Supplementary data

A simple and efficient approach for preparing indazole compounds by palladium-catalyzed Suzuki-Miyaura cross-coupling

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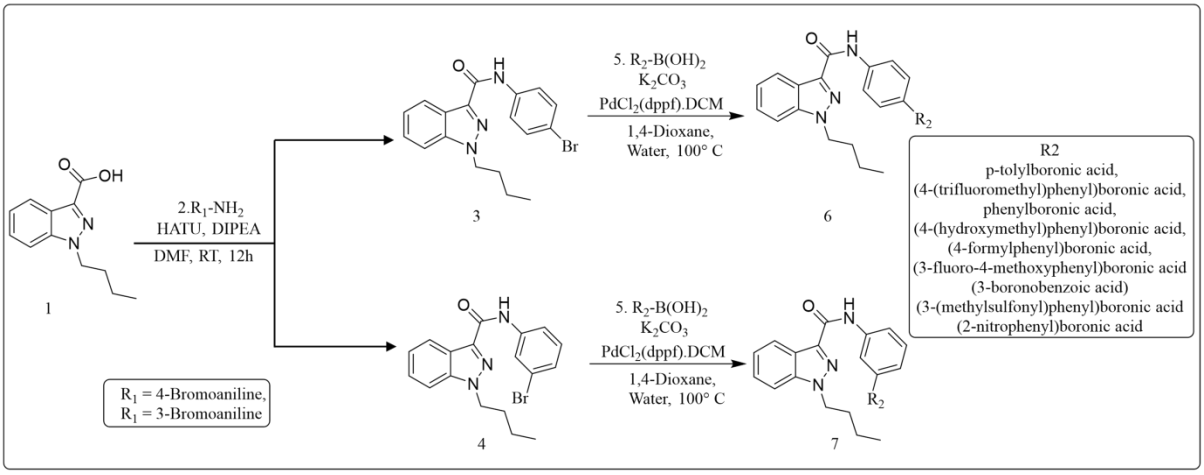
1. General methods

All the necessary chemicals and solvents used in the experiment were purchased from commercially available chemical suppliers and used as received without further purification. The solvents DMF and 1,4-dioxane were obtained from Finar chemical suppliers, while the remaining chemicals were purchased from Avra Chemicals and Sigma Aldrich. All the reactions were carried out in round bottom flasks. The infrared absorption spectra were recorded on an Affinity-1 (4000-200 cm^{-1}). The 1-butyl-1*H*-indazole-3-carboxamide was prepared according to the reported protocols. The ^{1}H-NMR and ^{13}C-NMR spectra were recorded at room temperature on a Brucker Avance III (400 MHz) spectrometer using $CDCl_3$ as a solvent and TMS as an internal standard and are referred to the residual solvent signal $CDCl_3$: (7.26) for ^{1}H and (77.16) for ^{13}C NMR: dimethyl sulfoxide-d_6 (2.50) for ^{1}H and (39.50) for ^{13}C NMR: chemical shift (δ) is 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. Colum chromatography uses a glass column of silica gel (100-200 mesh). Analytical TLC was carried out on Macherey-Nagel 60 F245 aluminium-backed silica gel plates.

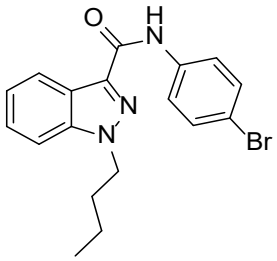
2. Scheme and Experimental procedure for indazole derivative



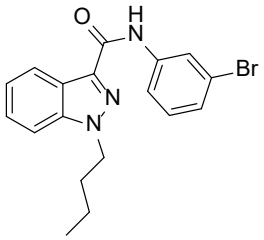
General procedure for the synthesis of 3, 4

To a stirred solution of 1-butyl-1*H*-indazole-3-carboxylic acid (250 mg, 1.146mmol) was dissolved in DMF (10 mL), HATU (2 equivalents), and DIPEA (3 equivalents) was added to the reaction mixture, then commercial amines (2 equivalents) were added. The reaction mixture was stirred at room temperature for 8-16 hours. After completion of the reaction, the

resultant reaction mixture was poured into ice-cold water, and solid precipitated and filtered through the Buchner funnel under a high vacuum dried to obtain pure compound 3,4.

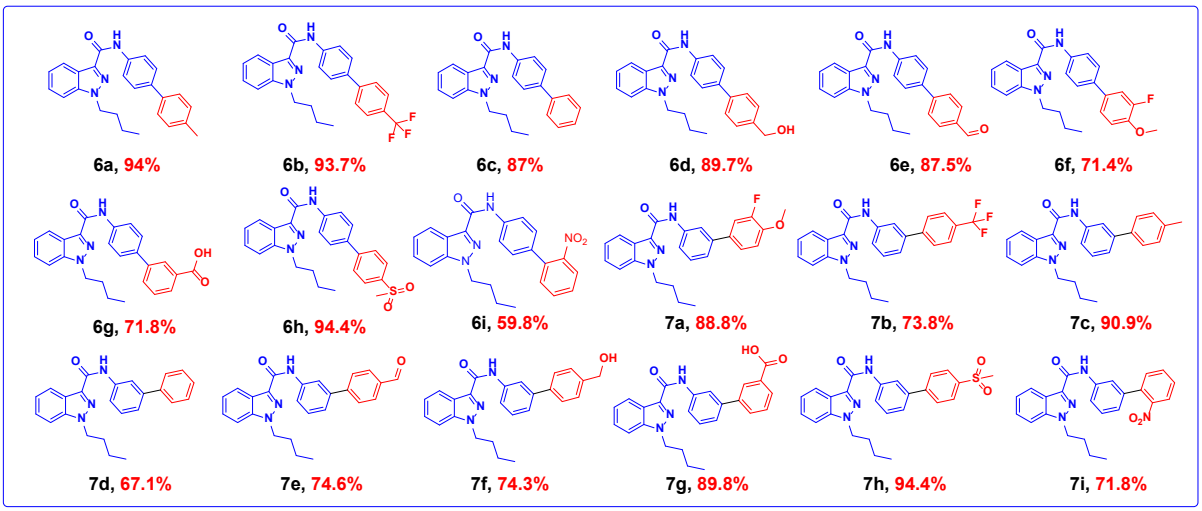


1-Butyl-1*H*-indazole-3-carboxylic acid to N-(4-bromophenyl)-1-butyl-1*H*-indazole-3-carboxamide (3). Appearance: Brown solid (melting point = 96°-99°C, yield = 82.5 %, weight = 210.6 mg). **^{1}H NMR** [400 MHz, DMSO-d_6]: δ 10.41 (s, 1H), 8.23 (d, *J* = 8.40 Hz, 1H), 7.90 (d, *J* = 8.80 Hz, 2H), 7.83 (d, *J* = 8.40 Hz, 1H), 7.55-7.52 (m, 3H), 7.32 (t, *J* = 7.60 Hz, 1H), 4.55 (t, *J* = 7.20 Hz, 2H), 1.90 (q, *J* = 7.20 Hz, 2H), 1.34-1.32 (m, 2H), 0.91 (t, *J* = 7.20 Hz, 3H). **^{13}C NMR** [100 MHz, DMSO-d_6]: δ 161.16, 141.18, 138.68, 137.23, 131.82, 127.24, 123.18, 122.74, 122.18, 111.04, 55.37, 31.99, 19.92, 14.01. **IR STRECHING** (cm^{-1}): 3272 (N-H), 1655 (C=O). **HRMS (ESI) m/z: [M+H]** calculated $C_{18}H_{18}BrN_3O$ 372.0711 + found 372.0707[M+H].



1-Butyl-1H-indazole-3-carboxylic acid to N-(3-bromophenyl)-1-butyl-1*H*-indazole-3-carboxamide (4). Appearance**:** Brown solid melting point = 96°-99°C, yield = 78.4%, weight = 200 mg). **^{1}H NMR** [400 MHz, $CDCl_3$]: δ 8.78 (s, 1H), 8.32 (d, *J* = 8.40 Hz, 1H), 7.95 (d, *J* = 1.60 Hz, 1H), 7.60-7.59 (m, 1H), 7.37-7.36 (m, 2H), 7.16 (t, *J* = 7.20 Hz, 2H), 4.34 (t, *J* = 7.20 Hz, 2H), 1.87 (q, *J* = 7.60 Hz, 2H), 1.34-1.32 (m, 2H), 0.89 (t, *J* = 7.20 Hz, 3H). **^{13}C NMR** [100 MHz, $CDCl_3$]: δ 160.51, 141.11, 139.38, 136.73, 126.99, 126.83, 123.03, 122.94, 122.73, 122.44, 118.03, 109.48, 49.38, 31.38, 20.07, 13.66**.** **IR STRECHING** (cm^{-1}): 3272 (N-H), 1655 (C=O). **HRMS (ESI) m/z: [M+H]** calculated $C_{18}H_{18}BrN_3O$ 372.0711 + found 372.0707 [M+H].

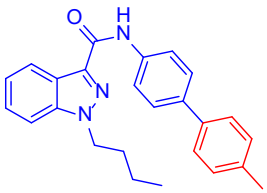
Indazole derivatives from 6a-6i, 7a-7i



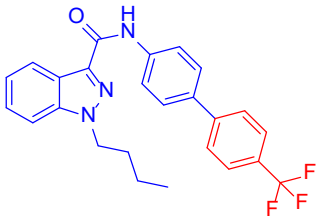
General procedure for Suzuki reaction (6a-6i and 7a-7i).

To a stirred solution of N-(3-bromophenyl)-1-butyl-1*H*-indazole-3-carboxamide (150 mg) was dissolved in 1,4-dioxane/water (6/2 mL), K_2CO_3(3eq), and Pd(dppf)Cl_2.DCM (0.05eq) was added to the reaction mixture, and commercial boronic acids (3 eq) were added. The reaction mixture was stirred at room temperature for 8-12 hours. After completion of the reaction the resultant reaction mixture was filtered through a celite pad with a Buchner funnel under a high vacuum, the filtrate was extracted with water and ethyl acetate (4 x 20 mL). The organic layer was dried with anhydrous sodium sulphate and the

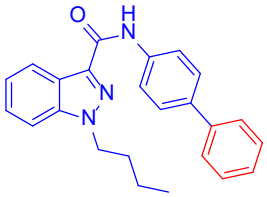
solvent was removed under reduced pressure to afford crude product. The crude was purified by silica gel chromatography to obtain a pure compound.



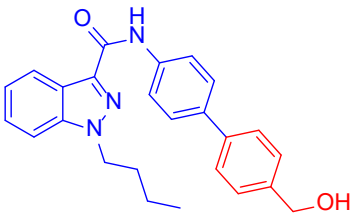
1-Butyl-N-(4-methyl-[1,1-biphenyl]-4-yl)-1*H*-indazole-3-carboxamide (6a). Appearance: off white solid, yield = 94%, weight = 145 mg, melting point = 94°-97°C, (Eluent = 15% Ethyl acetate/Hexane). **^{1}H NMR** [400 MHz, $CDCl_3$]: δ 8.83 (s, 1H), 8.37 (d, *J* = 8.00 Hz, 1H), 7.75 (d, *J* = 8.40 Hz, 2H), 7.52 (d, *J* = 8.80 Hz, 2H), 7.43 (t, *J* = 8.40 Hz, 2H), 7.36 (t, *J* = 2.00 Hz, 2H), 7.17 (t, *J* = 5.60 Hz, 2H), 4.35 (t, *J* = 7.20 Hz, 3H), 2.31 (s, 2H), 1.88 (q, *J* = 7.60 Hz, 2H), 1.26-1.27 (m, 2H), 0.90 (t, *J* = 7.20 Hz, 3H). **^{13}C NMR** [100 MHz, $CDCl_3$]: δ 160.54, 141.11, 137.78, 137.16, 137.14, 136.79, 136.71, 129.51, 127.45, 126.91, 126.68, 123.00, 122.91, 122.88, 119, 109.41, 49.34, 31.85, 21.11, 20.09, 13.68. **DEPT-135 NMR** [100 MHz, $CDCl_3$]: δ 129.51, 127.45, 126.91, 122.91, 122.88, 119.94, 109.42, 49.35, 31.85, 21.11, 20.09, 13.69. **FT-IR** (cm^{-1}): 3358 (N-H), 1659 (C=O). **HRMS (ESI) m/z: [M+H]** calculated $C_{25}H_{25}N_3O$ 384.2076 + found 384.2078 [M+H].



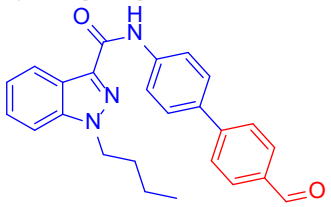
11-Butyl-N-(4-(trifluoromethyl)-[1,1-biphenyl]-4-yl)-1*H*-indazole-3-carboxamide (6b). Appearance: off white solid, yield = 93.7%, weight = 165 mg, melting point = 101°-105°C, (Eluent = 15% Ethyl acetate/Hexane), **^{1}H NMR** [400 MHz, $CDCl_3$]: δ 8.88 (s, 1H), 8.37 (d, J = 8.00 Hz, 1H), 7.80 (d, *J* = 8.80 Hz, 2H), 7.59-7.61 (m, 4H), 7.55 (d, *J* = 8.40 Hz, 2H), 7.37 (t, *J* = 1.60 Hz, 2H), 4.36 (t, *J* = 7.20 Hz, 2H), 1.89 (q, *J* = 7.20 Hz, 2H), 1.26-1.28 (m, 2H), 0.90 (t, *J* = 7.20 Hz, 3H). **^{13}C NMR** [100 MHz, $CDCl_3$]: δ 160.60, 144.11, 141.12, 138.29, 136.98, 135.06, 129.18, 128.85, 127.85, 127.02, 126.98, 125.70, 122.98, 122.83, 120.00, 109.46, 49.38, 31.84, 20.08, 13.67. **DEPT-135 NMR** [100 MHz, $CDCl_3$]: δ 127.085, 127.02, 126.98, 125.70, 122.98, 120.00, 109.46, 109.46, 49.38, 31.84, 20.08, 13.67. **FT-IR** (cm^{-1}): 3351(N-H), 1664 (C=O). **HRMS (ESI) m/z: [M+H]** calculated $C_{25}H_{22}F_3N_3O$ 438.1793 + found 438.1794 [M+H].



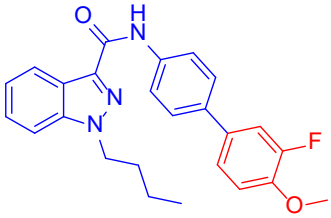
N-([1,1-Biphenyl]-4-yl)-1-butyl-1*H*-indazole-3-carboxamide (6c). Appearance**:** off white solid, yield = 87%, weight = 130 mg, melting point = 83°-88°C, (Eluent = 10% Ethyl acetate/Hexane), **^{1}H NMR** [400 MHz, $CDCl_3$]: δ 8.85 (s, 1H), 8.37 (d, *J* = 8.00 Hz, 1H), 7.77 (d, *J* = 8.40 Hz, 2H), 7.53-7.54 (m, 4H), 7.34-7.36 (m, 4H), 4.35 (t, *J* = 6.80 Hz, 2H), 1.89 (q, *J* = 7.60 Hz, 2H), 1.36-1.34 (m, 2H), 0.90 (t, *J* = 7.20 Hz, 3H). **^{13}C NMR** [100 MHz, $CDCl_3$]: δ 160.55, 141.12, 140.66, 137.43, 137.12, 136.75, 128.78, 127.03, 126.92, 126.85, 123.01, 122.91, 119.94, 109.41, 49.35, 31.84, 20.08, 13.67. **DEPT-135 NMR** [100 MHz, $CDCl_3$]: δ 128.78, 127.67, 127.03, 126.86, 122.91, 122.89 119.93, 109.41, 49.35, 31.85, 20.09, 13.68. **FT-IR** (cm^{-1}): N-H (3363), C=O (1660). **HRMS (ESI) m/z: [M+H]** calculated $C_{24}H_{22}N_3O$ 370.1919 + found 370.1924[M+H].



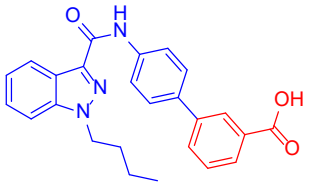
1-Butyl-N-(4-(hydroxymethyl)-[1,1-biphenyl]-4-yl)-1*H*-indazole-3-carboxamide (6d). Appearance: off white solid (yield = 89.7%, weight = 145 mg, melting point = 81°-86°C, (Eluent = 25% Ethyl acetate/Hexane), **^{1}H NMR** [400 MHz, $CDCl_3$]: δ 8.86 (s, 1H), 8.37 (d, *J* = 7.60 Hz, 1H), 7.76 (d, *J* = 7.20 Hz, 2H), 7.53 (s, 3H), 7.46 (d, *J* = 6.40 Hz, 1H), 7.36 (d, *J* = 9.20 Hz, 3H), 7.25 (d, *J* = 5.60 Hz, 2H), 4.69 (s, 2H), 4.35 (s, 2H), 1.88 (s, 2H), 1.31 (d, *J* = 6.80 Hz, 2H), 0.90 (t, *J* = 6.80 Hz, 3H). **^{13}C NMR** [100 MHz, $CDCl_3$]: δ 160.59, 141.50, 141.09, 137.48, 137.06, 136.46, 136.46, 129.02, 127.66, 126.94, 126.10, 125.64, 125.42, 122.99, 122.93, 122.87, 119.94, 109.44, 65.37, 49.35, 31.85, 20.08, 13.69. **DEPT-135 NMR** [100 MHz, $CDCl_3$]: δ 129.02, 127.66, 126.94, 126.10, 125.65, 125.42, 122.93, 122.86, 119.94, 109.44, 65.37, 49.35, 31.85, 20.09, 13.69. **FT-IR** (cm^{-1}): 3403 (OH), 3250 (N-H), 1645 (C=O). **HRMS (ESI) m/z: [M+H]** calculated $C_{25}H_{25}N_3O_2$ 400.2025 + found 400.2037 [M+H].



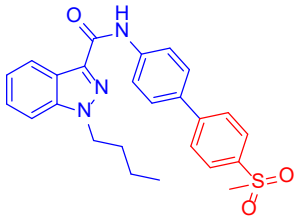
1-Butyl-N-(4-formyl-[1,1-biphenyl]-4-yl)-1*H*-indazole-3-carboxamide (6e). Appearance: Off white solid, yield = 87.5%, weight = 140 mg, melting point = 93°-97°C, (Eluent = 25% Ethyl acetate/Hexane), **^{1}H NMR** [400 MHz, $CDCl_3$]: δ 10.01 (s, 1H), 8.89 (s, 1H), 8.37 (d, *J* = 8.00 Hz, 1H), 8.03 (s, 1H), 7.75-7.77 (m, 4H), 7.58 (d, *J* = 8.64 Hz, 2H), 7.52 (t, *J* = 8.00 Hz, 1H), 7.37-7.38 (m, 2H), 4.36 (t, *J* = 7.20 Hz, 2H), 1.89 (q, *J* = 7.20 Hz, 2H), 1.26-1.28 (m, 2H), 0.00 (t, *J* = 7.20 Hz, 3H). **^{13}C NMR** [100 MHz, $CDCl_3$]: δ 192.45, 160.61, 141.56, 138.12, 136.98, 136.94, 135.04, 129.52, 128.38, 127.81, 127.70, 126.97, 122.97, 122.83, 122.05, 109.46, 49.38, 31.84, 20.08, 13.67. **DEPT-135 NMR** [100 MHz, $CDCl_3$]: δ 132.74, 129.52, 128.39, 127.81, 127.70, 126.97, 122.97, 122.82, 120.05, 109.46, 49.38, 31.84, 20.08, 13.68. **FT-IR** (cm^{-1}): 2955 (CHO), 3301 (N-H), 1693 (C=O). **HRMS (ESI) m/z: [M+H]** calculated $C_{25}H_{23}N_3O_2$ 398.1868 + found 398.1868 [M+H].



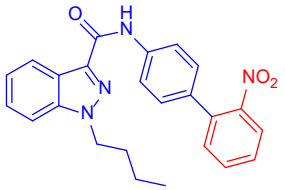
1-Butyl-N-(3-fluoro-4-methoxy-[1,1-biphenyl]-4-yl)-1*H*-indazole-3-carboxamide (6f). Appearance: Off white solid, yield = 71.4%, weight = 120 mg, melting point = 80°-85°C, (Eluent = 15% Ethyl acetate/Hexane), **^{1}H NMR** [400 MHz, $CDCl_3$]: δ 8.84 (s, 1H), 8.37 (d, *J* = 8.00 Hz, 1H), 7.76 (d, *J* = 8.00 Hz, 2H), 7.48 (d, *J* = 7.60 Hz, 2H), 7.39 (s, 2H), 7.19-7.26 (m, 4H), 6.95 (t, *J* = 8.00 Hz, 1H), 4.37 (t, *J* = 6.80 Hz, 2H), 3.86 (s, 3H), 1.90 (t, *J* = 7.20 Hz, 2H), 1.32 (q, *J* = 6.80 Hz, 2H), 0.912 (t, *J* = 6.80 Hz, 3H). **^{13}C NMR** [100 MHz, $CDCl_3$]: δ 160.65, 141.11, 138.62, 137.04, 129.51, 127.20, 126.39, 122.97, 122.91, 122.85, 122.26, 119.98, 118.41, 117.92, 115.00, 114.81, 113.58, 109.43, 56.37, 49.36, 31.84, 20.08, 13.68. **DEPT-135 NMR** [100 MHz, $CDCl_3$]: δ 129.51, 127.20, 126.93, 122.91, 122.86, 122.26, 119.98, 118.41, 117.92, 115.00, 114.81, 113.56, 109.44, 56.37, 49.36, 31.85, 20.08, 13.68. **FT-IR** (cm^{-1}): 3380 (N-H), 2955 (-OCH_3), 1681 (C=O). **HRMS (ESI) m/z: [M+H]** calculated $C_{25}H_{24}FN_3O_2$ 418.1931 + found 418.1933 [M+H].



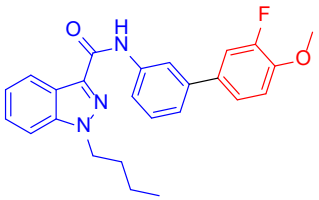
4-(1-Butyl-1*H*-indazole-3-carboxamido)-[1,1-biphenyl]-3-carboxylic acid (6g). Appearance: Off white solid, yield = 71.8%, weight = 120 mg, melting point = 159°-164°C, (Eluent = 30% Ethyl acetate/Hexane) **^{1}H NMR** [400 MHz, DMSO-d_6]: δ 10.39 (s, 1H), 8.26 (d, *J* = -8.40 Hz, 1H), 8.22 (s, 1H), 8.05 (d, *J* = 8.40 Hz, 2H), 7.92 (t, *J* = 8.40 Hz, 2H), 7.84 (d, *J* = 8.40 Hz, 1H), 7.73 (d, *J* = 8.80 Hz, 2H), 7.60 (t, *J* = 7.60 Hz, 1H), 7.51 (t, *J* = 8.00 Hz, 1H), 7.34 (t, *J* = 7.60 Hz, 1H), 4.57 (t, *J* = 7.20 Hz, 2H), 0.00 (q, *J* = 7.20 Hz, 2H), 1.27-1.28 (m, 2H), 0.92 (t, *J* = 7.60 Hz, 3H). **^{13}C NMR** [100 MHz, $CDCl_3$]: δ 167.18, 161.14, 141.9, 140.54, 139.14, 137.37, 134.62, 132.00, 131.14, 129.77, 128.32, 127.39, 127.24, 123.16, 122.91, 122.22, 121.22, 111.02, 49.11, 31.99, 19.93, 14.02. **DEPT-135 NMR** [100 MHz, $CDCl_3$]: δ 131.14, 129.77, 128.33, 127.39, 127.36, 127.25, 123.17, 122.22, 121.22, 111.03, 49.11, 31.99, 19.93, 14.02. **FT-IR** (cm^{-1}): 3281(N-H), 1715(C=O). **HRMS (ESI) m/z: [M+H]** calculated $C_{25}H_{23}N_3O_3$ 414.1817 + found 414.1818 [M+H].



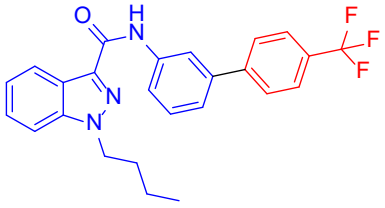
1-Butyl-N-(4-(methylsulfonyl)-[1,1-biphenylyl]-4-yl)-1*H*-indazole-3-carboxamide (6h). Appearance: Off white solid, yield = 94.4%, weight = 170 mg, melting point = 79°-84°C, (Eluent = 15% Ethyl acetate/Hexane), **^{1}H NMR** [400 MHz, $CDCl_3$]: δ 8.98 (s, 1H), 8.44 (d, *J* = -8.00 Hz, 1H), 8.00 (d, *J* = 8.00 Hz, 2H), 7.91 (d, *J* = 8.40 Hz, 2H), 7.79 (d, *J* = 8.40 Hz, 2H), 7.65 (d, *J* = 8.40 Hz, 2H), 7.47 (d, *J* = 4.80 Hz, 2H), 7.32-7.32 (m, 1H), 4.45 (t, *J* = 7.20 Hz, 2H), 3.10 (s, 3H), 1.98 (q, *J* = 7.20 Hz, 2H), 1.35-1.37 (m, 2H), 0.99 (t, *J* = 7.20 Hz, 3H). **^{13}C NMR** [100 MHz, $CDCl_3$]: δ 160.61, 1466.10, 141.15, 138.79, 138.75, 136.93, 134.33, 128.02, 127.94, 127.54, 127.01, 123.02, 122.99, 122.80, 120.06, 109.47, 49.40, 44.67, 31.83, 20.07, 13.65. **DEPT-135 NMR** [100 MHz, $CDCl_3$]: δ 128.28, 126.96, 126.86, 126.46, 125.97, 122.00, 121.73, 119.91, 119.01, 116.73, 48.32, 43.53, 30.78, 28.66, 19.02, 12.63. **FT-IR** (cm^{-1}): 3075 (N-H), 1676 (C=O). **HRMS (ESI) m/z: [M+H]** calculated $C_{25}H_{23}N_3O_3S$ 448.1695 + found 448.1697 [M+H].



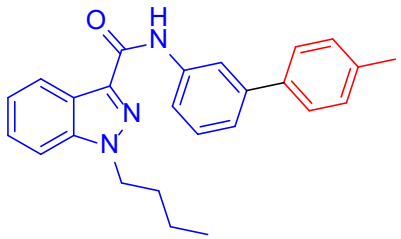
1-Butyl-N-(2-nitro[1,1-biphenyl]-4-1*H*-indazole-3-carboxamide (6i). Appearance: Off white solid, yield = 59.8%, weight = 100 mg, melting point = 88°-94°C, (Eluent = 15% Ethyl acetate/Hexane), **^{1}H NMR** [400 MHz, $CDCl_3$]: δ 8.86 (s, 1H), 8.37 (d , *J* = 8.00 Hz, 1H), 7.77 (d, *J* = 7.60 Hz, 3H), 7.54 (t, *J* = 7.60 Hz, 1H), 7.40 (d, *J* = 9.20 Hz, 4H), 7.28 (s, 1H), 4.37 (t, *J* = 7.20 Hz, 2H), 1.90 (q, *J* = 7.20 Hz, 2H), 1.30 (d, *J* = 35.60 Hz, 2H), 0.91 (t, *J* = 7.20 Hz, 3H). **^{13}C NMR** [100 MHz, $CDCl_3$]: δ 160.57, 149.36, 141.14, 138.27, 137, 135.87, 132.69, 132.24, 132, 128.7, 126.94, 124.1, 123, 122.93, 122.87, 119.76, 109.43, 49.36, 31.81, 20.06, 13.64. **DEPT-135 NMR** [100 MHz, $CDCl_3$]: δ 132.24, 132, 128.7, 127.97, 126.94, 124.1, 122.93, 122.87, 119.76, 109.43, 49.36, 31.81, 20.06, 13.64. **FT-IR** (cm^{-1}): 3390 (N-H), 1671(C=O), 1521(NO_2). **HRMS (ESI) m/z: [M+H]** calculated $C_{25}H_{22}N_4O_3$ 415.1770 + found 415.1773 [M+H].



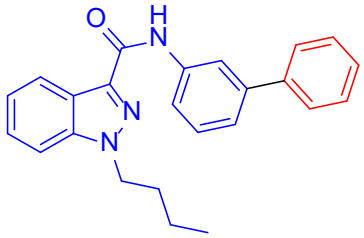
1-Butyl-N-(3-fluoro-4-methoxy-[1,1-biphenyl]-3-yl)-1*H*-indazole-3-carboxamide (7a). Appearance: Off white solid, yield = 88.8%, weight = 150 mg, melting point = 96°-100°C, (Eluent = 15% Ethyl acetate/Hexane), **^{1}H NMR** [400 MHz, $CDCl_3$]: δ 8.86 (s, 1H), 8.37 (d, *J* = 8.00 Hz, 1H), 7.93 (s, 1H), 7.63 (d, *J* = 8.00 Hz, 1H), 7.30-7.31 (m, 5H), 7.18-7.21 (m, 2H), 6.95 (t, *J* = 8.80 Hz, 1H), 4.36 (t, *J* = 6.80 Hz, 2H), 3.86 (s, 3H), 1.90 (q, *J* = 7.20 Hz, 2H), 1.27-1.29 (m, 2H), 0.904(t, *J* = 7.60 Hz, 3H). **^{13}C NMR** [100 MHz, $CDCl_3$]: δ 160.66, 153.77, 147.24, 141.11, 140.66, 138.62, 137.35, 137.04, 129.51, 127.19, 126.93,122.97, 122.83, 122.26, 119.99, 118.42, 117.92, 114.99, 109.44, 56.37, 49.36, 31.84, 20.08, 13.67. **DEPT-135 NMR** [100 MHz, $CDCl_3$]: δ 129.51, 127.20, 126.93, 122.91, 122.83, 122.26, 119.99, 118.42, 117.92, 114.99, 114.80, 113.59, 113.57, 109.44 56.37, 49.36, 31.85, 20.08, 13.68. **FT-IR** (cm^{-1}): 3277(N-H), 2767 (OCH_3), 1664 (C=O). **HRMS (ESI) m/z: [M+H]** calculated $C_{25}H_{24}FN_3O_2$ 418.1931+ found 418.1931 [M+H].



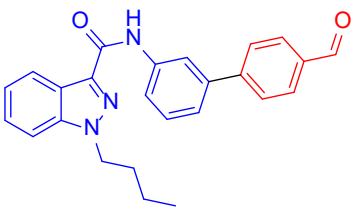
1-Butyl-N-(4-(trifluoromethyl)-[1,1-biphenyl]-3-yl)-1*H*-indazole-3-carboxamide (7b). Appearance: Off white solid, yield = 73.8%, weight = 130 mg, melting point = 66°-70°C, (Eluent = 15% Ethyl acetate/Hexane), **^{1}H NMR** [400 MHz, $CDCl_3$]: δ 8.89 (s, 1H), 8.37 (d, *J* = 8.00 Hz, 1H), 8.05 (s, 1H), 7.61-7.64 (m, 5H), 7.38-7.39 (m, 3H), 7.18 (d, *J* = 3.60 Hz, 1H), 4.37 (t, *J* = 6.80 Hz, 2H), 1.90 (q, *J* = 7.20 Hz, 2H), 1.27-1.29 (m, 2H), 0.91 (t, *J* = 7.60 Hz, 3H). **^{13}C NMR** [100 MHz, $CDCl_3$]: δ 160.69, 144.40, 141.14, 140.71, 138.77, 136.99, 129.64, 127.58, 126.97, 125.69, 125.65, 122.97, 122.77, 119.30, 118.50, 109.45, 49.38, 31.84, 20.08, 13.66. **DEPT-135 NMR** [100 MHz, $CDCl_3$]: δ 129.64, 127.58, 126.97, 125.69, 122.97, 122.83, 122.78, 119.30, 118.50, 109.45, 49.38, 31.84, 20.08, 13.66. **FT-IR** (cm^{-1}): 3289 (N-H), 1668 (C=O). **HRMS (ESI) m/z: [M+H]** calculated $C_{25}H_{22}F_3N_3O$ 438.1793 + found 438.1795 [M+H].



1-Butyl-N-(4-methyl-[1,1-biphenyl]-3-yl)-1*H*-indazole-3-carboxamide (7c). Appearance**:** Off white solid, yield = 90.9%, weight = 140 mg, melting point = 107°-110°C, (Eluent = 15% Ethyl acetate/Hexane), **^{1}H NMR** [400 MHz, $CDCl_3$]: δ 8.86 (s, 1H), 8.38 (d, *J* = 8.00 Hz, 1H), 7.92 (s, 1H), 7.68 (d, *J* = 8.00 Hz, 1H), 7.49 (d, *J* = 8.00 Hz, 2H), 7.34-7.36 (m, 3H), 7.29 (s, 1H), 7.18 (t, *J* = 4.40 Hz, 2H), 4.37 (t, *J* = 7.20 Hz, 2H), 2.33 (s, 3H), 1.90 (q, *J* = 7.60 Hz, 2H), 1.27-1.29 (m, 2H), 0.91 (t, *J* = 7.60 Hz, 3H). **^{13}C NMR** [100 MHz, $CDCl_3$]: δ 160.61, 142.11, 141.11, 138.50, 137.94, 137.24, 137.15, 129.45, 129.39, 127.10, 126.90, 122.99, 122.91, 122.85, 122.57, 118.27, 118.17, 109.40, 49.34, 31.85, 21.14, 20.09, 13.68. **DEPT-135 NMR** [100 MHz, $CDCl_3$]: δ 129.46, 129.40, 127.10, 126.90, 122.91, 122.86, 122.57, 118.27, 118.17, 109.40, 49.34, 31.85, 21.14, 20.09, 13.68. **FT-IR** (cm^{-1}): 3289 (N-H), 1668 (C=O). **HRMS (ESI) m/z: [M+H]** calculated $C_{25}H_{25}N_3O$ 384.2076 + found 384.2080 [M+H].

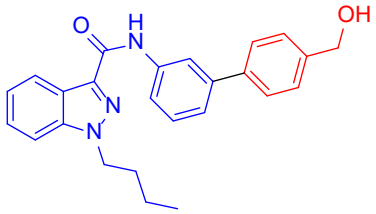


N-([1,1-Biphenyl]-3-yl)-1-butyl-1*H*-indazole-3-carboxamide (7d). Appearance: Off white solid, yield = 67.1%, weight = 100 mg, melting point = 65°-68°C, (Eluent = 10% Ethyl acetate/Hexane), **^{1}H NMR** [400 MHz, $CDCl_3$]: δ 8.94 (s, 1H), 8.45 (d, *J* = 6.80 Hz, 1H), 8.02 (s, 1H), 7.76 (d, *J* = 6.00 Hz, 1H), 7.66 (d, *J* = 5.60 Hz, 2H), 7.33-7.36 (m, 8H), 4.43 (s, 2H), 1.97 (s, 2H), 1.38 (d, *J* = 6.00 Hz, 2H), 0.97 (s, 3H). **^{13}C NMR** [100 MHz, $CDCl_3$]: δ 160.63, 142.21, 141.12**,** 140.86, 138.55, 137.12, 129.44, 128.74, 127.46, 127.29, 123.00, 122.90, 122.88, 118.52, 118.41, 109.42, 49.35, 31.85, 20.09, 13.68. **DEPT-135 NMR** [100 MHz, $CDCl_3$]: δ 129.44, 128.74, 127.29, 126.91, 122.88, 122.75, 118.52, 118.41, 109.42, 49.35, 31.85, 20.09, 13.68. **FT-IR** (cm^{-1}): 3014 (N-H), 1670 (C=O). **HRMS (ESI) m/z: [M+H]** calculated $C_{24}H_{24}N_3O$ 370.1919 + found 370.1920 [M+H].

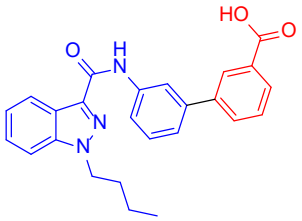


1-Butyl-N-(4-formyl-[1,1-biphenyl]-3-yl)-1*H*-indazole-3-carboxamide (7e). Appearance: off white solid, yield = 74.6%, weight = 120 mg, melting point = 67°-72°C, (Eluent = 25% Ethyl acetate/Hexane) **^{1}H NMR** [400 MHz, $CDCl_3$]: δ 10.10 (s, 1H), 9.00 (s, 1H), 8.44 (d, *J* = 6.40 Hz, 1H), 8.13 (d, *J* = 14.40 Hz, 2H), 7.76-7.78 (m, 3H), 7.61 (s, 1H), 7.26-7.33 (m, 5H), 4.45 (s, 2H), 1.98 (s, 2H), 1.39 (d, *J* = 5.20 Hz, 2H), 0.98 (s, 3H). **^{13}C NMR** [100 MHz, $CDCl_3$]: δ 192.47, 160.76, 141.82, 140.66, 138.73, 136.93, 136.87, 133.29, 129.71, 129.51, 128.72, 128.44, 126.98, 122.96, 122.78, 122.72, 119.21, 118.40, 109.48, 49.40, 31.85, 20.09, 13.68. **DEPT-135 NMR** [100 MHz, $CDCl_3$]: δ 133.28, 129.71, 129.51, 128.72, 128.44, 126.98, 122.99, 122.71,

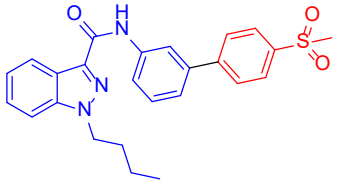
119.21, 118.39, 109.48, 49.40, 31.85, 20.09, 13.68. **FT-IR** (cm-^{1}): 3257 (N-H), 2952(CHO), 1690 (C=O). **HRMS (ESI) m/z: [M+H]** calculated $C_{25}H_{23}N_3O_2$ 398.1868 + found 398.1873 [M+H].



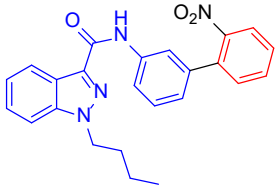
1-Butyl-N-(4-(hydroxymethyl)-[1,1-biphenyl]-3-yl)-1*H*-indazole-3-carboxamide (7f). Appearance: Off white solid, yield = 74.3%, weight = 120 mg, melting point = 79°-82°C, (Eluent = 25% Ethyl acetate/Hexane), **^{1}H NMR** [400 MHz, $CDCl_3$]: δ 8.97 (s, 1H), 8.43 (d, *J* = 7.60 Hz, 1H), 8.01 (s, 1H), 7.74 (d, *J* = 7.20 Hz, 1H), 7.64 (s, 1H), 7.57 (d, *J* = 7.60 Hz, 1H), 7.42-7.44 (m, 4H), 7.26-7.31 (m, 3H), 4.76 (s, 2H), 4.58 (s, 1H), 4.43 (t, *J* = 6.40 Hz, 2H), 1.95-1.97 (m, 2H), 1.36-1.37 (m, 2H), 0.97 (t, *J* = 7.20 Hz, 3H)**. ^{13}C NMR** [100 MHz, $CDCl_3$]: δ 160.71, 141.94, 141.39, 141.12, 138.47, 137.03, 129.76, 129.46, 128.99, 126.95, 126.57, 126.10, 125.87, 122.97, 122.94, 122.84, 122.81, 118.67, 118.44, 114.65, 113.84, 109.44, 49.37, 31.85, 20.08, 13.68. **DEPT-135 NMR** [100 MHz, $CDCl_3$]: δ 129.76, 129.47, 128.99, 126.95, 126.57, 126.10, 125.87, 122.94, 122.84, 122.81, 118.82, 118.67, 118.44, 114.66, 113.84, 109.44, 65.04, 49.38, 31.85, 20.09, 13.68. **FT-IR** (cm-^{1}): 3383 (O-H), 1663 (C=O). **HRMS (ESI) m/z: [M+H]** calculated $C_{25}H_{25}N_3O_2$ 400.2025 + found 400.2027 [M+H].



3-(1-Butyl-1*H*-indazole-3-carboxamido)-[1,1-biphenyl]-3-carboxylic acid (7g). Appearance: Off white solid, yield = 89.8%, weight = 150 mg, melting point = 145°-148°C, (Eluent = 30% Ethyl acetate/Hexane), **^{1}H NMR** [400 MHz, $CDCl_3$]: δ 8.95 (s, 1H), 8.38 (d, *J* = 8.00 Hz, 1H), 8.33 (s, 1H), 8.04 (d, *J* = 7.60 Hz, 1H), 7.95 (s, 1H), 7.84 (d, *J* = 7.60 Hz, 1H), 7.78 (d, *J* = 8.00 Hz, 1H), 7.48 (t, *J* = 7.60 Hz, 1H), 7.32-7.34 (m, 4H), 4.37 (t, *J* = 7.20 Hz, 2H), 1.90 (q, *J* = 7.20 Hz, 2H), 1.27-1.29 (m, 2H), 0.90 (t, *J* = 7.20 Hz, 3H). **^{13}C NMR** [100 MHz, $CDCl_3$]: δ 175.23, 160.68, 141.29, 141.12, 140.91, 138.71, 132.56, 129.67, 129.17, 129.00, 128.90, 126.94, 122.99, 122.93, 122.88, 122.75, 119.08, 118.37, 109.43, 49.38, 31.86, 20.09, 13.68. **DEPT-135 NMR** [100 MHz, $CDCl_3$]: δ 135.56, 129.67, 129.17, 129.00, 128.89, 126.95, 122.94, 122.88, 122.76, 119.08, 118.37, 109.43, 49.38, 31.86, 20.09, 13.68. **FT-IR** (cm-^{1}): 3281 (N-H), 1715 (C=O). **HRMS (ESI) m/z: [M+H]** calculated $C_{25}H_{23}N_3O_3$ 414.1817 + found 414.1818 [M+H].



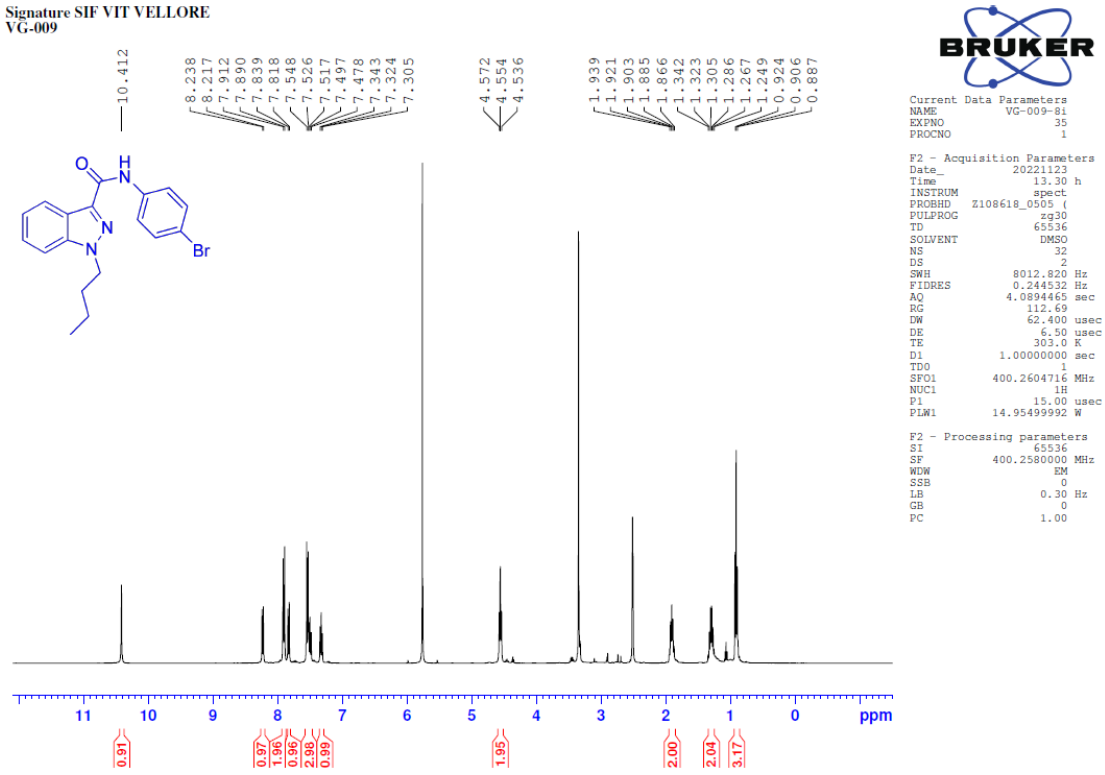
1-Butyl-N-(4-(methylsulfonyl)-[1,1-biphenyl]-3-yl)-1*H*-indazole-3-carboxamide (7h). Appearance**:** Off white solid, yield = 94.4 %, weight = 170 mg, melting point = 110°-106°C, (Eluent = 25% Ethyl acetate/Hexane), **^{1}H NMR** [400 MHz, $CDCl_3$]: δ 8.91 (s, 1H), 8.36 (d, *J* = 8.00 Hz, 1H), 8.12 (d, *J* = Hz, 1H), 7.94 (d, *J* = 8.40 Hz, 2H), 7.77 (d, *J* = 8.00 Hz, 2H), 7.65 (d, *J* = 7.60 Hz, 1H), 7.38-7.40 (m, 3H), 7.30 (d, *J* = 7.60 Hz, 1H), 7.19 (s, 1H), 4.38 (t, *J* = 7.20 Hz, 2H), 3.03 (s, 3H), 0.91 (q, *J* = 7.20 Hz, 2H), 1.27-1.29 (m, 2H), 0.91 (t, *J* = 7.20 Hz, 3H). **^{13}C NMR** [100 MHz, $CDCl_3$]: δ 159.70, 145.41, 140.13, 139.08, 138.27, 137.88, 135.90, 128.73, 127.16, 125.98, 121.99, 121.96, 121.82, 121.76, 118.71, 108.45, 48.37, 43.65, 30.81, 19.05, 12.63. **DEPT-135 NMR** [100 MHz, $CDCl_3$]: δ 128.72, 127.15, 126.85, 125.97, 121.98, 121.81, 121.72, 118.68, 117.57, 108.46, 48.36, 43.64, 30.81, 19.04, 12.64. **FT-IR** (cm-^{1}): N-H (3336), 1669 (C=O). **HRMS (ESI) m/z: [M+H]** calculated $C_{25}H_{25}N_3O_3S$ 448.1695 + found 448.1876 [M+H].



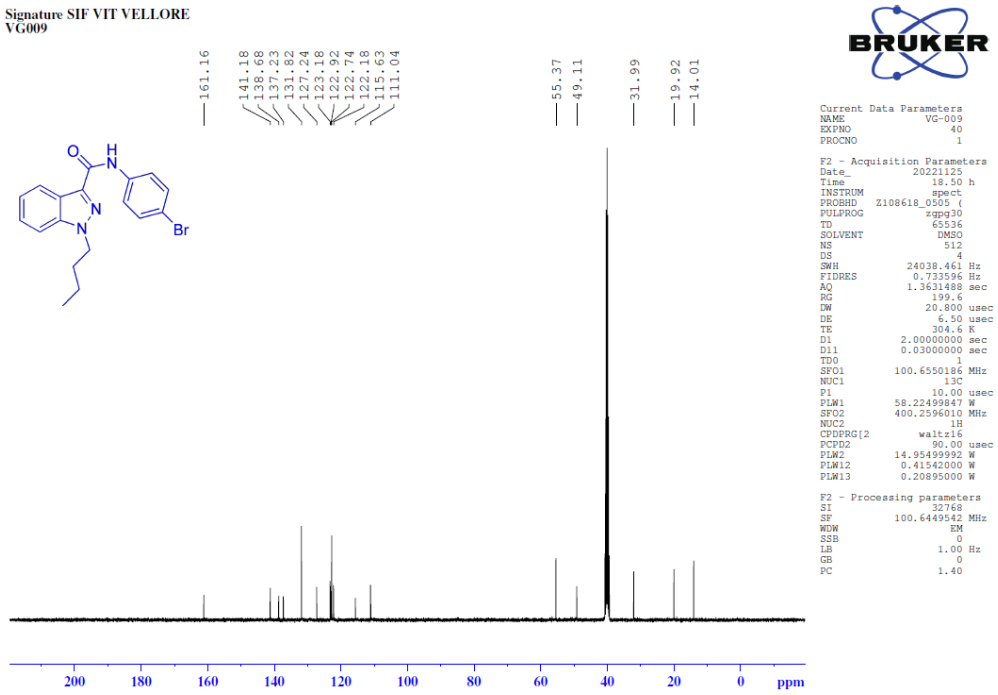
1-Butyl-N-(2-nitro-[1,1-biphenyl]-3-yl]-1*H*-indazole-3-carboxamide (7i). Appearance: Off white solid, yield = 71.8%, weight = 120 mg, melting point = 99°-104°C, (Eluent = 15% Ethyl acetate/Hexane), **^{1}H NMR** [400 MHz, $CDCl_3$]: δ 8.93 (s, 1H), 8.42

(d, *J* = 8.00 Hz, 1H), 7.89 (d, *J* = 8.00 Hz, 1H), 7.80 (d, *J* = 9.20 Hz, 1H), 7.62 (d, *J* = 7.20 Hz, 1H), 7.52 (d, *J* = 6.00 Hz, 1H), 7.43-7.44 (m, 3H), 7.32 (t, *J* = 6.00 Hz, 1H), 7.26 (s, 1H), 7.07 (d, *J* = 7.60 Hz, 1H), 4.44 (t, *J* = 7.20 Hz, 2H), 0.00 (q, *J* = 7.60 Hz, 2H), 1.33-1.35 (m, 2H), 0.98 (t, *J* = 7.20 Hz, 3H). **^{13}C NMR** [100 MHz, $CDCl_3$]: δ 160.61, 149.20, 141.11, 138.43, 138.39, 136.92, 136.16, 132.35, 129.36, 128.30, 126.91, 124.10, 123.39, 122.96, 122.82, 119.37, 119.12, 109.44, 49.36, 31.82, 20.07, 13.67. **DEPT-135 NMR** [100 MHz, $CDCl_3$]: δ 132.35, 132.15, 129.37, 128.30, 126.92, 124.11, 123.39, 122.92, 122.82, 119.37, 119.12, 109.14. **FT-IR** (cm^{-1}): N-H (3384), C=O (1676), NO_2 (1524). **HRMS (ESI) m/z: [M+H]** calculated $C_{25}H_{22}N_3O_3$ 414.1770 + found 415.1771 [M+H].

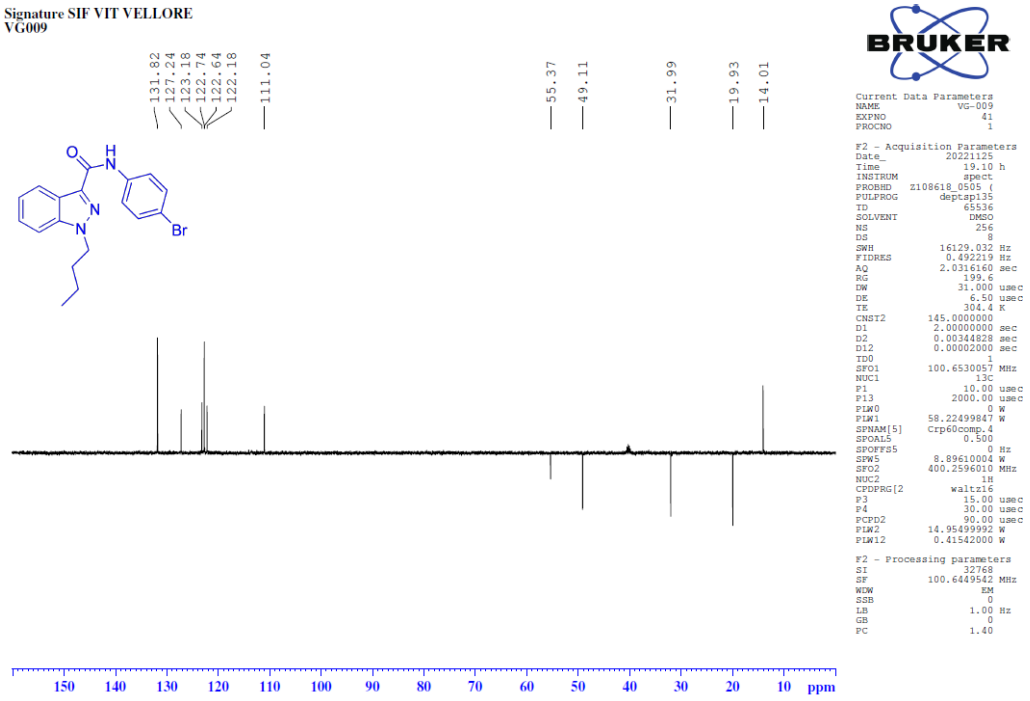
^{1}H-NMR [400MHz, DMSO-d_6] spectrum of N-(4-Bromophenyl)-1-butyl-1*H*-indazole-3-carboxamide (3).



