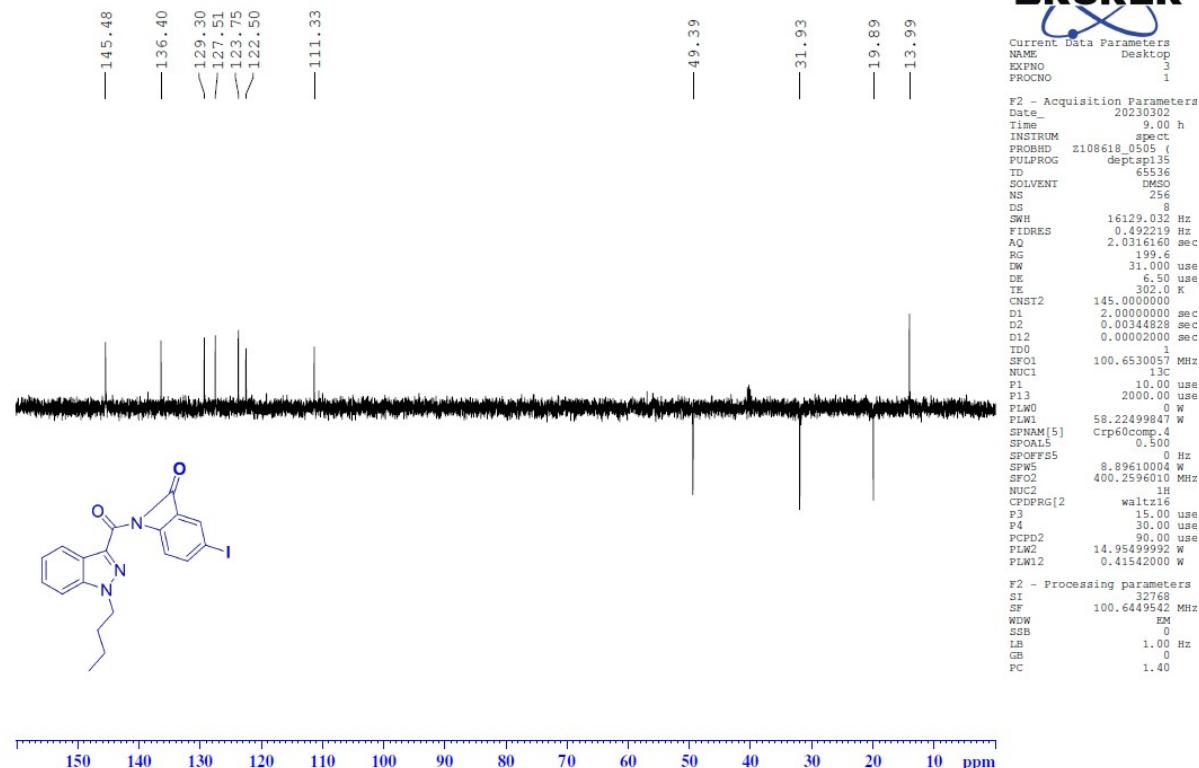
¹H-NMR [100MHz, DMSO-d₆] spectrum of 2-(1-butyl-1H-indazole -3-carboxamido)-5-iodobenzoic acid (8e).

Signature SIF VIT VELLORE
VG-005



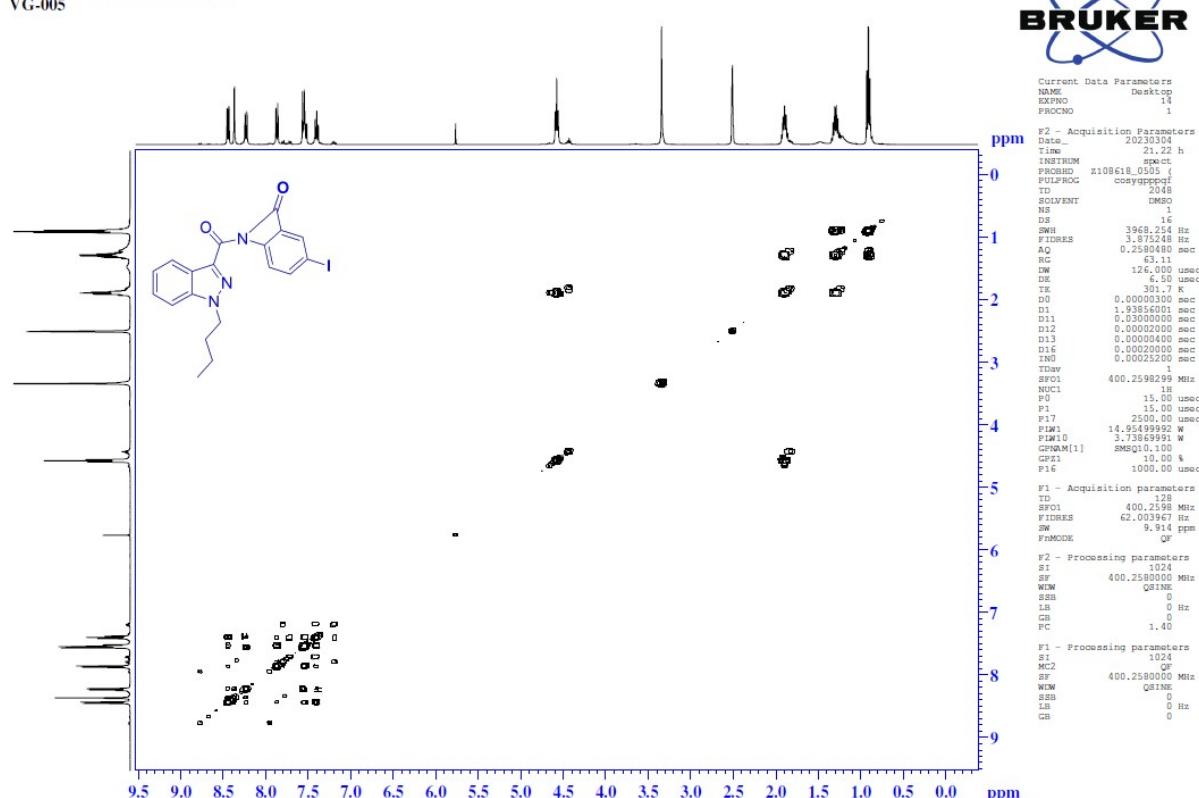
¹³C-NMR [100MHz, DMSO-d₆] spectrum of 2-(1-butyl-1H-indazole -3-carboxamido)-5-iodobenzoic acid (8e).

Signature SIF VIT VELLORE
VG-005

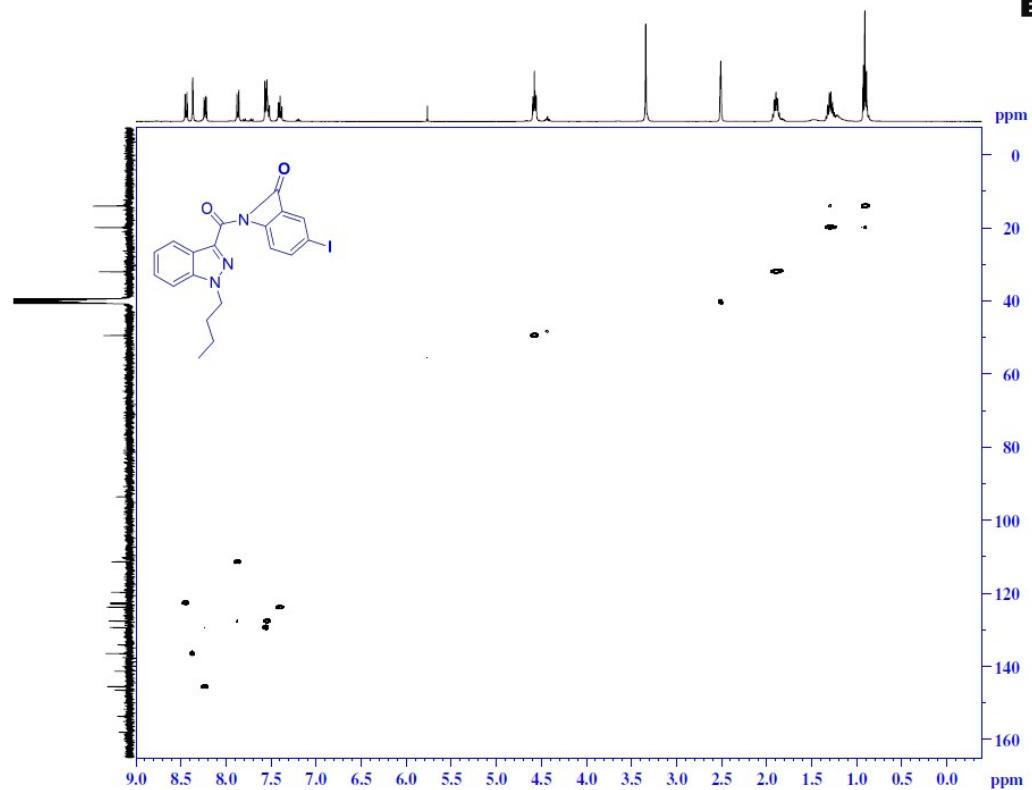


COSY-NMR [400MHz, DMSO-d₆] spectrum of 2-(1-butyl-1H-indazole -3-carboxamido)-5-iodobenzoic acid (8e).

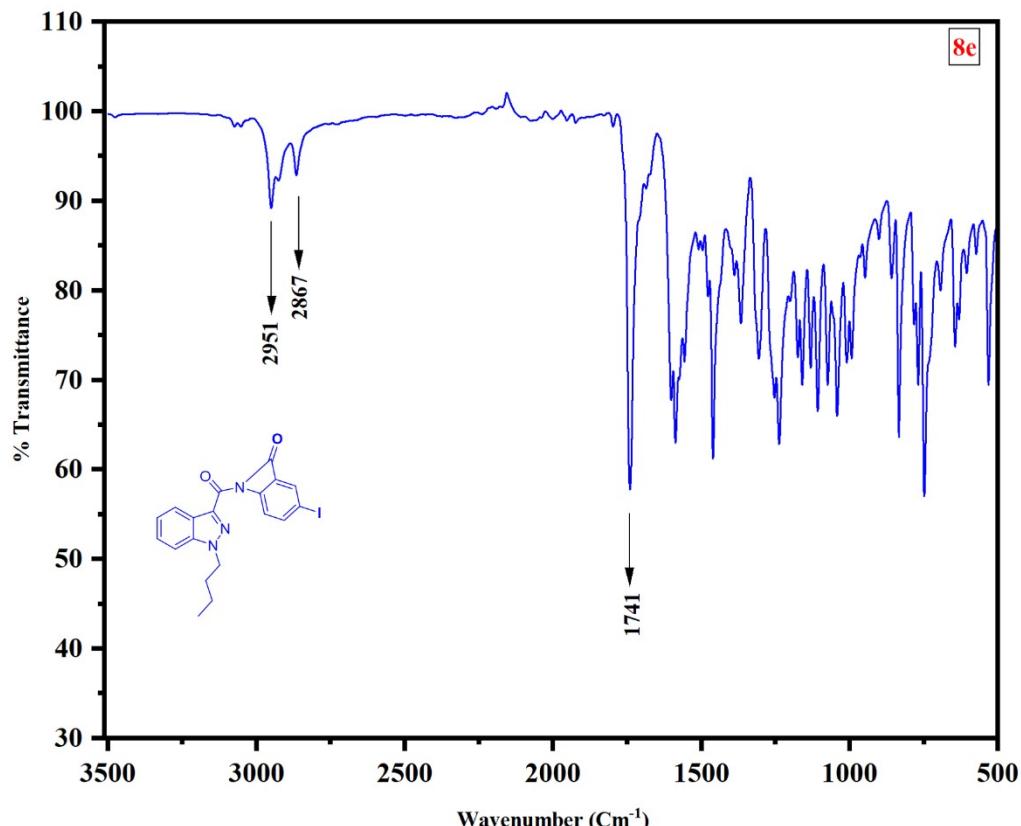
Signature SIF VIT VELLORE
VG-005



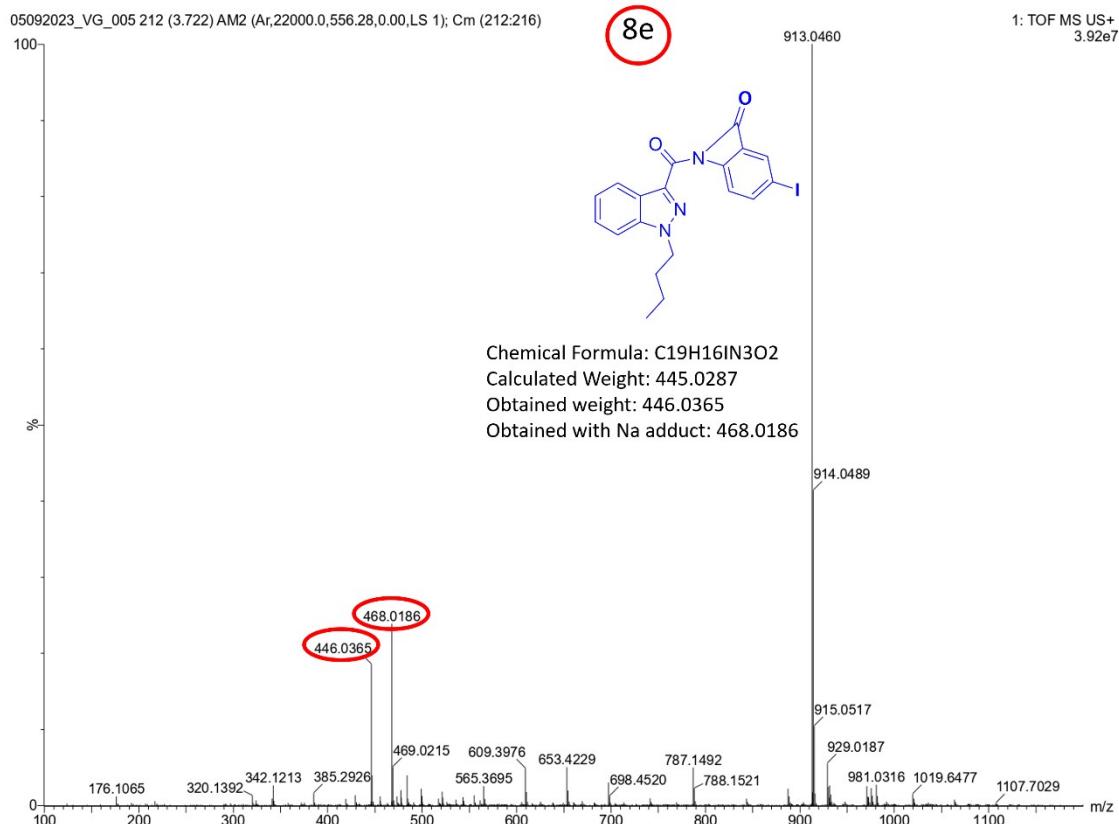
HSQC-NMR [400MHz, DMSO-d₆] spectrum of 2-(1-butyl-1H-indazole -3-carboxamido)-5-iodobenzoic acid (8e).



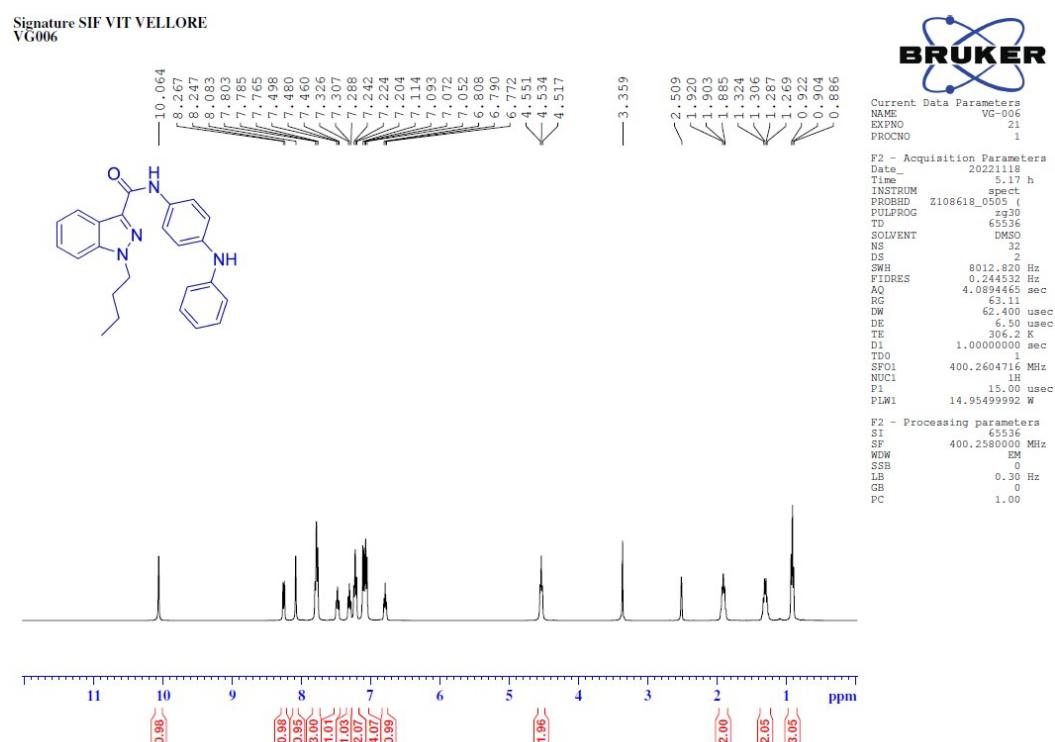
FT-IR spectrum of 2-(1-butyl-1H-indazole-3-carboxamido)-5-iodobenzoic acid (8e).



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

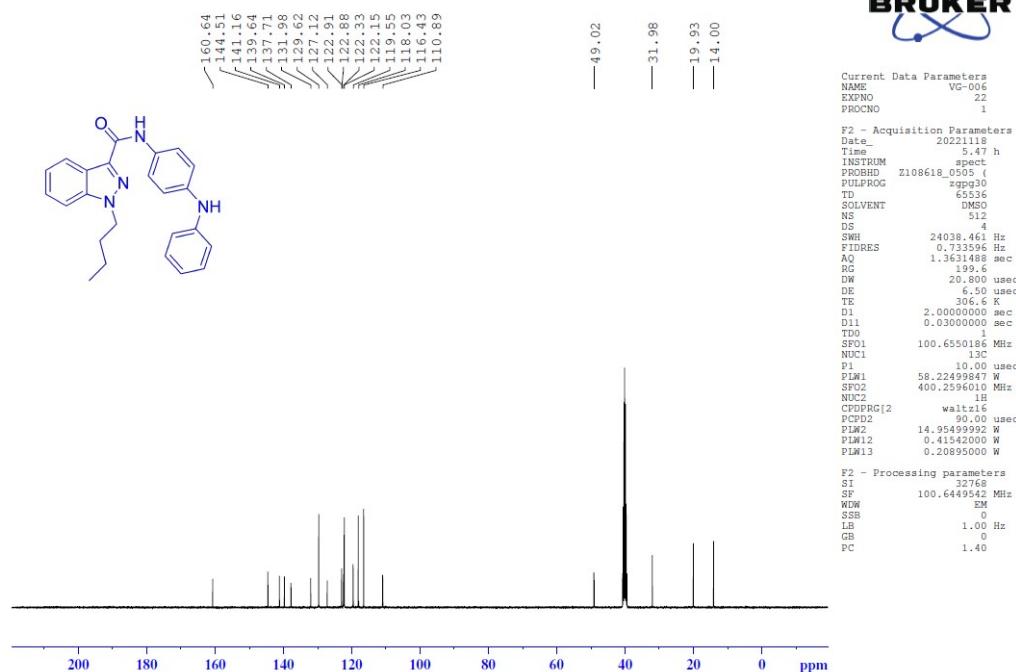


¹H-NMR [400MHz, DMSO-d₆] spectrum of 1-butyl-N-(4-(phenylamino) phenyl)-1H-indazole-3-carboxamide (8f).



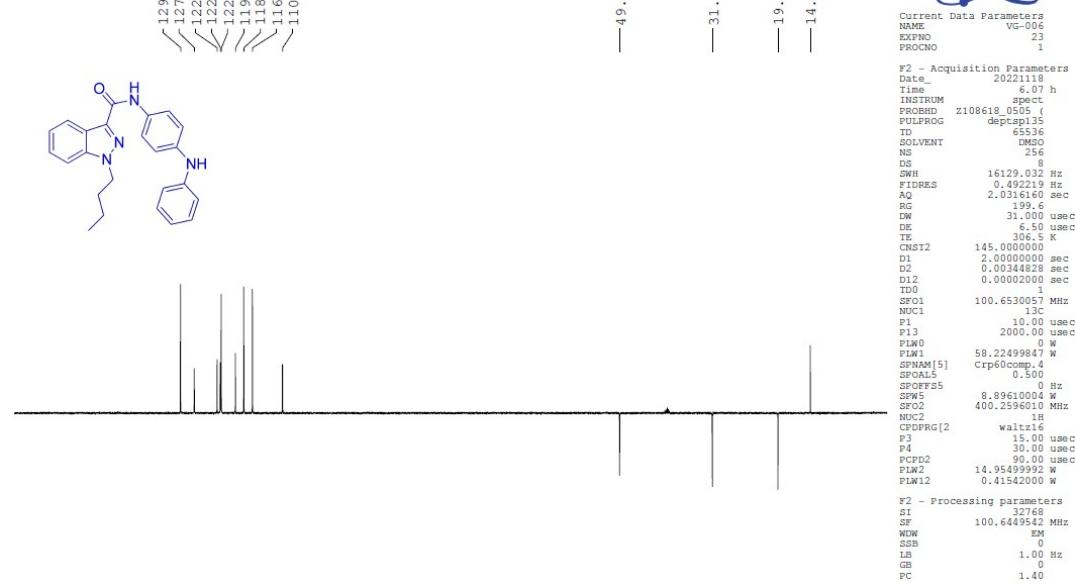
¹³C-NMR [100MHz, DMSO-d₆] spectrum of 1-butyl-N-(4-(phenylamino) phenyl)-1H-indazole-3-carboxamide (8f).

Signature SIF VIT VELLORE
VG006



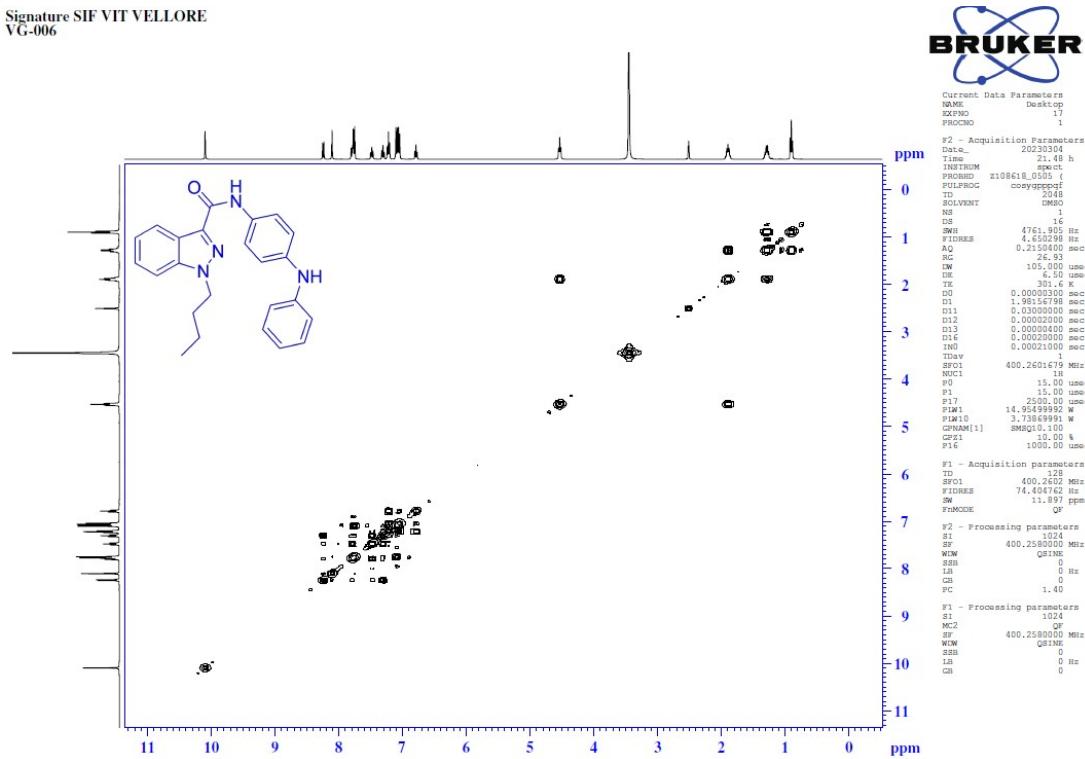
¹³⁵-DEPT-NMR [100MHz, DMSO-d₆] spectrum of 1-butyl-N-(4-(phenylamino)phenyl)-1H-indazole-3-carboxamide (8f).

Signature SIF VIT VELLORE
VG006



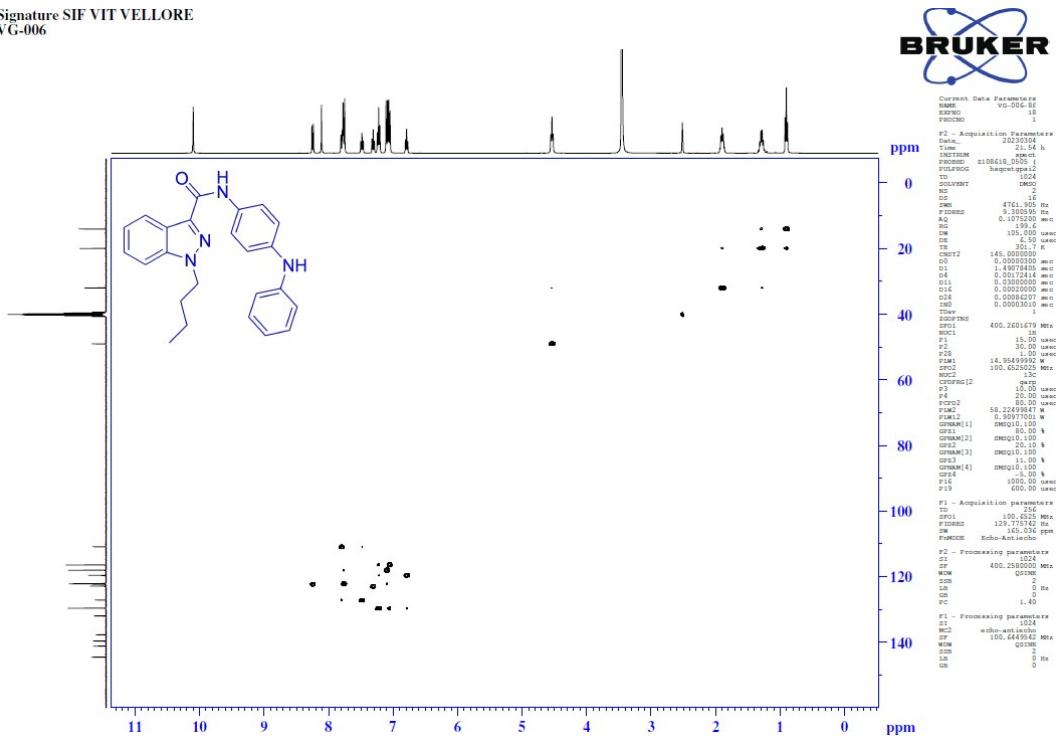
¹COSY-NMR [400MHz, DMSO-d₆] spectrum of 1-butyl-N-(4-(phenylamino)phenyl)-1H-indazole-3-carboxamide (8f).

Signature SIF VIT VELLORE
VG-006

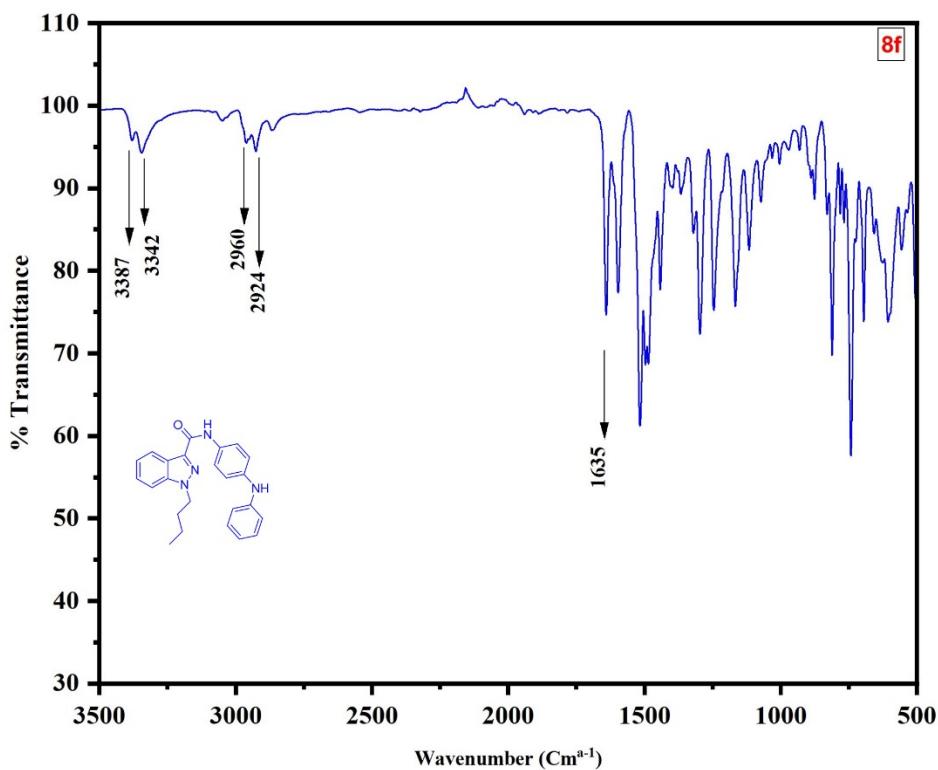


HSQC-NMR [400MHz, DMSO-d₆] spectrum of 1-butyl-N-(4-(phenylamino)phenyl)-1H-indazole-3-carboxamide (8f).

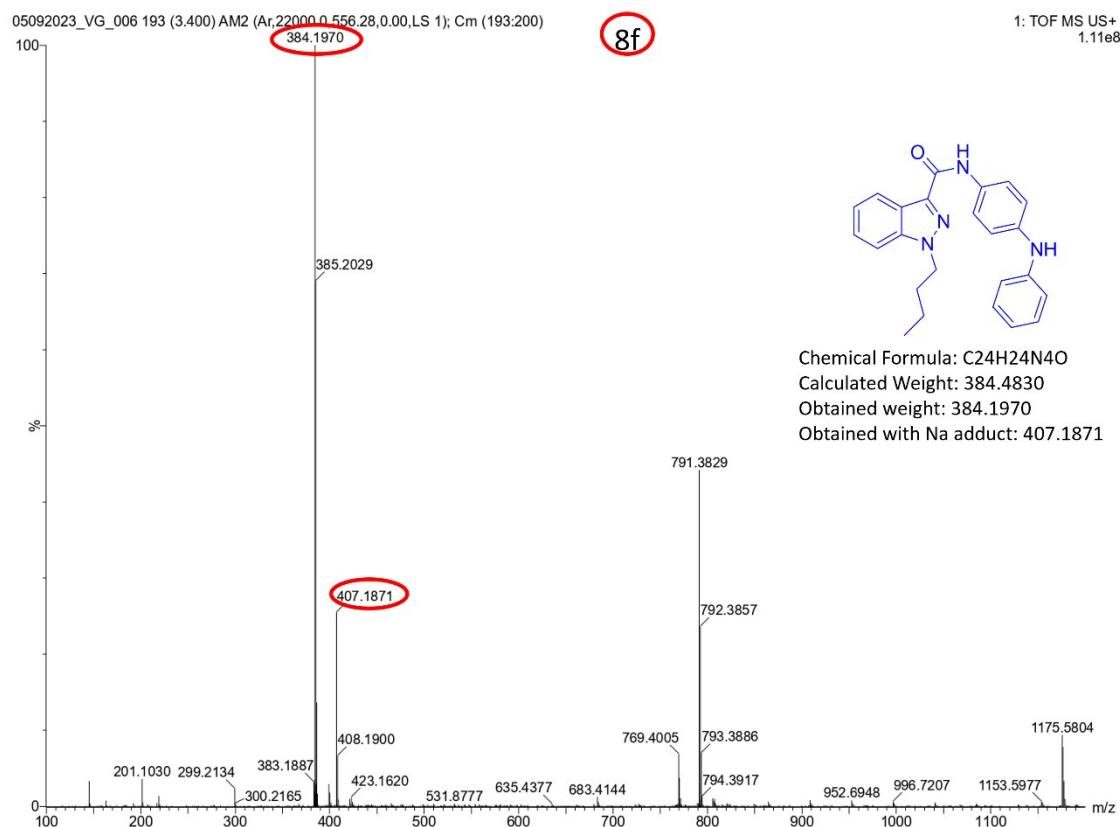
Signature SIF VIT VELLORE
VG-006



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

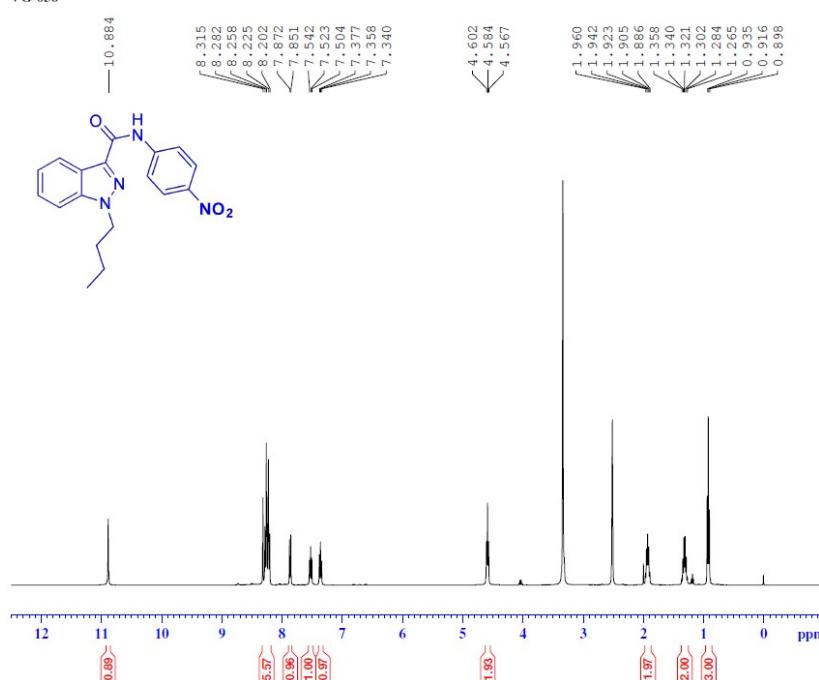


HRMS of 1-butyl-N-(4-(phenylamino)phenyl)-1H-indazole-3-carboxamide (8f).



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

Signature SIF VIT VELLORE
VG-036



Current Data Parameters
NAME VG-036
EXPNO 70
PROCNO 1

F2 - Acquisition Parameters
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Time 15.38 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 4.0894165 sec
RG 143.7
DW 62.400 usec
DE 6.50 usec
TE 305.9 K
D1 1.00000000 sec
TDO 400.260716 MHz
SF01 400.260716 MHz
NUC1 1H
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PLW1 14.95499992 W
PC 1.00

F2 - Processing parameters

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SP 400.2579980 MHz

WDW EM

SSB 0

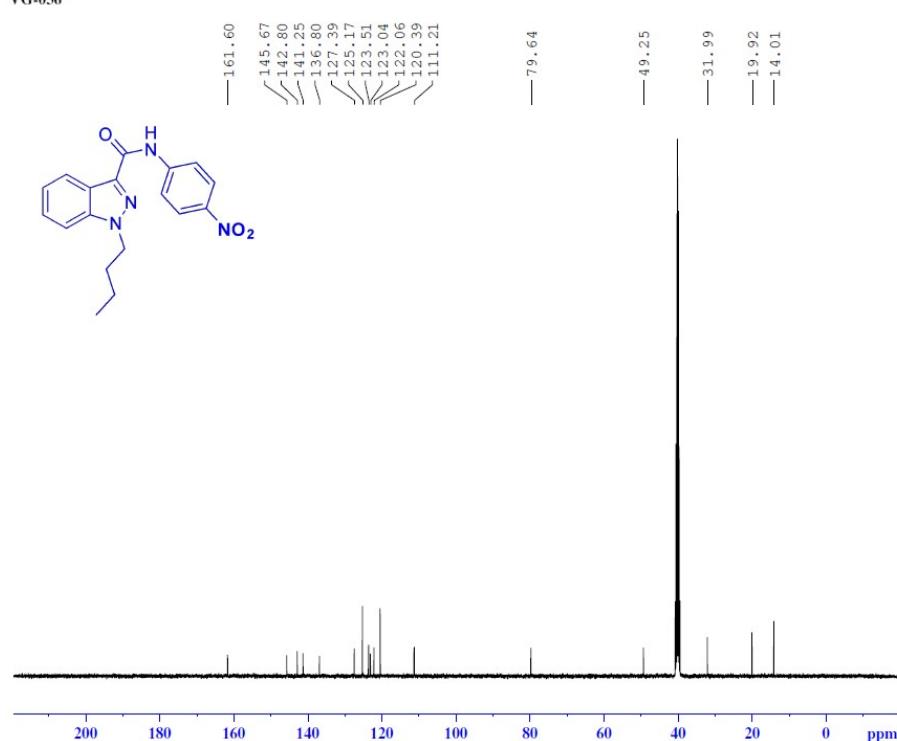
LB 0.30 Hz

GB 0

PC 1.00

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

Signature SIF VIT VELLORE
VG-036



Current Data Parameters
NAME Dr.VVR160523
EXPNO 58
PROCNO 1

F2 - Acquisition Parameters
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Time 1.18 h
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TD 65536
SOLVENT DMSO
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.1996 Hz
AQ 1.363148 sec
RG 199.6
DW 20.800 usec
DE 6.50 usec
TE 305.0 K
D1 2.0000000 sec
D11 0.03000000 sec
TDO 1
SF01 100.6550186 MHz
NUC1 13C
P1 10.00 usec
PLW1 58.2249980 W
SF02 400.2596010 MHz
NUC2 1H
CPDPG[2] waltz16
CPDPG[2] 90.00 usec
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F2 - Processing parameters

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SP 100.6449542 MHz

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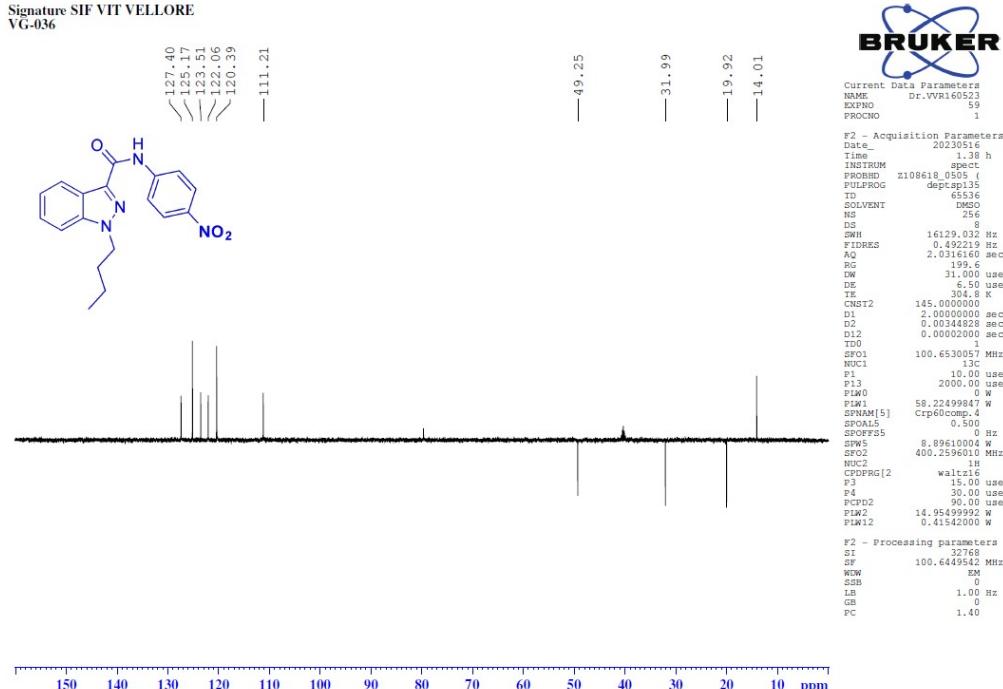
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LB 1.00 Hz

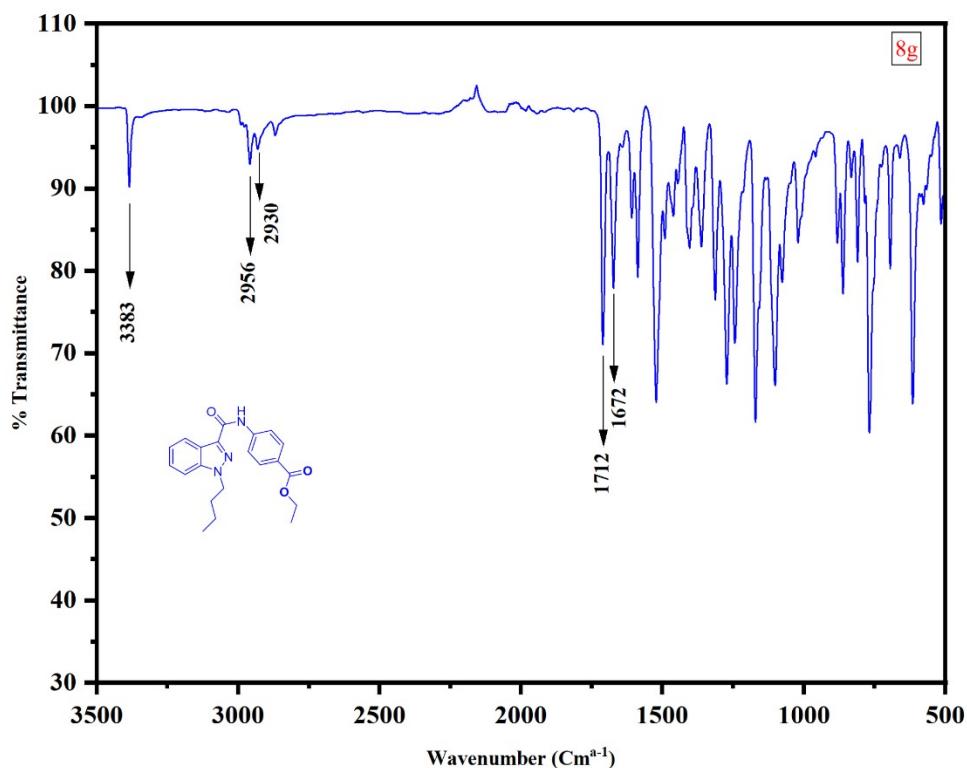
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PC 1.40

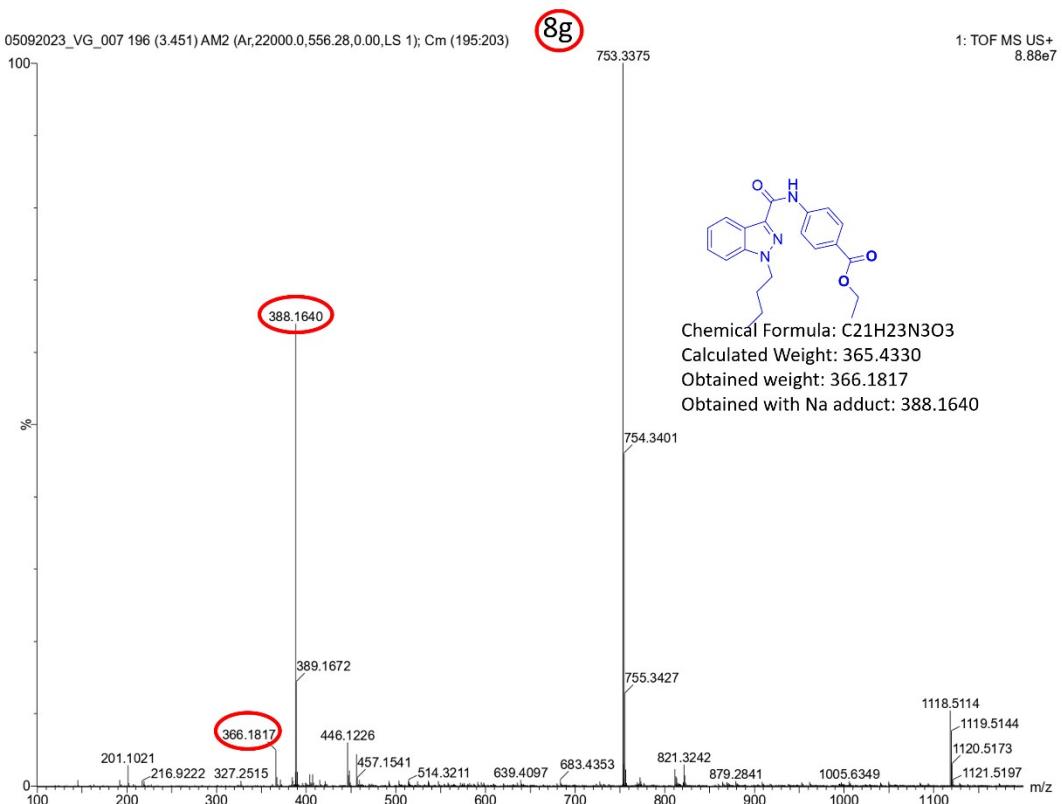
135-DEPT-NMR [400MHz, DMSO-d₆] spectrum of 1-butyl-N-(4-nitophenyl)-1H-indazole-3-carboxamide (8g).



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

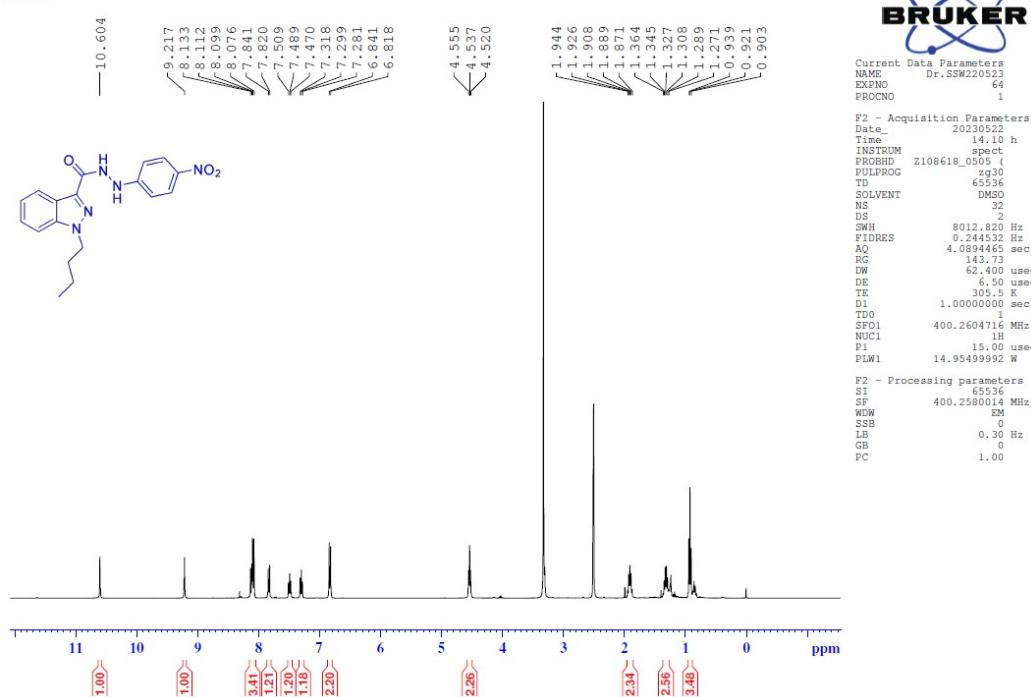


HRMS of 1-butyl-N-(4-nitrophenyl)-1H-indazole-3-carboxamide (8g).



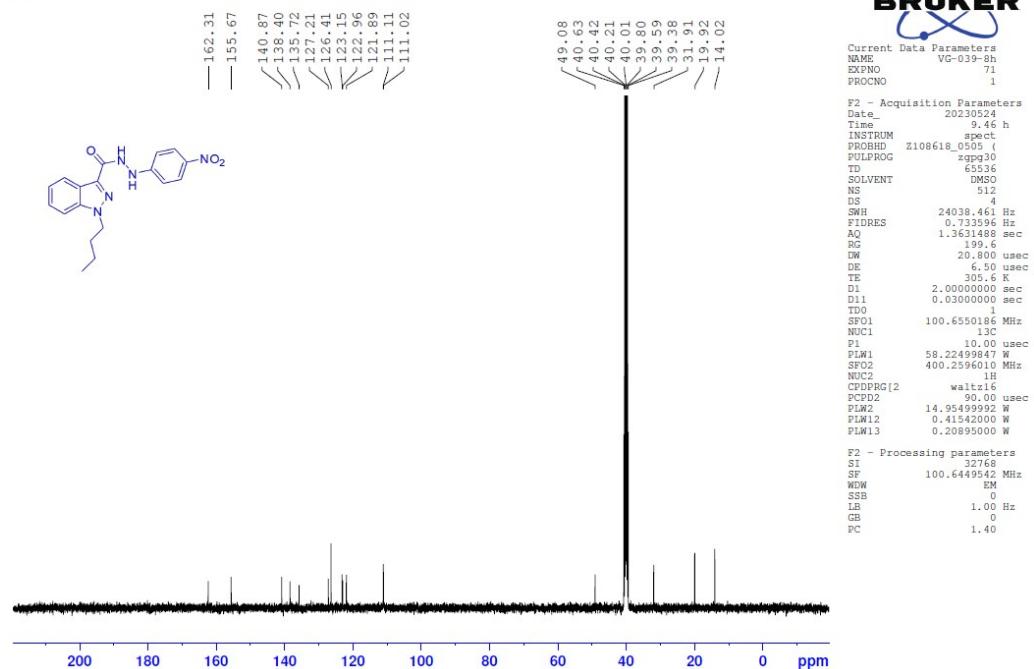
¹H-NMR [400MHz, DMSO-d₆] spectrum of 1-butyl-N-(4-nitrophenyl)-1H-indazole-3-carbohydrazide (8h).

Signature SIF VIT VELLORE
VG-039



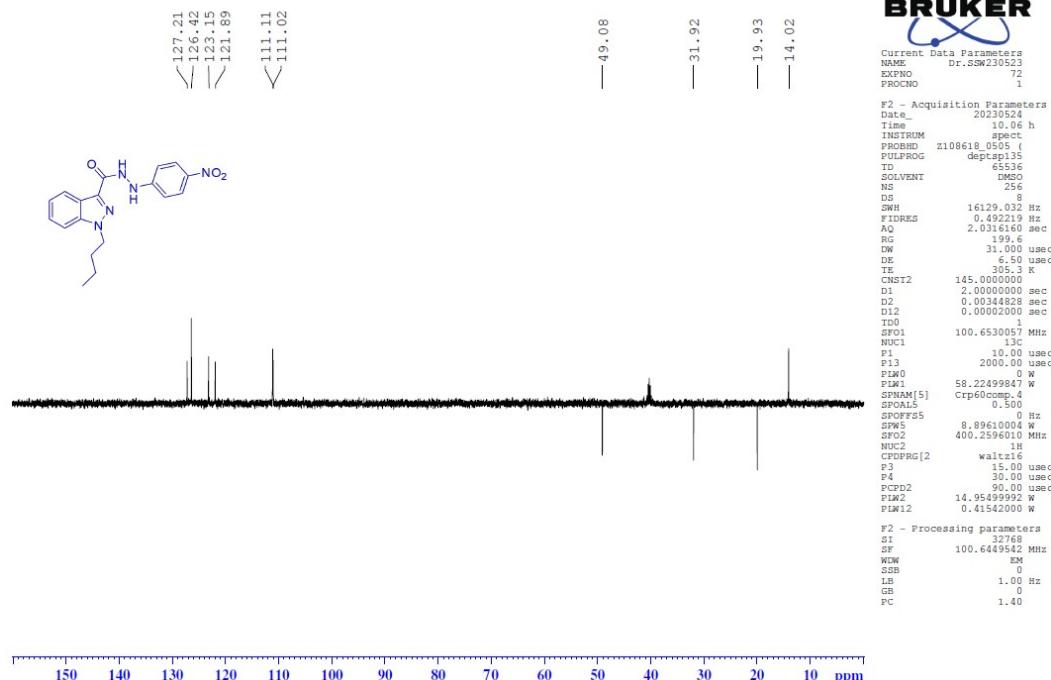
¹³C-NMR [100MHz, DMSO-d₆] spectrum of 1-butyl-N-(4-nitro phenyl)-1H-indazole-3-carbohydrazide (8h).

Signature SIF VIT VELLORE
VG-039

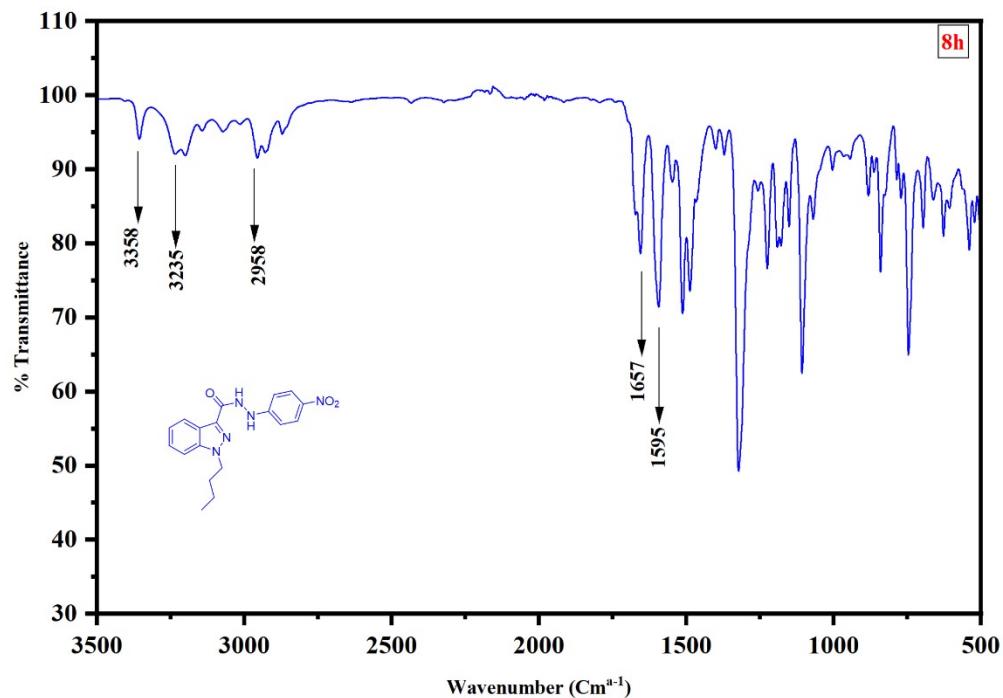


135-DEPT-NMR [100MHz, DMSO-d₆] spectrum of 1-butyl-N-(4-nitrophenyl)-1H-indazole-3-carbohydrazide (8h).