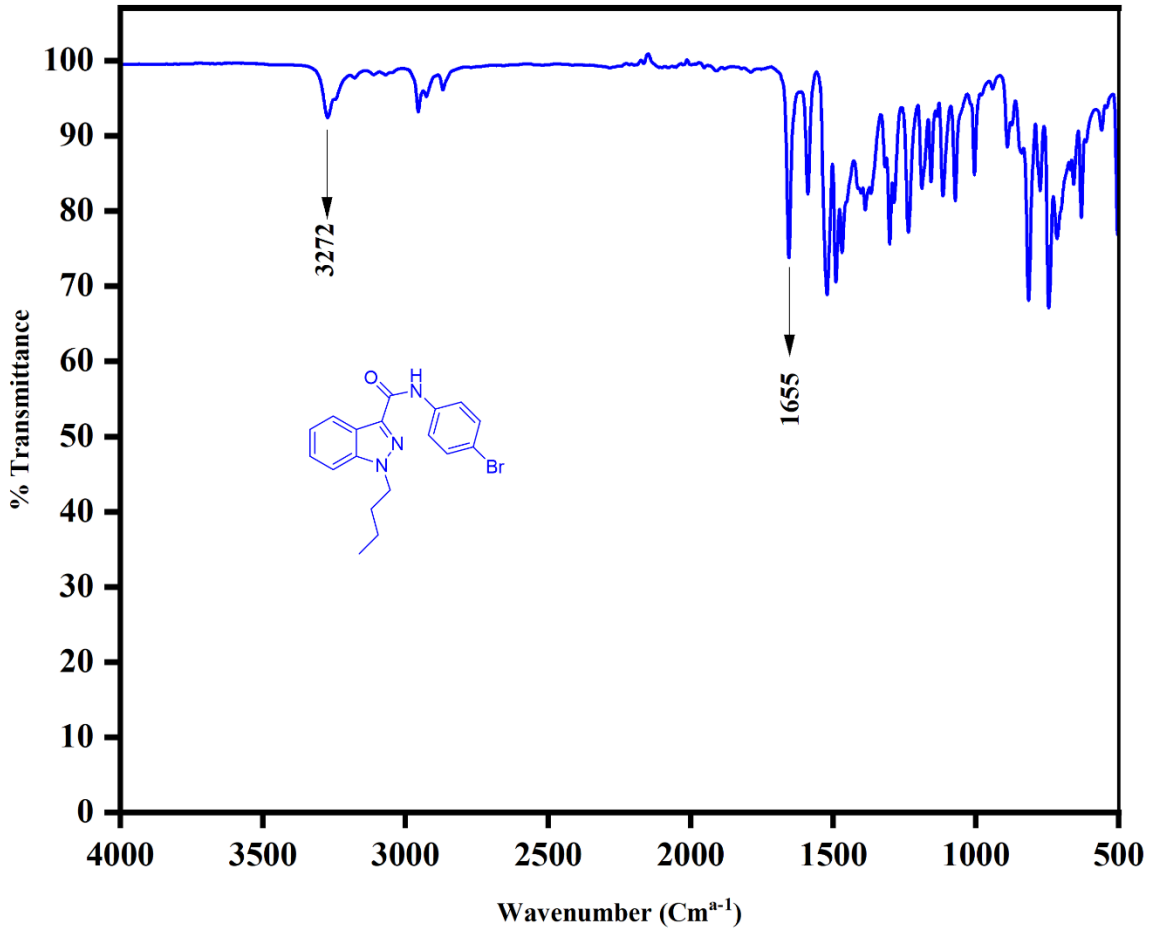
^{13}C-NMR [100MHz, DMSO-d_6] spectrum of N-(4-Bromophenyl)-1-butyl-1*H*-indazole-3-carboxamide (3).



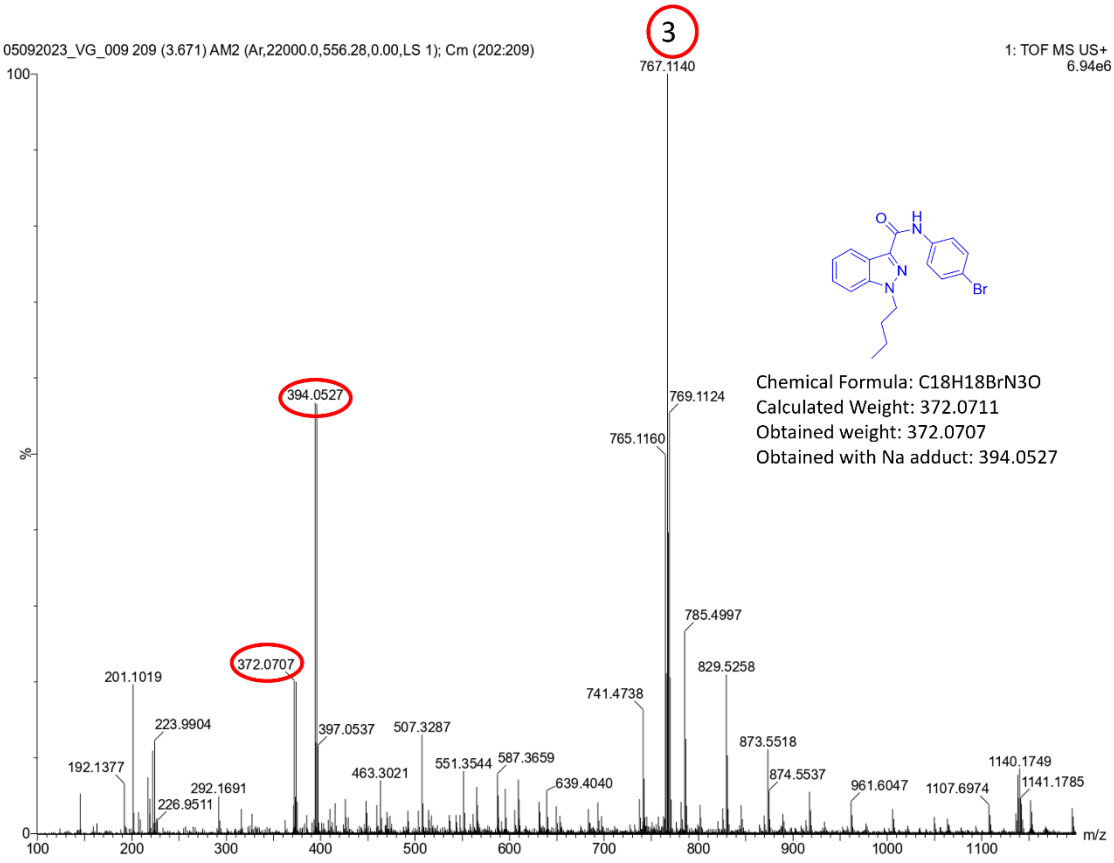
135-DEPT-NMR [100MHz, DMSO-d_6] spectrum of N-(4-Bromophenyl)-1-butyl-1*H*-indazole-3-carboxamide (3).



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



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



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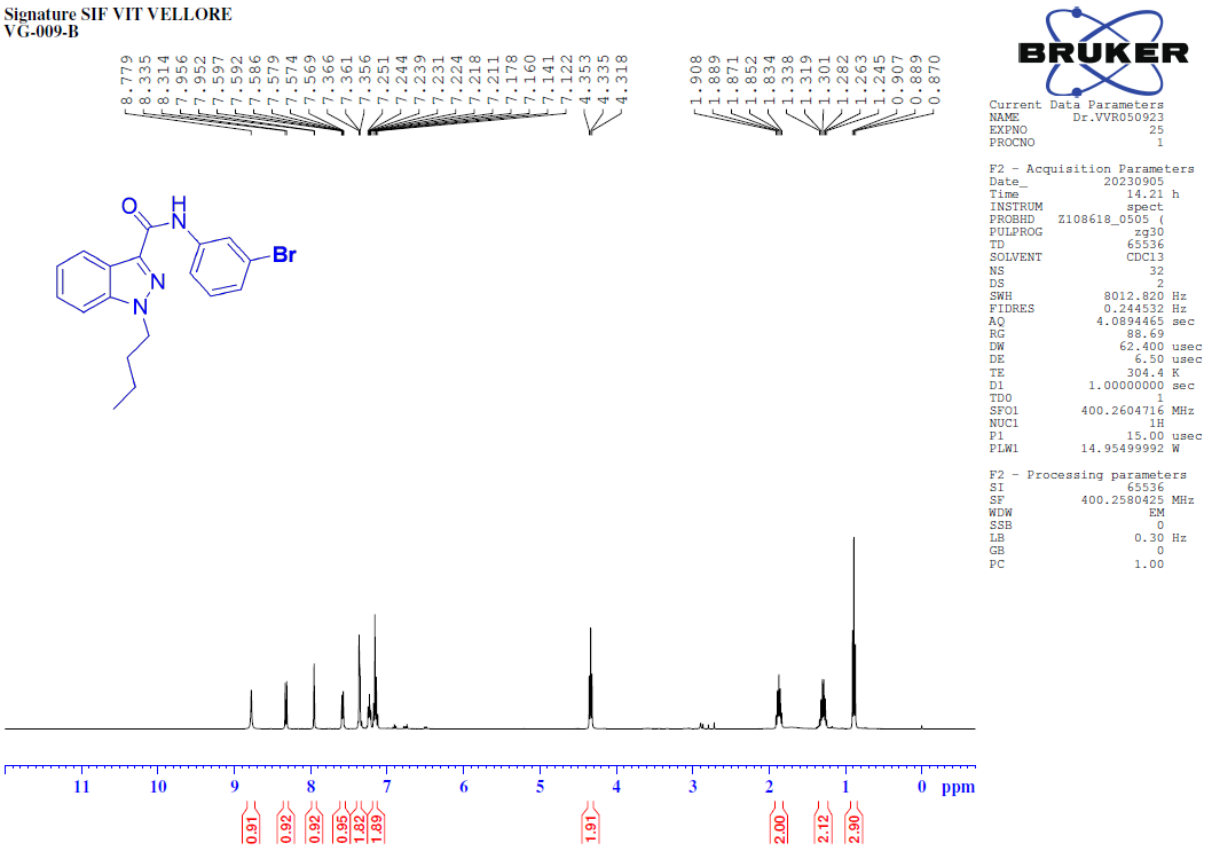
^{1}H-NMR [400MHz, DMSO-d_6] spectrum of 1-butyl-N-(6-methylpyridine-2yl)-1*H*-indazole-3-carboxamide (4).



BRUKER

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TE                304.4 K
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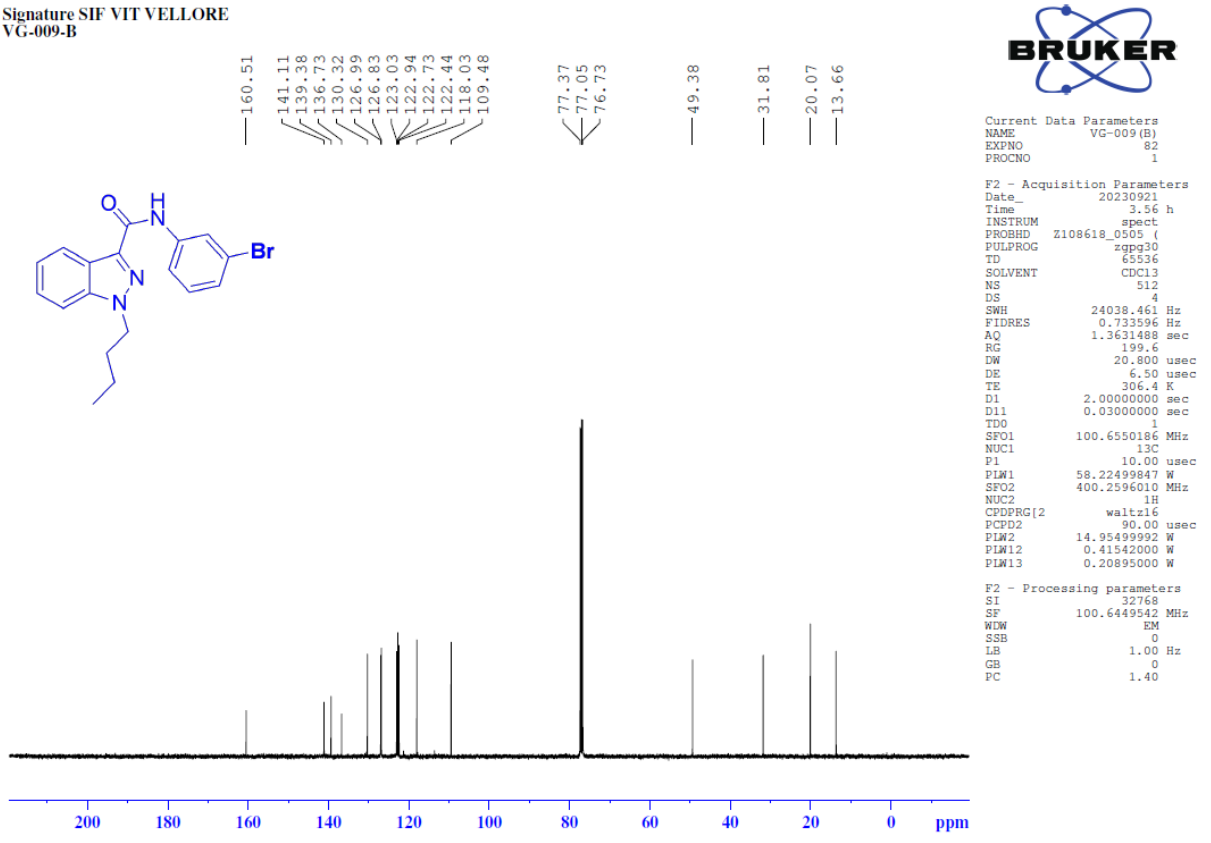
^{13}C-NMR [100MHz, DMSO-d_6] spectrum of 1-butyl-N-(6-methylpyridine-2yl)-1*H*-indazole-3-carboxamide (4).



BRUKER

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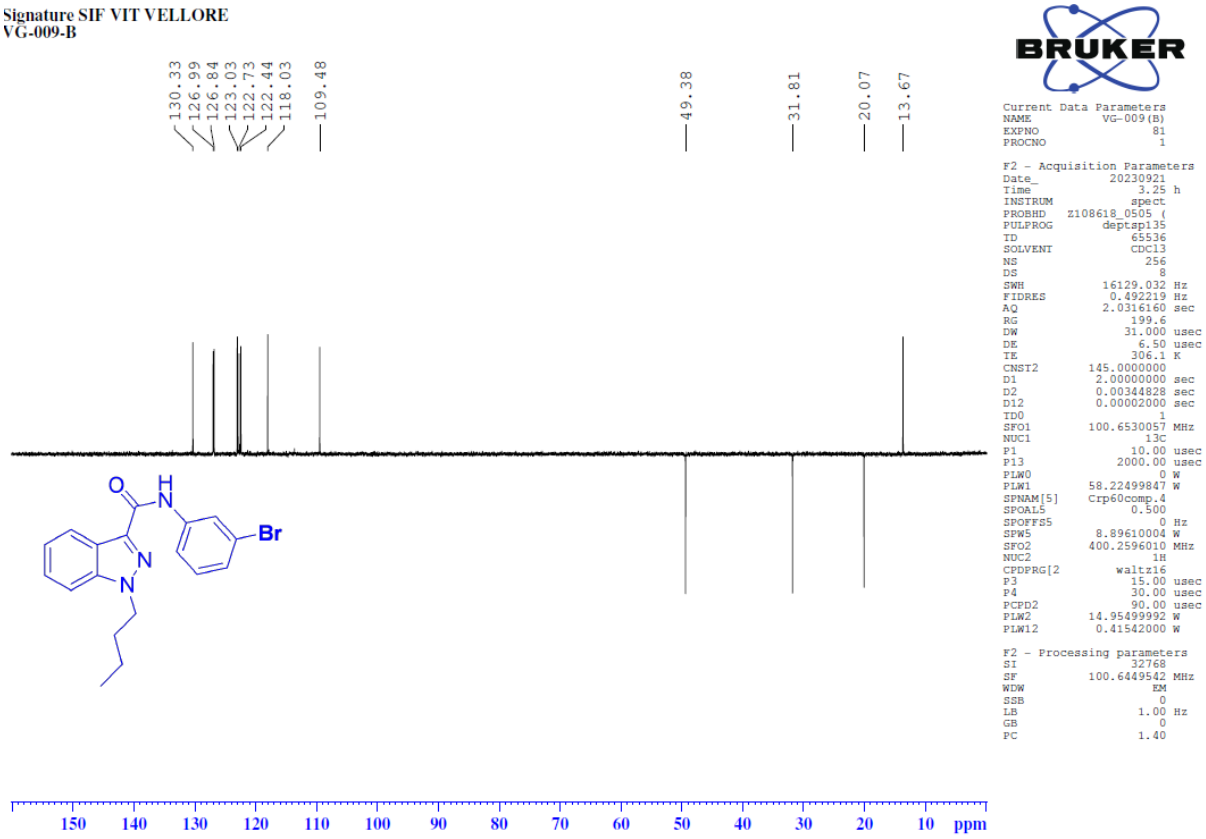
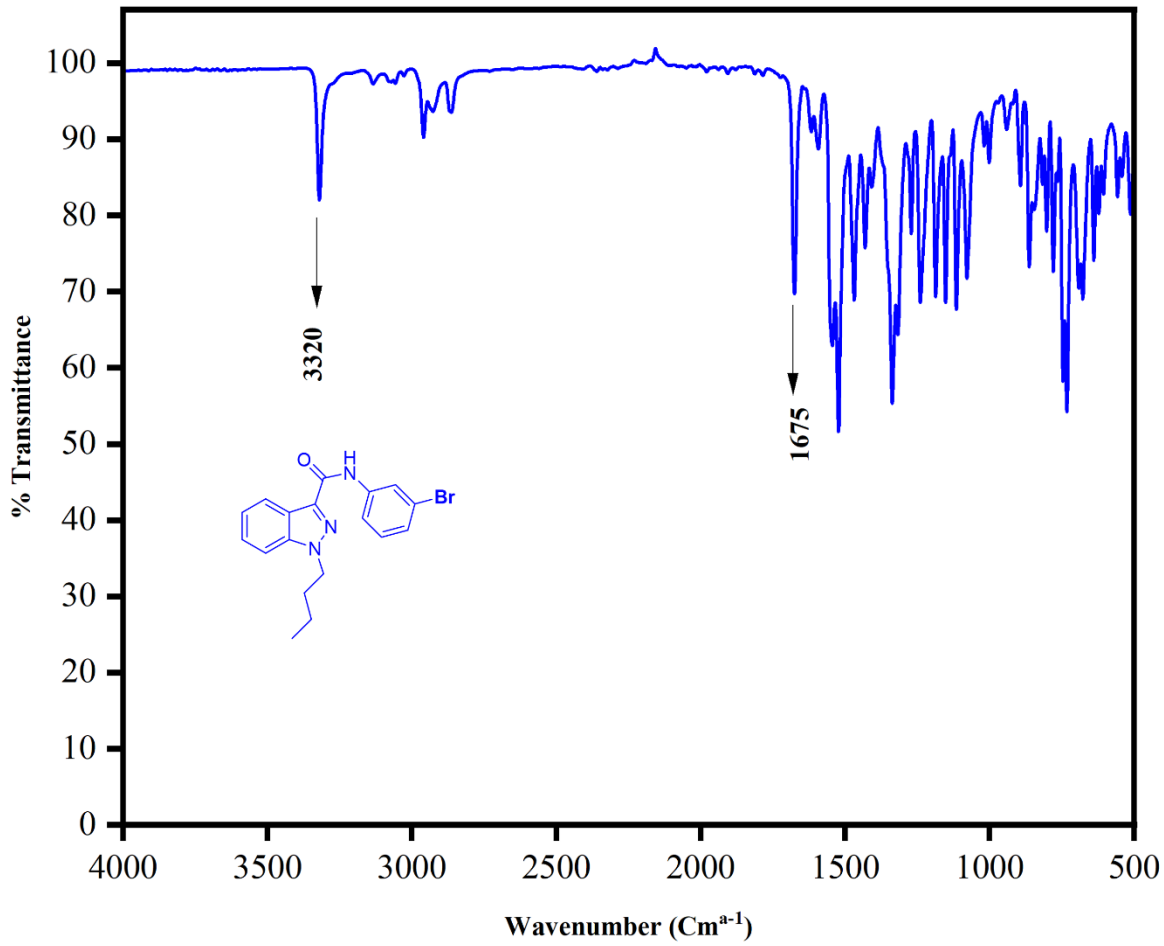
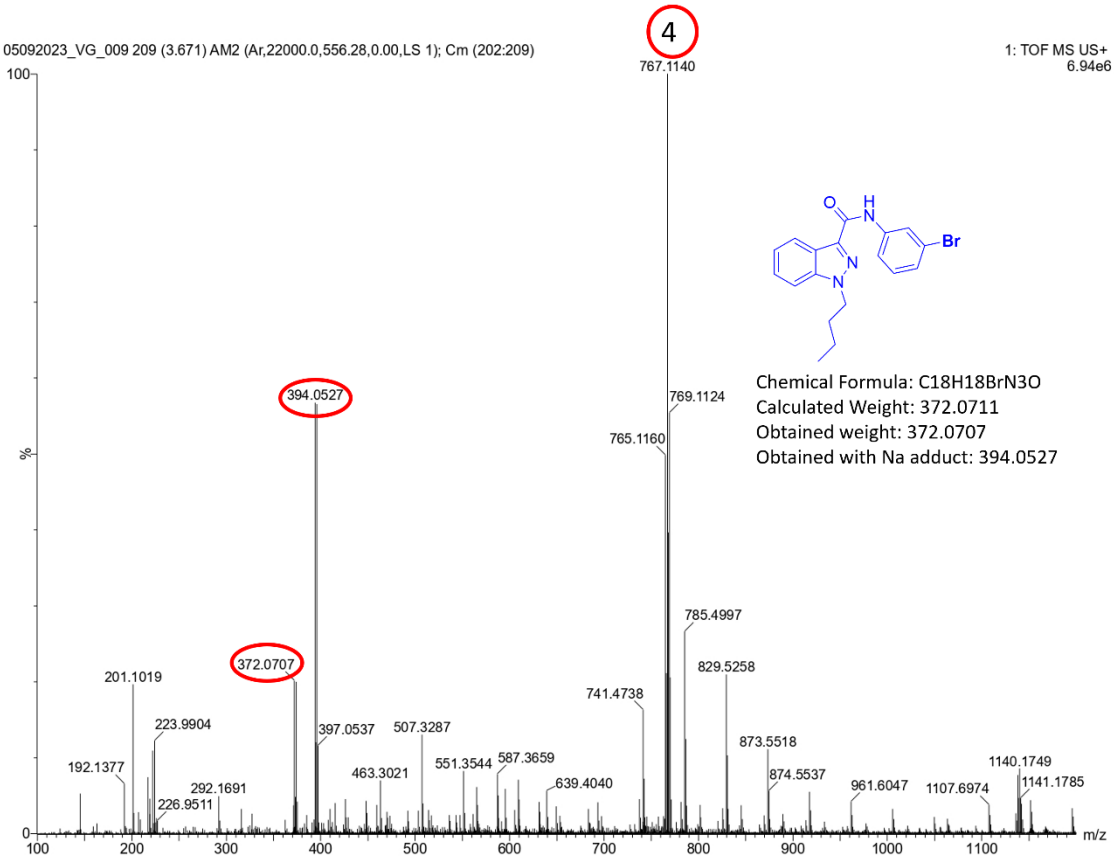
135-DEPT-NMR [100MHz, DMSO-d_6] spectrum of 1-butyl-N-(6-methylpyridine-2yl)-1*H*-indazole-3-carboxamide (4).



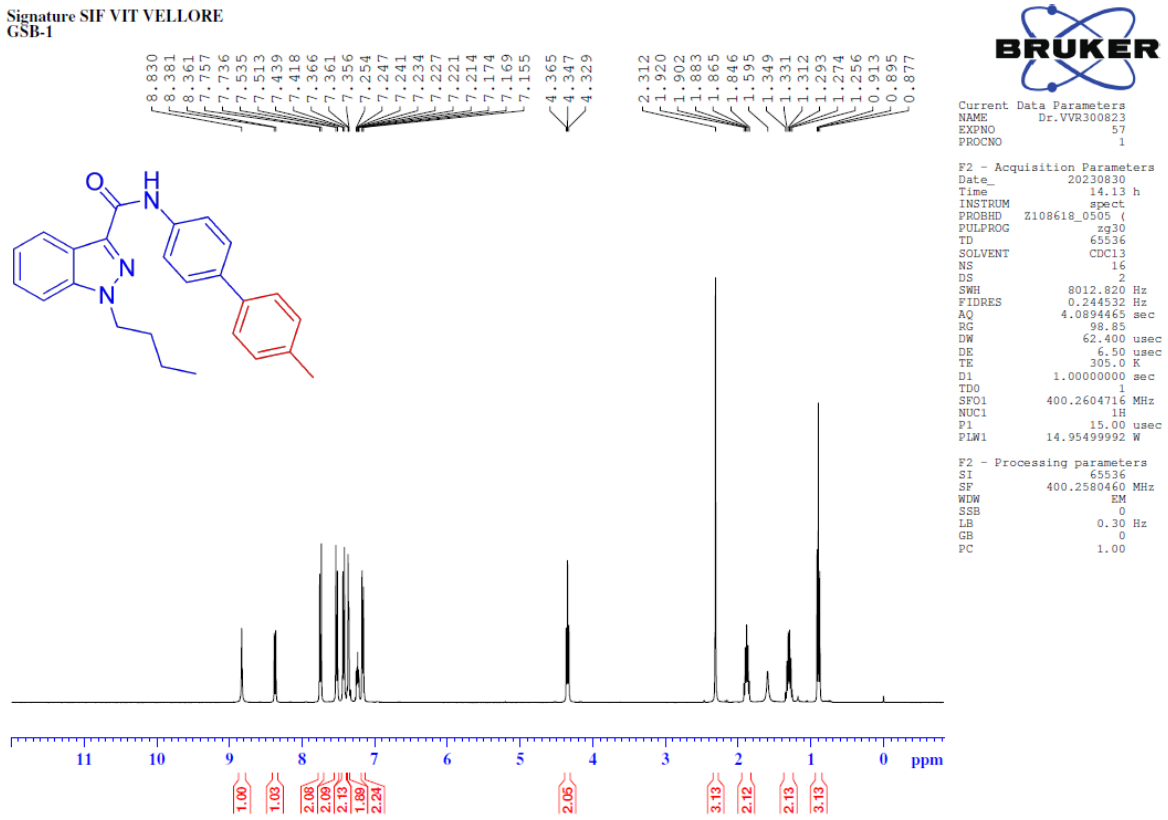
FT-IR spectrum of 1-butyl-N-(6-methylpyridine-2yl)-1*H*-indazole-3-carboxamide (4).



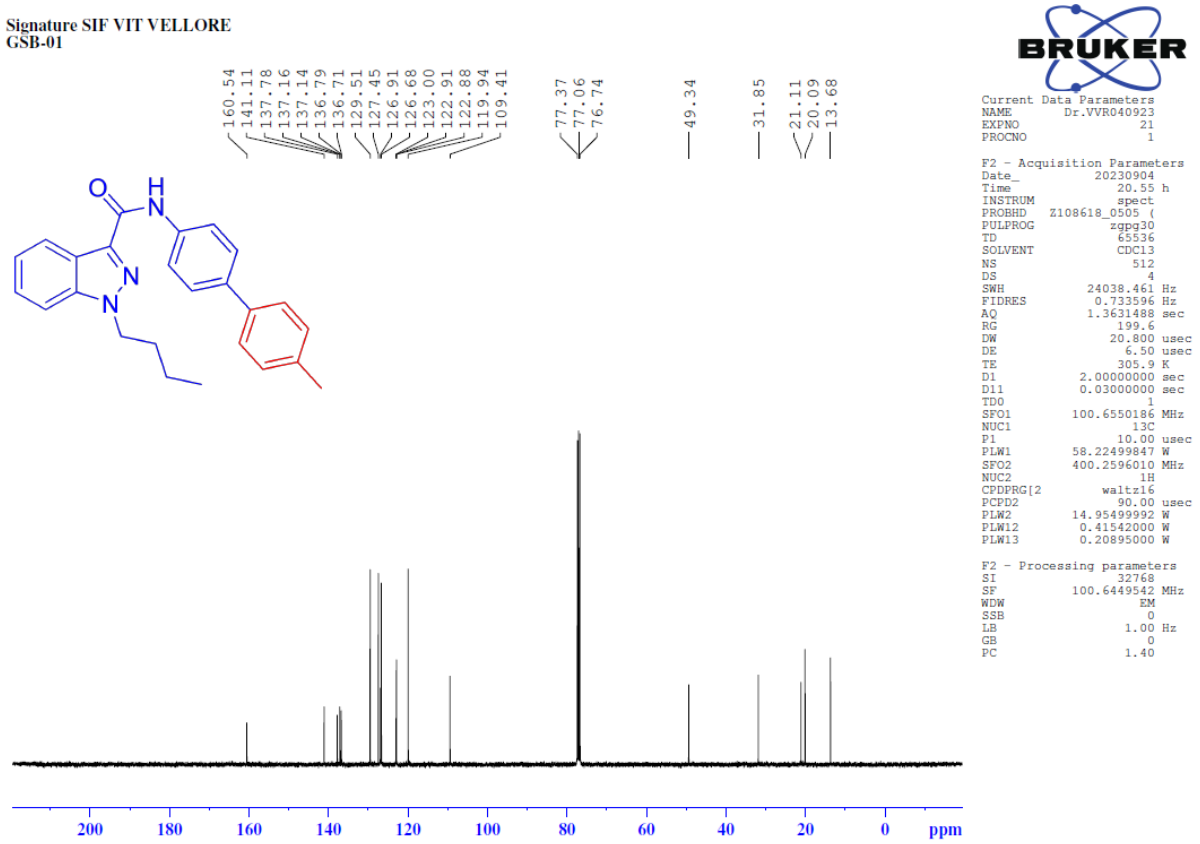
HRMS of 1-butyl-N-(6-methylpyridine-2yl)-1*H*-indazole-3-carboxamide (4).



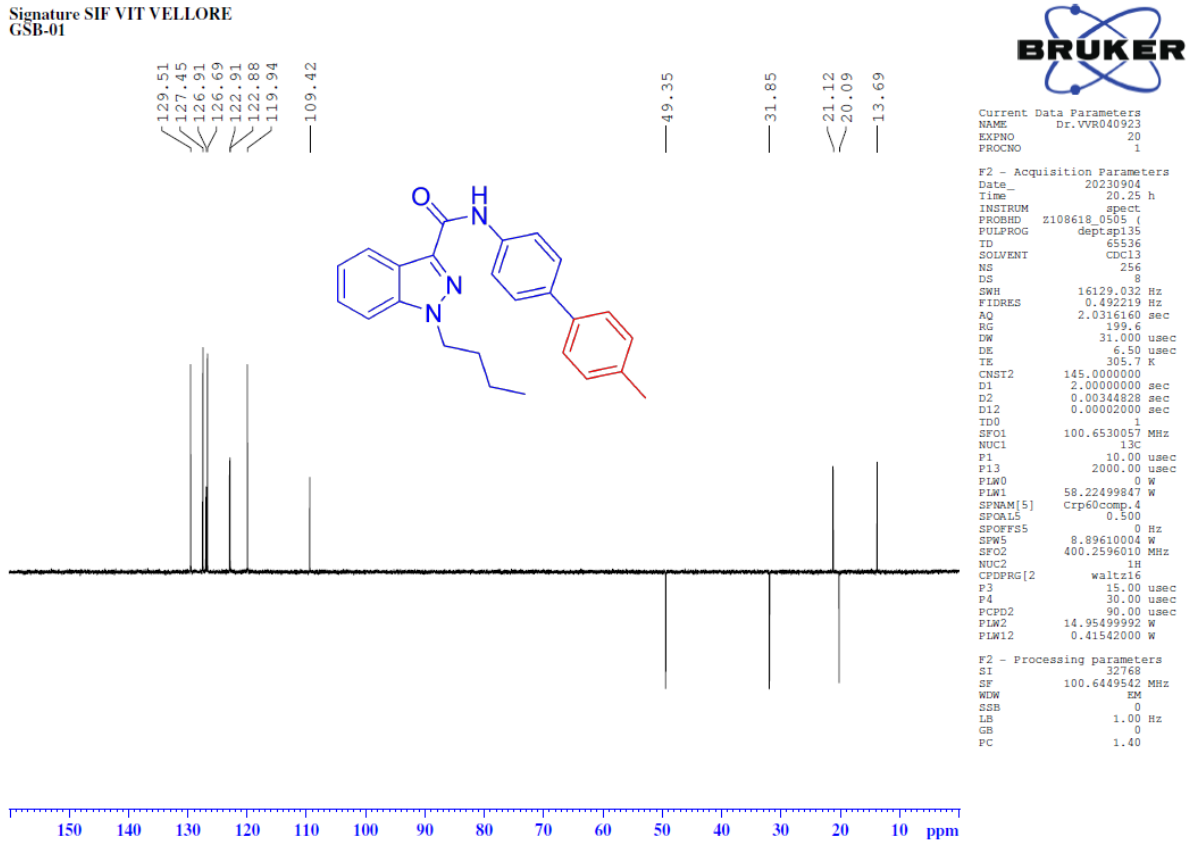
^{1}H-NMR [400MHz, $CDCl_3$] spectrum of 1-butyl-N-(4-methyl-[1,1-biphenyl]-4-yl)-1*H*-indazole-3-carboxamide (6a).



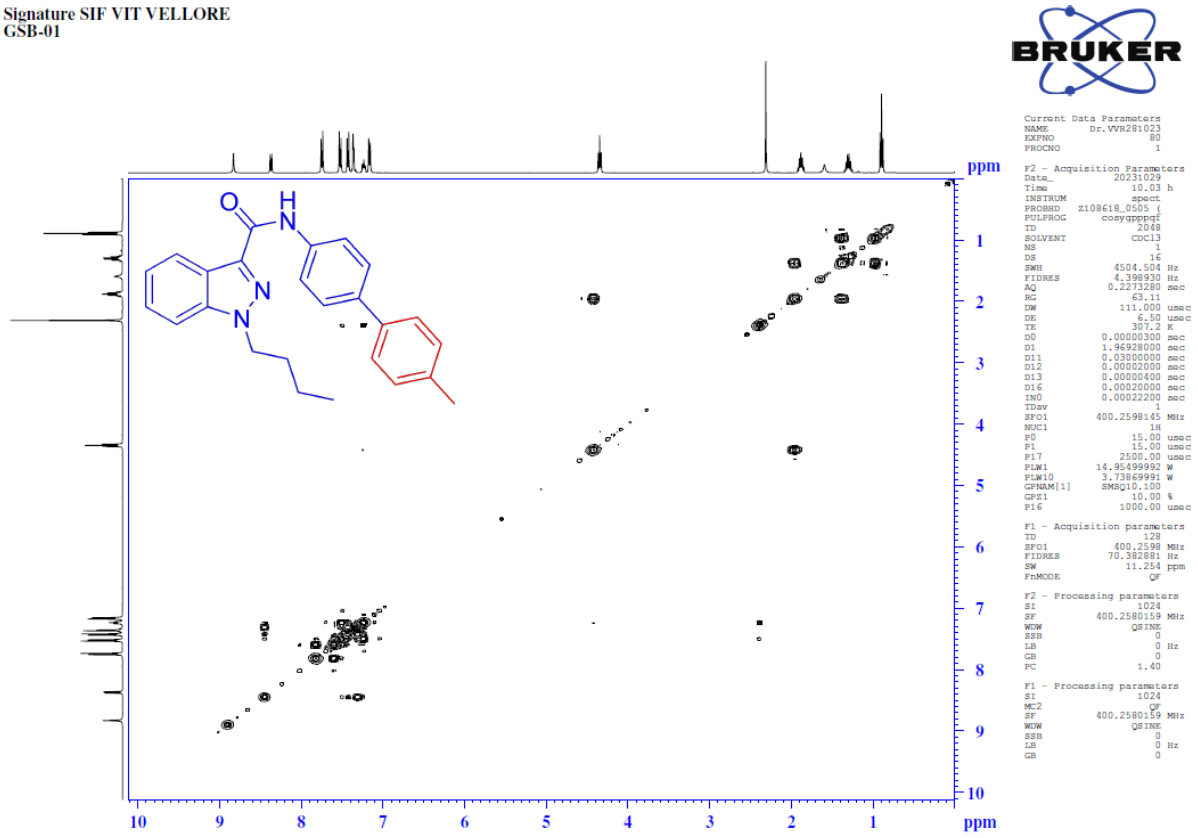
^{13}C-NMR [100MHz, $CDCl_3$] spectrum of 1-butyl-N-(4-methyl-[1,1-biphenyl]-4-yl)-1*H*-indazole-3-carboxamide (6a).



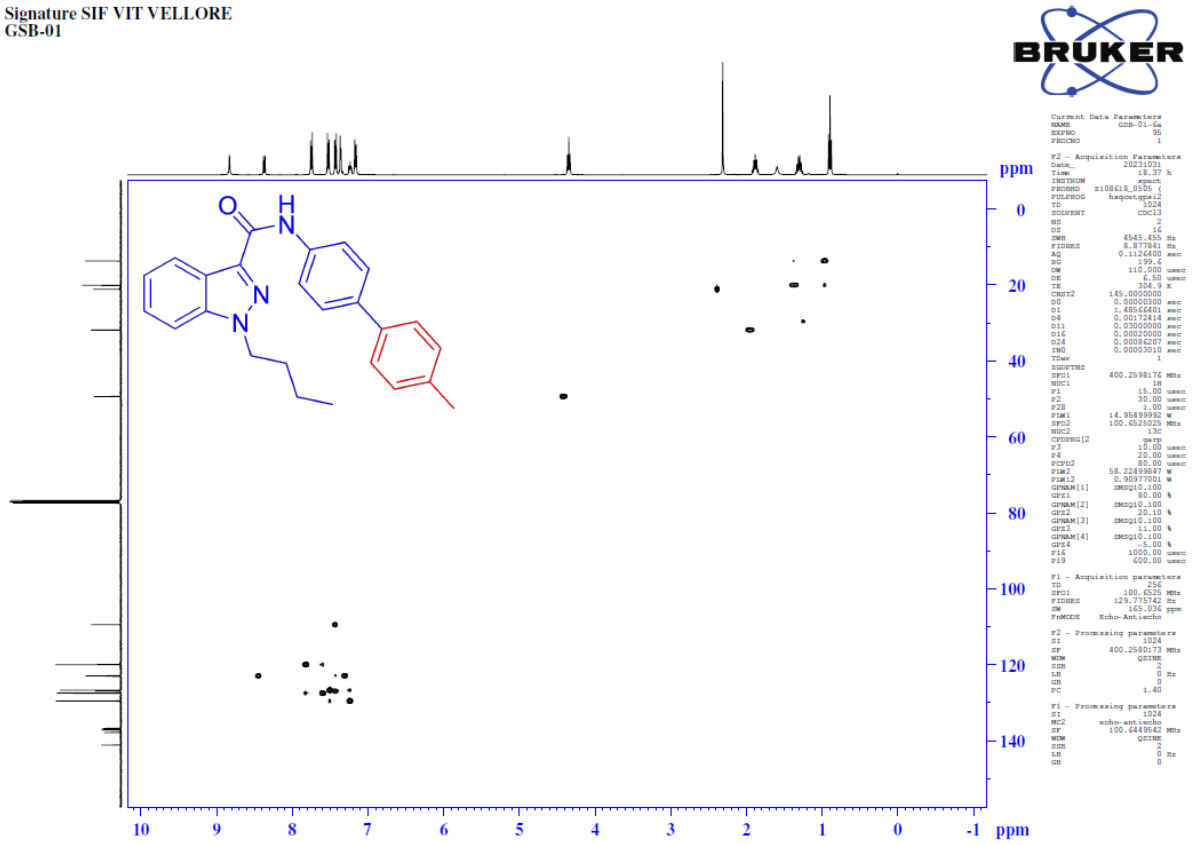
DEPT135-NMR [100MHz, $CDCl_3$] spectrum of 1-butyl-N-(4-methyl-[1,1-biphenyl]-4-yl)-1*H*-indazole-3-carboxamide (6a).



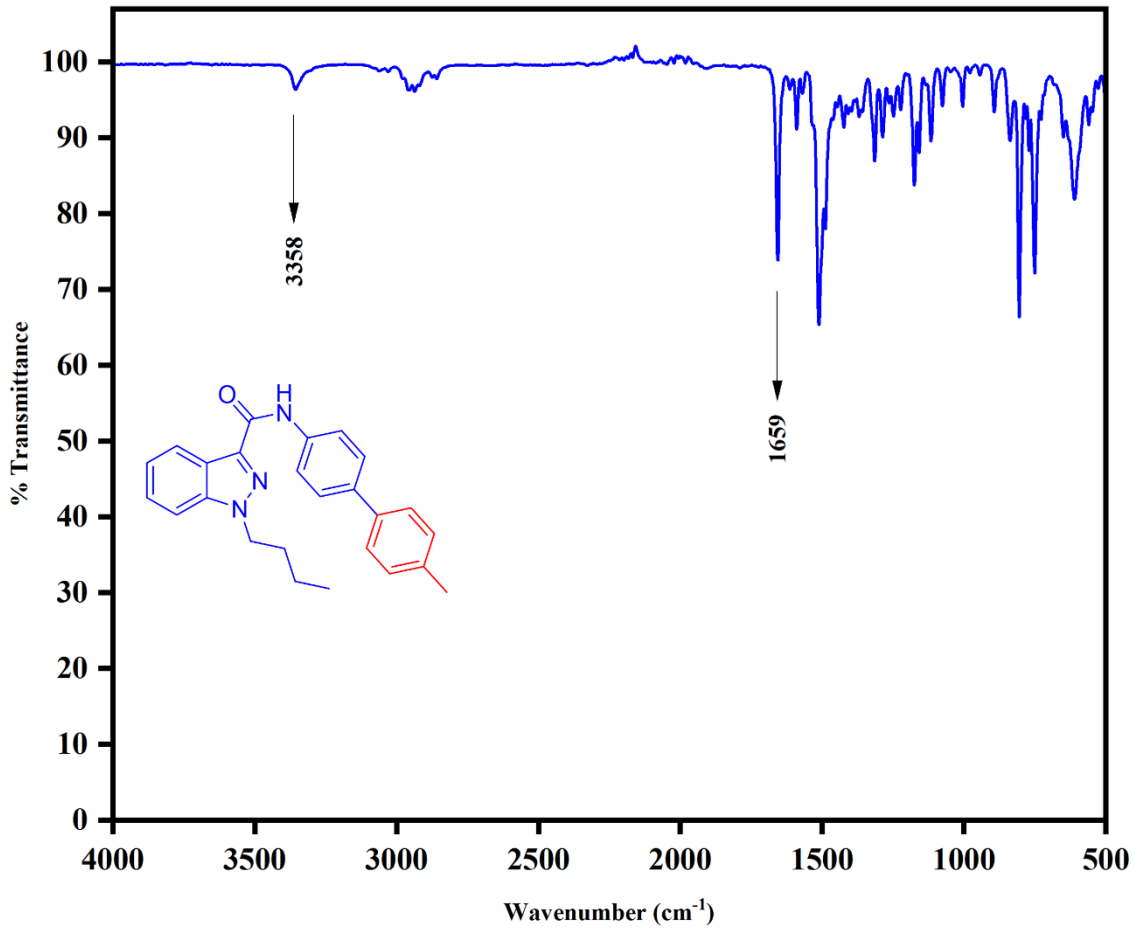
COSY-NMR [400MHz, $CDCl_3$] spectrum of 1-butyl-N-(4-methyl-[1,1-biphenyl]-4-yl)-1*H*-indazole-3-carboxamide (6a).



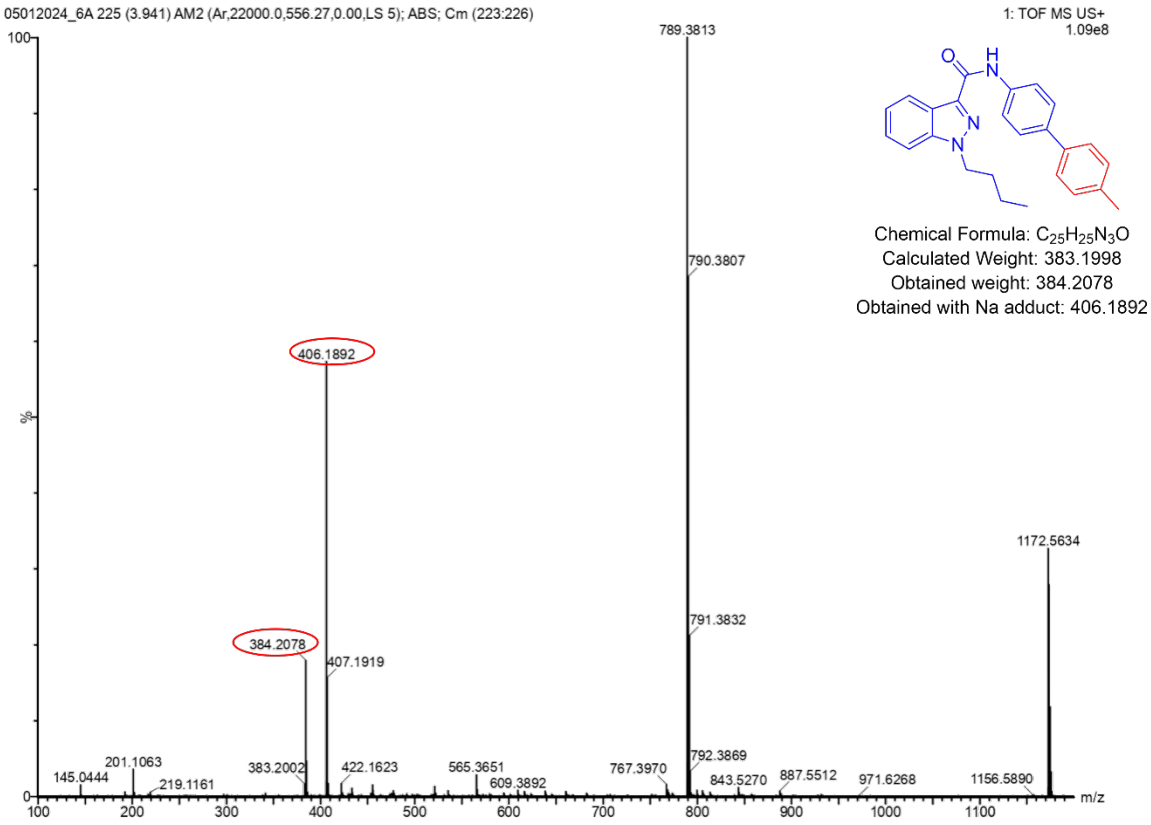
HSQC-NMR [400MHz, $CDCl_3$] spectrum of 1-butyl-N-(4-methyl-[1,1-biphenyl]-4-yl)-1*H*-indazole-3-carboxamide (6a).



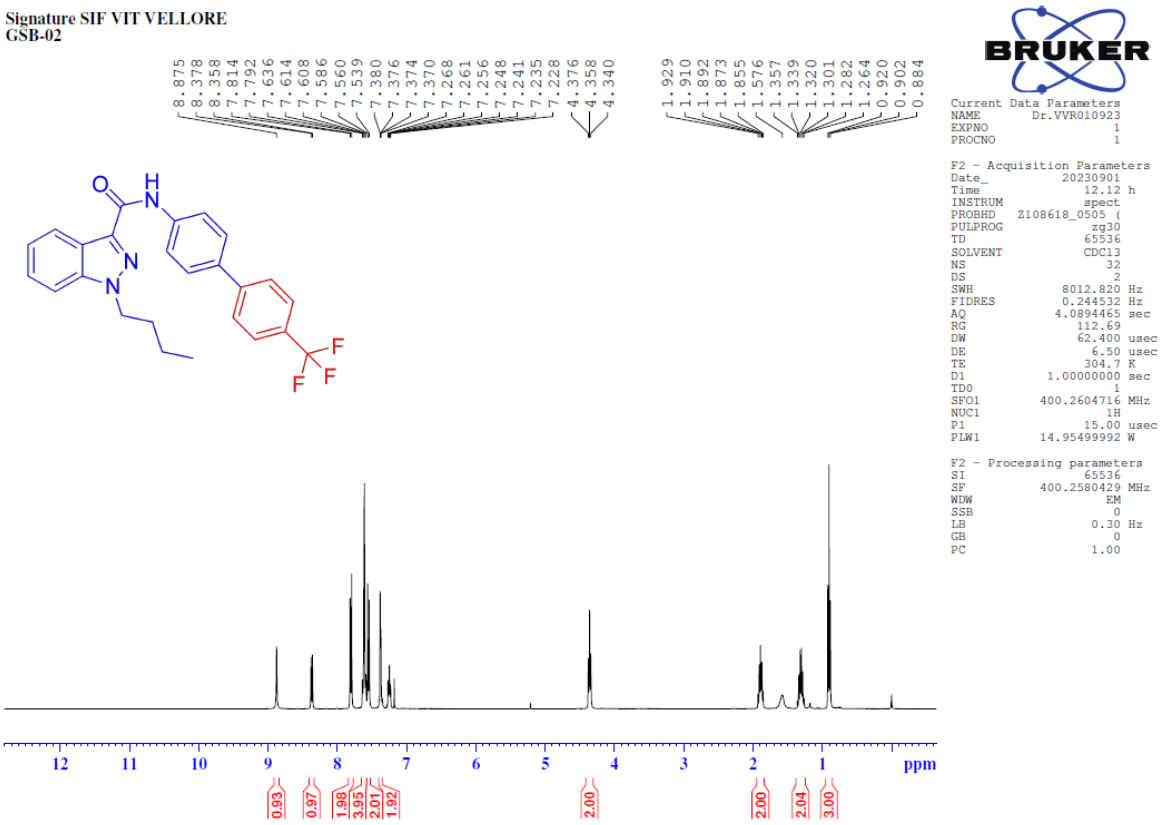
FT-IR Spectrum of 1-butyl-N-(4-methyl-[1,1-biphenyl]-4-yl)-1*H*-indazole-3-carboxamide (6a).



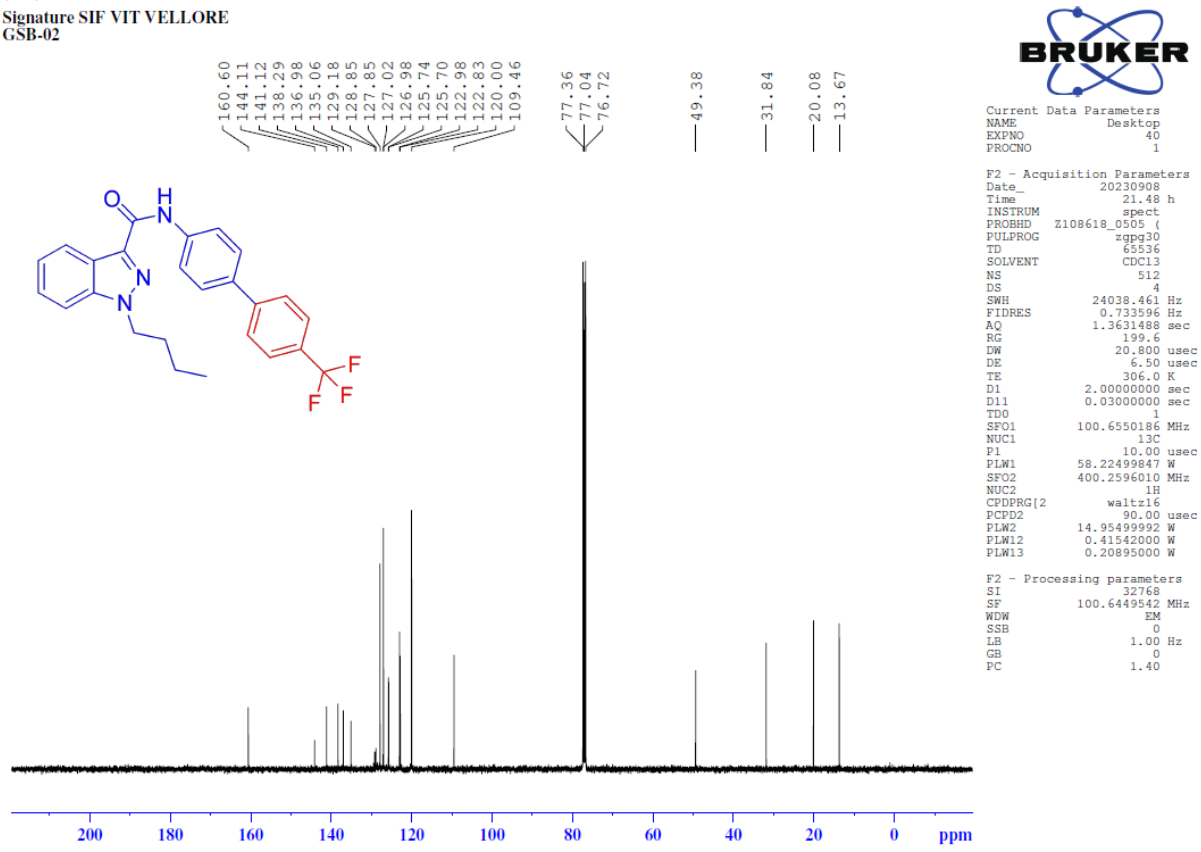
HRMS of 1-butyl-N-(4-methyl-[1,1-biphenyl]-4-yl)-1*H*-indazole-3-carboxamide (6a).