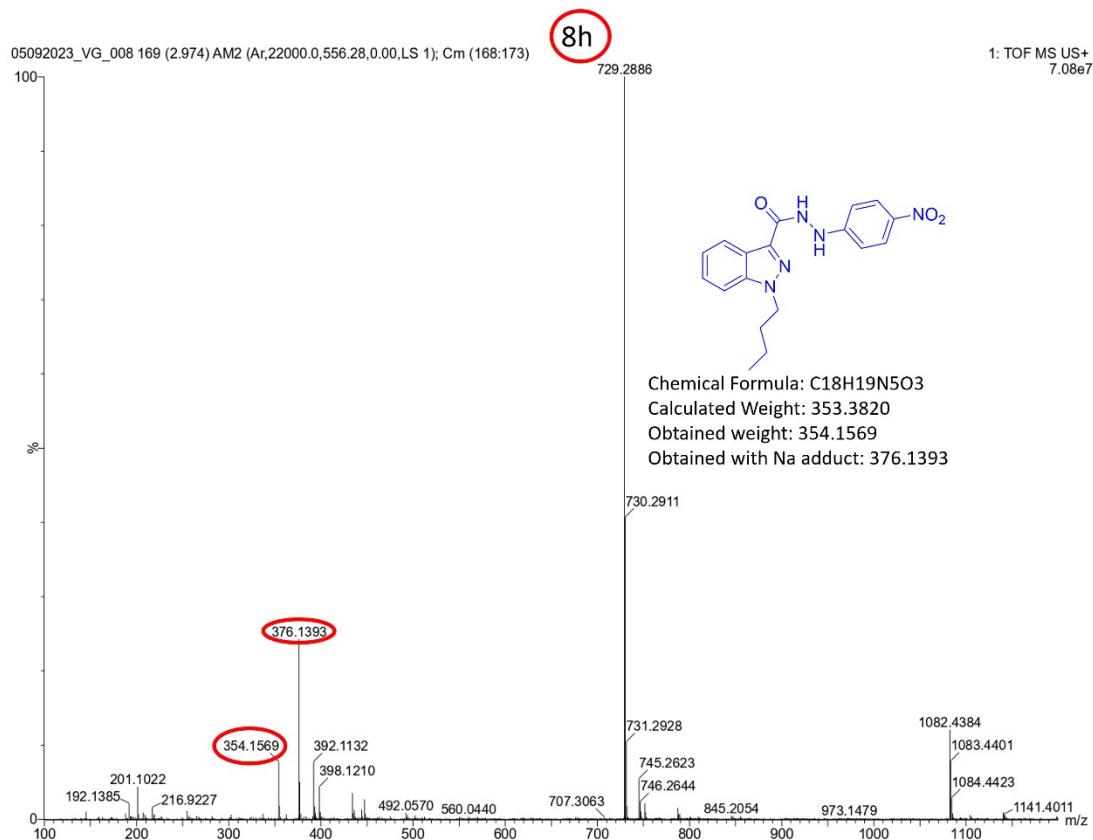
Signature SIF VIT VELLORE
VG-039



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

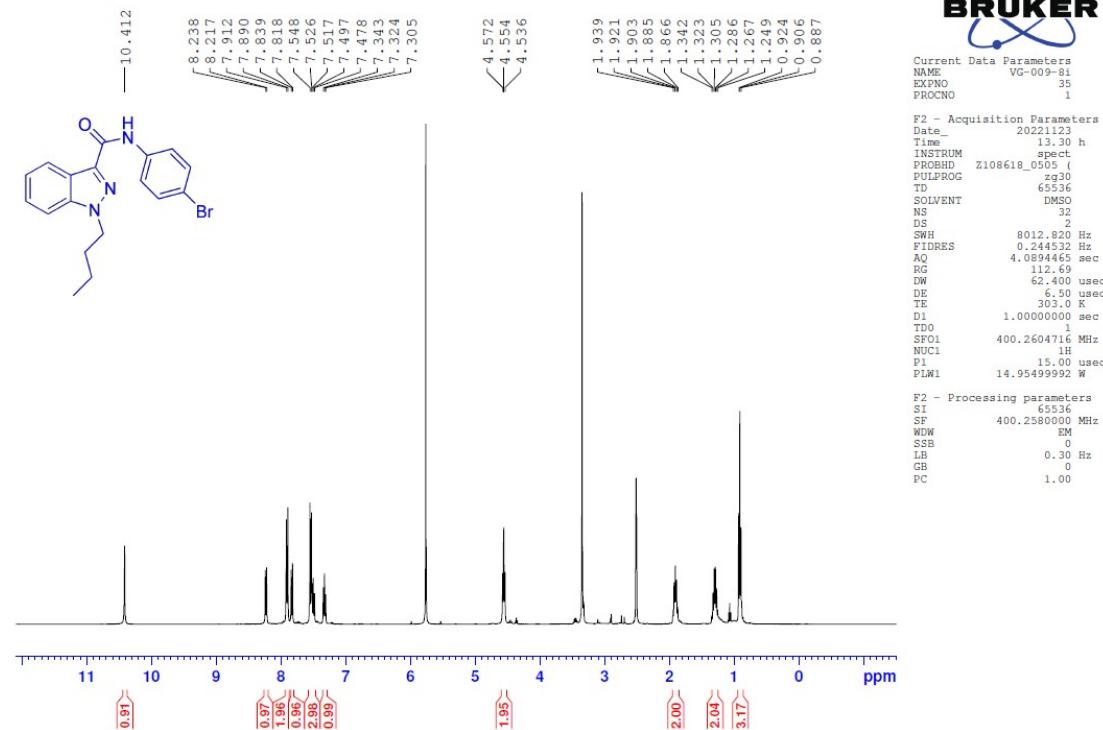


HRMS of **1-butyl-N-(4-nitrophenyl)-1H-indazole-3-carbohydrazide** (**8h**).



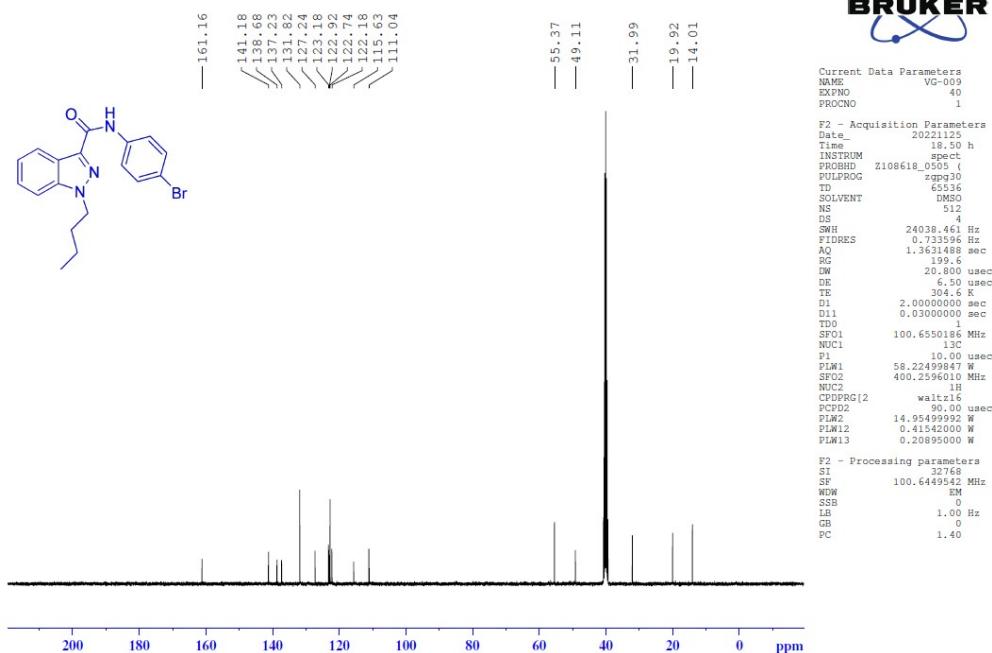
¹H-NMR [400MHz, DMSO-d₆] spectrum of N-(4-Bromophenyl)-1-butyl-1H-indazole-3-carboxamide (**8i**).

Signature SIF VIT VELLORE
VG-009



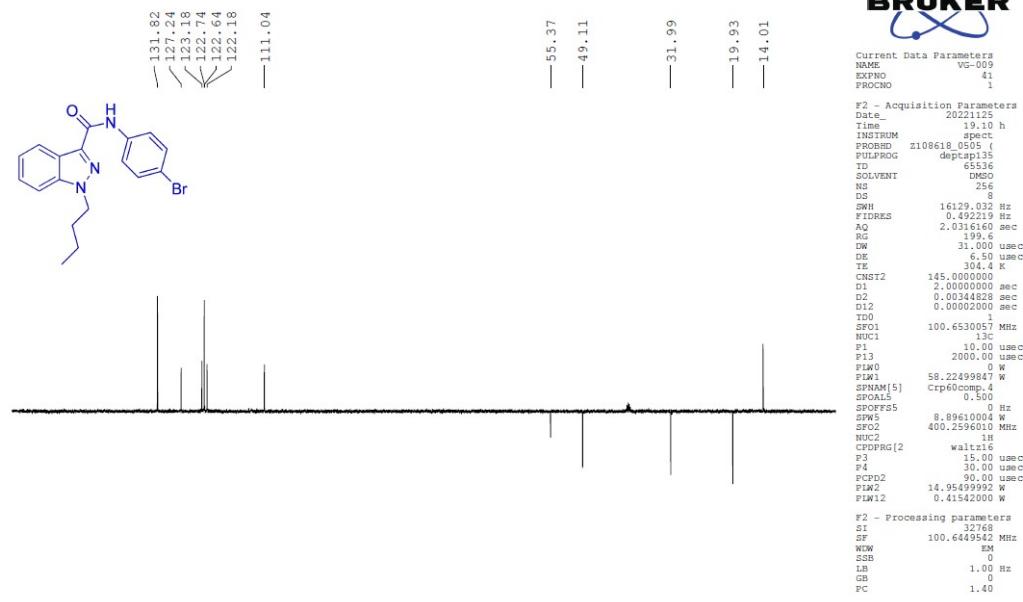
¹³C-NMR [100MHz, DMSO-d₆] spectrum of N-(4-Bromophenyl)-1-butyl-1H-indazole-3-carboxamide (8i).

Signature SIF VIT VELLORE
VG009



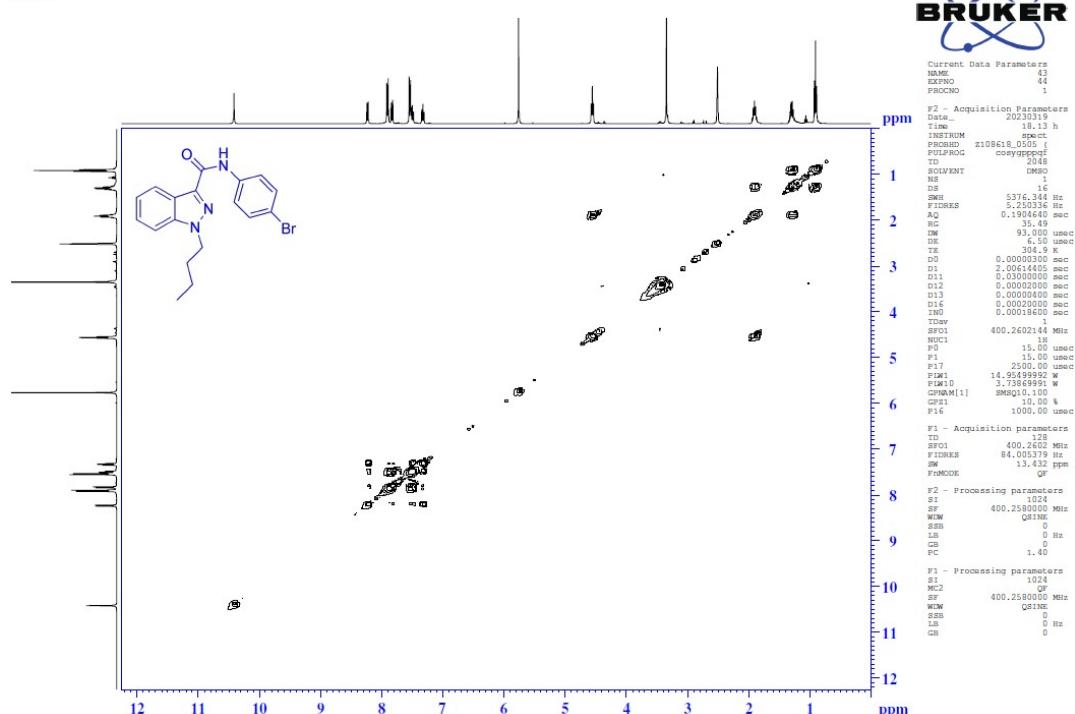
¹³⁵-DEPT-NMR [100MHz, DMSO-d₆] spectrum of N-(4-Bromophenyl)-1-butyl-1H-indazole-3-carboxamide (8i).

Signature SIF VIT VELLORE
VG009

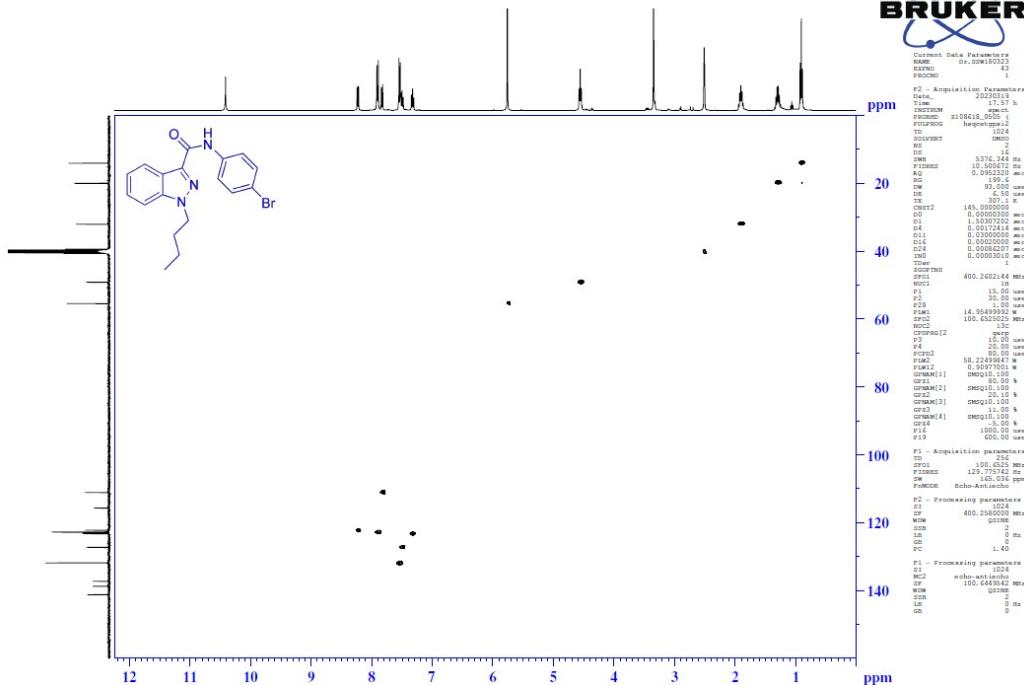


COSY-NMR [400MHz, DMSO-d₆] spectrum of N-(4-Bromophenyl)-1-butyl-1H-indazole-3-carboxamide (8i).

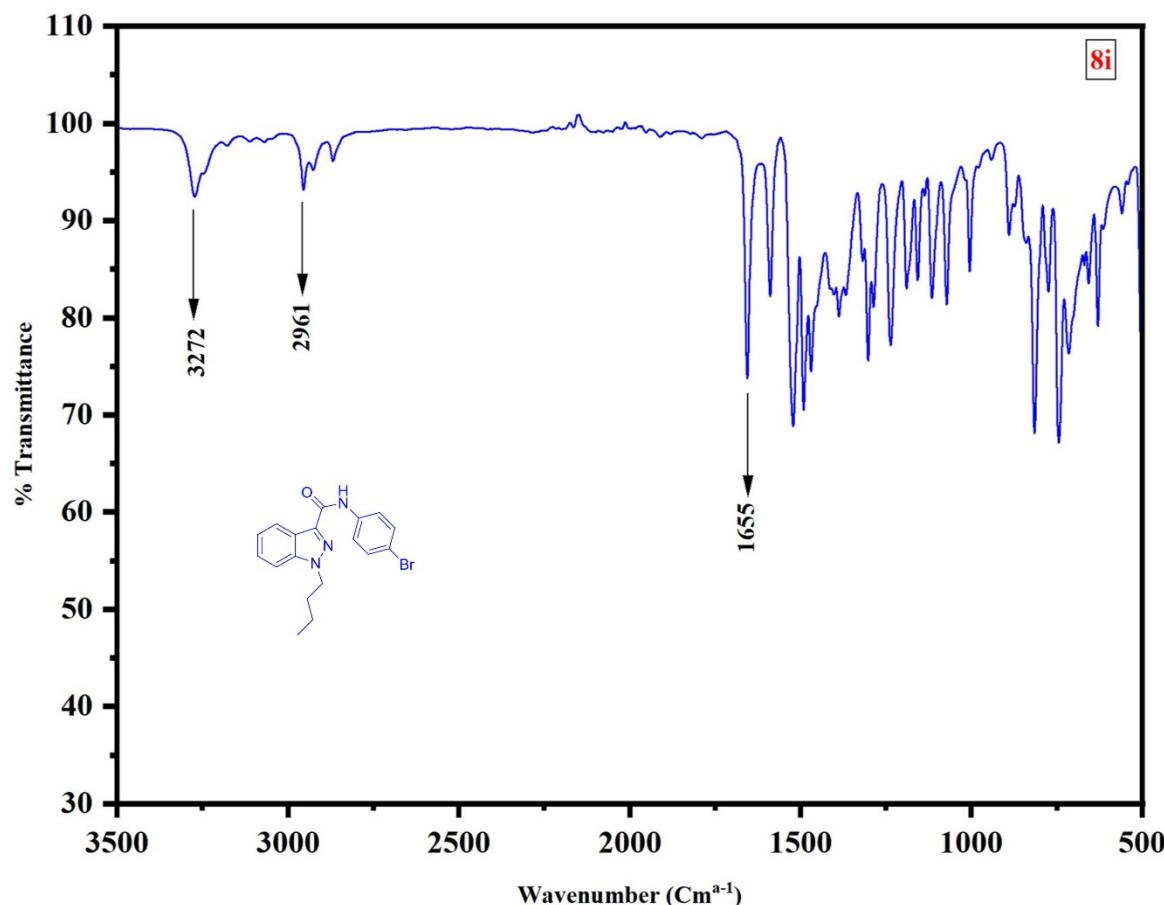
Signature SIF VIT VELLORE
VG-009



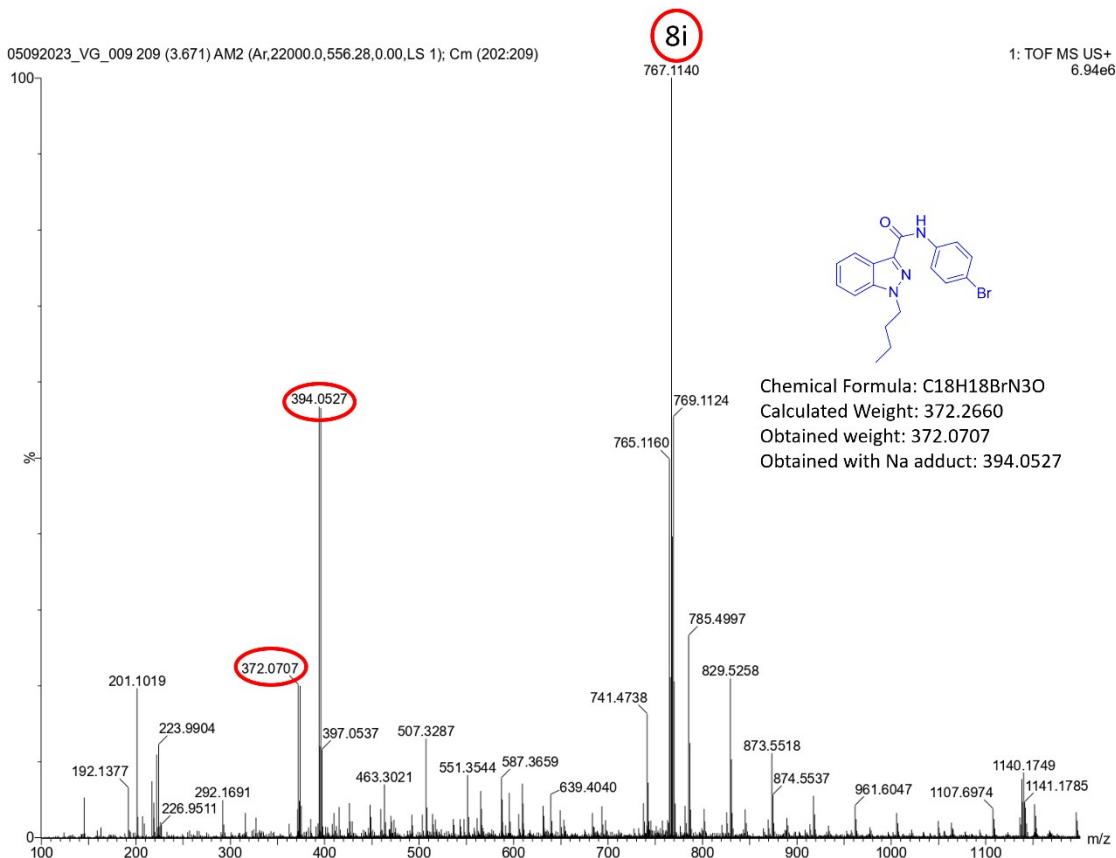
HSQC-NMR [400MHz, DMSO-d₆] spectrum of N-(4-Bromophenyl)-1-butyl-1H-indazole-3-carboxamide (8i).



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

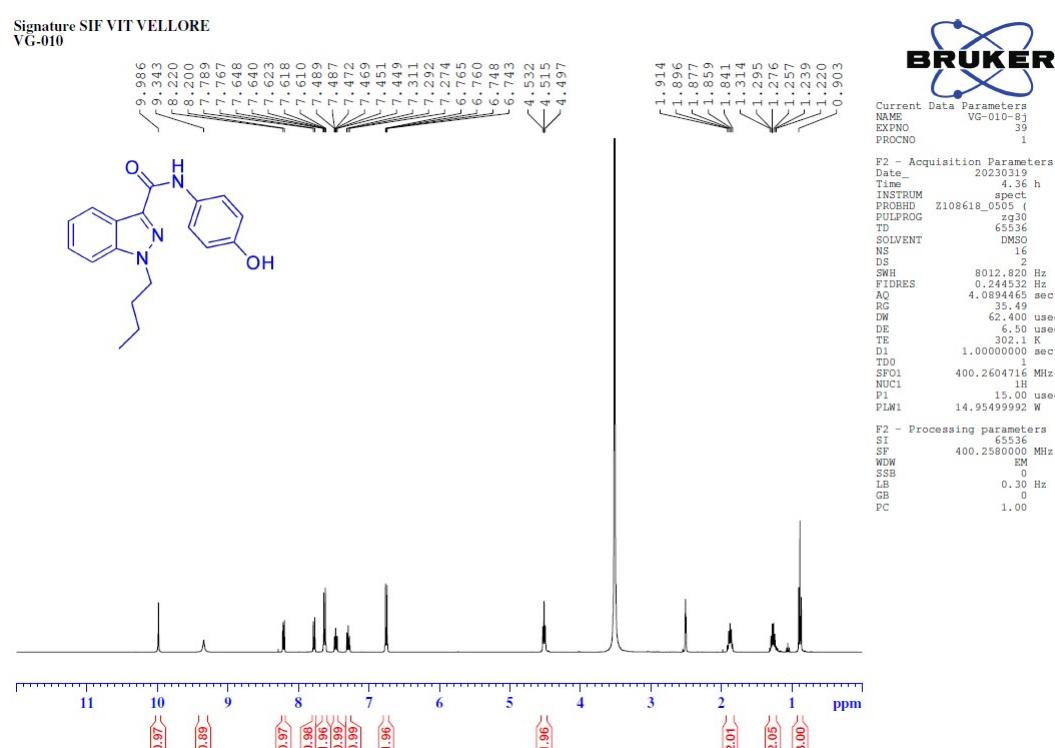


HRMS of N-(4-Bromophenyl)-1-butyl-1H-indazole-3-carboxamide (8i).



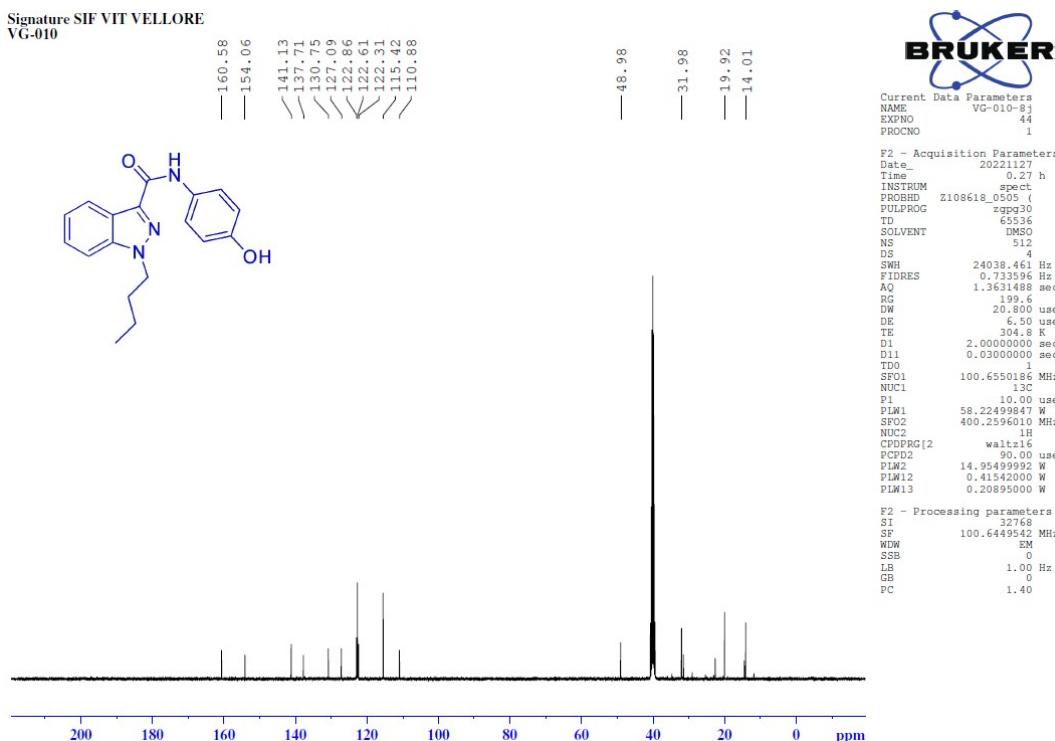
¹H-NMR [400MHz, DMSO-d₆] spectrum of 1-butyl-N-(4-hydroxyphenyl)-1H-indazole-3-carboxamide (8j).

Signature SIF VIT VELLORE
VG-010



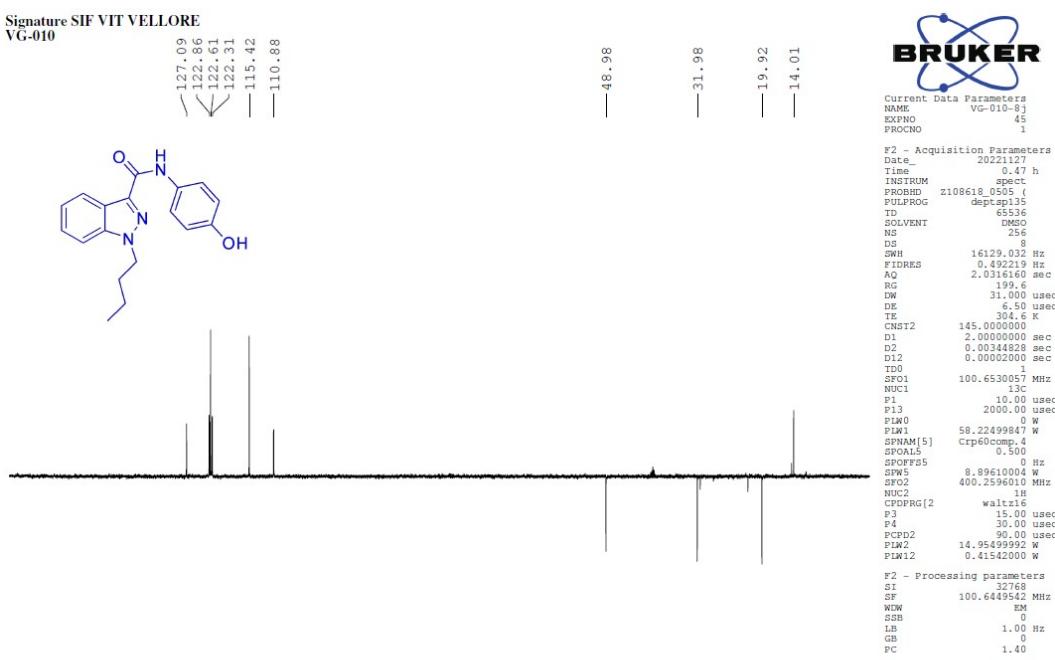
¹³C-NMR [100MHz, DMSO-d₆] spectrum of 1-butyl-N-(4-hydroxyphenyl)-1H-indazole-3-carboxamide (8j).

Signature SIF VIT VELLORE
VG-010



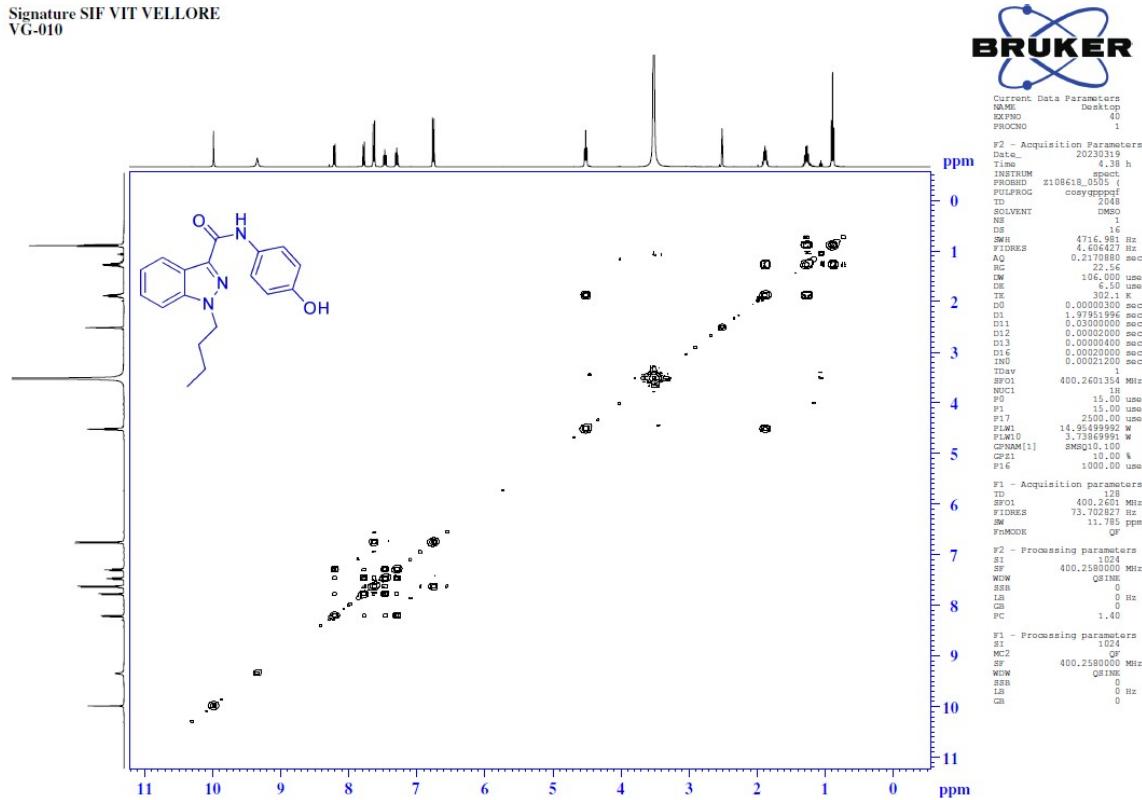
¹³⁵-DEPT-NMR [100MHz, DMSO-d₆] spectrum of 1-butyl-N-(4-hydroxyphenyl)-1H-indazole-3-carboxamide (8j).

Signature SIF VIT VELLORE
VG-010



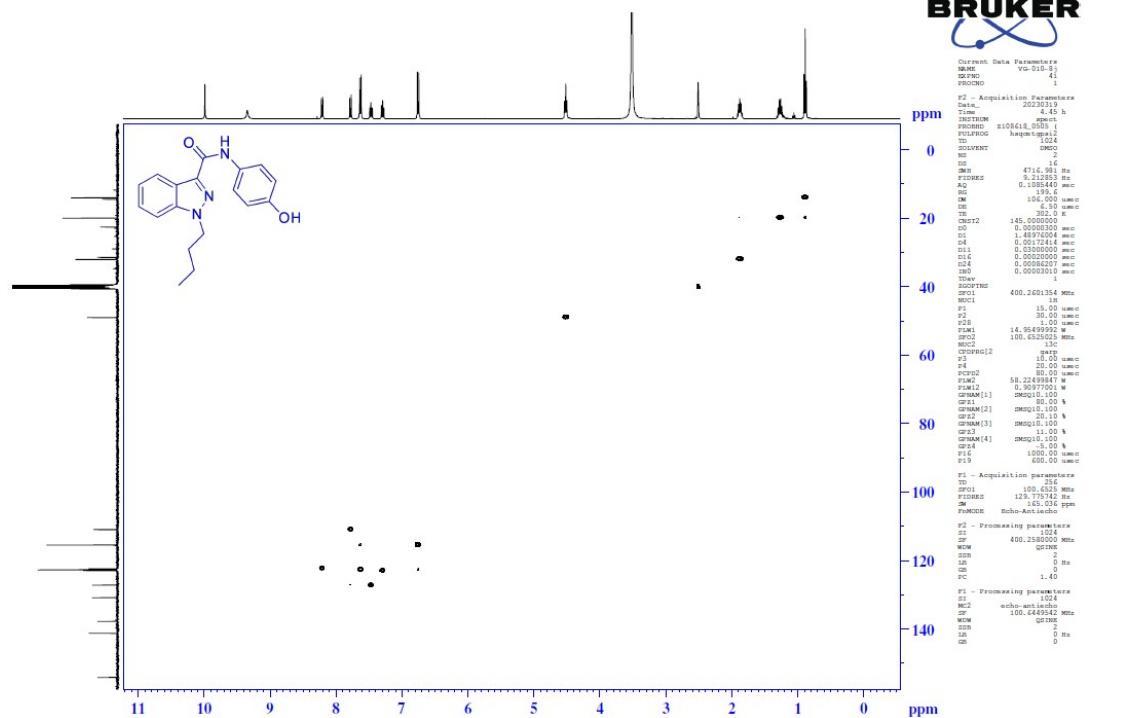
COSY-NMR [400MHz, DMSO-d₆] spectrum of 1-butyl-N-(4-hydroxyphenyl)-1H-indazole-3-carboxamide (8j).

**Signature SIF VIT VELLORE
VG-010**

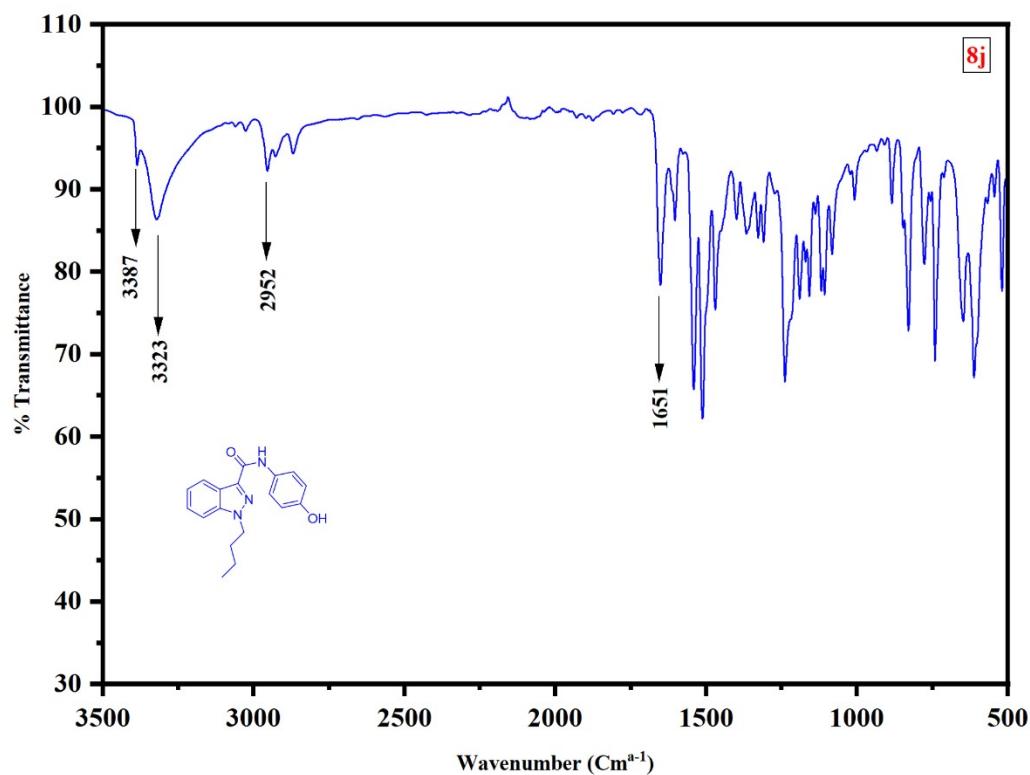


HSQC-NMR [400MHz, DMSO-d₆] spectrum of 1-butyl-N-(4-hydroxyphenyl)-1H-indazole-3-carboxamide (8j).

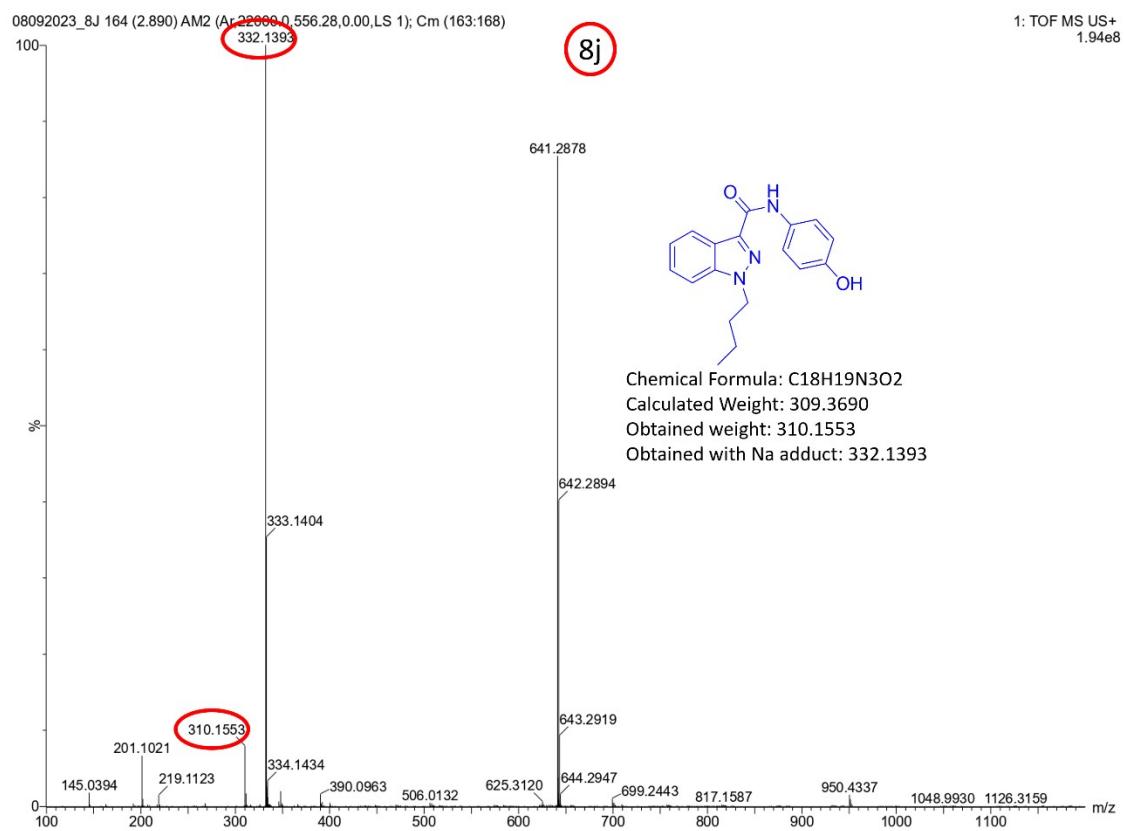
**Signature SIF VIT VELLORE
VG-010**



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

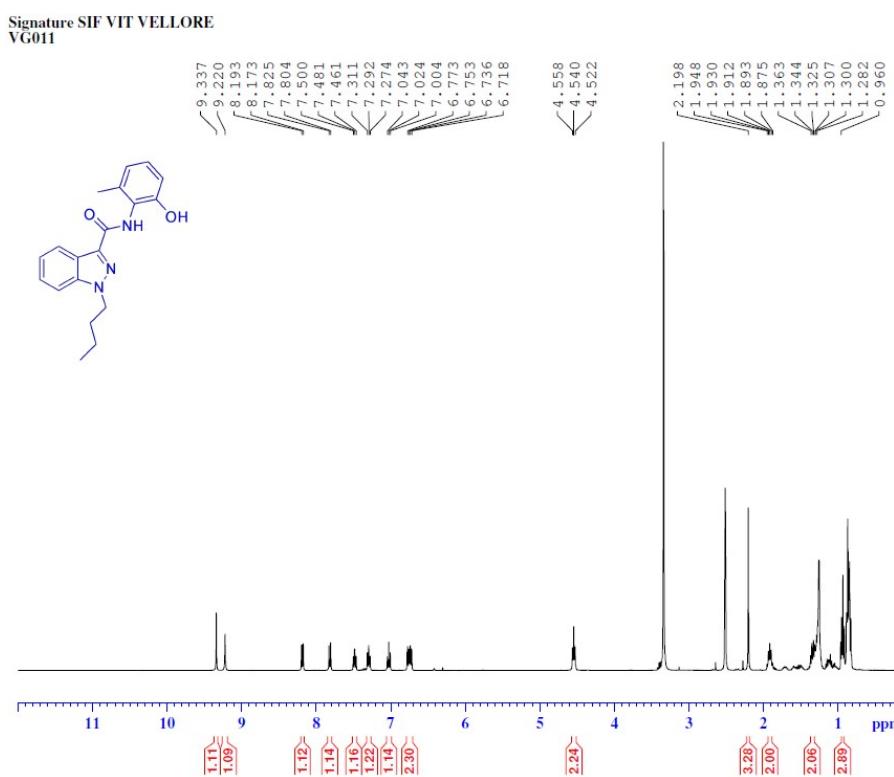


HRMS of 1-butyl-N-(4-hydroxyphenyl)-1H-indazole-3-carboxamide (8j).



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

**Signature SIF VIT VELLORE
VG011**



BRUKER

Current Data Parameters
NAME VG-011-8k
EXPNO 57
PROCNO 1

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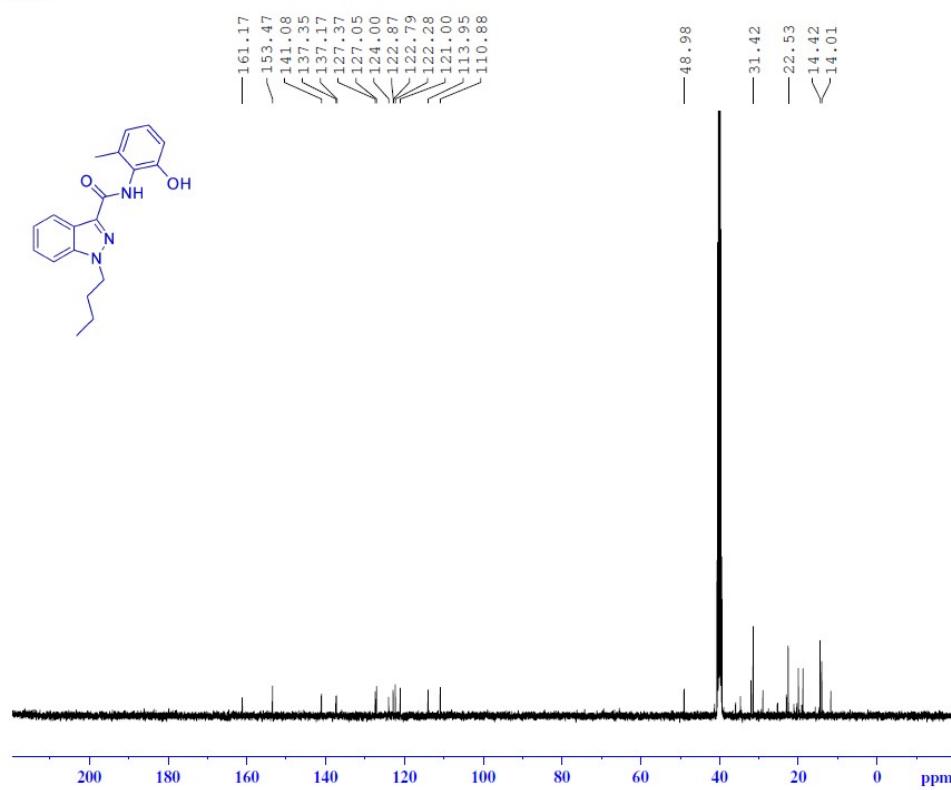
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FIDRES   0.244532 Hz
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DE        6.500 usec
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NUC1      1H
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PLW1     14.05499992 W

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F2 - Processing parameters
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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-hydroxy-6-methylphenyl)-1H-indazole-3-carboxamide (8k).

**Signature SIF VIT VELLORE
VG011**



 BRUKER

Current Data Parameter
NAME VG-01
EXPNO 5
PROCNO

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ETDRES 0.733333 Hz
AQ_    1.3631468 sec
RG_    199.6
DW_    20.800 used
DE_    6.50 used
TE_    306.1 K
D1_    2.0000000 sec
D11_   0.03000000 sec
TDO_   100.6550186 MHz
NUC1_  13C
P1_    10.00 used
PLW1_  58.22499847 W
SF02_  400.2596010 MHz
NUC2_  1H
CPDPBG[2] waltz16
CPDPRG[2] 0.00 used
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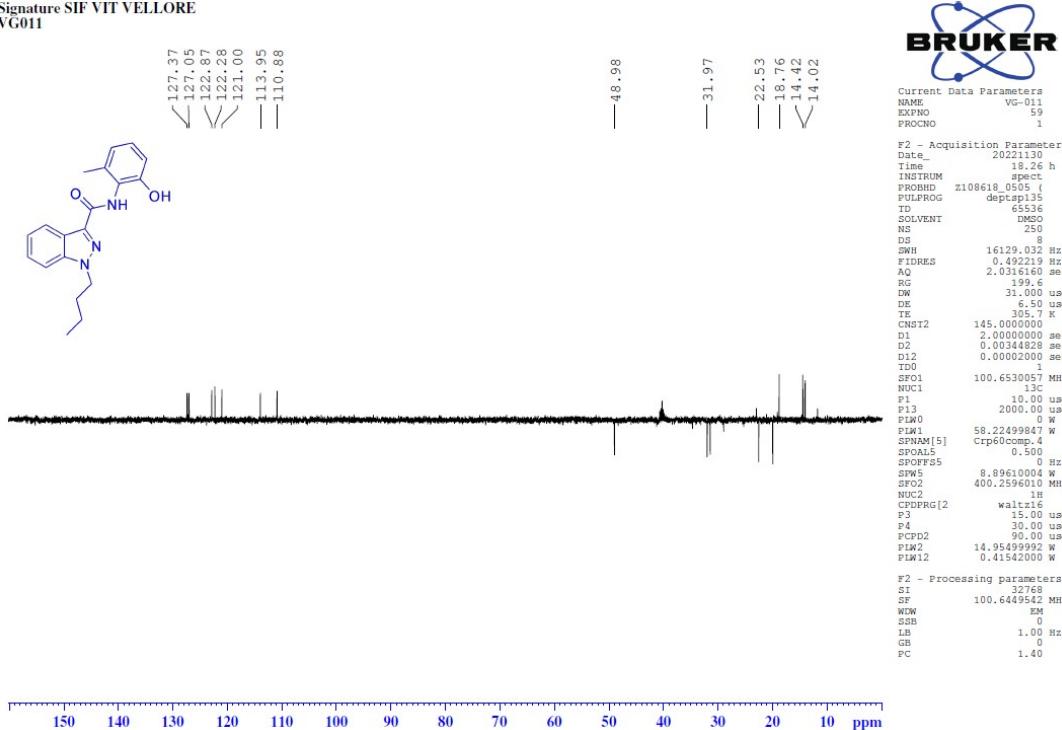
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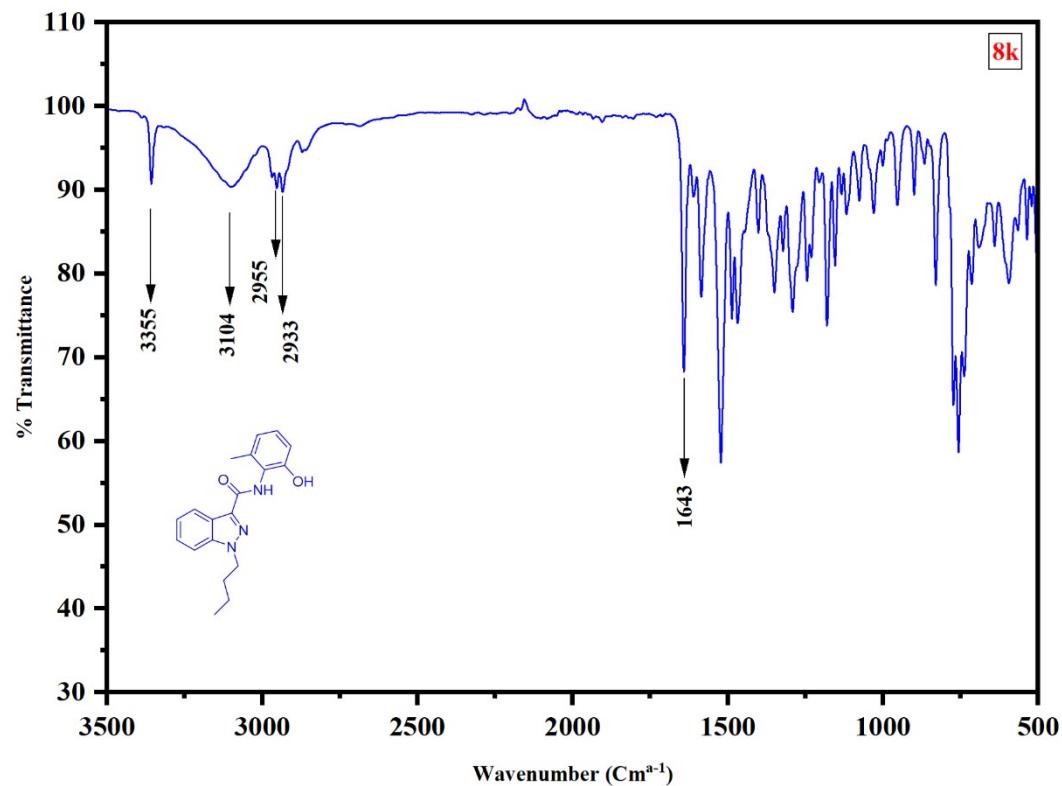
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5-DEPT-NMR [100MHz, DMSO- d_6] spectrum of 1-butyl-N-(2-hydroxy-6-methylphenyl)-1H-indazole-3-carboxamide (8k).

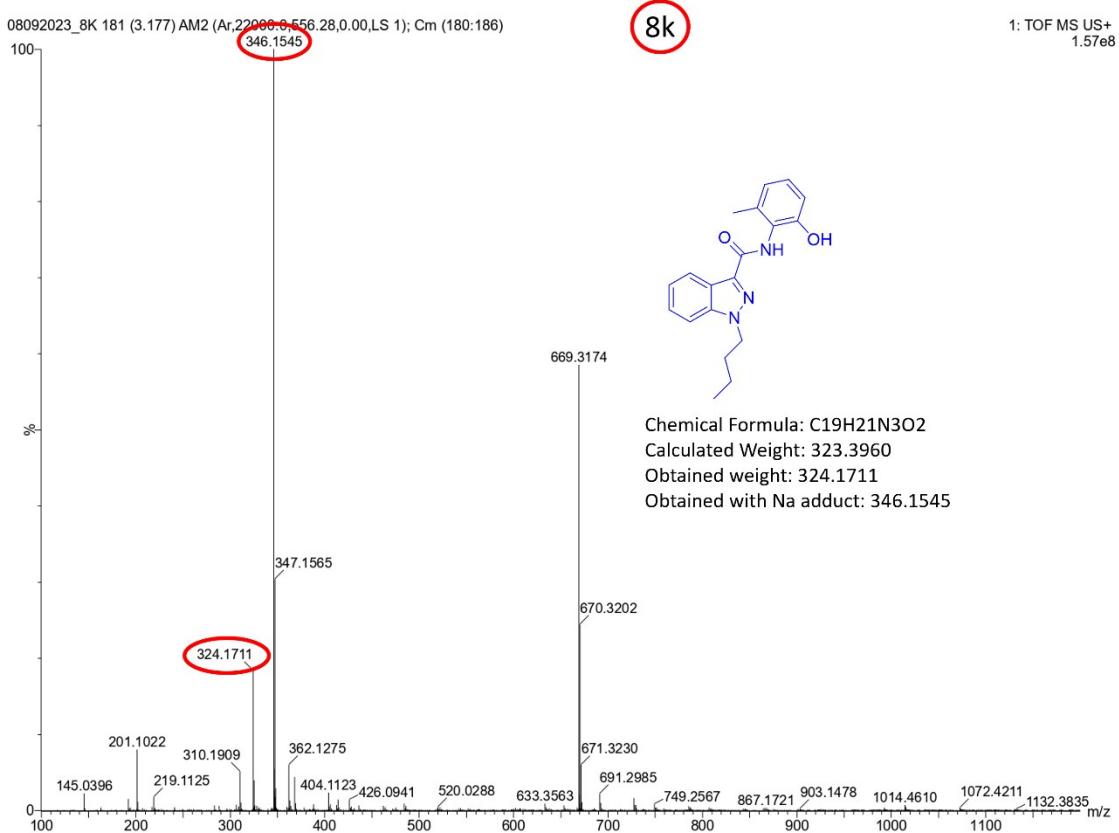
**Signature SIF VIT VELLORE
VG011**



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

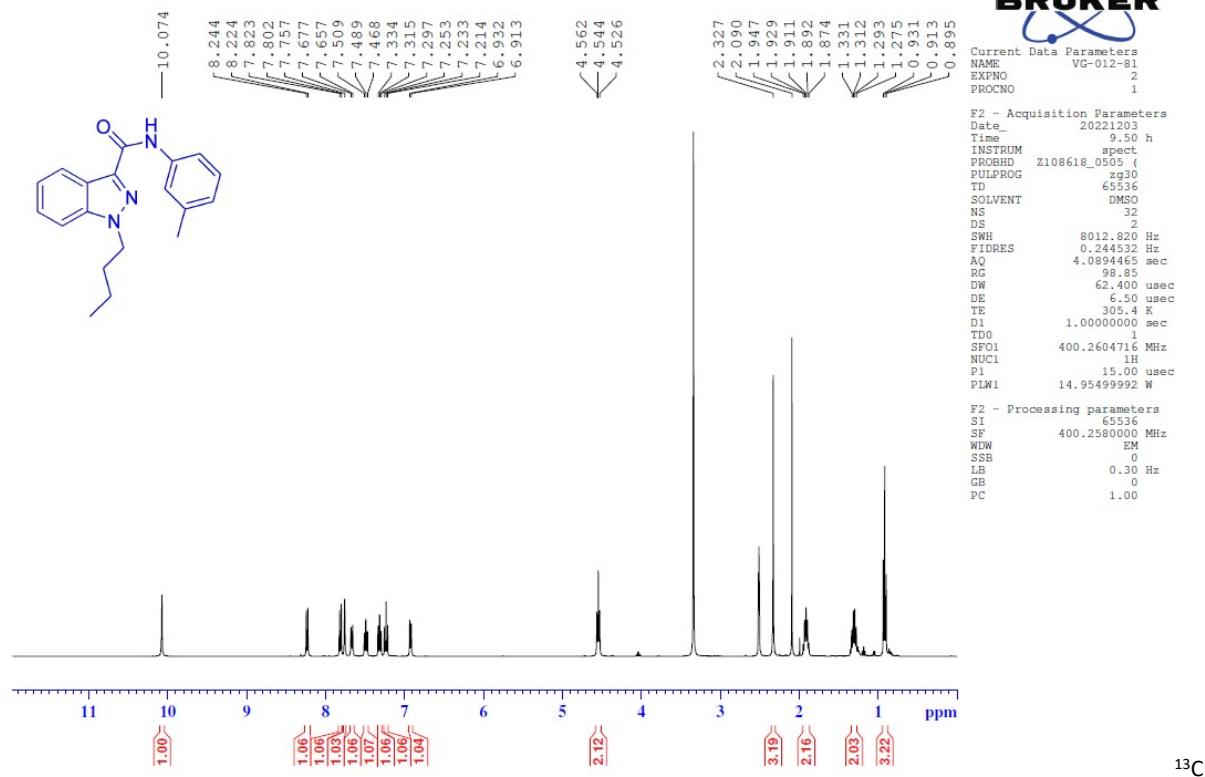


HRMS of 1-butyl-N-(2-hydroxy-6-methylphenyl)-1H-indazole-3-carboxamide (8k).



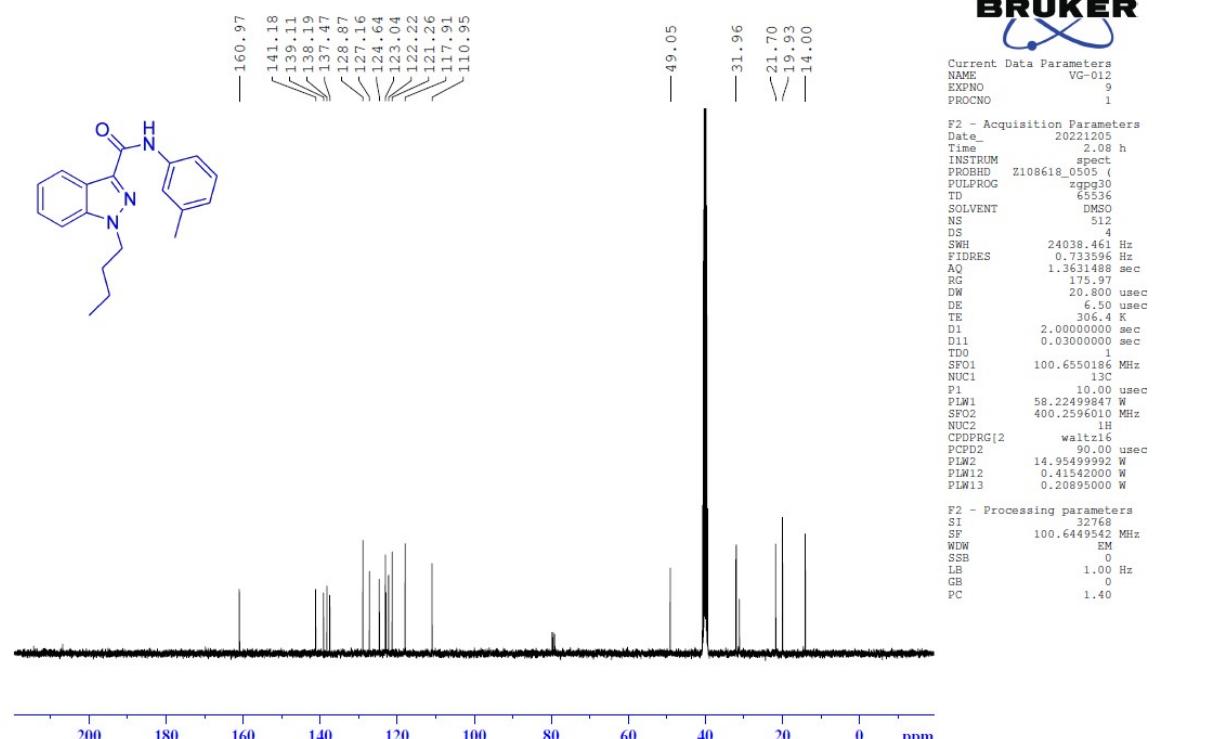
¹H-NMR [400MHz, DMSO-d₆] spectrum of 1-butyl-N-(m-tolyl)-1H-indazole-3-carboxamide (8l).

Signature SIF VIT VELLORE
VG012



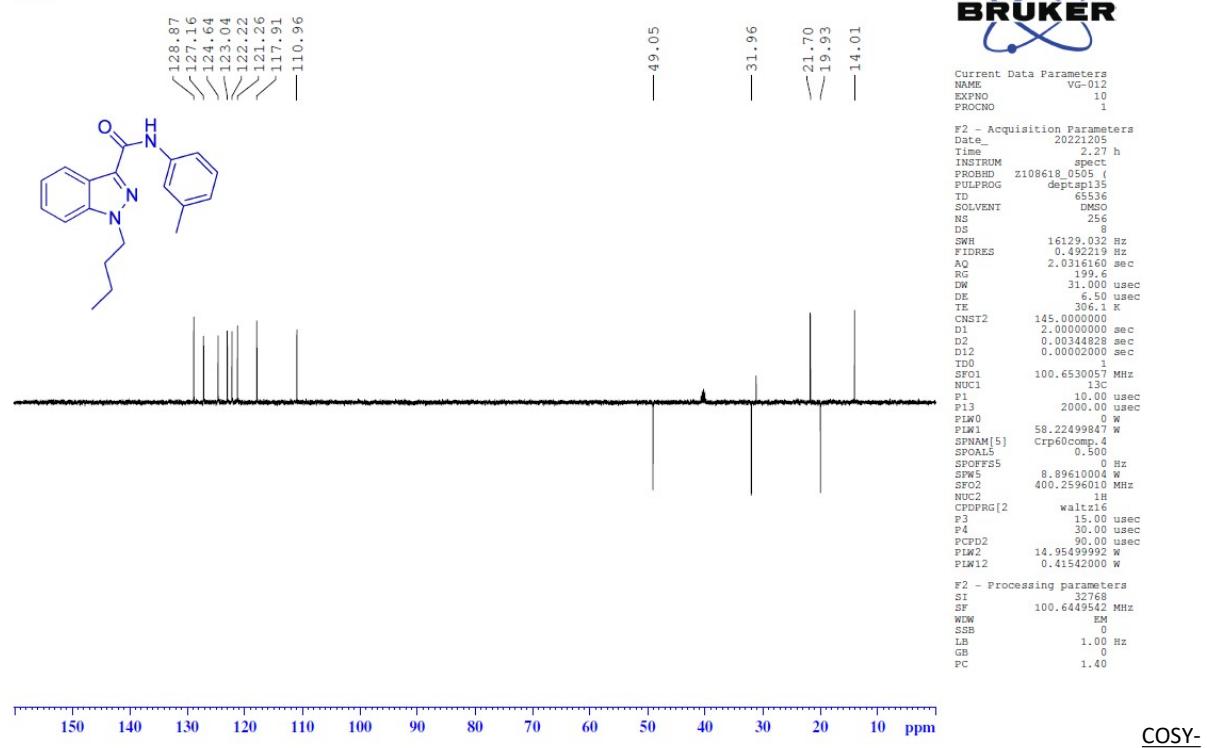
¹³C-NMR [100MHz, DMSO-d₆] spectrum of 1-butyl-N-(m-tolyl)-1H-indazole-3-carboxamide (8l).

Signature SIF VIT VELLORE
VG012



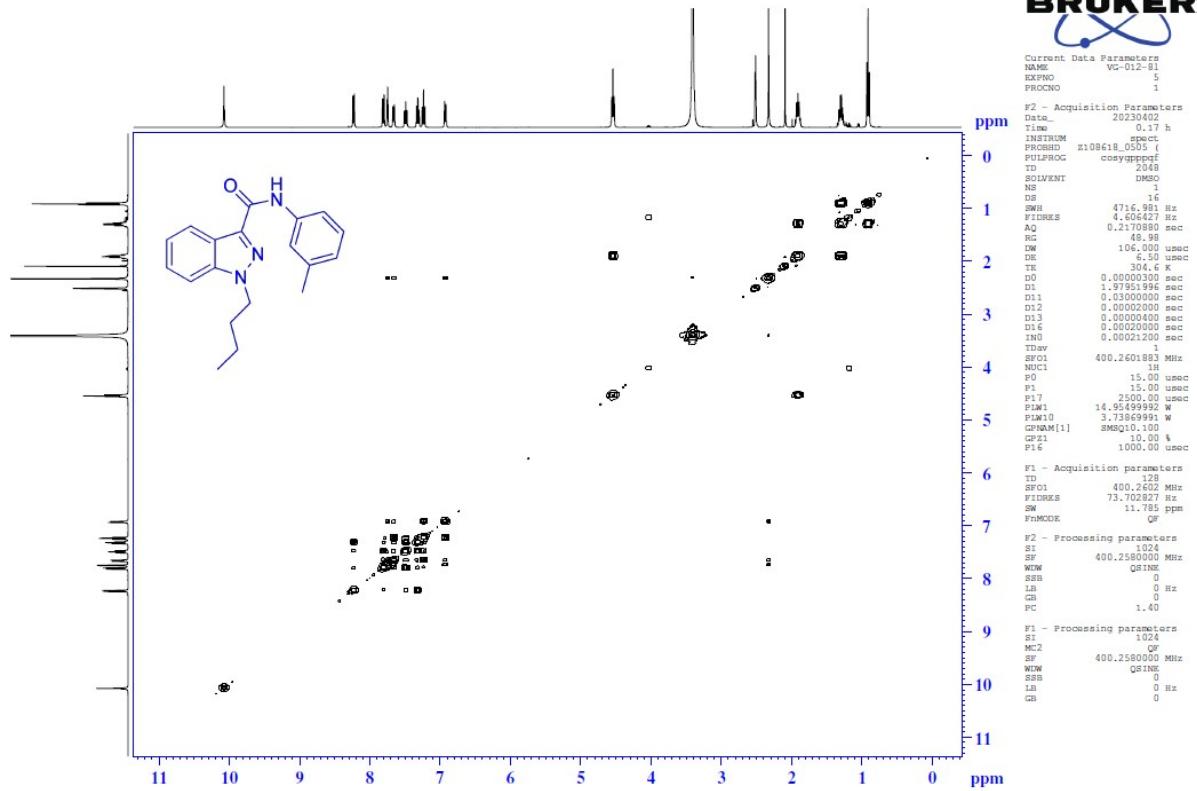
135-DEPT-NMR [100MHz, DMSO-d₆] spectrum of 1-butyl-N-(m-tolyl)-1H-indazole-3-carboxamide (8l).

Signature SIF VIT VELLORE
VG012



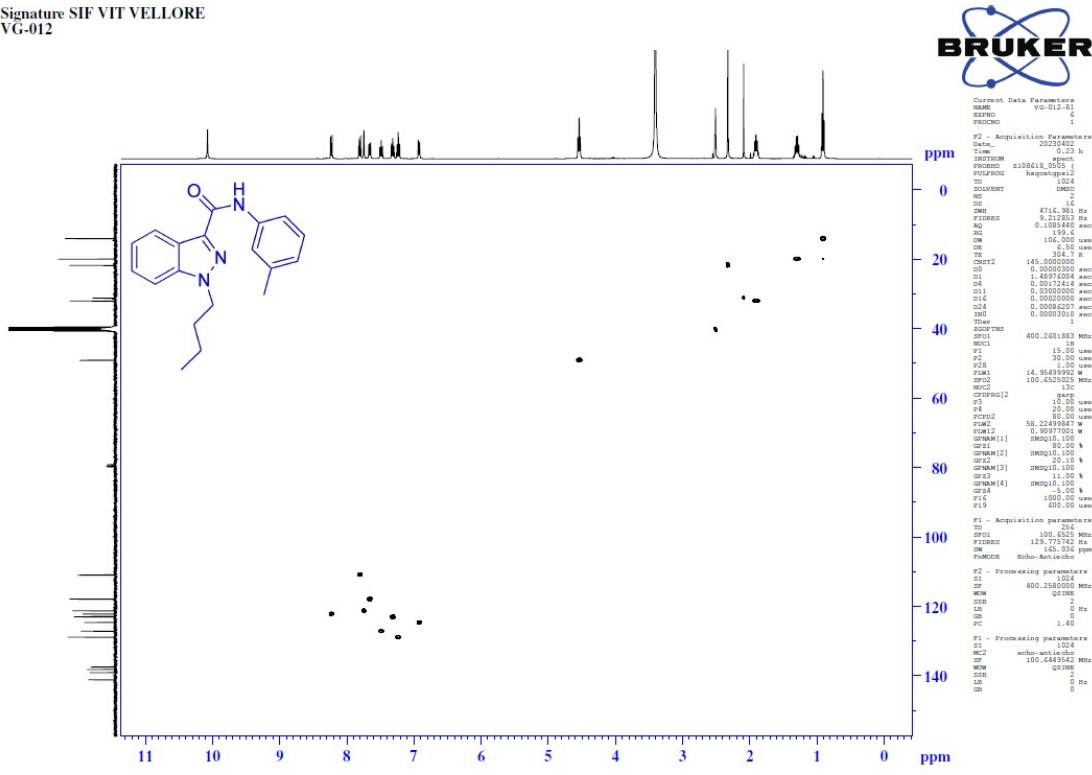
NMR [400MHz, DMSO-d₆] spectrum of 1-butyl-N-(m-tolyl)-1H-indazole-3-carboxamide (8I).

Signature SIF VIT VELLORE
VG-012

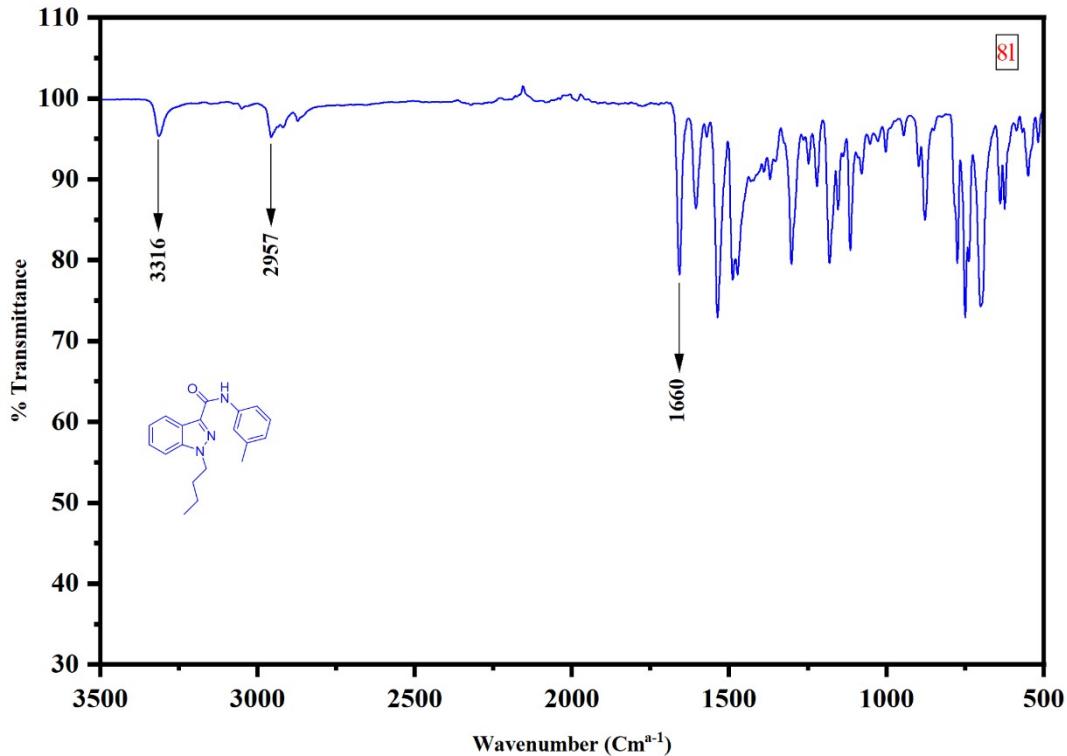


HSQC-NMR [400MHz, DMSO-d₆] spectrum of 1-butyl-N-(m-tolyl)-1H-indazole-3-carboxamide (8I).

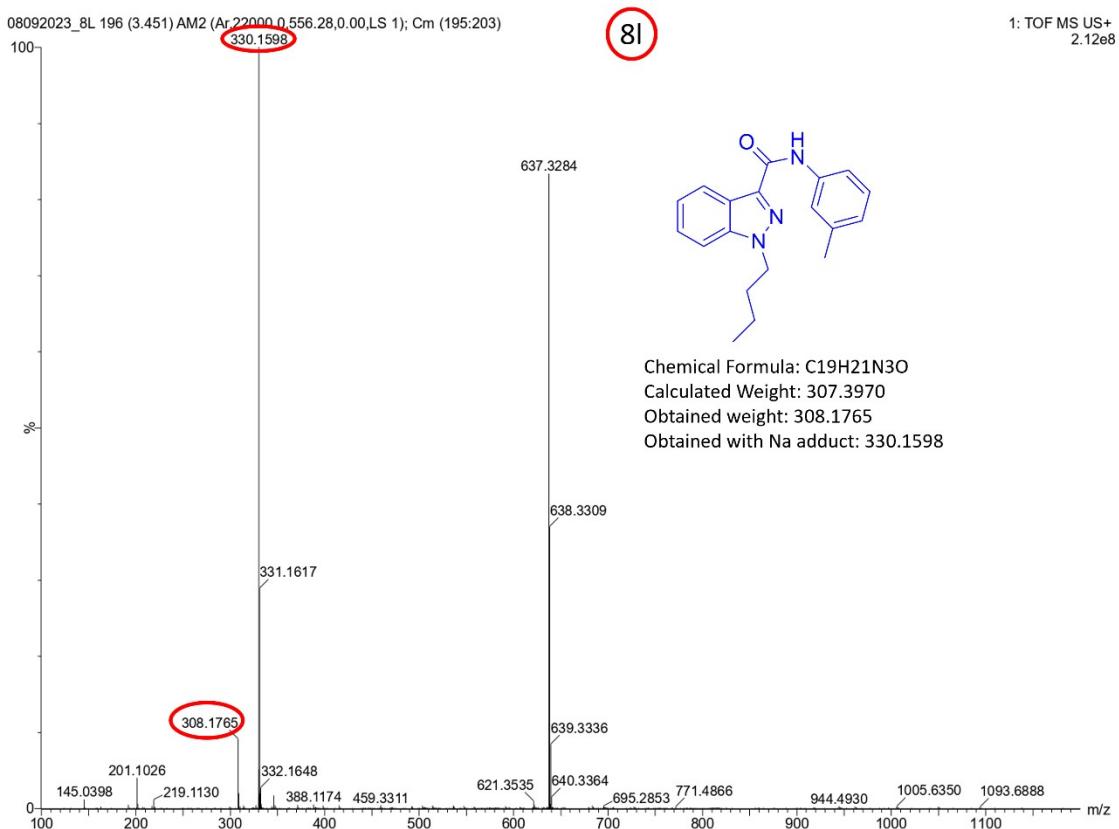
**Signature SIF VIT VELLORE
VG-012**



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

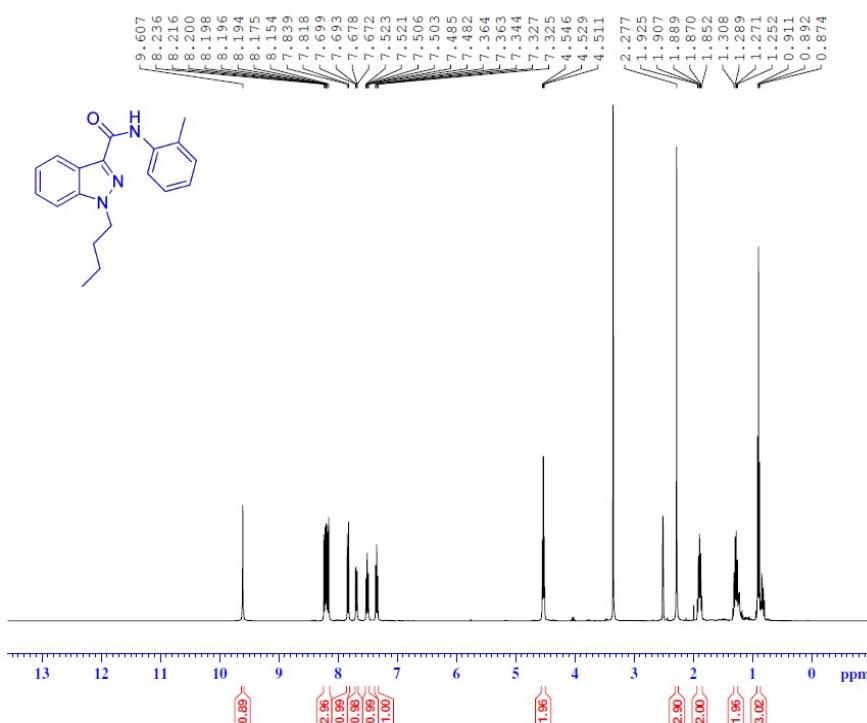


HRMS of 1-butyl-N-(m-tolyl)-1H-indazole-3-carboxamide (8I).



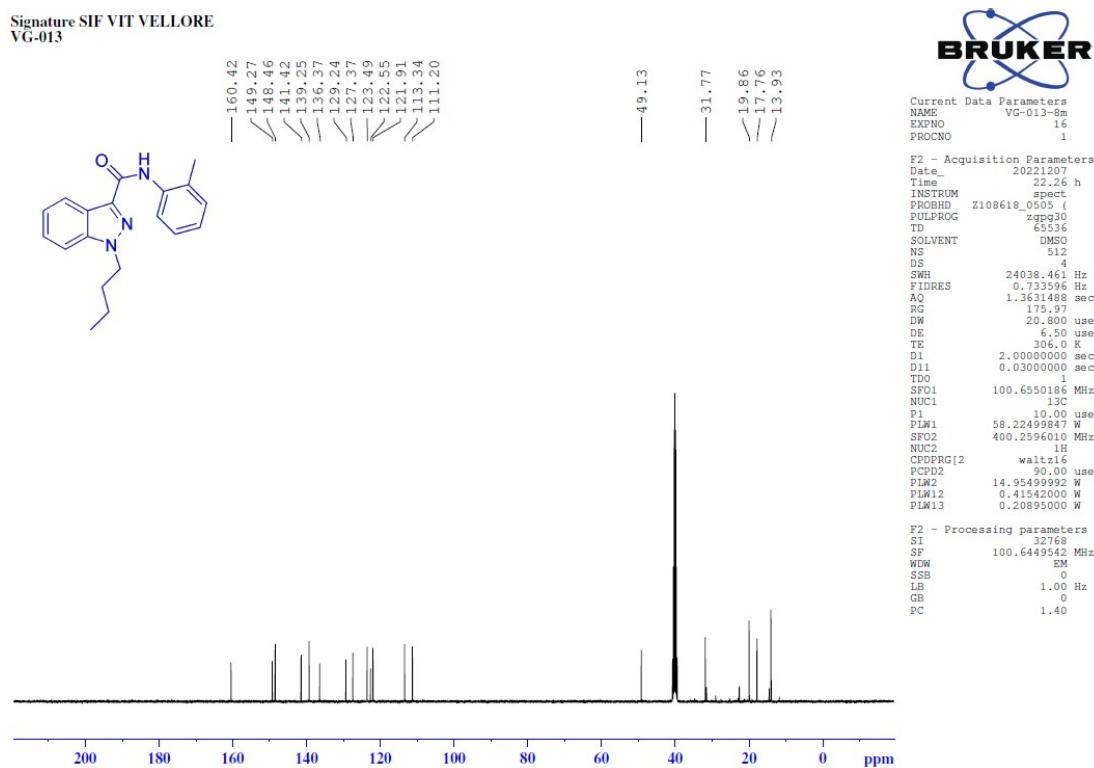
¹H-NMR [400MHz, DMSO-d₆] spectrum of 1-butyl-N-(tolyl)-1H-indazole-3-carboxamide (8m).

Signature SIF VIT VELLORE
VG-013



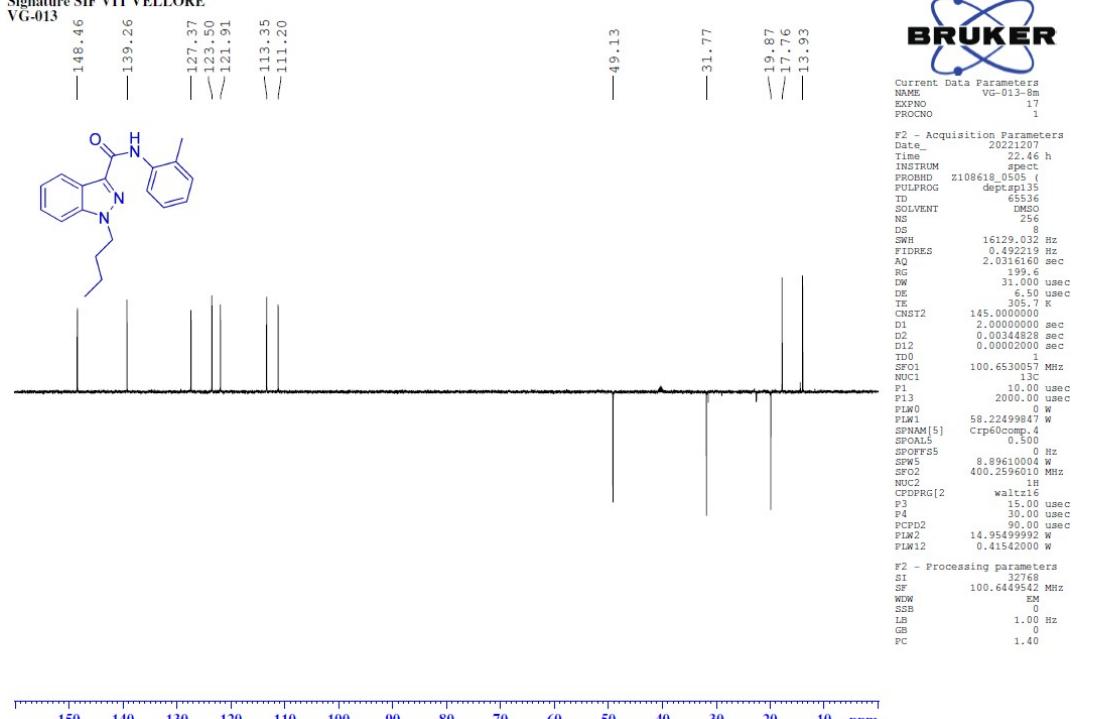
¹³C-NMR [100MHz, DMSO-d₆] spectrum of 1-butyl-N-(o-tolyl)-1H-indazole-3-carboxamide (8m).

Signature SIF VIT VELLORE
VG-013



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

Signature SIF VIT VELLORE
VG-013



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

Signature SIF VIT VELLORE
VG-013



Current Data Parameters
NAME: VG-013-
EXPNO: 28
PROCNO: 1

P1 - Acquisition Parameters

Date: 20221210
Time: 13.03 h

TE(MS): 90.000000 ms

P1BPPM: 2108618.0503 (

PULPROG: cosypppdpf

TSP: 30000.000000 ms

SOLVENT: DMSO

NS: 1

DS: 16

SWH: 4672.897 Hz

FIDRES: 4.56315 Hz

AQ: 0.12500 sec

RG: 39.08

DW: 107.000 usec

D1: 1.000000 sec

TDR: 304.1 K

D0: 0.0000000 sec

D11: 1.97747195 sec

D12: 0.03000000 sec

D13: 0.00000000 sec

D14: 0.00020000 sec

D15: 0.00024000 sec

D16: 0.00024000 sec

D17: 1 sec

SP1C1: 400.260274 MHz

NUC1: 13 C

PC1: 15.00 usec

P1: 15.00 usec

P17: 2.000000 sec

P1M10: 14.95499992 w

P1M10: 3.73889991 w

CPDGM11: 30000.000000

CPDGM11: 10.00 %

GP11: 1000.00 usec

P16: 1000.00 usec

F1 - Acquisition parameters

TD: 65536

SP1C1: 400.260274 MHz

FIDRES: 400.26156 Hz

SW: 11.11 ppm

PR1: 90

PC: 1.40

F1 - Processing parameters

SI: 1024

SF: 400.2580000 MHz

WM: QSIINE

SSB: 0

LB: 0 Hz

GB: 0

TC: 1024

TD: 65536

SP1C1: 400.260274 ms

NUC1: 13 C

PC1: 15.00 usec

P1: 15.00 usec

P17: 1.000000 sec

TD: 1024

SP1C1: 400.260274 ms

NUC1: 13 C

PC1: 15.00 usec

P1: 15.00 usec

P17: 1.000000 sec

TD: 1024

SP1C1: 400.260274 ms

NUC1: 13 C

PC1: 15.00 usec

P1: 15.00 usec

P17: 1.000000 sec

TD: 1024

SP1C1: 400.260274 ms

NUC1: 13 C

PC1: 15.00 usec

P1: 15.00 usec

P17: 1.000000 sec

TD: 1024

SP1C1: 400.260274 ms

NUC1: 13 C

PC1: 15.00 usec

P1: 15.00 usec

P17: 1.000000 sec

TD: 1024

SP1C1: 400.260274 ms

NUC1: 13 C

PC1: 15.00 usec

P1: 15.00 usec

P17: 1.000000 sec

TD: 1024

SP1C1: 400.260274 ms

NUC1: 13 C

PC1: 15.00 usec

P1: 15.00 usec

P17: 1.000000 sec

TD: 1024

SP1C1: 400.260274 ms

NUC1: 13 C

PC1: 15.00 usec

P1: 15.00 usec

P17: 1.000000 sec

TD: 1024

SP1C1: 400.260274 ms

NUC1: 13 C

PC1: 15.00 usec

P1: 15.00 usec

P17: 1.000000 sec

TD: 1024

SP1C1: 400.260274 ms

NUC1: 13 C

PC1: 15.00 usec

P1: 15.00 usec

P17: 1.000000 sec

TD: 1024

SP1C1: 400.260274 ms

NUC1: 13 C

PC1: 15.00 usec

P1: 15.00 usec

P17: 1.000000 sec

TD: 1024

SP1C1: 400.260274 ms

NUC1: 13 C

PC1: 15.00 usec

P1: 15.00 usec

P17: 1.000000 sec

TD: 1024

SP1C1: 400.260274 ms

NUC1: 13 C

PC1: 15.00 usec

P1: 15.00 usec

P17: 1.000000 sec

TD: 1024

SP1C1: 400.260274 ms

NUC1: 13 C

PC1: 15.00 usec

P1: 15.00 usec

P17: 1.000000 sec

TD: 1024

SP1C1: 400.260274 ms

NUC1: 13 C

PC1: 15.00 usec

P1: 15.00 usec

P17: 1.000000 sec

TD: 1024

SP1C1: 400.260274 ms

NUC1: 13 C

PC1: 15.00 usec

P1: 15.00 usec

P17: 1.000000 sec

TD: 1024

SP1C1: 400.260274 ms

NUC1: 13 C

PC1: 15.00 usec

P1: 15.00 usec

P17: 1.000000 sec

TD: 1024

SP1C1: 400.260274 ms

NUC1: 13 C

PC1: 15.00 usec

P1: 15.00 usec

P17: 1.000000 sec

TD: 1024

SP1C1: 400.260274 ms

NUC1: 13 C

PC1: 15.00 usec

P1: 15.00 usec

P17: 1.000000 sec

TD: 1024

SP1C1: 400.260274 ms

NUC1: 13 C

PC1: 15.00 usec

P1: 15.00 usec

P17: 1.000000 sec

TD: 1024

SP1C1: 400.260274 ms

NUC1: 13 C

PC1: 15.00 usec

P1: 15.00 usec

P17: 1.000000 sec

TD: 1024

SP1C1: 400.260274 ms

NUC1: 13 C

PC1: 15.00 usec

P1: 15.00 usec

P17: 1.000000 sec

TD: 1024

SP1C1: 400.260274 ms

NUC1: 13 C

PC1: 15.00 usec

P1: 15.00 usec

P17: 1.000000 sec

TD: 1024

SP1C1: 400.260274 ms

NUC1: 13 C

PC1: 15.00 usec

P1: 15.00 usec

P17: 1.000000 sec

TD: 1024

SP1C1: 400.260274 ms

NUC1: 13 C

PC1: 15.00 usec

P1: 15.00 usec

P17: 1.000000 sec

TD: 1024

SP1C1: 400.260274 ms

NUC1: 13 C

PC1: 15.00 usec

P1: 15.00 usec

P17: 1.000000 sec

TD: 1024

SP1C1: 400.260274 ms

NUC1: 13 C

PC1: 15.00 usec

P1: 15.00 usec

P17: 1.000000 sec

TD: 1024

SP1C1: 400.260274 ms

NUC1: 13 C

PC1: 15.00 usec

P1: 15.00 usec

P17: 1.000000 sec

TD: 1024

SP1C1: 400.260274 ms

NUC1: 13 C

PC1: 15.00 usec

P1: 15.00 usec

P17: 1.000000 sec

TD: 1024

SP1C1: 400.260274 ms

NUC1: 13 C

PC1: 15.00 usec

P1: 15.00 usec

P17: 1.000000 sec

TD: 1024

SP1C1: 400.260274 ms

NUC1: 13 C

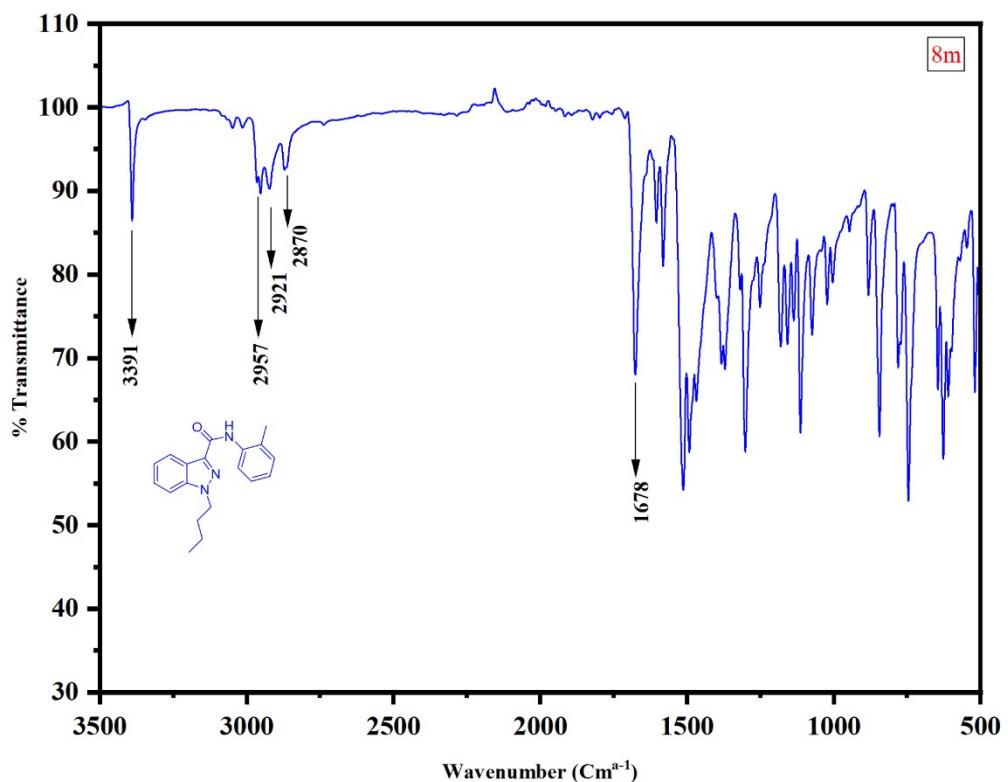
PC1: 15.00 usec

P1: 15.00 usec

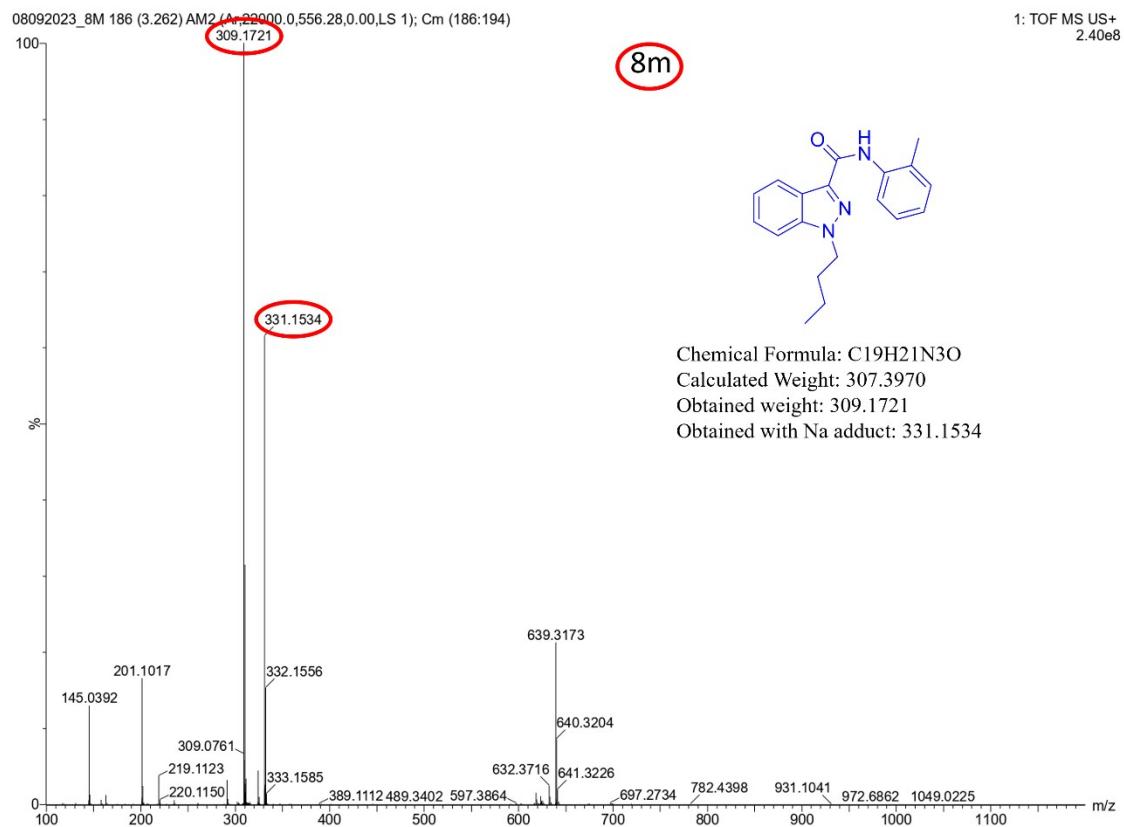
P17: 1.000000 sec

TD: 1024

SP1C1: 400.260274 ms

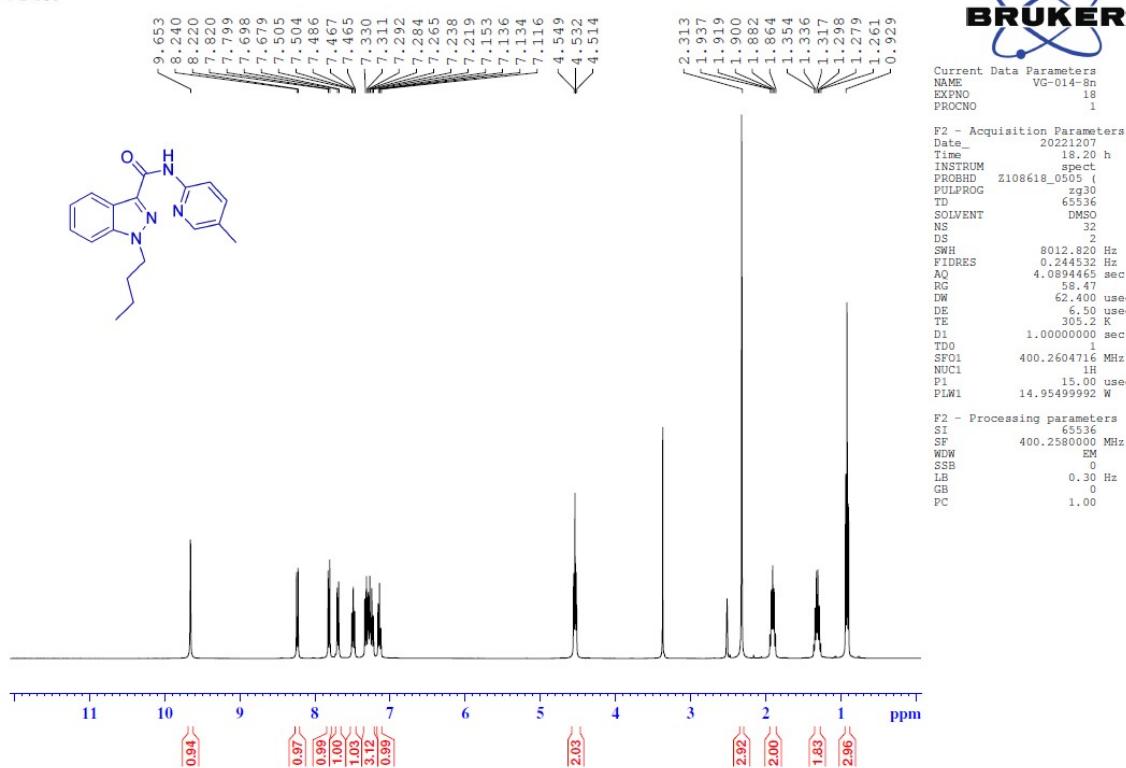


HRMS of 1-butyl-N-(o-tolyl)-1H-indazole-3-carboxamide (8m).



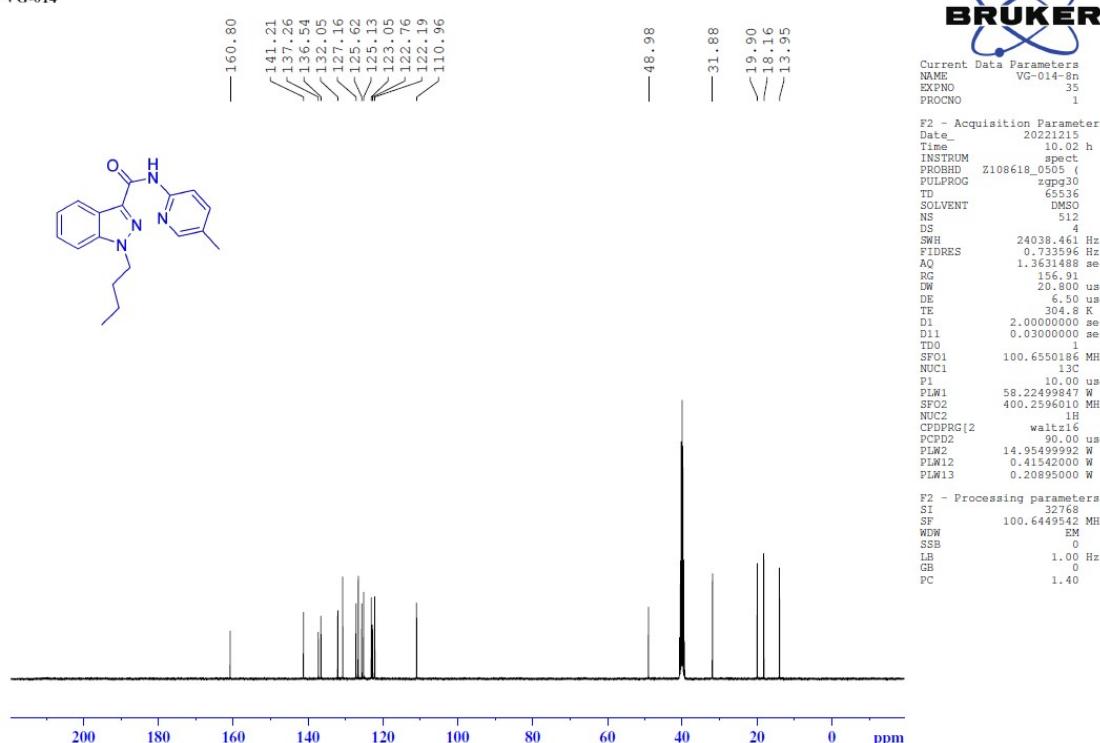
¹H-NMR [400MHz, DMSO- d_6] spectrum of 1-butyl-N-(5-methylpyridin-2-yl)-1H-indazole-3-carboxamide (8n).

**Signature SIF VIT VELLORE
VG-014**



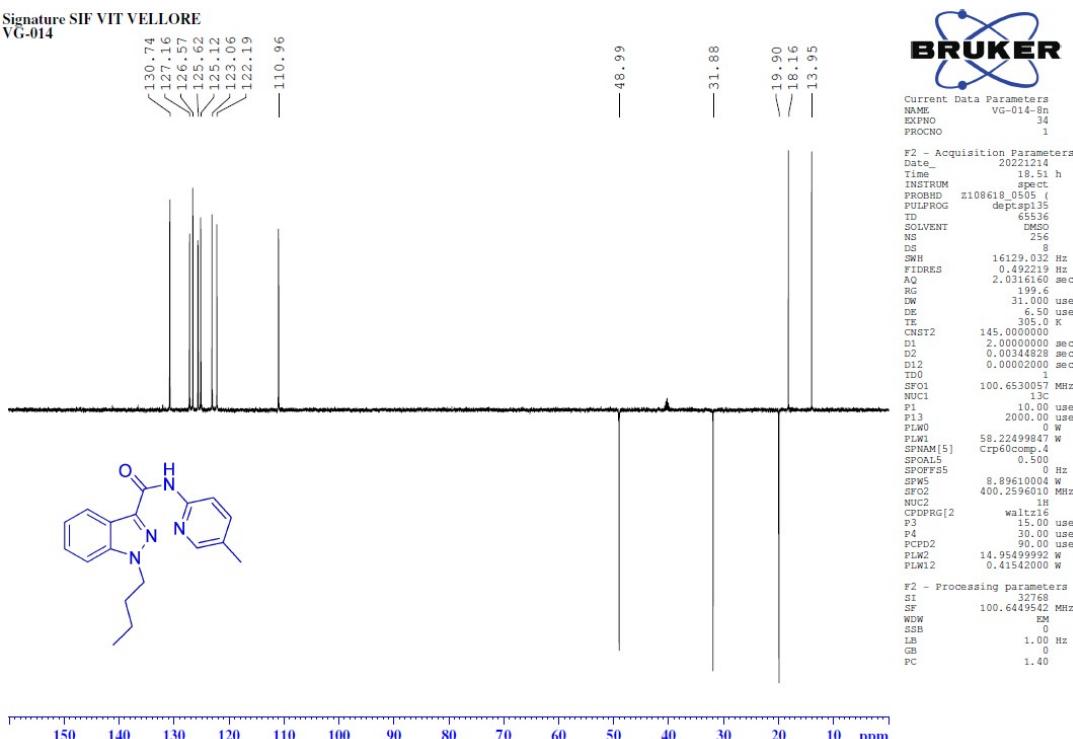
¹³C-NMR [100MHz, DMSO-d₆] spectrum of 1-butyl-N-(5-methylpyridin-2-yl)-1H-indazole-3-carboxamide (8n).

**Signature SIF VIT VELLORE
VG-014**



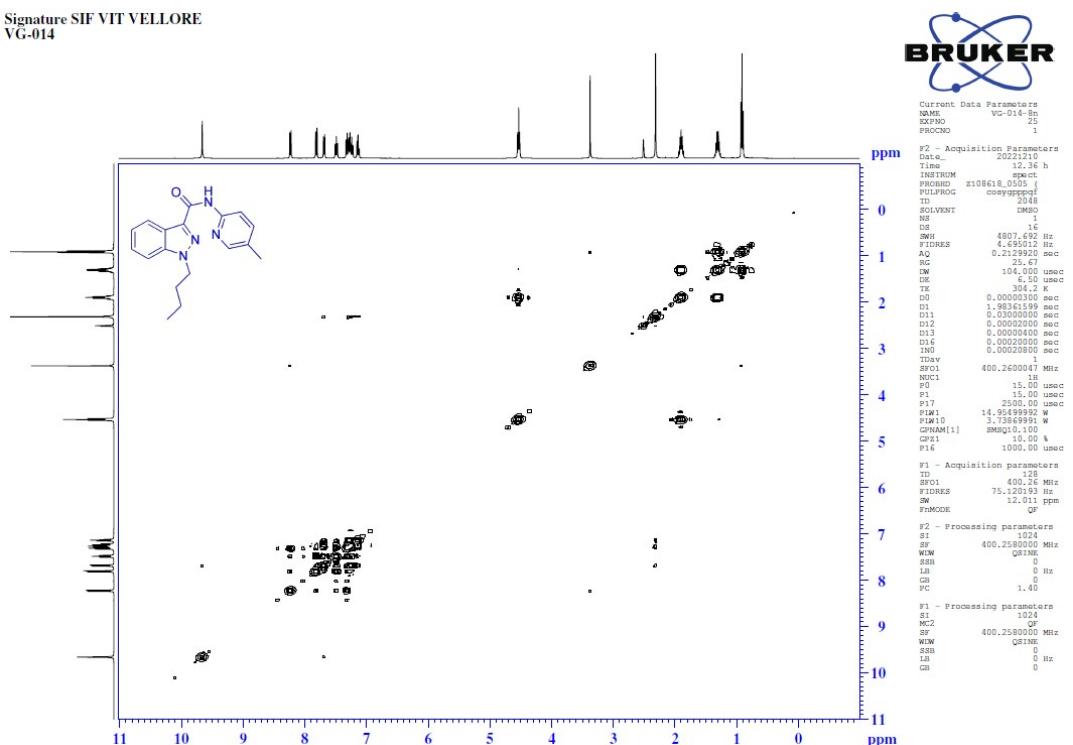
135-DEPT-NMR [100MHz, DMSO-d₆] spectrum of 1-butyl-N-(5-methylpyridin-2-yl)-1H-indazole-3-carboxamide (8n).

Signature SIF VIT VELLORE
VG-014

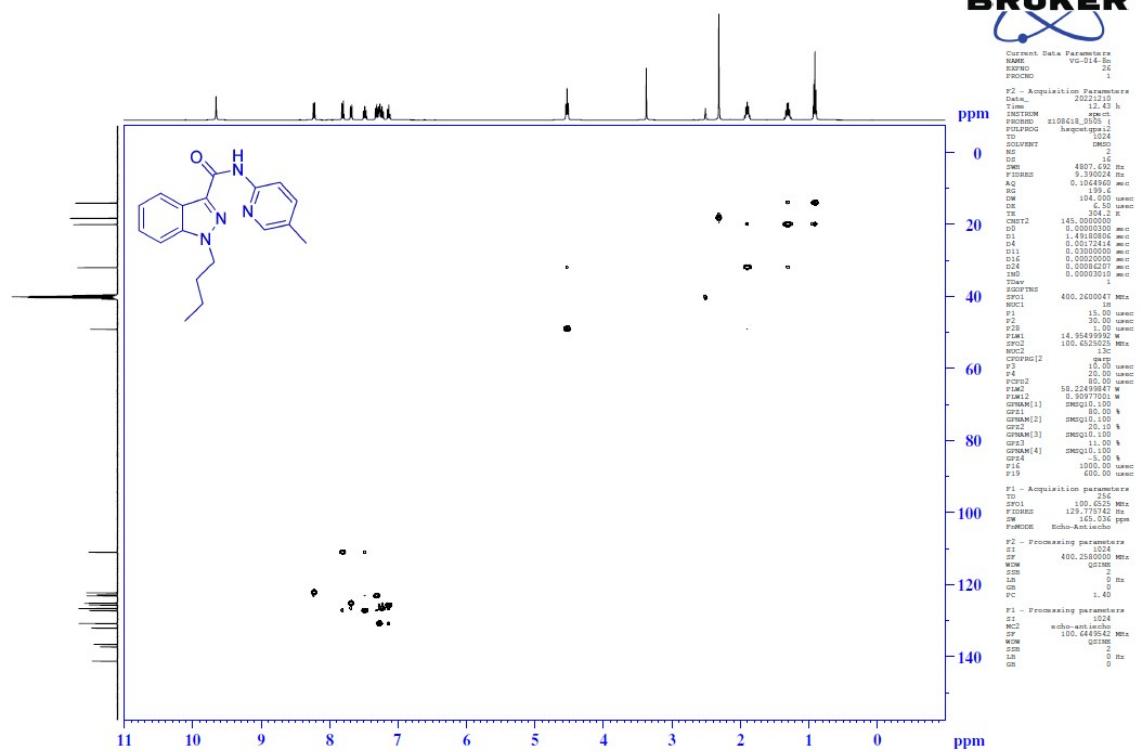


COSY-NMR [400MHz, DMSO-d₆] spectrum of 1-butyl-N-(5-methylpyridin-2-yl)-1H-indazole-3-carboxamide (8n).