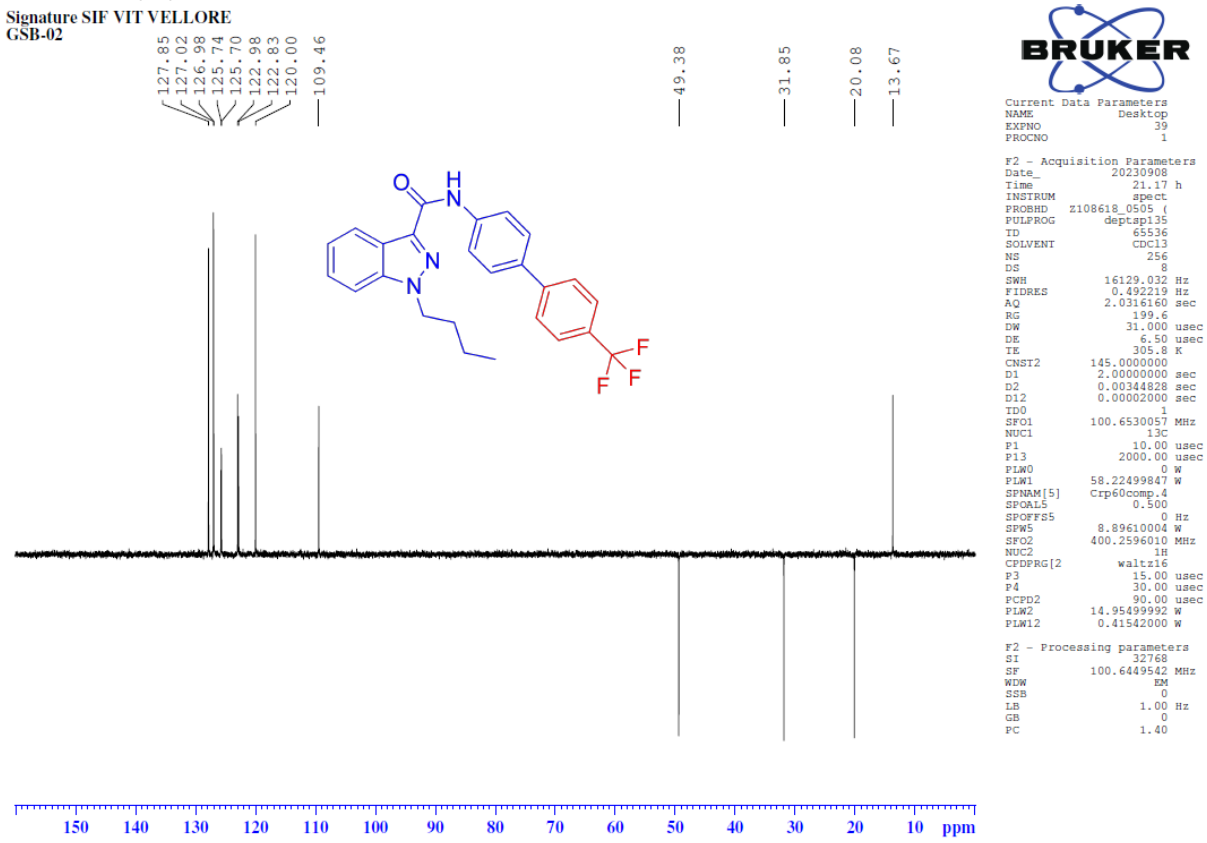
[1]H-NMR [400MHz, $CDCl_3$] spectrum of 1-butyl-N-(4-(trifluoromethyl)-[1,1-biphenyl]-4-yl)-1*H*-indazole-3-carboxamide (6b).



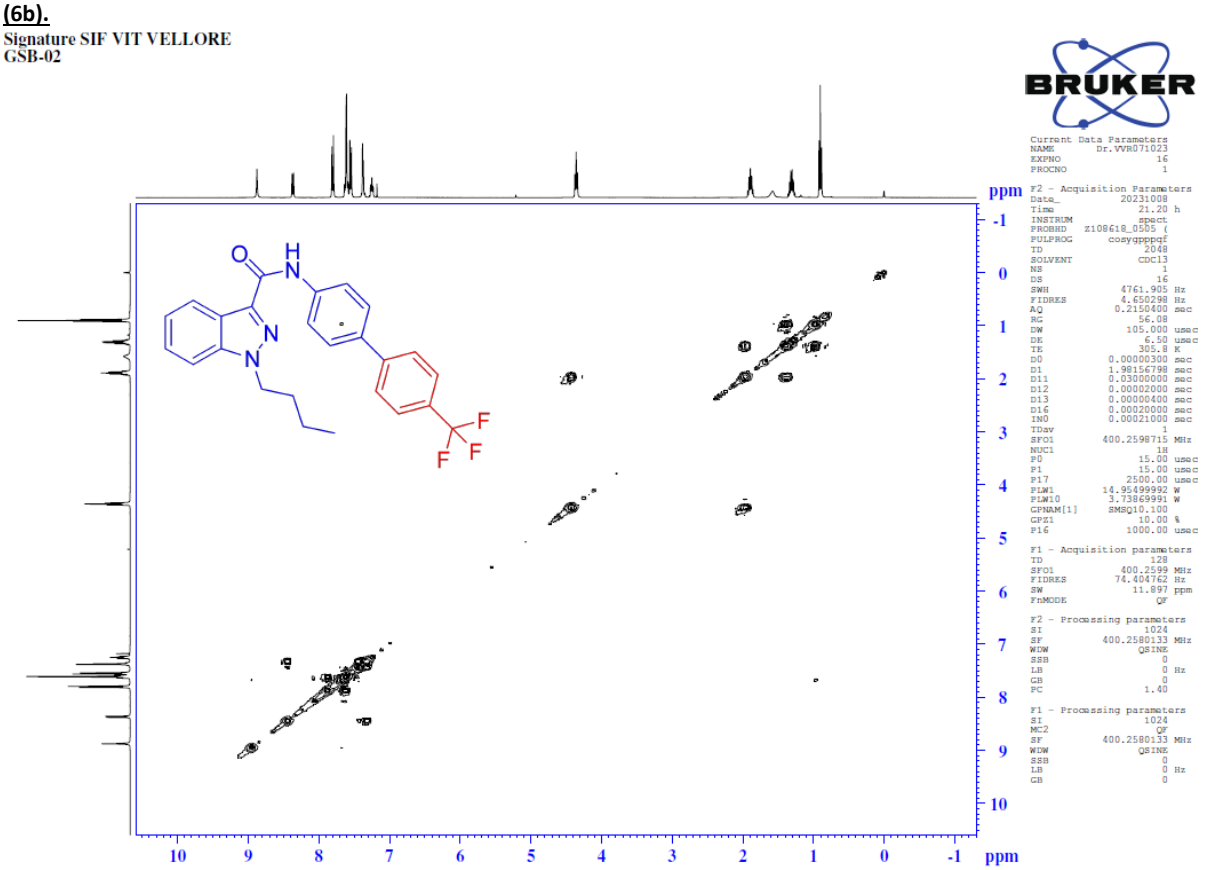
<u>^{13}C-NMR [100MHz, $CDCl_3$] spectrum of 1-butyl-N-(4-(trifluoromethyl)-[1,1-biphenyl]-4-yl)-1*H*-indazole-3-carboxamide (6b).</u>



DEPT135-NMR [100MHz, $CDCl_3$] spectrum of 1-butyl-N-(4-(trifluoromethyl)-[1,1-biphenyl]-4-yl)-1*H*-indazole-3-carboxamide (6b).

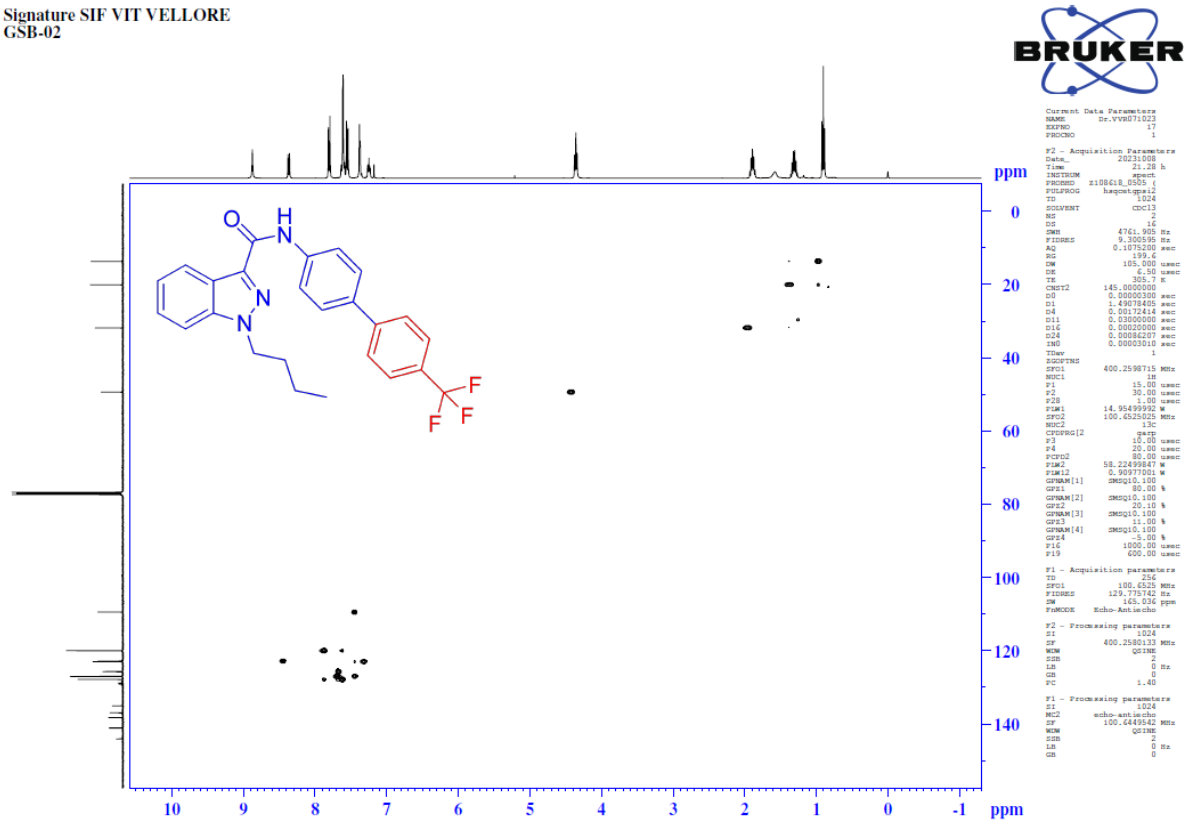


COSY-NMR [400MHz, $CDCl_3$] spectrum of 1-butyl-N-(4-(trifluoromethyl)-[1,1-biphenyl]-4-yl)-1*H*-indazole-3-carboxamide (6b).

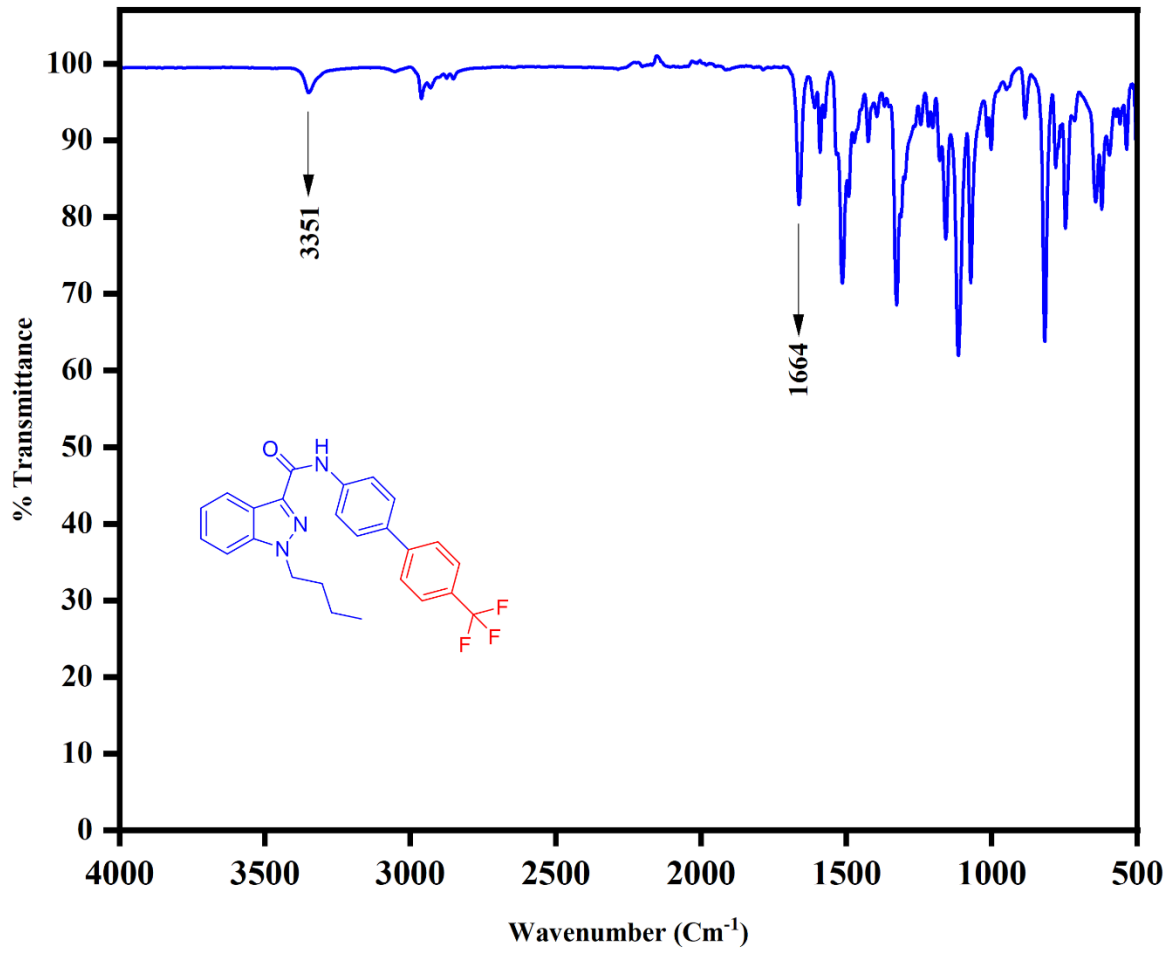


HSQC-NMR [400MHz, $CDCl_3$] spectrum of 1-butyl-N-(4-(trifluoromethyl)-[1,1-biphenyl]-4-yl)-1*H*-indazole-3-carboxamide

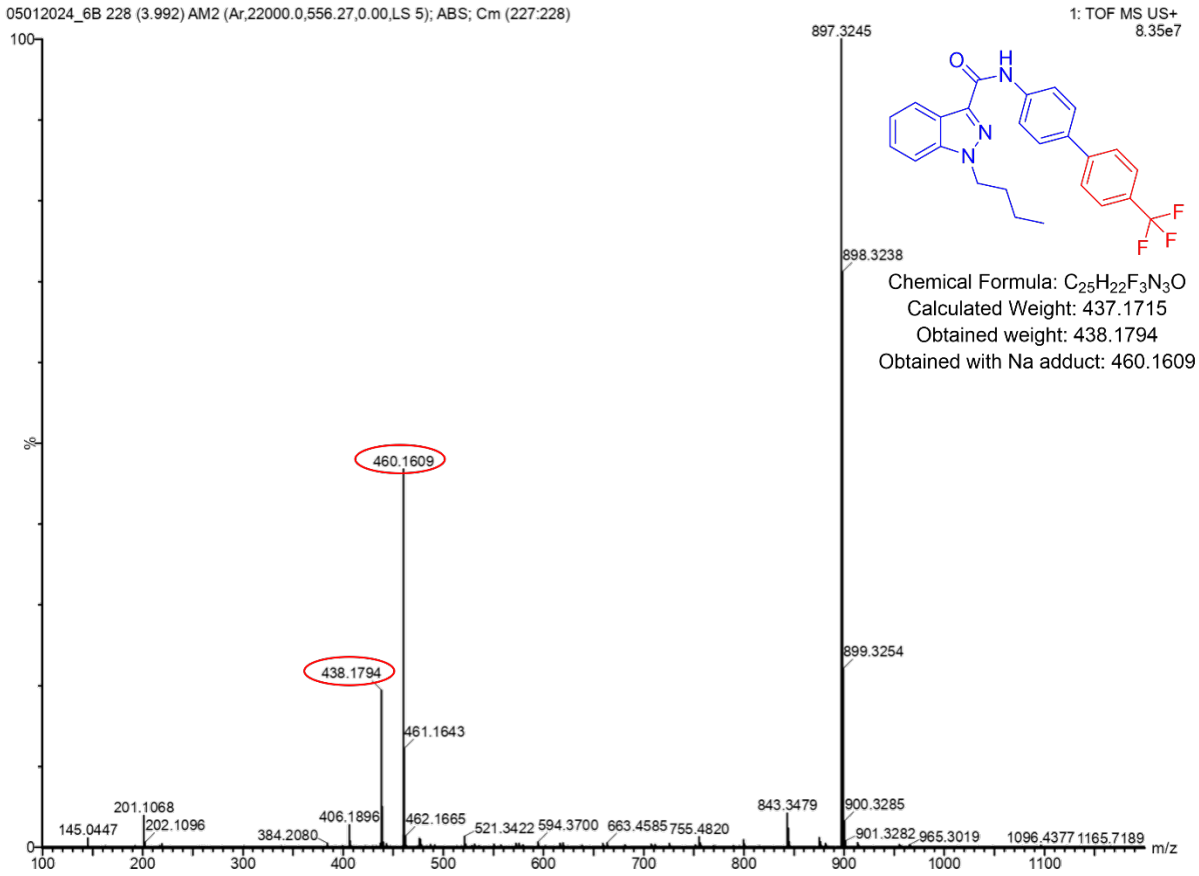
(6b).



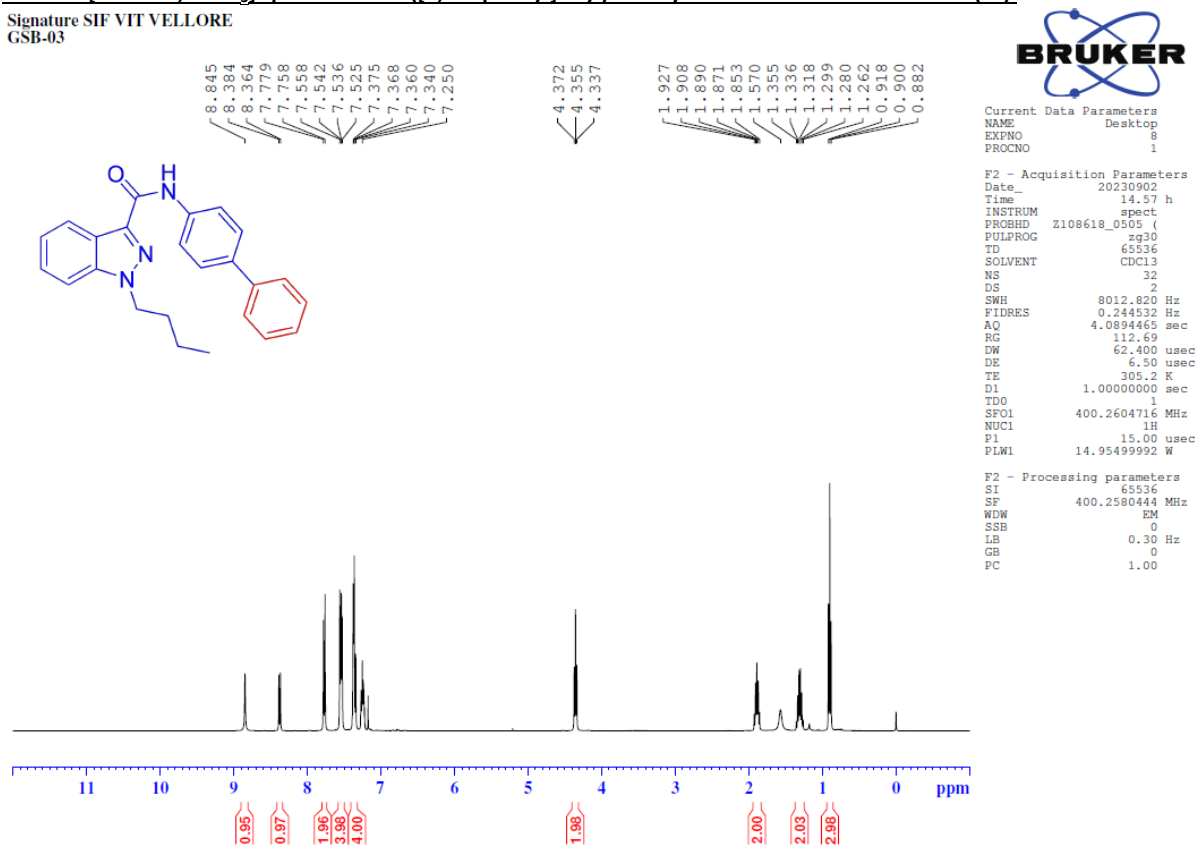
FT-IR spectrum of 1-butyl-N-(4-(trifluoromethyl)-[1,1-biphenyl]-4-yl)-1*H*-indazole-3-carboxamide (6b).



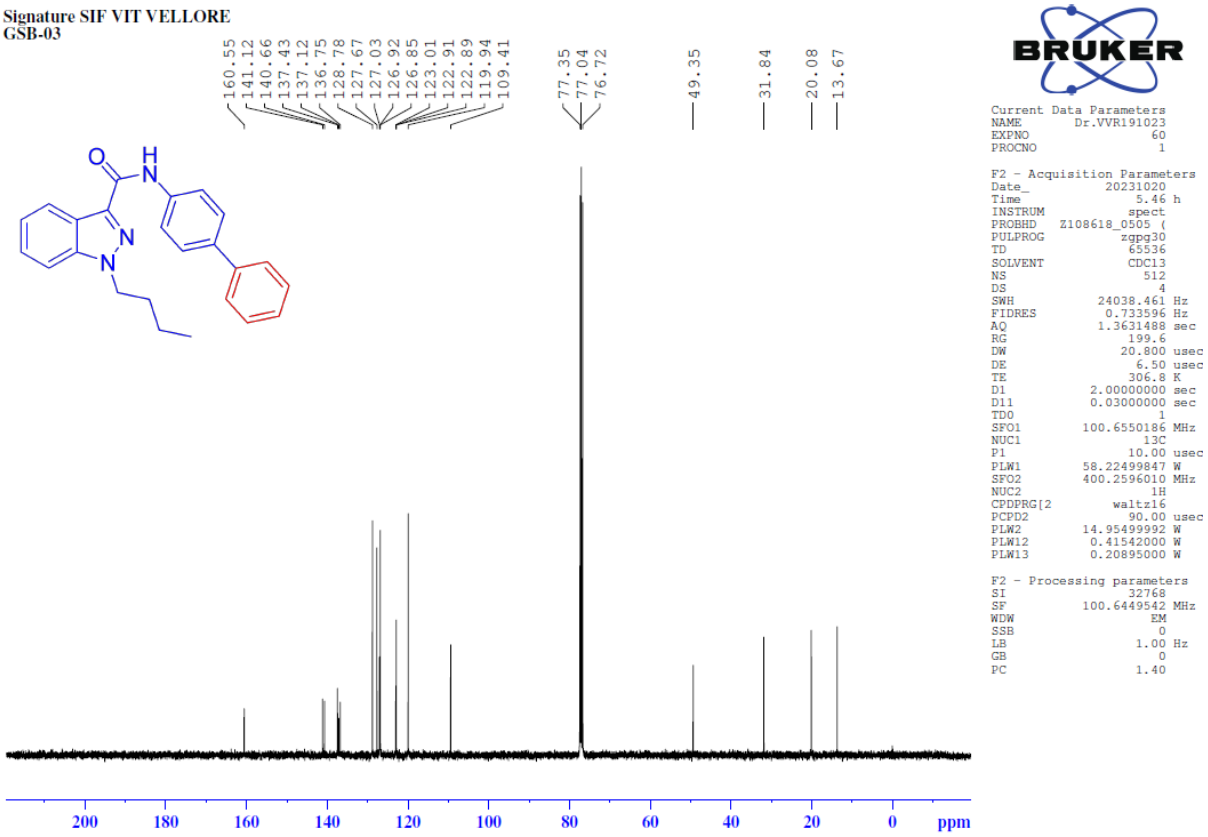
HRMS of 1-butyl-N-(4-(trifluoromethyl)-[1,1-biphenyl]-4-yl)-1*H*-indazole-3-carboxamide (6b).



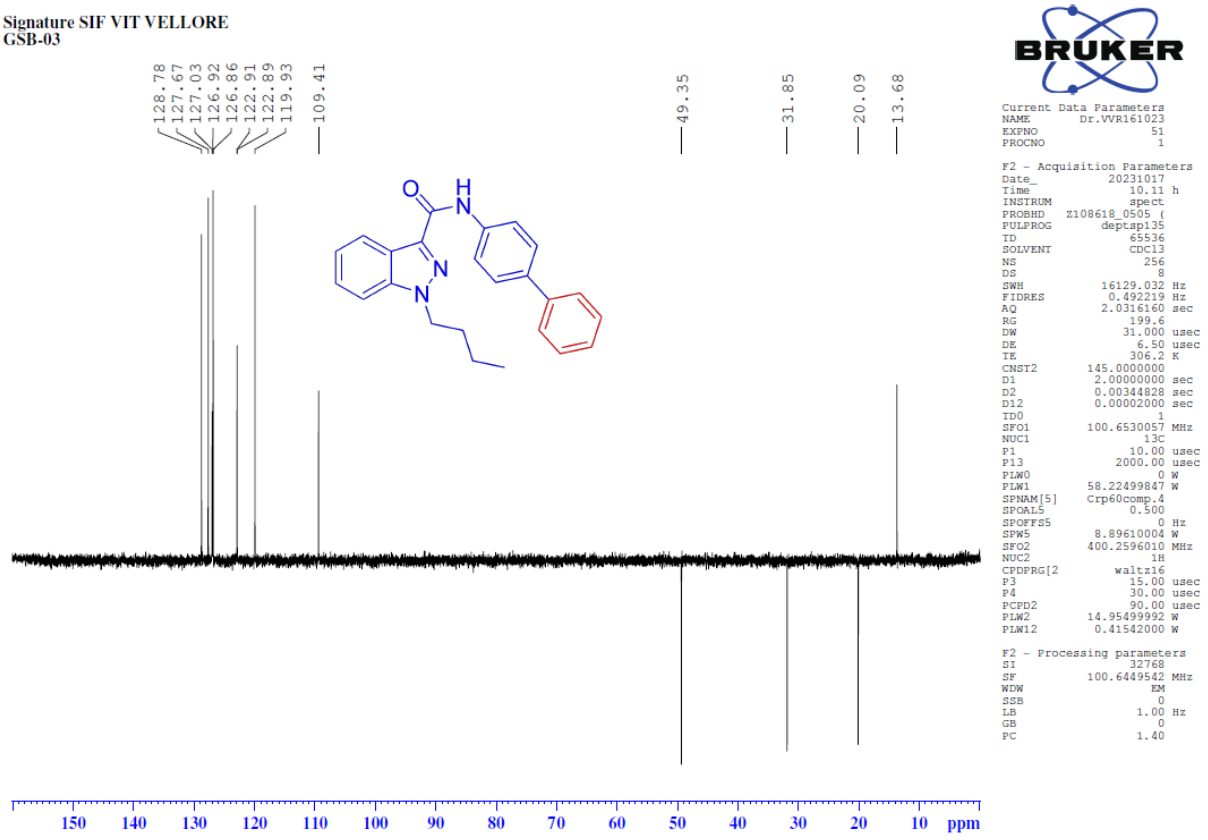
^{1}H-NMR [400MHz, $CDCL_3$] spectrum of N-([1,1-biphenyl]-4-yl)-1-butyl-1*H*-indazole-3-carboxamide (6c).



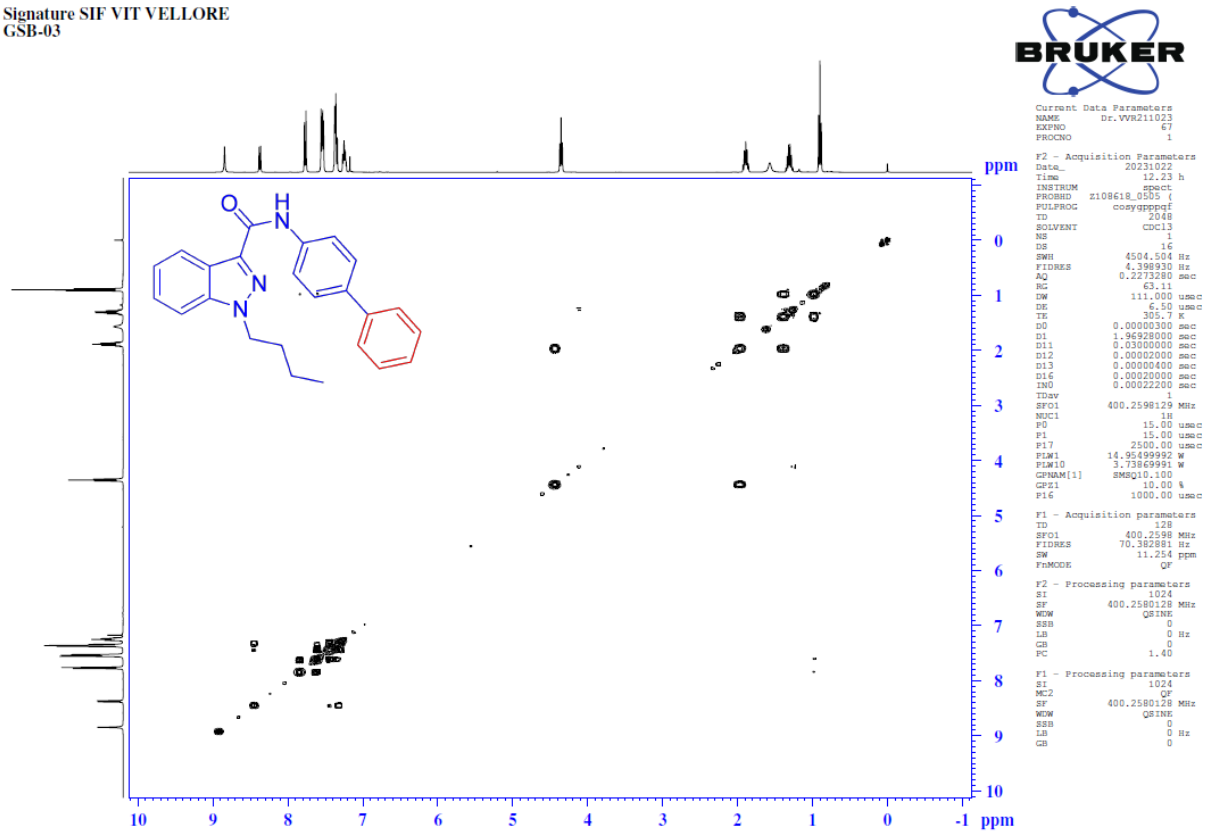
^{13}C-NMR [100MHz, $CDCL_3$] spectrum of N-([1,1-biphenyl]-4-yl)-1-butyl-1*H*-indazole-3-carboxamide (6c).



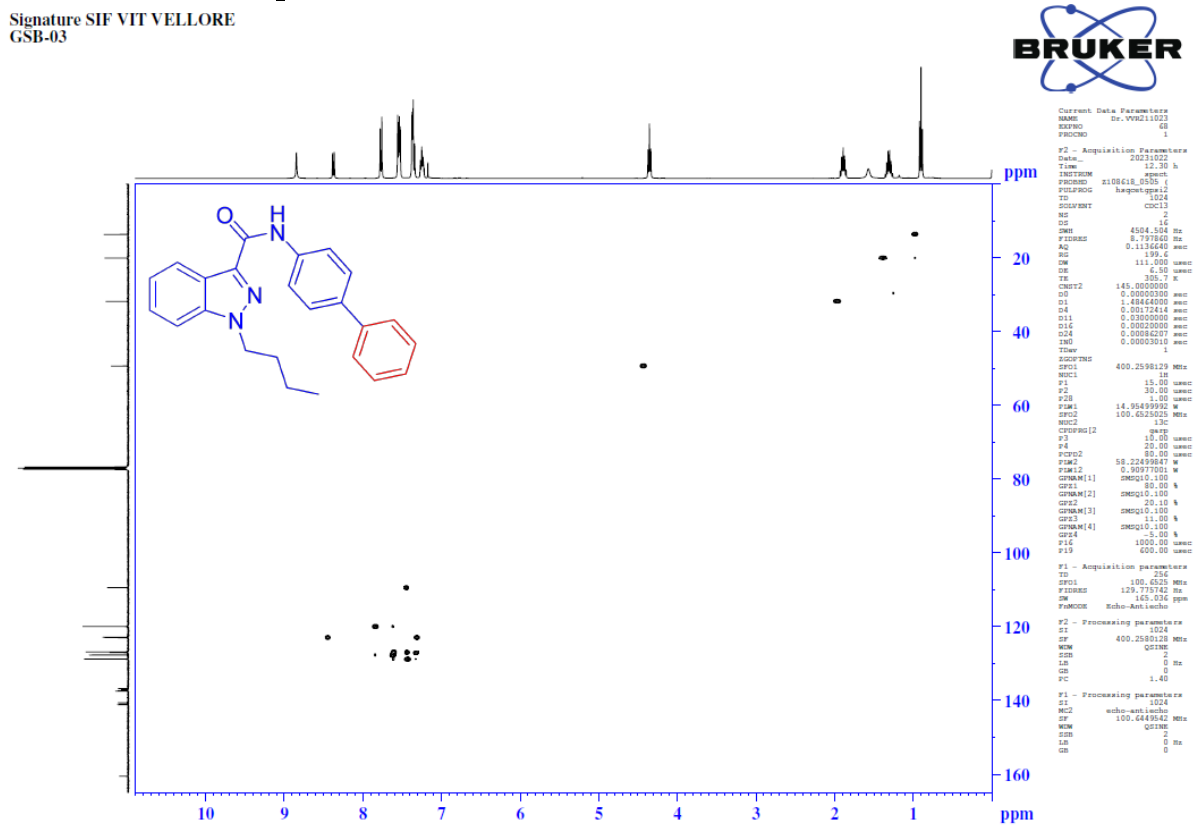
DEPT135-NMR [100MHz, $CDCL_3$] spectrum of N-([1,1-biphenyl]-4-yl)-1-butyl-1*H*-indazole-3-carboxamide (6c).



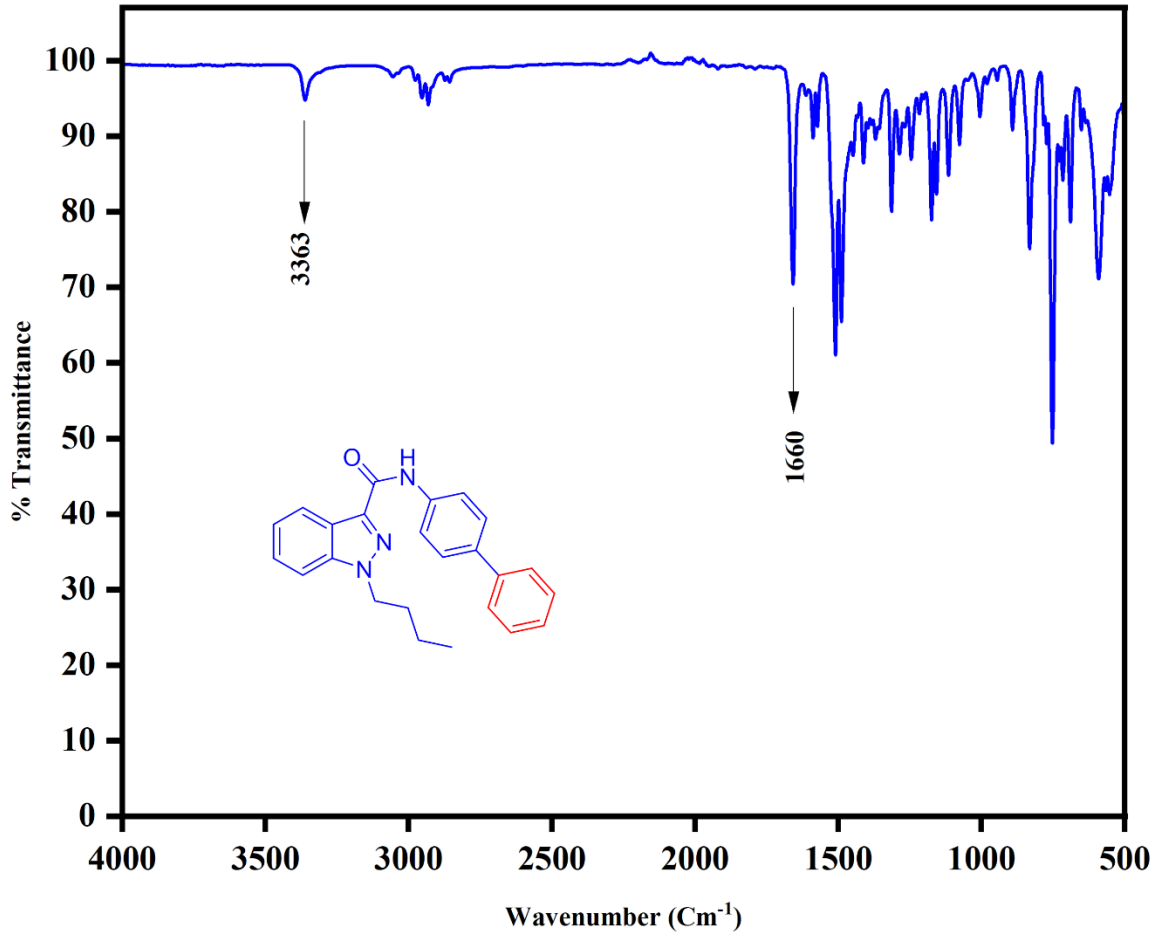
COSY-NMR [400MHz, $CDCL_3$] spectrum of N-([1,1-biphenyl]-4-yl)-1-butyl-1*H*-indazole-3-carboxamide (6c)



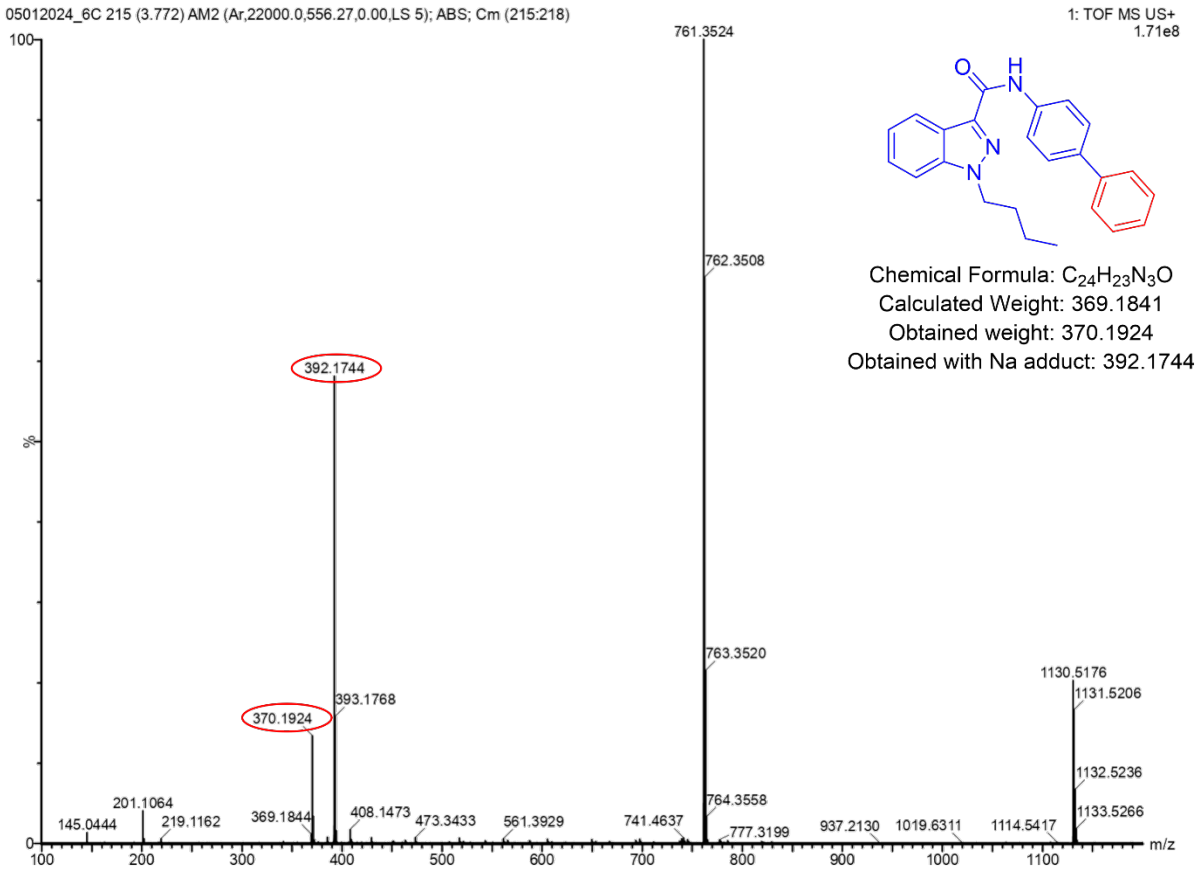
HSQC-NMR [100MHz, $CDCL_3$] spectrum of N-([1,1-biphenyl]-4-yl)-1-butyl-1*H*-indazole-3-carboxamide (6c)



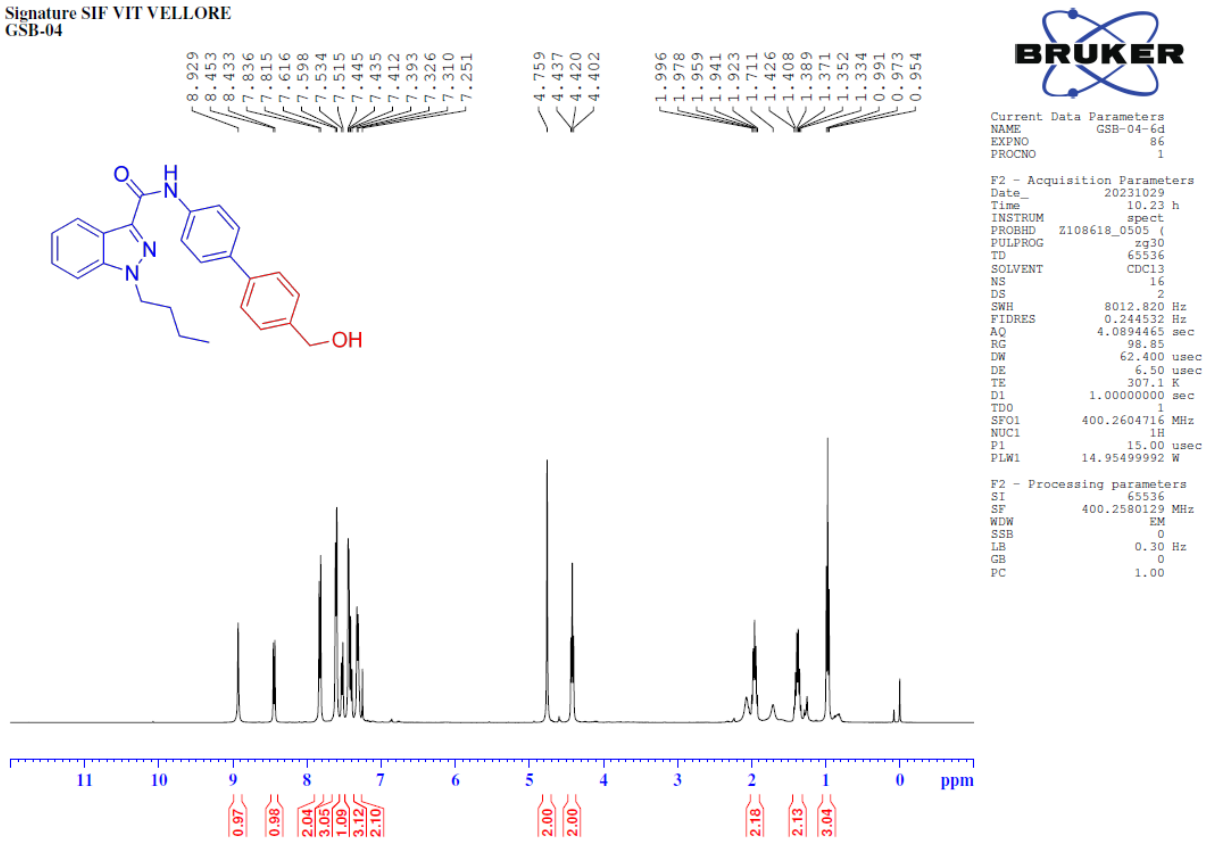
FT-IR spectrum of N-([1,1-biphenyl]-4-yl)-1-butyl-1*H*-indazole-3-carboxamide (6c).



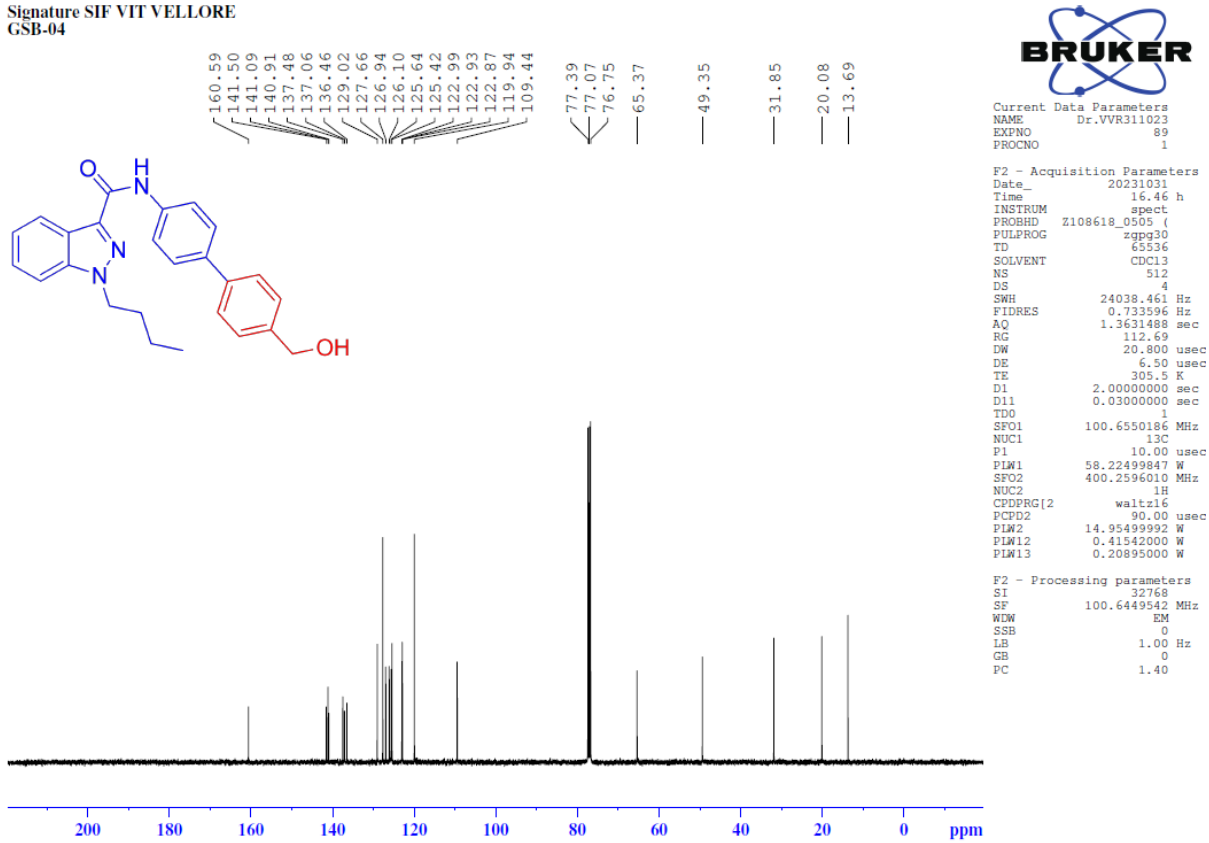
HRMS of N-([1,1-biphenyl]-4-yl)-1-butyl-1*H*-indazole-3-carboxamide (6c).



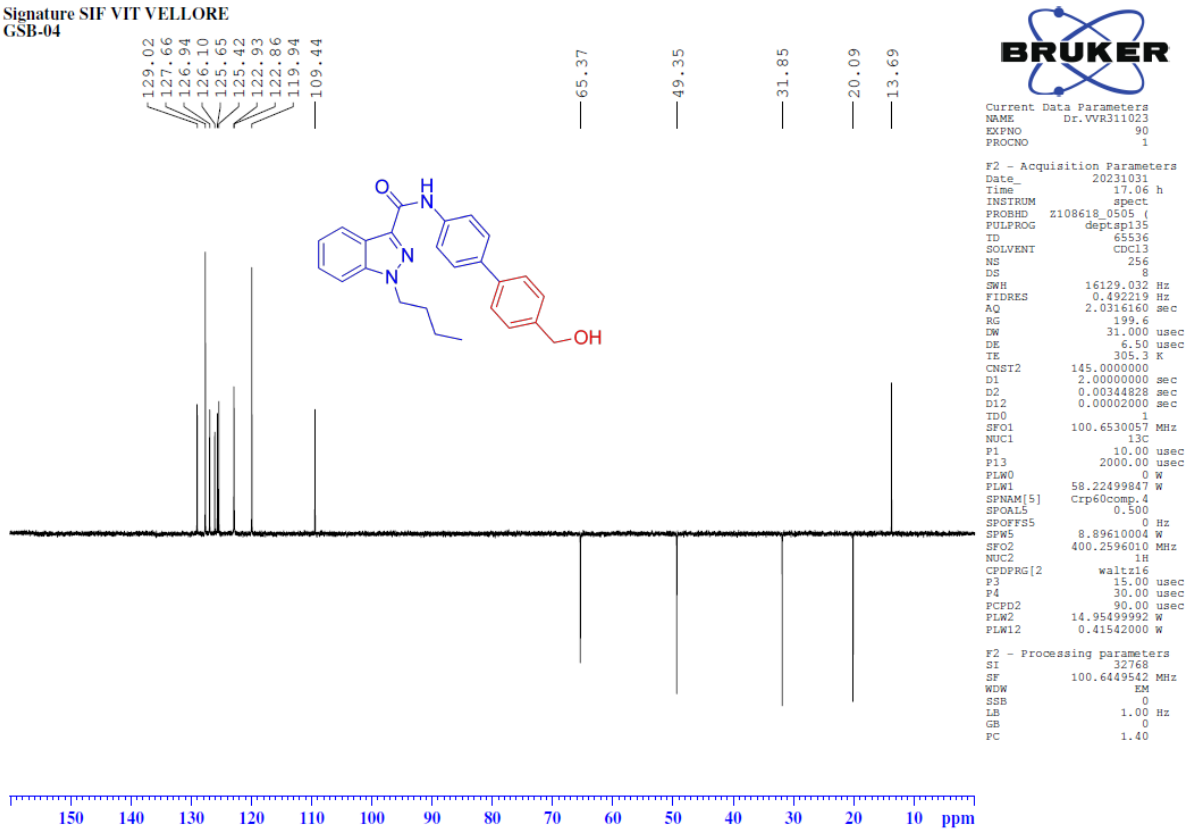
^{1}H-NMR [400MHz, $CDCl_3$] spectrum of 1-butyl-N-(4-(hydroxymethyl)-[1,1-biphenyl]-4-yl)-1*H*-indazole-3-carboxamide (6d).



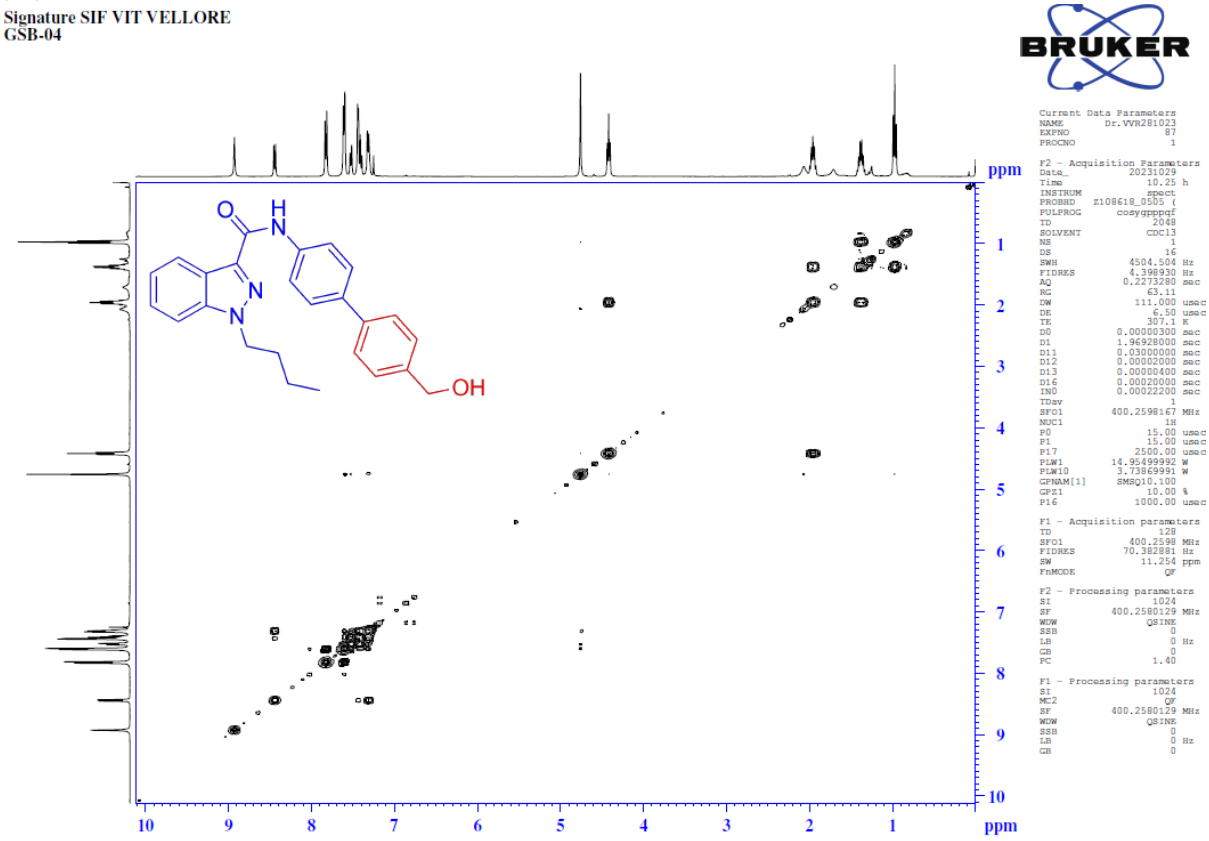
^{13}C-NMR [100MHz, $CDCl_3$] spectrum of 1-butyl-N-(4-(hydroxymethyl)-[1,1-biphenyl]-4-yl)-1*H*-indazole-3-carboxamide (6d).