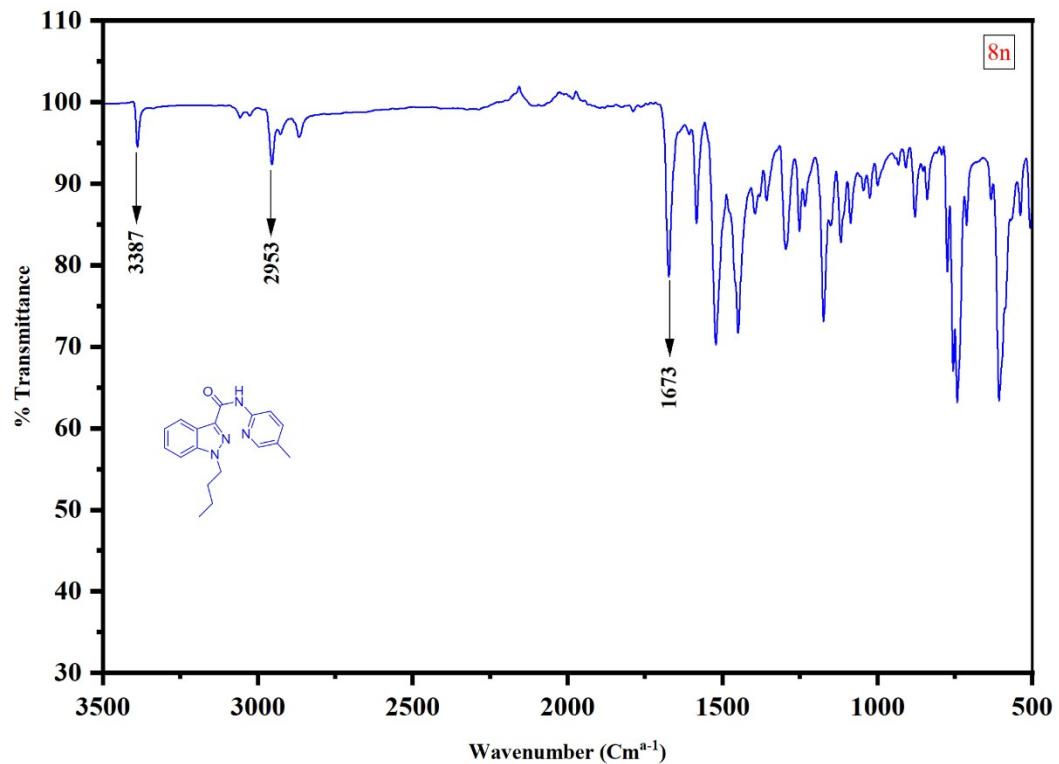
Signature SIF VIT VELLORE
VG-014



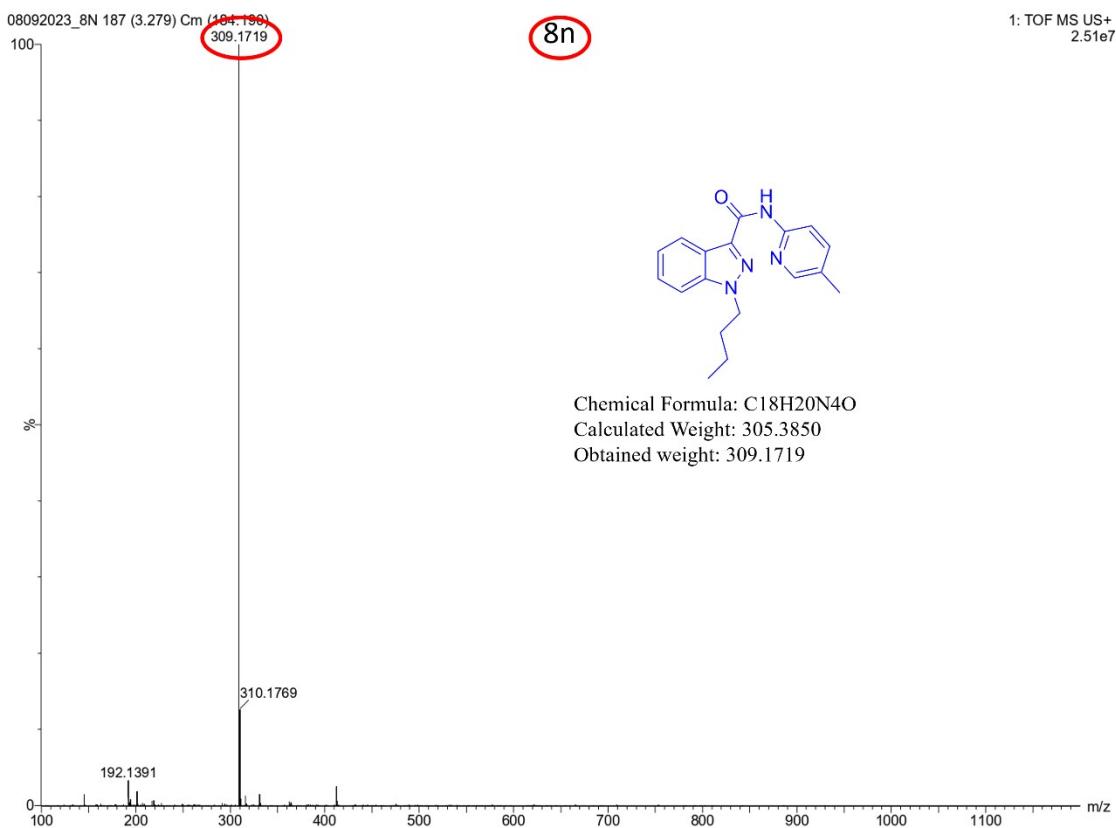
HSQC-NMR [400MHz, DMSO-d₆] spectrum of 1-butyl-N-(5-methylpyridin-2-yl)-1H-indazole-3-carboxamide (8n).



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

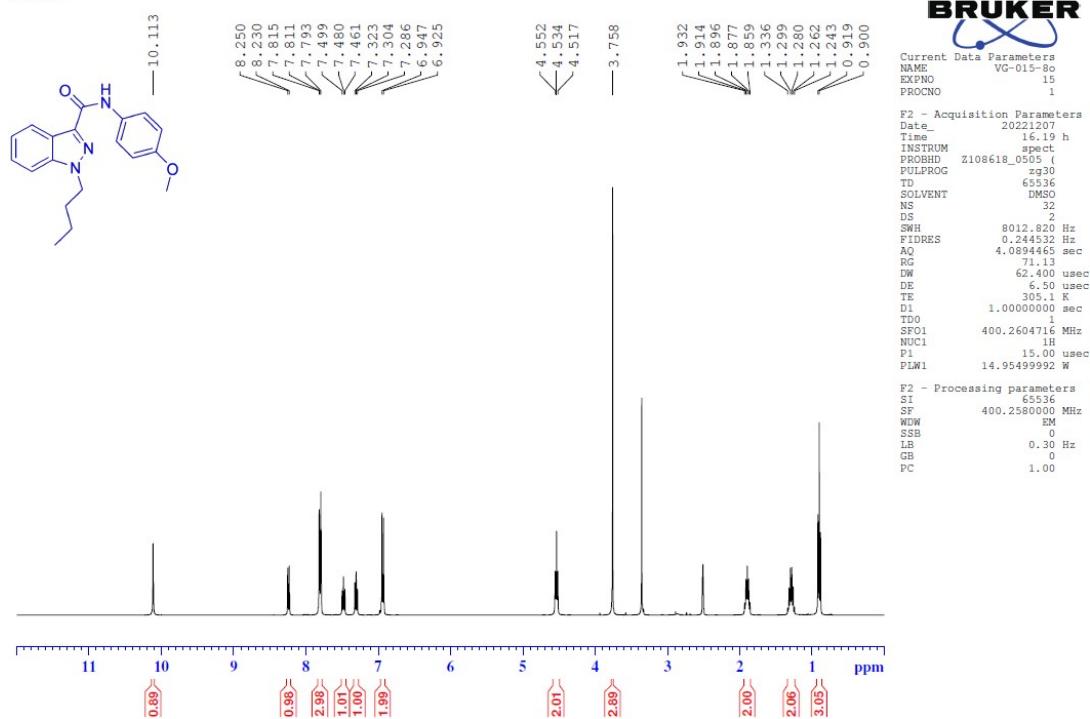


HRMS of 1-butyl-N-(5-methylpyridin-2-yl)-1H-indazole-3-carboxamide (8n).



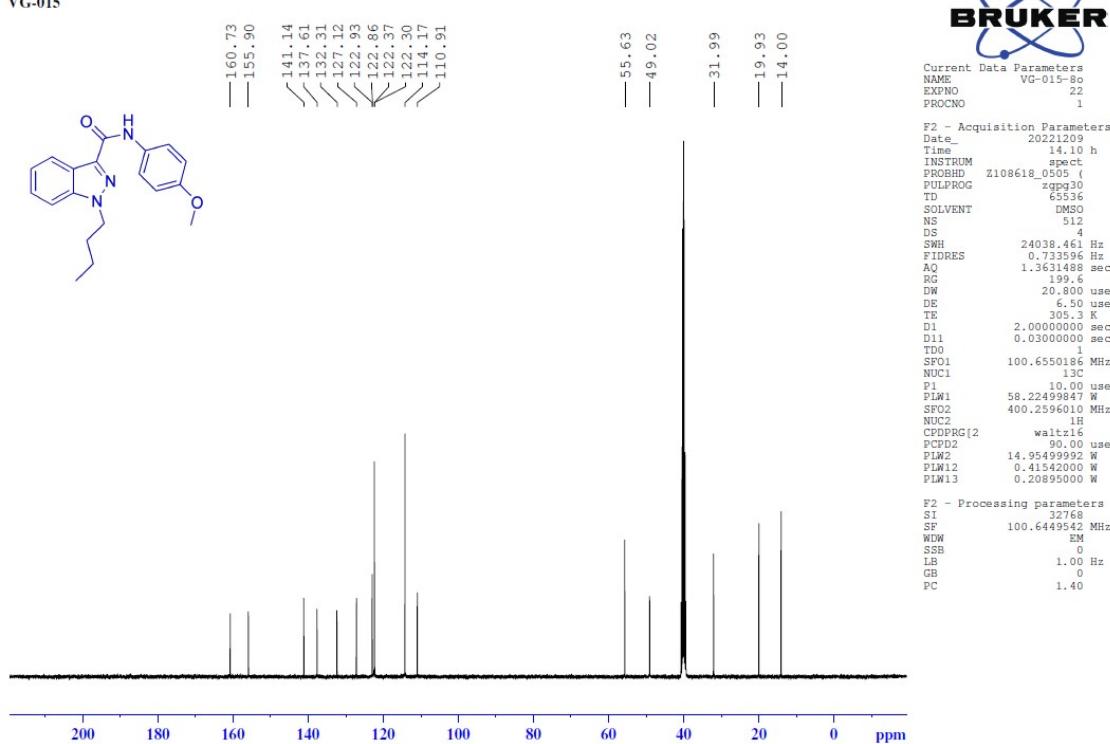
¹H-NMR [400MHz, DMSO-d₆] spectrum of 1-butyl-N-(4-methoxyphenyl)-1H-indazole-3-carboxamide (8o).

Signature SIF VIT VELLORE
VG-015



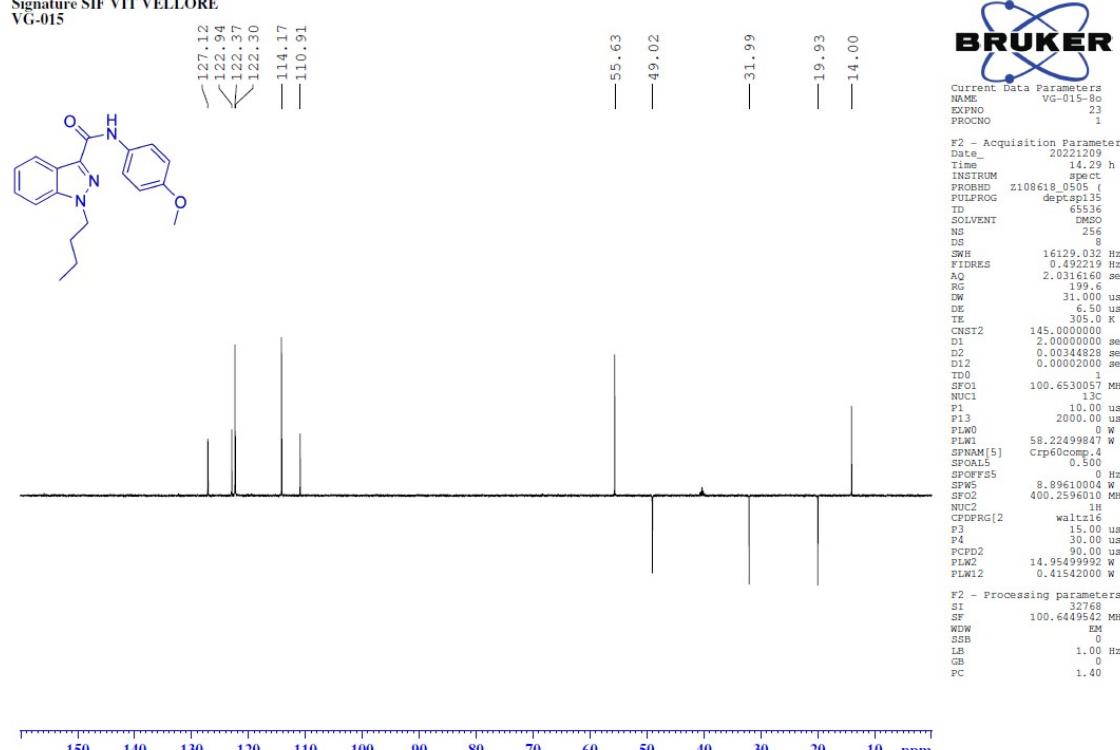
¹³C-NMR [400MHz, DMSO-d₆] spectrum of 1-butyl-N-(4-methoxyphenyl)-1H-indazole-3-carboxamide (8o).

Signature SIF VIT VELLORE
VG-015



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).

Signature SIF VIT VELLORE
VG-015



Current Data Parameters
NAME: VG-015-Bo
EXPNO: 2
PRCHNC: 1

p2 - Acquisition Parameters
Data_1D: 20230401
Time: 23.51 h
TE: 300.00 ms
PROBDRY: z108618_0505 {
POLYPFG: eceeyggppftt
TD: 32768
SOLVENT: DMSO
NS: 1
DS: 16
SWH: 4761.900 Hz
FIDRES: 4.530000 Hz
AQ: 0.2150400 sec
RG: 20
DM: 105.000 usc
DE: 6.500 usc
TE: 300.00 ms
D1: 0.0000300 sec
D11: 1.9815799 sec
D13: 0.0000200 sec
D12: 0.0000200 sec
D14: 0.0000200 sec
D16: 0.0000200 sec
IN1D: 0.00021000 sec
TDppw: 400,2401921. Mix:
SWC1: 15.00 usc
P1: 15.00 usc
P11: 200.00 usc
P1M1: 14.9549999 sec
P1MM1[1]: 3.7384999 sec
SWC2: 10.00 usc
CP13: 10.00 usc
P1E2: 1000.00 usc

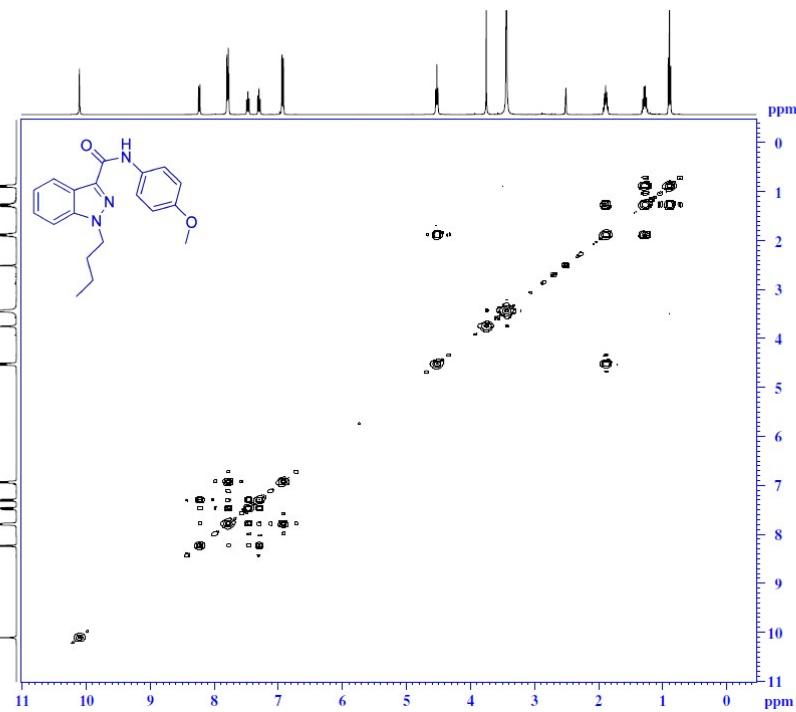
P1 - Acquisition parameters
TE: 300.00 ms
SF01: 400.2602 MHz
FIDRES: 74.404762 Hz
SW: 11.200 KHz
PrwCODE: QF

p2 - Processing parameters
SI: 1024
SF: 400.2580000 MHz
WM: Q31ME
SSB: 0
LB: 0 Hz
GB: 0
PC: 1.40

P1 - Processing parameters
SI: 1024
SF: 400.2602 MHz
WM: Q31ME

9 SW: 250.0000000 MHz
SSB: 0

10 LB: 0 Hz
GB: 0



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

Signature SIF VIT VELLORE
VG-015



Current Data Parameters

NAME: VG-015-Bo
EXPNO: 2
PRCHNC: 1

p2 - Acquisition Parameters
Data_1D: 20230401
Time: 23.58 h
PROBDRY: z108618_0512
POLYPFG: hexagppftt
TD: 32768
SOLVENT: DMSO
NS: 1
DS: 16
SWH: 4761.900 Hz
FIDRES: 9.300995 Hz
AQ: 0.1970300 sec
RG: 199.6
DM: 105.000 usc
DE: 6.500 usc
TE: 300.00 ms
D1: 1.9815799 sec
C1: 145.0000000 sec
D2: 0.0000300 sec
D11: 1.9973744 sec
D13: 0.0000200 sec
D12: 0.0000200 sec
D14: 0.0000200 sec
D16: 0.0000200 sec
IN1D: 0.00003010 sec
TDppw: 400,2401921. Mix:
SWC1: 15.00 usc
P1: 15.00 usc
P12: 15.00 usc
P1M1: 14.9549999 sec
P1MM1[2]: 100.6520003 sec
SWC2: 15.00 usc
CP13: 15.00 usc
P1E2: 20.00 usc
P1C2: 20.00 usc
P1M2: 58.22499847 sec
TE1D: 1.9973744 sec
GR1M[1]: 3.7384999 sec
GR1M[2]: 3.7384999 sec
GR1M[3]: 3.7384999 sec
GR1M[4]: 3.7384999 sec
P19: 1000.00 usc
P19: 600.00 usc

P1 - Acquisition parameters
TD: 32768
SF01: 400.2602 MHz
FIDRES: 128.0000000 Hz
SW: 165.036 ppm
PrwCODE: Echo-Ave

p2 - Processing parameters
SI: 1024
SF: 400.2580000 MHz
WM: Q31ME

80 SSB: 0

80 GR1M[1]: 3.7384999 sec

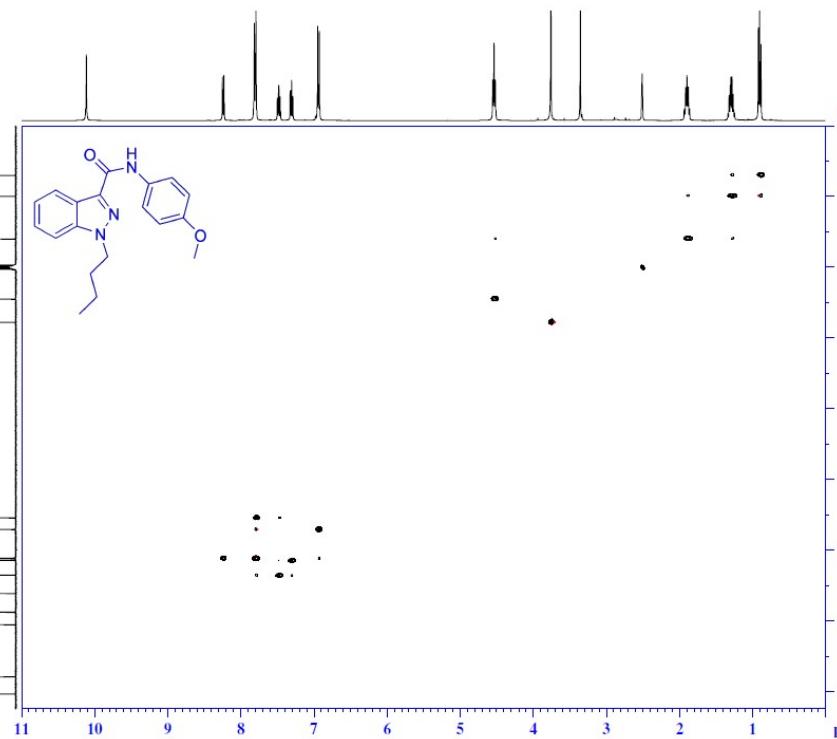
80 GR1M[2]: 3.7384999 sec

80 GR1M[3]: 3.7384999 sec

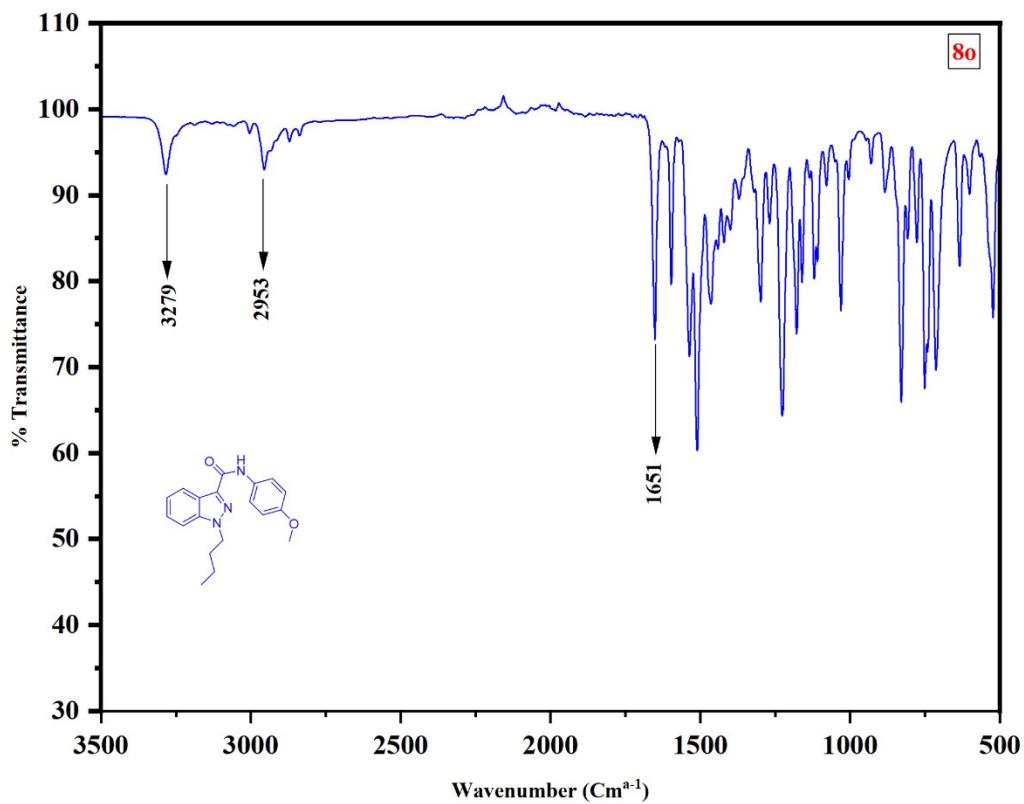
80 GR1M[4]: 3.7384999 sec

100 P1: 1000.00 usc

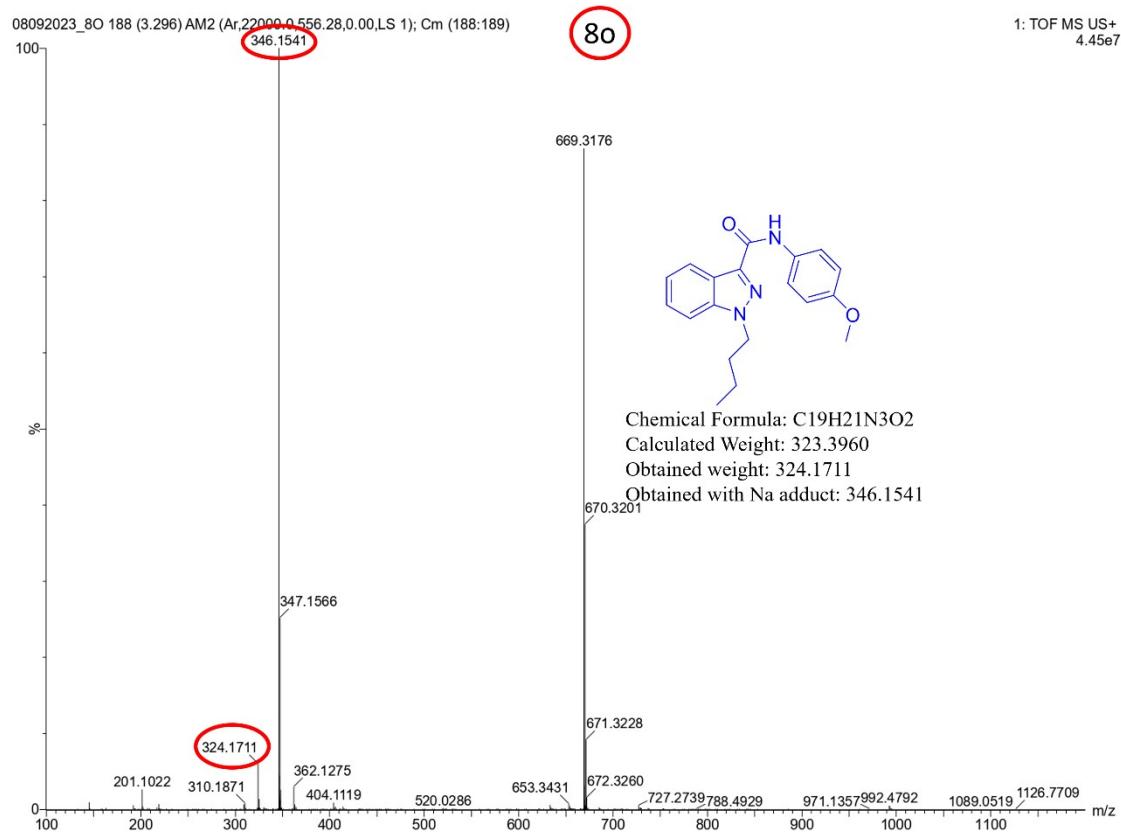
100 P19: 600.00 usc



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

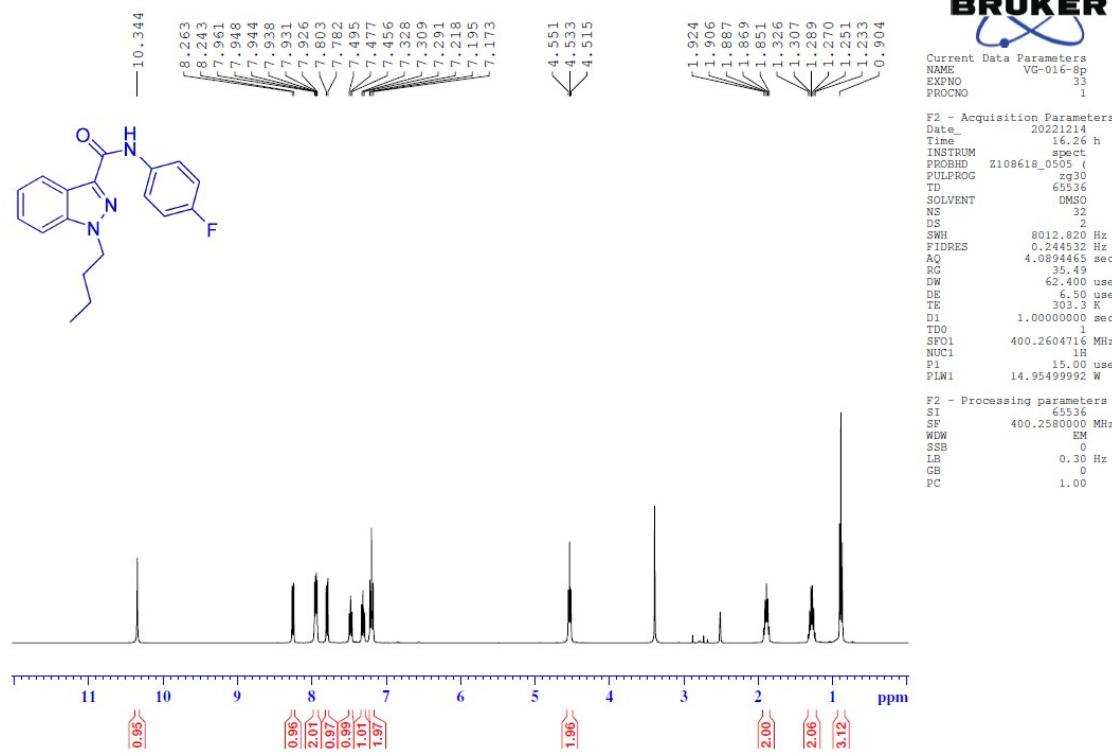


HRMS of **1-butyl-N-(4-methoxyphenyl)-1H-indazole-3-carboxamide (8o).**



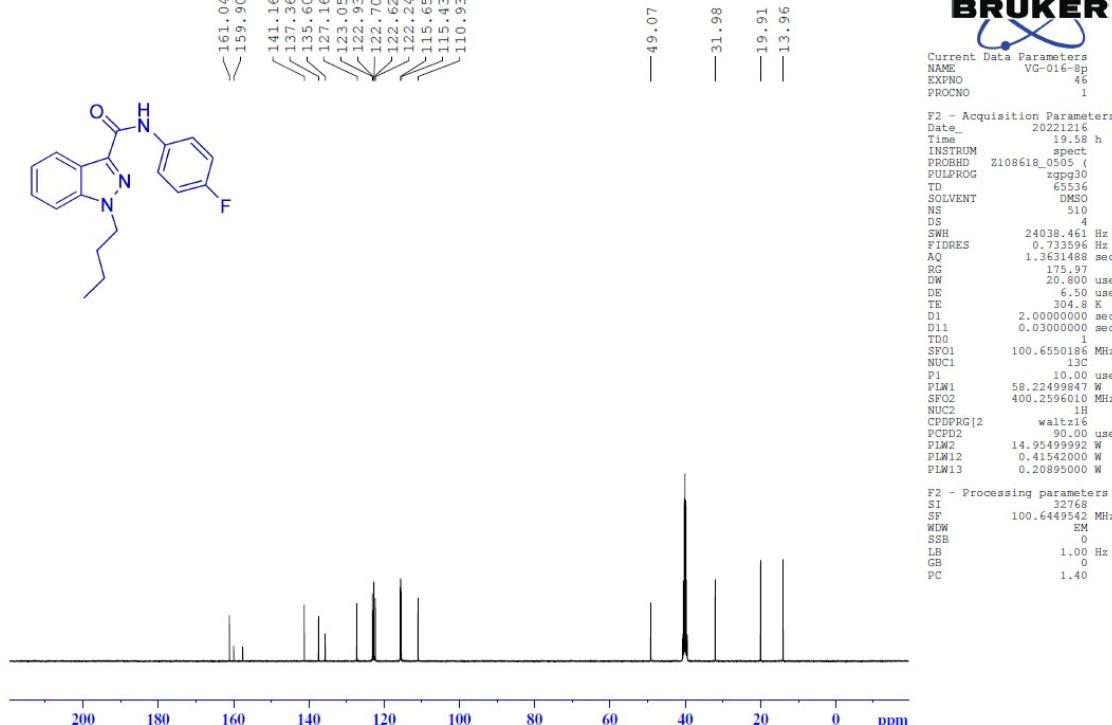
¹H-NMR [400MHz, DMSO-d₆] spectrum of 1-butyl-N-(4-fluorophenyl)-1H-indazole-3-carboxamide (8p).

Signature SIF VIT VELLORE
VG-016



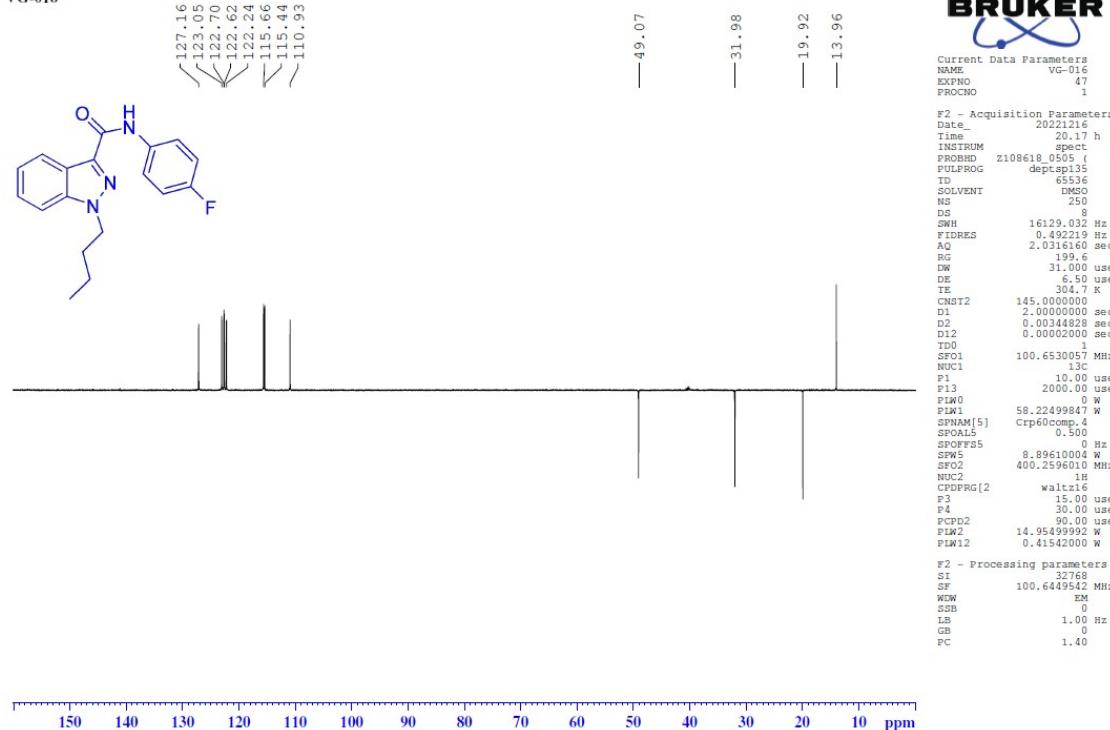
¹³C-NMR [100MHz, DMSO-d₆] spectrum of 1-butyl-N-(4-fluorophenyl)-1H-indazole-3-carboxamide (8p).

Signature SIF VIT VELLORE
VG-016

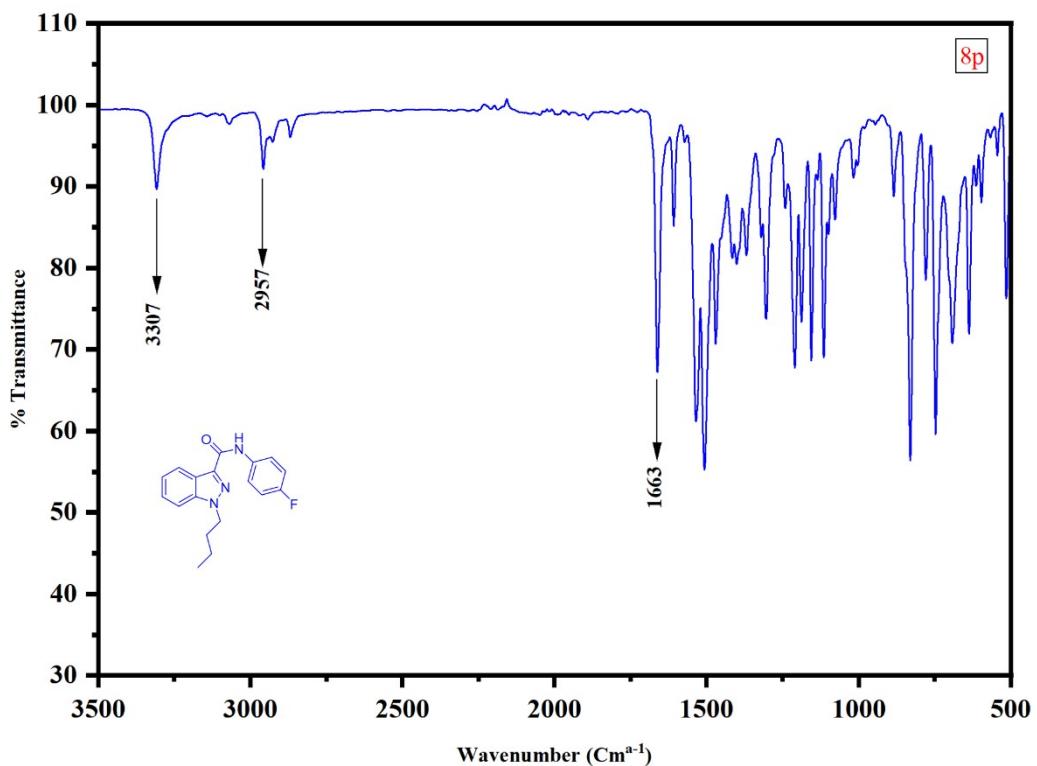


135-DEPT-NMR [100MHz, DMSO-d₆] spectrum of 1-butyl-N-(4-fluorophenyl)-1H-indazole-3-carboxamide (8p).

Signature SIF VIT VELLORE
VG-016



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

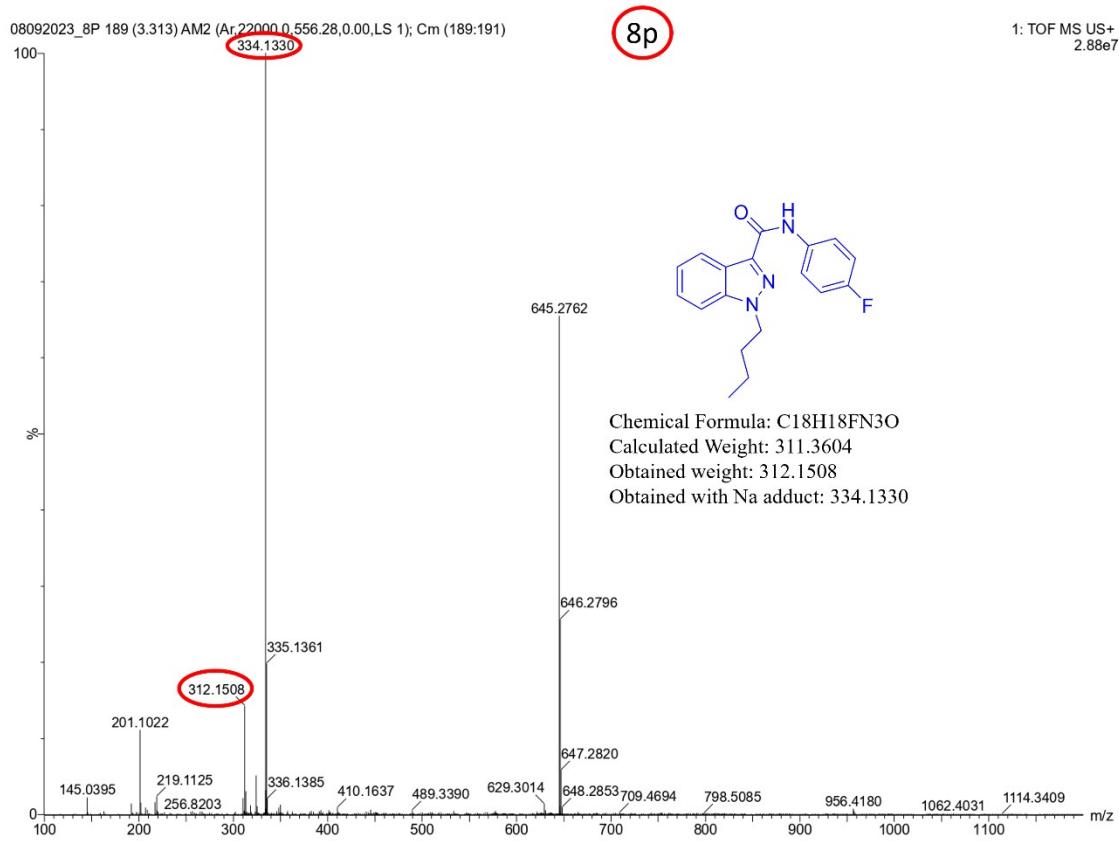
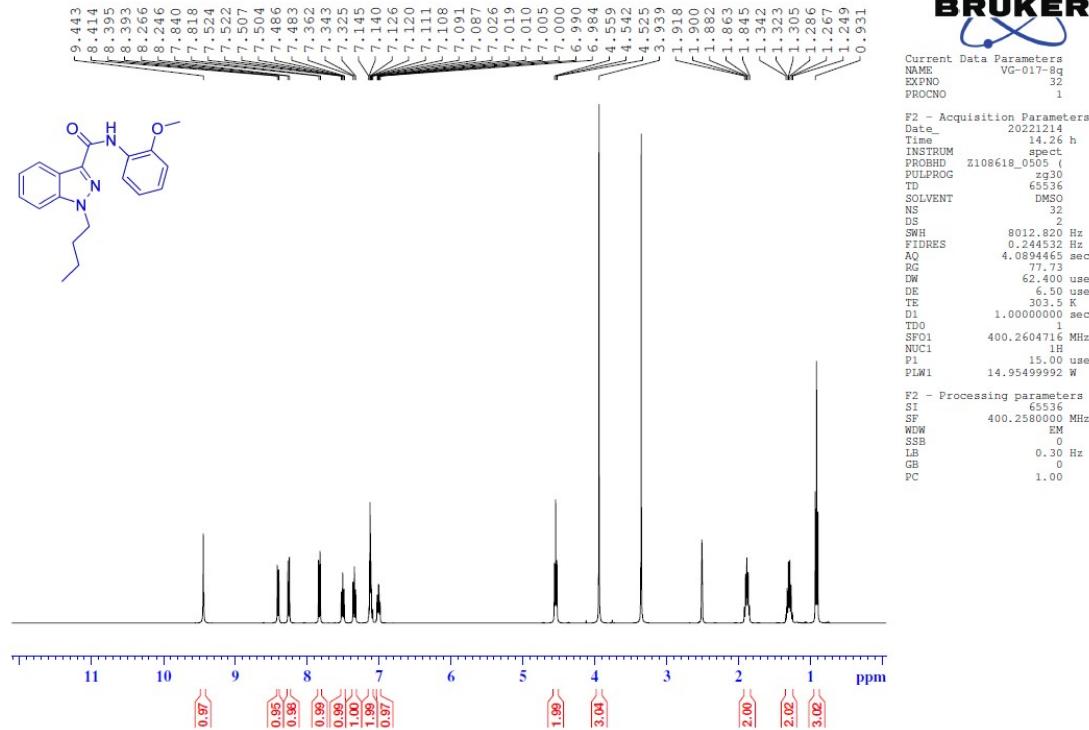


HRMS

of

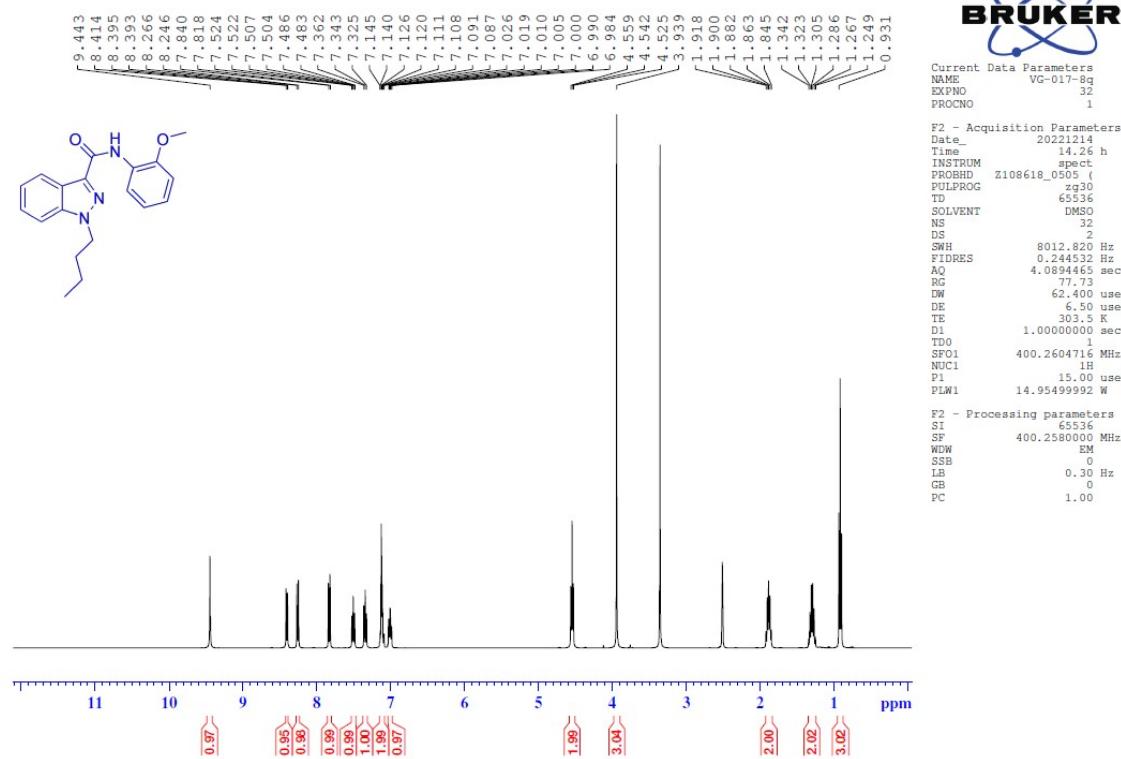
1-butyl-N-(4-fluorophenyl)-1H-indazole-3-carboxamide

(8p).

¹H-NMR [100MHz, DMSO-d₆] spectrum of 1-butyl-N-(2-methoxyphenyl)-1H-indazole-3-carboxamide (8q).Signature SIF VIT VELLORE
VG-017

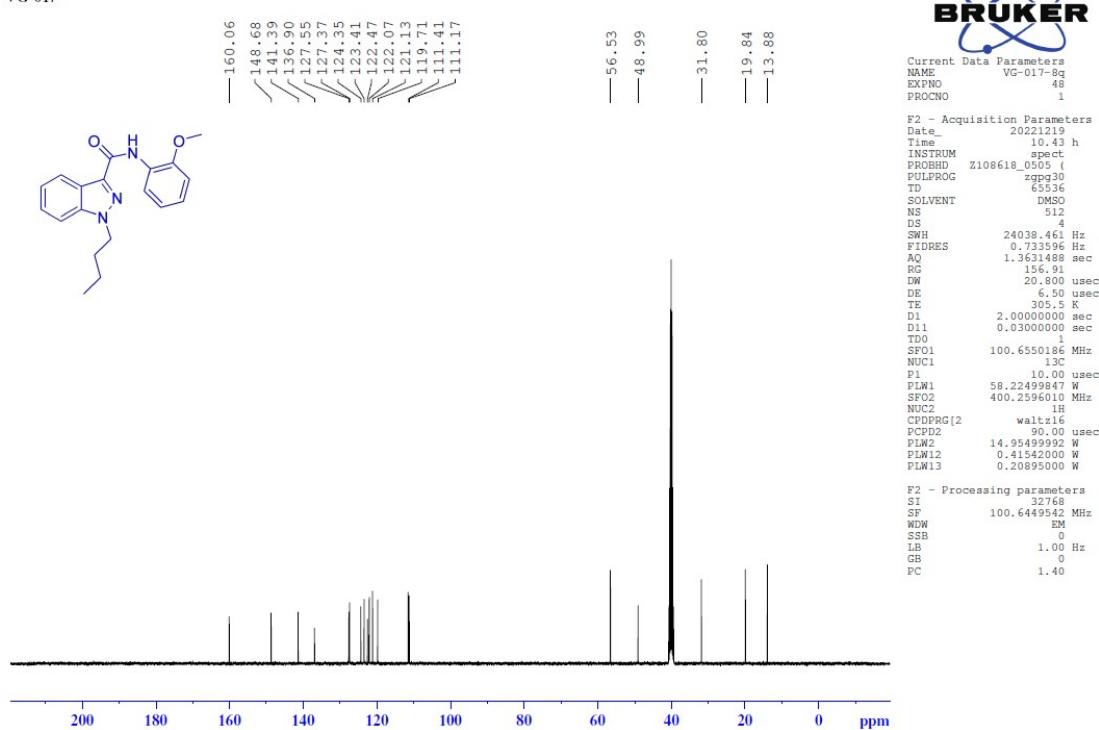
¹H-NMR [400MHz, DMSO-d₆] spectrum of 1-butyl-N-(2-methoxyphenyl)-1H-indazole-3-carboxamide (8q).

Signature SIF VIT VELLORE
VG-017



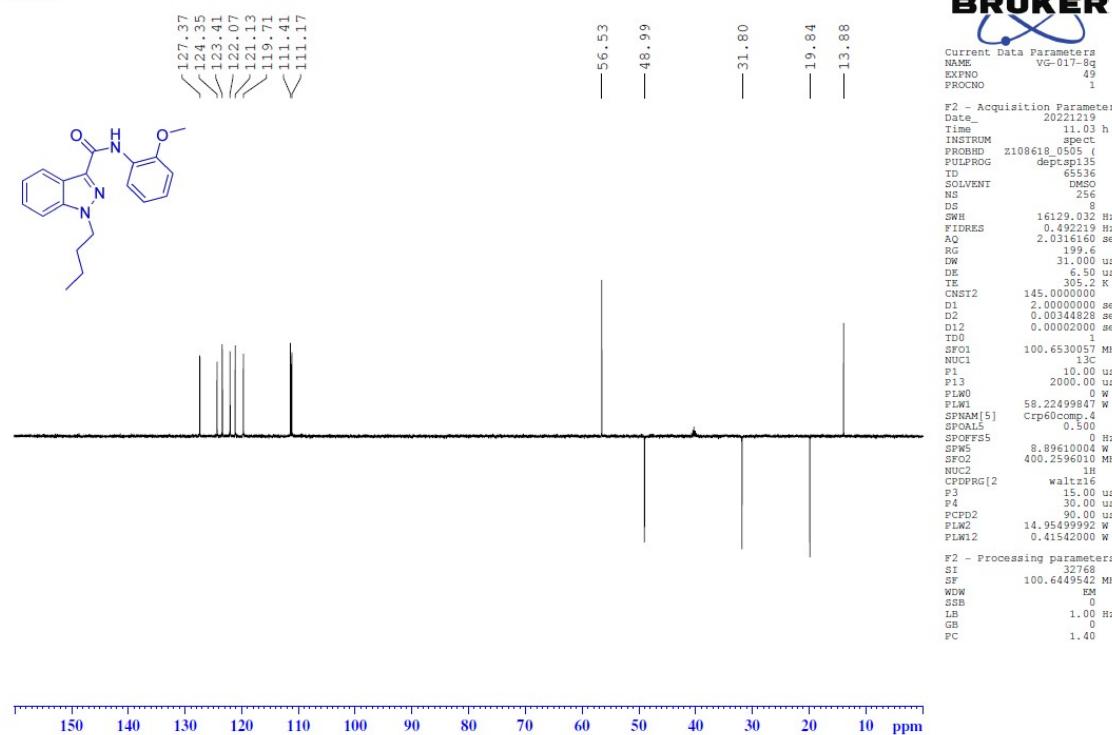
¹³C-NMR [100MHz, DMSO-d₆] spectrum of 1-butyl-N-(2-methoxyphenyl)-1H-indazole-3-carboxamide (8q).

Signature SIF VIT VELLORE
VG-017

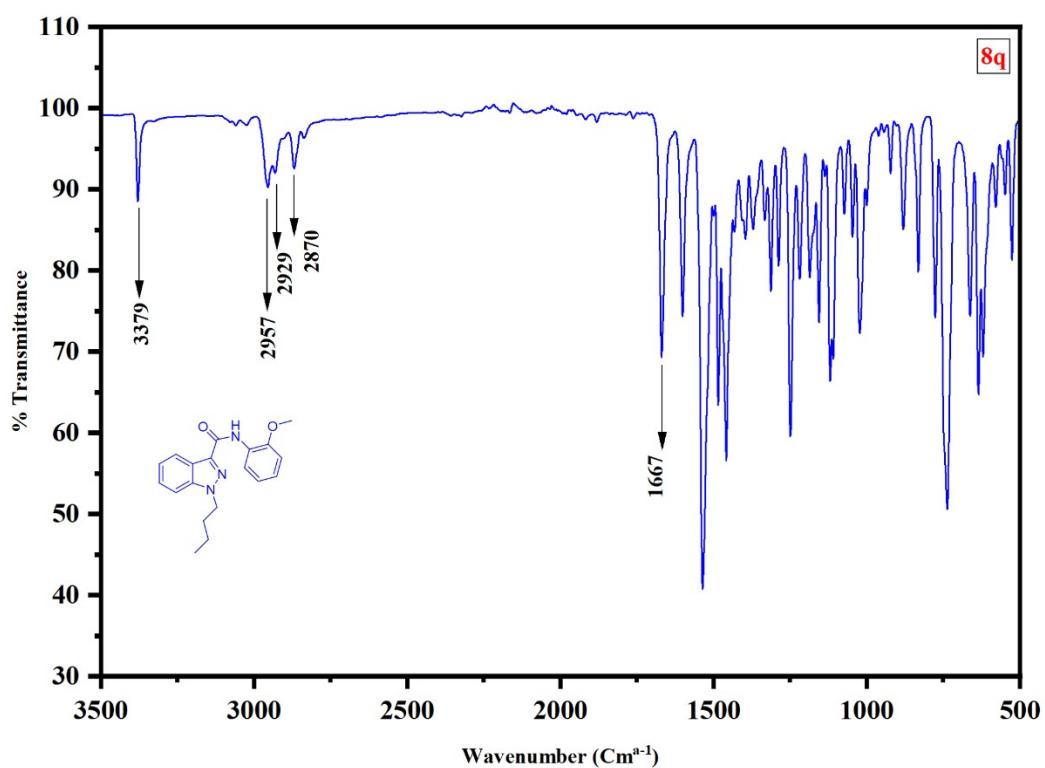


¹³⁵-DEPT-NMR [100MHz, DMSO-d₆] spectrum of 1-butyl-N-(2-methoxyphenyl)-1H-indazole-3-carboxamide (8q).

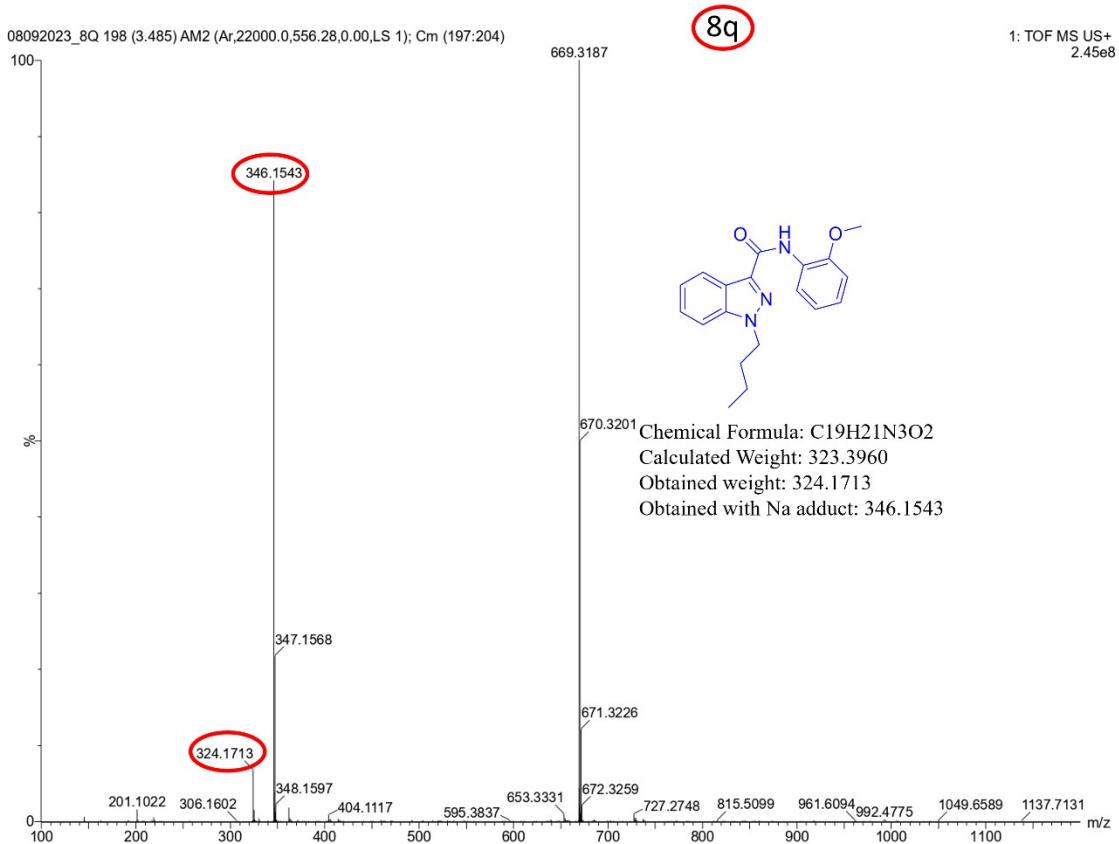
Signature SIF VIT VELLORE
VG-017



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

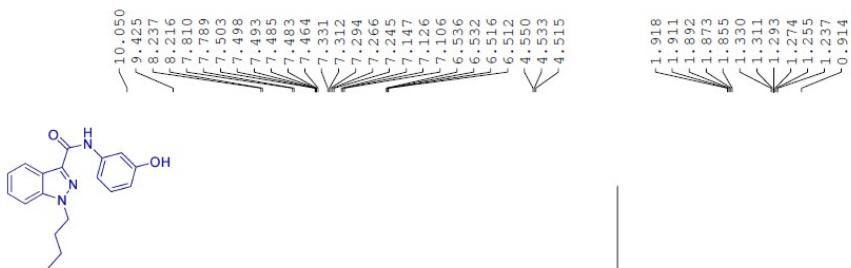


HRMS of 1-butyl-N-(2-methoxyphenyl)-1H-indazole-3-carboxamide (8q).



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

Signature SIF VIT VELLORE
VG-018



BRUKER

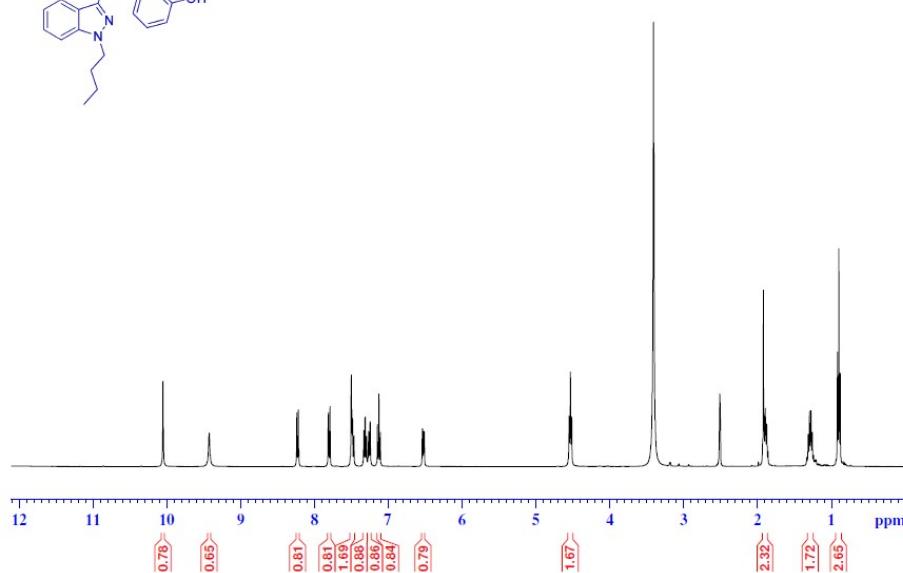
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Current Data Parameters
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EXPNO         36
PROCNO        1

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Date_        20230122
Time_        14.32 h
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PROBHD      PULPROG zg30
TD           65536
SOLVENT      DMSO
NS           16
DS           2
SWH          8012.82 Hz
FIDRES      0.244532 Hz
AQ           4.094465 sec
RG           63.11
DW           62.4000 usec
DE           6.50 usec
TE           303.3 K
D1           1.0000000 sec
TD0          1
SF01        400.2604716 MHz
NUC1         1H
P1           15.00 usec
PLW1        14.95499992 W

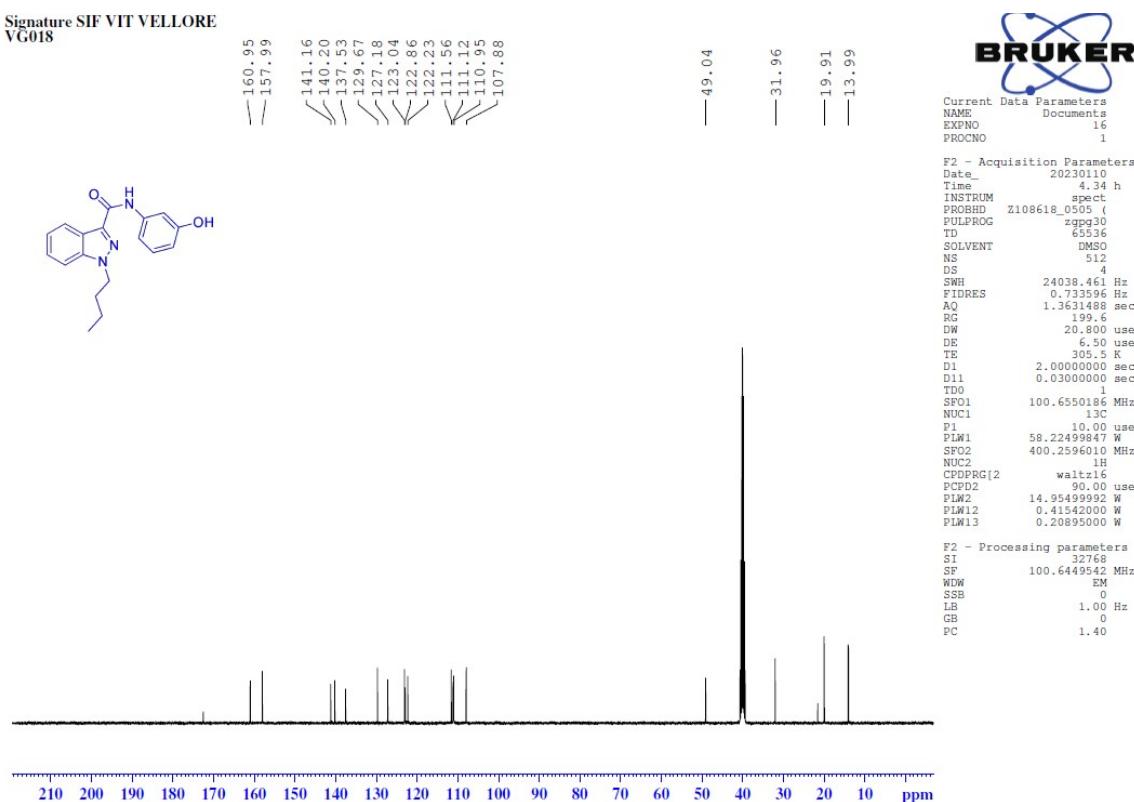
F2 - Processing parameters
SI            65536
SF           400.2580000 MHz
WDW          EM
SSB           0
LB           0.30 Hz
GB           0
PC           1.0

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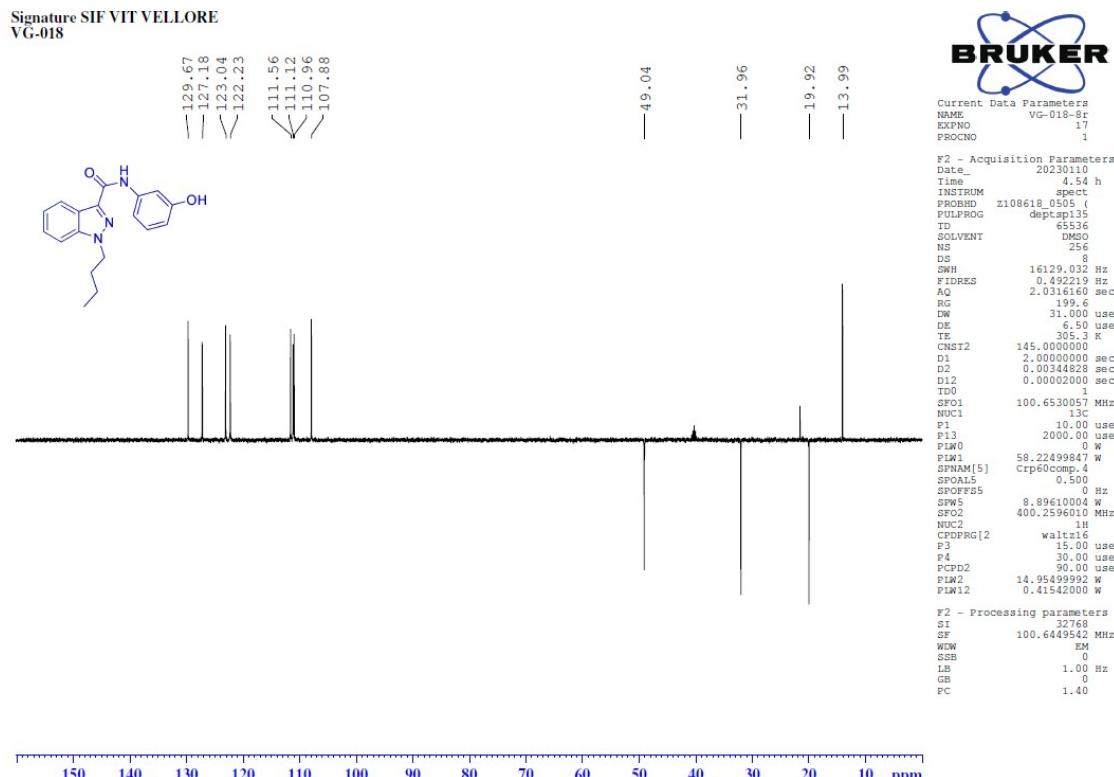
¹³C-NMR [100MHz, DMSO-d₆] spectrum of 1-butyl-N-(3-hydroxyphenyl)-1H-indazole-3-carboxamide (8r).

Signature SIF VIT VELLORE
VG018



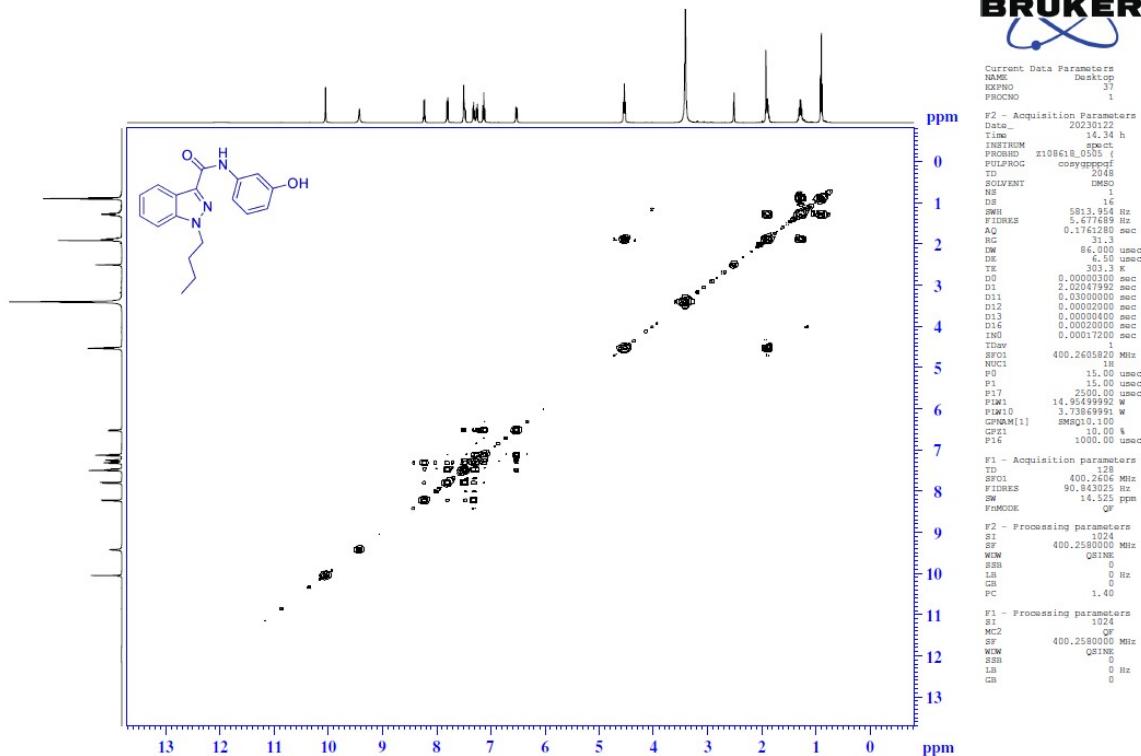
¹³⁵-DEPT-NMR [100MHz, DMSO-d₆] spectrum of 1-butyl-N-(3-hydroxyphenyl)-1H-indazole-3-carboxamide (8r).

Signature SIF VIT VELLORE
VG-018



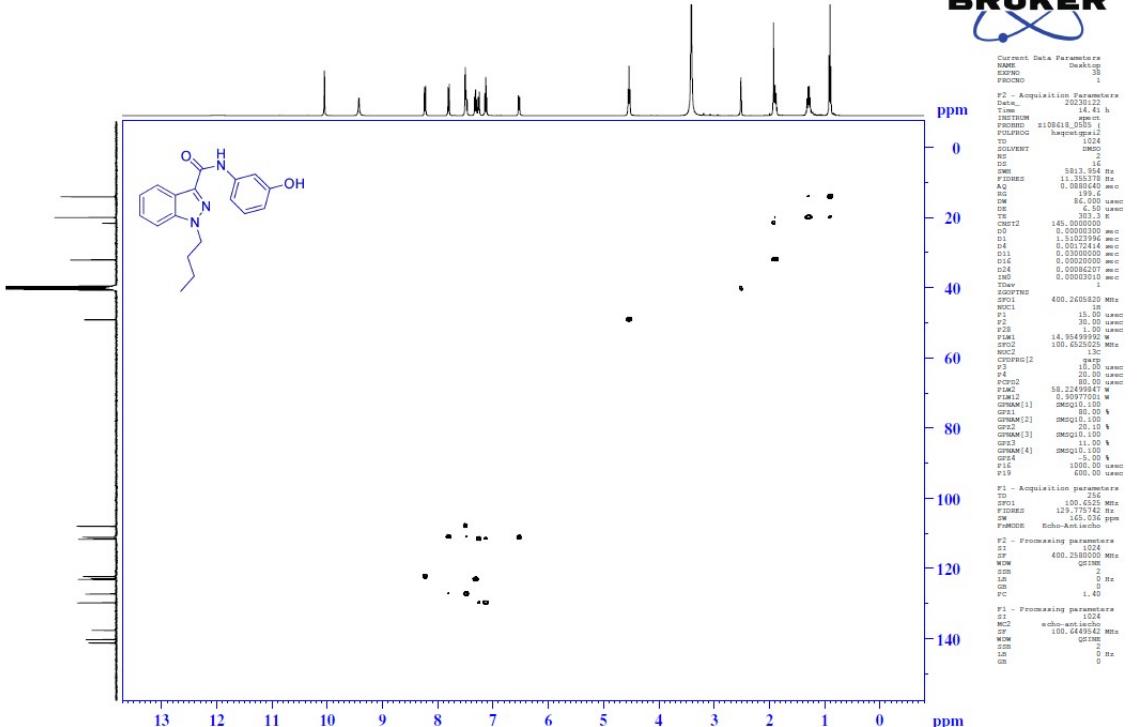
COSY-NMR [400MHz, DMSO-d₆] spectrum of 1-butyl-N-(3-hydroxyphenyl)-1H-indazole-3-carboxamide (8r).

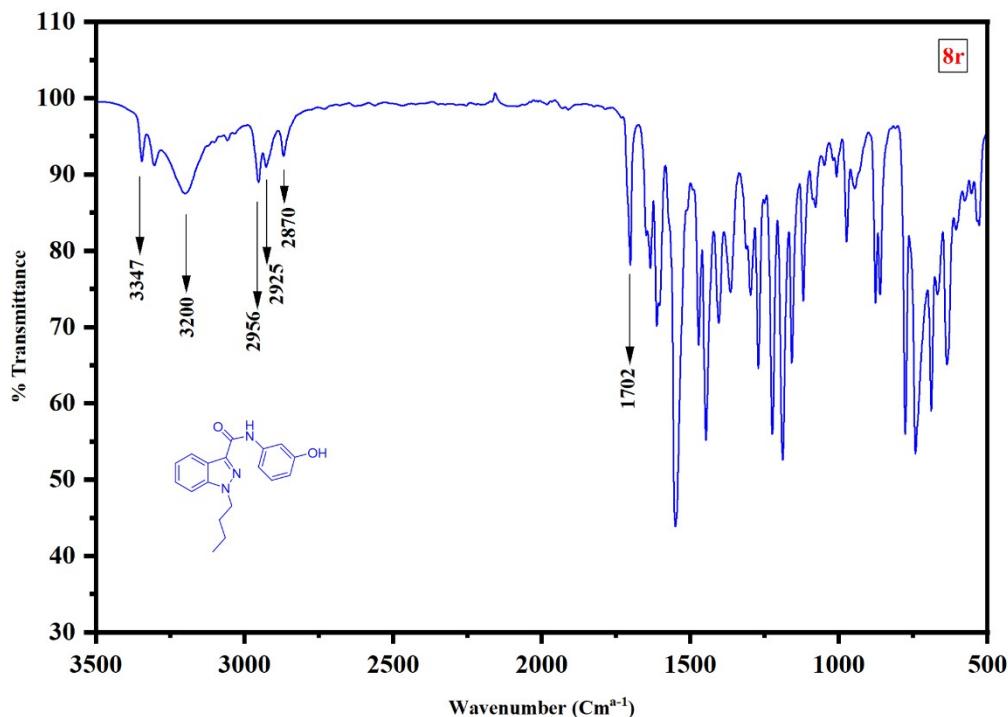
Signature SIF VIT VELLORE
VG-018



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

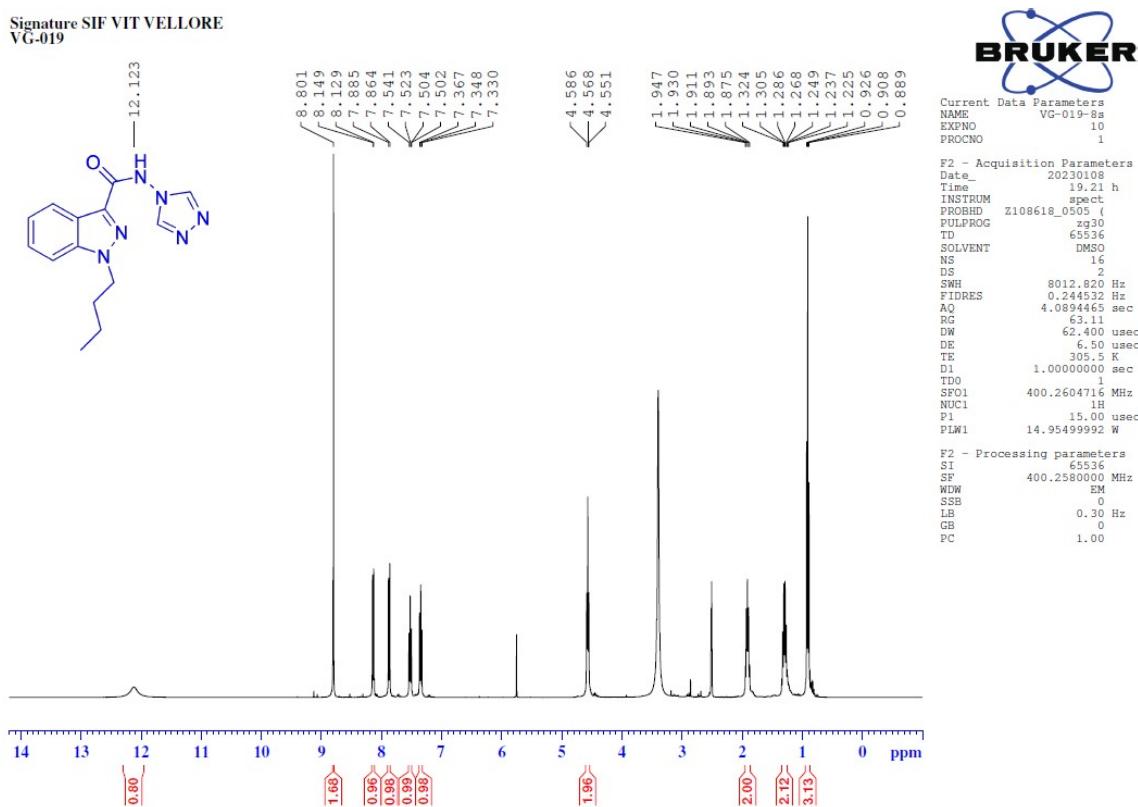
Signature SIF VIT VELLORE
VG-018





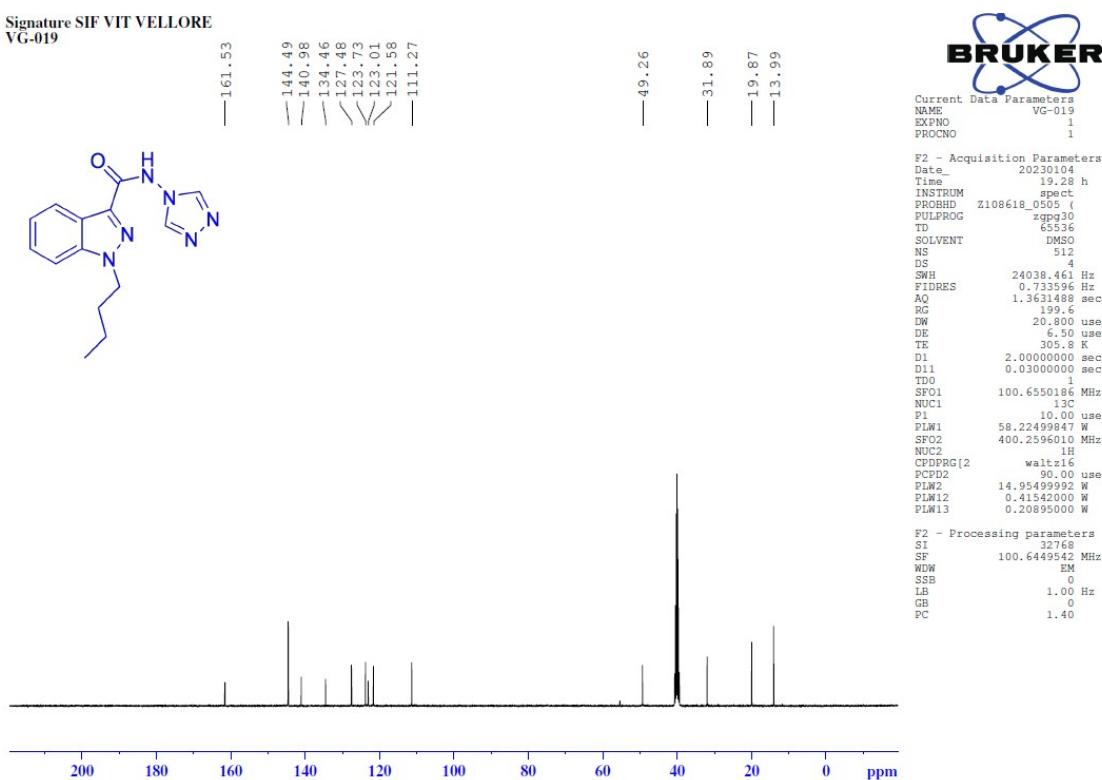
HRMS of 1-butyl-N-(3-hydroxyphenyl)-1H-indazole-3-carboxamide (8r).

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



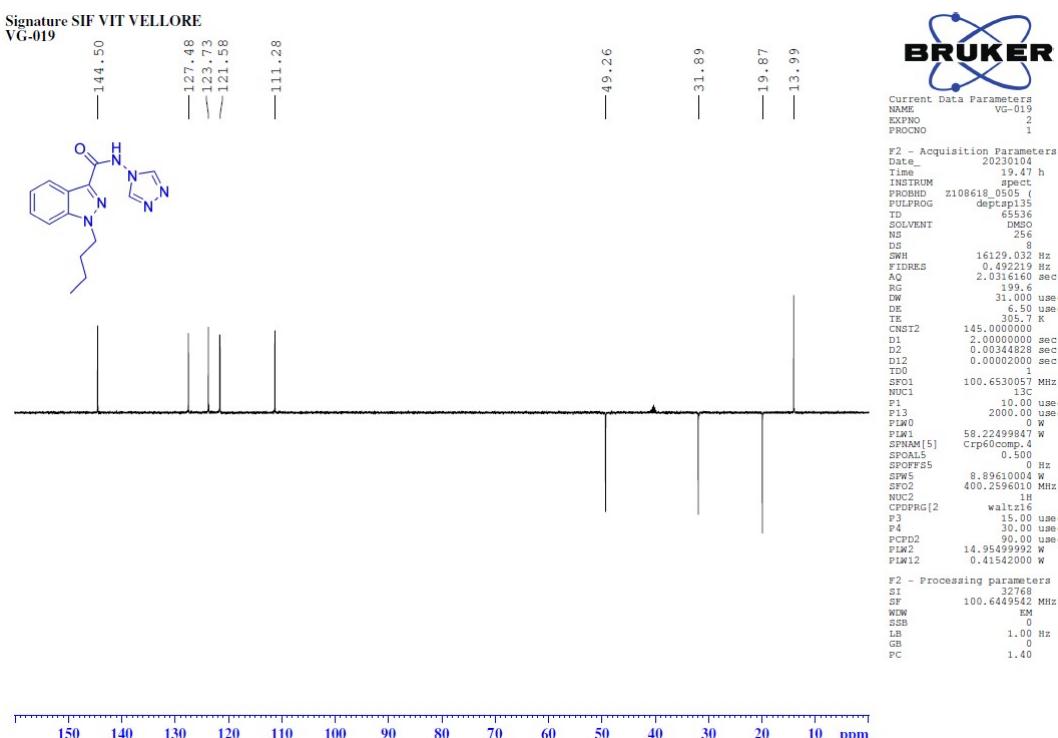
¹³C-NMR [100MHz, DMSO-d₆] spectrum of 1-butyl-N-(4H-1,2,4-triazol-4-yl)-1H-indazole-3-carboxamide (8s).

Signature SIF VIT VELLORE
VG-019



¹³⁵-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



Current Data Parameters

NAME VG-019_Ba

EXPTNO 12

PROCNO 1

F2 - Acquisition Parameters

Date_ 2023-07-18

Time_ 15:38:00 h

INSTRUM spect

PROBHD z108618_0505

PULPROG cogwheels

TD 2048

SW1 200.1333 MHz

DS 16

TE 30.00 sec

D0 0.00000300 sec

D1 2.02867198 sec

D11 0.00000000 sec

D12 0.00000200 sec

D13 0.00000040 sec

D14 0.00000000 sec

IN0 0.00014400 sec

TDRW 400.2606232 Min

NUC1 1H

P0 15.00 usec

P1 1.00 usec

P17 2500.00 usec

P18A 14.7358399 sec

P1W1D 3.7358399 sec

CPDPR1M[1] SWQU10.100

G2Z1 10.00 %

P1E 1000.00 usec

F1 - Acquisition parameters

TD 1024

SF 400.2606232 MHz

FW1ES 95.2748000 Hz

SW 15.231 ppm

FOV 0.00000000

F2 - Processing parameters

S1 1024

MC2 0

SF 400.2606232 MHz

WW 0.00000000

SB 0

LB 0 Hz

GB 0

PC 1.40

F1 - Processing parameters

S1 1024

MC2 0

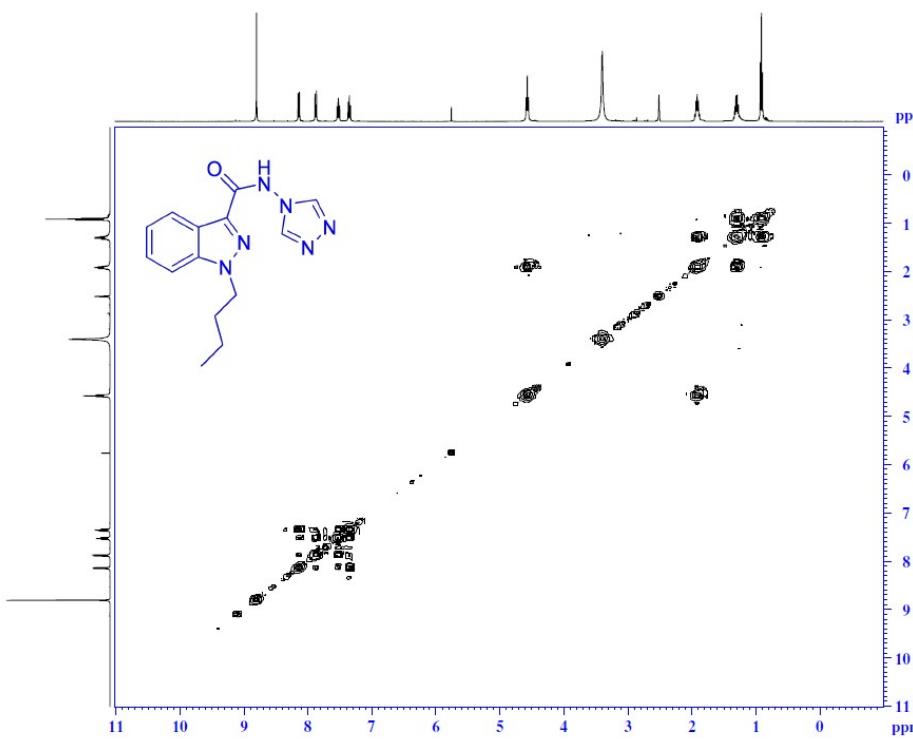
SF 400.2606232 MHz

WW 0.00000000

SB 0

LB 0 Hz

GB 0



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



Current Data Parameters

NAME VG-019_Ba

EXPTNO 11

PROCNO 1

F2 - Acquisition Parameters

TD 2048

Time_ 15.23 h

INSTRUM spect

PROBHD z108618_0505

PULPROG hechospe1

TD 2048

SW1 200.1333 MHz

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TE 30.00 sec

D0 0.00000300 sec

D1 11.00000000 sec

AQ 0.00000000 sec

RG 199.00 usec

DE 6.50 usec

TM 0.00000000 sec

CR0T2 145.00000000 sec

D0 1.00000000 sec

D1 1.43230000 sec

D4 0.00172414 sec

D11 0.00020000 sec

D14 0.00020000 sec

D24 0.00030100 sec

TDW 400.2606232 Min

NUC1 1H

P0 15.00 usec

P1 2.00 usec

P2 0.00000000 sec

P2M2 58.22499847 sec

P1M2 0.00000000 sec

GR4M[1] 0.00000000 sec

GR4M[2] 0.00000000 sec

GR4M[3] 0.00000000 sec

GR4M[4] 0.00000000 sec

GR4 0.00000000 sec

P1 1.00000000 sec

P19 0.00000000 sec

F1 - Acquisition parameters

TD 1024

SF 400.2606232 MHz

FW1ES 129.0000000 Hz

SW 165.0000000 Hz

FOV Echo-Antiecho

F2 - Processing parameters

S1 1024

MC2 0

SF 400.2606232 MHz

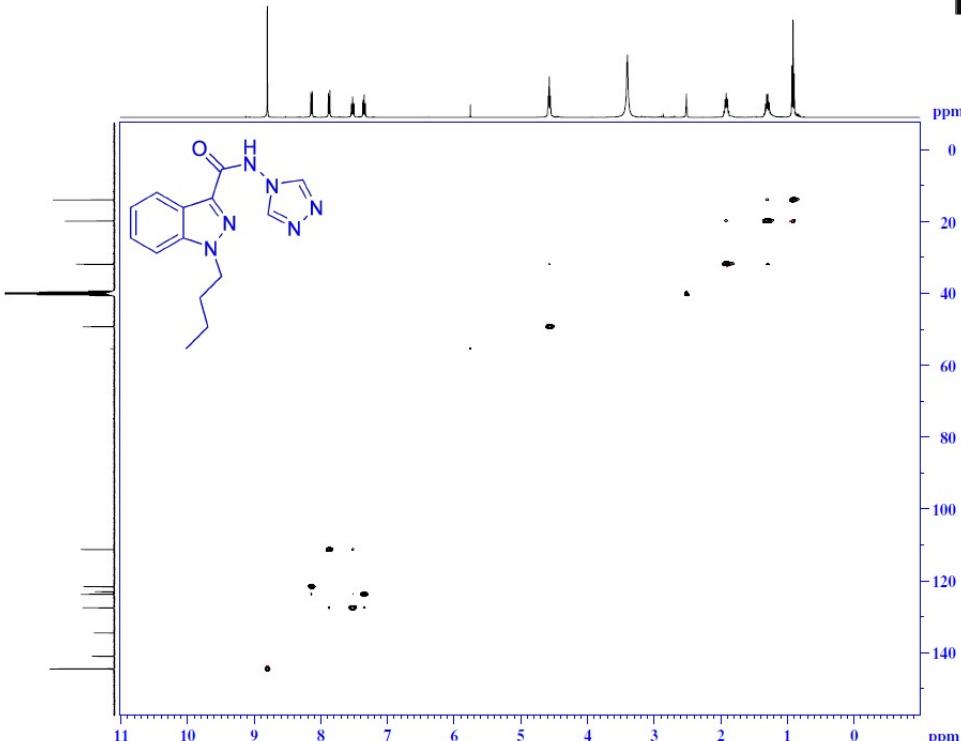
WW 0.00000000

SB 0

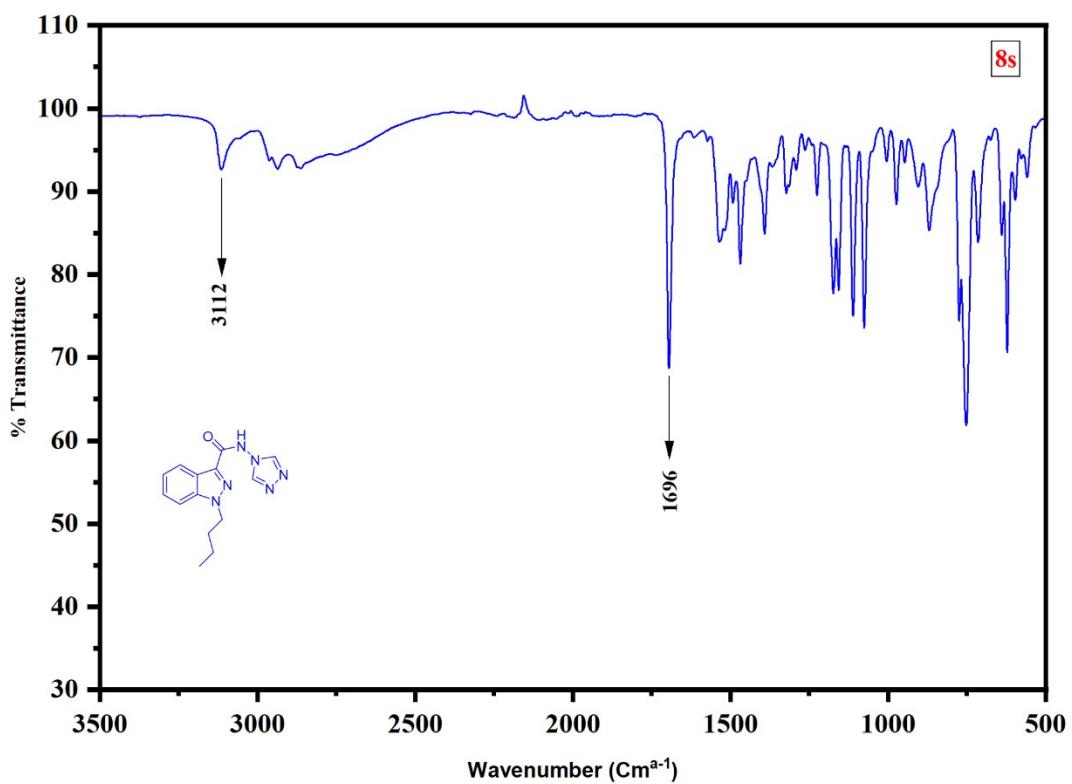
LB 0 Hz

GB 0

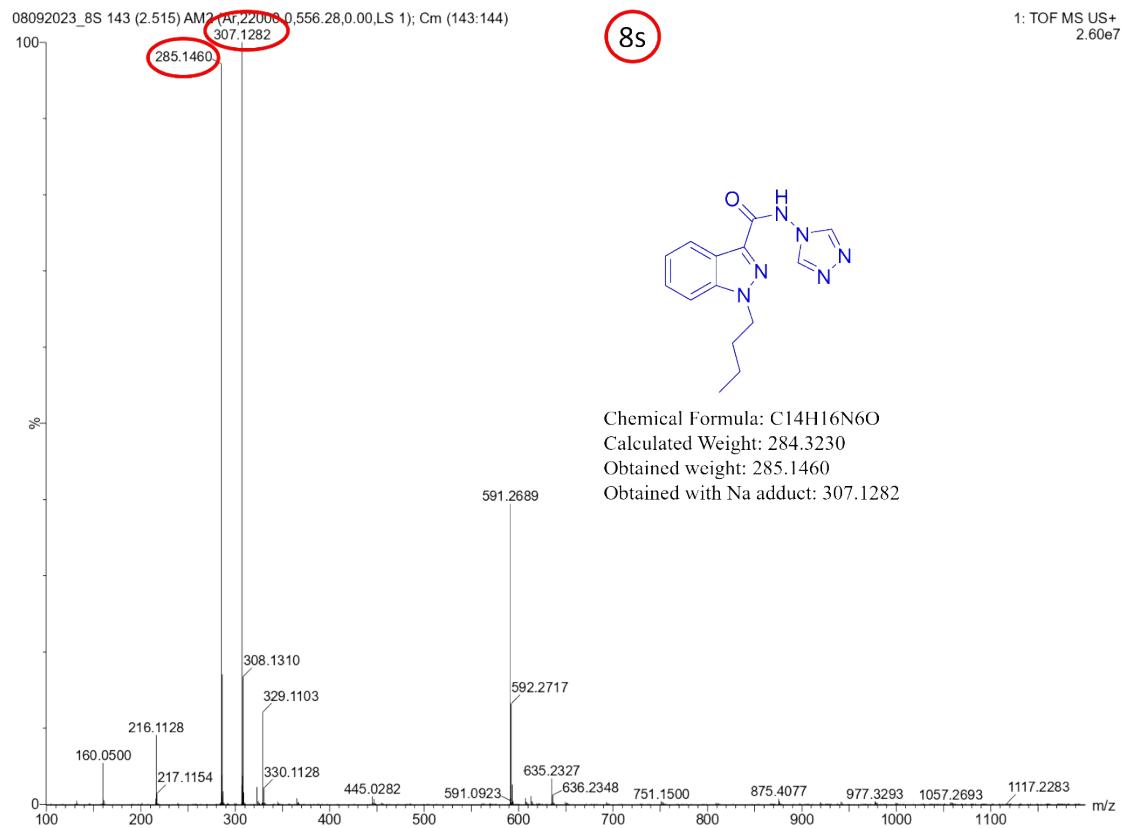
PC 1.40



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

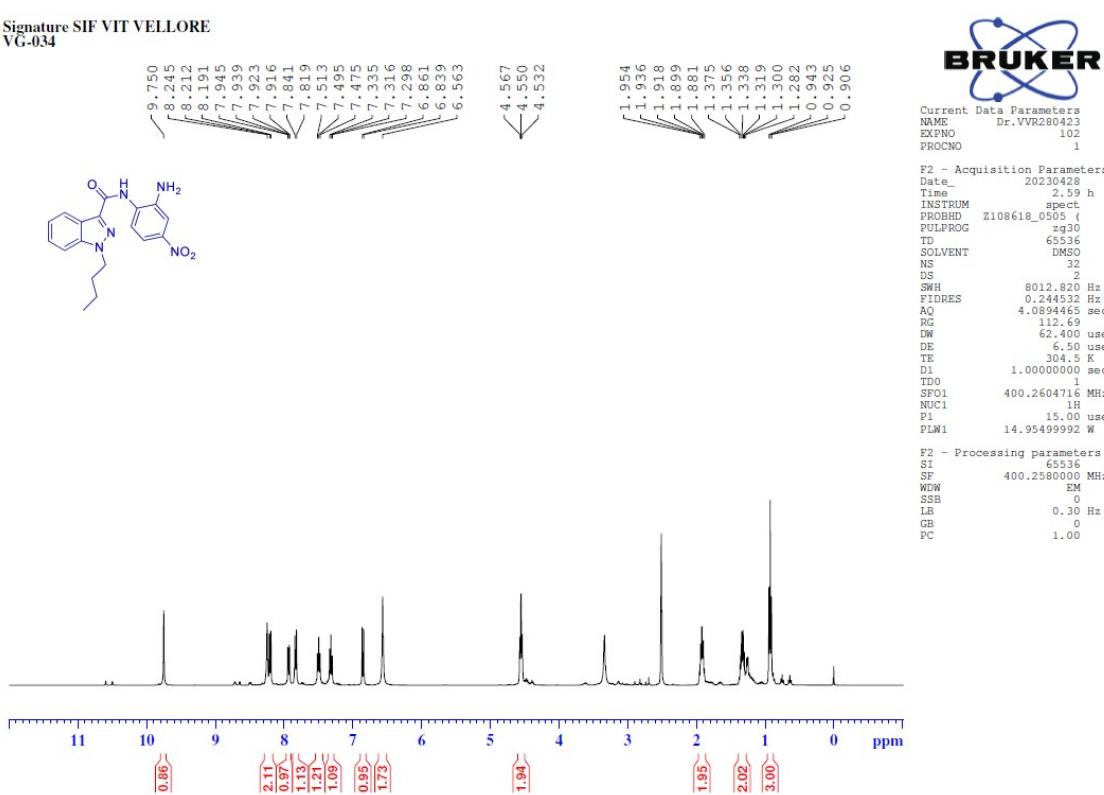


HRMS of 1-butyl-N-(4H-1,2,4-triazol-4-yl)-1H-indazole-3-carboxamide (8s).



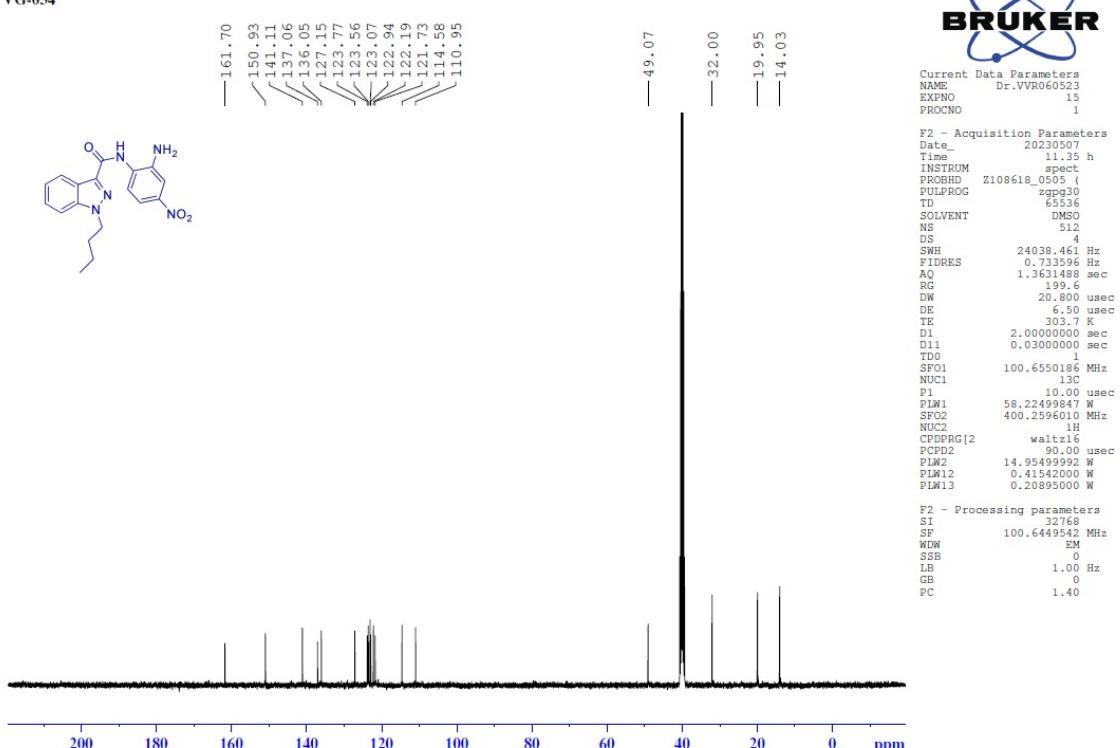
¹H-NMR [400MHz, DMSO-d₆] spectrum of N-(2-amino-4-nitrophenyl)-1-butyl-1H-indazole-3-carboxamide (8t).

Signature SIF VIT VELLORE
VG-034

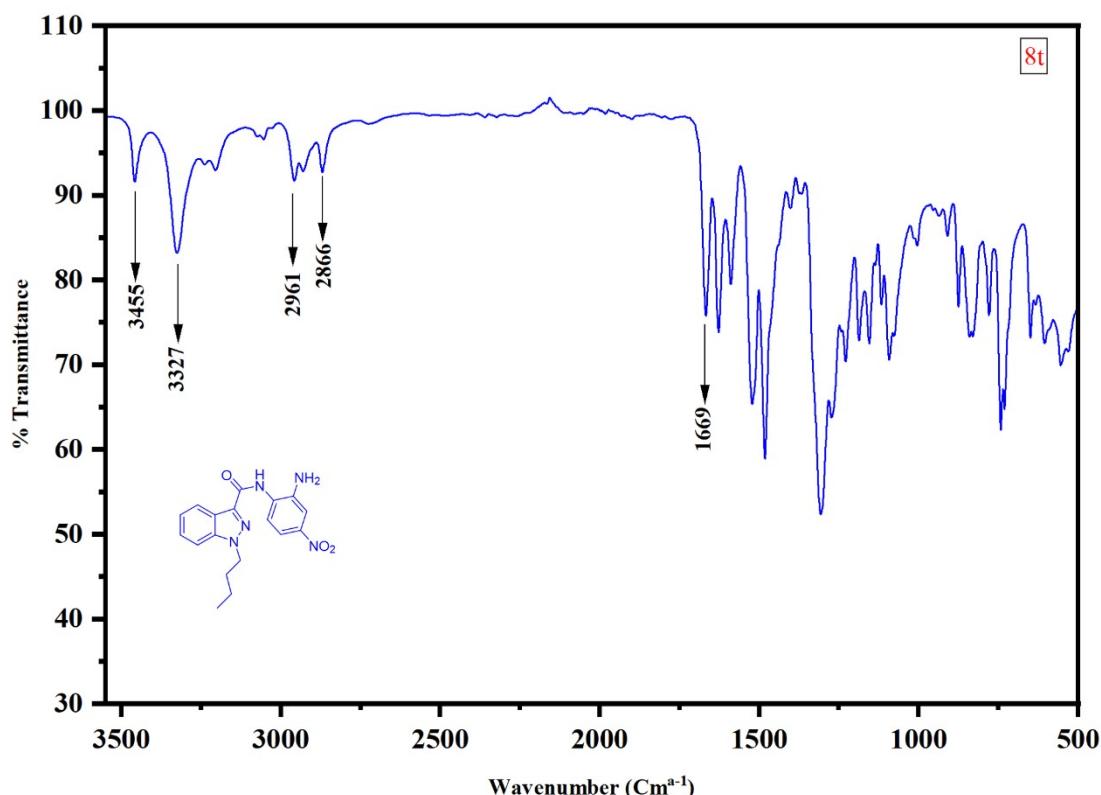


¹³C-NMR [400MHz, DMSO-d₆] spectrum of N-(2-amino-4-nitrophenyl)-1-butyl-1H-indazole-3-carboxamide (8t).

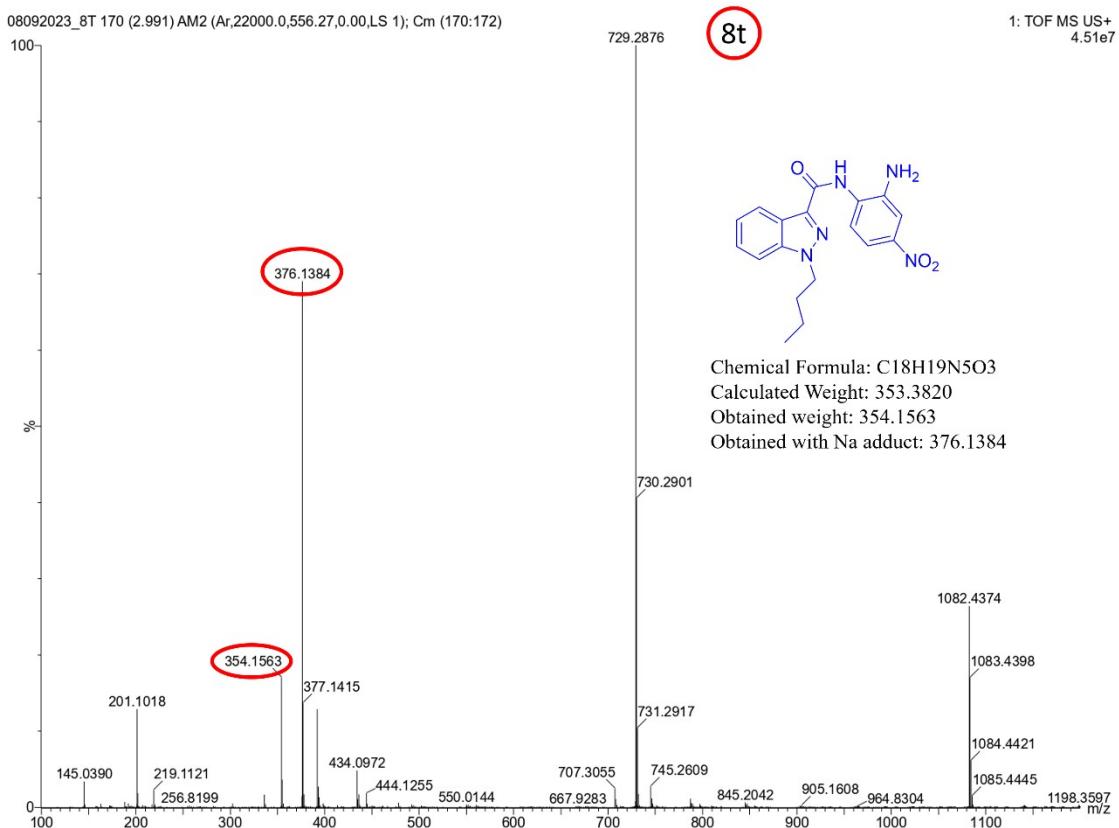
Signature SIF VIT VELLORE
VG-034



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

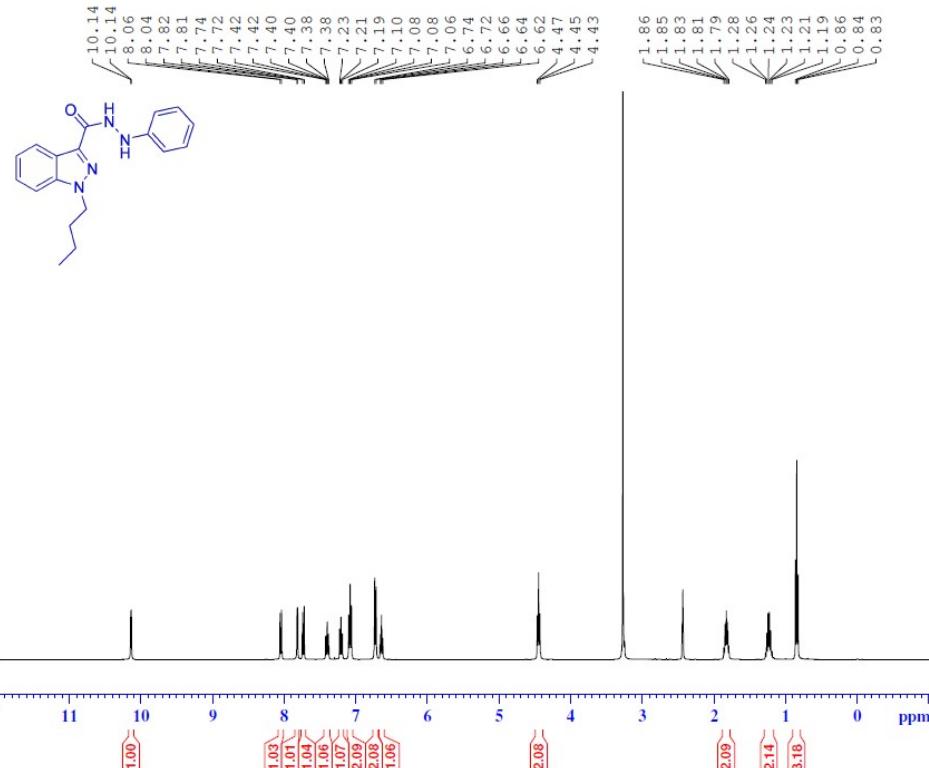


HRMS of N-(2-amino-4-nitrophenyl)-1-butyl-1H-indazole-3-carboxamide (8t).