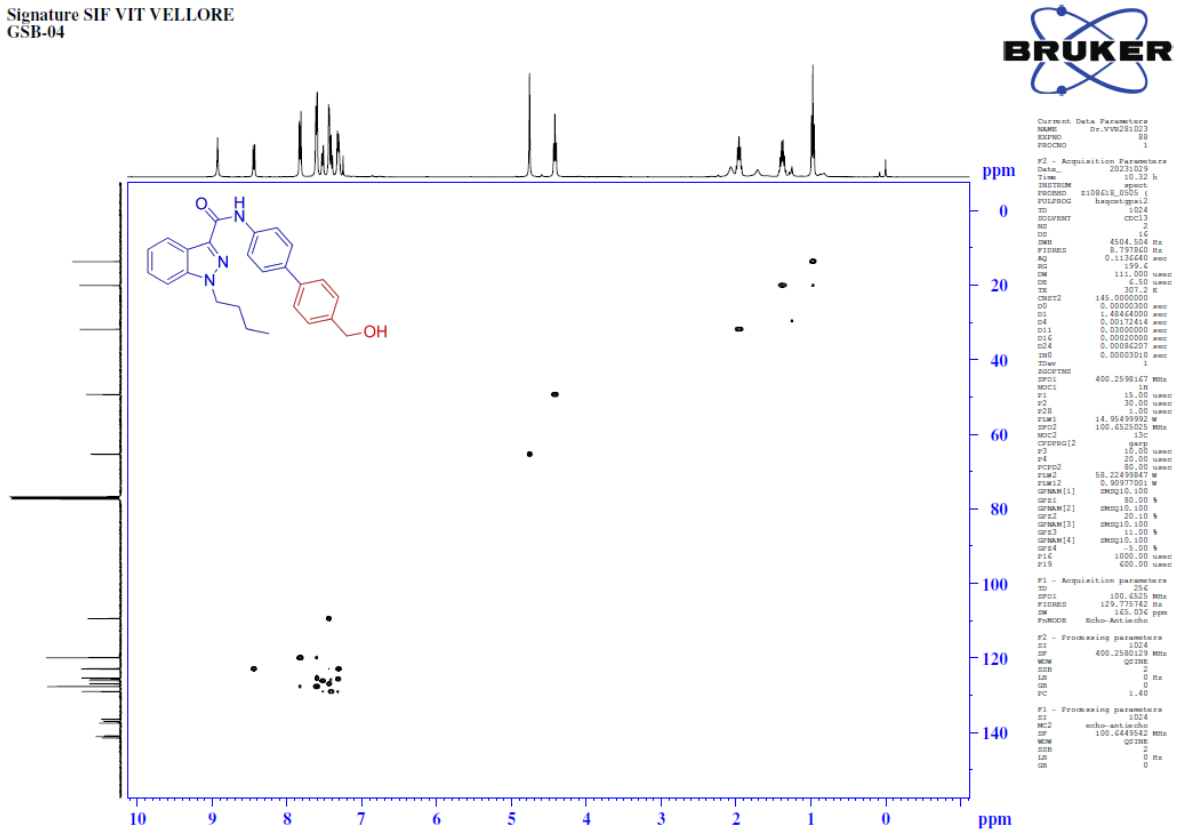
DEPT135-NMR [400MHz, $CDCl_3$] spectrum of 1-butyl-N-(4-(hydroxymethyl)-[1,1-biphenyl]-4-yl)-1*H*-indazole-3-carboxamide (6d).



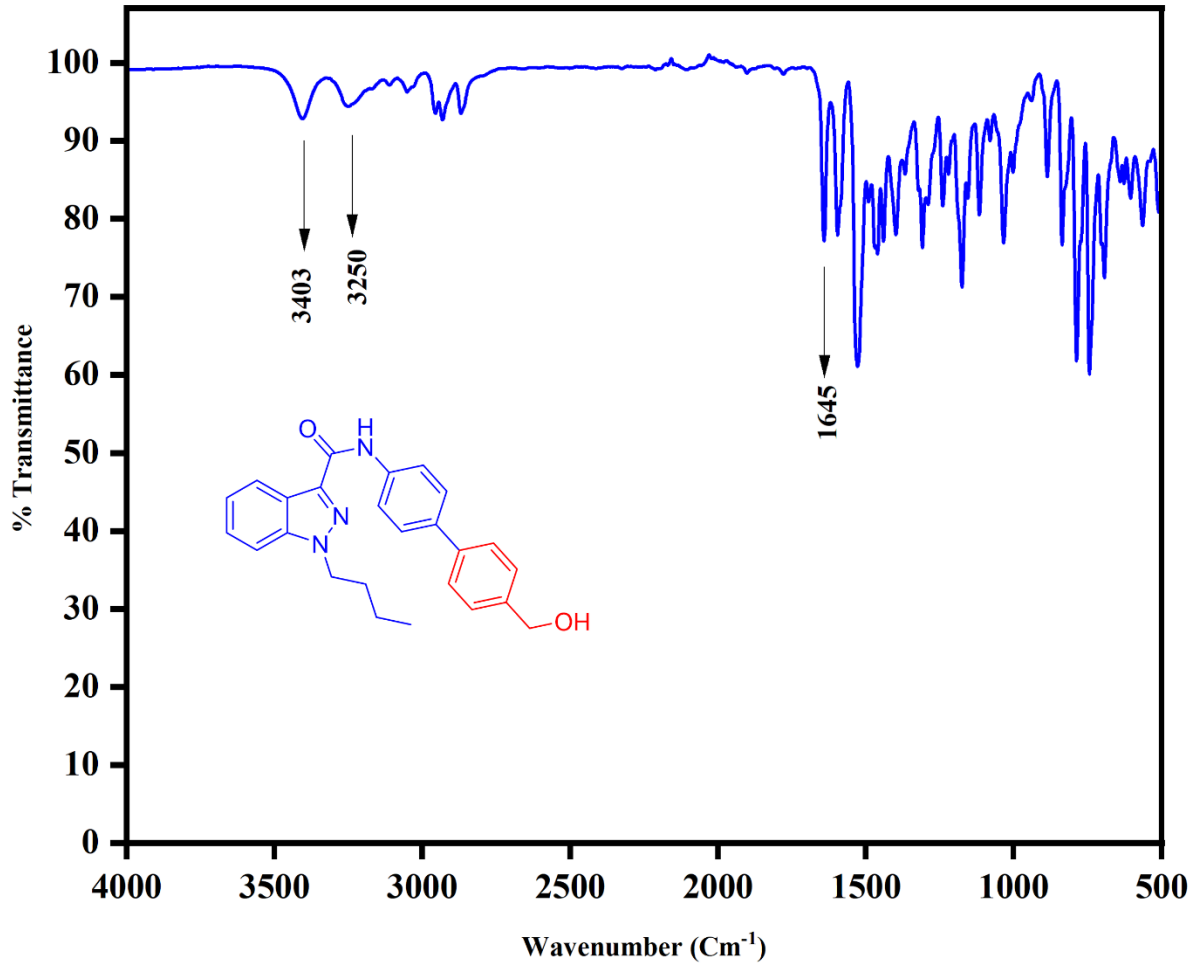
COSY-NMR [400MHz, $CDCl_3$] spectrum of 1-butyl-N-(4-(hydroxymethyl)-[1,1-biphenyl]-4-yl)-1*H*-indazole-3-carboxamide (6d).



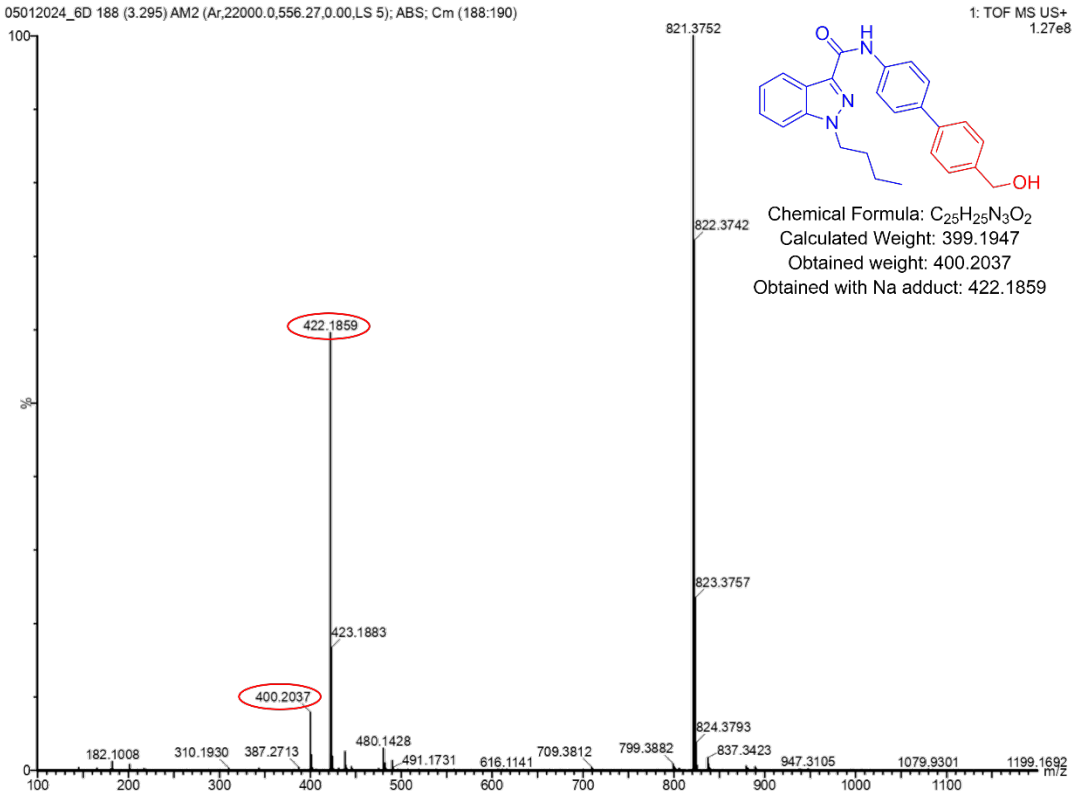
HSQC-NMR [400MHz, $CDCl_3$] spectrum of 1-butyl-N-(4-(hydroxymethyl)-[1,1-biphenyl]-4-yl)-1*H*-indazole-3-carboxamide (6d).



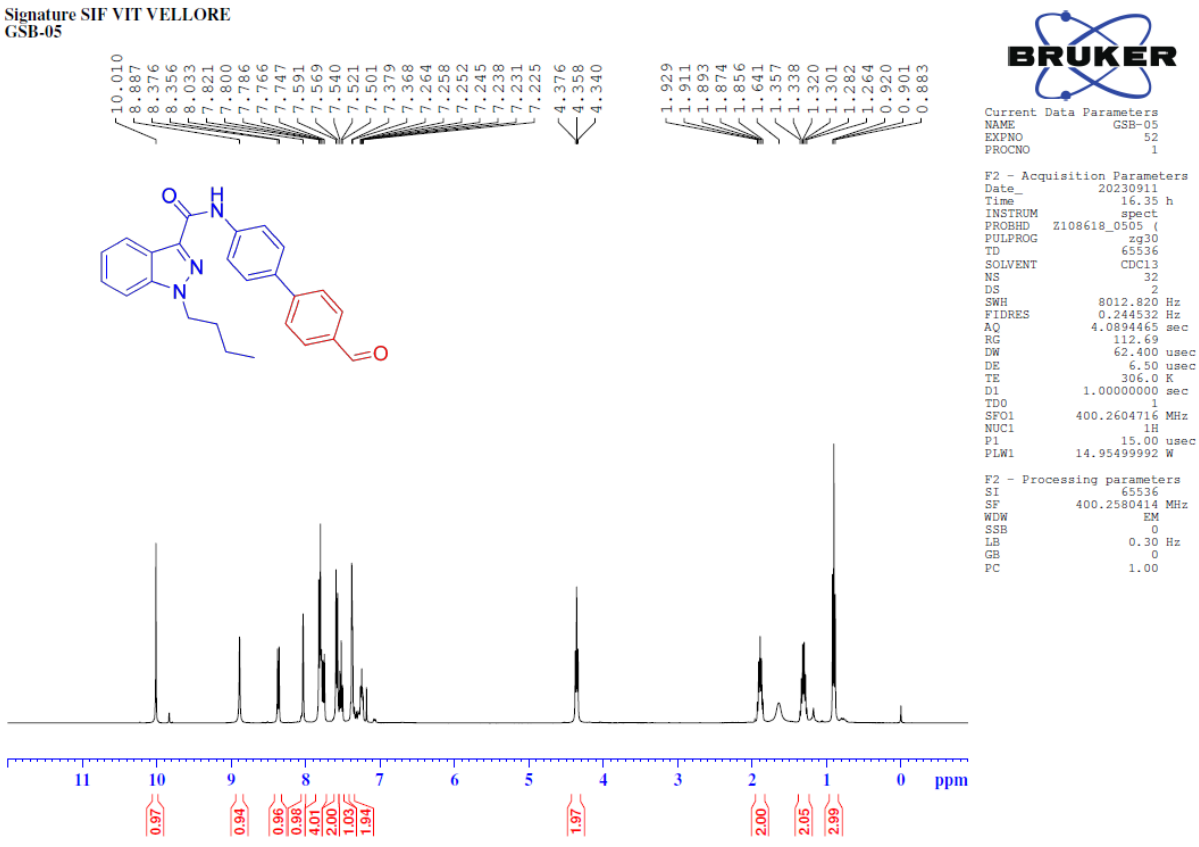
FT-IR spectrum of 1-butyl-N-(4-(hydroxymethyl)-[1,1-biphenyl]-4-yl)-1*H*-indazole-3-carboxamide (6d).



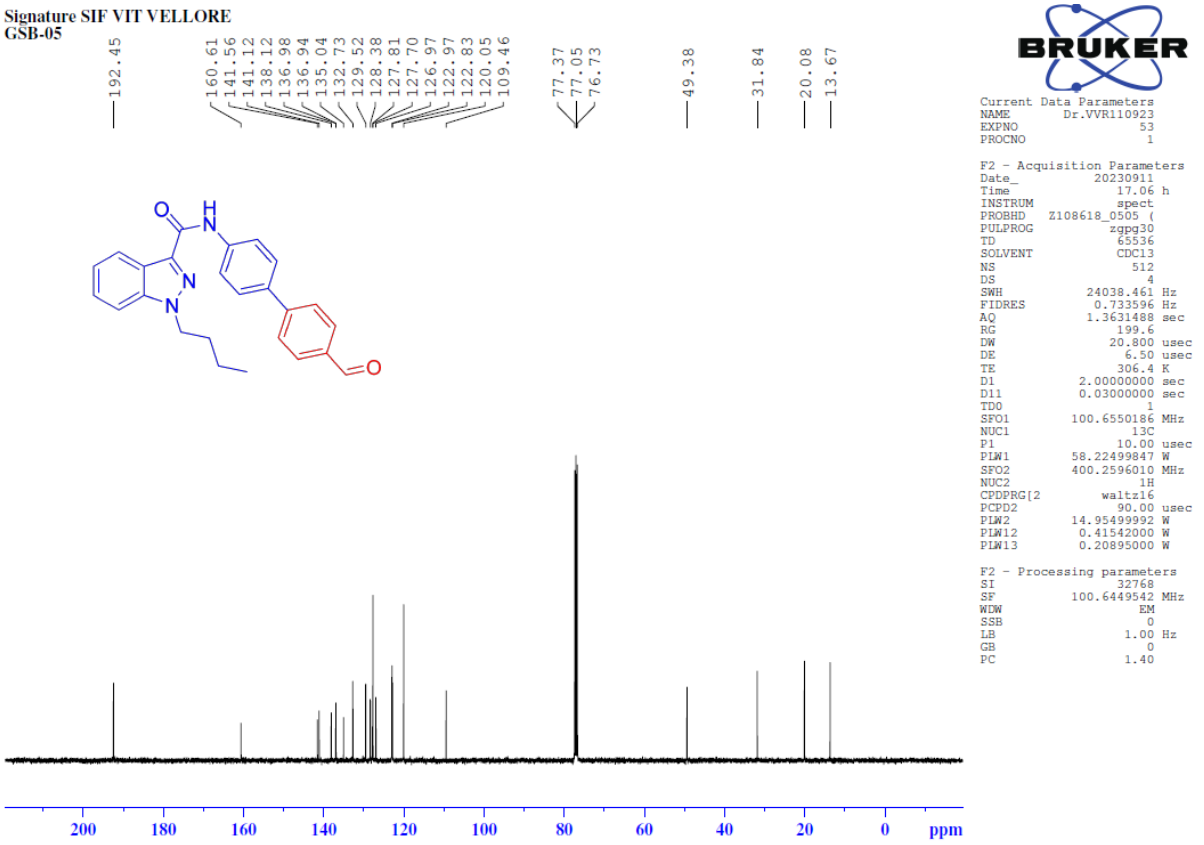
HRMS of 1-butyl-N-(4-(hydroxymethyl)-[1,1-biphenyl]-4-yl)-1*H*-indazole-3-carboxamide (6d).



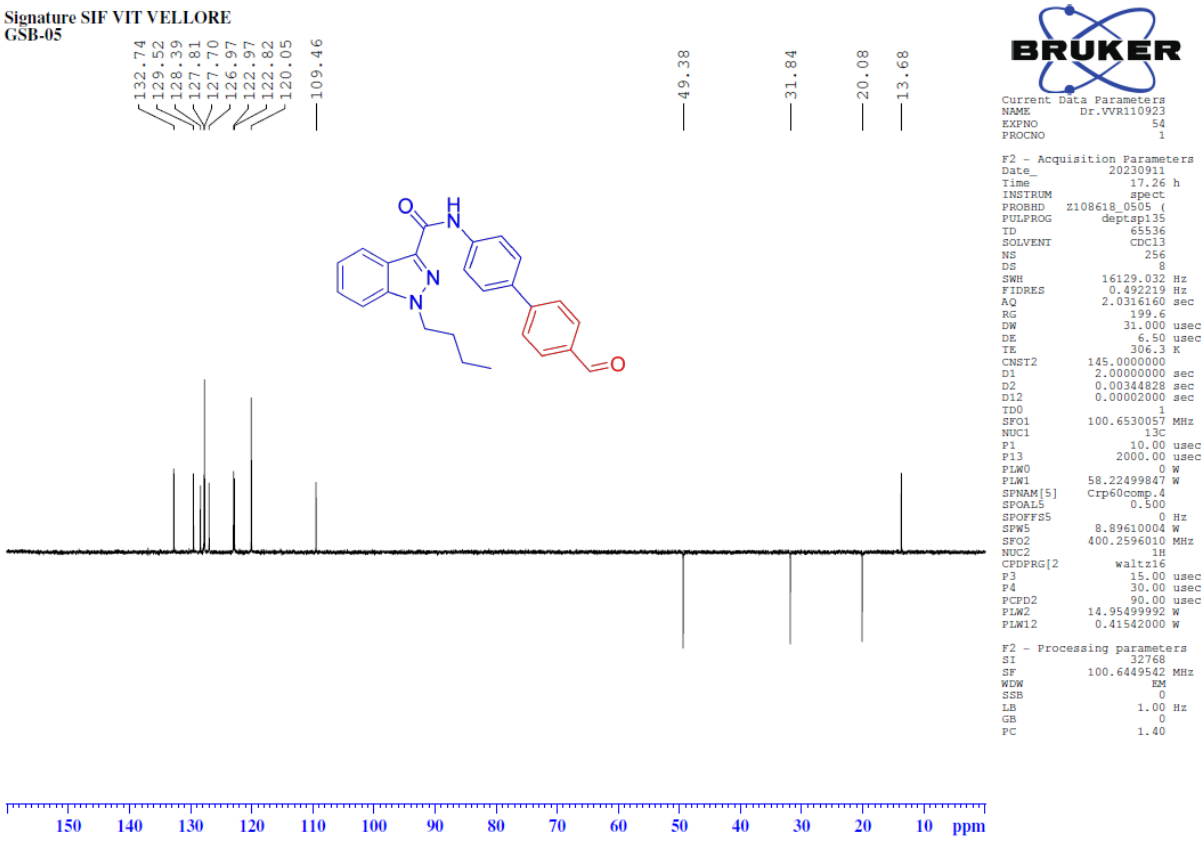
^{1}H-NMR [400MHz, $CDCl_3$] spectrum of 1-butyl-N-(4-formyl-[1,1-biphenyl]-4-yl)-1*H*-indazole-3-carboxamide (6e).



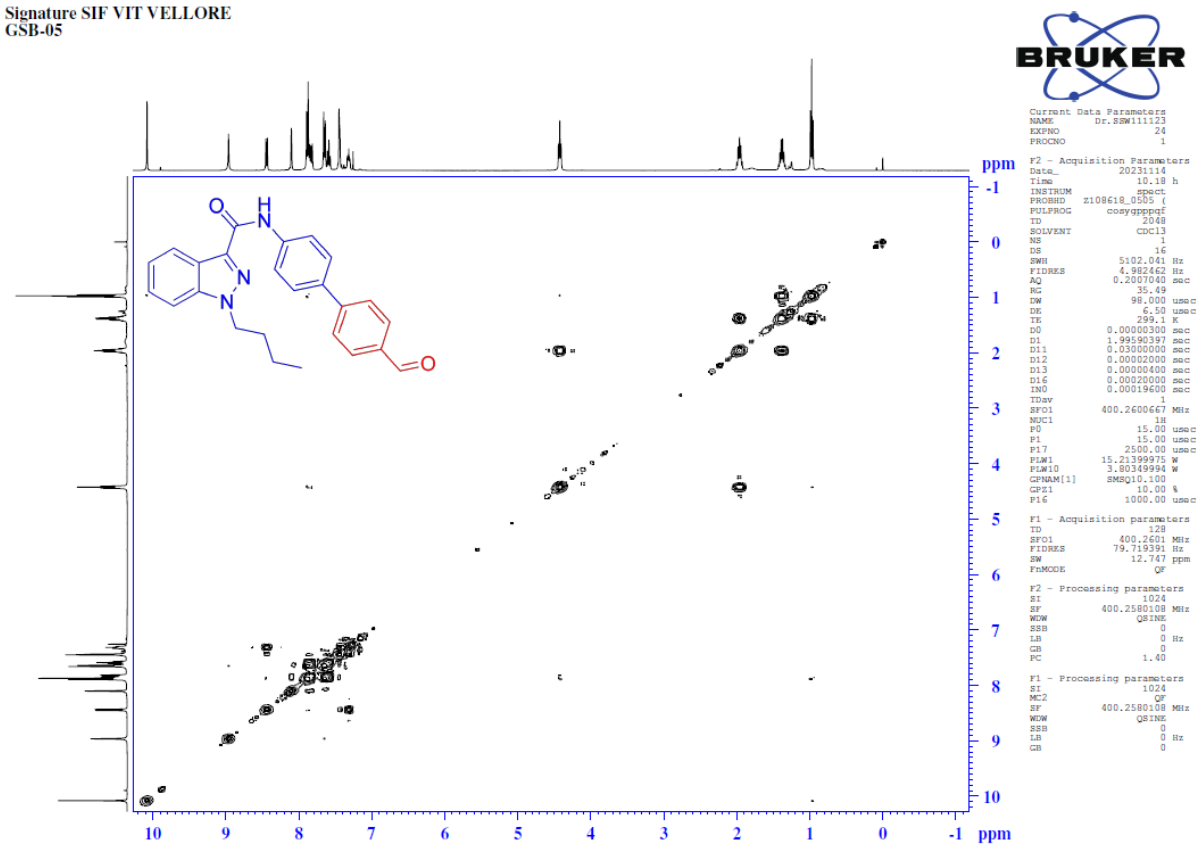
^{13}C-NMR [100MHz, $CDCl_3$] spectrum 1-butyl-N-(4-formyl-[1,1-biphenyl]-4-yl)-1*H*-indazole-3-carboxamide (6e).



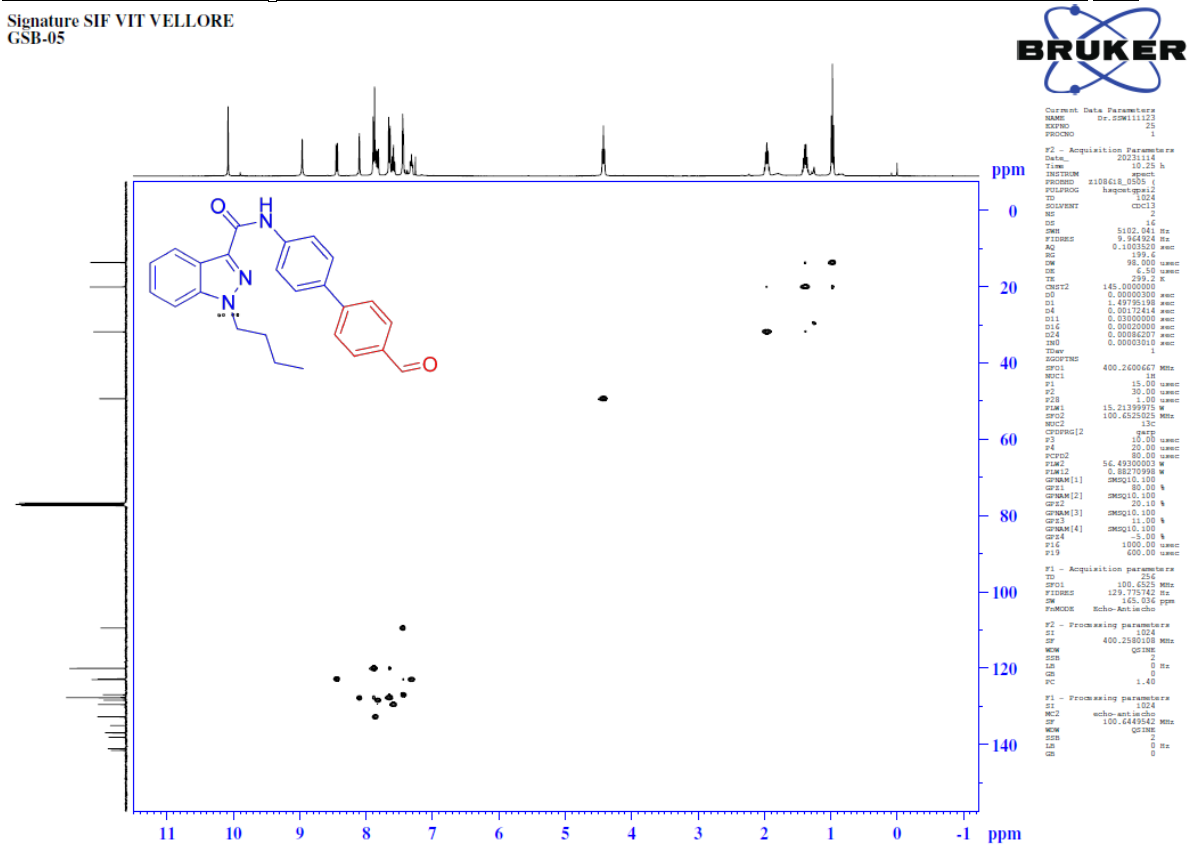
DEPT135-NMR [100MHz, $CDCl_3$] spectrum of 1-butyl-N-(4-formyl-[1,1-biphenyl]-4-yl)-1*H*-indazole-3-carboxamide (6e).



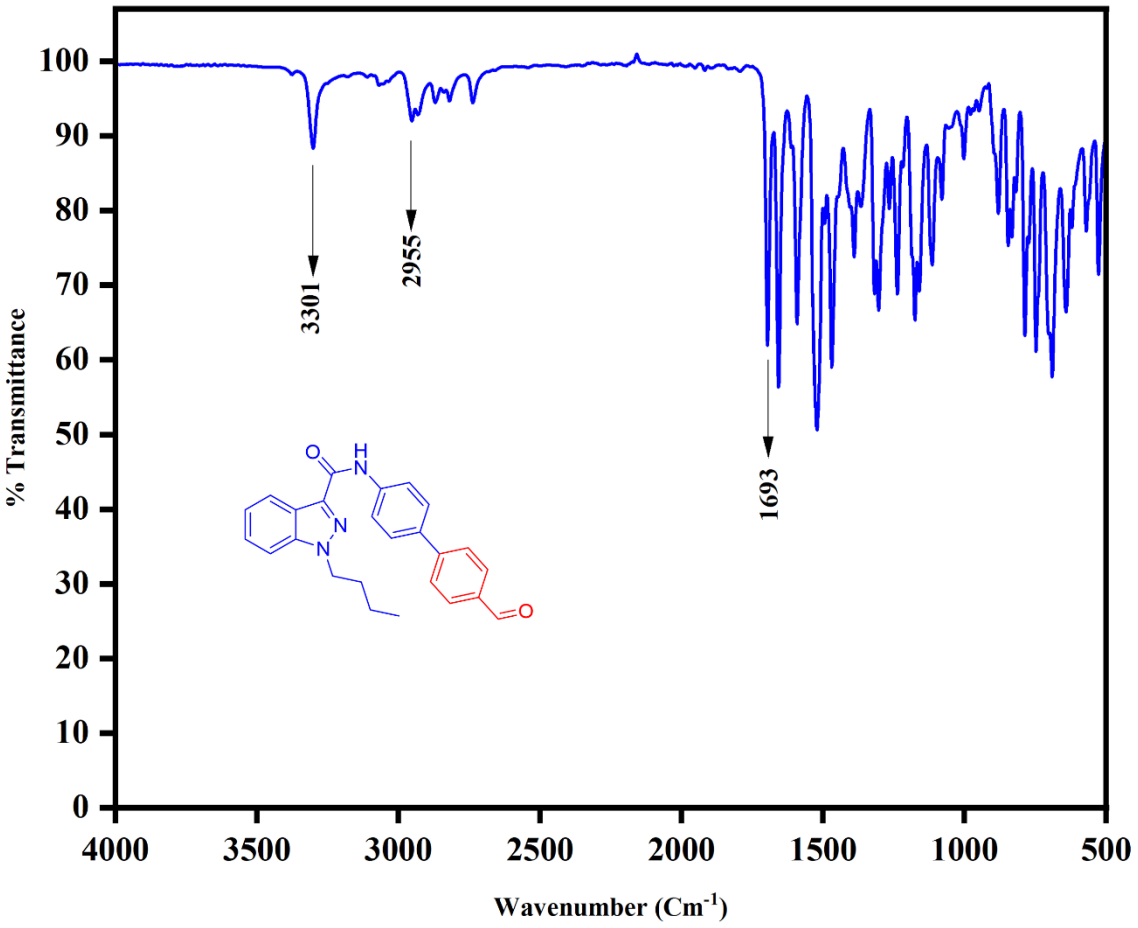
COSY-NMR [400MHz, $CDCl_3$] spectrum of 1-butyl-N-(4-formyl-[1,1-biphenyl]-4-yl)-1*H*-indazole-3-carboxamide (6e).



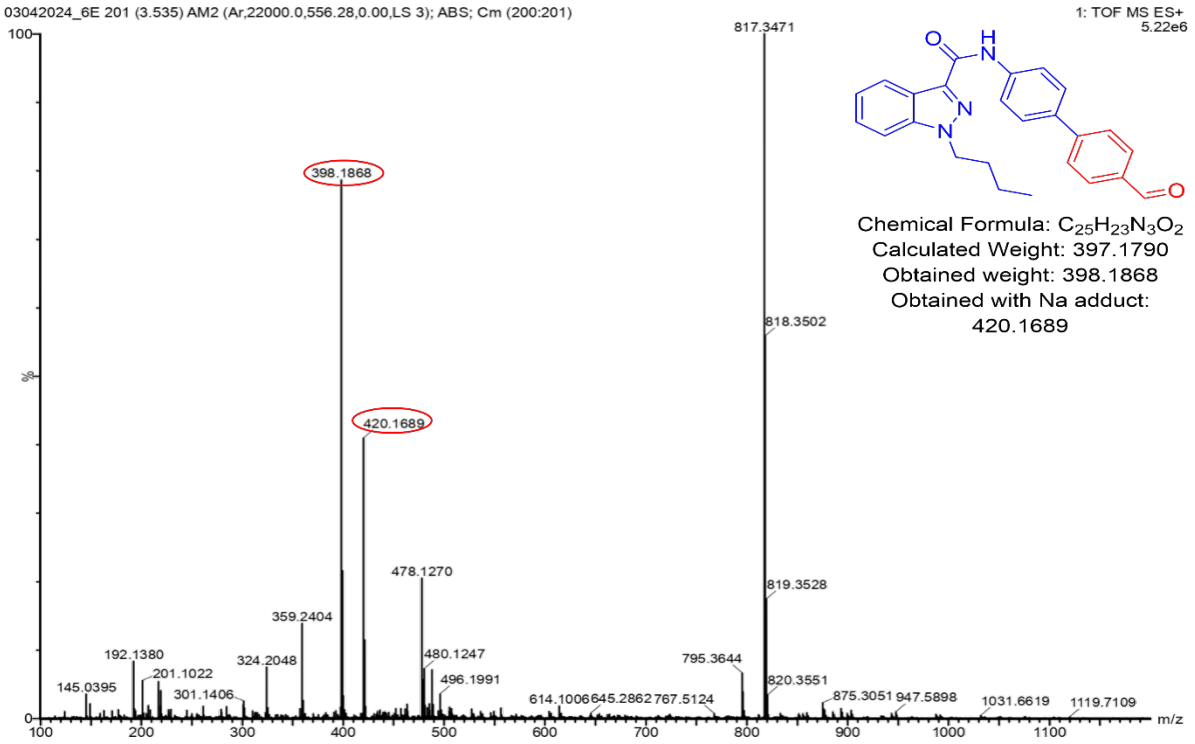
HSQC-NMR [400MHz, $CDCl_3$] spectrum of 1-butyl-N-(4-formyl-[1,1-biphenyl]-4-yl)-1*H*-indazole-3-carboxamide (6e).



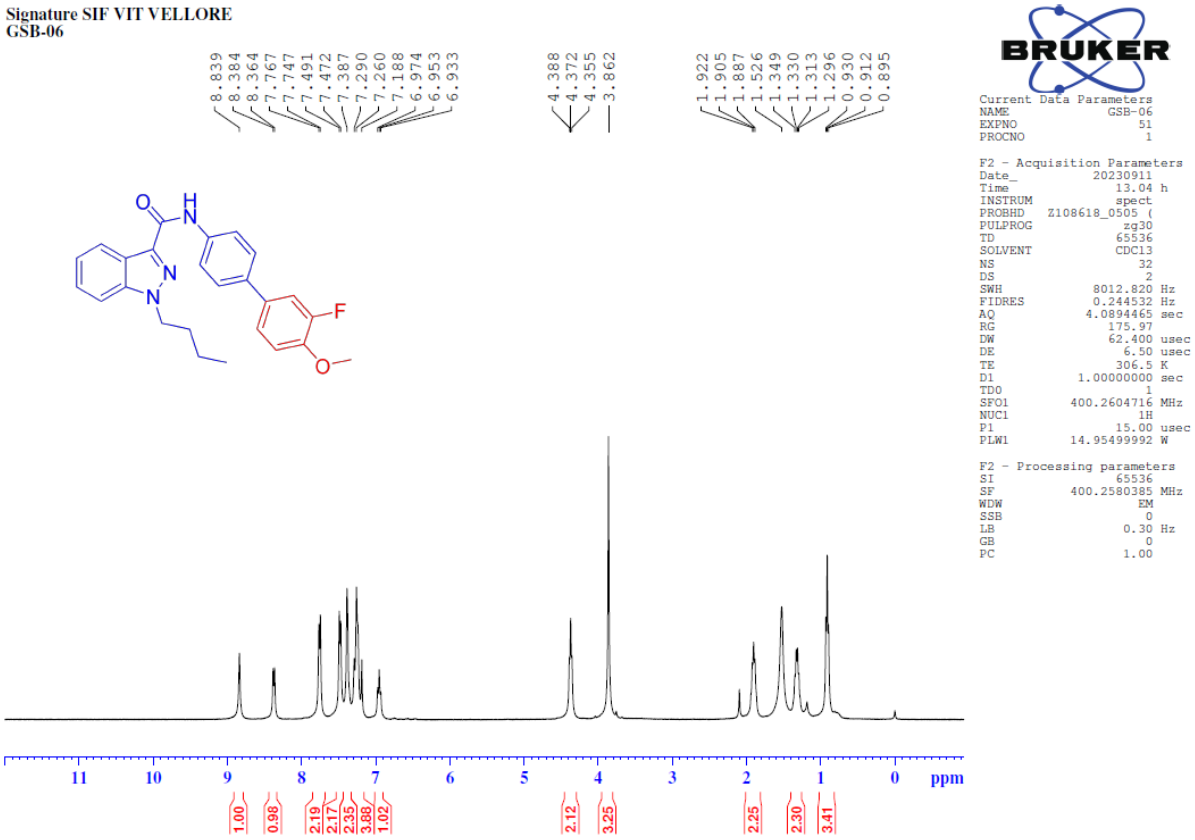
FT-IR spectrum of 1-butyl-N-(4-formyl-[1,1-biphenyl]-4-yl)-1*H*-indazole-3-carboxamide (6e).



HRMS of 1-butyl-N-(4-formyl-[1,1-biphenyl]-4-yl)-1*H*-indazole-3-carboxamide (6e).



^{1}H-NMR [400MHz, $CDCl_3$] spectrum of 1-butyl-N-(3-fluoro-4-methoxy-[1,1-biphenyl]-4-yl)-1*H*-indazole-3-carboxamide (6f).

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Current Data Parameters
NAME                  GSB-06
EXPNO                     51
PROCNO                     1

F2 - Acquisition Parameters
Date_              20230911
Time                  13.04 h
INSTRUM                spect
PROBHD    Z108618_0505 (
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       32
DS                        2
SWH                8012.820 Hz
FIDRES                0.244532 Hz
AQ                 4.0894465 sec
RG                    175.97
DW                    62.400 usec
DE                     6.50 usec
TE                    306.5 K
D1                 1.00000000 sec
TD0                        1
SFO1              400.2604716 MHz
NUC1                      1H
P1                    15.00 usec
PLW1              14.95499992 W

F2 - Processing parameters
SI                    65536
SF                400.2580385 MHz
WDW                       EM
SSB                        0
LB                     0.30 Hz
GB                         0
PC                      1.00
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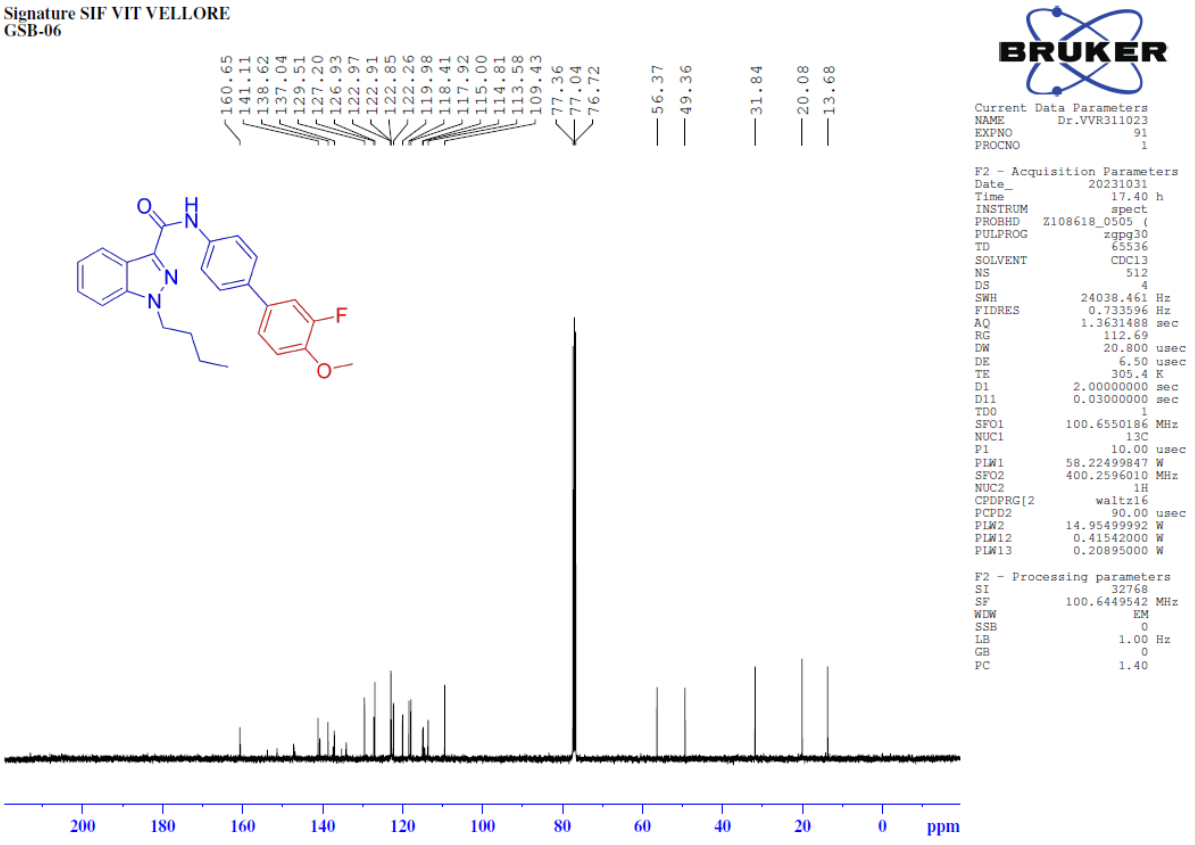
^{13}C-NMR [100MHz, $CDCl_3$] spectrum of 1-butyl-N-(3-fluoro-4-methoxy-[1,1-biphenyl]-4-yl)-1*H*-indazole-3-carboxamide (6f).

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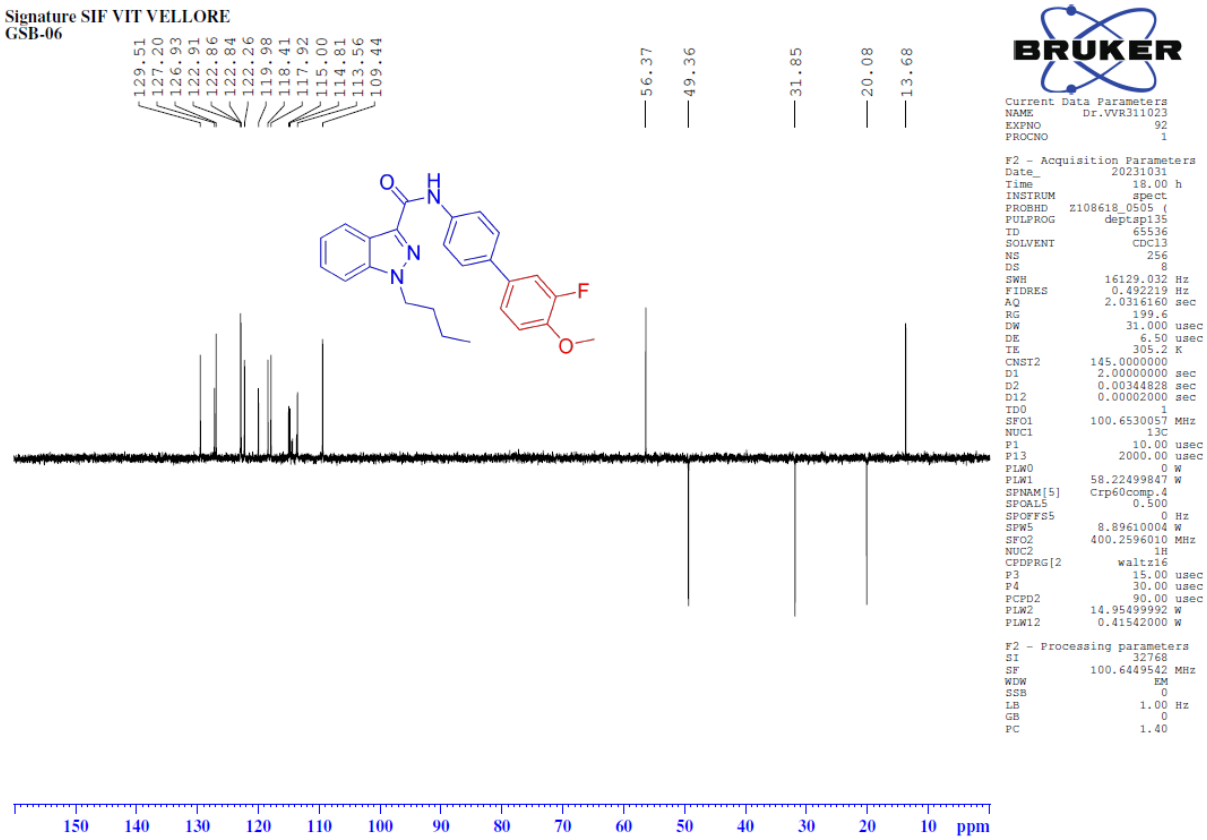
Current Data Parameters
NAME              Dr.VVR311023
EXPNO                     91
PROCNO                     1

F2 - Acquisition Parameters
Date_              20231031
Time                  17.40 h
INSTRUM                spect
PROBHD    Z108618_0505 (
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                      512
DS                        4
SWH               24038.461 Hz
FIDRES                0.733596 Hz
AQ                 1.3631488 sec
RG                    112.69
DW                    20.800 usec
DE                     6.50 usec
TE                    305.4 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                        1
SFO1              100.6550186 MHz
NUC1                      13C
P1                    10.00 usec
PLW1              58.22499847 W
SFO2              400.2596010 MHz
NUC2                      1H
CPDPRG[2              waltz16
PCPD2                 90.00 usec
PLW2              14.95499992 W
PLW12              0.41542000 W
PLW13              0.20895000 W

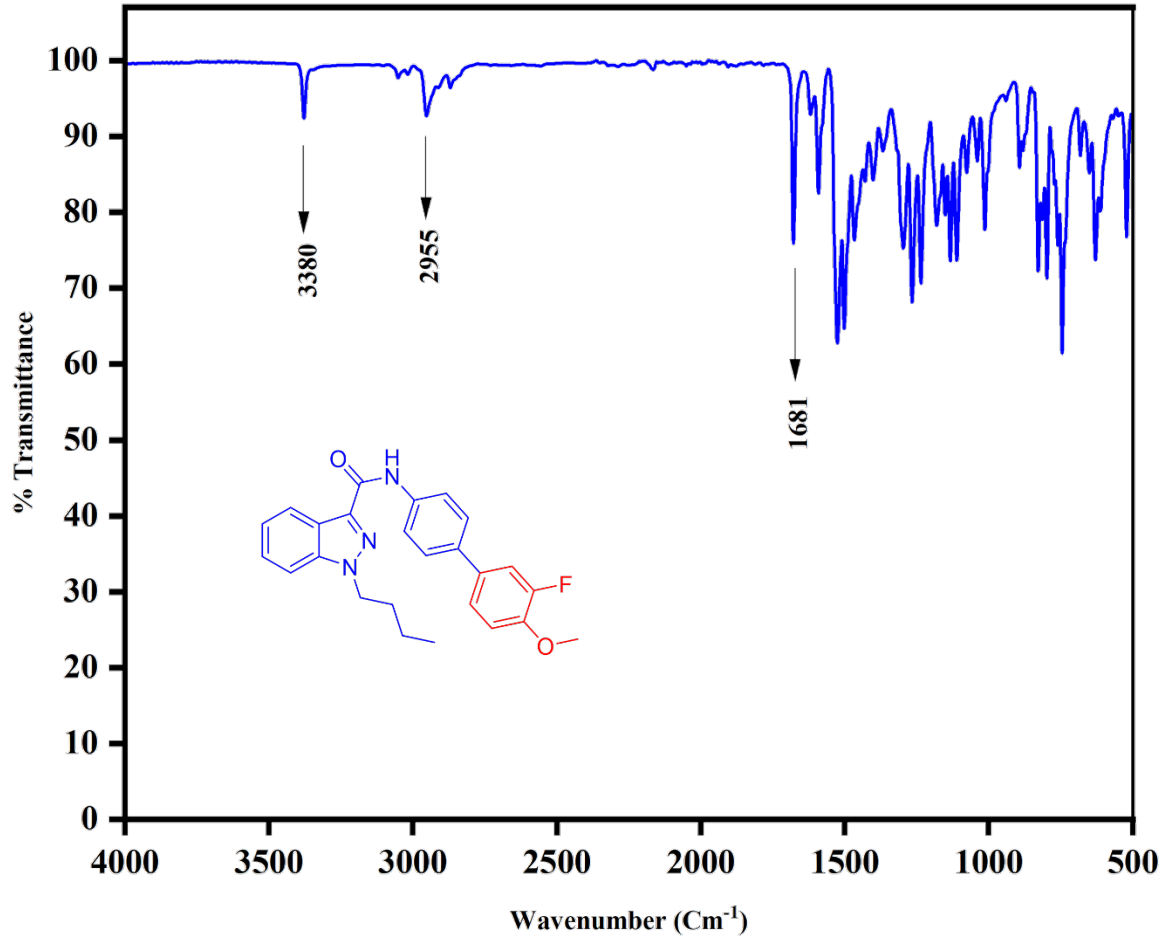
F2 - Processing parameters
SI                    32768
SF                100.6449542 MHz
WDW                       EM
SSB                        0
LB                     1.00 Hz
GB                         0
PC                      1.40
```

DPET135-NMR [100MHz, $CDCl_3$] spectrum of 1-butyl-N-(3-fluoro-4-methoxy-[1,1-biphenyl]-4-yl)-1*H*-indazole-3-

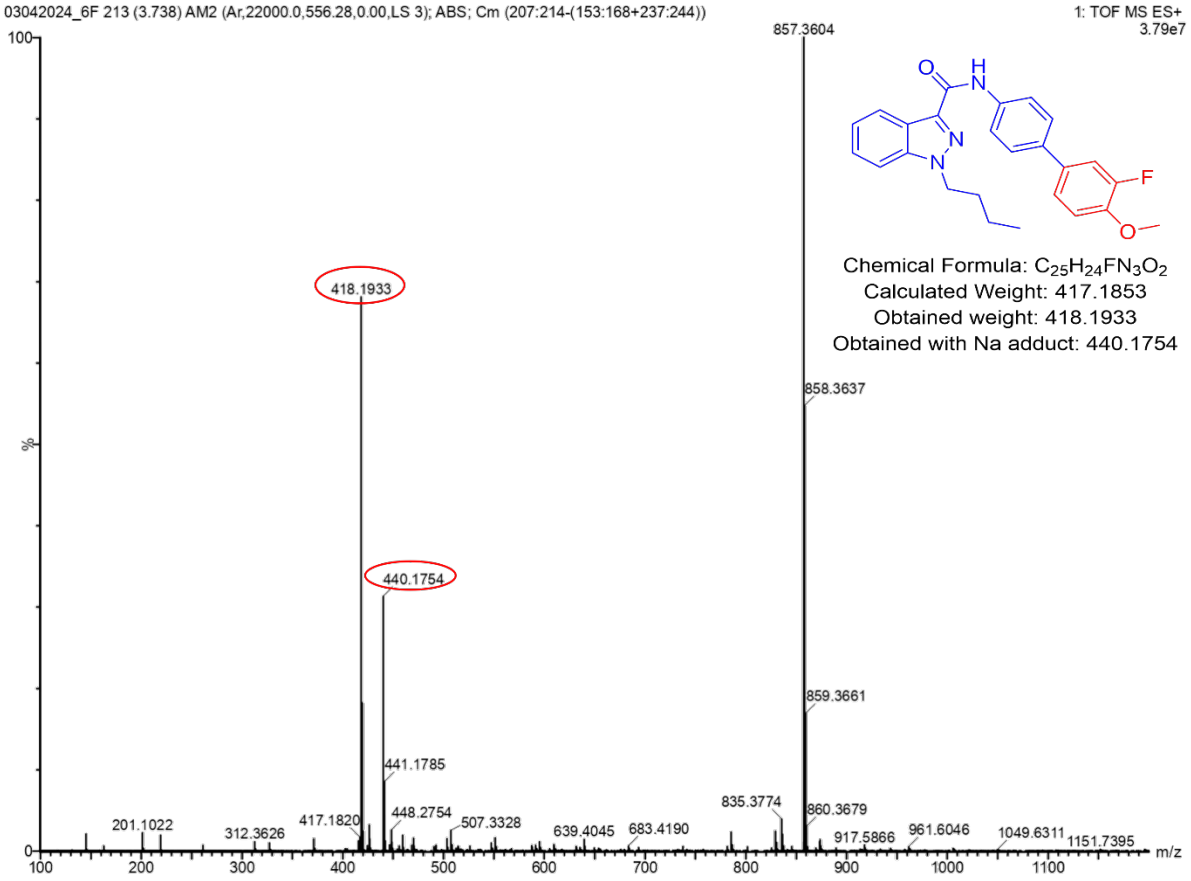
carboxamide (6f).



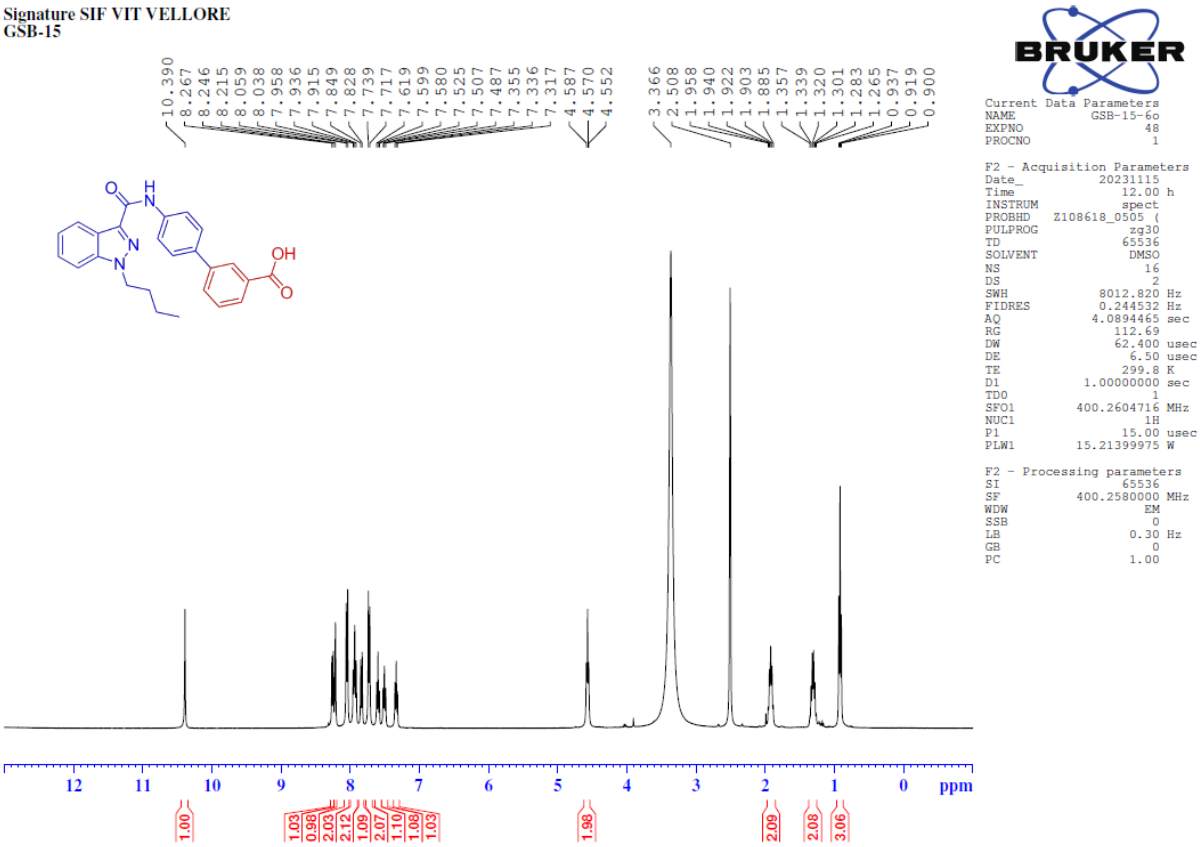
FT-IR spectrum of 1-butyl-N-(3-fluoro-4-methoxy-[1,1-biphenyl]-4-yl)-1*H*-indazole-3-carboxamide (6f).



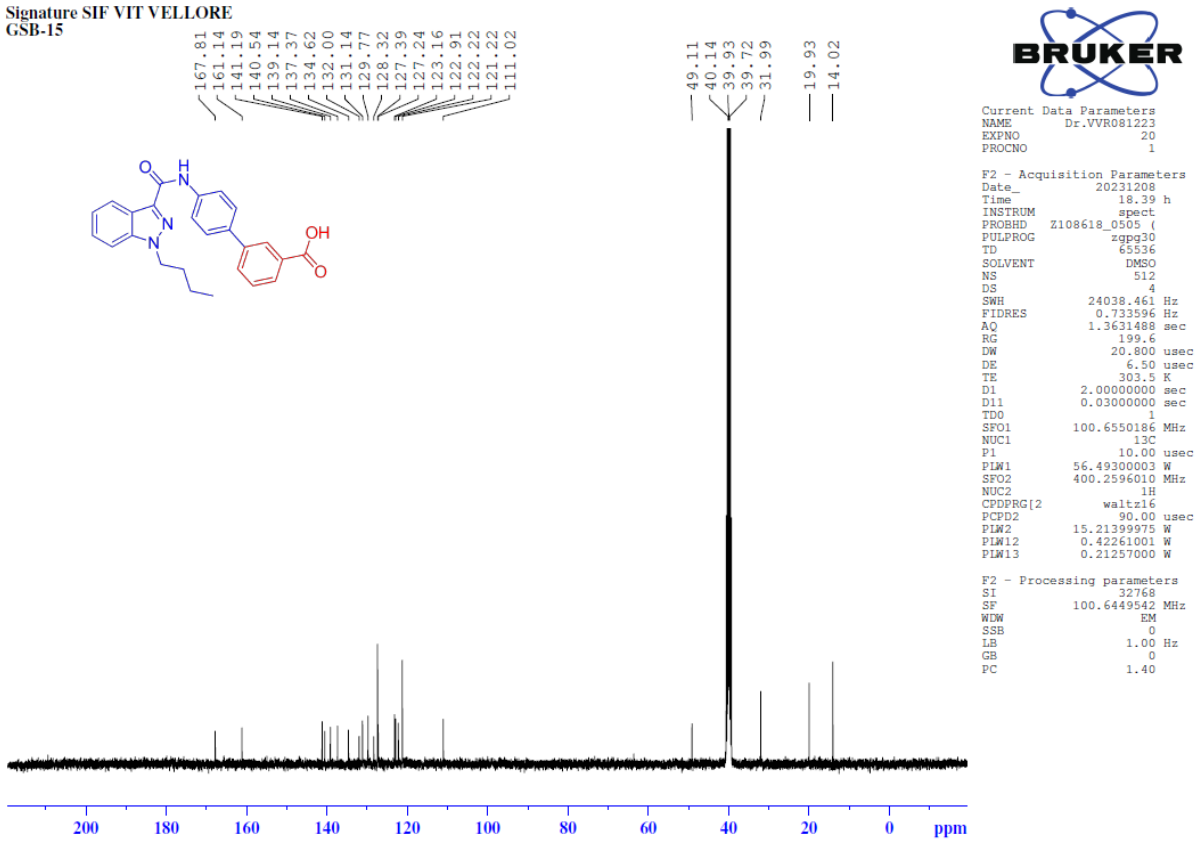
HRMS of 1-butyl-N-(3-fluoro-4-methoxy-[1,1-biphenyl]-4-yl)-1*H*-indazole-3-carboxamide (6f).



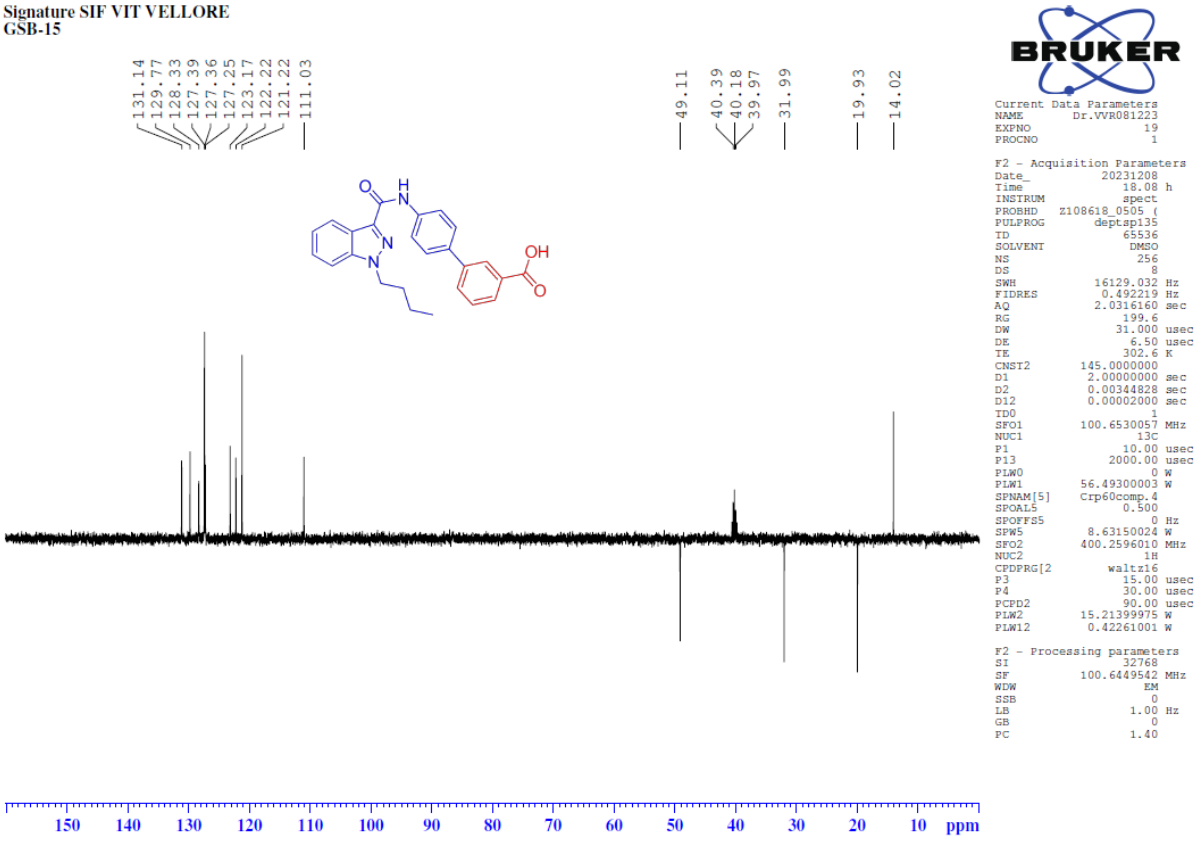
^{1}H-NMR [400MHz, $CDCl_3$] spectrum of 4-(1-butyl-1*H*-indazole-3-carboxamido)-[1,1-biphenyl]-3-carboxylic acid (6g).



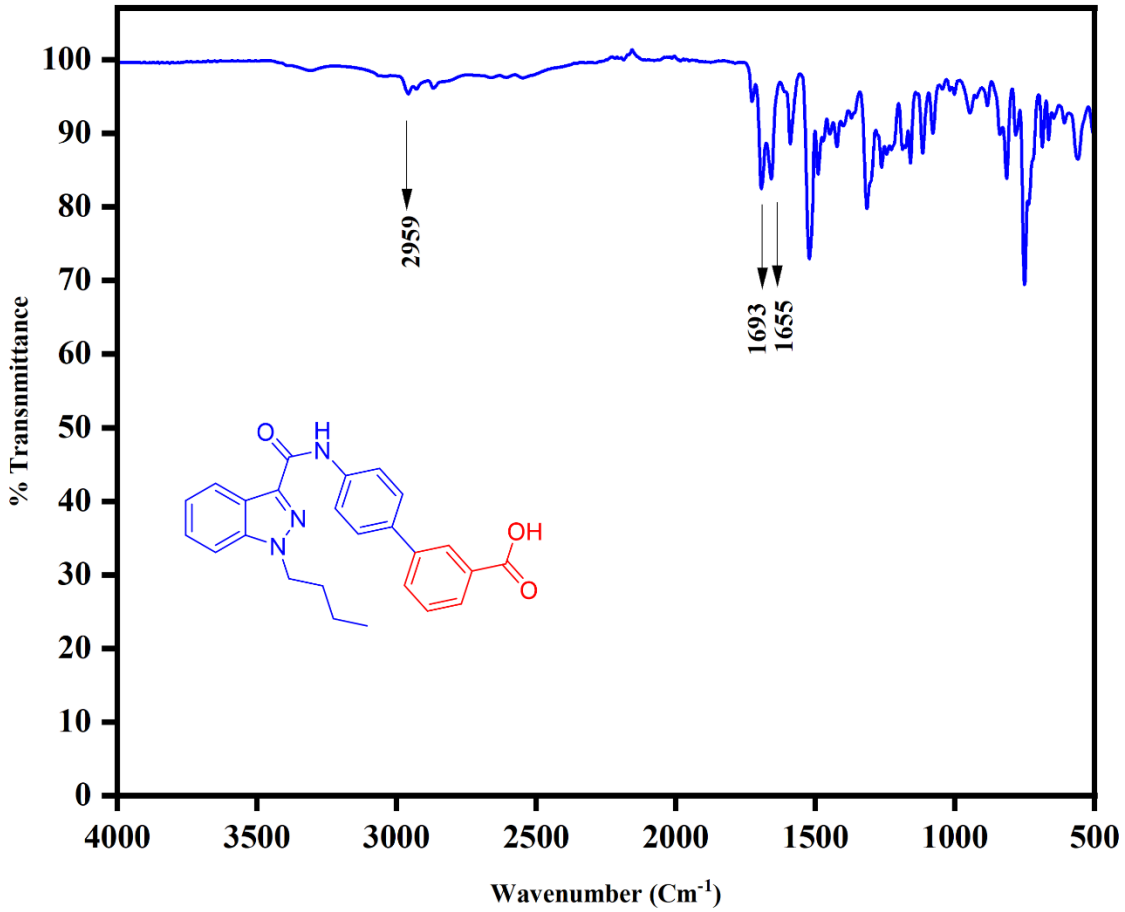
^{13}C-NMR [100MHz, $CDCl_3$] spectrum of 4-(1-butyl-1*H*-indazole-3-carboxamido)-[1,1-biphenyl]-3-carboxylic acid (6g).



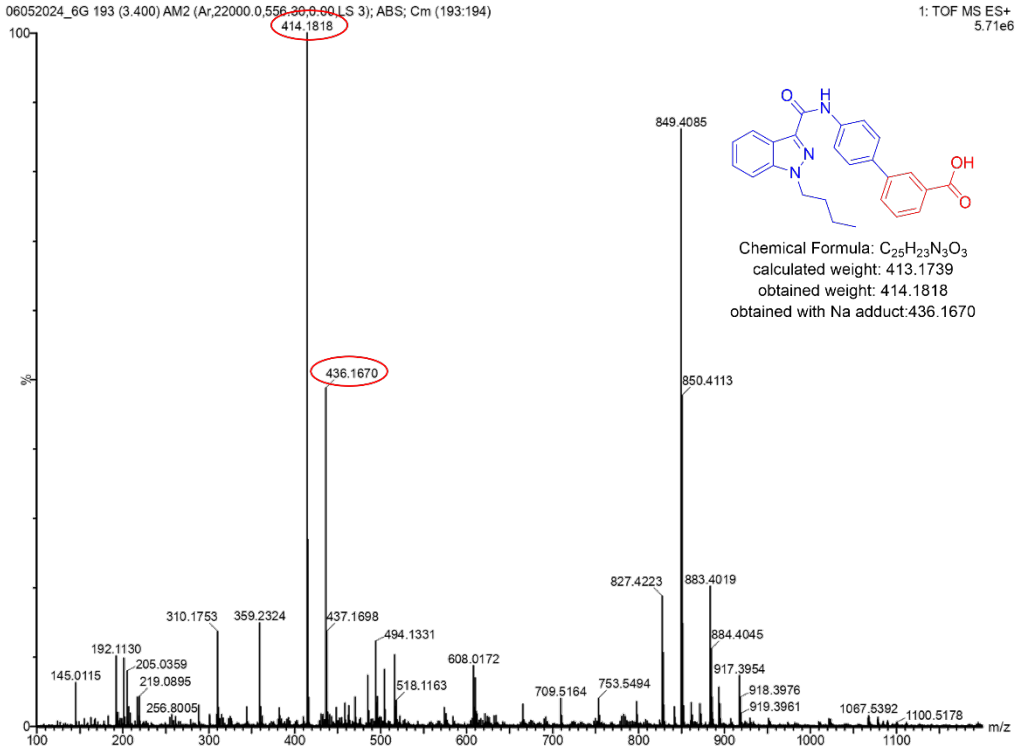
DEPT135-NMR [100MHz, $CDCl_3$] spectrum of 4-(1-butyl-1*H*-indazole-3-carboxamido)-[1,1-biphenyl]-3-carboxylic acid (6g).



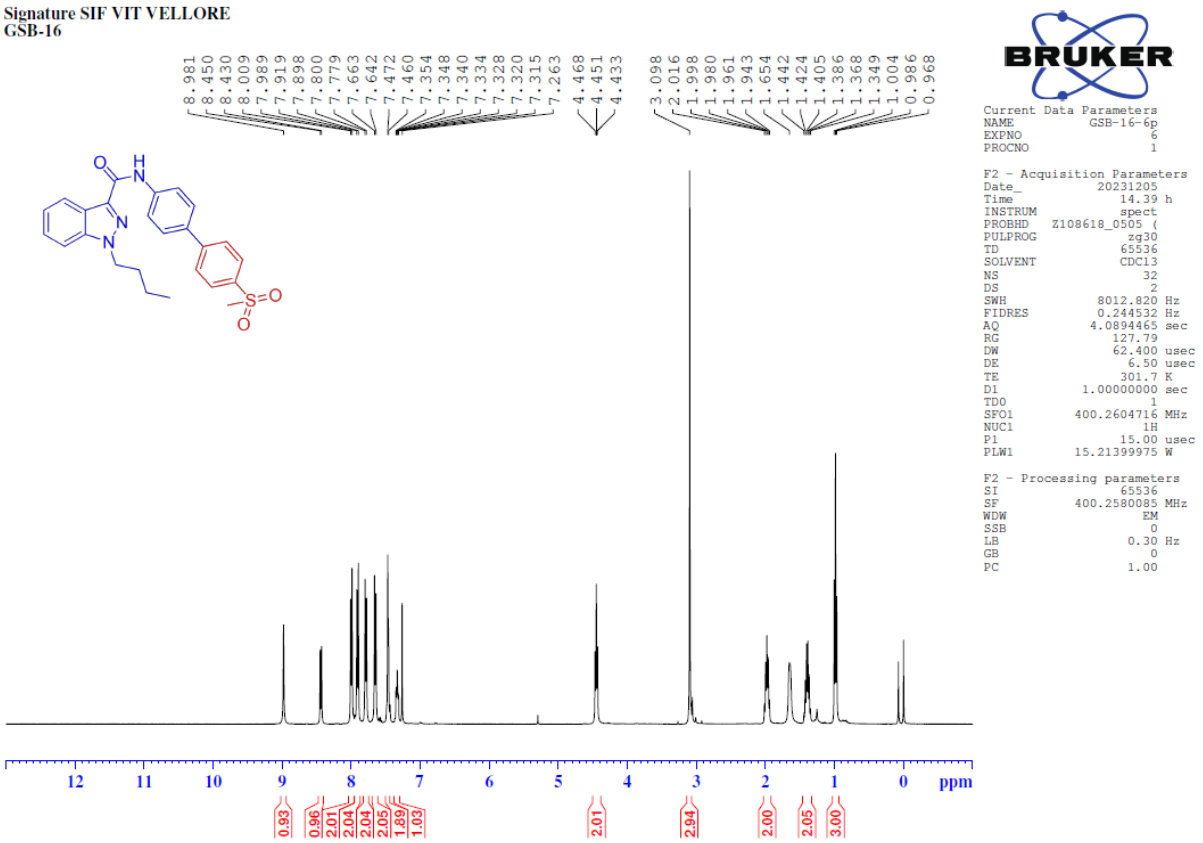
FT-IR spectrum of 4-(1-butyl-1*H*-indazole-3-carboxamido)-[1,1-biphenyl]-3-carboxylic acid (6g).



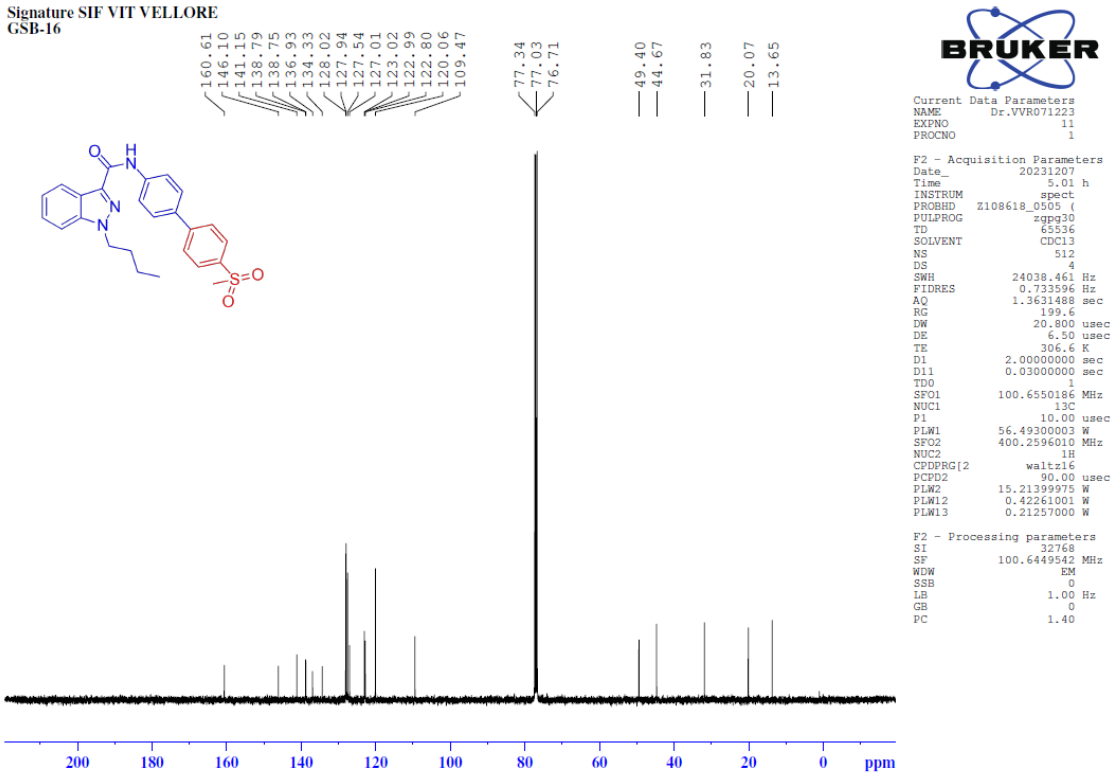
HRMS of 4-(1-butyl-1*H*-indazole-3-carboxamido)-[1,1-biphenyl]-3-carboxylic acid (6g).



^{1}H-NMR [400MHz, $CDCl_3$] spectrum of 1-butyl-N-(4-(methylsulfonyl)-[1,1-biphenylyl]-4-yl)-1*H*-indazole-3-carboxamide (6h).



^{13}C-NMR [100MHz, $CDCl_3$] spectrum of 1-butyl-N-(4-(methylsulfonyl)-[1,1-biphenylyl]-4-yl)-1*H*-indazole-3-carboxamide(6h).

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Current Data Parameters
NAME        Dr.VVR071223
EXPNO                 11
PROCNO                 1

F2 - Acquisition Parameters
Date_           20231207
Time                5.01 h
INSTRUM            spect
PROBHD    Z108618_0505 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
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               306.6 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1
SFO1        100.6550186 MHz
NUC1               13C
P1               10.00 usec
PLW1         56.49300003 W
SFO2        400.2596010 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2            90.00 usec
PLW2         15.21399975 W
PLW12         0.42261001 W
PLW13         0.21257000 W

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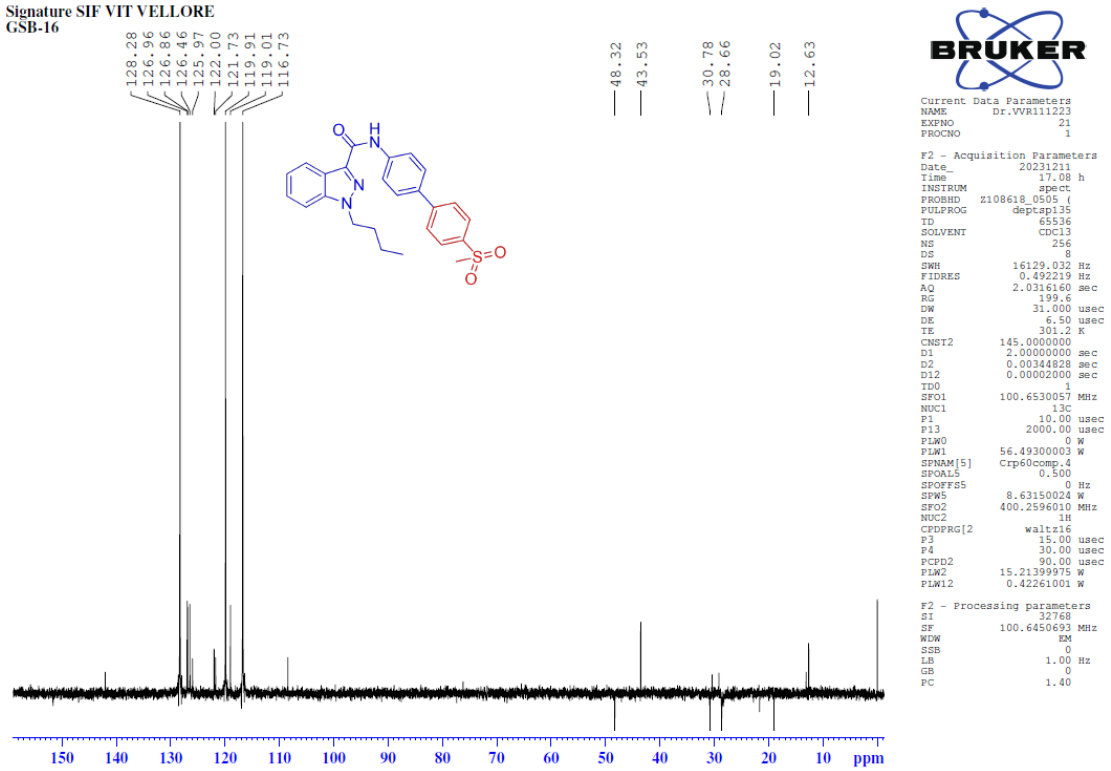

DEPT135-NMR [100MHz, $CDCl_3$] spectrum of 1-butyl-N-(4-(methylsulfonyl)-[1,1-biphenylyl]-4-yl)-1*H*-indazole-3-carboxamide (6h).

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Current Data Parameters
NAME        Dr.VVR111223
EXPNO                 21
PROCNO                 1

F2 - Acquisition Parameters
Date_           20231211
Time               17.08 h
INSTRUM            spect
PROBHD    Z108618_0505 (
PULPROG        deptsp135
TD                65536
SOLVENT           CDCl3
NS                  256
DS                    8
SWH           16129.032 Hz
FIDRES         0.492219 Hz
AQ             2.0316160 sec
RG                199.6
DW               31.000 usec
DE                6.50 usec
TE               301.2 K
CNST2        145.0000000
D1            2.00000000 sec
D2            0.00344828 sec
D12           0.00002000 sec
TD0                   1
SFO1        100.6530057 MHz
NUC1               13C
P1               10.00 usec
P13            2000.00 usec
PLW0                  0 W
PLW1         56.49300003 W
SPNAM[5]    Crp60comp.4
SPOAL5             0.500
SPOFF5                0 Hz
SPW5          8.63150024 W
SFO2        400.2596010 MHz
NUC2               1H
CPDPRG[2        waltz16
P3               15.00 usec
P4               30.00 usec
PCPD2            90.00 usec
PLW2         15.21399975 W
PLW12         0.42261001 W

F2 - Processing parameters
SI                32768
SF          100.6450693 MHz
WDW                EM
SSB                 0
LB                1.00 Hz
GB                  0
PC                1.40
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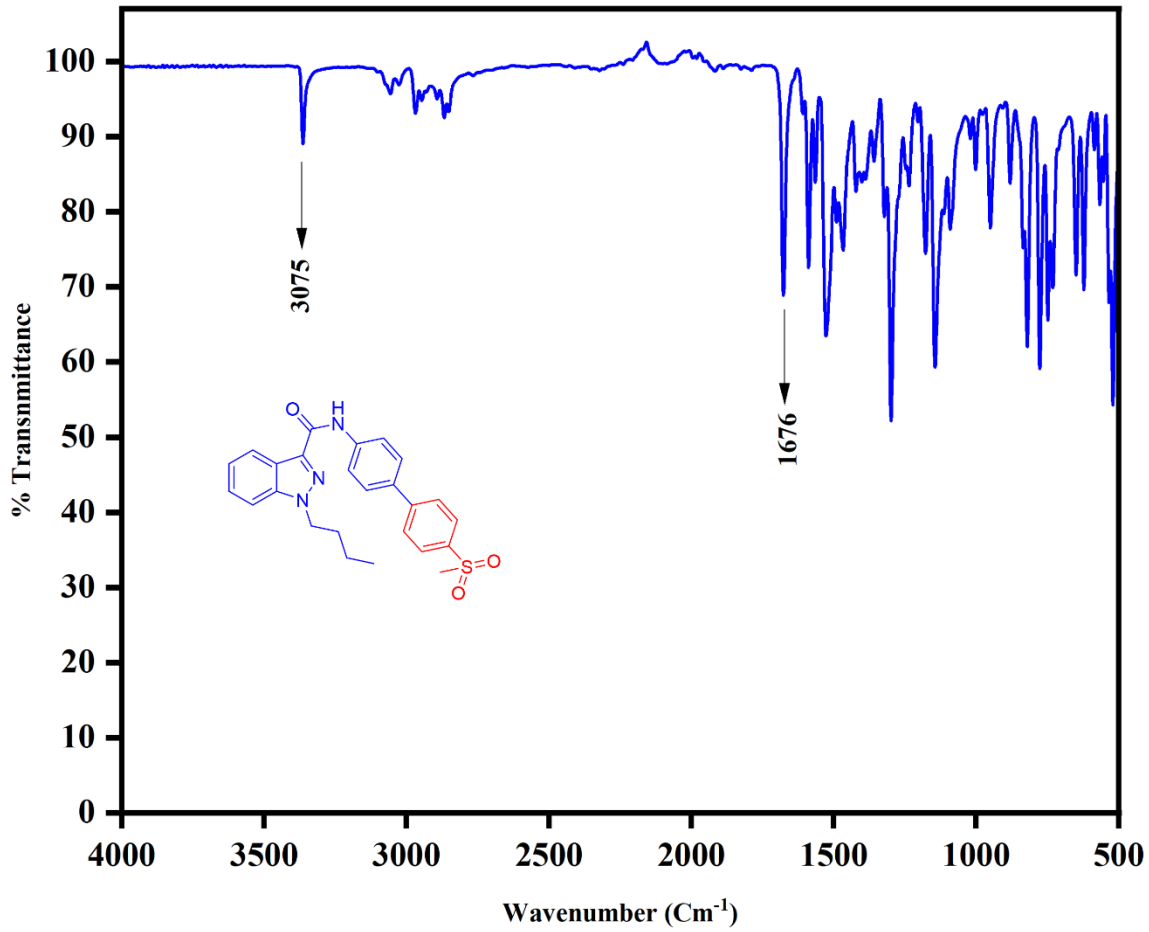
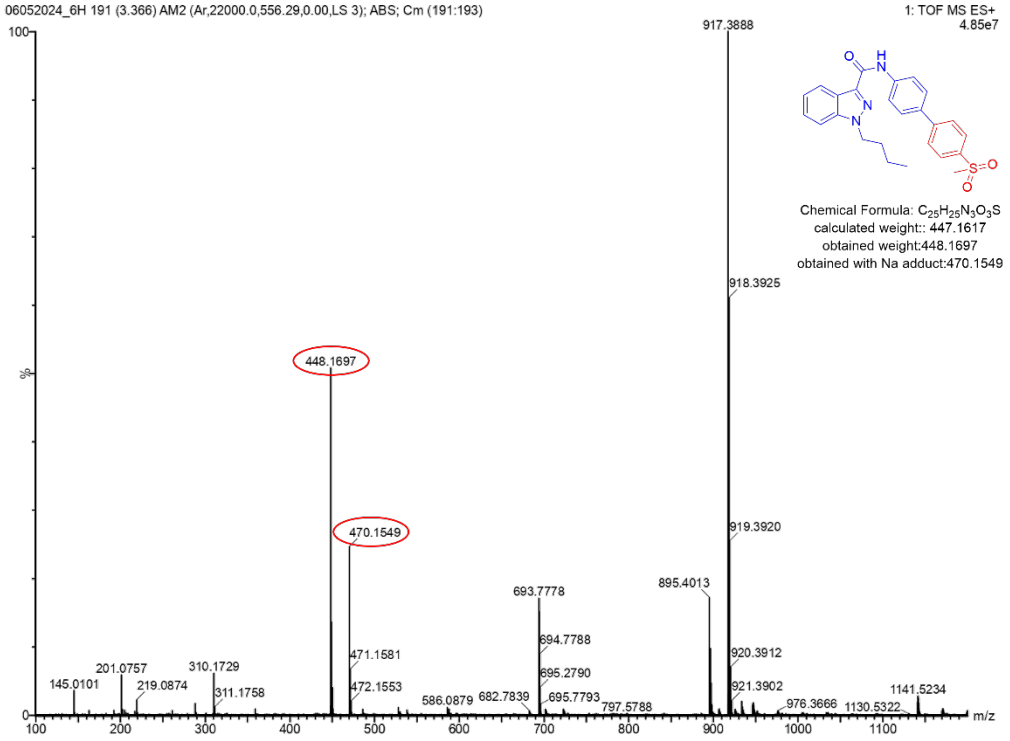
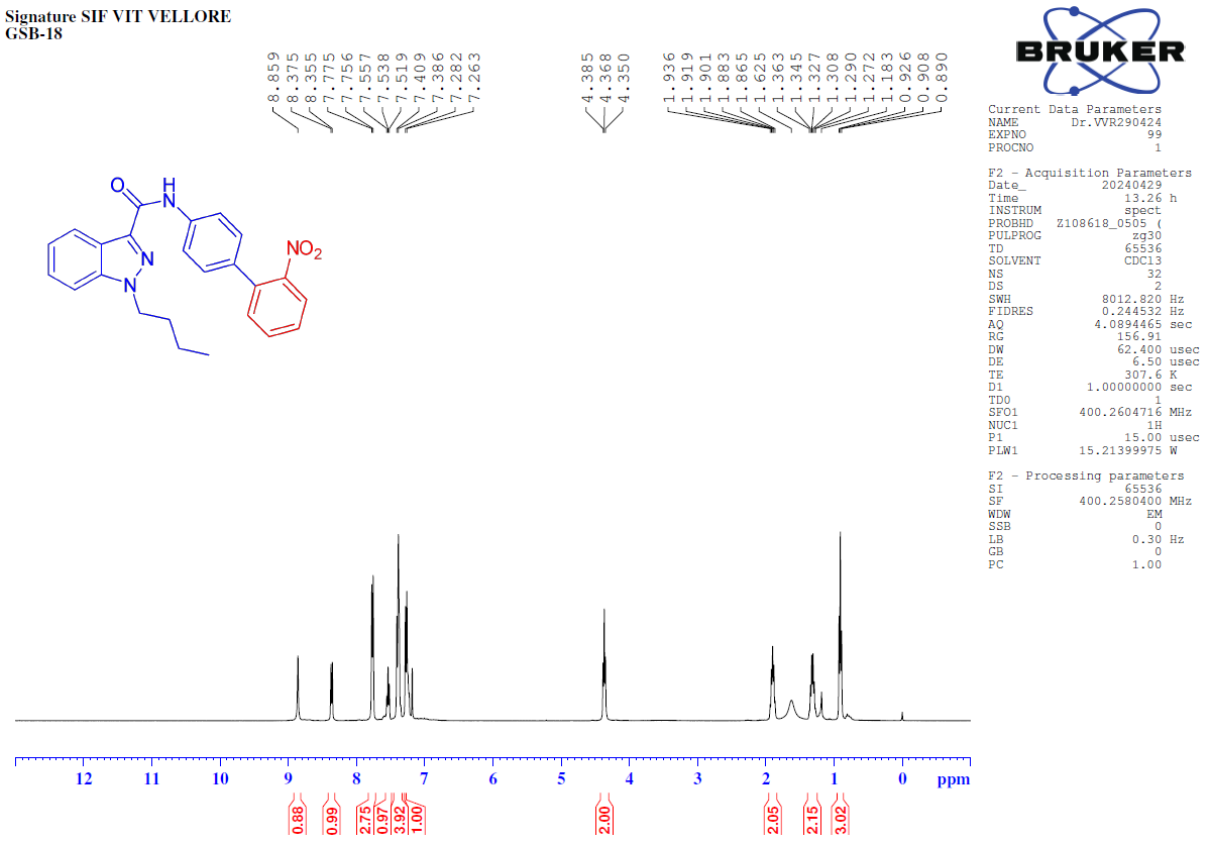
FT-IR spectrum of 1-butyl-N-(4-(methylsulfonyl)-[1,1-biphenylyl]-4-yl)-1*H*-indazole-3-carboxamide (6h).



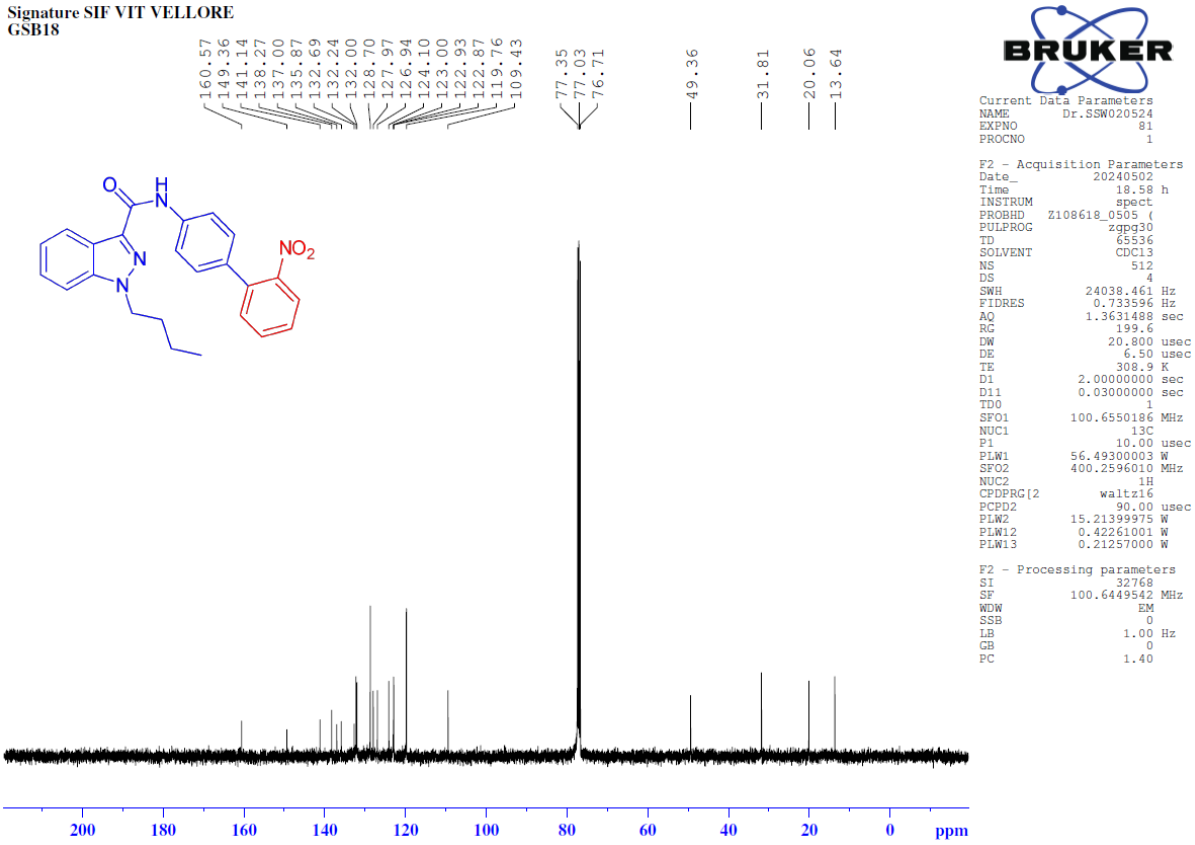
HRMS of 1-butyl-N-(4-(methylsulfonyl)-[1,1-biphenylyl]-4-yl)-1*H*-indazole-3-carboxamide (6h).



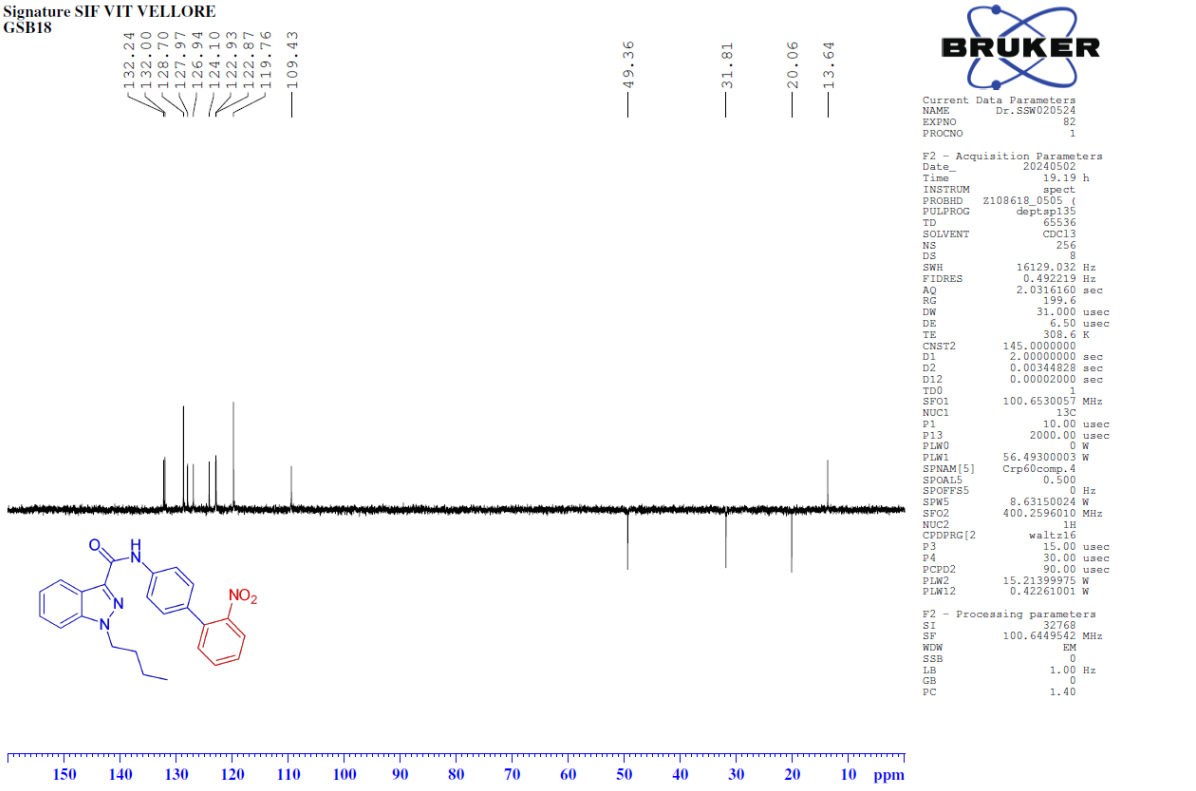
[1]H-NMR [400MHz, $CDCl_3$] spectrum of 1-butyl-N-(2-nitro[1,1-biphenyl]-4-1*H*-indazole-3-carboxamide (6i).



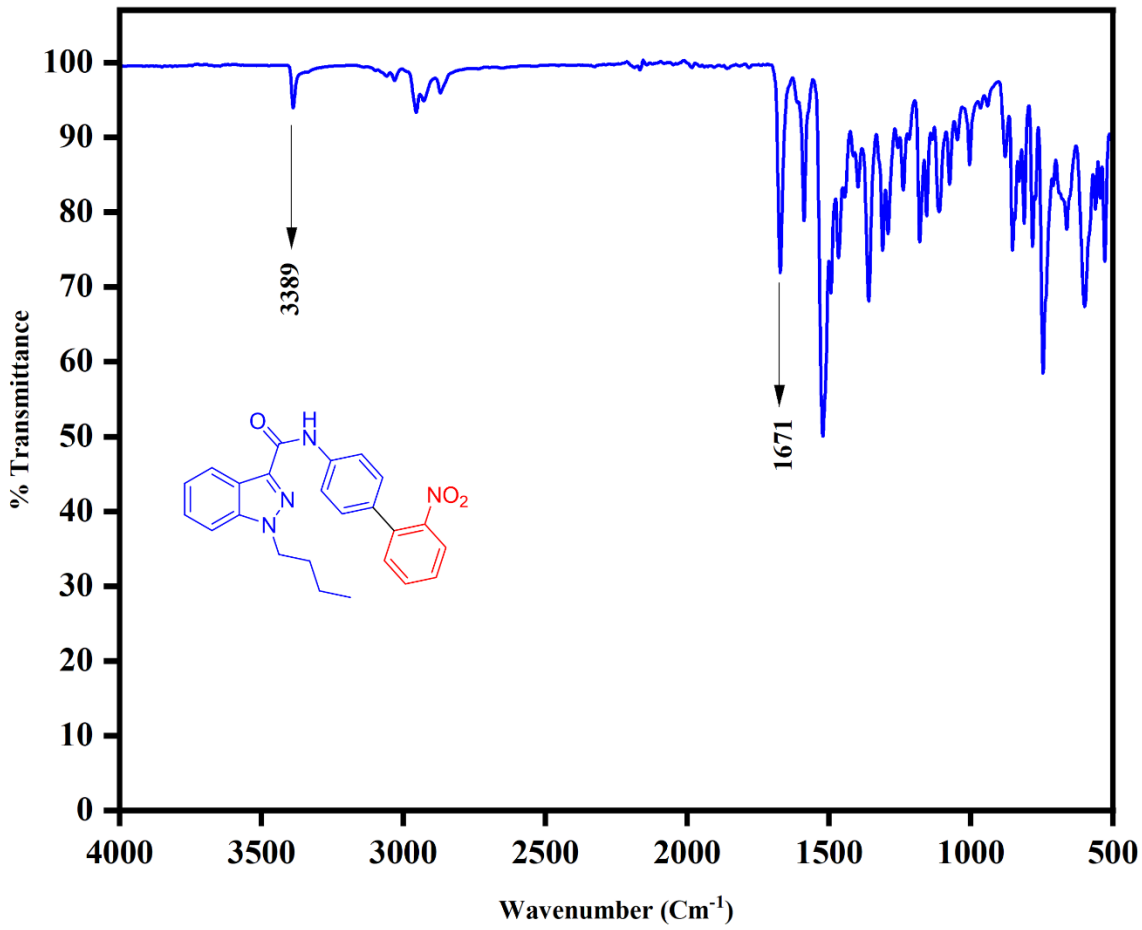
^{13}C-NMR [100MHz, $CDCl_3$] spectrum of 1-butyl-N-(2-nitro[1,1-biphenyl]-4-1*H*-indazole-3-carboxamide (6i).



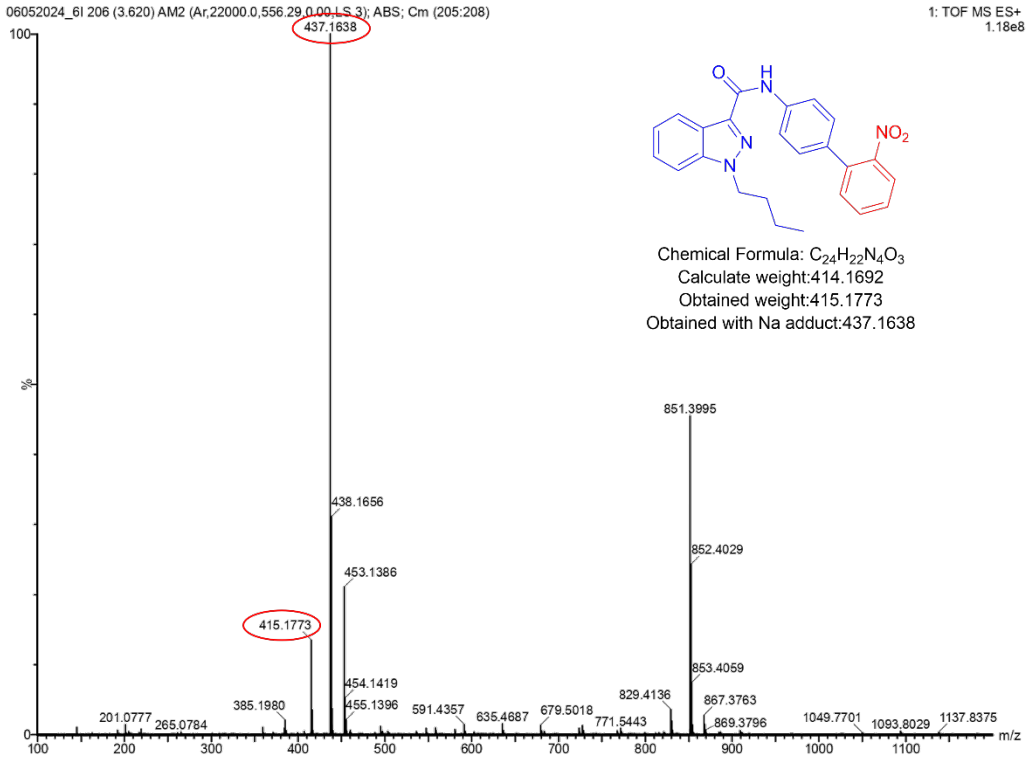
DEPT135-NMR [100MHz, $CDCl_3$] spectrum of 1-butyl-N-(2-nitro[1,1-biphenyl]-4-1*H*-indazole-3-carboxamide (6i).



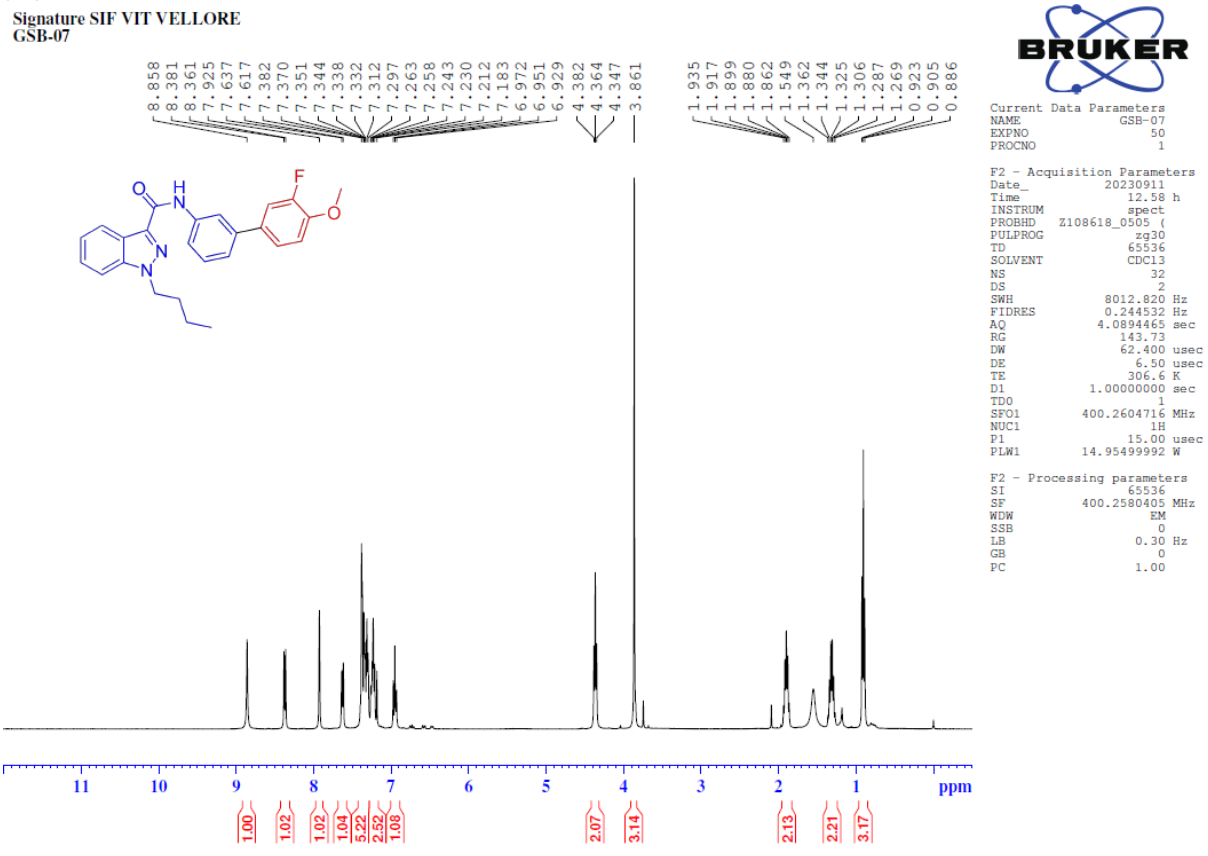
FT-IR spectrum of 1-butyl-N-(2-nitro[1,1-biphenyl]-4-1*H*-indazole-3-carboxamide (6i).



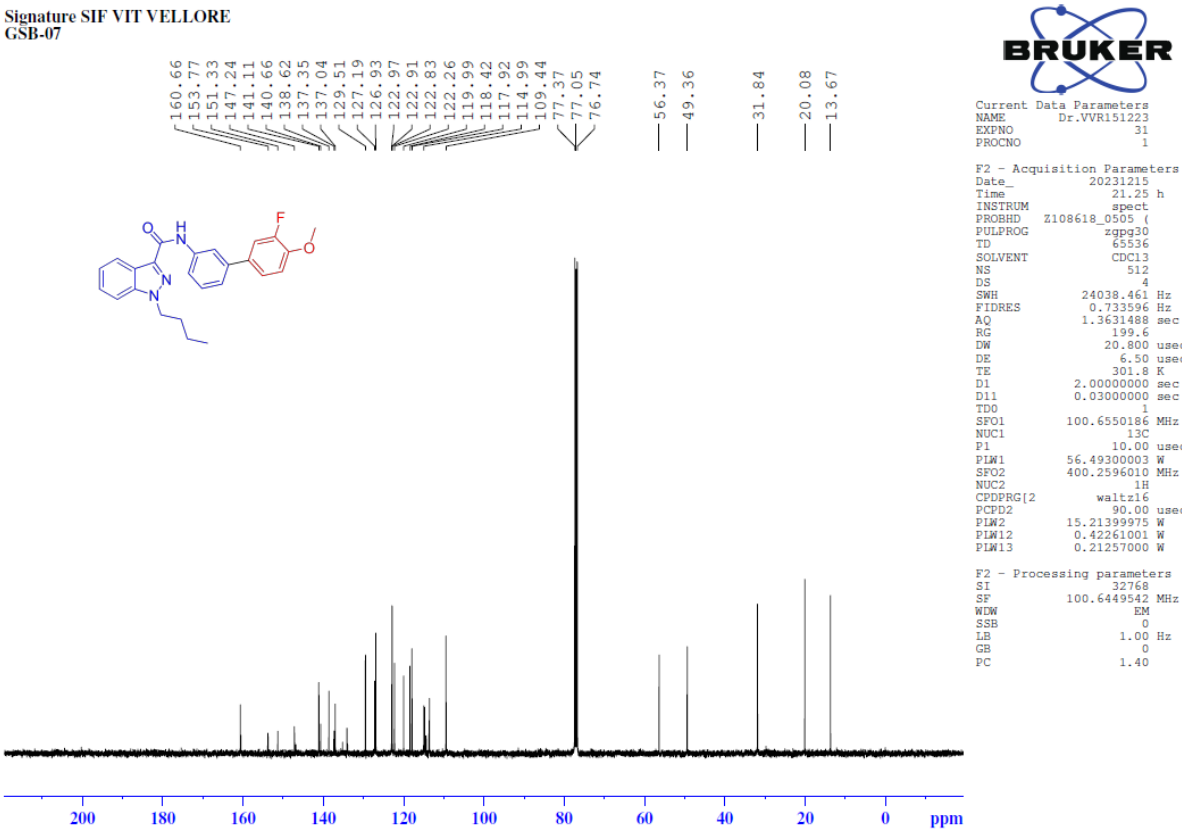
HRMS of1-butyl-N-(2-nitro[1,1-biphenyl]-4-1*H*-indazole-3-carboxamide (6i).



[1]H-NMR [400MHz, $CDCl_3$] spectrum of 1-butyl-N-(3-fluoro-4-methoxy-[1,1-biphenyl]-3-yl)-1*H*-indazole-3-carboxamide (7a).



^{13}C-NMR [100MHz, $CDCl_3$] spectrum of 1-butyl-N-(3-fluoro-4-methoxy-[1,1-biphenyl]-3-yl)-1*H*-indazole-3-carboxamide (7a).

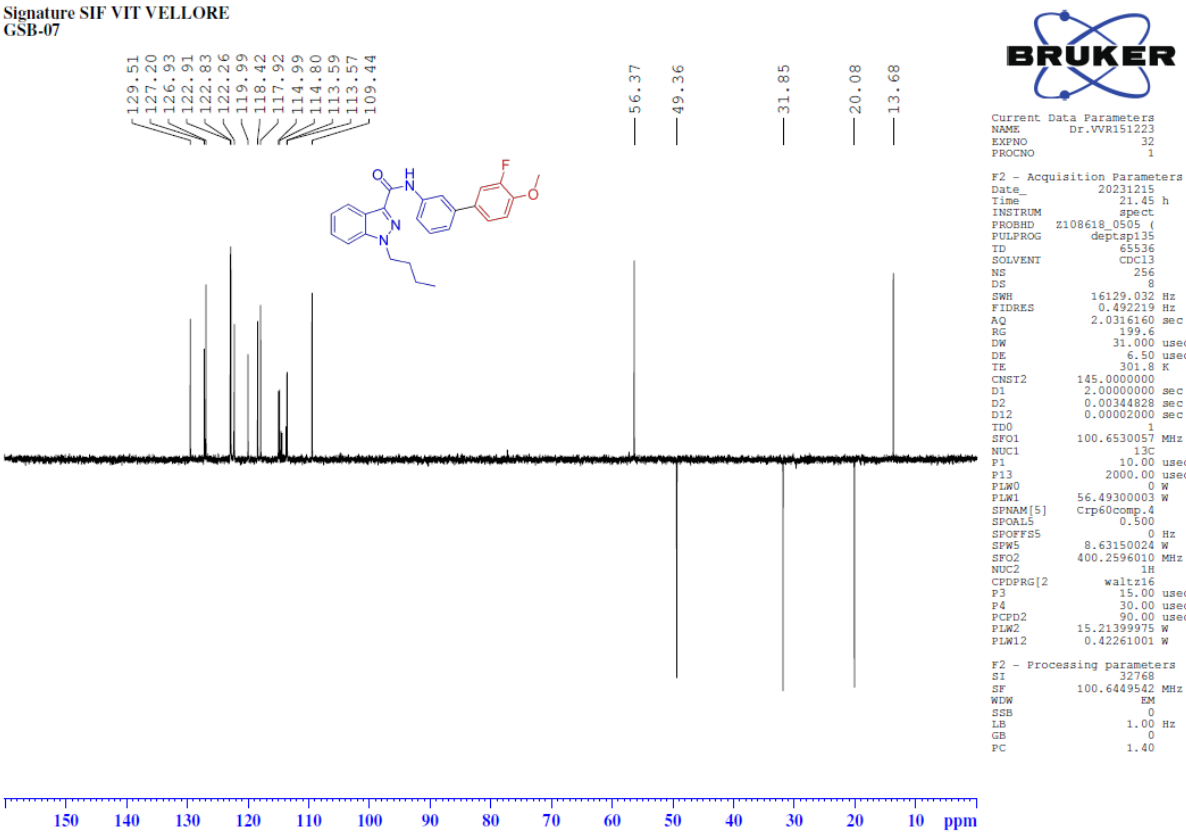


Current Data Parameters