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

Signature SIF VIT VELLORE
VG-027



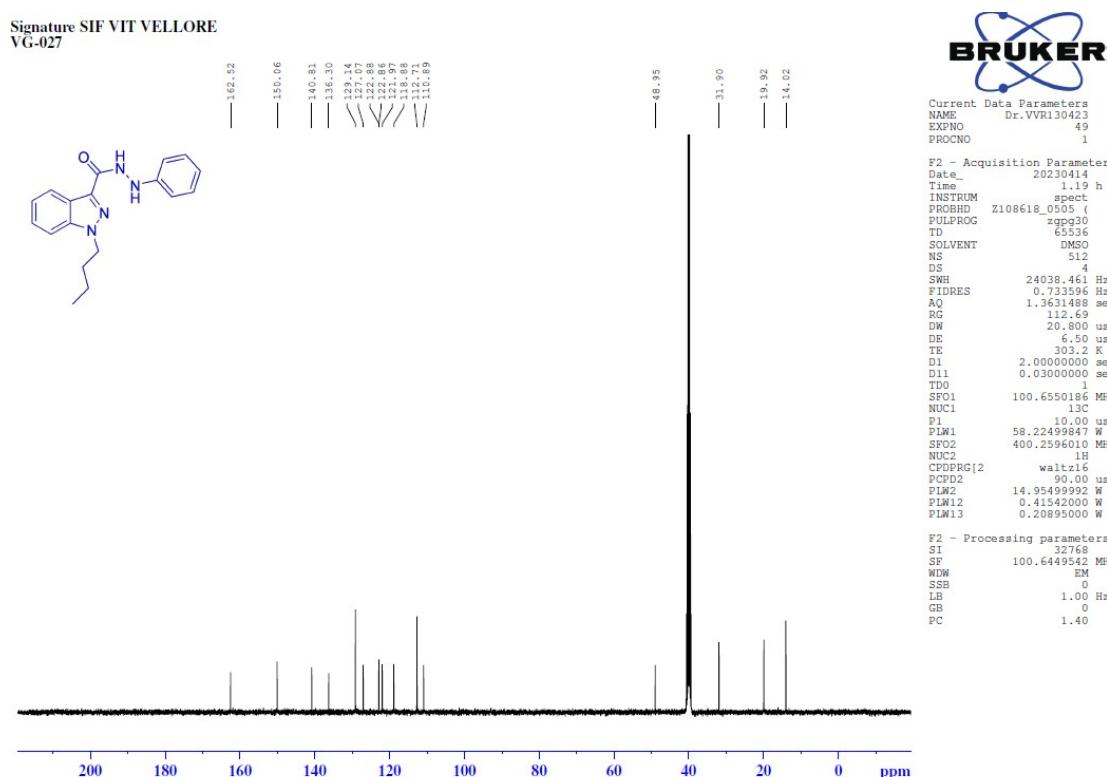
Current Data Parameters
NAME VG-027-8u
EXPNO 39
PROCNO 1

F2 - Acquisition Parameters
Date 20230411
Time 11:42 h
INSTRUM spect
PROBHD Z108618_0505_1
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.68 Hz
FIDRES 0.244532 Hz
AQ 4.0594465 sec
RG 127.79
DW 62.400 usec
DE 6.50 usec
TE 303.8 K
D1 1.0000000 sec
TD0 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

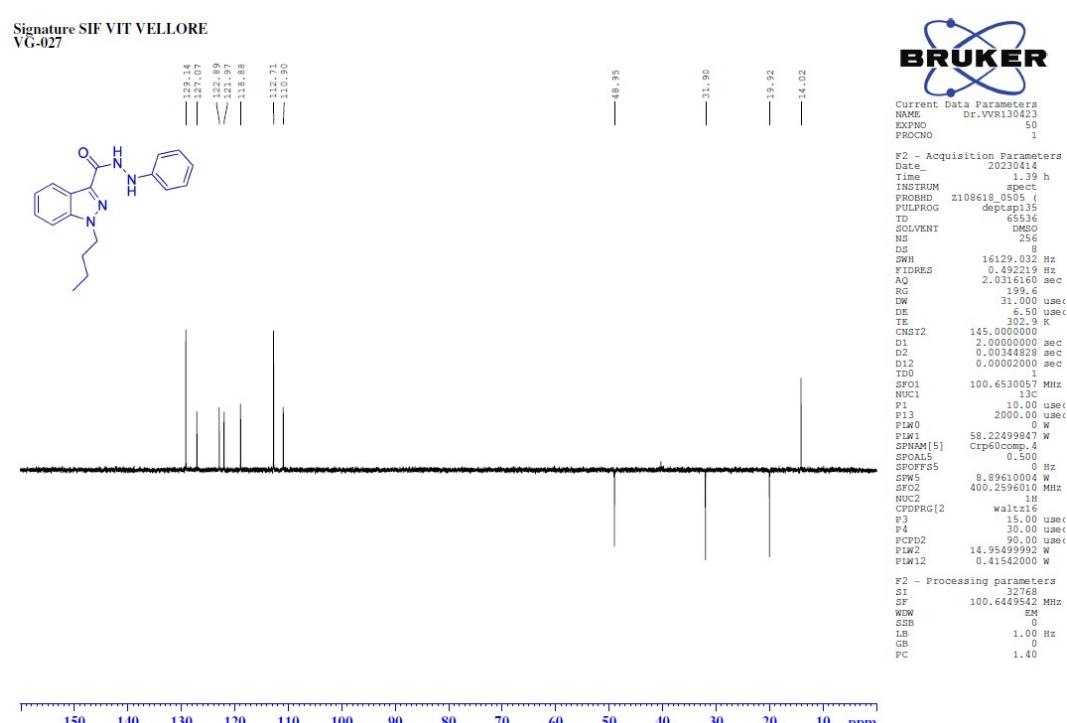
¹³C-NMR [100MHz, DMSO-d₆] spectrum of 1-butyl-N-phenyl-1H-indazole-3-carbohydrazide (8u).

Signature SIF VIT VELLORE
VG-027

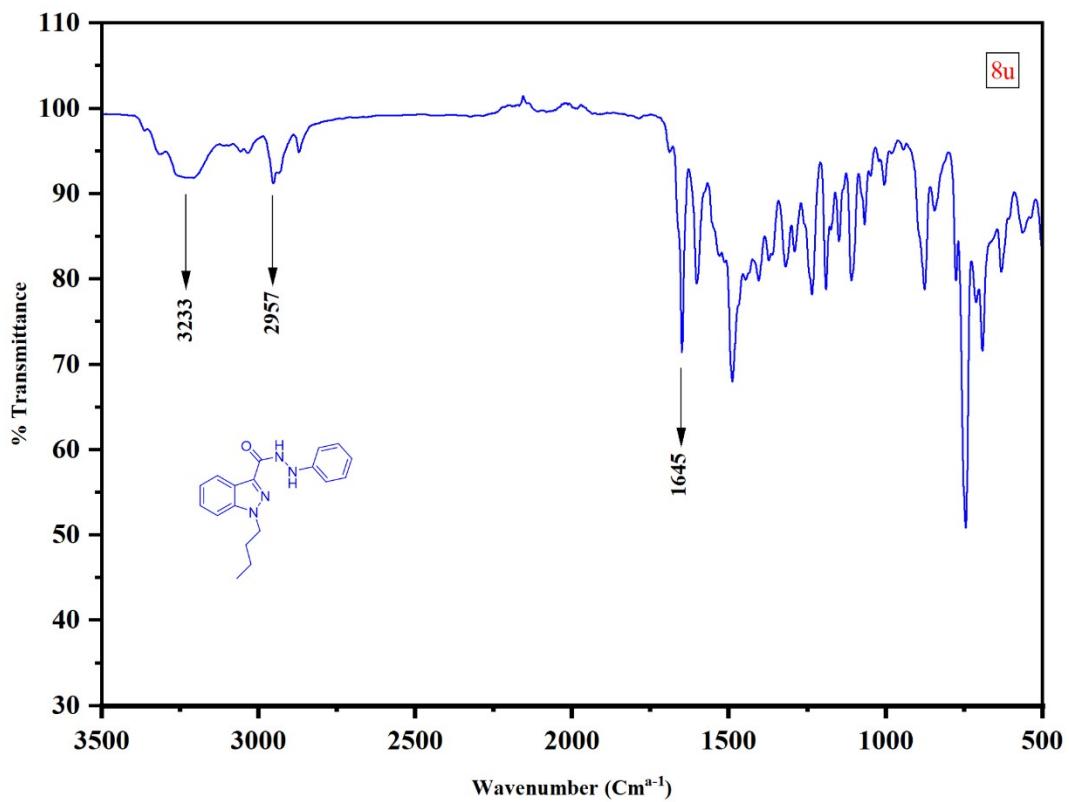


¹³⁵-DEPT-NMR [100MHz, DMSO-d₆] spectrum of 1-butyl-N-phenyl-1H-indazole-3-carbohydrazide (8u).

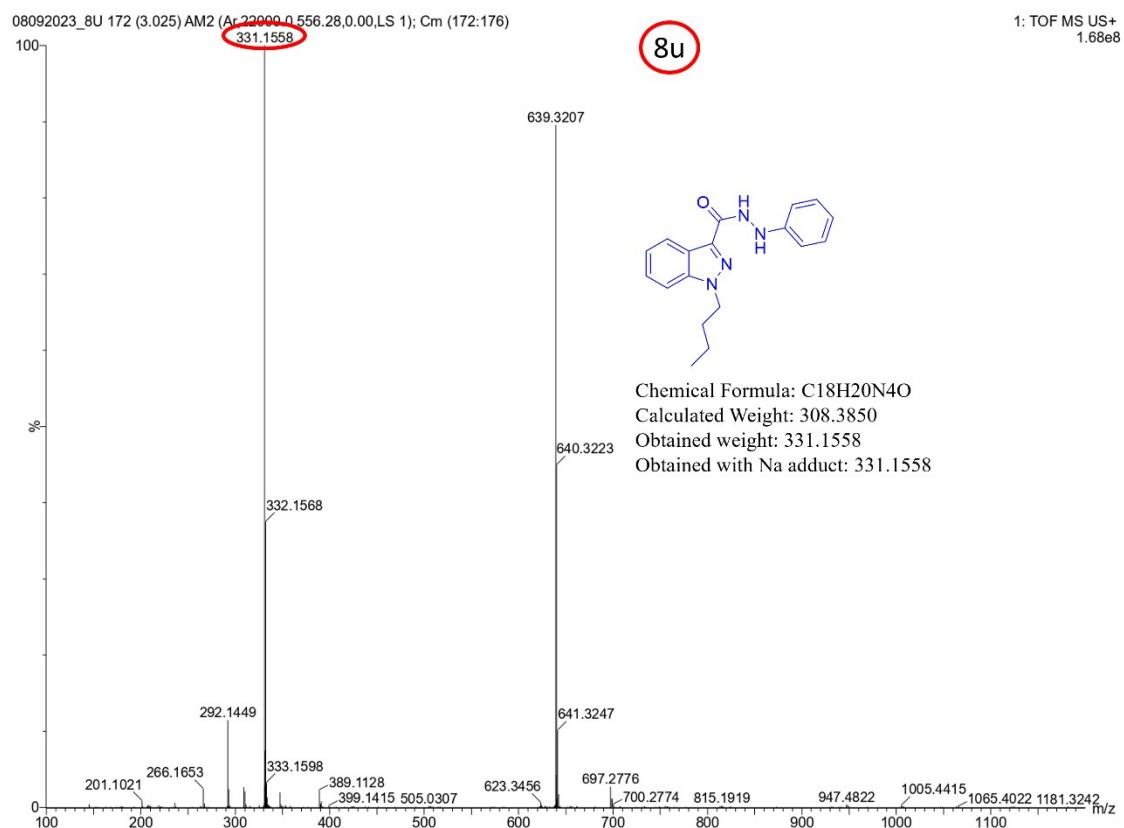
Signature SIF VIT VELLORE
VG-027



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

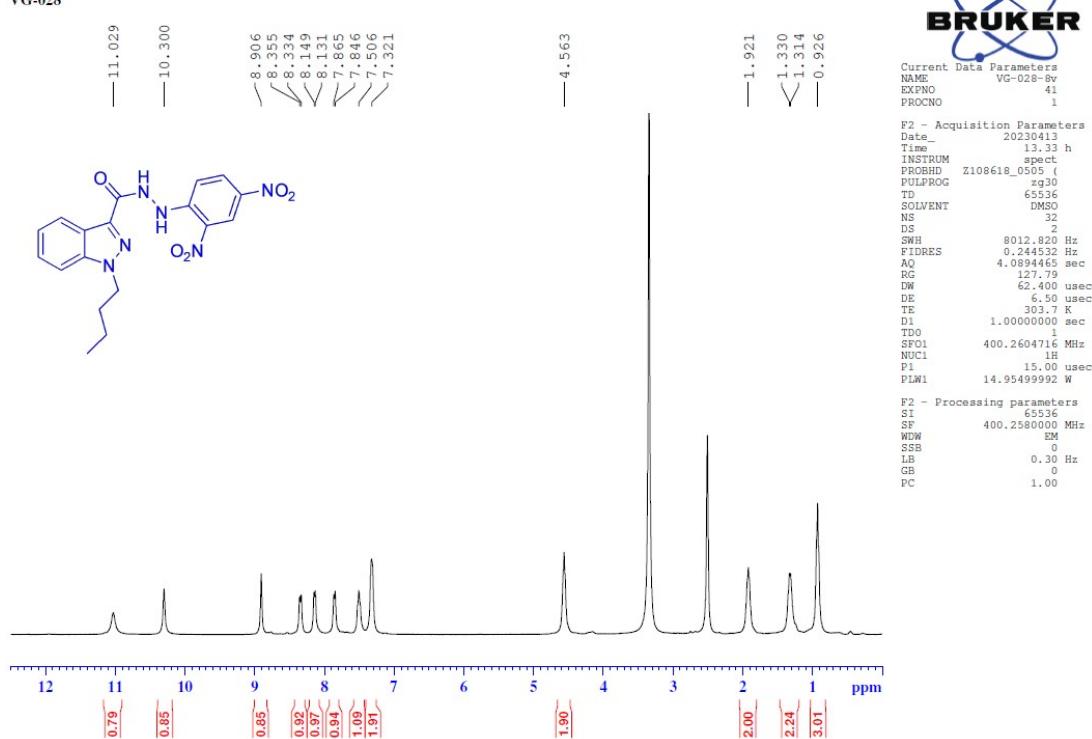


HRMS of 1-butyl-N-phenyl-1H-indazole-3-carbohydrazide (**8u**).



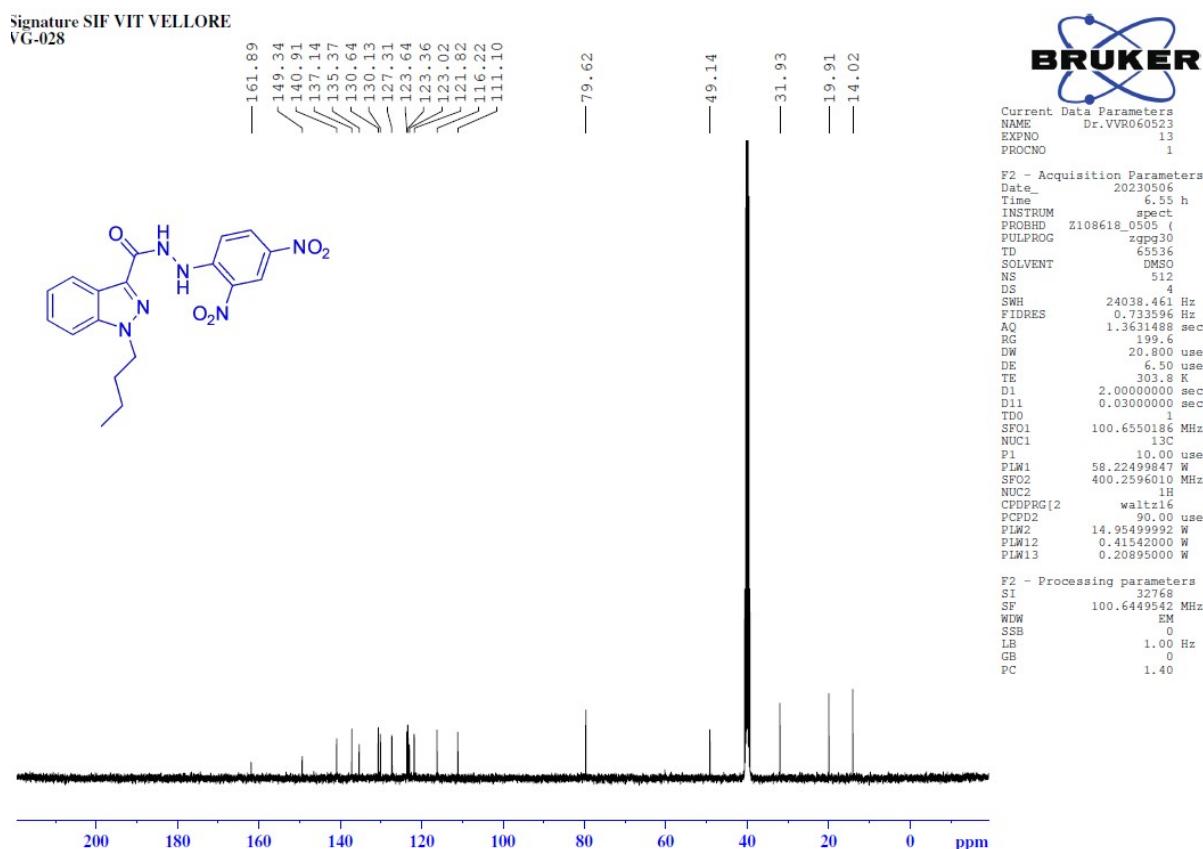
¹H-NMR [400MHz, DMSO-d₆] spectrum of 1-butyl-N-(2,4-dinitrophenyl)-1H-indazole-3-carbohydrazide (8v).

Signature SIF VIT VELLORE
VG-028



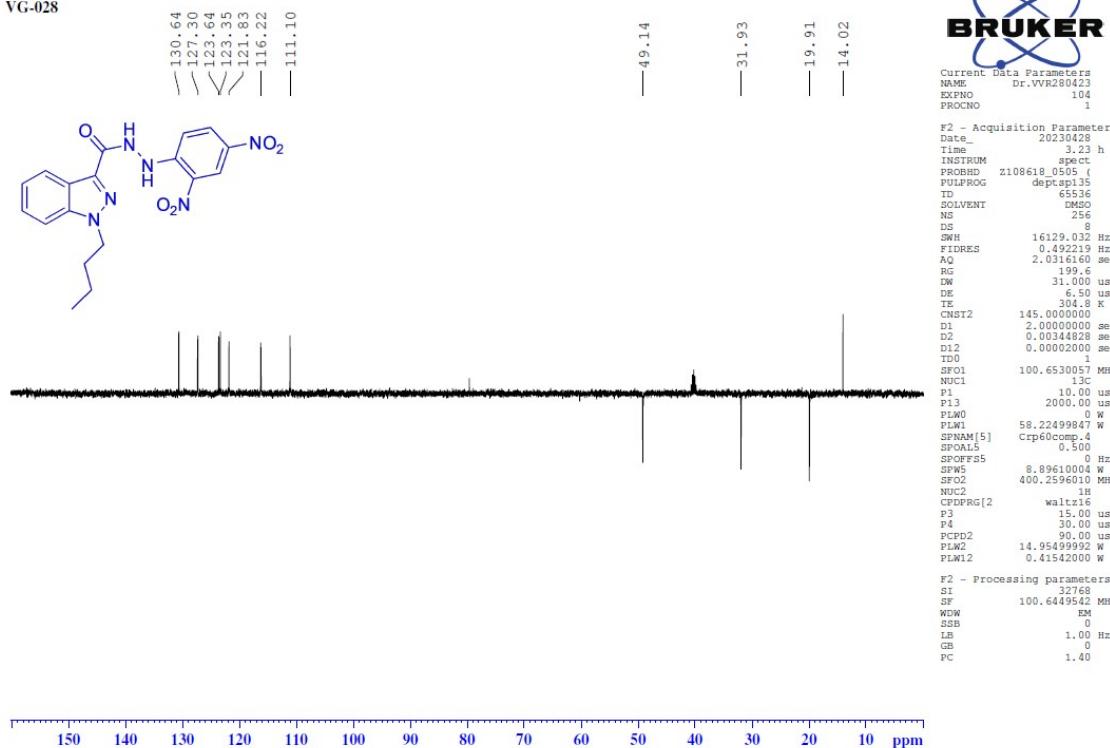
¹³C-NMR [100MHz, DMSO-d₆] spectrum of 1-butyl-N-(2,4-dinitrophenyl)-1H-indazole-3-carbohydrazide (8v).

Signature SIF VIT VELLORE
VG-028

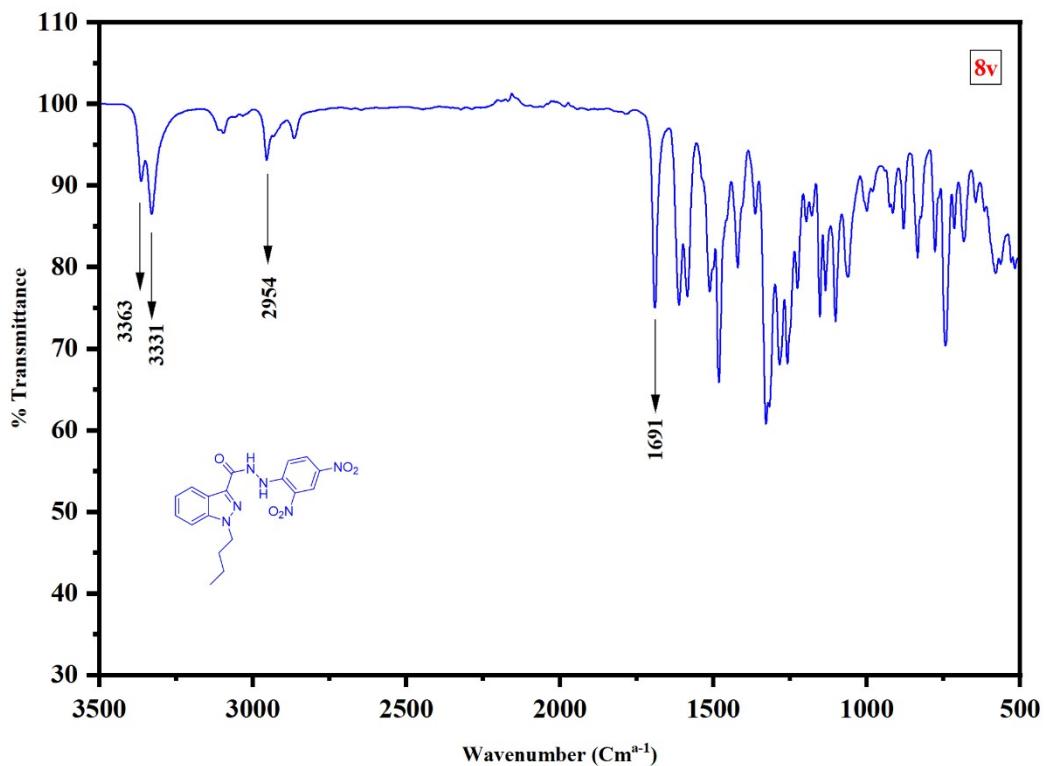


¹³⁵-DEPT-NMR [100MHz, DMSO-d₆] spectrum of 1-butyl-N-(2,4-dinitrophenyl)-1H-indazole-3-carbohydrazide (8v).

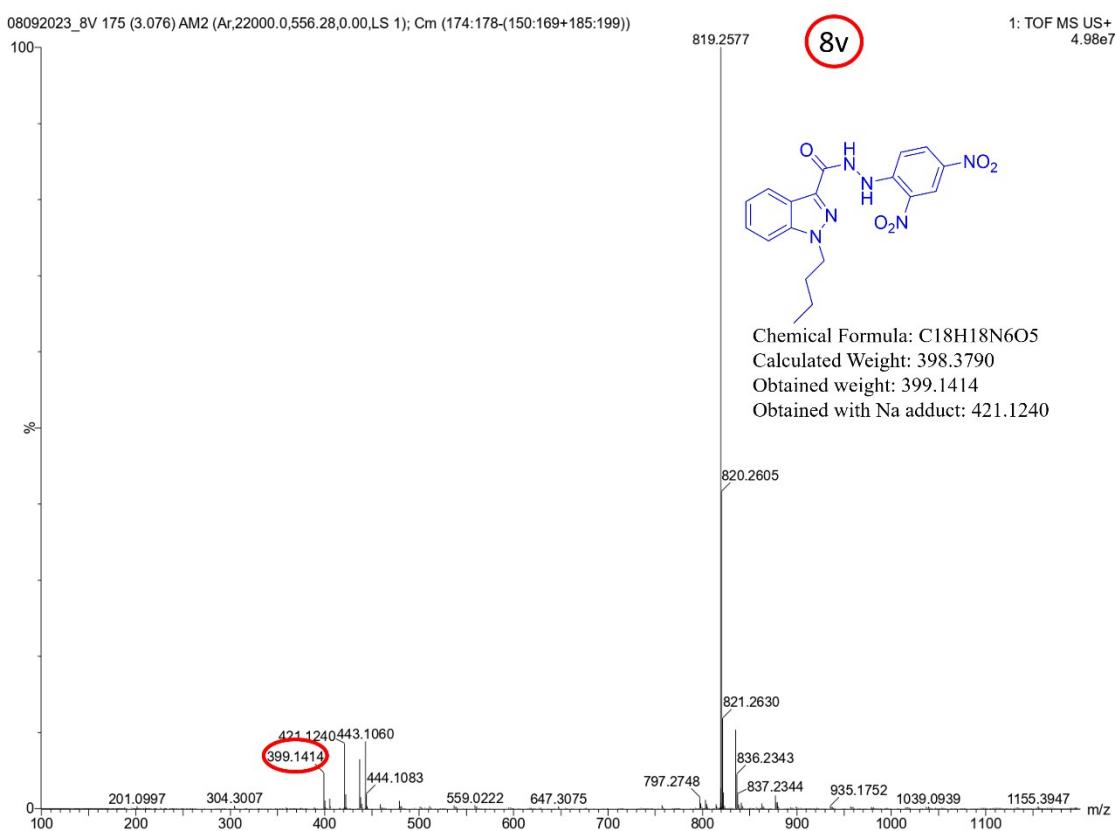
Signature SIF VIT VELLORE
VG-028



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

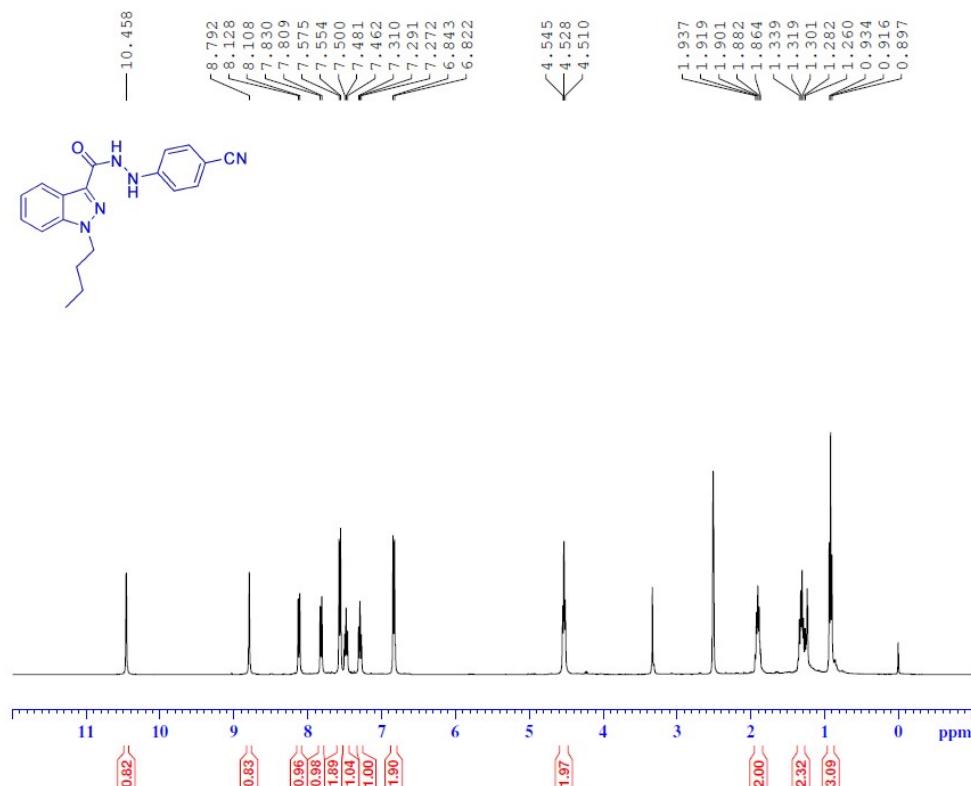


HRMS of 1-butyl-N-(2,4-dinitrophenyl)-1H-indazole-3-carbohydrazide (8v).



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

Signature SIF VIT VELLORE
VG-030



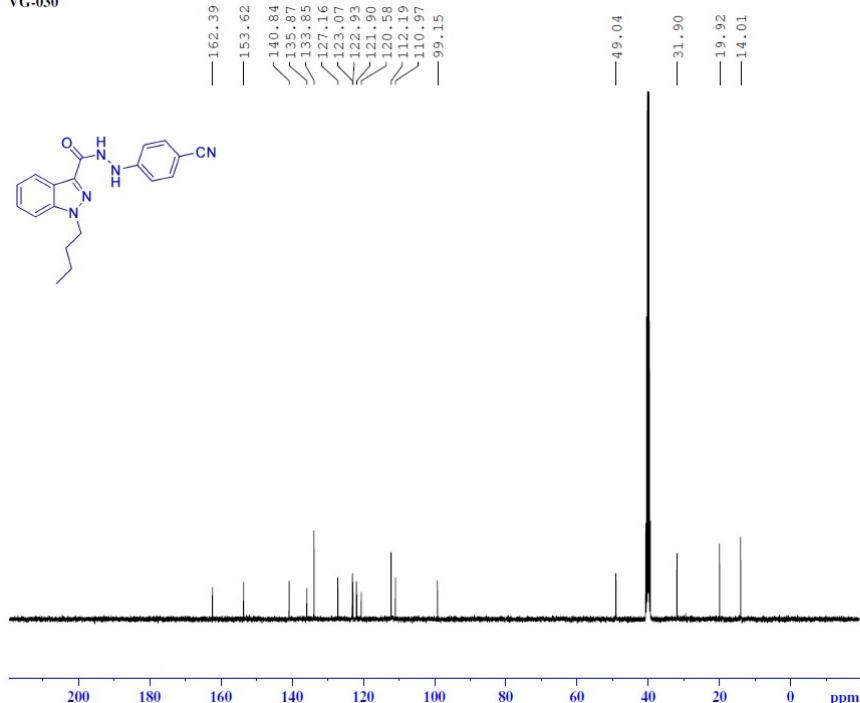
Current Data Parameters
NAME VG-30_8w
EXPNO 77
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230419
Time 10:30 h
INSTRUM spect
PROBHD Z108618_0505_1
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.24452 Hz
AQ 4.089446 sec
RG 127.79
DW 62.400 usec
DE 6.50 usec
TE 304.3 K
D1 1.0000000 sec
TDO 1
SF01 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PLW1 14.9549992 W

F2 - Processing parameters
SI 65536
SF 400.2580003 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-cyanophenyl)-1H-indazole-3-carbohydrazide (8W).

Signature SIF VIT VELLORE
VG-030



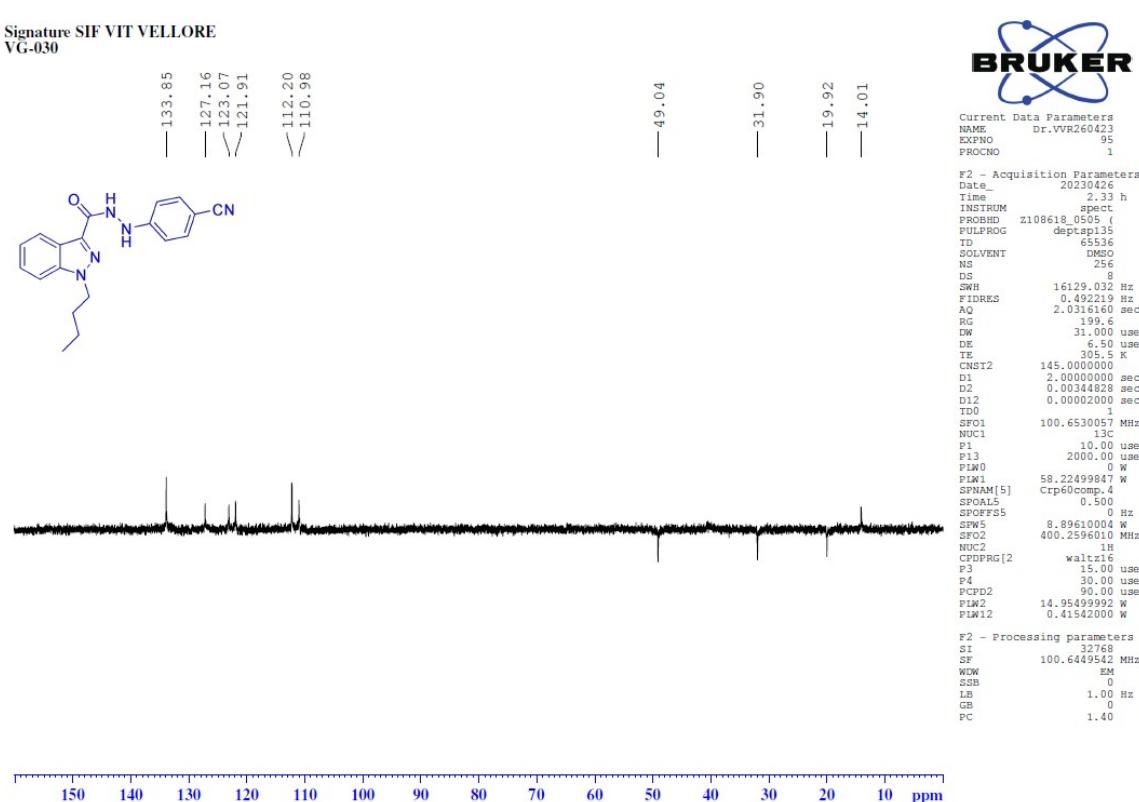
Current Data Parameters
NAME Desktop
EXPNO 88
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230422
Time 20:07 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 1.363100 sec
RG 199.6
DW 20.800 usec
DE 6.50 usec
TE 304.8 K
D1 2.0000000 sec
D11 0.03000000 sec
TDO 1
SF01 100.6550186 MHz
NUC1 13C
P1 10.00 usec
PLW1 58.22499847 W
SF02 400.2596010 MHz
NUC2 1H
CPDPG[2 1.0000000 sec
CPDQ2 90.00 usec
PLW2 14.95499992 W
PLW12 0.41542000 W
PLW13 0.20895000 W

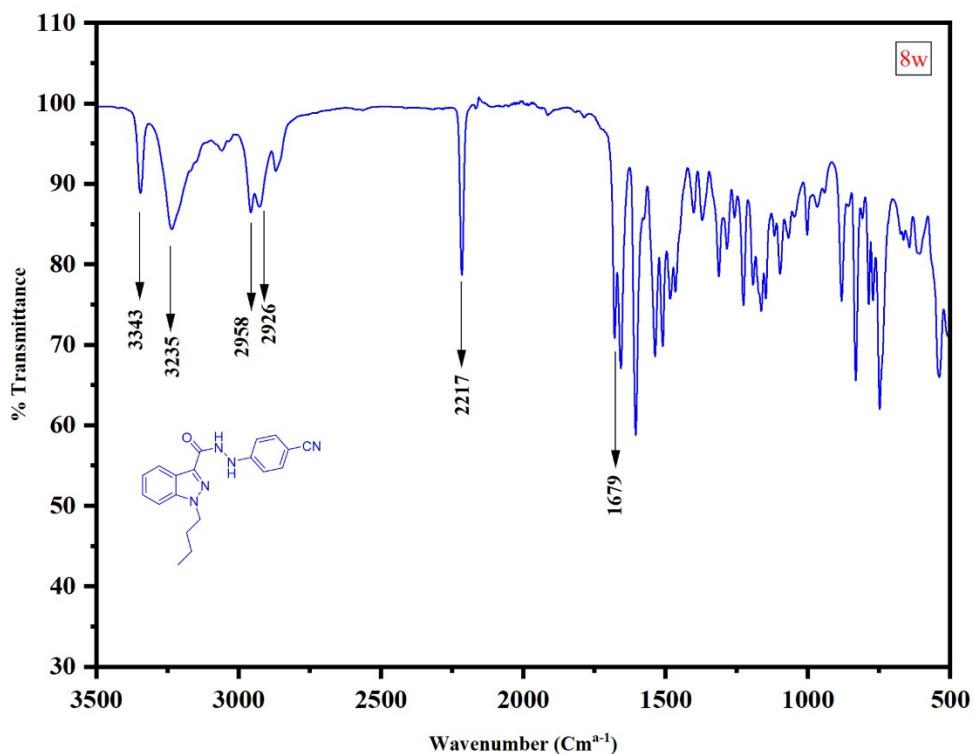
F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

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

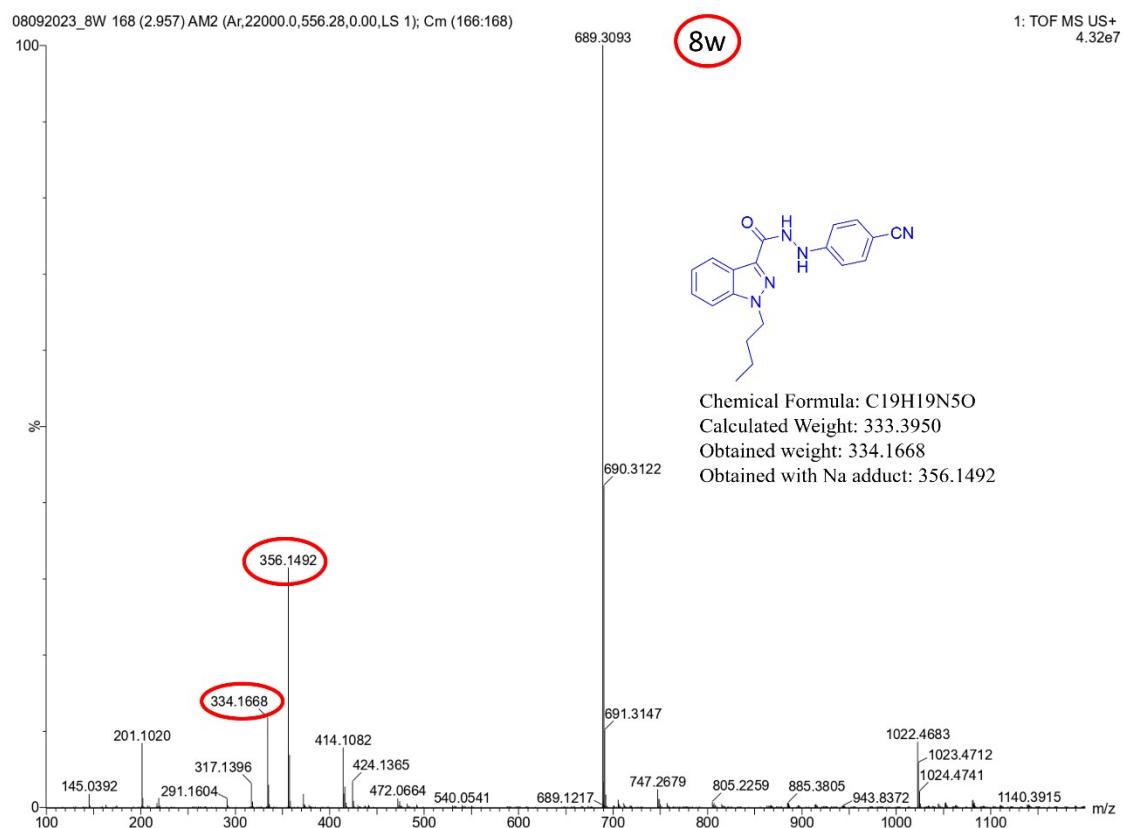
Signature SIF VIT VELLORE
VG-030



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

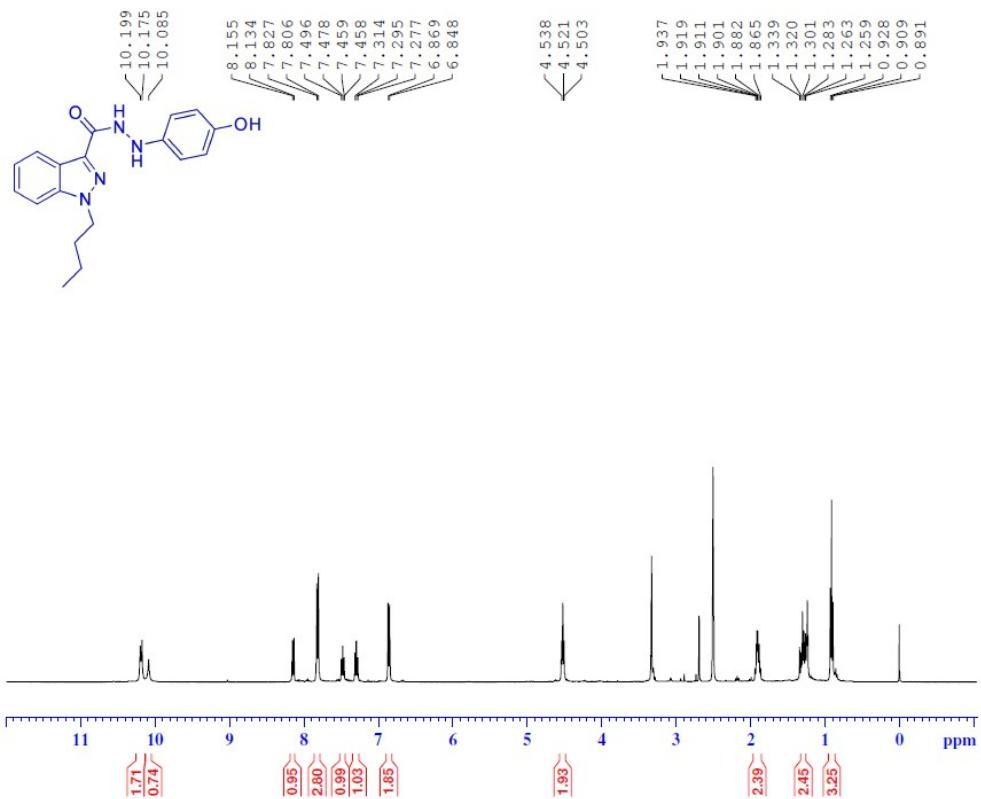


HRMS of 1-butyl-N-(4-cyanophenyl)-1H-indazole-3-carbohydrazide (8W).



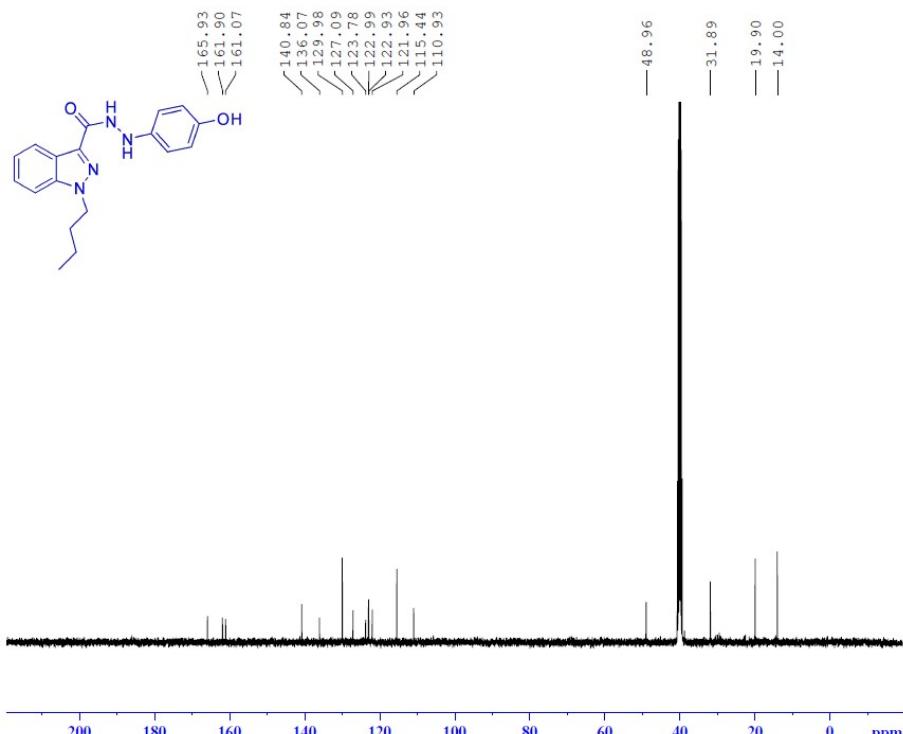
¹H-NMR [400MHz, DMSO-d₆] spectrum of 1-butyl-N-(4-hydroxyphenyl)-1H-indazole-3-carbohydrazide (8x).

Signature SIF VIT VELLORE
VG-031



¹H-NMR [100MHz, 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).



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

F2 - Acquisition Parameters
Date 20230419
Time 19.36 h
INSTRUM spect
PROBHD Z108618_0505 (bruker)
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 143
DW 62.400 usec
DE 6.50 usec
TE 304.3 K
D1 1.0000000 sec
TD0 1
SF01 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PLW1 14.95499992 W

F2 - Processing parameters
SI 65536
SF 400.258022 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

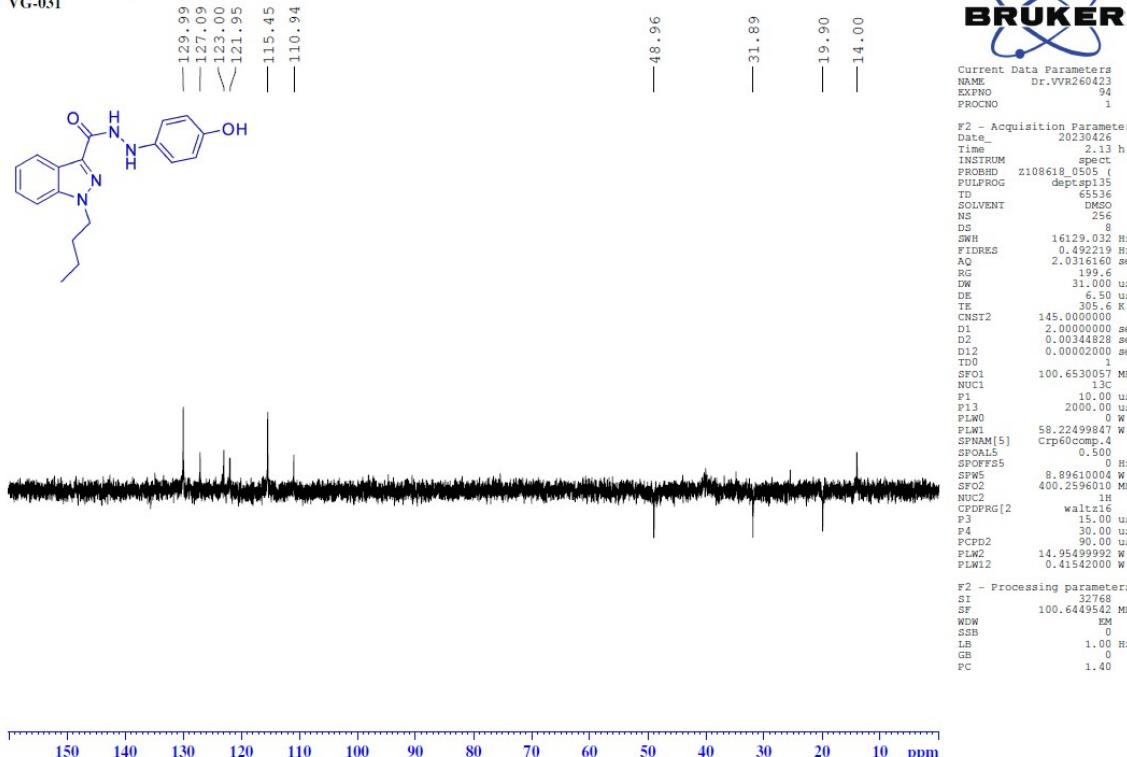


Current Data Parameters
NAME Desktop
EXPNO 87
PROCNO 1

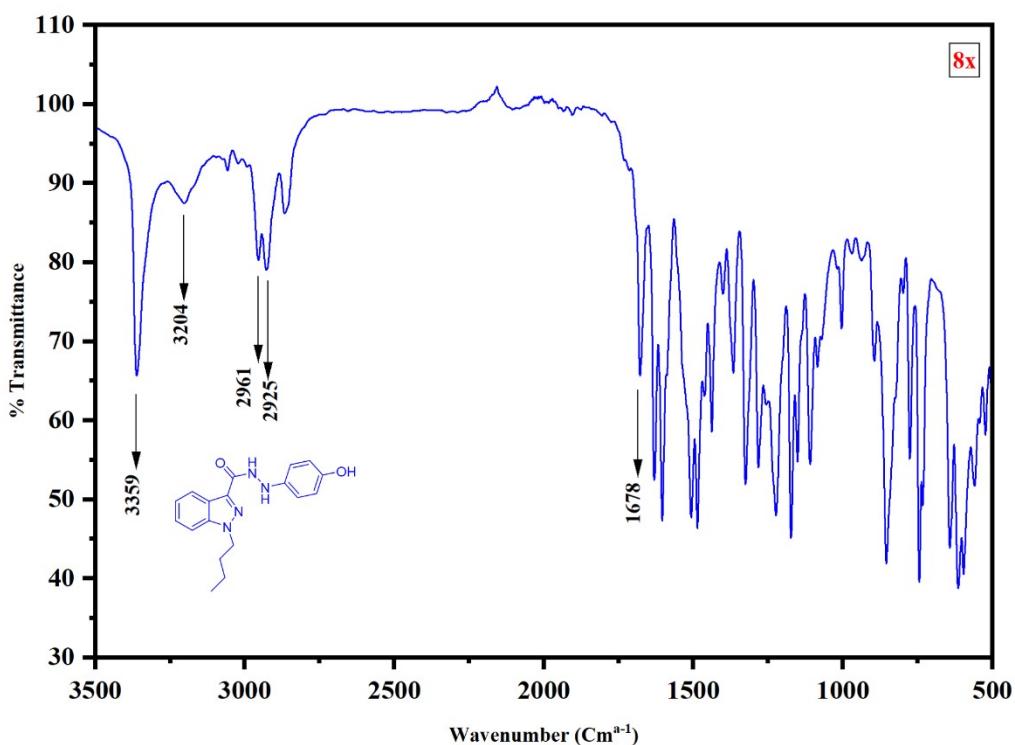
F2 - Acquisition Parameters
Date 20230422
Time 19.36 h
INSTRUM spect
PROBHD Z108618_0505 (bruker)
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 199.6
DW 20.800 usec
DE 6.50 usec
TE 304.3 K
D1 2.0000000 sec
D11 0.03000000 sec
TD0 1
SF01 100.6550186 MHz
NUC1 13C
P1 10.00 usec
PLW1 58.22499847 W
SF02 400.2596010 MHz
NUC2 1H
CPDPG[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

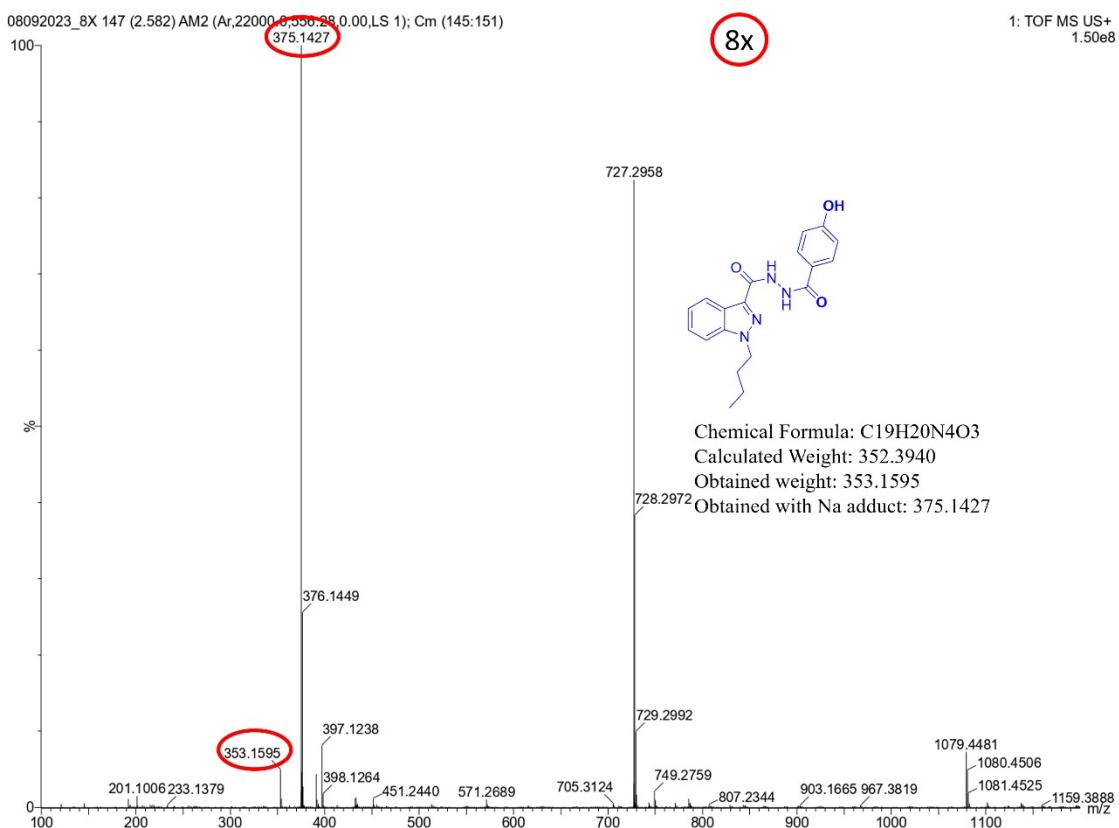
Signature SIF VIT VELLORE
VG-031



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

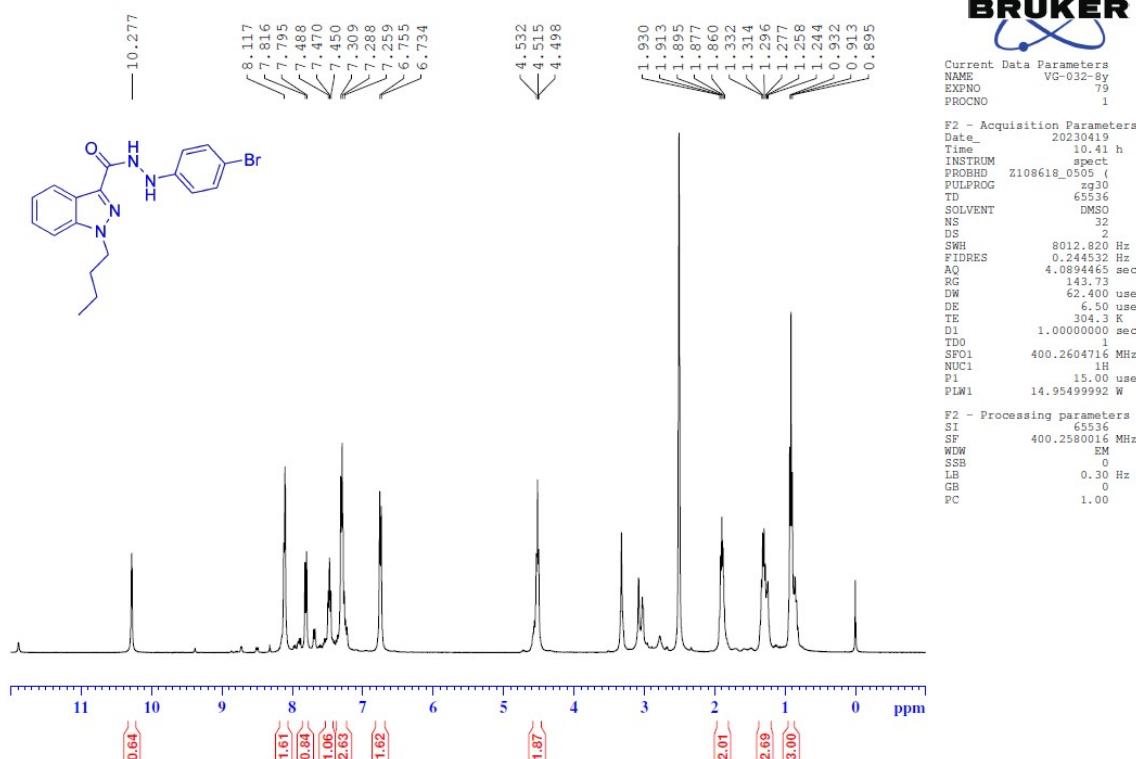


HRMS of 1-butyl-N-(4-hydroxyphenyl)-1H-indazole-3-carbohydrazide (8x).