NAME Dr.VVR151223
EXPNO 31
PROCNO 1

F2 - Acquisition Parameters
Date_ 20231215
Time 21.25 h
INSTRUM spect
PROBHD Z108618_0505 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
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 301.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6550186 MHz
NUC1 13C
P1 10.00 usec
PLW1 56.49300003 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 15.21399975 W
PLW12 0.42261001 W
PLW13 0.21257000 W

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

DPET135-NMR [100MHz, $CDCl_3$] spectrum of 1-butyl-N-(3-fluoro-4-methoxy-[1,1-biphenyl]-3-yl)-1*H*-indazole-3-carboxamide (7a).

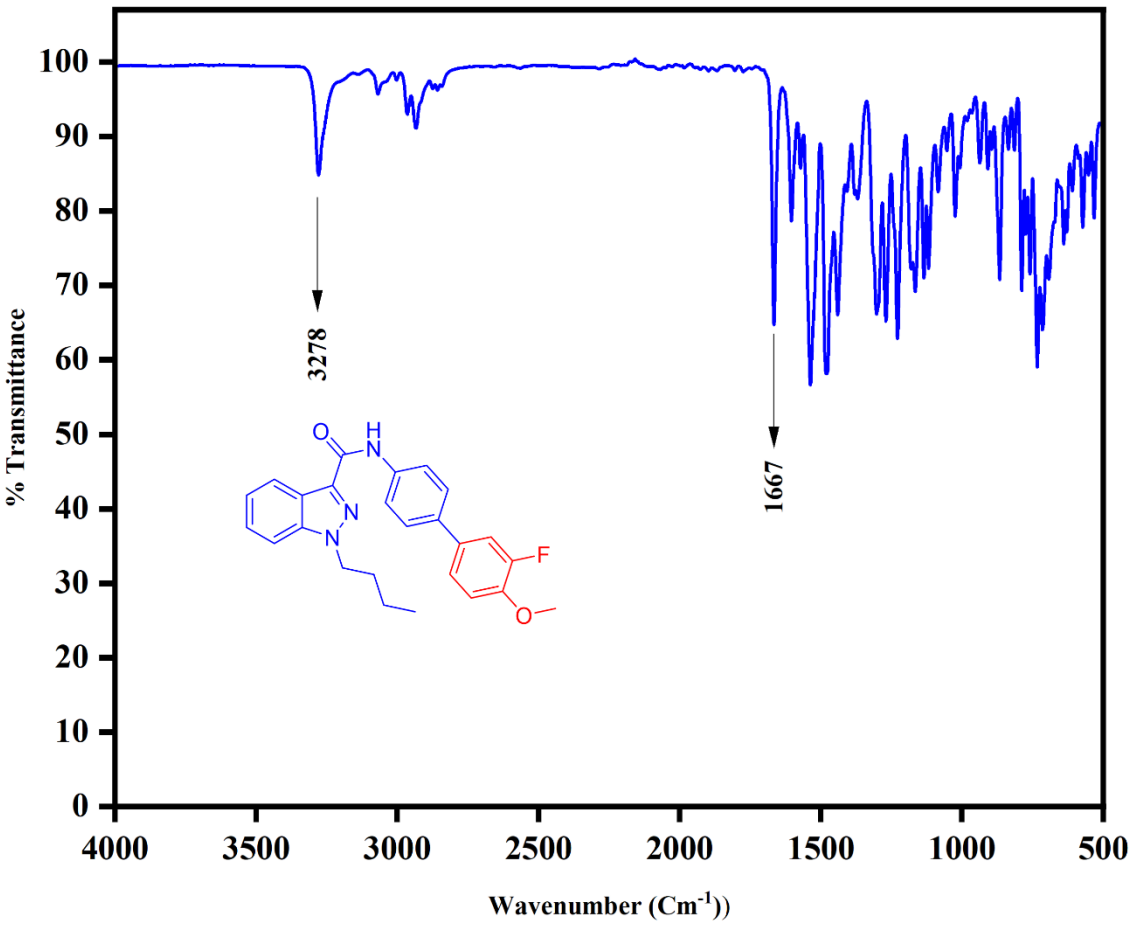


Current Data Parameters
NAME Dr.VVR151223
EXPNO 32
PROCNO 1

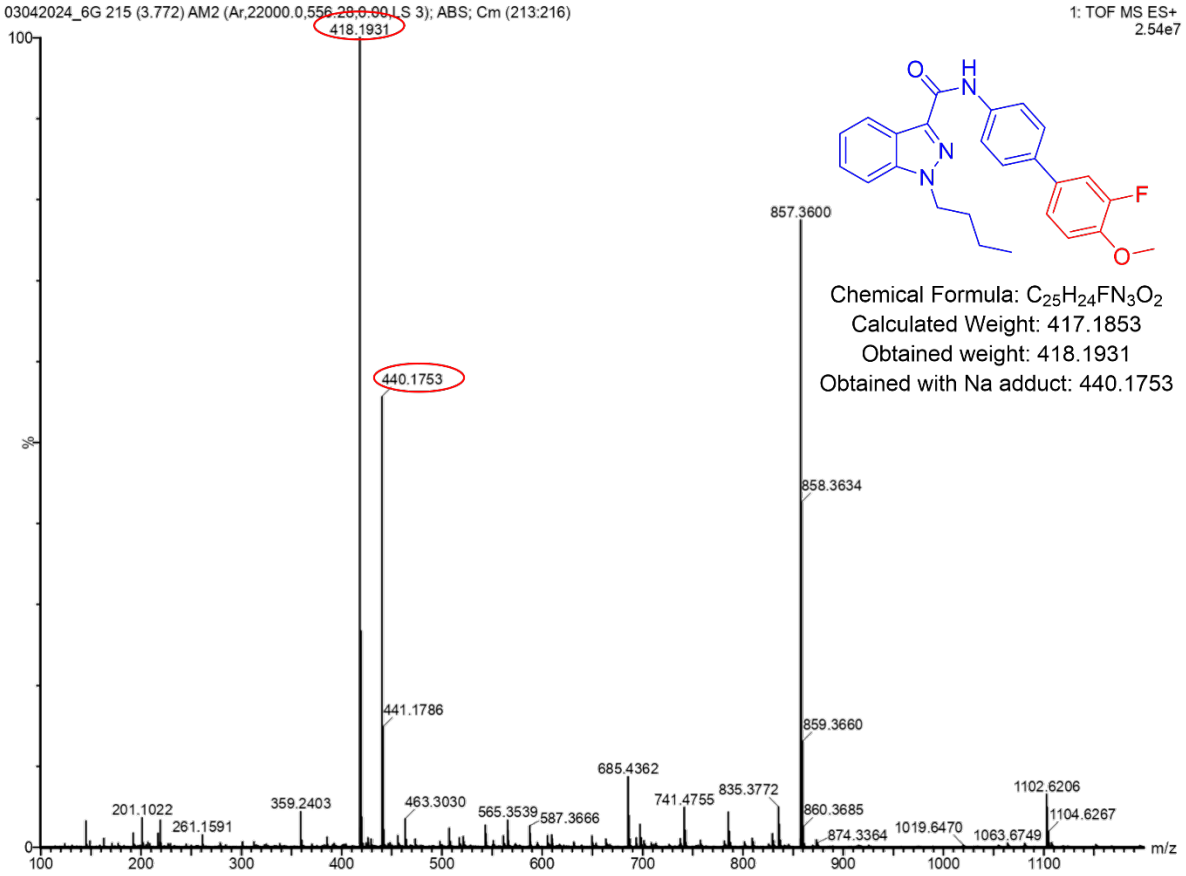
F2 - Acquisition Parameters
Date_ 20231215
Time 21.45 h
INSTRUM spect
PROBHD Z108618_0505 (
PULPROG deptsp135
TD 65536
SOLVENT CDCl3
NS 256
DS 8
SWH 16129.032 Hz
FIDRES 0.492219 Hz
AQ 2.0316160 sec
RG 199.6
DW 31.000 usec
DE 6.50 usec
TE 301.8 K
CNST2 145.0000000
D1 2.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1
SFO1 100.6530057 MHz
NUC1 13C
P1 10.00 usec
P13 2000.00 usec
PLW0 0 W
PLW1 56.49300003 W
SPNAM[5] Crp60comp.4
SPOAL5 0.500
SPOFFS5 0 Hz
SPW5 8.63150024 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG[2 waltz16
P3 15.00 usec
P4 30.00 usec
PCPD2 90.00 usec
PLW2 15.21399975 W
PLW12 0.42261001 W

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

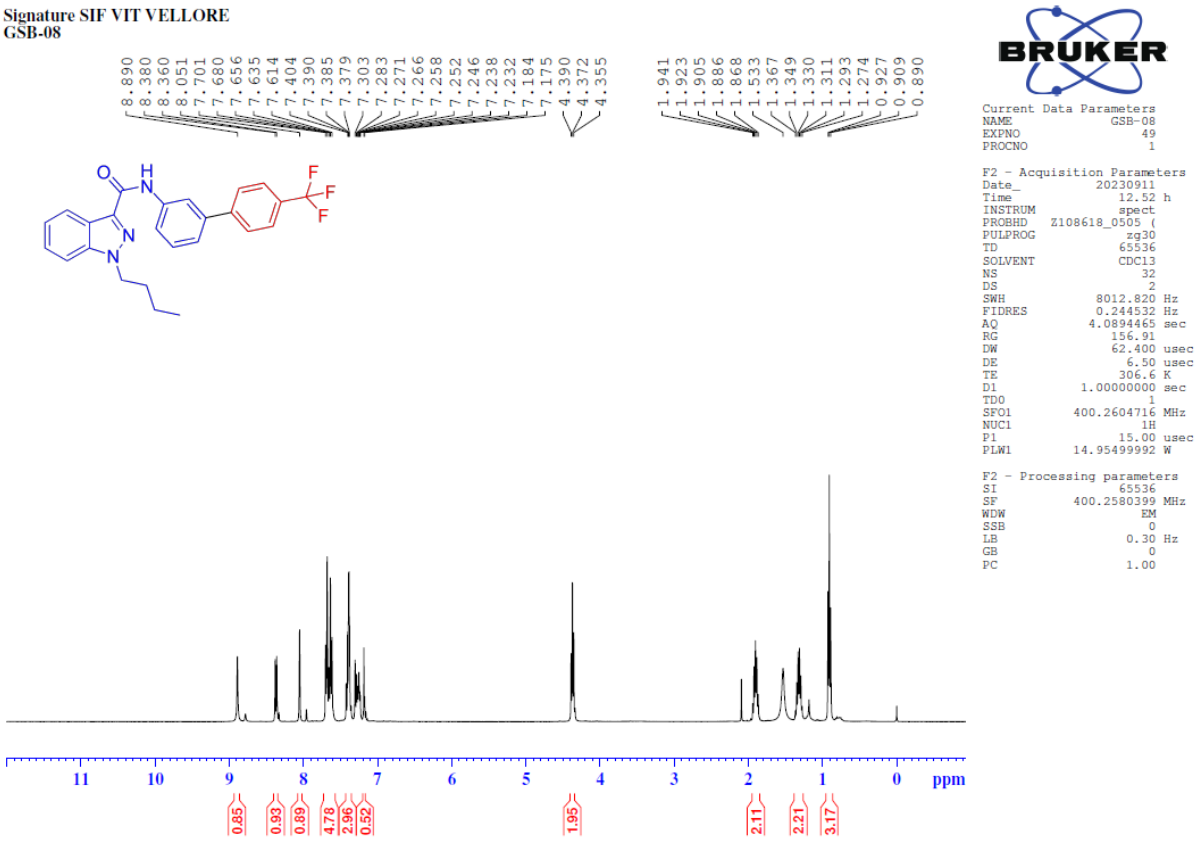
FT-IR spectrum of 1-butyl-N-(3-fluoro-4-methoxy-[1,1-biphenyl]-3-yl)-1*H*-indazole-3-carboxamide (7a).



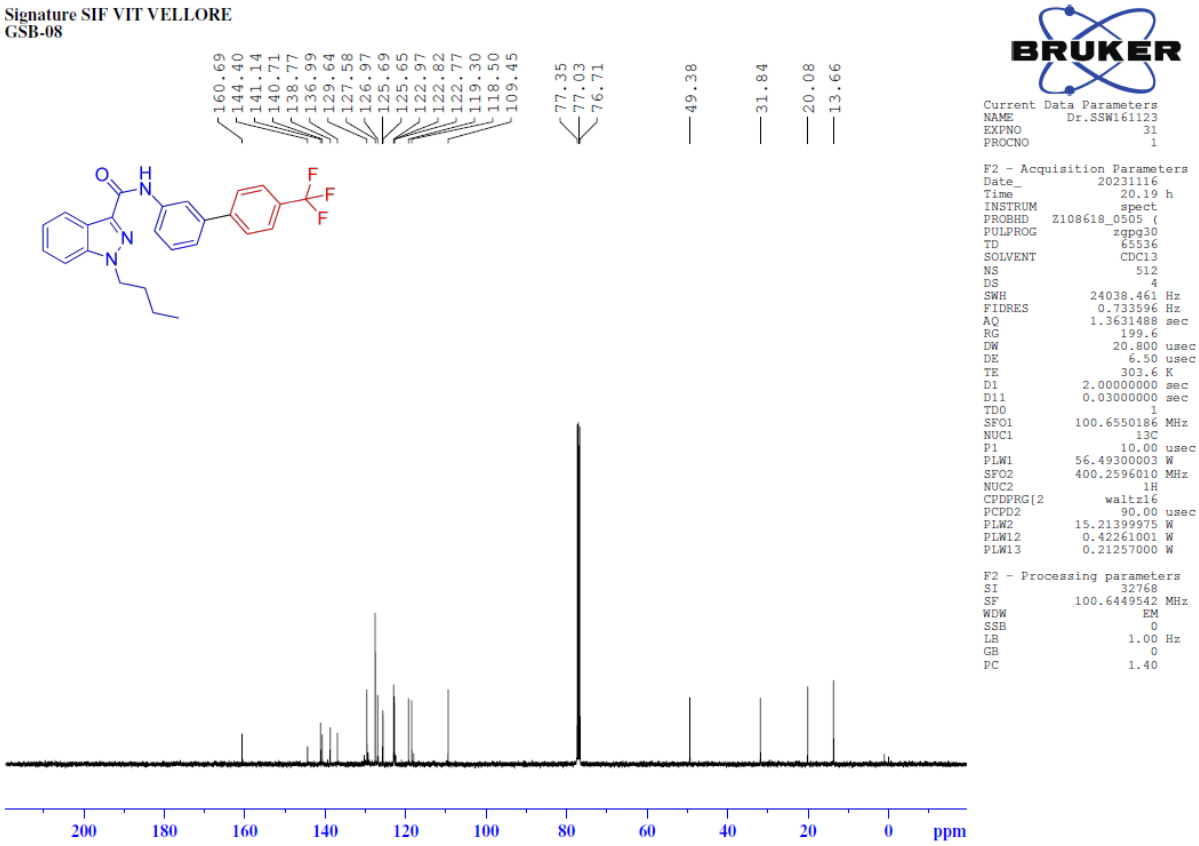
HRMS of 1-butyl-N-(3-fluoro-4-methoxy-[1,1-biphenyl]-3-yl)-1*H*-indazole-3-carboxamide (7a).



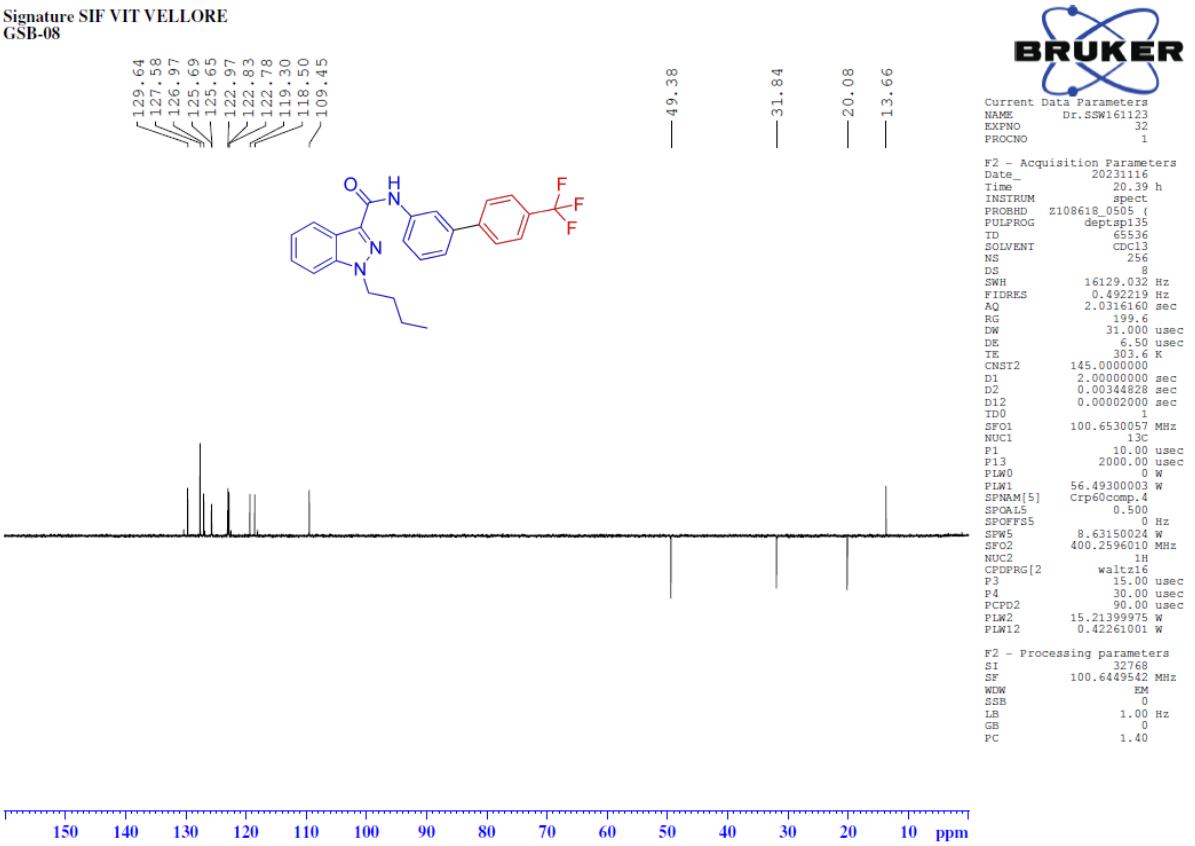
^{1}H-NMR [400MHz, $CDCl_3$] spectrum of 1-butyl-N-(4-(trifluoromethyl)-[1,1-biphenyl]-3-yl)-1*H*-indazole-3-carboxamide (7b).



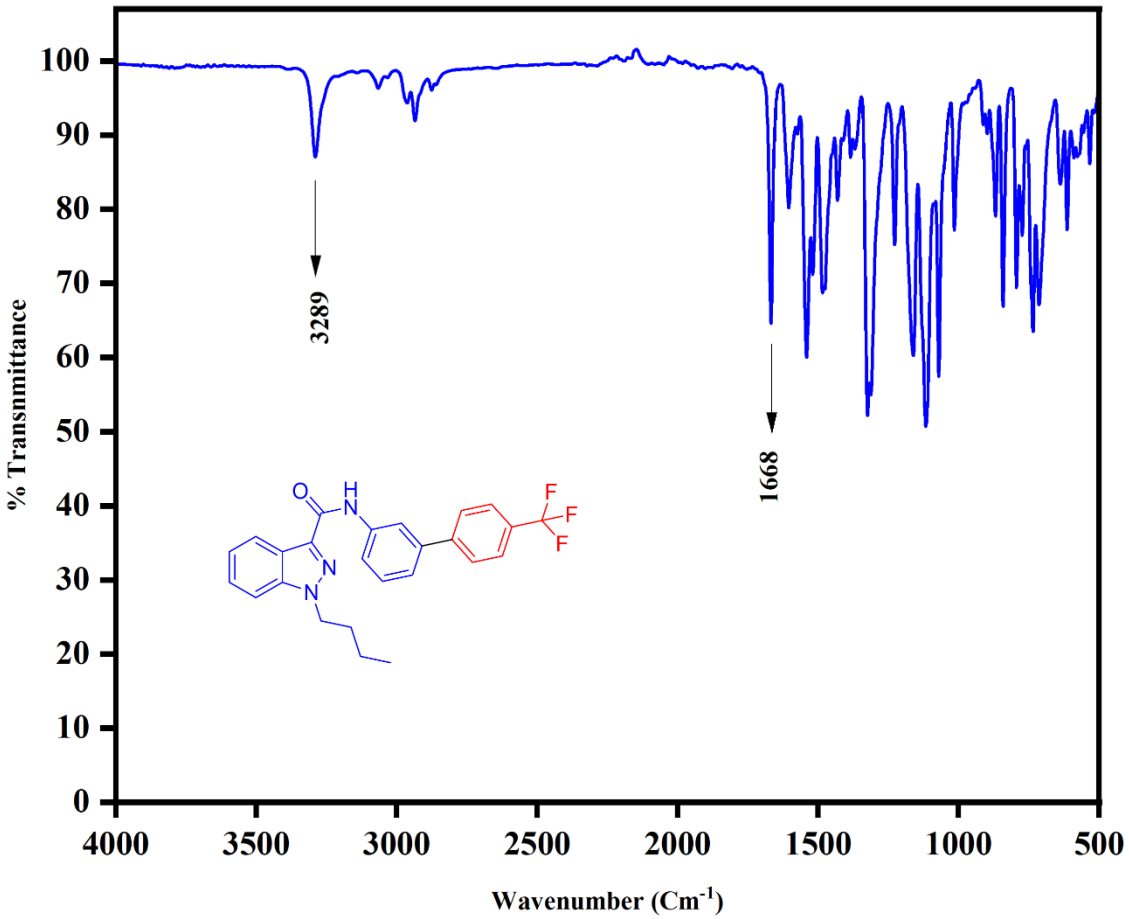
^{13}C-NMR [100MHz, $CDCl_3$] spectrum of 1-butyl-N-(4-(trifluoromethyl)-[1,1-biphenyl]-3-yl)-1*H*-indazole-3-carboxamide (7b).



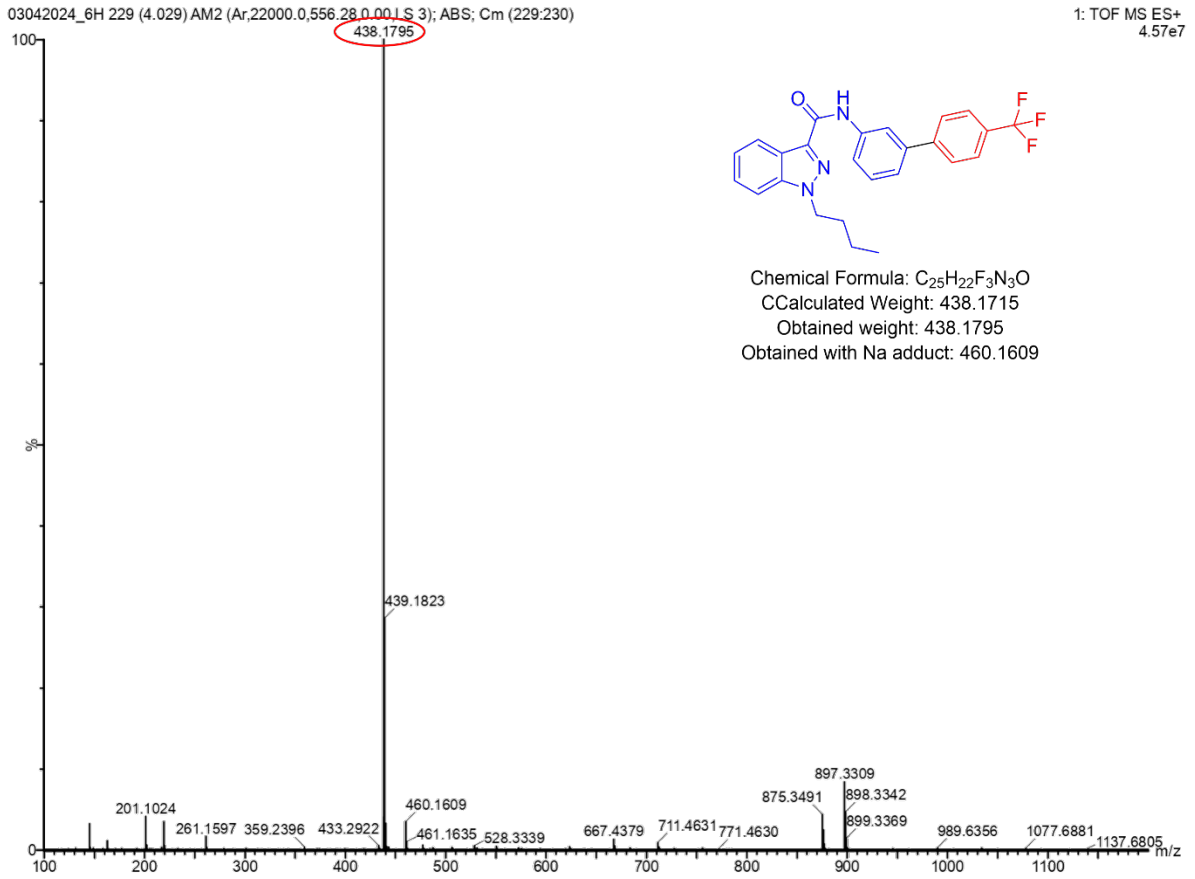
DEPT135-NMR [100MHz, $CDCl_3$] spectrum of 1-butyl-N-(4-(trifluoromethyl)-[1,1-biphenyl]-3-yl)-1*H*-indazole-3-carboxamide (7b).



FT-IR spectrum of 1-butyl-N-(4-(trifluoromethyl)-[1,1-biphenyl]-3-yl)-1*H*-indazole-3-carboxamide (7b).

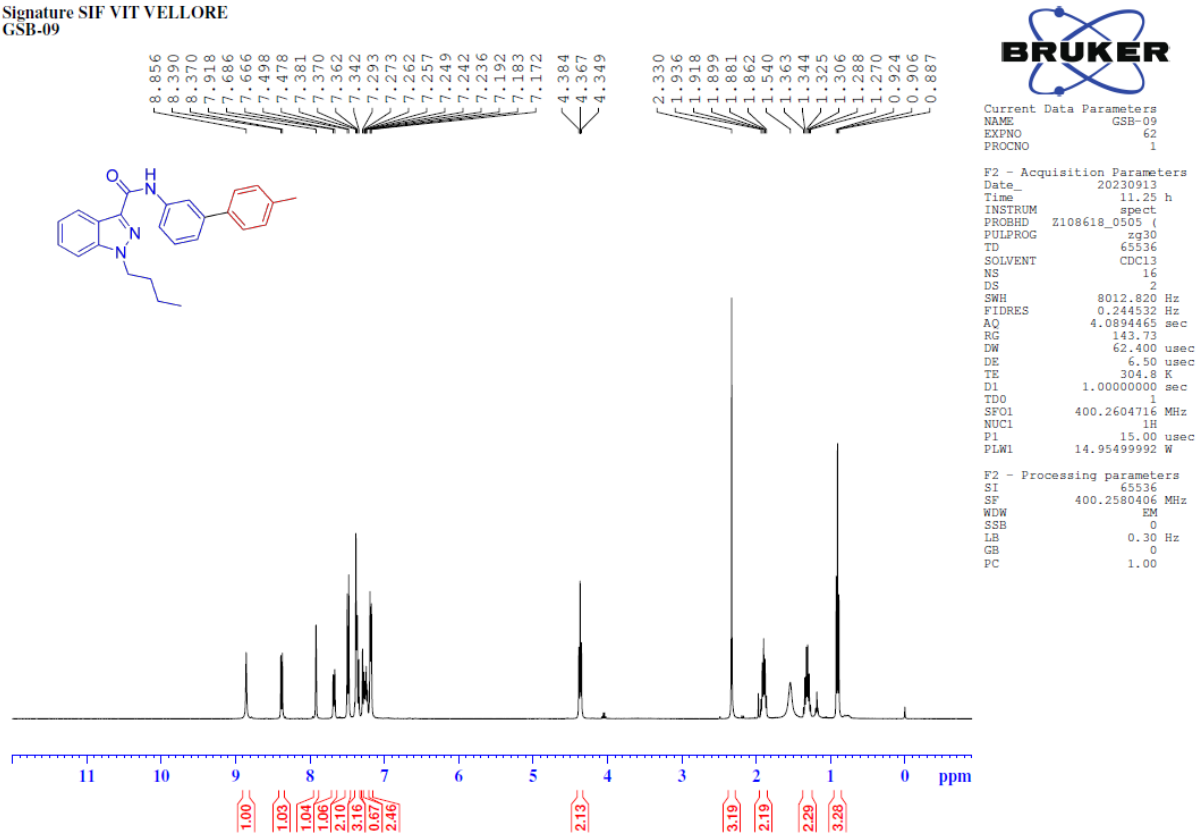


HRMS of 1-butyl-N-(4-(trifluoromethyl)-[1,1-biphenyl]-3-yl)-1*H*-indazole-3-carboxamide (7b).

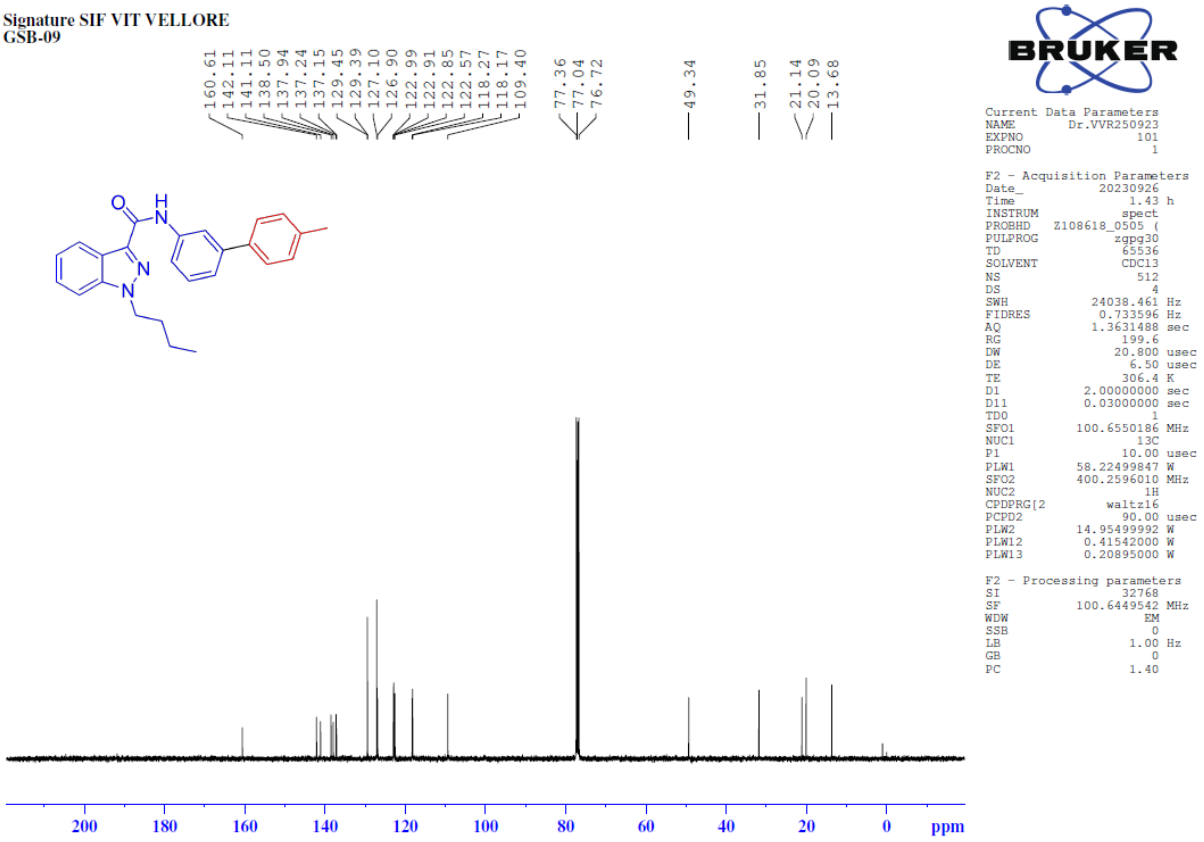


Chemical Formula: $C_{25}H_{22}F_3N_3O$
CCalculated Weight: 438.1715
Obtained weight: 438.1795
Obtained with Na adduct: 460.1609

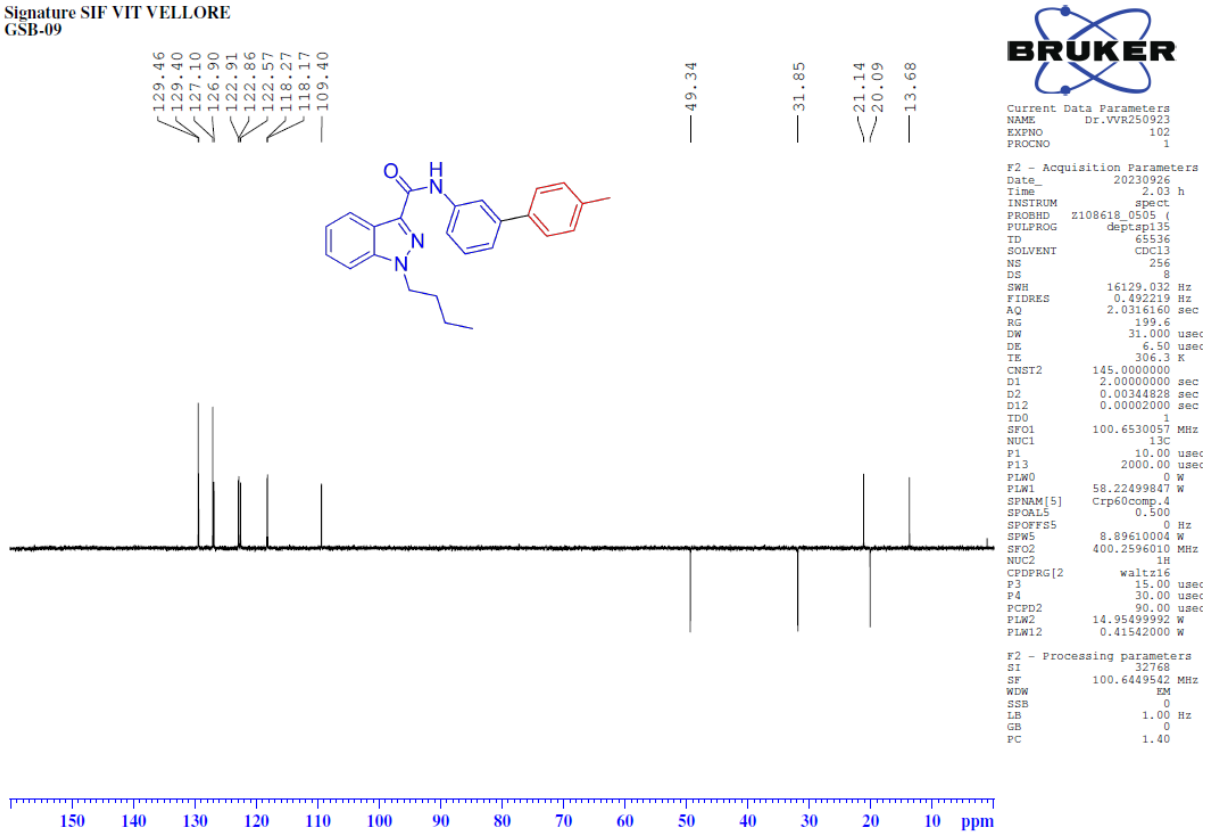
^{1}H-NMR [400MHz, $CDCl_3$] spectrum of 1-butyl-N-(4-methyl-[1,1-biphenyl]-3-yl)-1*H*-indazole-3-carboxamide (7c).



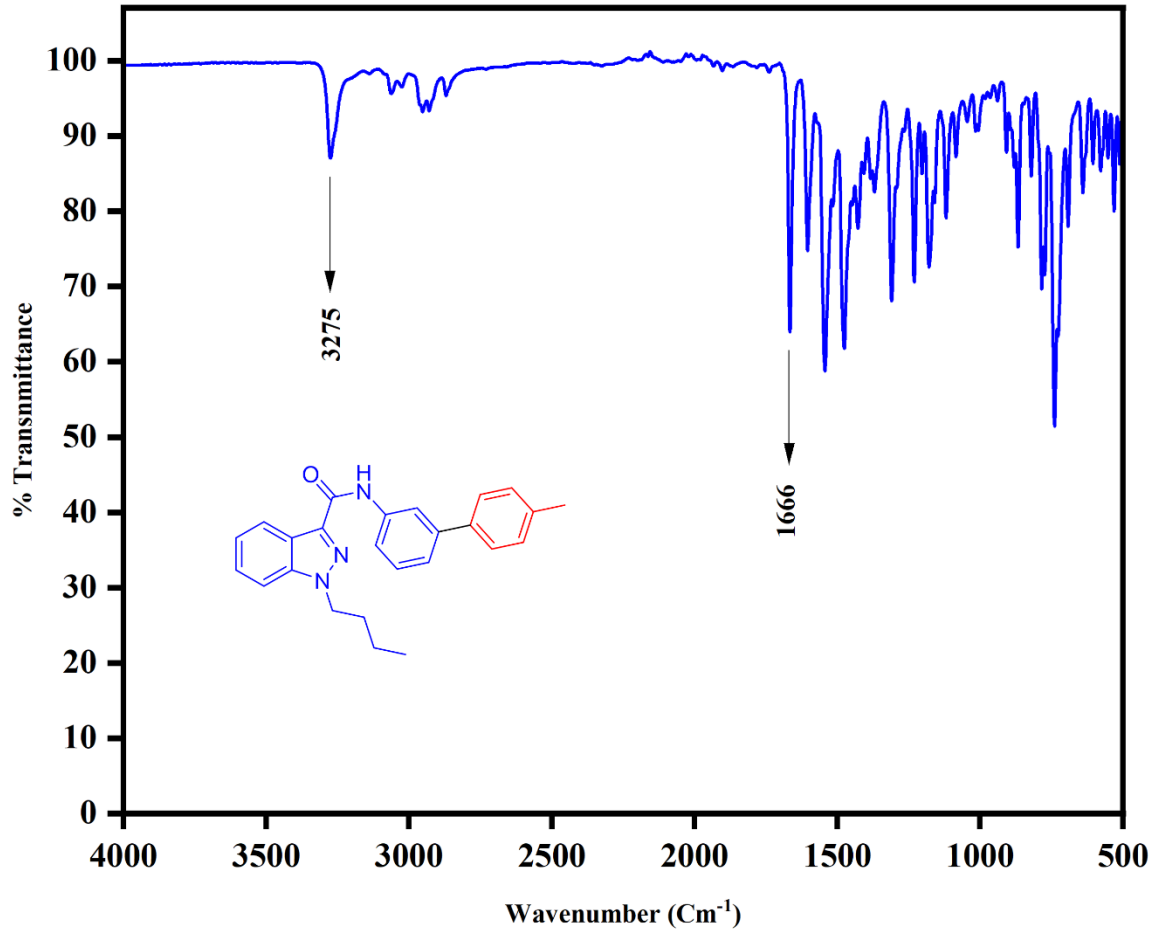
^{13}C-NMR [100MHz, $CDCl_3$] spectrum of 1-butyl-N-(4-methyl-[1,1-biphenyl]-3-yl)-1*H*-indazole-3-carboxamide (7c).



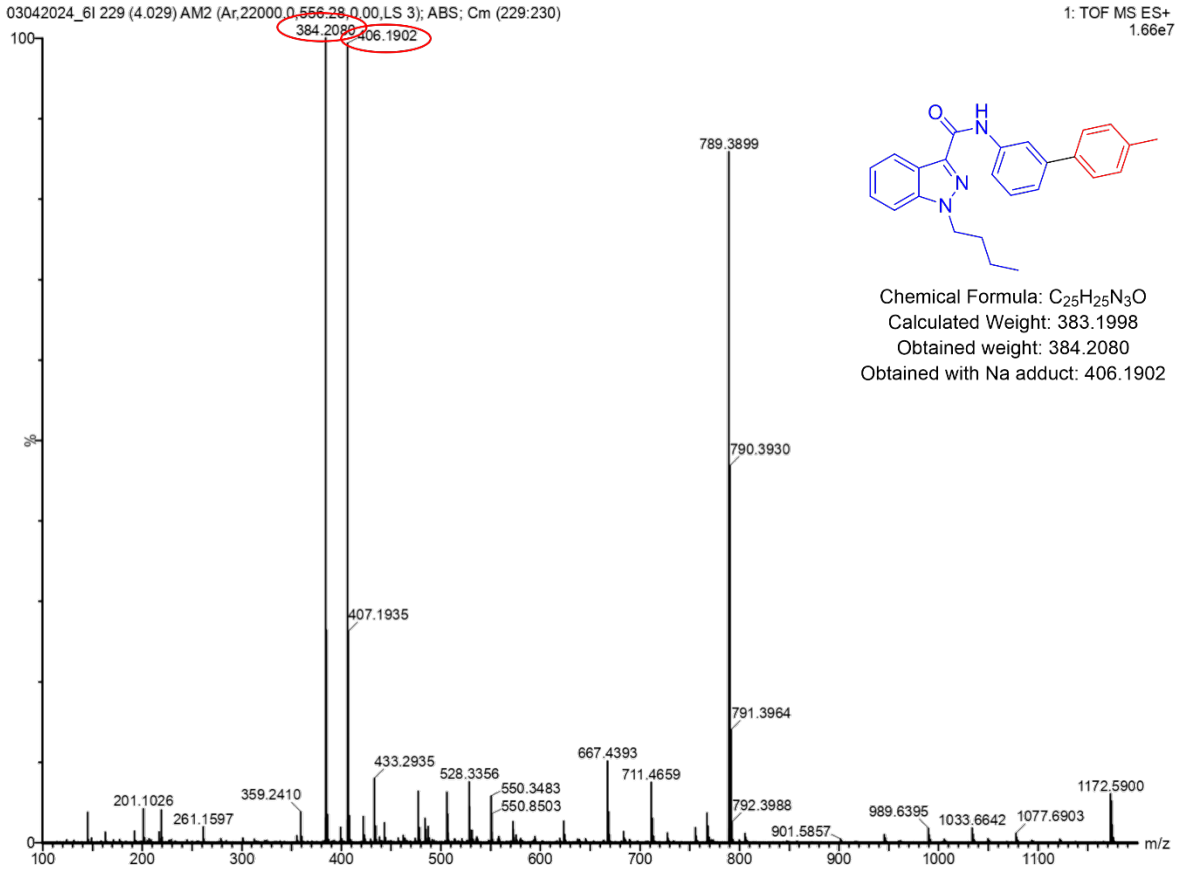
DEPT135-NMR [100MHz, $CDCl_3$] spectrum of 1-butyl-N-(4-methyl-[1,1-biphenyl]-3-yl)-1*H*-indazole-3-carboxamide (7c).



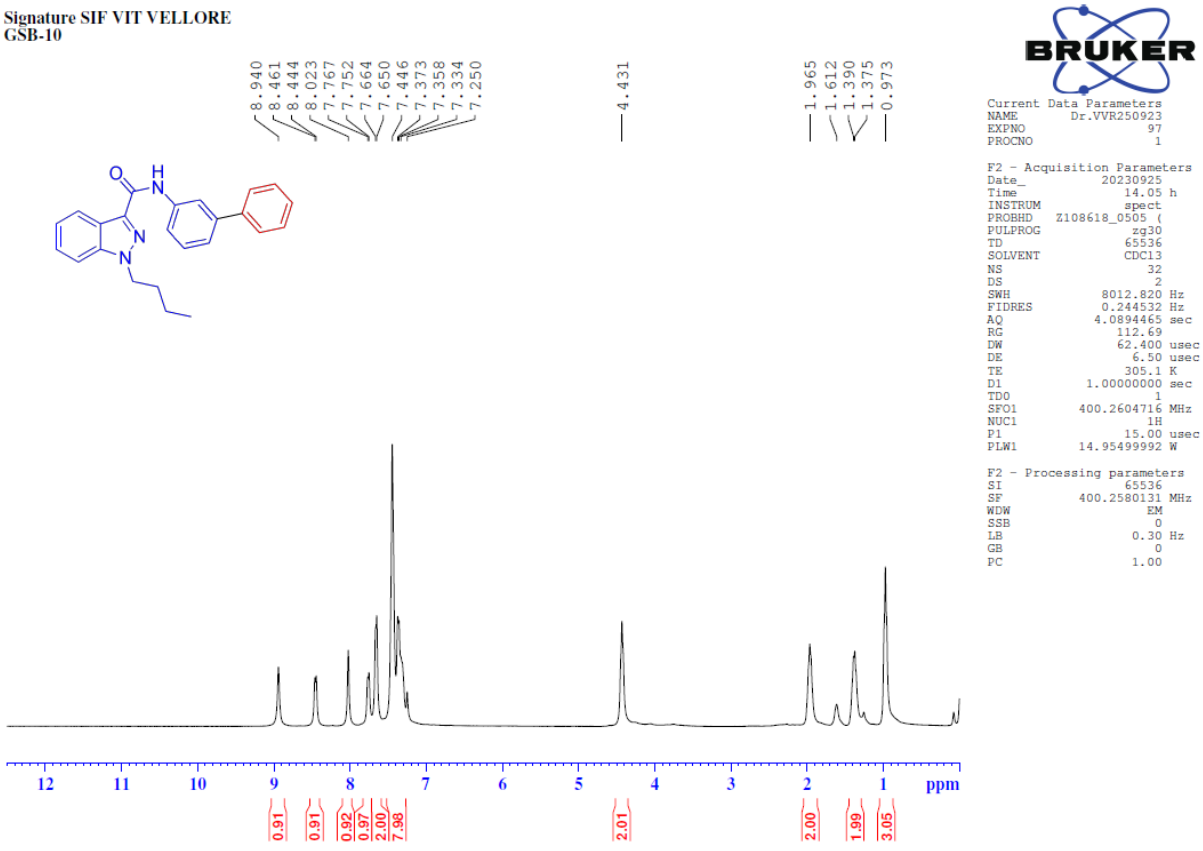
FT-IR spectrum of 1-butyl-N-(4-methyl-[1,1-biphenyl]-3-yl)-1*H*-indazole-3-carboxamide (7c).



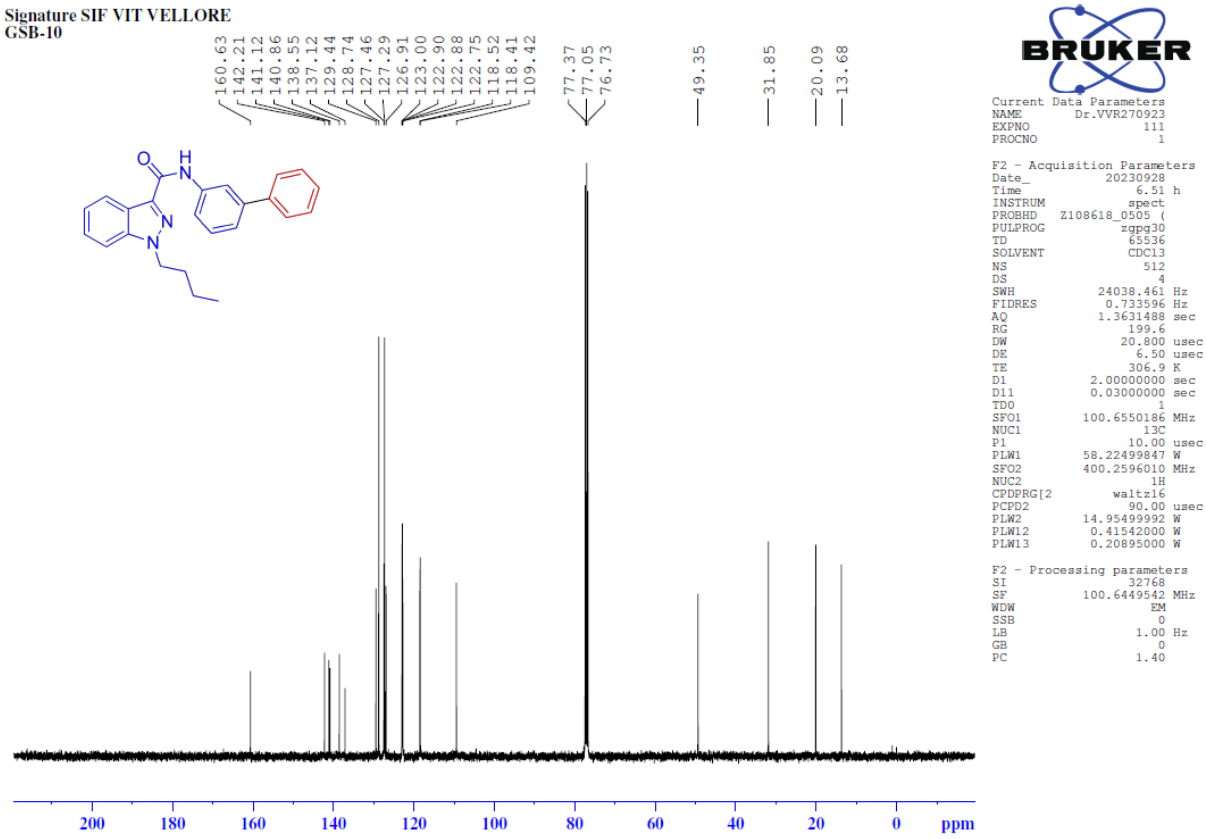
HRMS of 1-butyl-N-(4-methyl-[1,1-biphenyl]-3-yl)-1*H*-indazole-3-carboxamide (7c).



[1]H-NMR [400MHz, $CDCl_3$] spectrum of N-([1,1-biphenyl]-3-yl)-1-butyl-1*H*-indazole-3-carboxamide (7d).



[13]C-NMR [100MHz, $CDCl_3$] spectrum of N-([1,1-biphenyl]-3-yl)-1-butyl-1*H*-indazole-3-carboxamide (7d).



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PROCNO                           1

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TD                             65536
SOLVENT                      CDCl3
NS                               512
DS                                 4
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FIDRES                        0.733596 Hz
AQ                        1.3631488 sec
RG                              199.6
DW                             20.800 usec
DE                              6.50 usec
TE                             306.9 K
D1                        2.00000000 sec
D11                       0.03000000 sec
TD0                                1
SFO1                    100.6550186 MHz
NUC1                             13C
P1                              10.00 usec
PLW1                   58.22499847 W
SFO2                    400.2596010 MHz
NUC2                             1H
CPDPRG[2                    waltz16
PCPD2                          90.00 usec
PLW2                   14.95499992 W
PLW12                   0.41542000 W
PLW13                   0.20895000 W

F2 - Processing parameters
SI                             32768
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WDW                               EM
SSB                                0
LB                              1.00 Hz
GB                                 0
PC                              1.40
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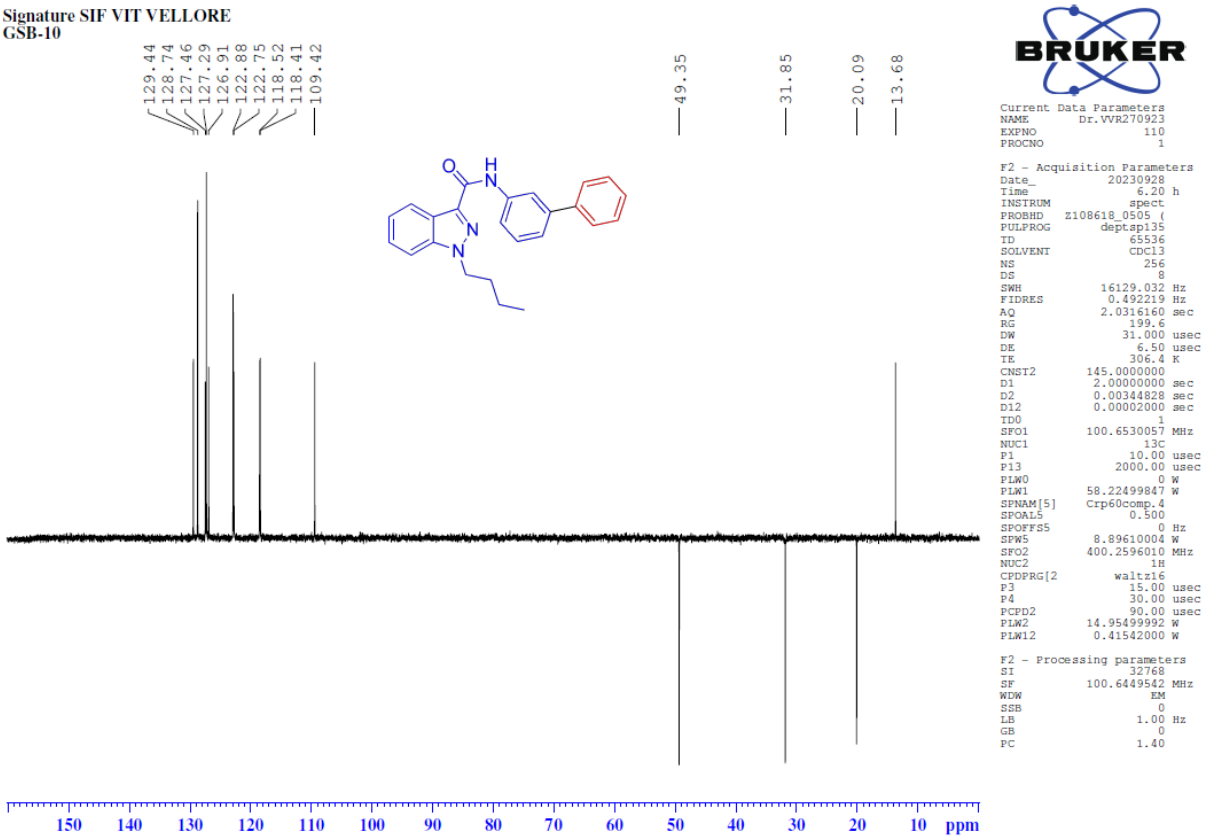
DEPT135-NMR [400MHz, $CDCl_3$] spectrum of N-([1,1-biphenyl]-3-yl)-1-butyl-1*H*-indazole-3-carboxamide (7d).



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PROCNO                           1

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PULPROG                 deptsp135
TD                             65536
SOLVENT                      CDCl3
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DS                                 8