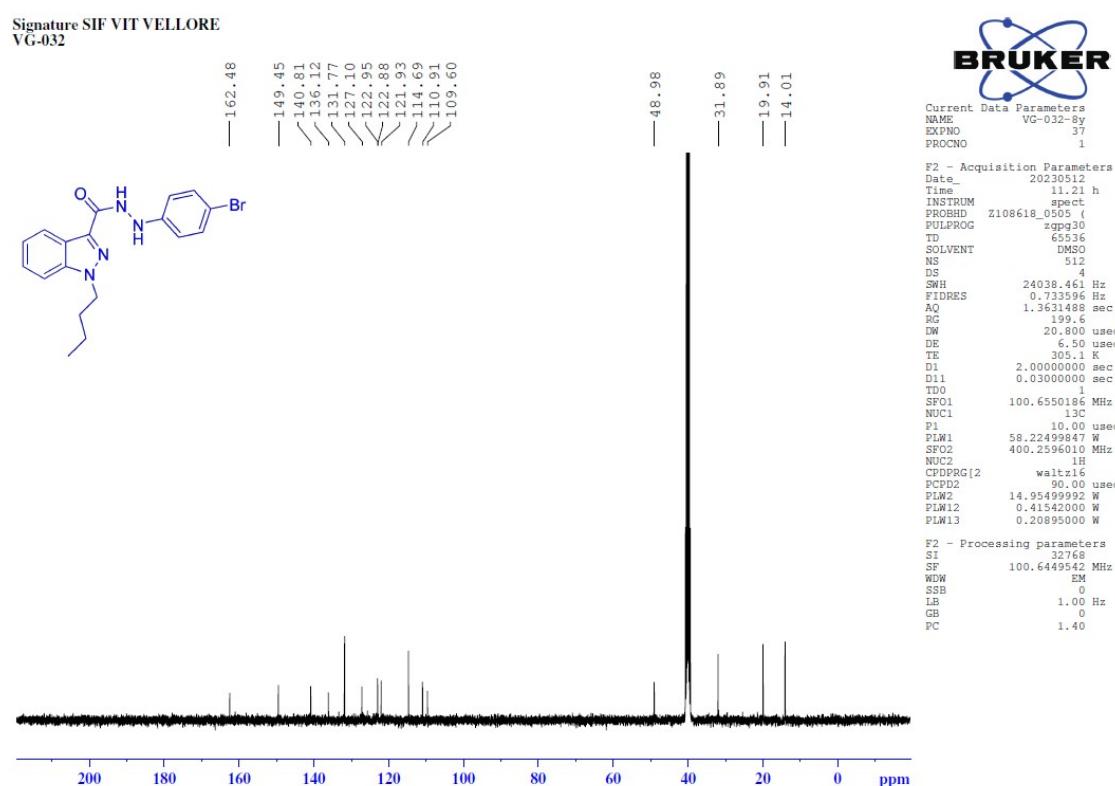
¹H-NMR [400MHz, DMSO-d₆] spectrum of N-(4-bromophenyl)1butyl-1H-indazole-3-carbohydrazide (8y).

Signature SIF VIT VELLORE
 VG-032



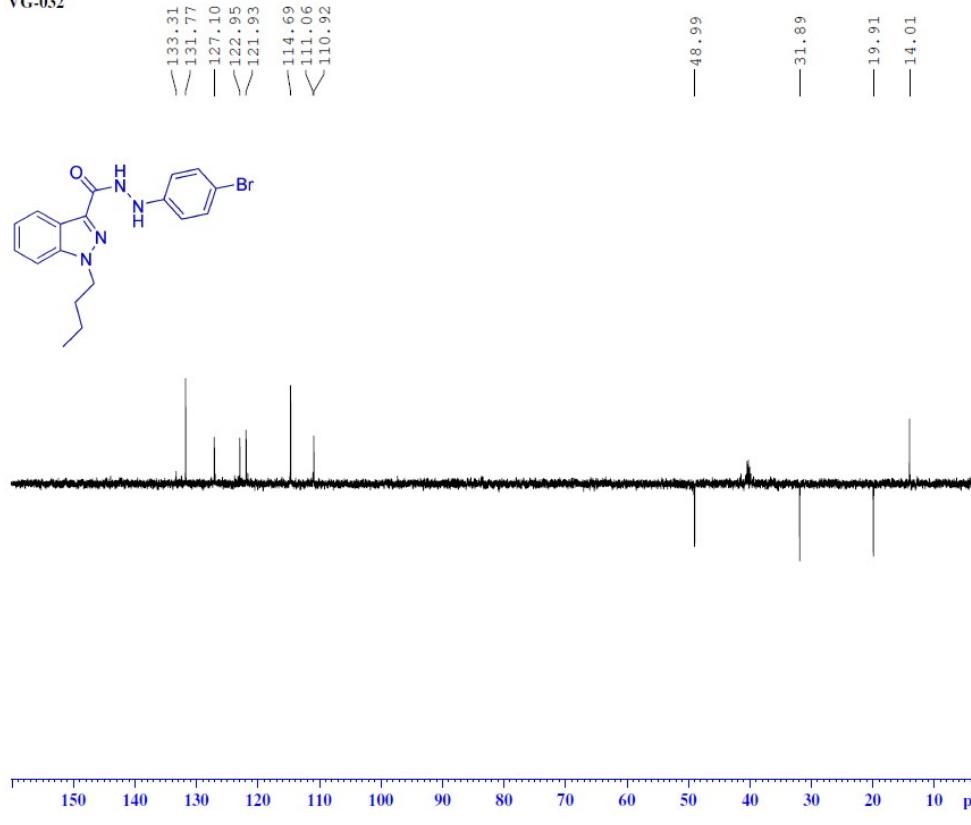
¹³C-NMR [100MHz, DMSO-d₆] spectrum of N-(4-bromophenyl)1butyl-1H-indazole-3-carbohydrazide (8y).

Signature SIF VIT VELLORE
VG-032

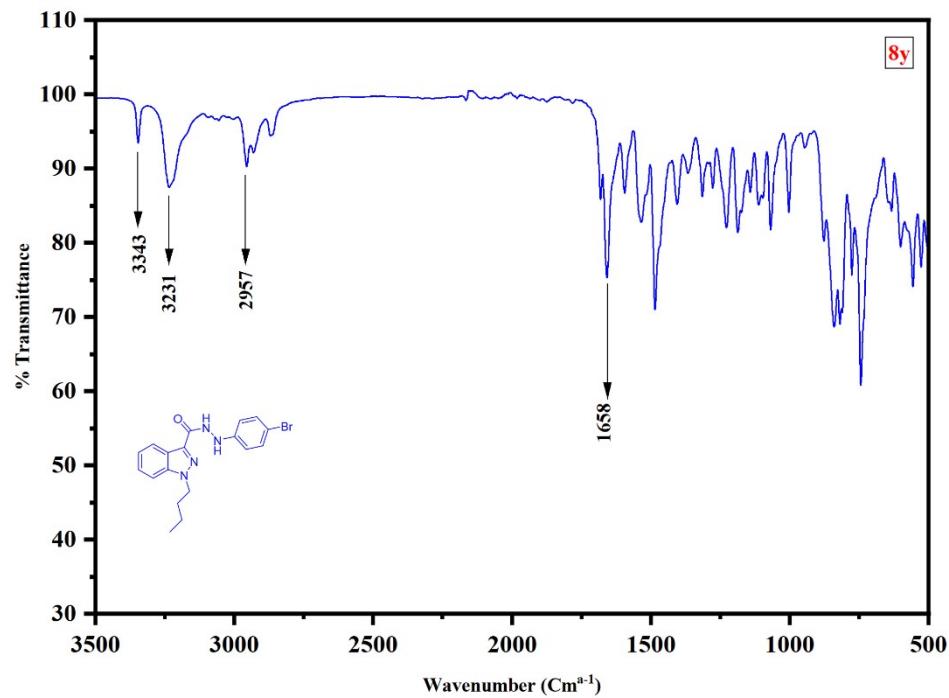


¹³⁵-DEPT-NMR [100MHz, DMSO-d₆] spectrum of N-(4-bromophenyl)1butyl-1H-indazole-3-carbohydrazide (8y).

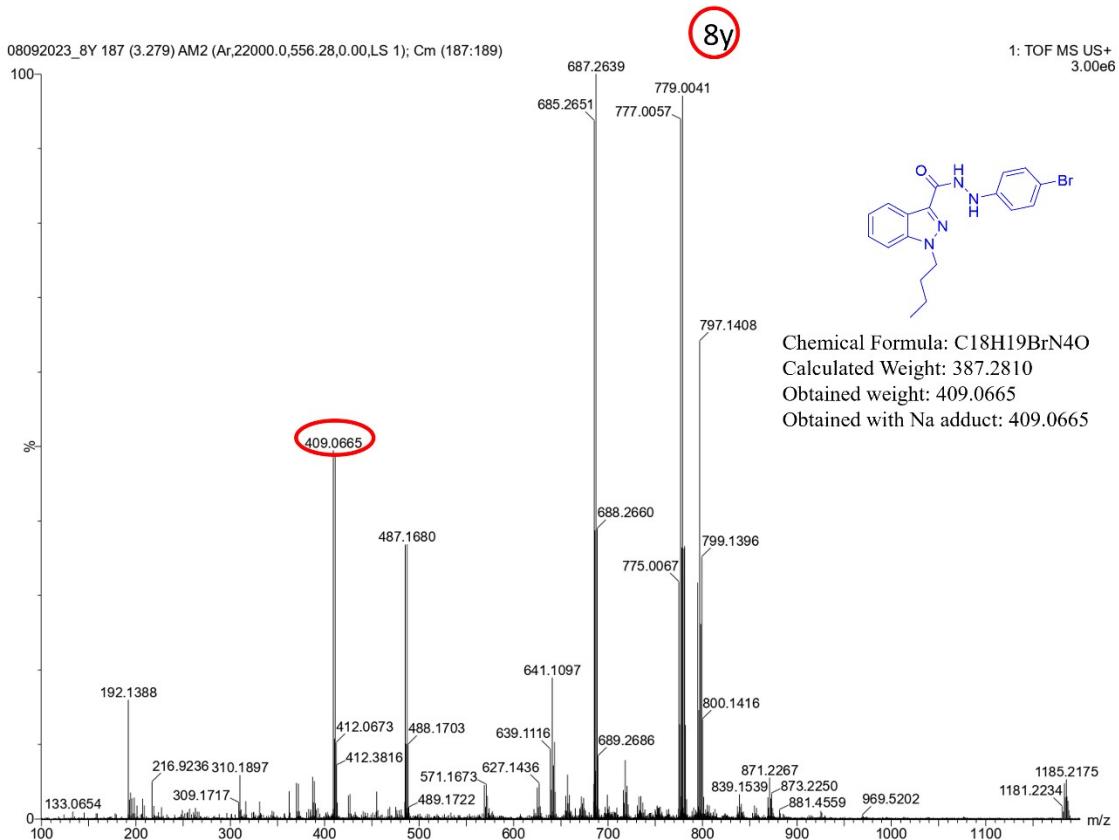
Signature SIF VIT VELLORE
VG-032



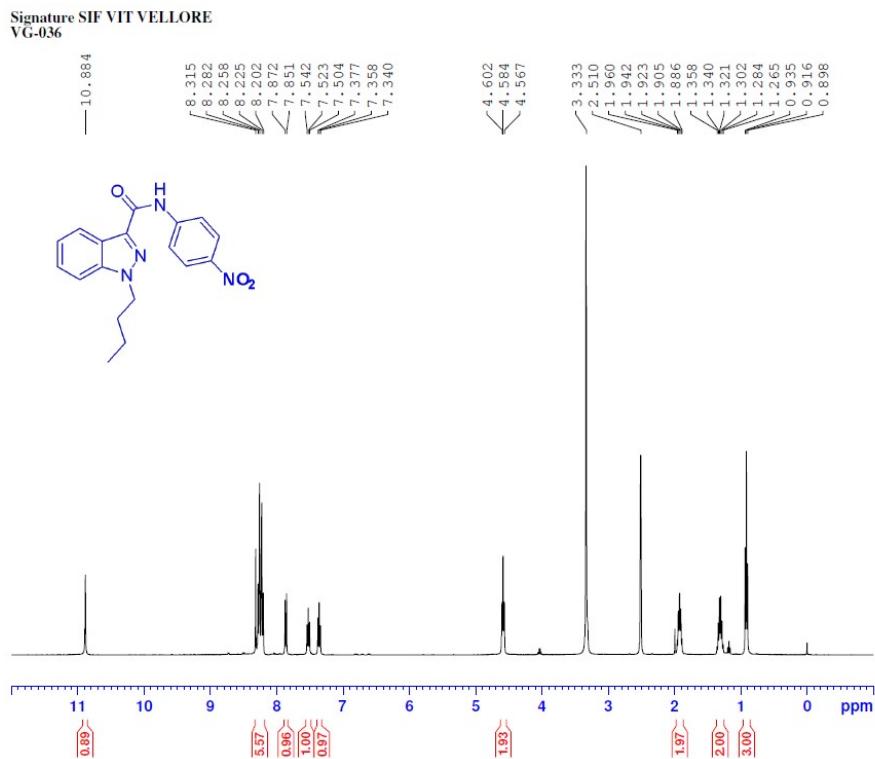
FT-IR spectrum of N-(4-bromophenyl)1butyl-1H-indazole-3-carbohydrazide (8y).



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

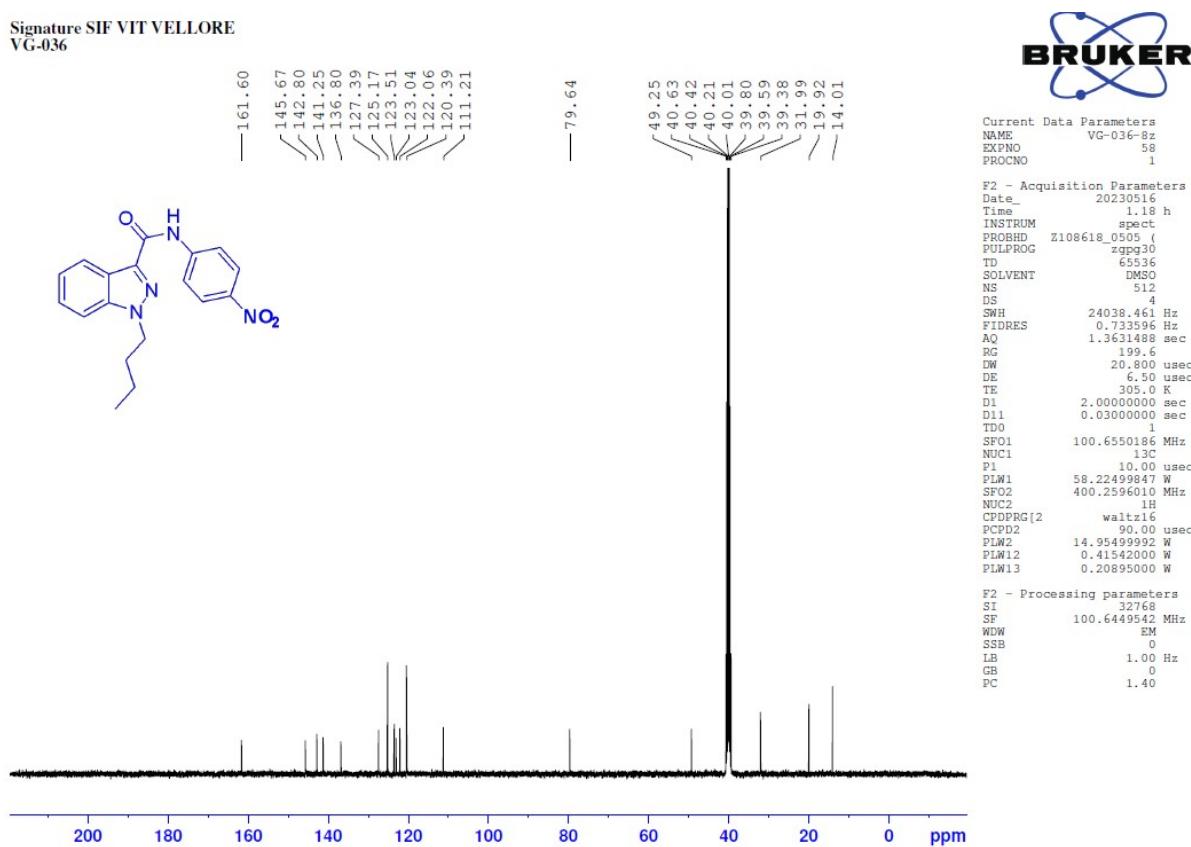


¹H-NMR [400MHz, DMSO-d₆] 1-Butyl-1H-indazole-3-carboxylic acid to 1-butyl-N-(4-nitrophenyl)-1H-indazole-3-carboxamide (8z).



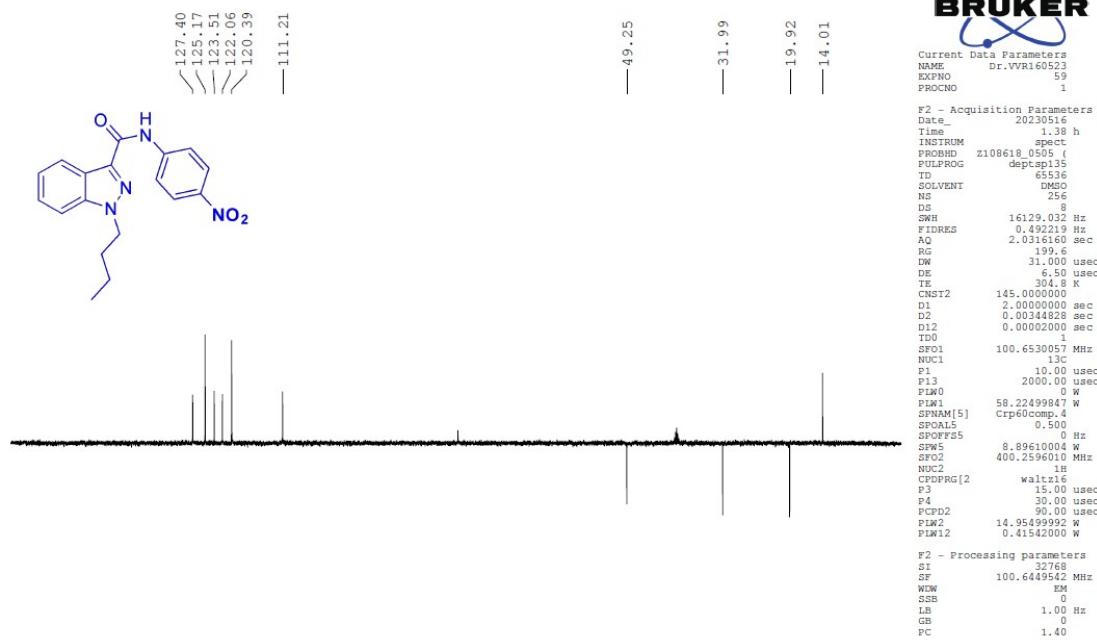
¹³C-NMR [100MHz, DMSO-d₆] 1-Butyl-1H-indazole-3-carboxylic acid to 1-butyl-N-(4-nitrophenyl)-1H-indazole-3-carboxamide (8z).

**Signature SIF VIT VELLORE
VG-036**

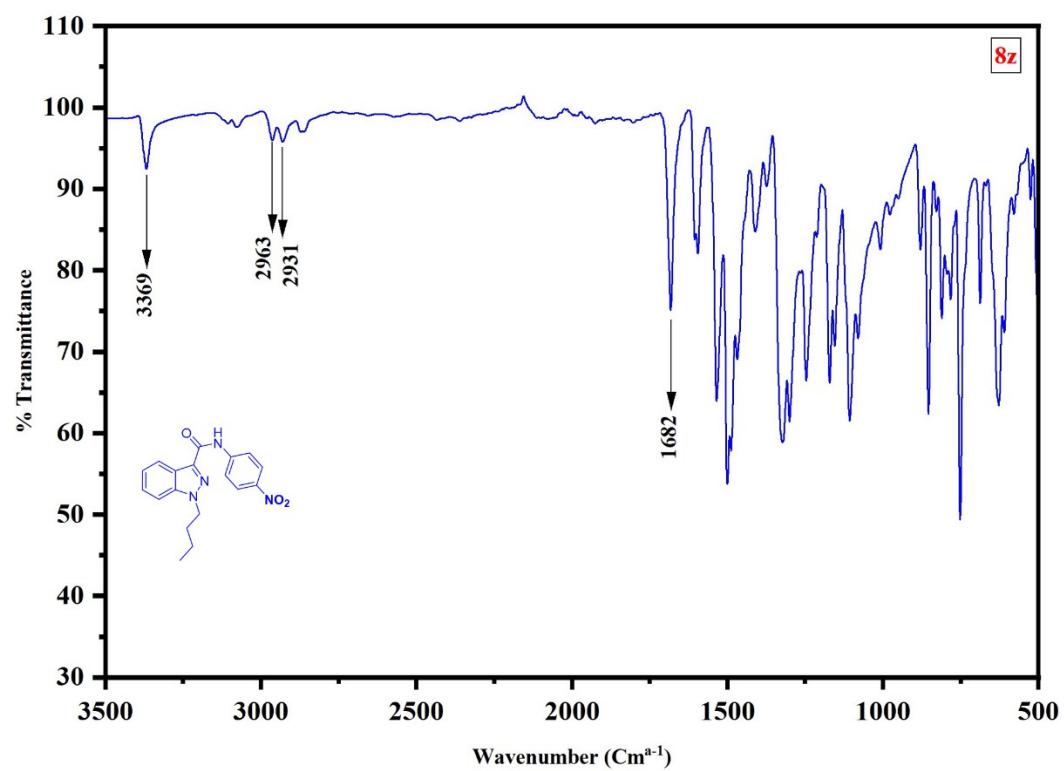


¹³⁵C-NMR [100MHz, DMSO-d₆] 1-Butyl-1H-indazole-3-carboxylic acid to 1-butyl-N-(4-nitrophenyl)-1H-indazole-3-carboxamide (8z).

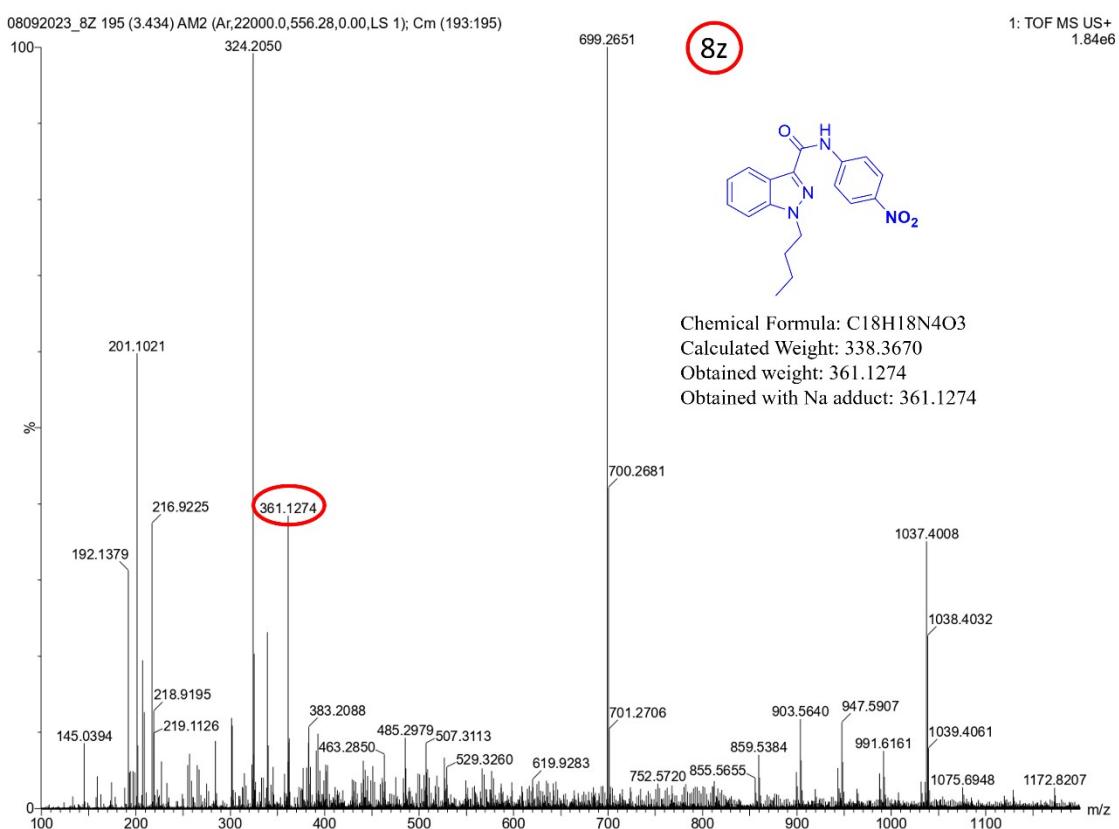
**Signature SIF VIT VELLORE
VG-036**



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).



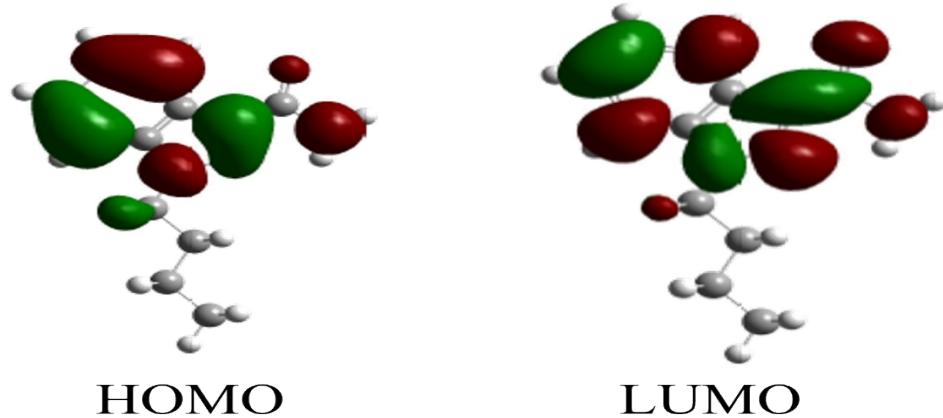
5.DFT studies indazole derivatives with HOMO and LUMO values

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

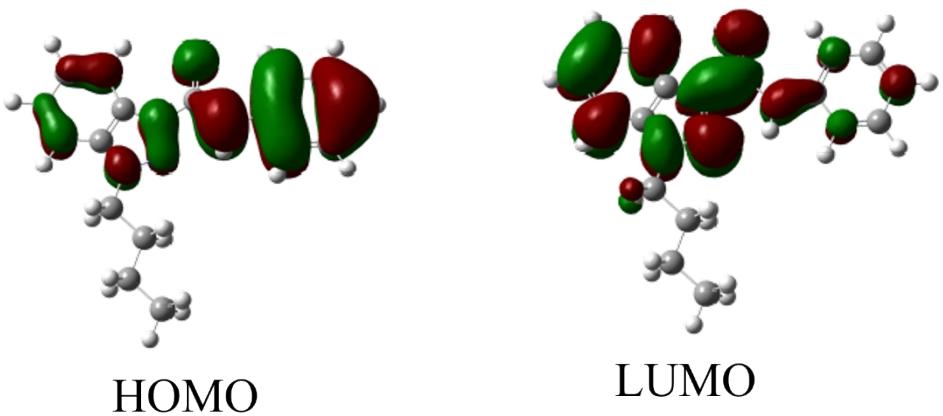
11	8k	-5.23692	-0.92853	4.30839
12	8l	-5.44563	-1.05111	4.39452
13	8m	-5.41485	-1.07244	4.34241
14	8n	-5.67216	-1.00143	4.67073
15	8o	-5.11137	-1.0287	4.08267
16	8p	-5.5039	-1.15128	4.35262
17	8q	-5.21937	-0.92529	4.29408
18	8r	-5.47317	-1.14426	4.32891
19	8s	-6.34878	-1.4283	4.92048
20	8t	-5.27715	-2.60523	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)

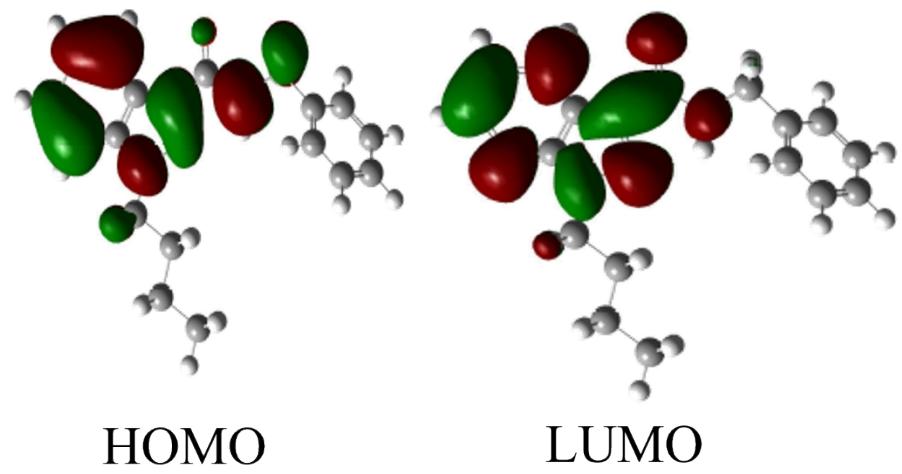
8a



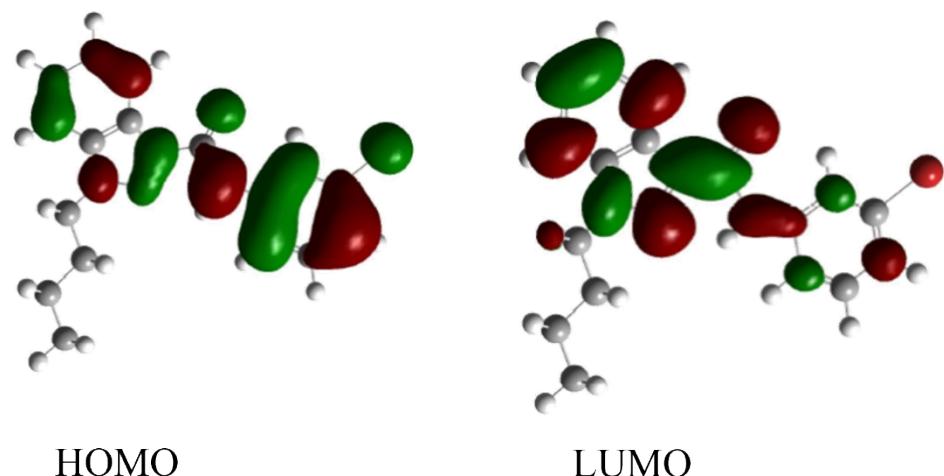
8b



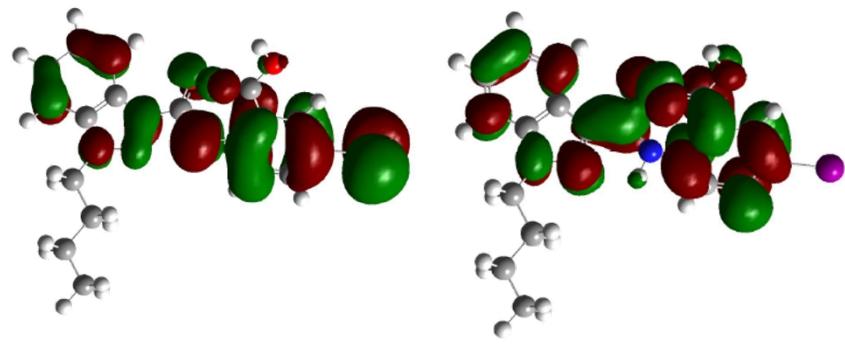
8c



8d



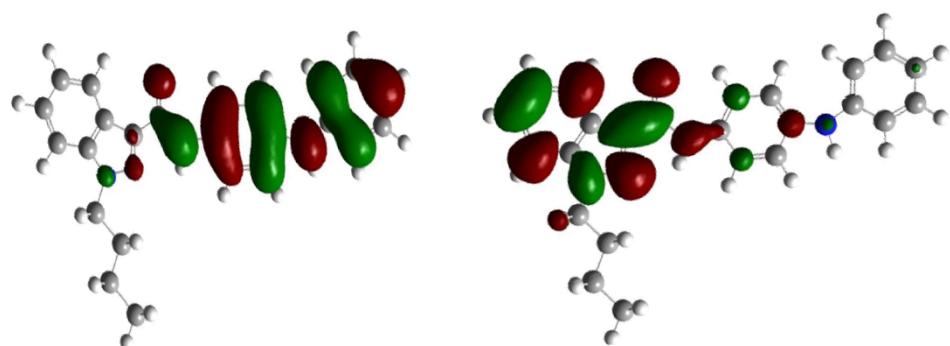
8e



HOMO

LUMO

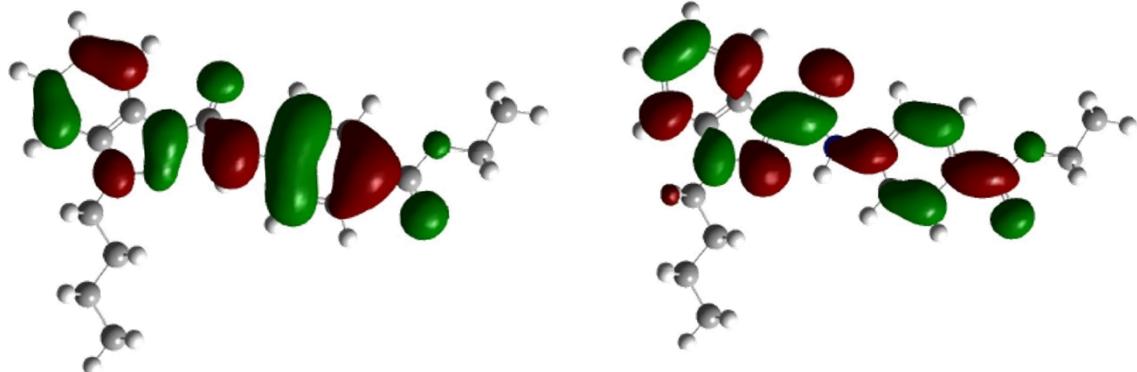
8f



HOMO

LUMO

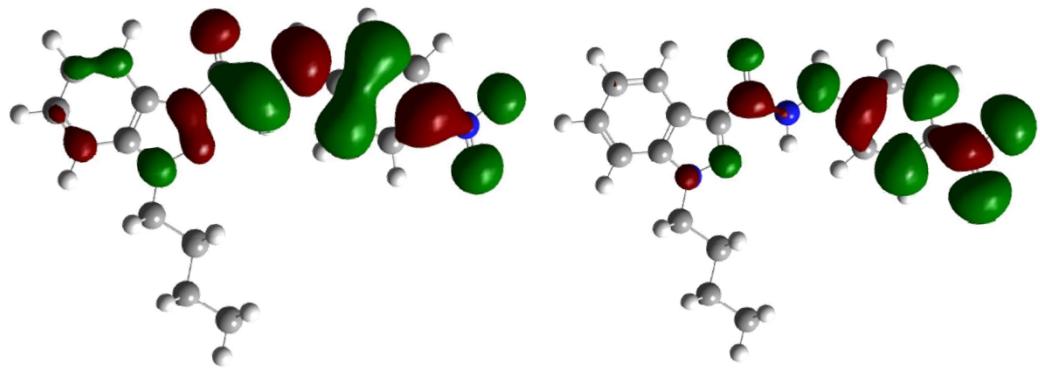
8g



HOMO

LUMO

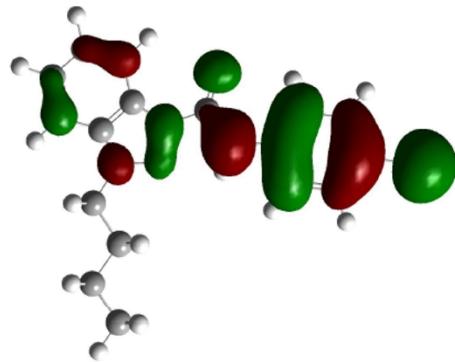
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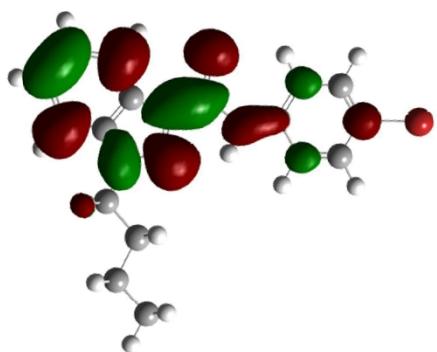
HOMO

LUMO

8i

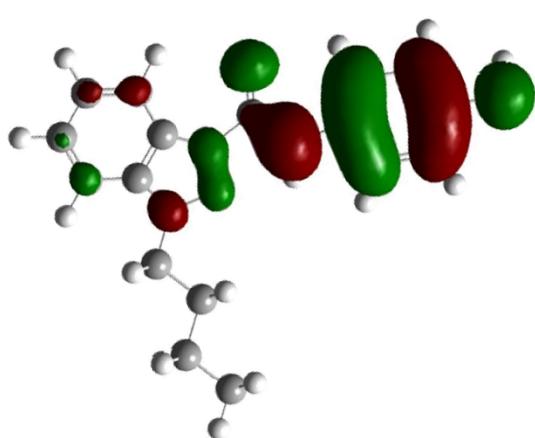


HOMO

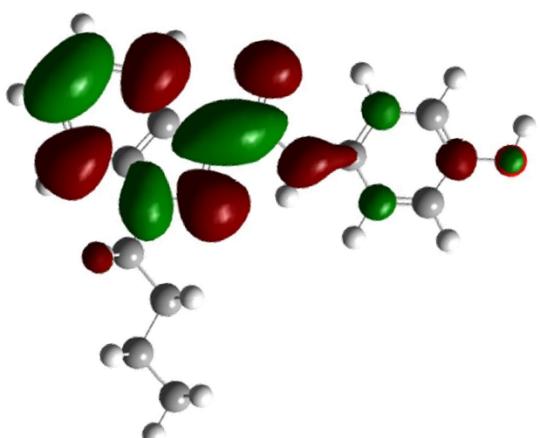


LUMO

8j

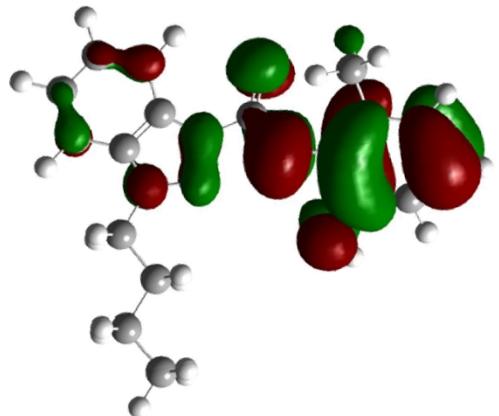


HOMO

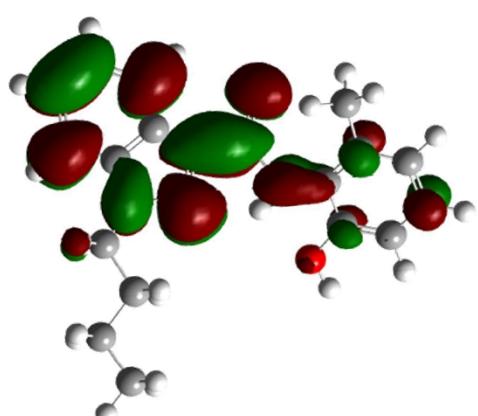


LUMO

8k

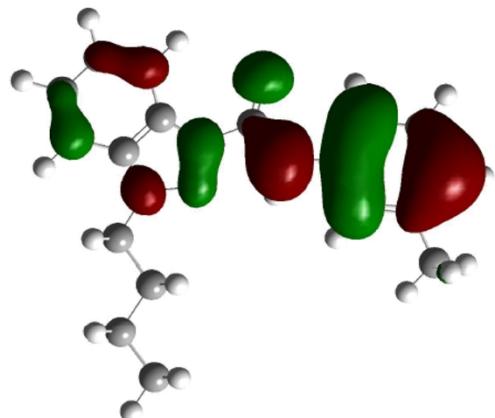


HOMO

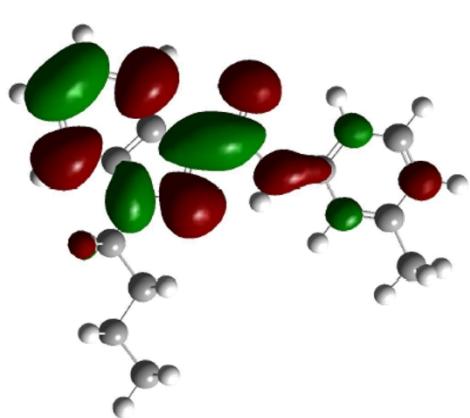


LUMO

8l

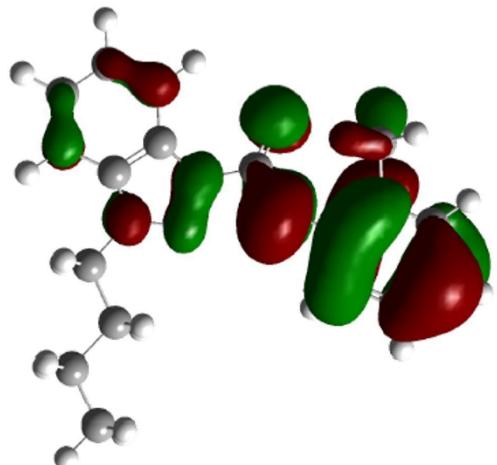


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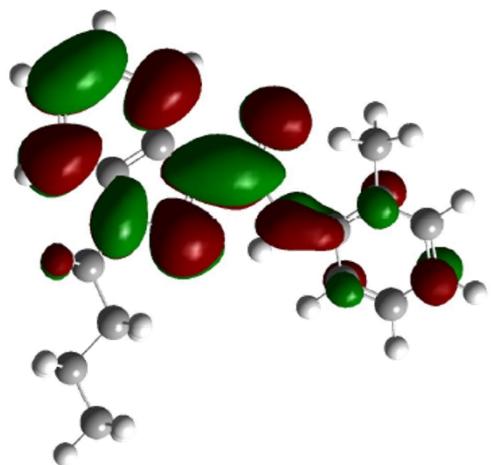


LUMO

8m

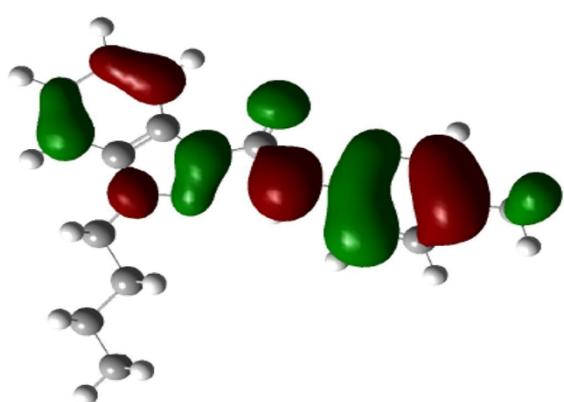


HOMO

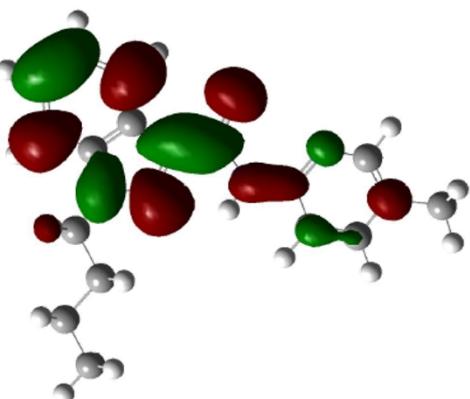


LUMO

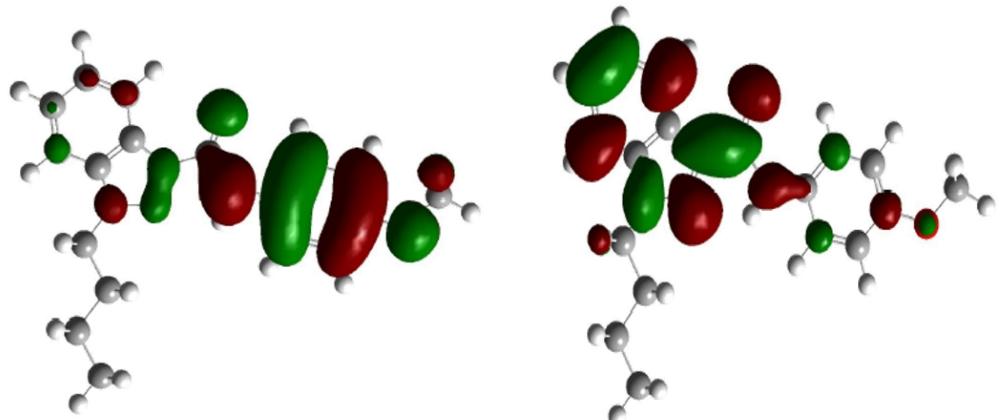
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HOMO



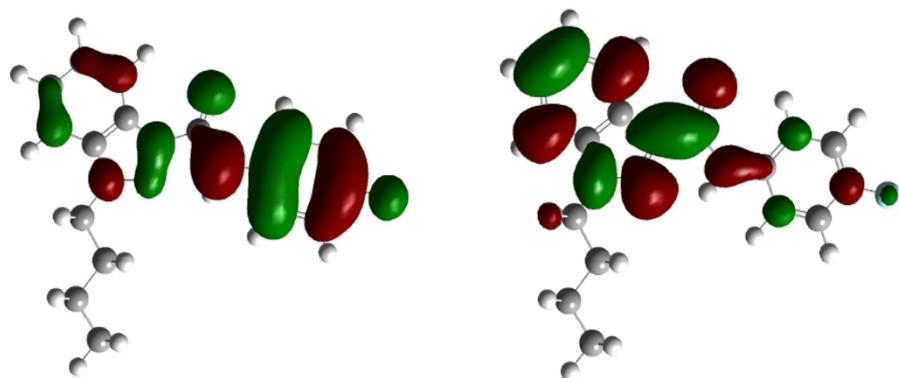
8o



HOMO

LUMO

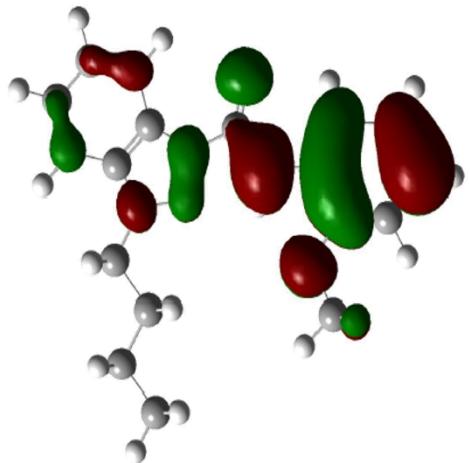
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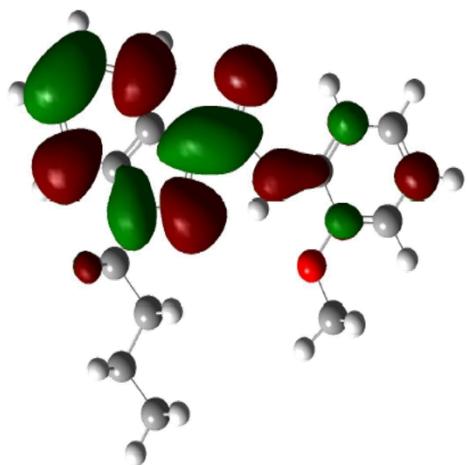
HOMO

LUMO

8q

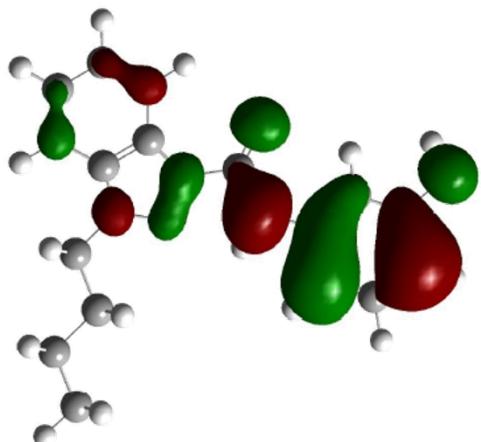


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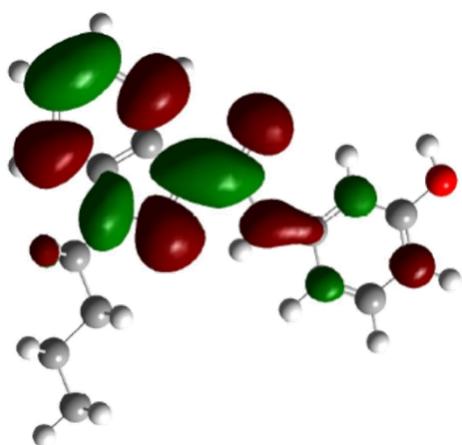


LUMO

8r

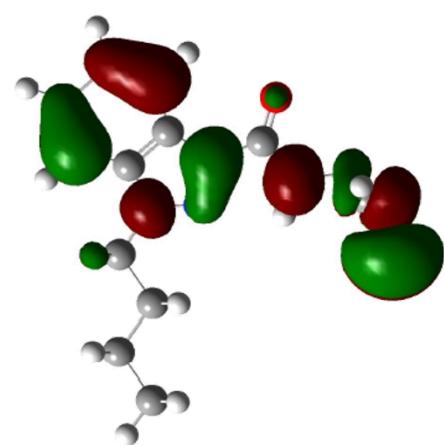


HOMO

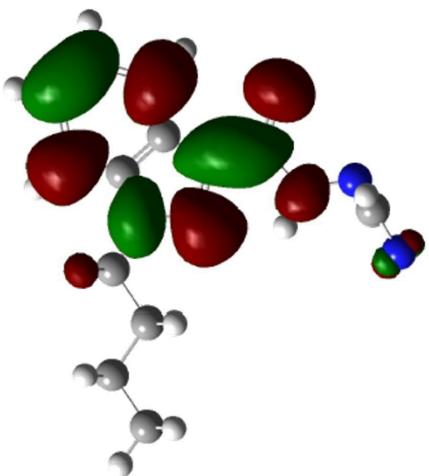


LUMO

8s

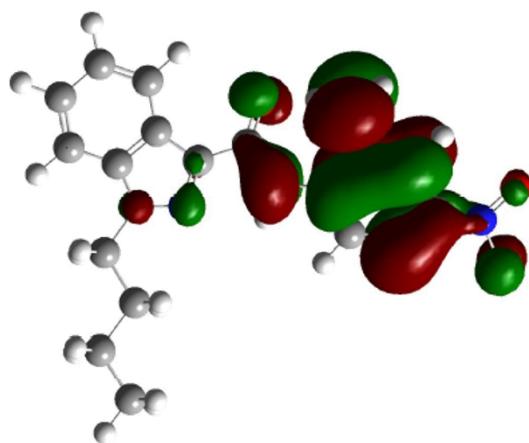


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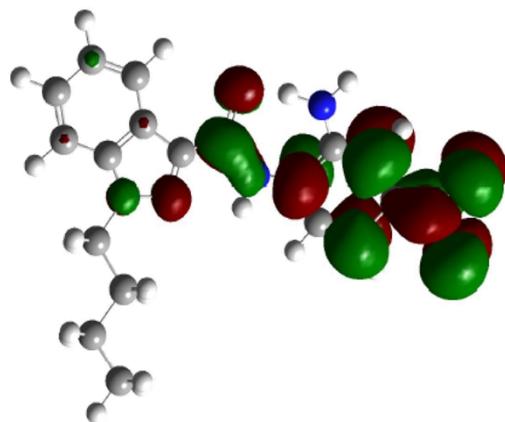


LUMO

8t

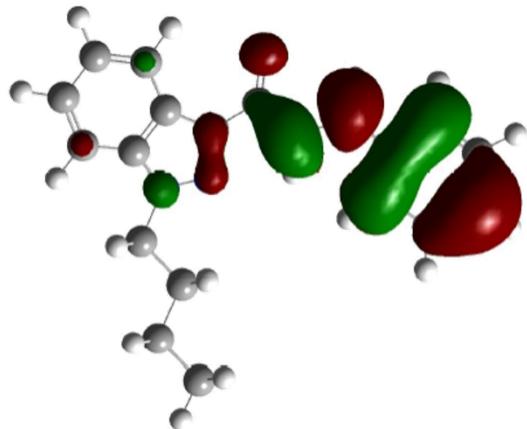


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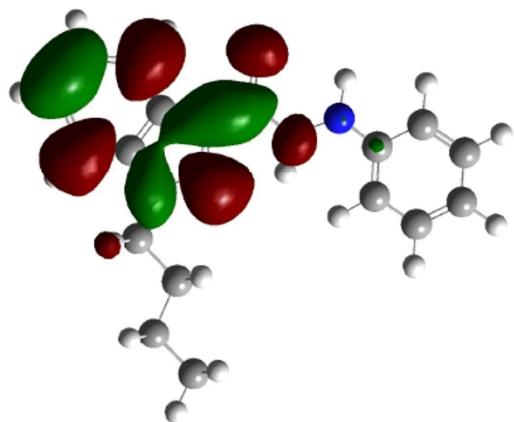


LUMO

8u

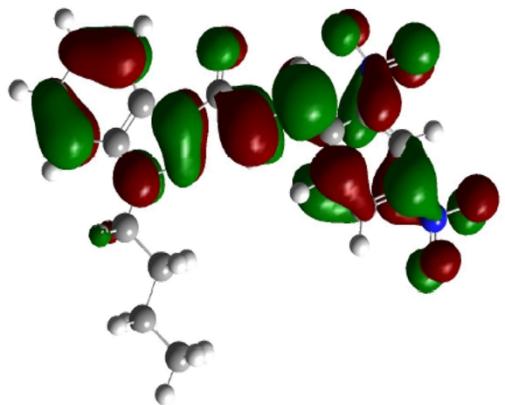


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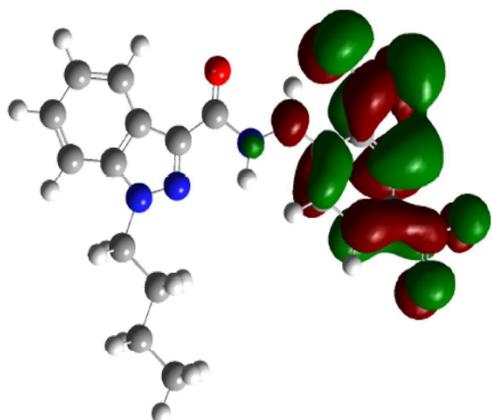


LUMO

8v

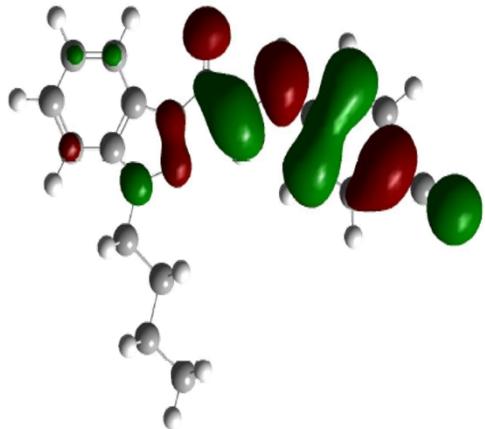


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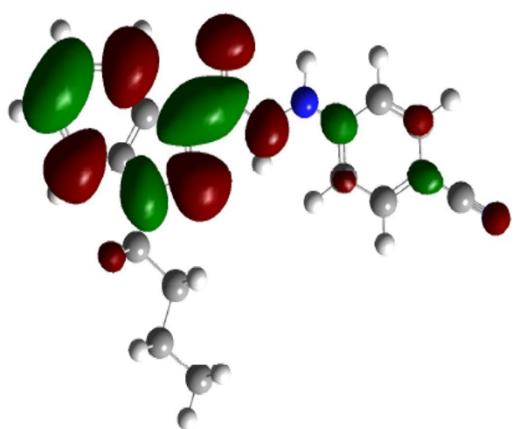


LUMO

8w

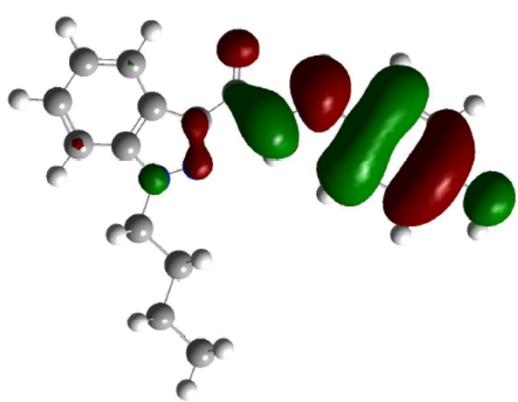


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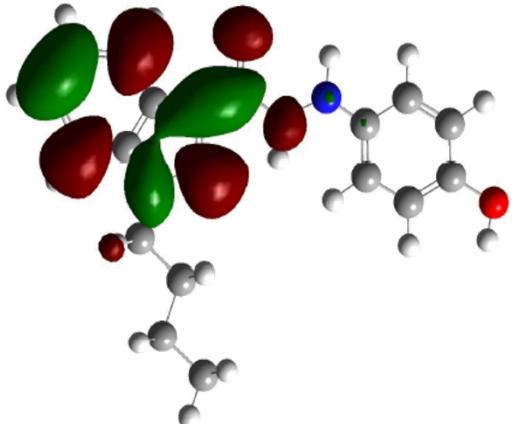


LUMO

8x

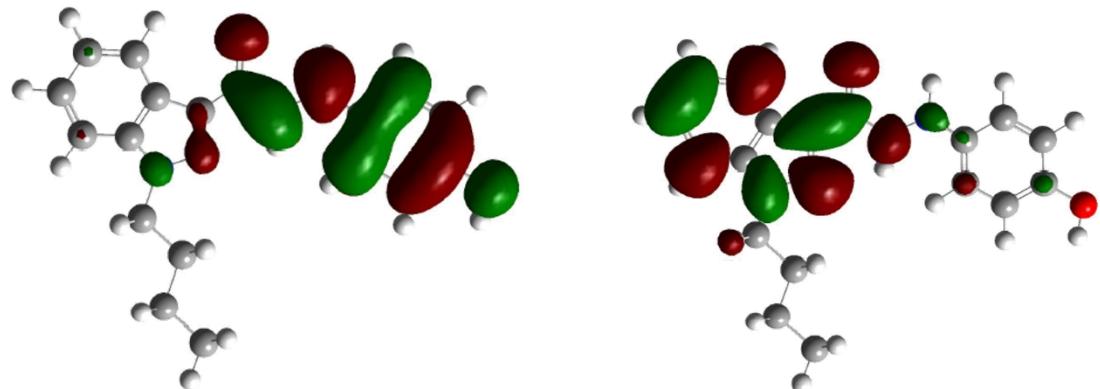


HOMO



LUMO

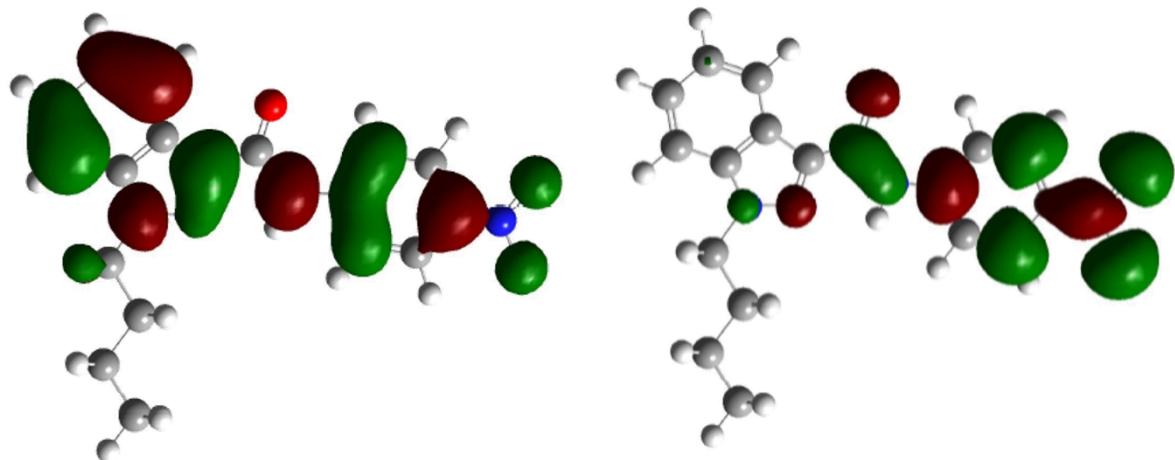
8y



HOMO

LUMO

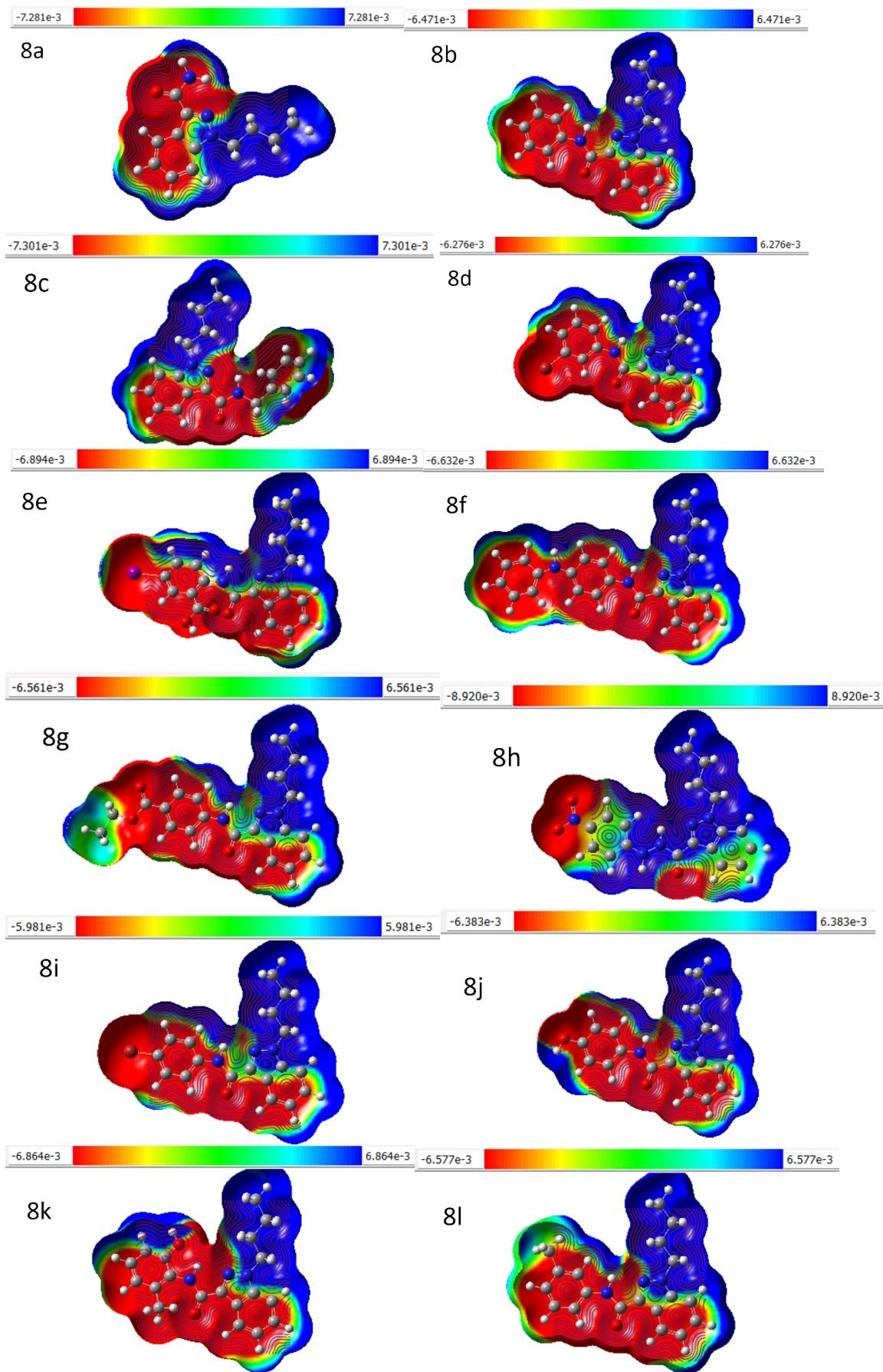
8z

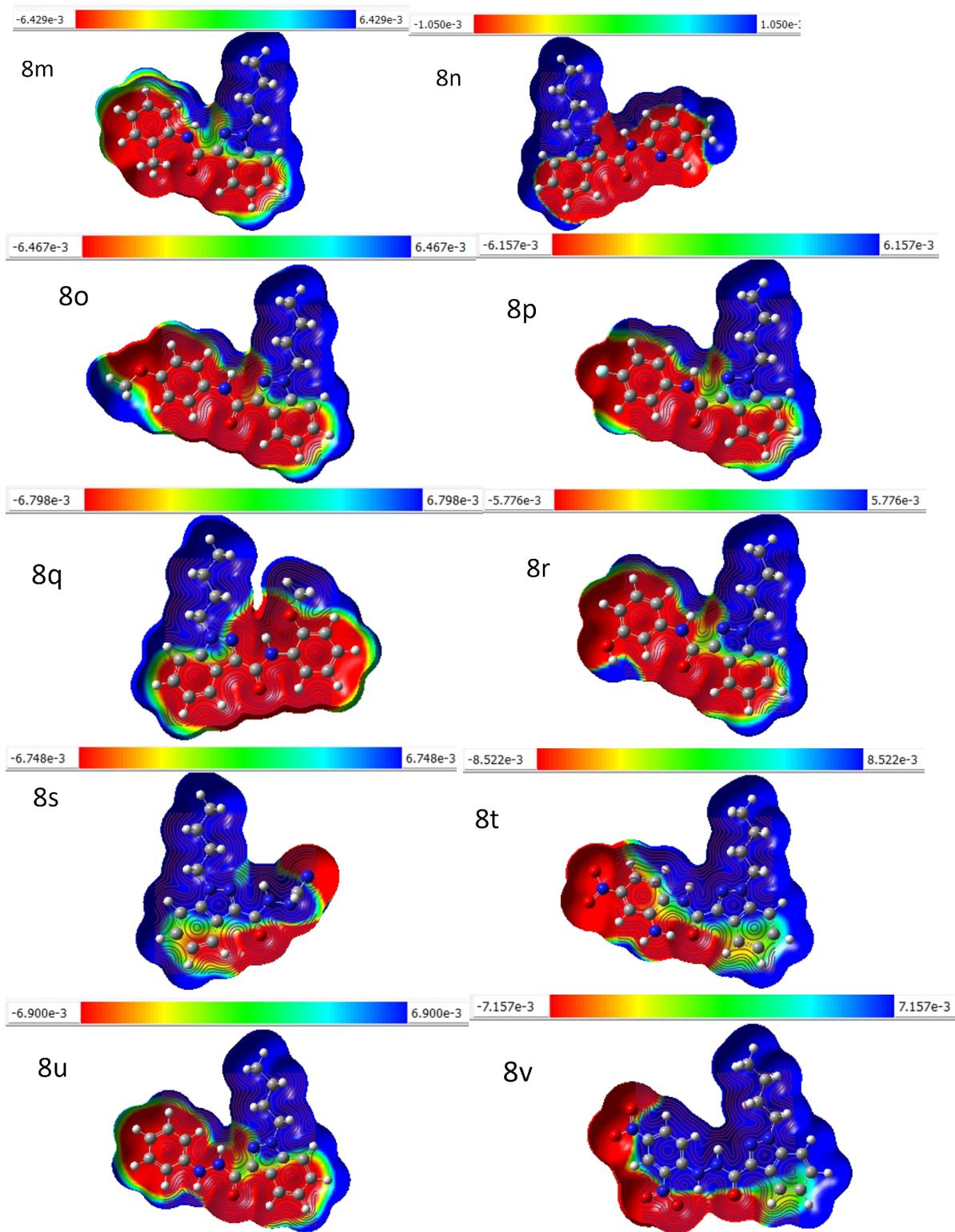


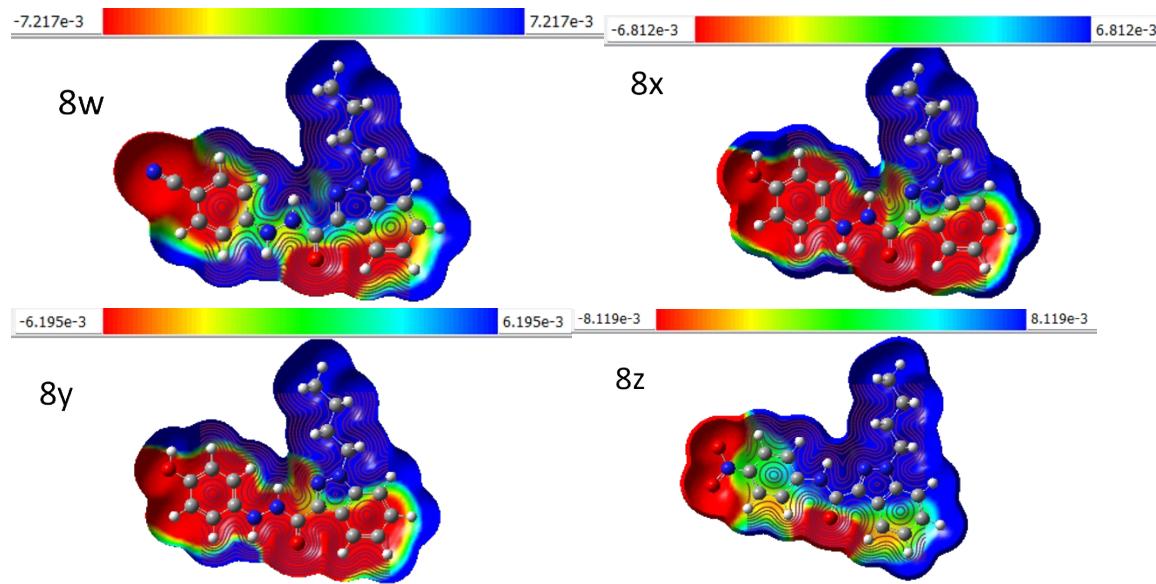
HOMO

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

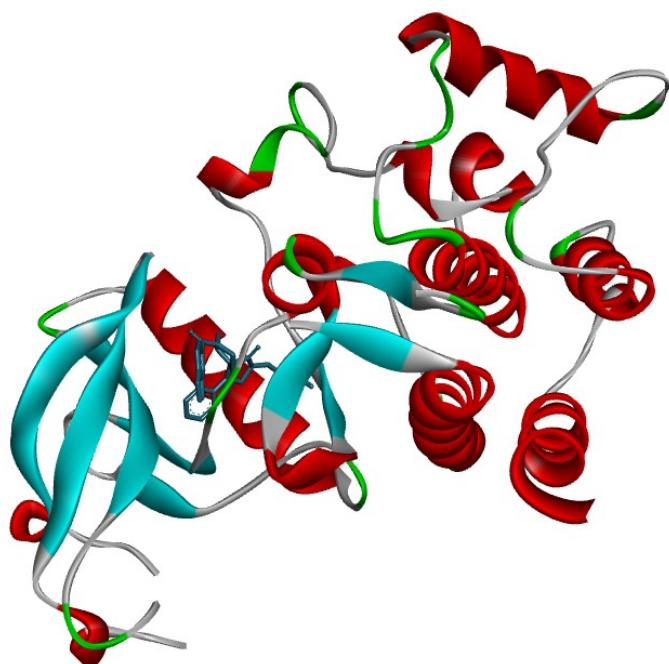
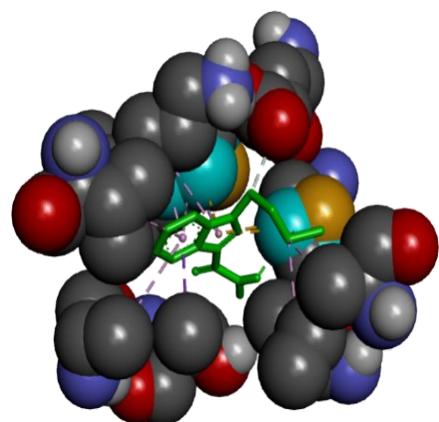


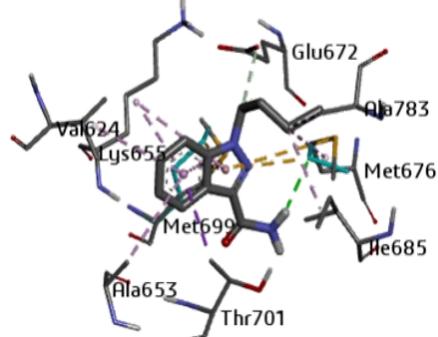
Fig 5. The crystal structure of DDR1, 2-[8-(1H-indazole-5-carbonyl)-4-oxo-1-phenyl-1,3,8-triazaspiro [4.5] decan-3-yl] -N-methyl acetamide (6FEW). 3D graphics were generated using Discovery Studio Visualizer 2021.

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

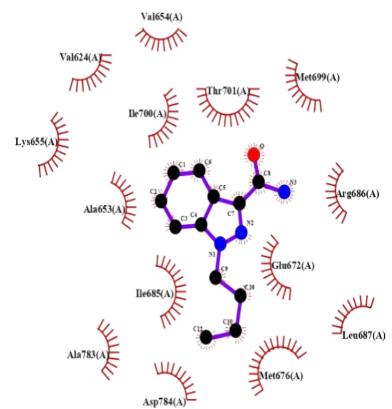
8a



A

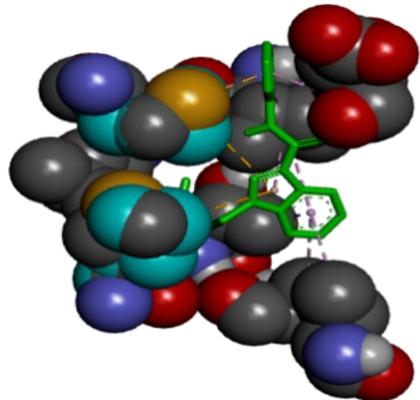


B

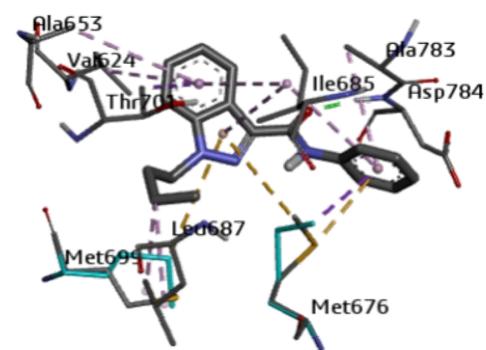


C

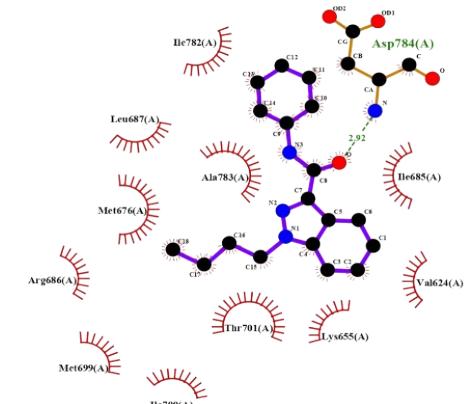
8b



A

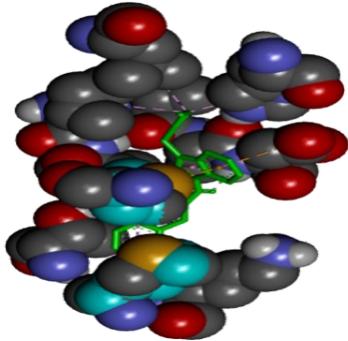


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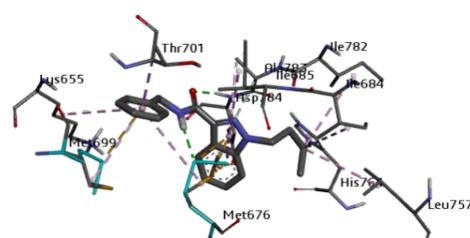


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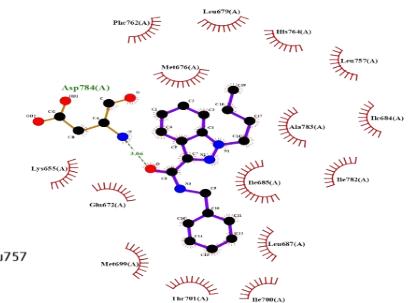
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A

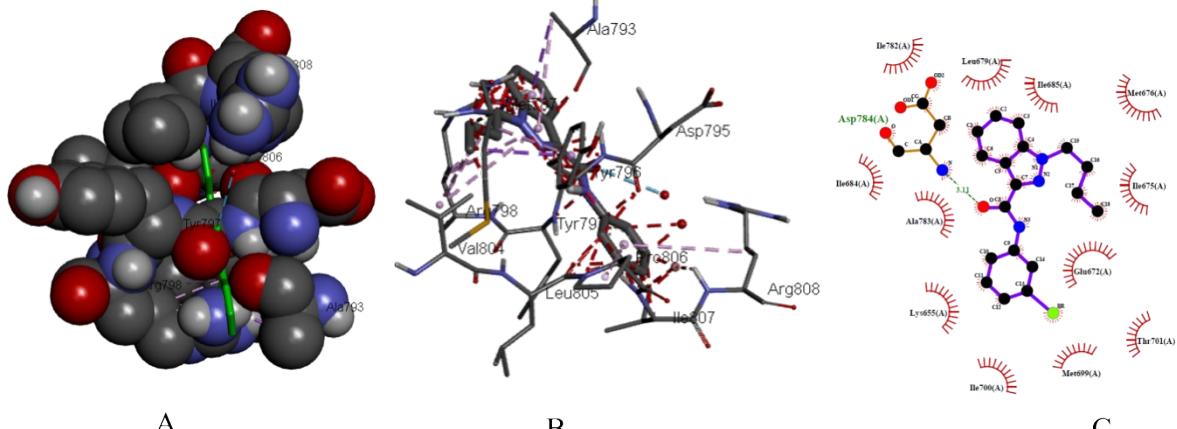


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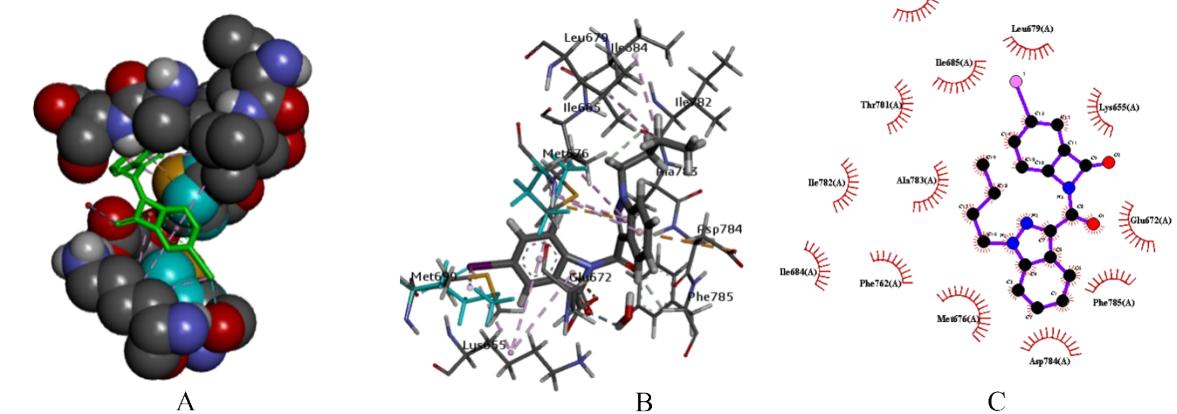


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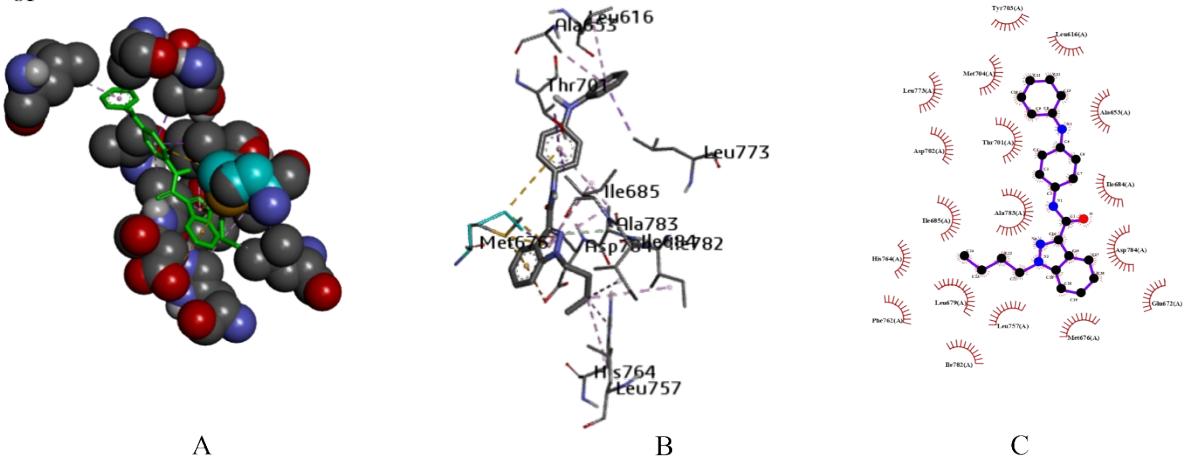
8d



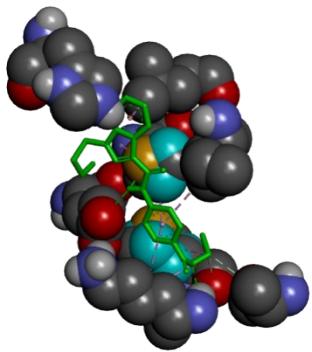
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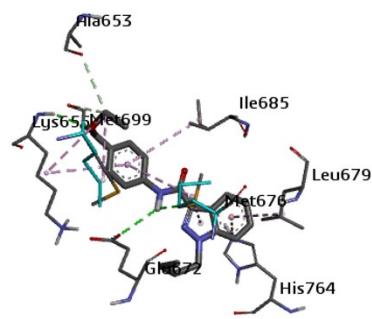
8f



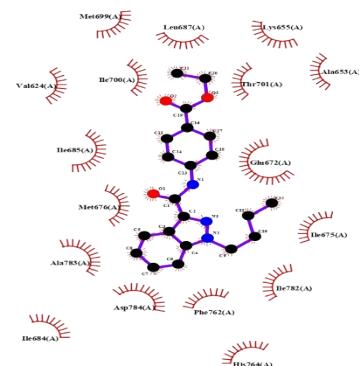
8g



A

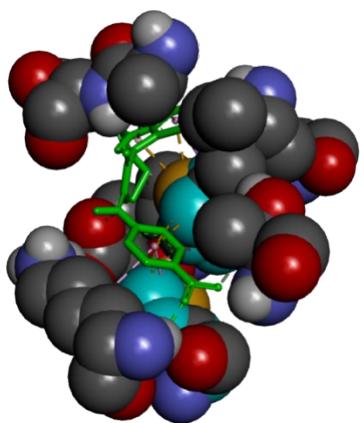


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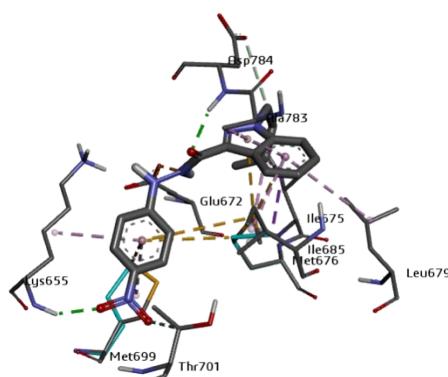


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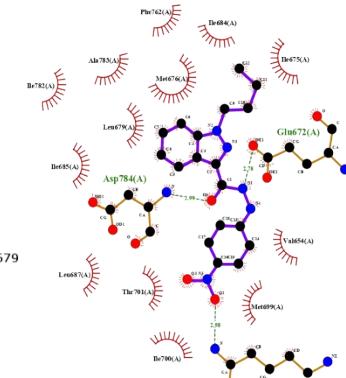
8h



A

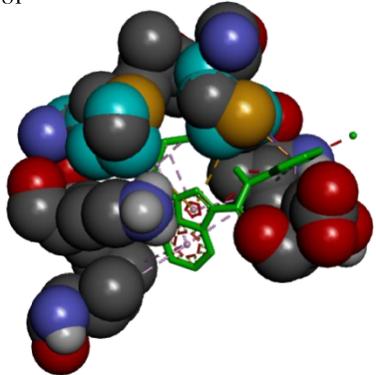


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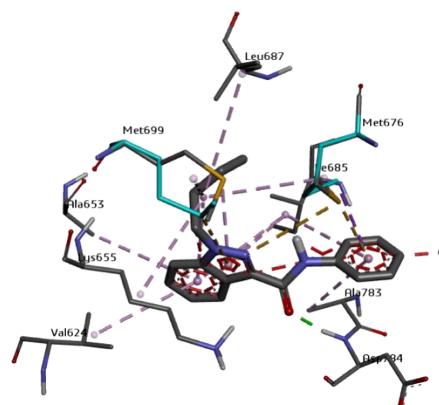


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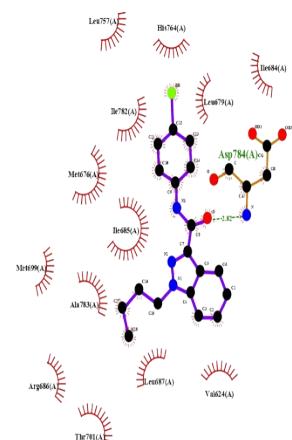
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A

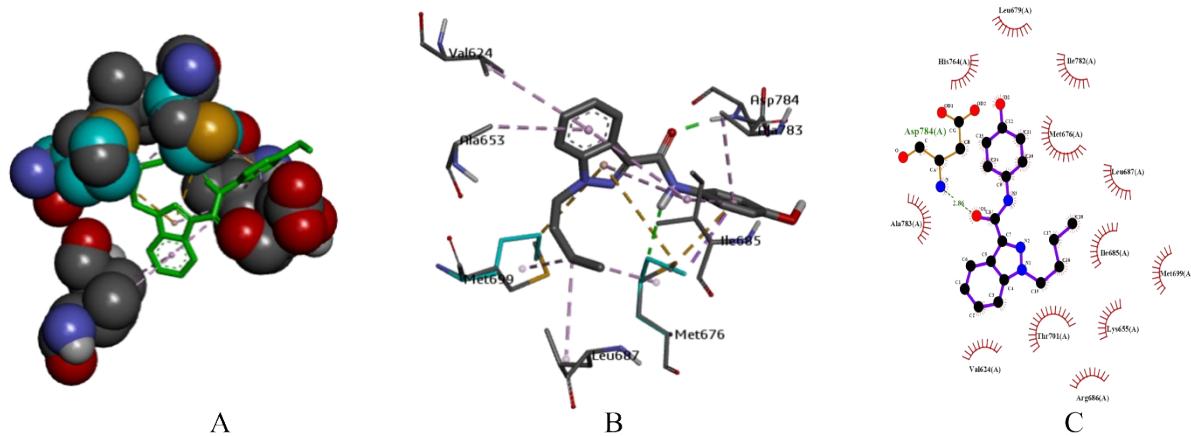


B

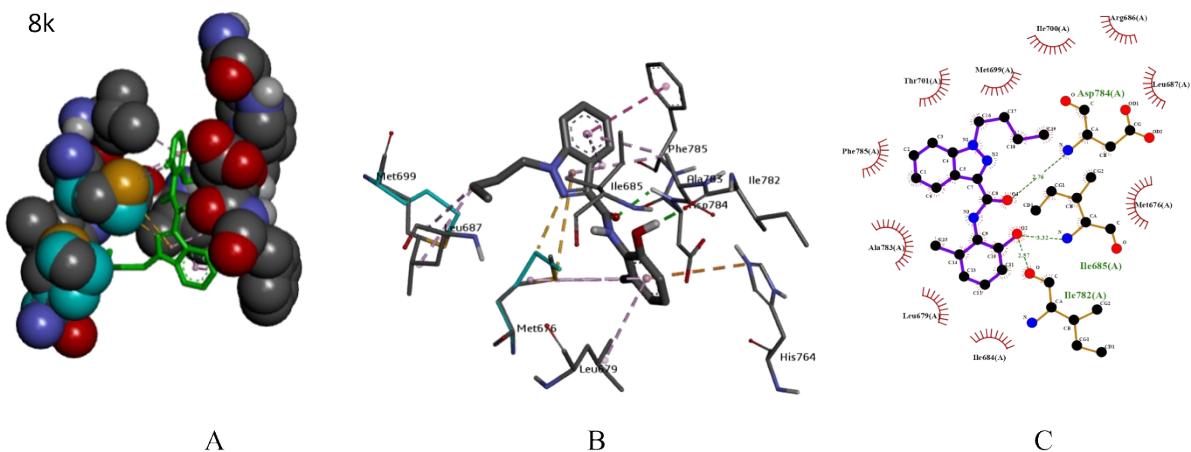


C

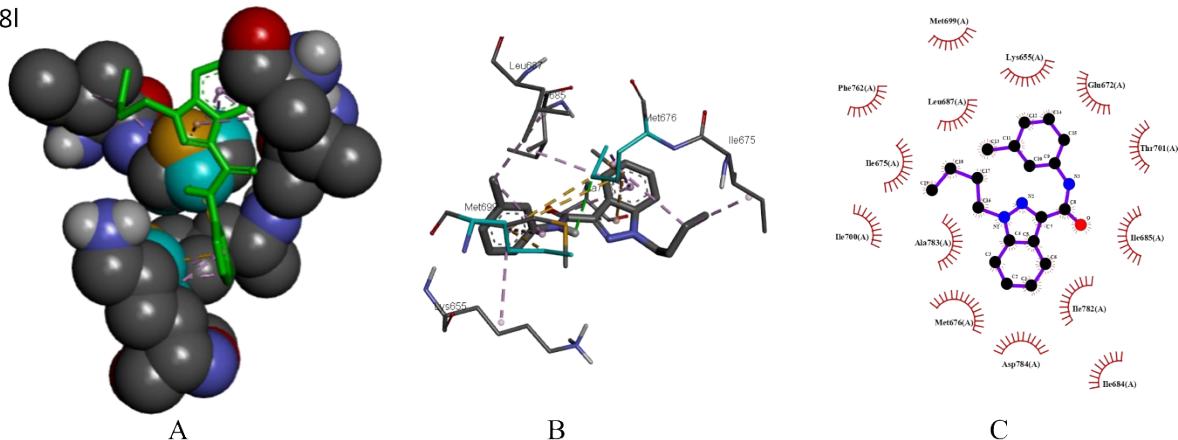
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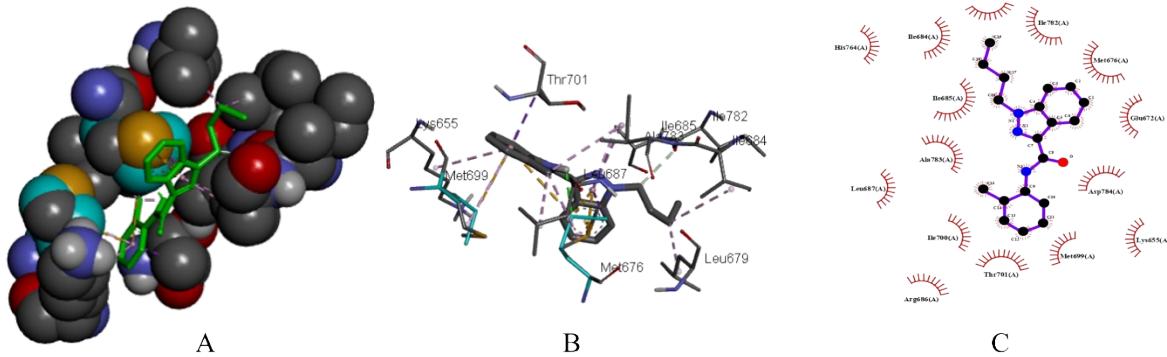
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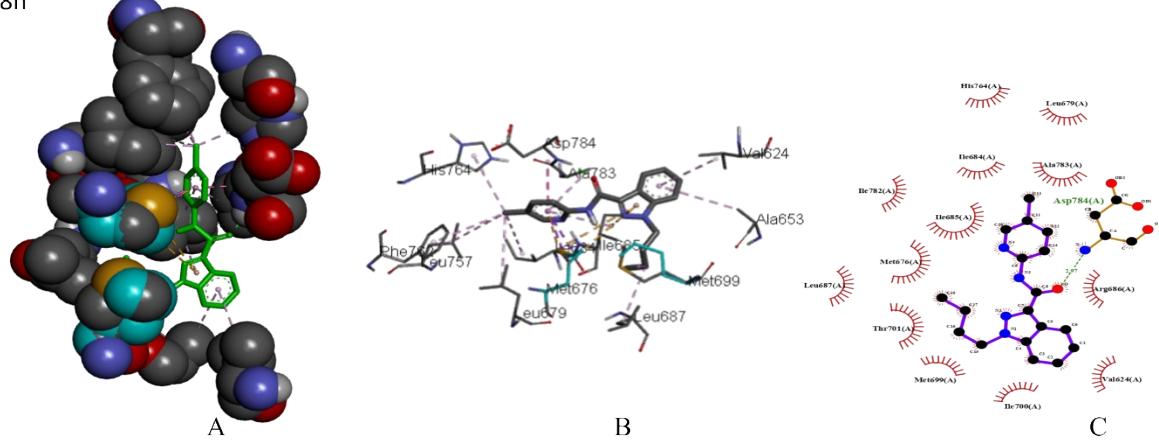
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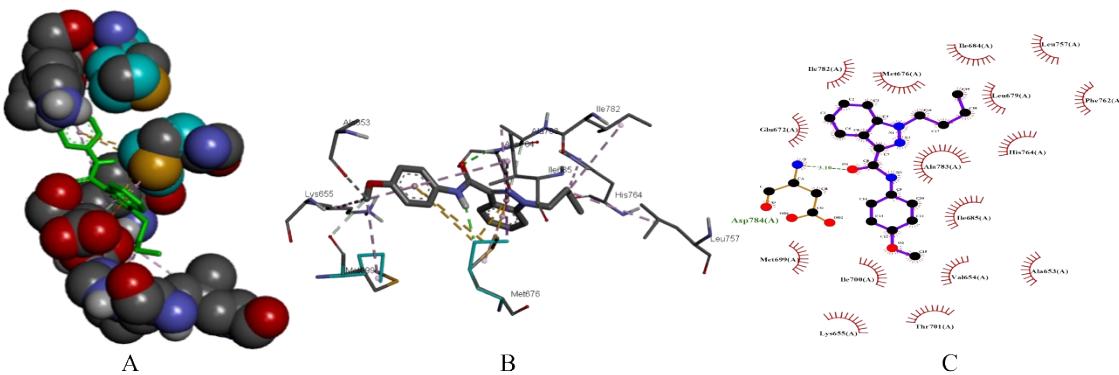
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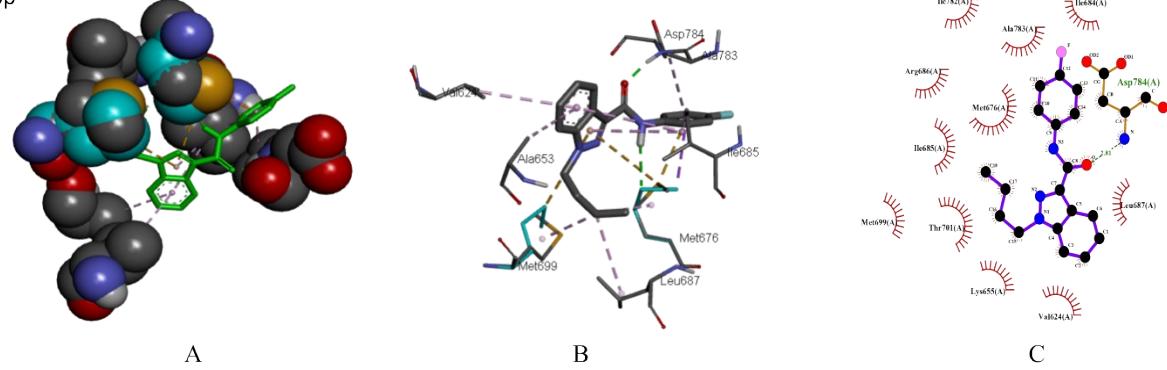
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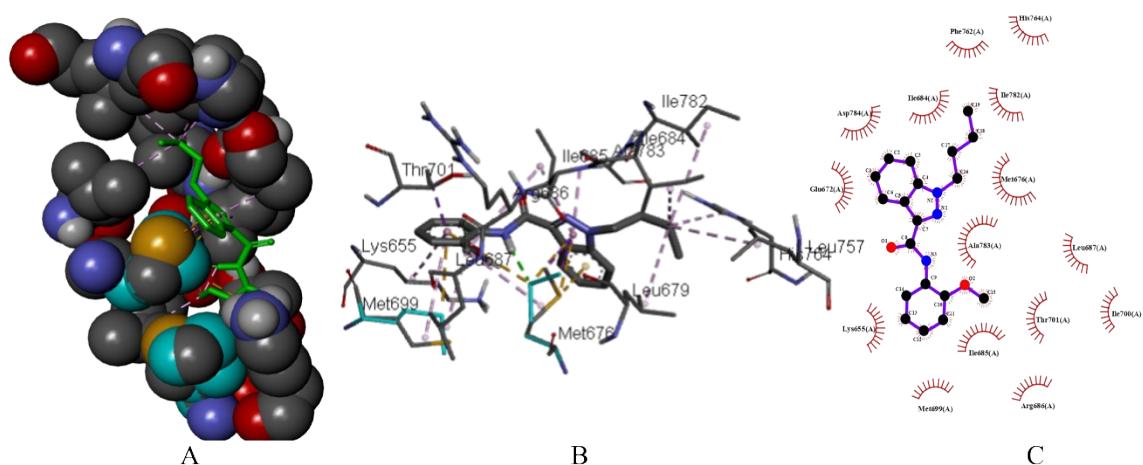
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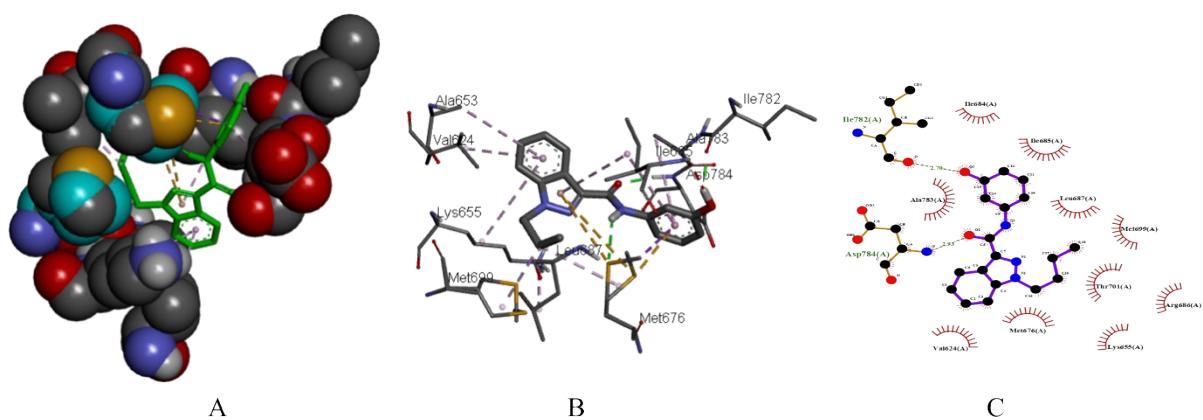
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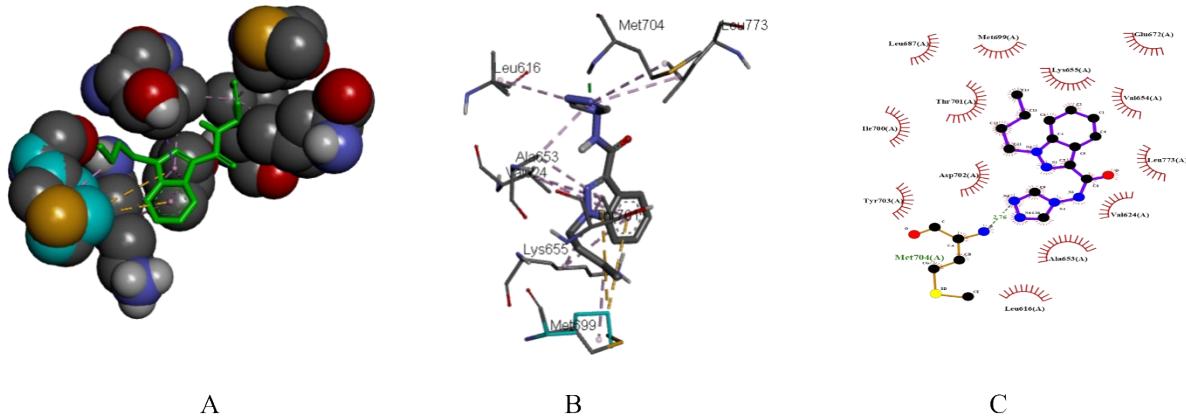
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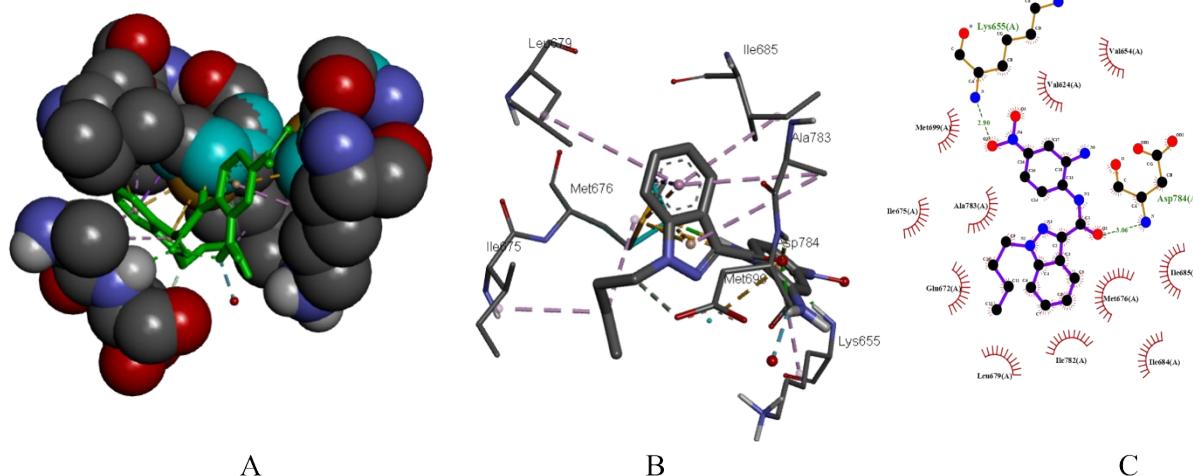
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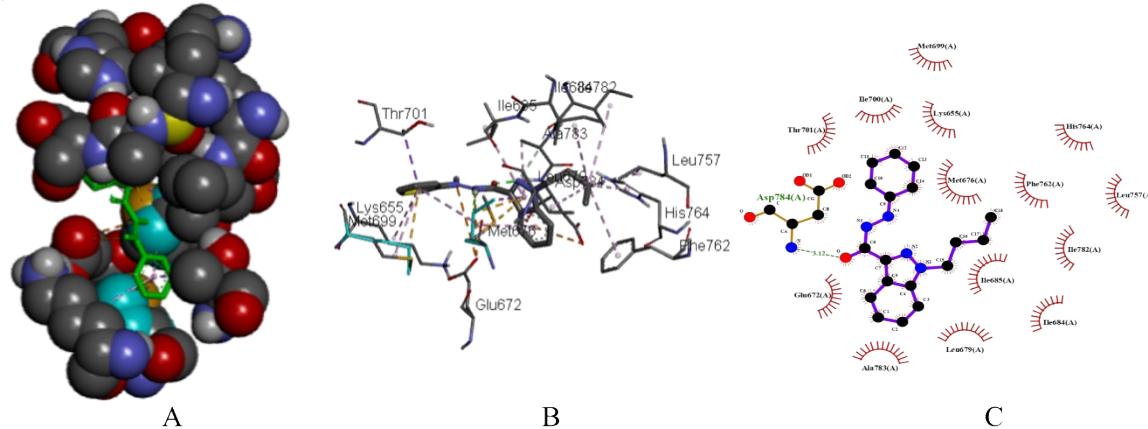
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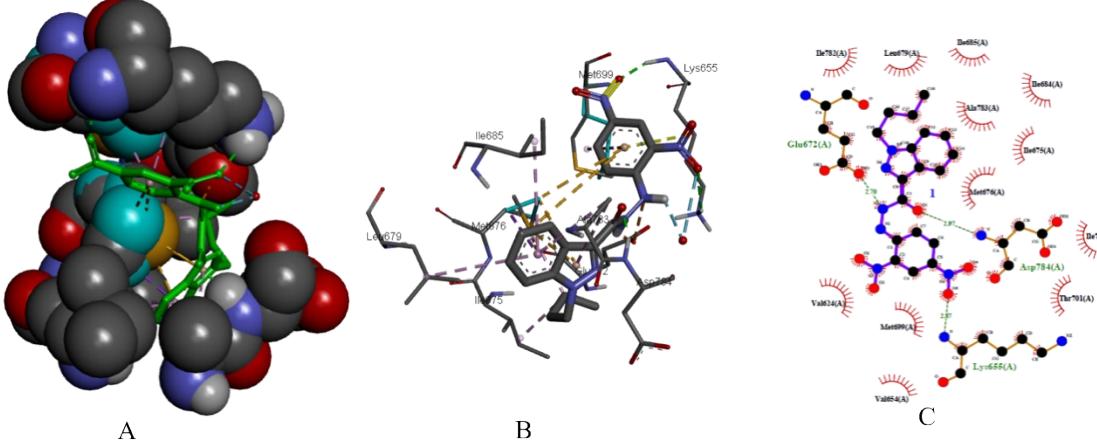
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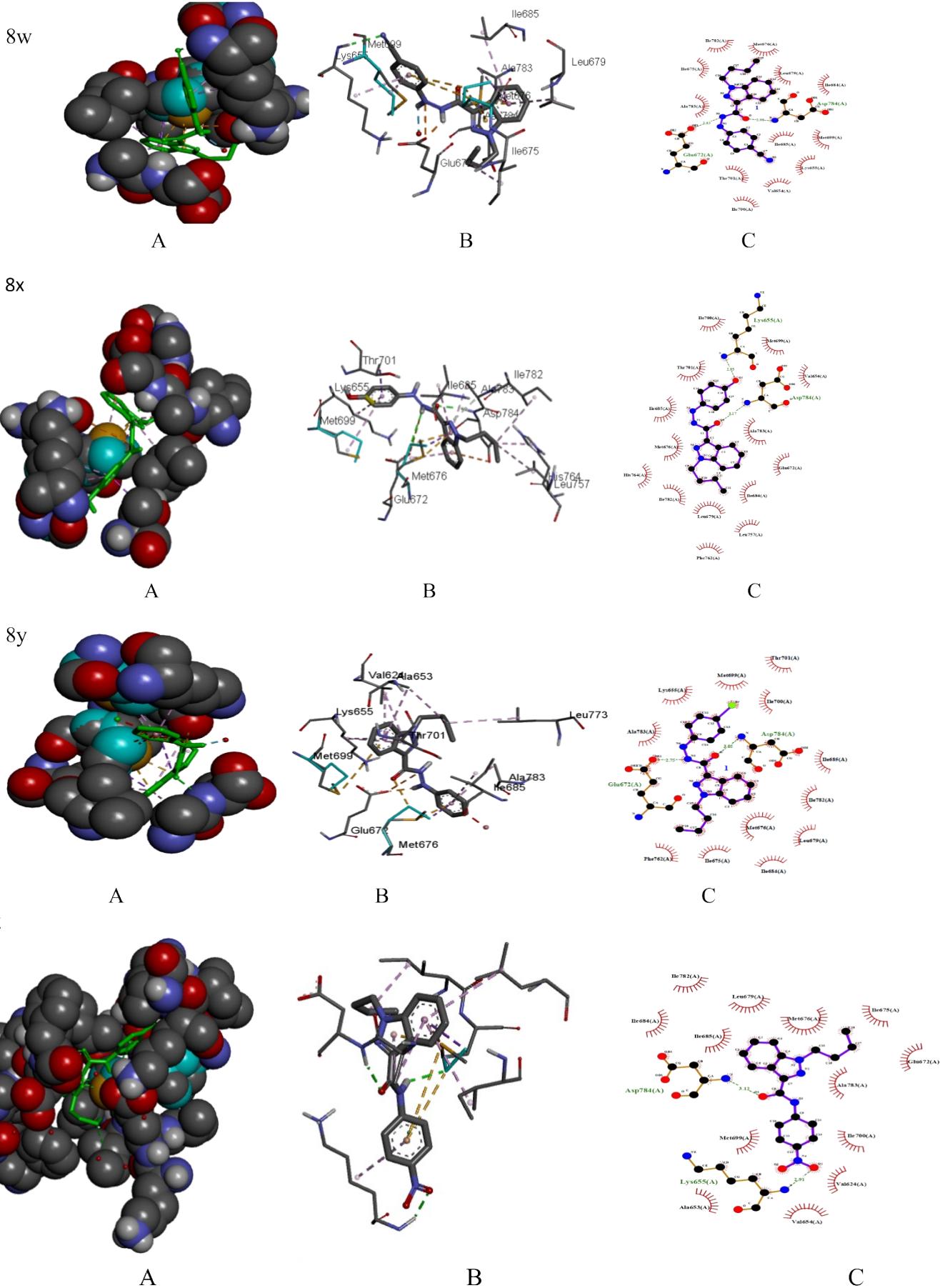


8u



8v





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