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FIDRES                        0.492219 Hz
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RG                              199.6
DW                             31.000 usec
DE                              6.50 usec
TE                             306.4 K
CNST2                   145.0000000
D1                        2.00000000 sec
D2                        0.00344828 sec
D12                       0.00002000 sec
TD0                                1
SFO1                    100.6530057 MHz
NUC1                             13C
P1                              10.00 usec
P13                           2000.00 usec
PLW0                               0 W
PLW1                   58.22499847 W
SPNAM[5]                Crp60comp.4
SPOAL5                         0.500
SPOFFS5                            0 Hz
SPW5                    8.89610004 W
SFO2                    400.2596010 MHz
NUC2                             1H
CPDPRG[2                    waltz16
P3                              15.00 usec
P4                              30.00 usec
PCPD2                          90.00 usec
PLW2                   14.95499992 W
PLW12                   0.41542000 W

F2 - Processing parameters
SI                             32768
SF                      100.6449542 MHz
WDW                               EM
SSB                                0
LB                              1.00 Hz
GB                                 0
PC                              1.40
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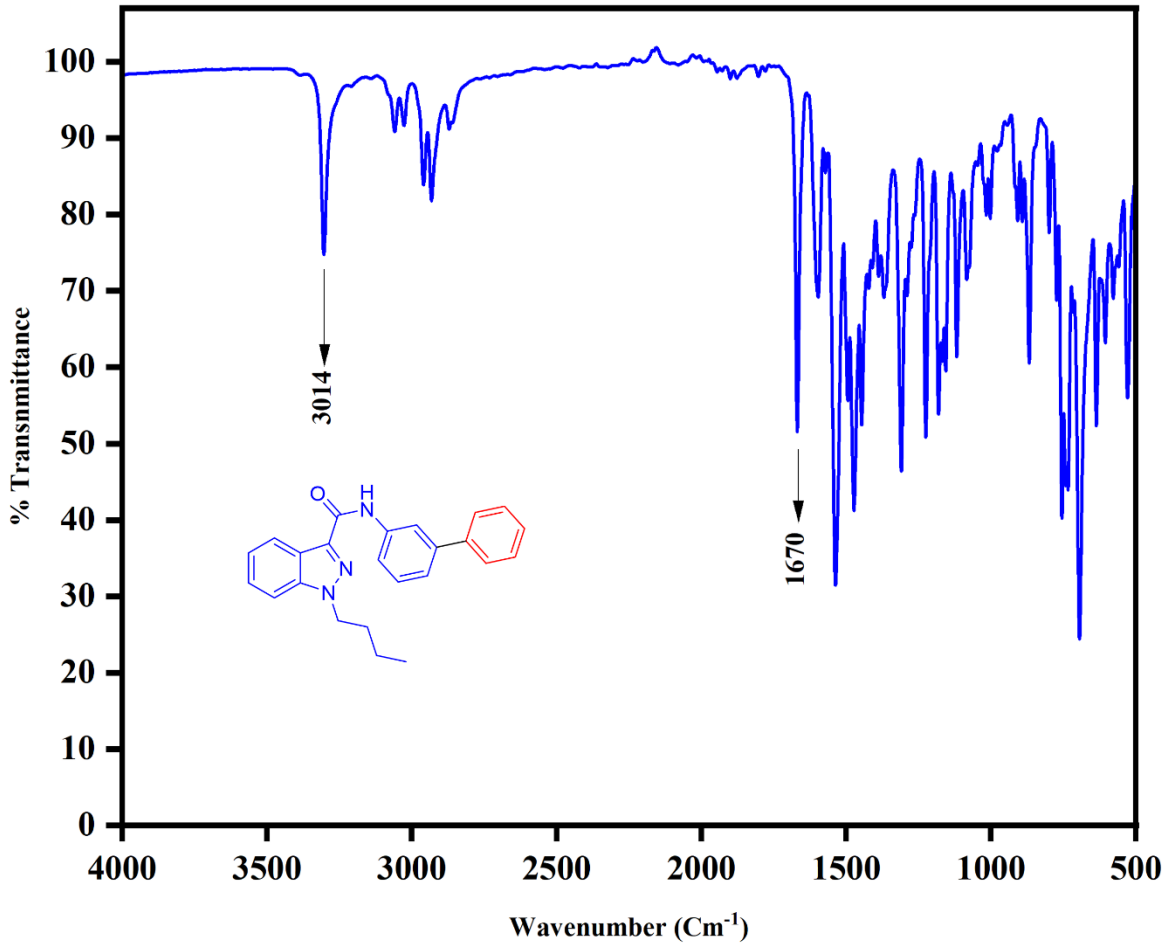
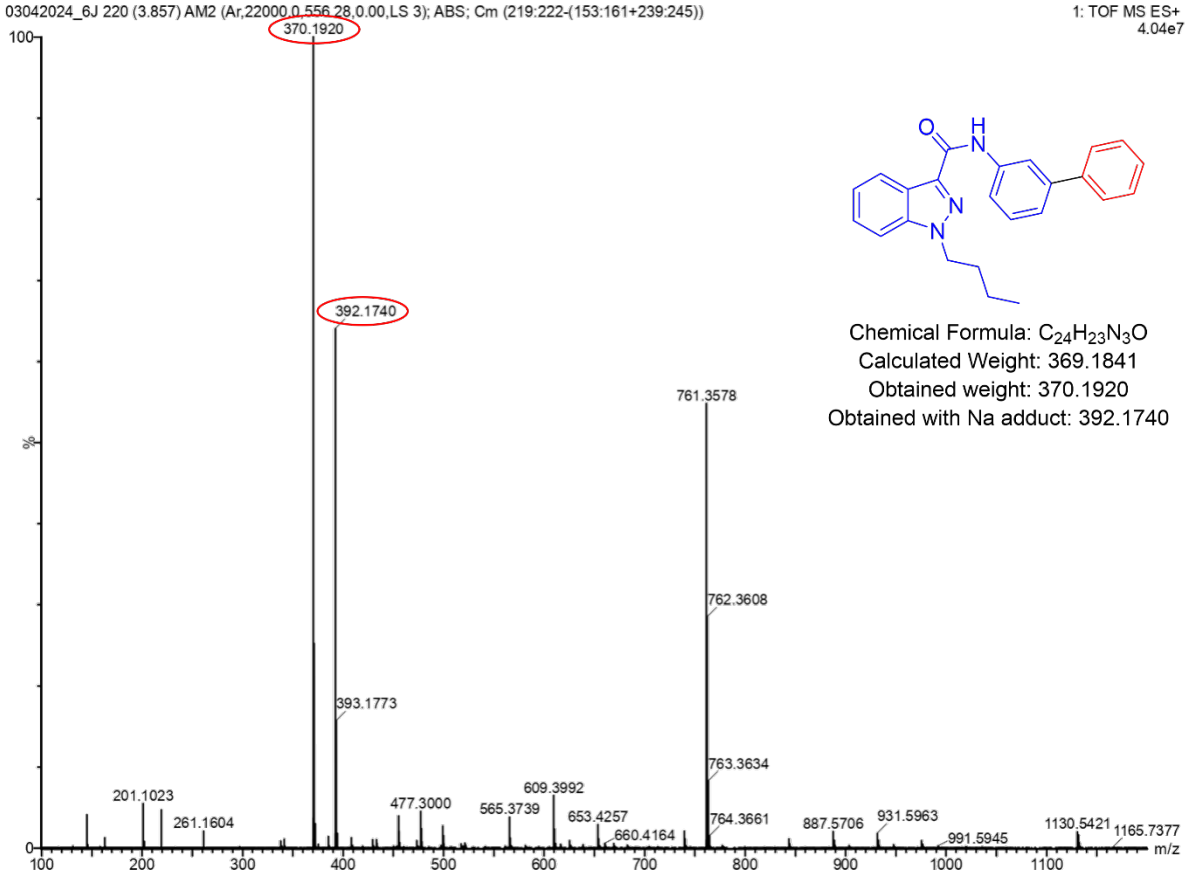
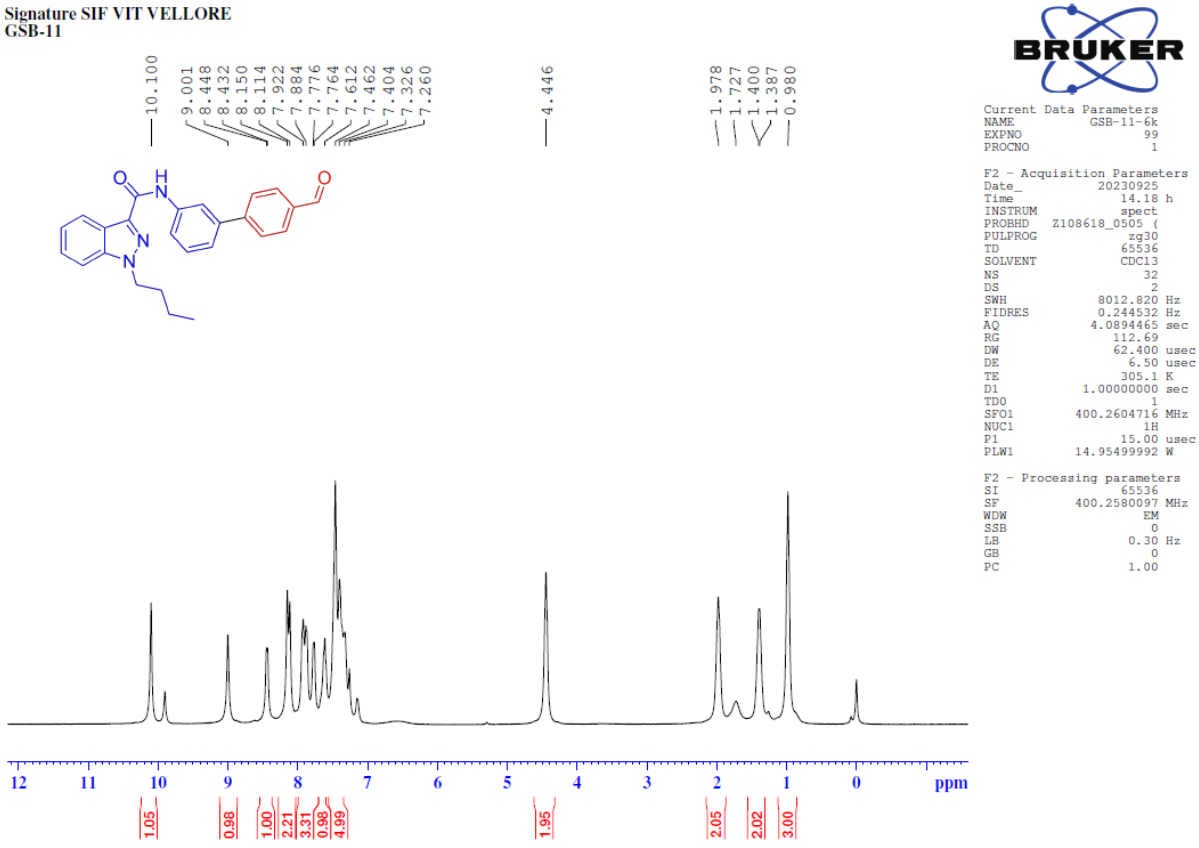
FT-IR spectrum of N-([1,1-biphenyl]-3-yl)-1-butyl-1*H*-indazole-3-carboxamide (7d).



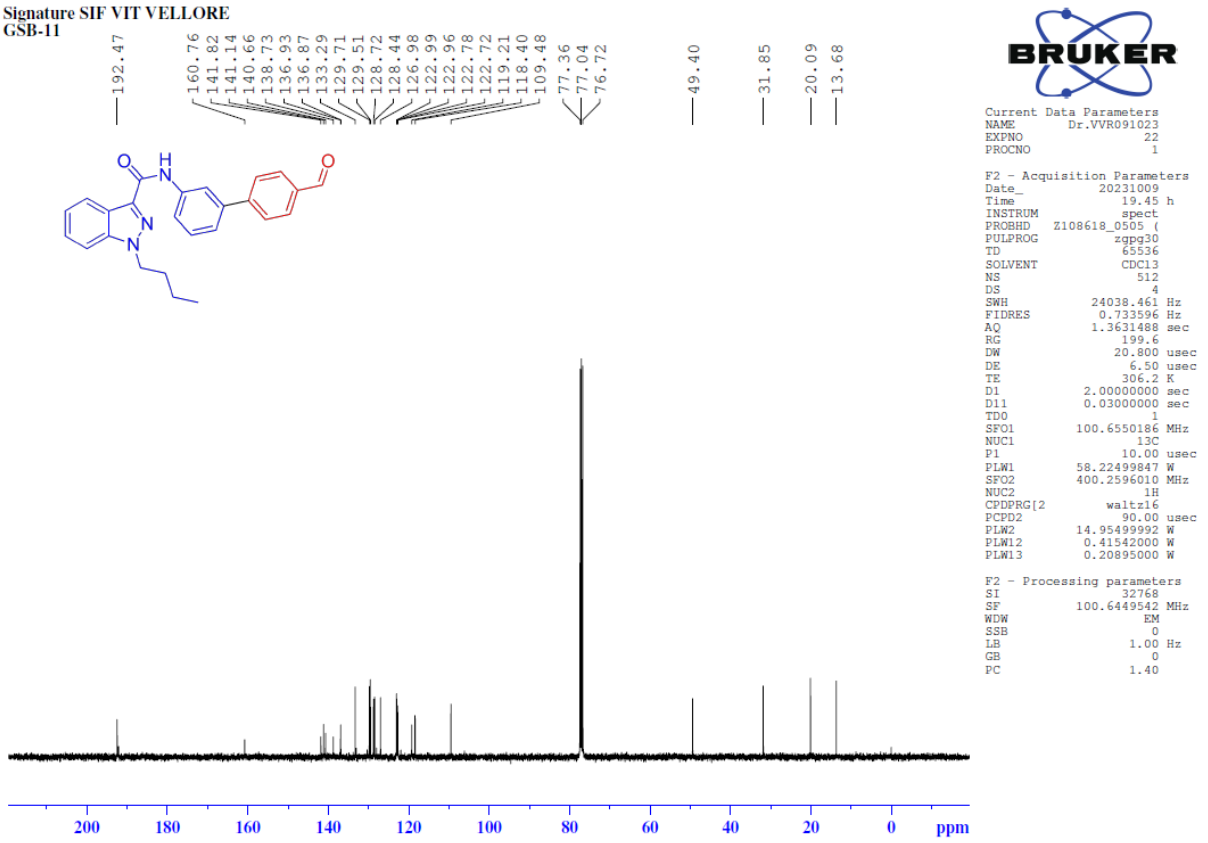
HRMS of N-([1,1-biphenyl]-3-yl)-1-butyl-1*H*-indazole-3-carboxamide (7d).



[1]H-NMR [400MHz, $CDCl_3$] spectrum of 1-butyl-N-(4-formyl-[1,1-biphenyl]-3-yl)-1*H*-indazole-3-carboxamide (7e).



[13]C-NMR [100MHz, $CDCl_3$] spectrum of 1-butyl-N-(4-formyl-[1,1-biphenyl]-3-yl)-1*H*-indazole-3-carboxamide (7e).



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PROCNO                 1

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INSTRUM             spect
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PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
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                306.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1
SFO1          100.6550186 MHz
NUC1                 13C
P1                 10.00 usec
PLW1          58.22499847 W
SFO2          400.2596010 MHz
NUC2                  1H
CPDPRG[2         waltz16
PCPD2              90.00 usec
PLW2          14.95499992 W
PLW12          0.41542000 W
PLW13          0.20895000 W

F2 - Processing parameters
SI                 32768
SF            100.6449542 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
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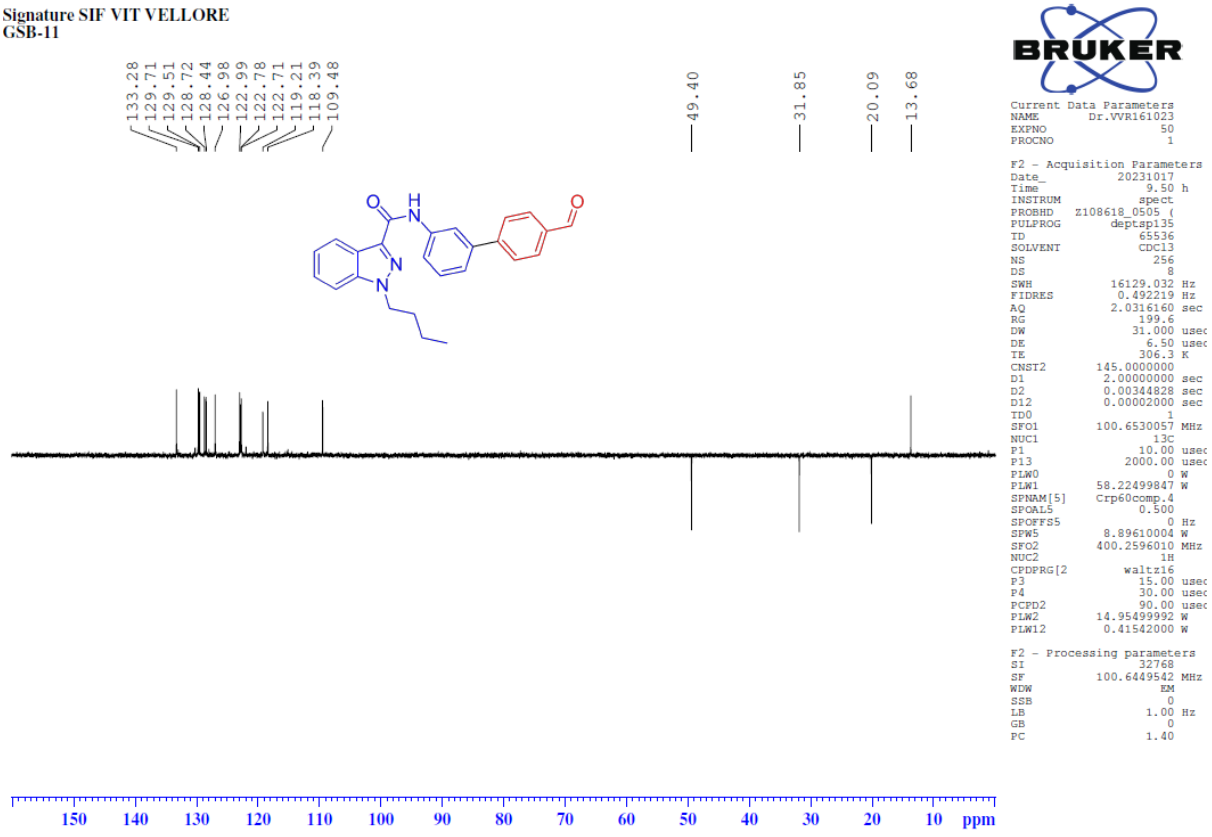
DEPT135-NMR [100MHz, $CDCl_3$] spectrum of 1-butyl-N-(4-formyl-[1,1-biphenyl]-3-yl)-1*H*-indazole-3-carboxamide (7e).



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PROCNO                 1

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INSTRUM             spect
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PULPROG        deptsp135
TD                65536
SOLVENT           CDCl3
NS                  256
DS                    8
SWH           16129.032 Hz
FIDRES         0.492219 Hz
AQ             2.0316160 sec
RG                199.6
DW               31.000 usec
DE                6.50 usec
TE                306.3 K
CNST2         145.0000000
D1            2.00000000 sec
D2            0.00344828 sec
D12           0.00002000 sec
TD0                   1
SFO1          100.6530057 MHz
NUC1                 13C
P1                 10.00 usec
P13              2000.00 usec
PLW0                0.00 W
PLW1          58.22499847 W
SPNAM[5]     Crp60comp.4
SPOAL5              0.500
SPOFFS5               0 Hz
SPW5           8.89610004 W
SFO2          400.2596010 MHz
NUC2                  1H
CPDPRG[2         waltz16
P3                 15.00 usec
P4                 30.00 usec
PCPD2              90.00 usec
PLW2          14.95499992 W
PLW12          0.41542000 W

F2 - Processing parameters
SI                 32768
SF            100.6449542 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
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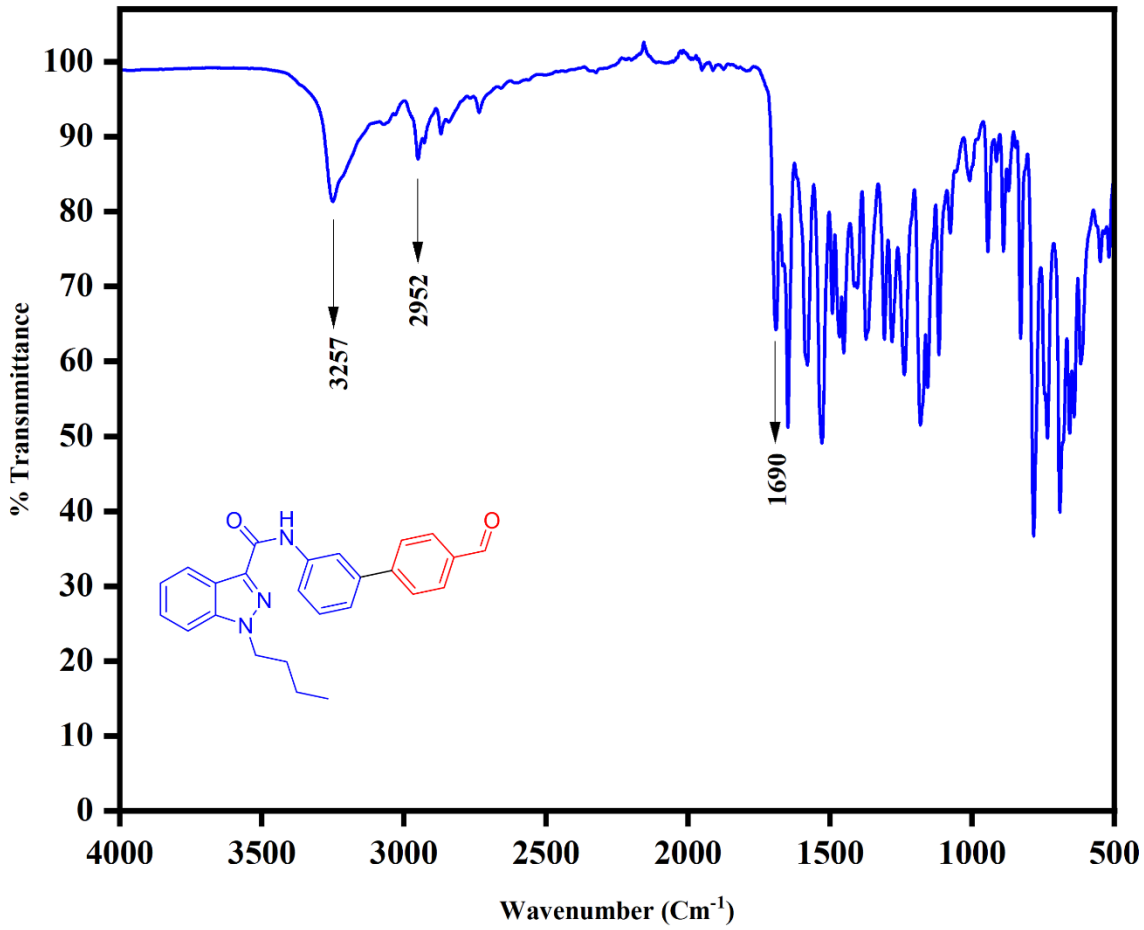
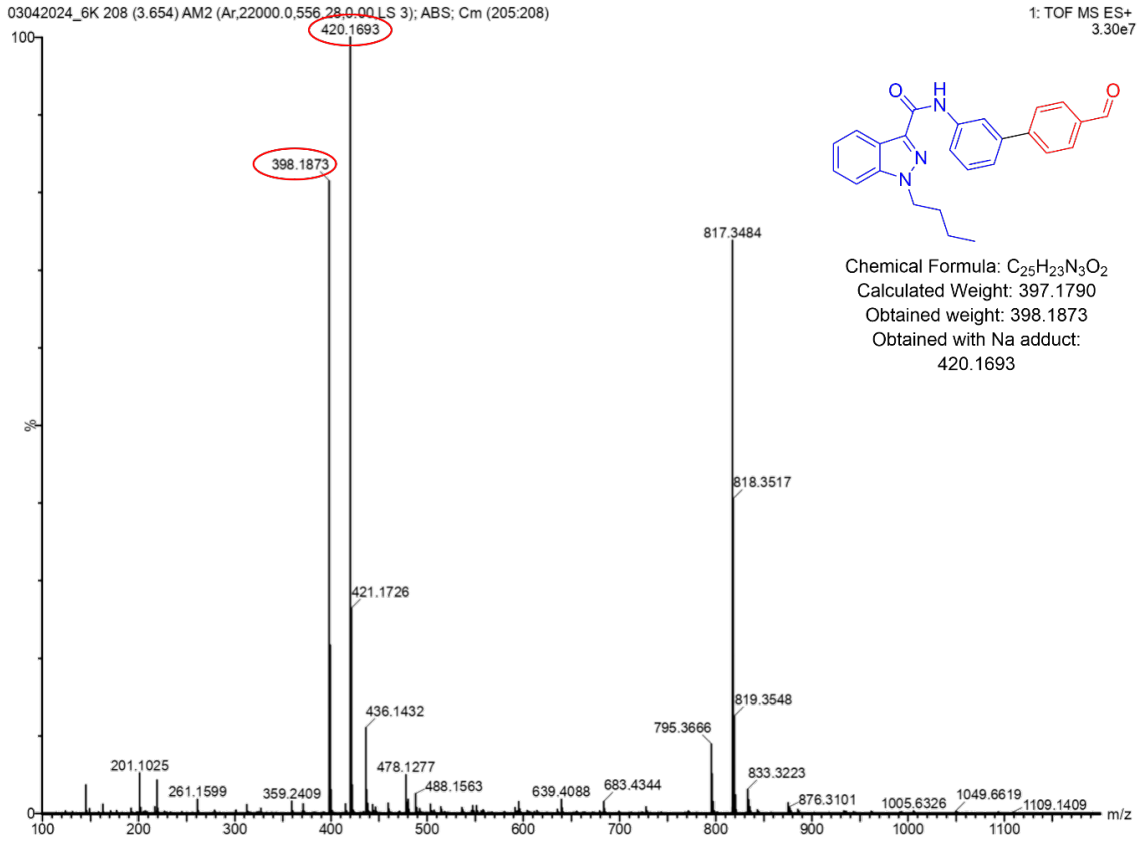
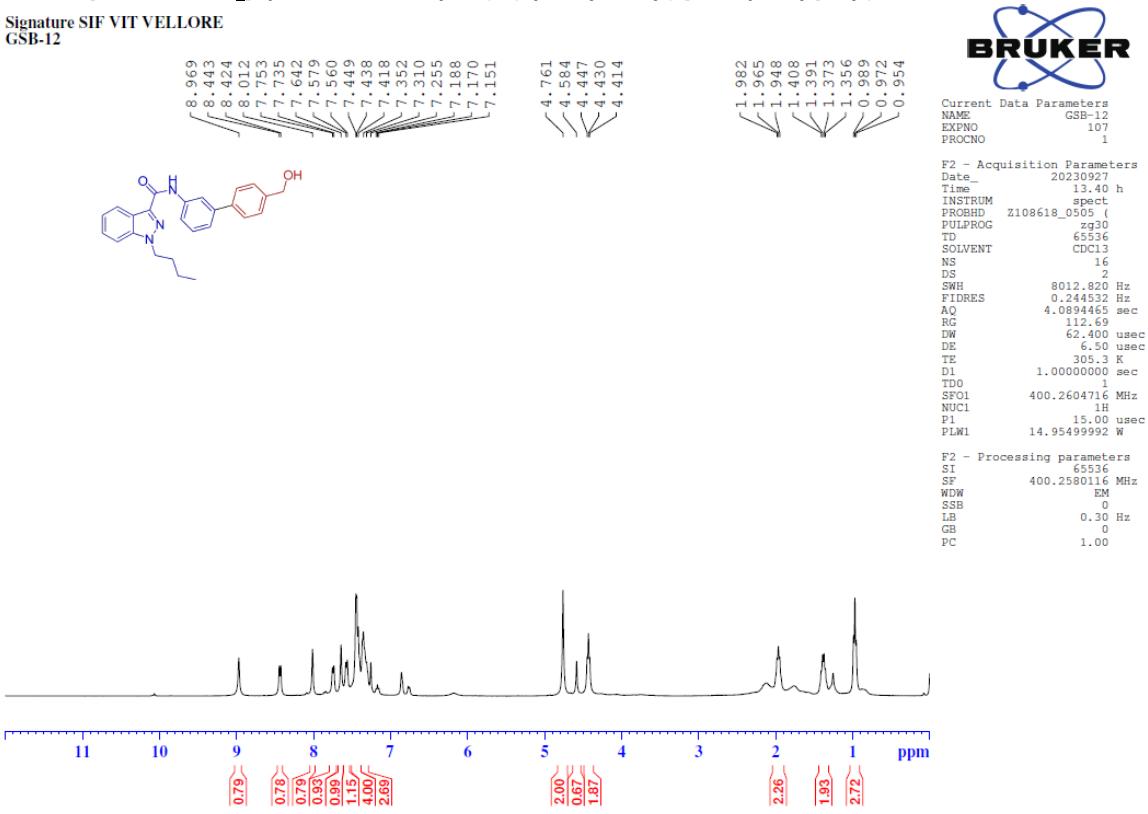
FT-IR spectrum of 1-butyl-N-(4-formyl-[1,1-biphenyl]-3-yl)-1*H*-indazole-3-carboxamide (7e).



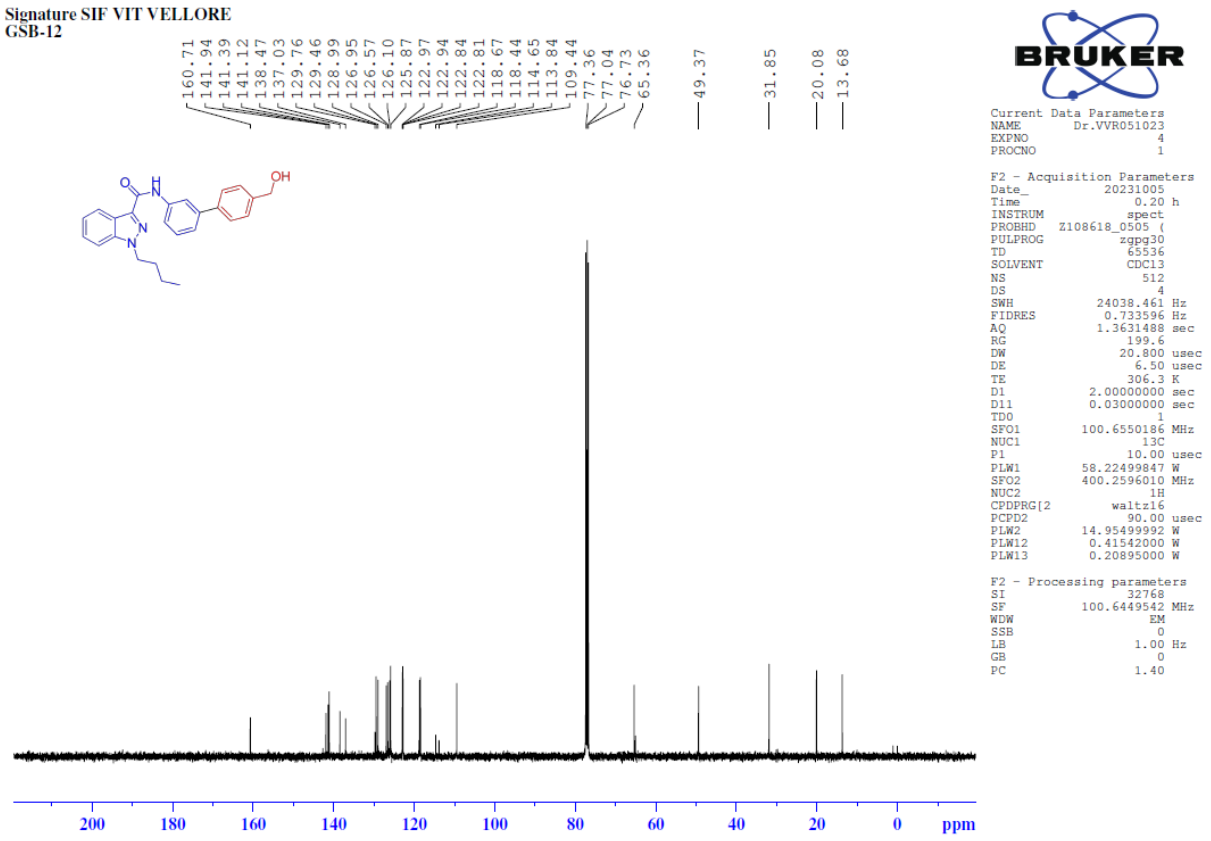
HRMS of 1-butyl-N-(4-formyl-[1,1-biphenyl]-3-yl)-1*H*-indazole-3-carboxamide (7e).



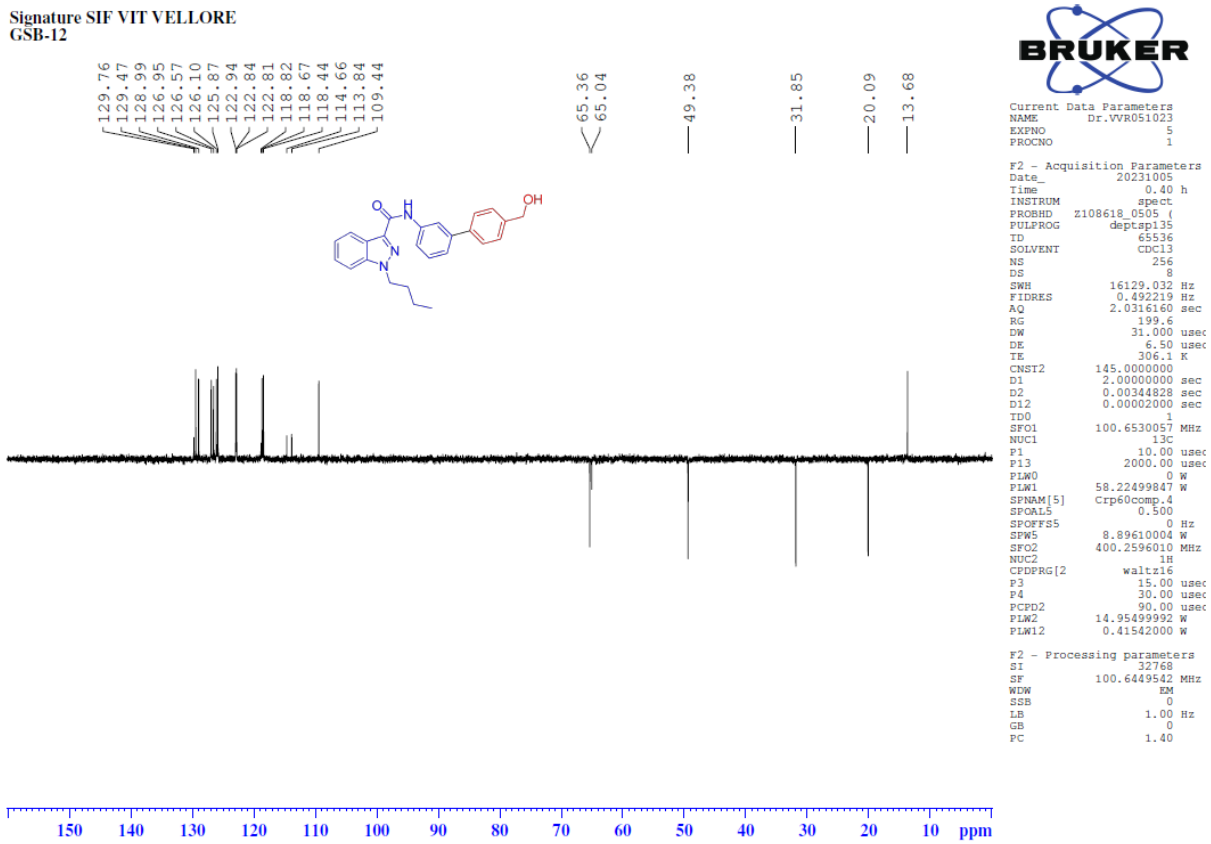
[1]H-NMR [400MHz, $CDCl_3$] spectrum of 1-butyl-N-(4-(hydroxymethyl)-[1,1-biphenyl]-3-yl)-1*H*-indazole-3-carboxamide(7f).



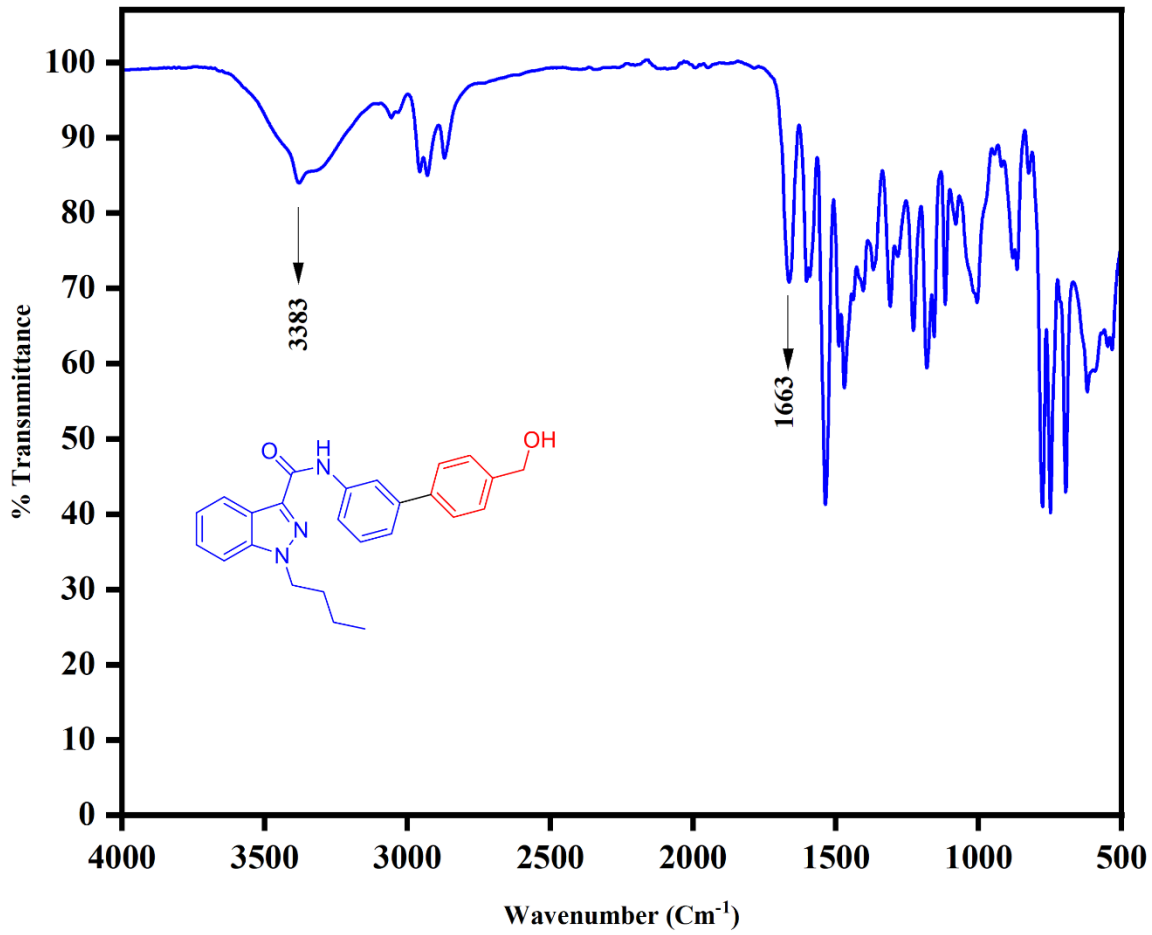
[13]C-NMR [100MHz, $CDCl_3$] spectrum of 1-butyl-N-(4-(hydroxymethyl)-[1,1-biphenyl]-3-yl)-1*H*-indazole-3-carboxamide (7f).



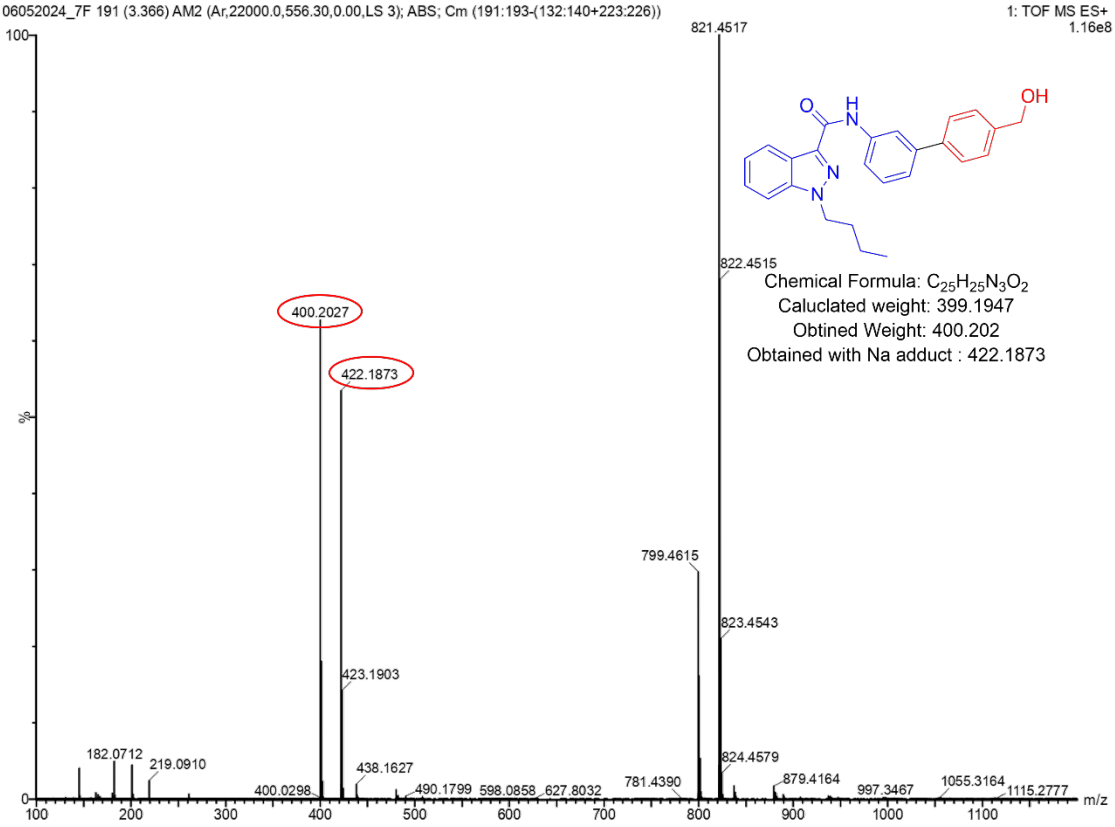
DEPT135-NMR [100MHz, $CDCl_3$] spectrum of 1-butyl-N-(4-(hydroxymethyl)-[1,1-biphenyl]-3-yl)-1*H*-indazole-3-carboxamide (7f).



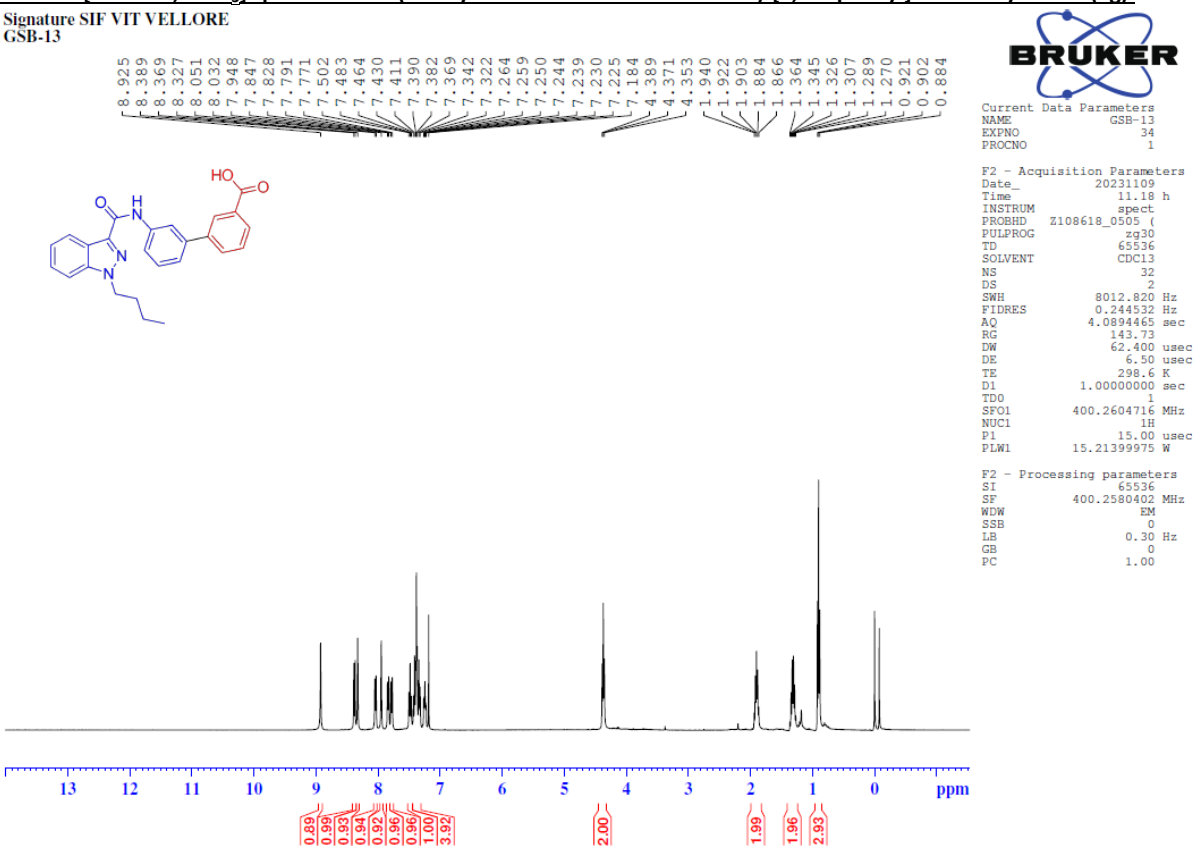
FT-IR spectrum of 1-butyl-N-(4-(hydroxymethyl)-[1,1-biphenyl]-3-yl)-1*H*-indazole-3-carboxamide (7f).



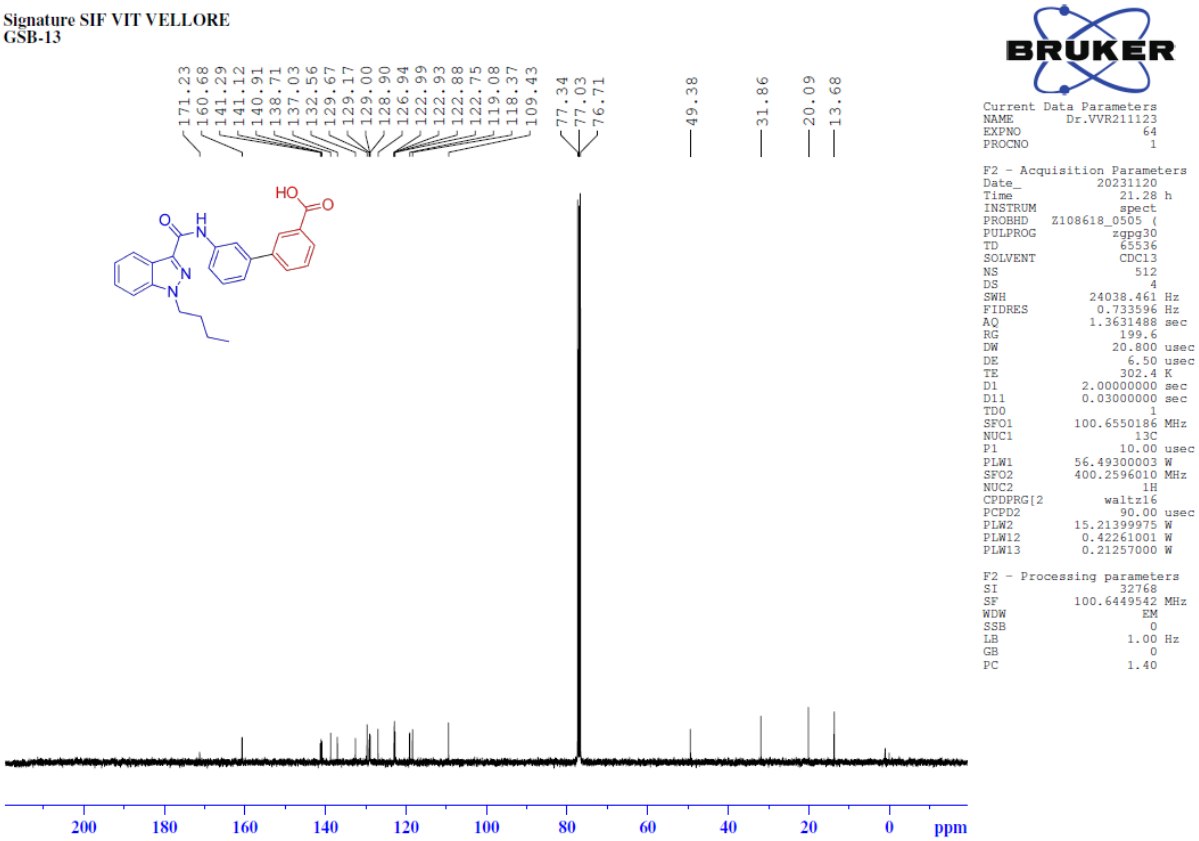
HRMS of 1-butyl-N-(4-(hydroxymethyl)-[1,1-biphenyl]-3-yl)-1*H*-indazole-3-carboxamide (7f).



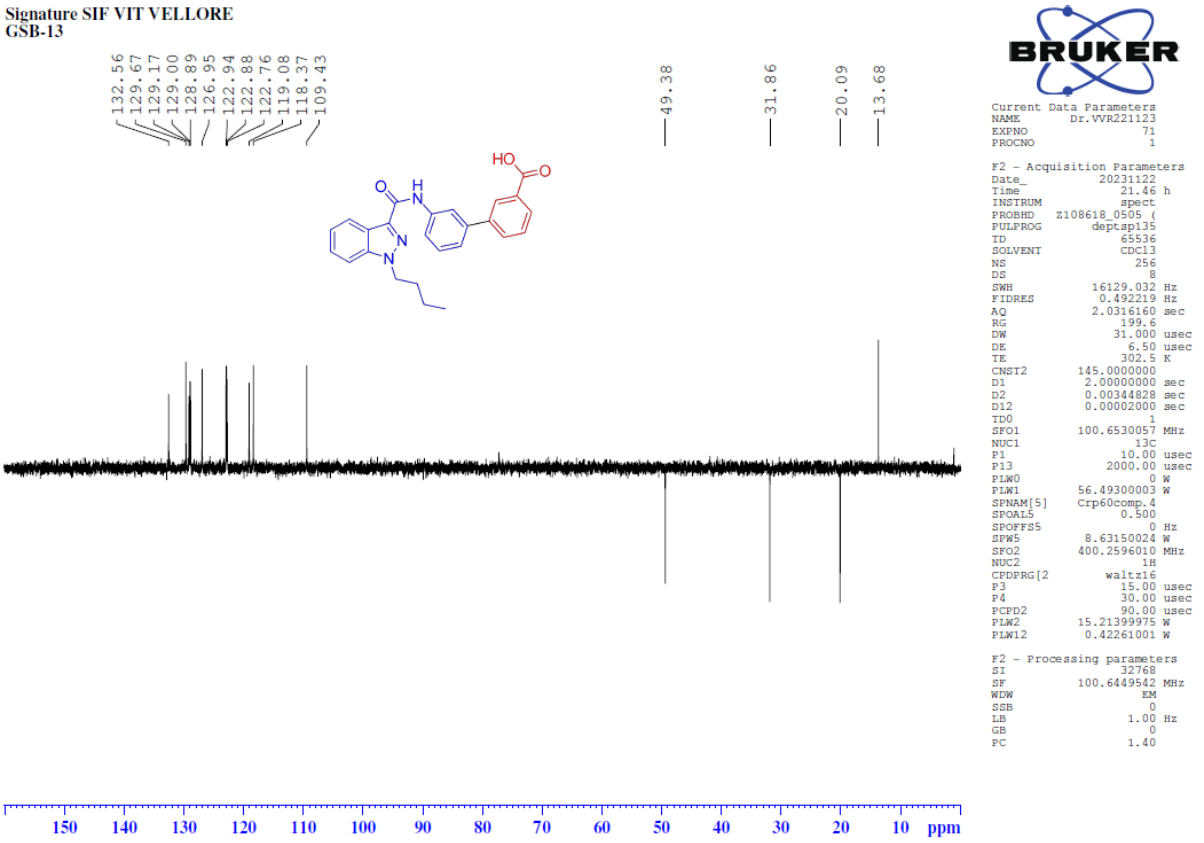
^{1}H-NMR [100MHz, $CDCl_3$] spectrum of 3-(1-butyl-1*H*-indazole-3-carboxamido)-[1,1-biphenyl]-3-carboxylic acid (7g).



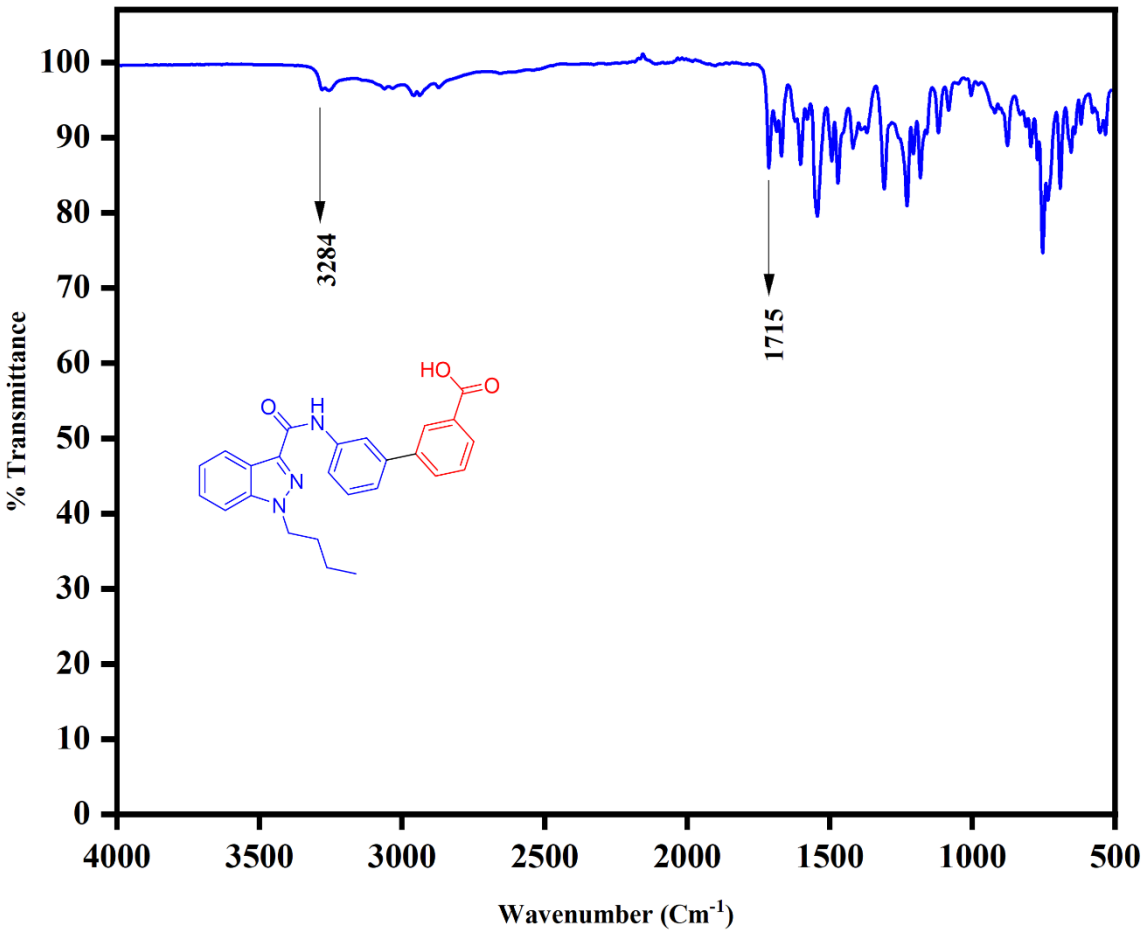
^{13}C-NMR [100MHz, $CDCl_3$] spectrum of 3-(1-butyl-1*H*-indazole-3-carboxamido)-[1,1-biphenyl]-3-carboxylic acid (7g).



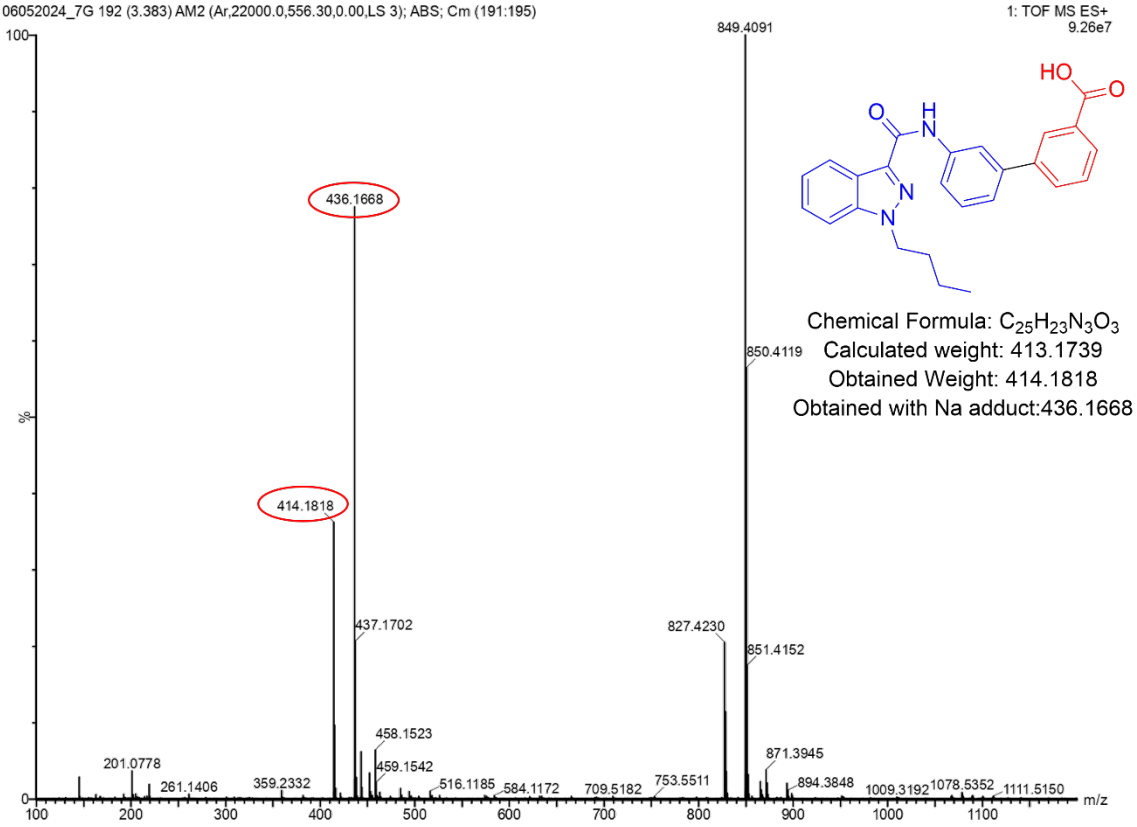
DEPT135-NMR [100MHz, $CDCl_3$] spectrum of 3-(1-butyl-1*H*-indazole-3-carboxamido)-[1,1-biphenyl]-3-carboxylic acid (7g).



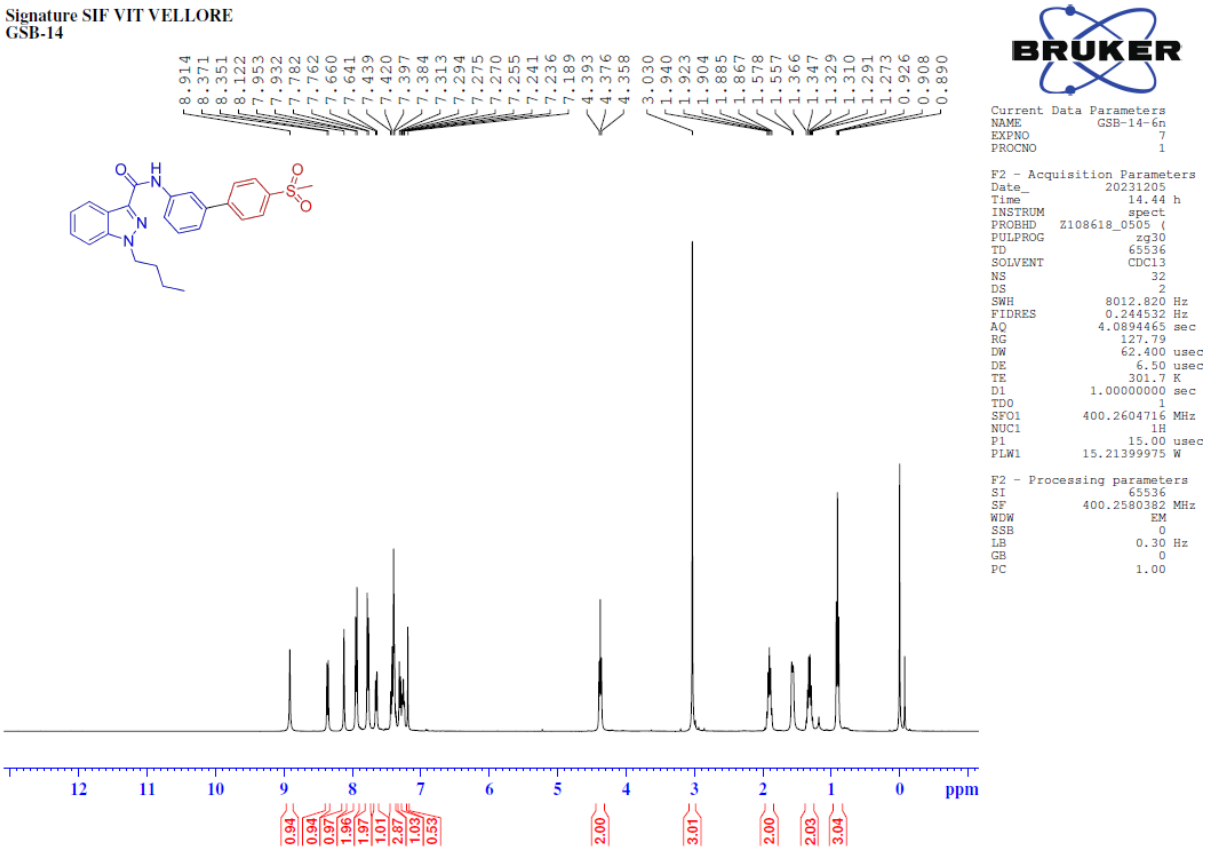
FT-IR spectrum of 3-(1-butyl-1*H*-indazole-3-carboxamido)-[1,1-biphenyl]-3-carboxylic acid (7g).



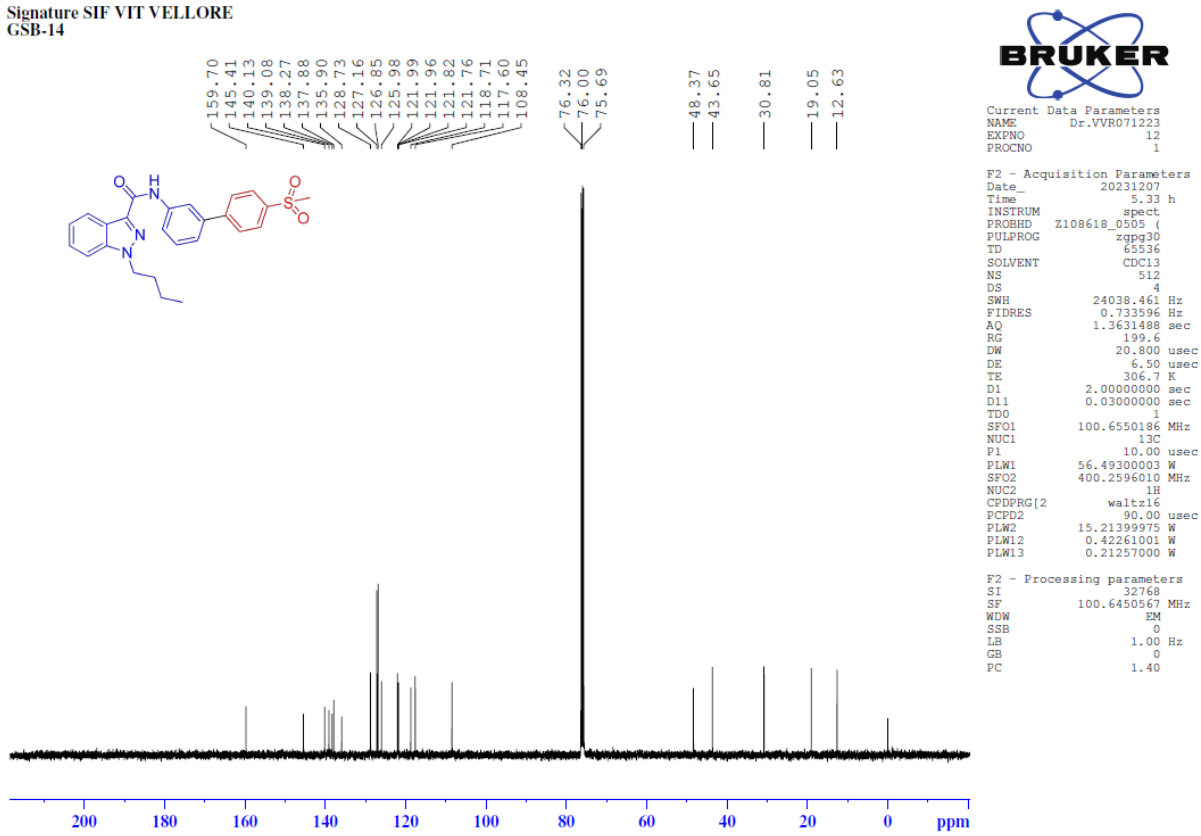
HRMS of 3-(1-butyl-1*H*-indazole-3-carboxamido)-[1,1-biphenyl]-3-carboxylic acid (7g).



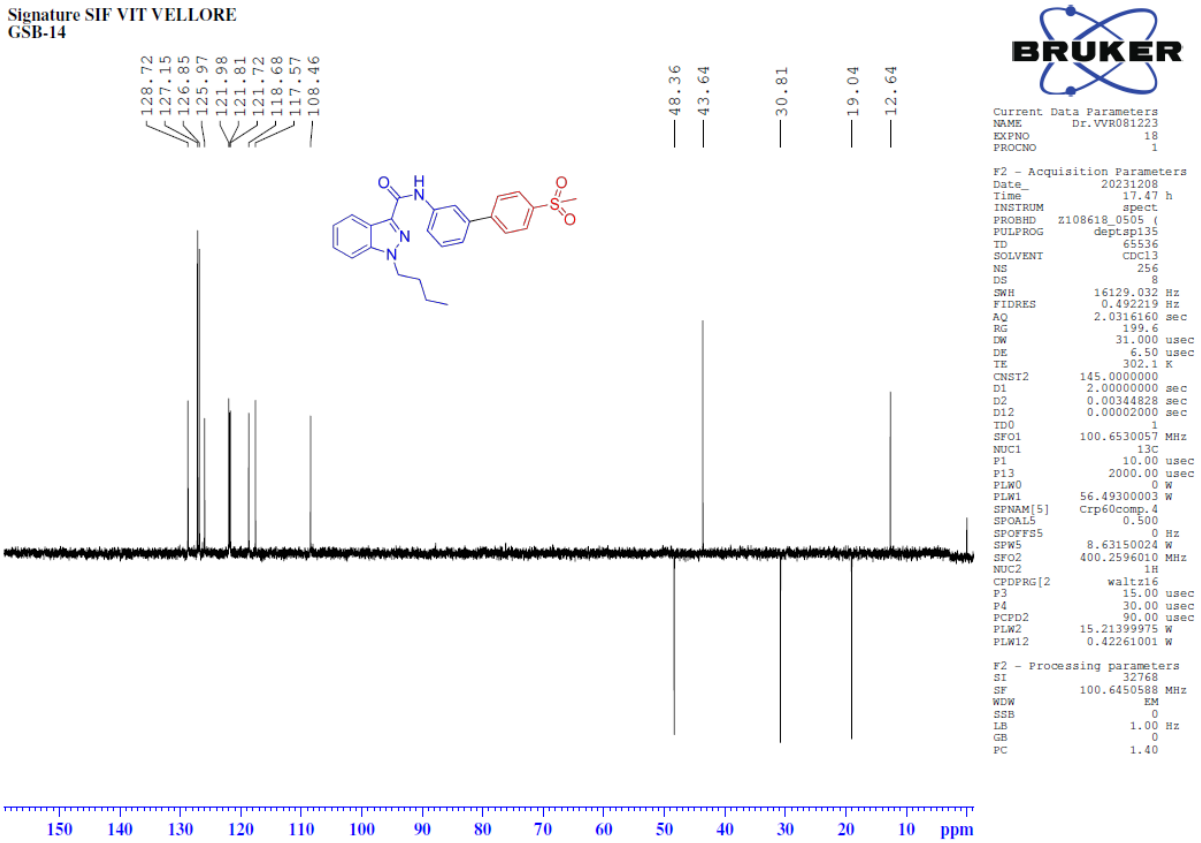
[1]H-NMR [400MHz, $CDCl_3$] spectrum of 1-butyl-N-(4-(methylsulfonyl)-[1,1-biphenyl]-3-yl)-1*H*-indazole-3-carboxamide (7h).



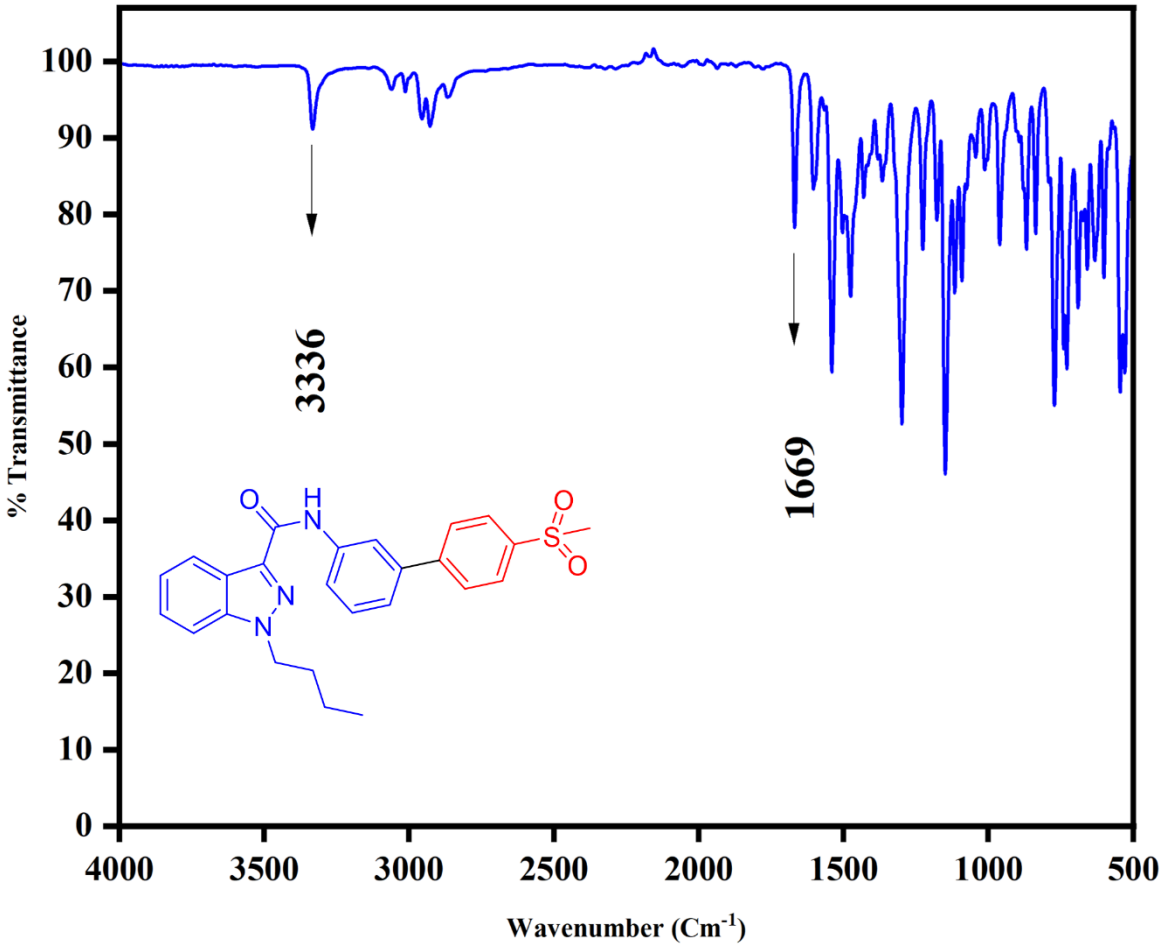
^{13}C-NMR [100MHz, $CDCl_3$] spectrum of 1-butyl-N-(4-(methylsulfonyl)-[1,1-biphenyl]-3-yl)-1*H*-indazole-3-carboxamide (7h).



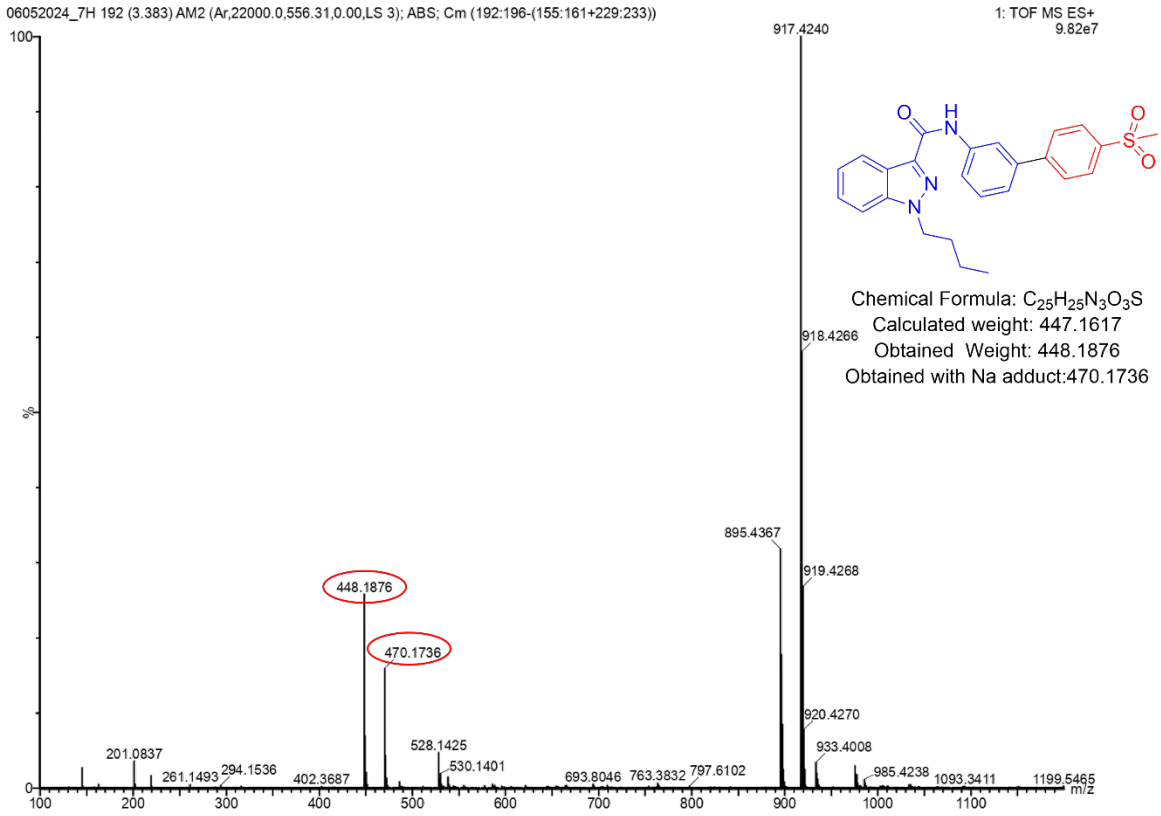
DEPT135-NMR [100MHz, $CDCl_3$] spectrum of 1-butyl-N-(4-(methylsulfonyl)-[1,1-biphenyl]-3-yl)-1*H*-indazole-3-carboxamide (7h).



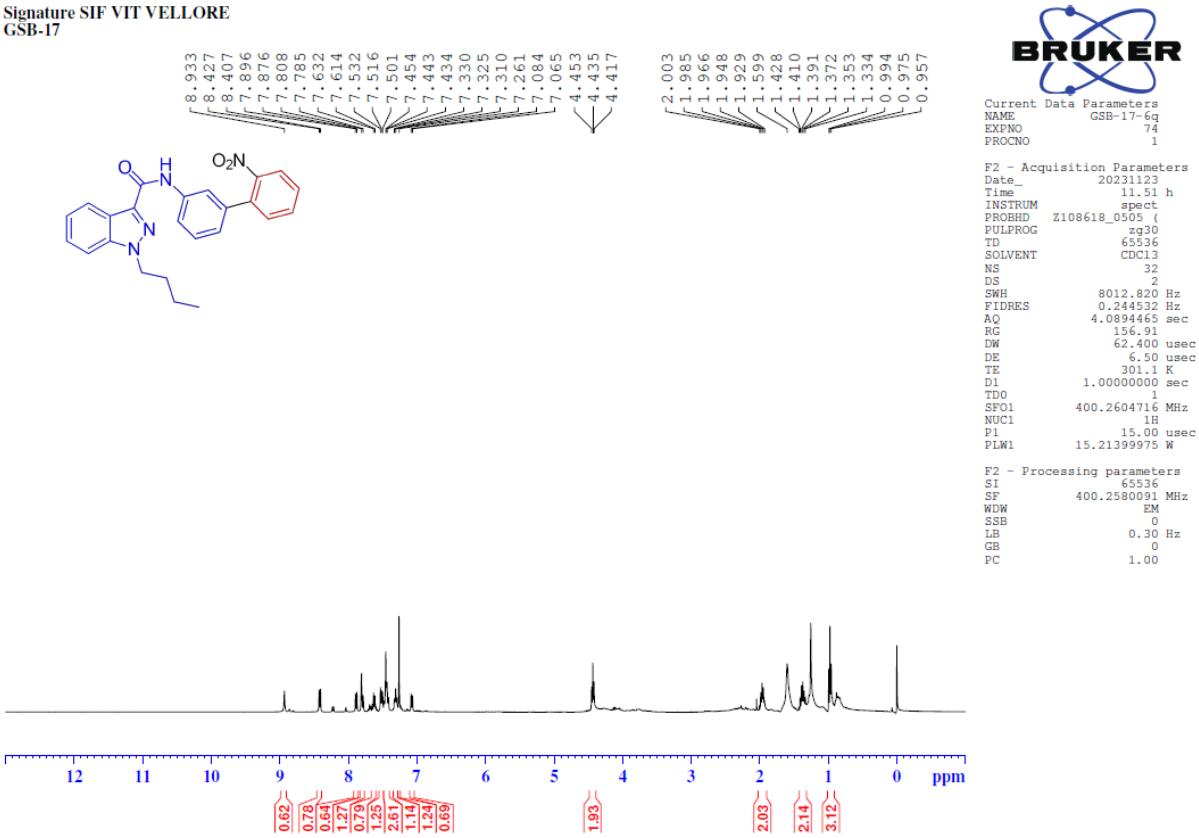
FT-IR spectrum of 1-butyl-N-(4-(methylsulfonyl)-[1,1-biphenyl]-3-yl)-1*H*-indazole-3-carboxamide (7h).



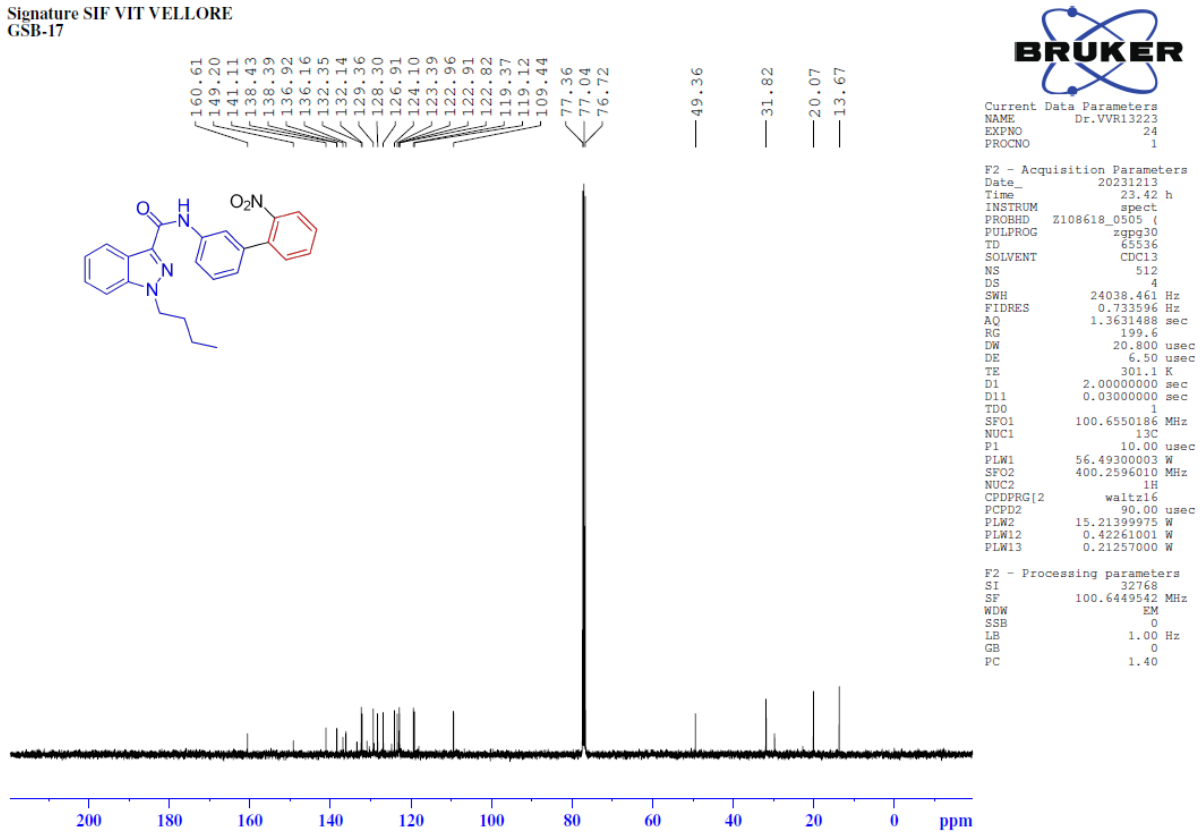
HRMS of 1-butyl-N-(4-(methylsulfonyl)-[1,1-biphenyl]-3-yl)-1*H*-indazole-3-carboxamide (7h).



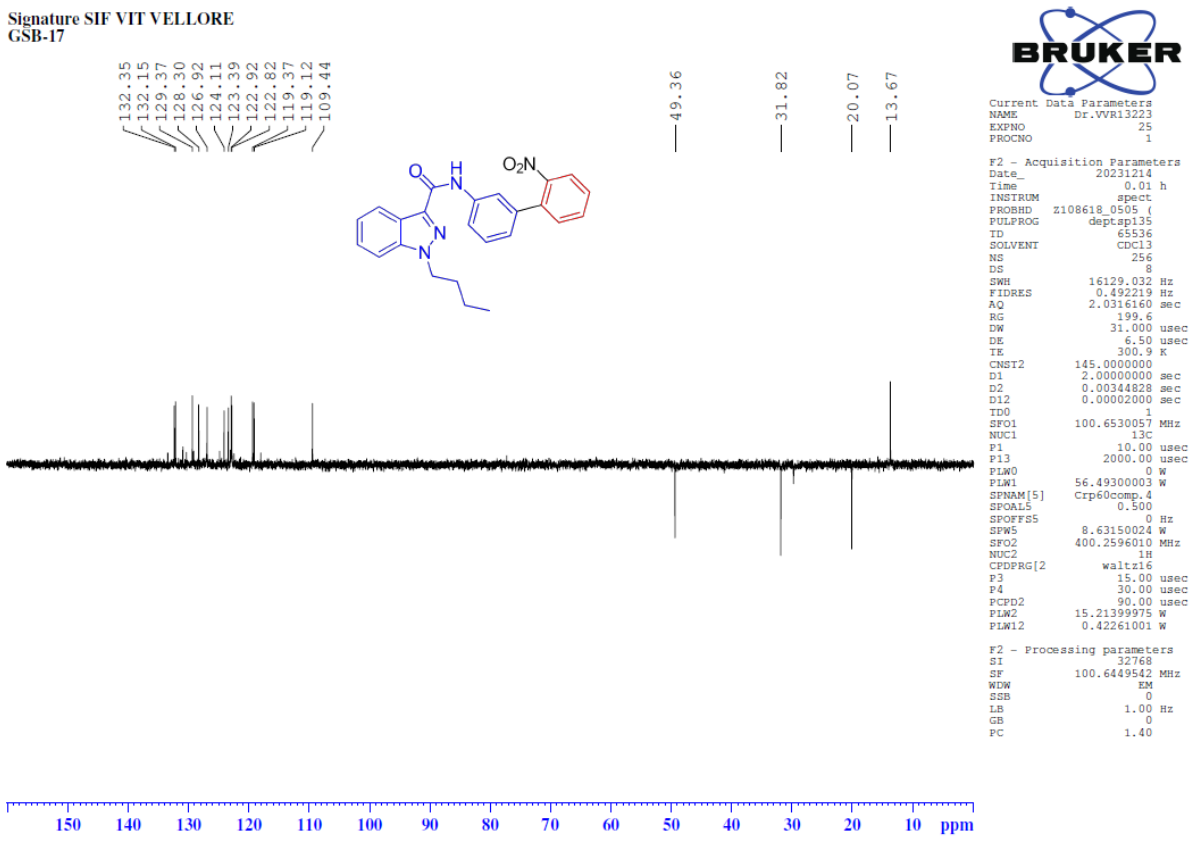
^{1}H-NMR [400MHz, $CDCl_3$] spectrum of 1-butyl-N-(2-nitro-[1,1-biphenyl]-3-yl]-1*H*-indazole-3-carboxamide (7i).



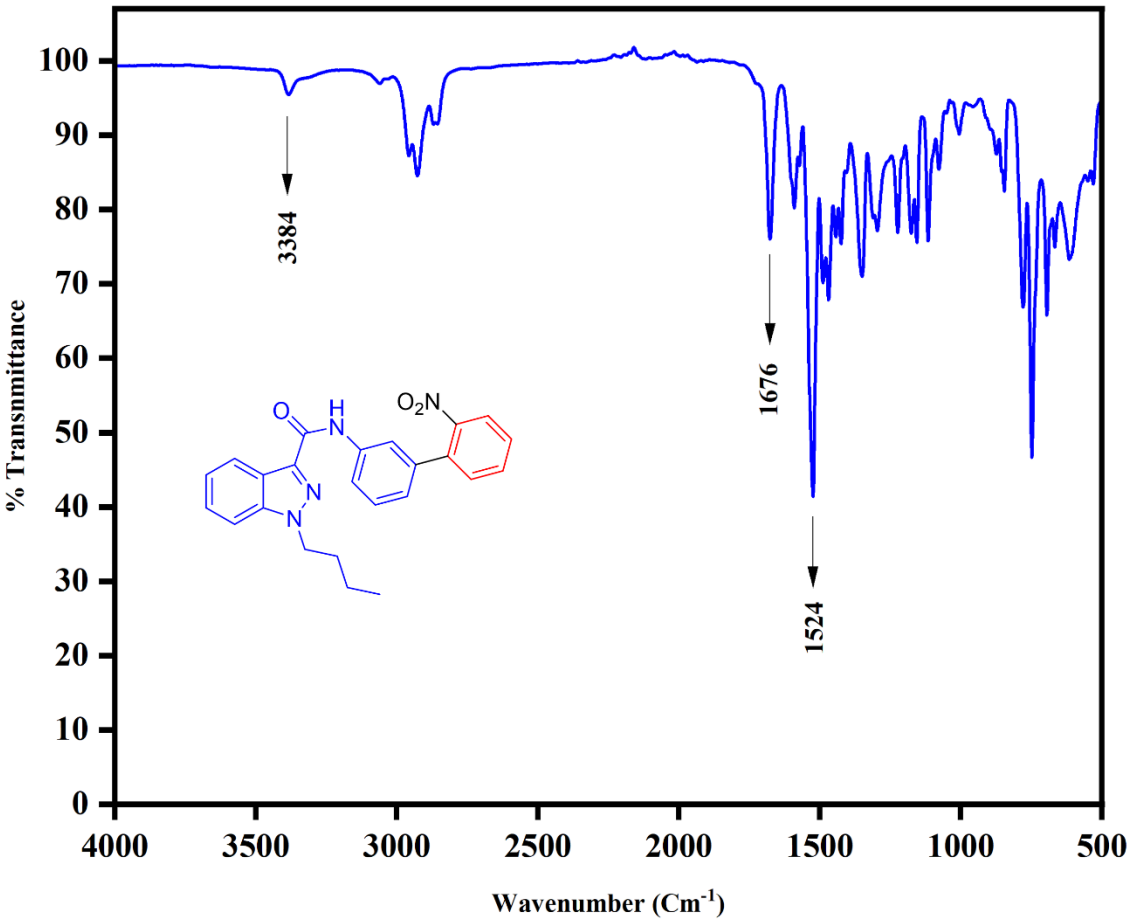
^{13}C-NMR [100MHz, $CDCl_3$] spectrum of 1-butyl-N-(2-nitro-[1,1-biphenyl]-3-yl]-1*H*-indazole-3-carboxamide (7i).



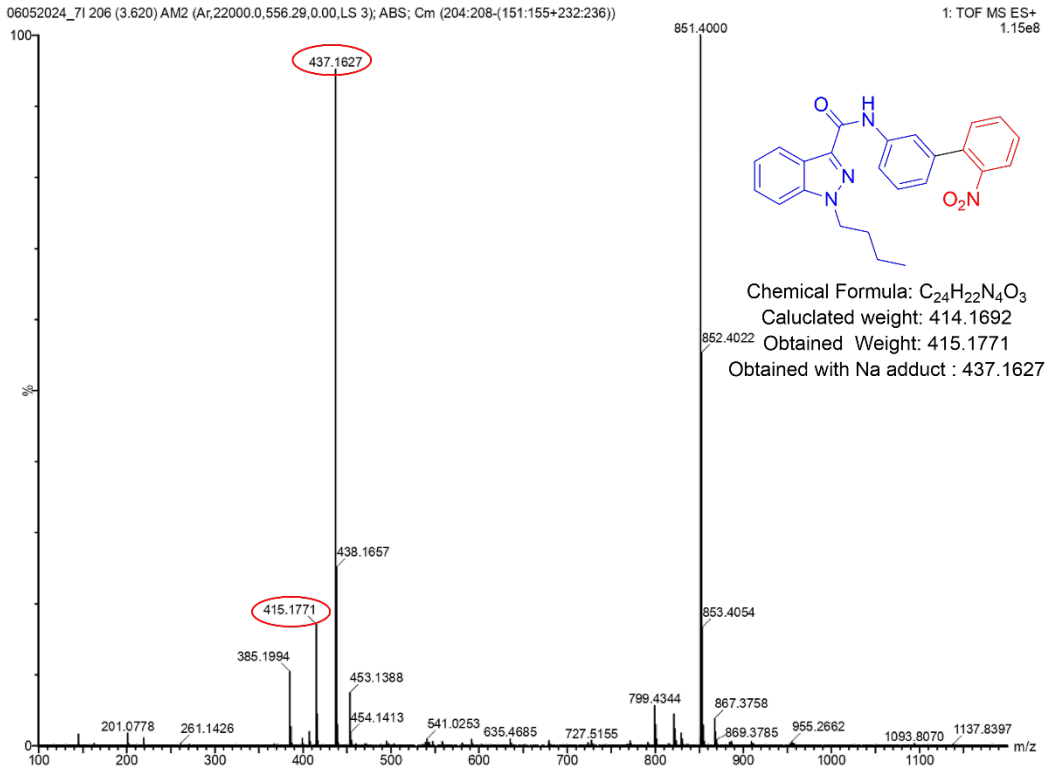
DEPT135-NMR [100MHz, $CDCl_3$] spectrum of 1-butyl-N-(2-nitro-[1,1-biphenyl]-3-yl]-1*H*-indazole-3-carboxamide (7i).



FT-IR spectrum of 1-butyl-N-(2-nitro-[1,1-biphenyl]-3-yl]-1*H*-indazole-3-carboxamide (7i).



HRMS of 1-butyl-N-(2-nitro-[1,1-biphenyl]-3-yl]-1*H*-indazole-3-carboxamide (7i).

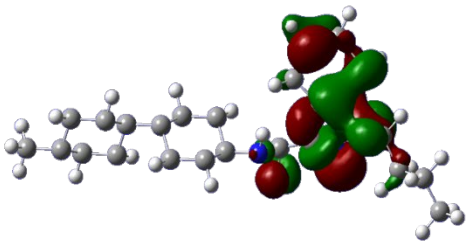


DFT STUDY, FMO Diagrams of synthesized indazole derivatives

s.no	HOMO (eV)	LUMO (eV)	ΔE = E_{LUMO}-E_{HOMO} (eV)	I = -E_{HOMO} (eV)	A =-E_{LUMO} (eV)	χ = (I+A)/2 (eV)	μ = - χ (eV)	η = (I-A)/2 (eV)	S = 1/η (eV)	ω = $\mu^2/2\eta$	ω^- = $(3I+A)^2/16(I-A)$	ω^+ = $(I+3A)^2/16(I-A)$
6a	-6.2721	-3.3780	2.8941	6.2721	3.3780	4.8250	-4.8250	1.4471	0.6911	16.8445	89.1004	48.6860
6b	-6.3887	-3.5149	2.8739	6.3887	3.5149	4.9518	-4.9518	1.4369	0.6959	17.6171	92.4009	51.5030
6c	-6.2948	-3.4050	2.8898	6.2948	3.4050	4.8499	-4.8499	1.4449	0.6921	16.9930	89.7310	49.2297
6d	-6.2670	-3.3734	2.8936	6.2670	3.3734	4.8202	-4.8202	1.4468	0.6912	16.8075	88.9235	48.5648
6e	-6.3893	-3.5151	2.8742	6.3893	3.5151	4.9522	-4.9522	1.4371	0.6959	17.6217	92.4250	51.5161
6f	-6.3347	-3.4520	2.8828	6.3347	3.4520	4.8933	-4.8933	1.4414	0.6938	17.2570	90.8583	50.1922
6g	**-5.5652**	**-1.3784**	**4.1869**	**5.5652**	**1.3784**	**3.4718**	**-3.4718**	**2.0934**	**0.4777**	**12.6165**	**85.4837**	**24.6230**
6h	**-6.0148**	**-1.7955**	**4.2193**	**6.0148**	**1.7955**	**3.9051**	**-3.9051**	**2.1096**	**0.4740**	**16.0862**	**103.7999**	**34.2789**
6i	-5.6781	-3.0040	2.6741	5.6781	3.0040	4.3411	-4.3411	1.3370	0.7479	12.5981	67.1084	36.0668
7a	-6.3439	-3.4368	2.9071	6.3439	3.4368	4.8904	-4.8904	1.4535	0.6880	17.3813	91.7255	50.3961
7b	-6.3933	-3.4952	2.8982	6.3933	3.4952	4.9442	-4.9442	1.4491	0.6901	17.7119	93.1334	51.6045
7c	-6.2799	-3.3599	2.9201	6.2799	3.3599	4.8199	-4.8199	1.4600	0.6849	16.9593	89.9422	48.8443
7d	-5.0431	-3.8351	1.2080	5.0431	3.8351	4.4391	-4.4391	0.6040	1.6557	5.9509	27.1526	20.6750
7e	-6.3893	-3.5195	2.8698	6.3893	3.5195	4.9544	-4.9544	1.4349	0.6969	17.6105	92.3212	51.5174
7f	-6.2616	-3.3701	2.8914	6.2616	3.3701	4.8159	-4.8159	1.4457	0.6917	16.7648	88.7014	48.4391
7g	**-5.9802**	**-1.4318**	**4.5484**	**5.9802**	**1.4318**	**3.7060**	**-3.7060**	**2.2742**	**0.4397**	**15.6177**	**106.6871**	**30.0165**
7h	**-6.1144**	**-1.6268**	**4.4877**	**6.1144**	**1.6268**	**3.8706**	**-3.8706**	**2.2438**	**0.4457**	**16.8079**	**111.8555**	**33.9051**
7i	-5.6303	-3.0653	2.5650	5.6303	3.0653	4.3478	-4.3478	1.2825	0.7797	12.1218	63.8447	35.2395

ionisation, A= EELECTRON AFFINITY, χ= ELECTRONEGITIVITY, μ = POTENTIAL EFFICIENCY, η = HARDNESS, S= SOFTNESS, ω= ELECTROPHILICITY, ω^- = e DONATING POWER, ω^+ = e ACCEPTING POWER

6a



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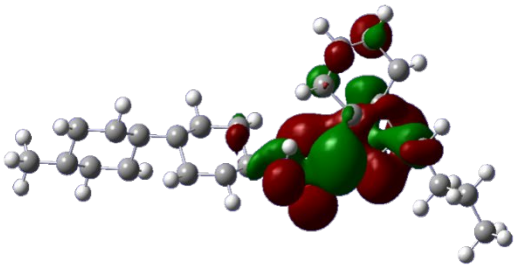
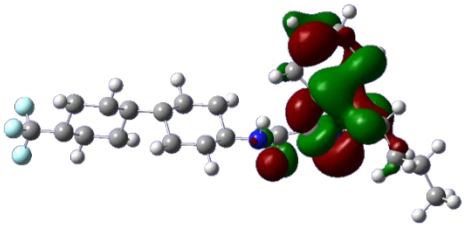


LUMO

6b



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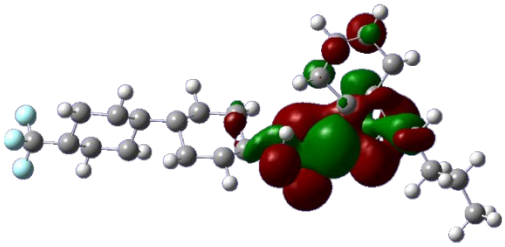

LUMO

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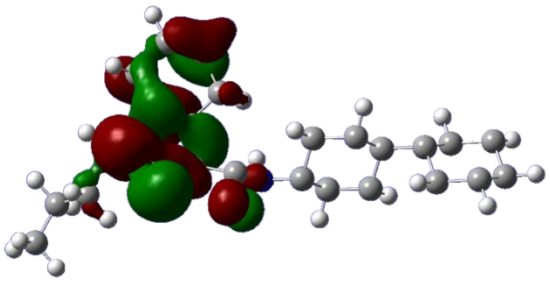

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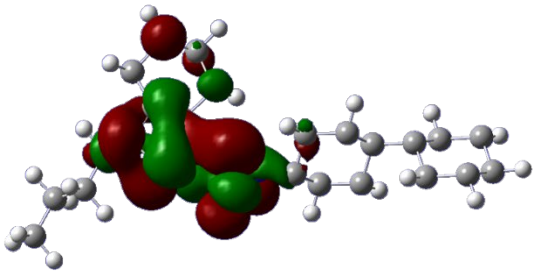

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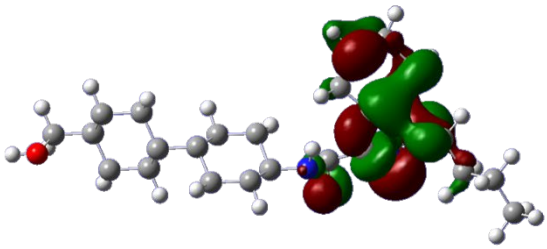

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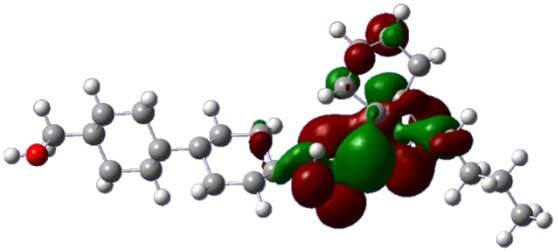

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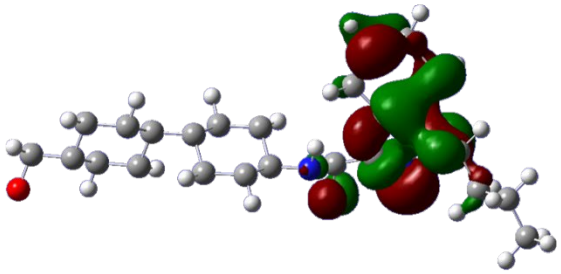

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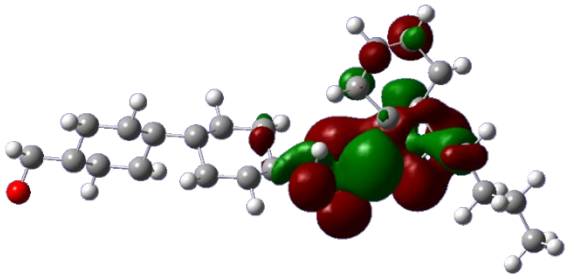

LUMO

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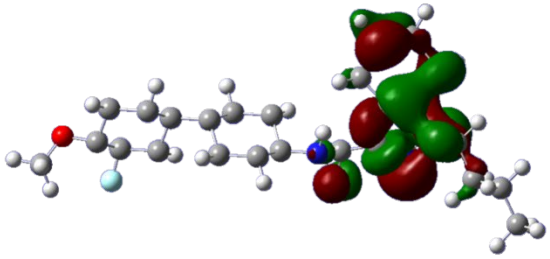

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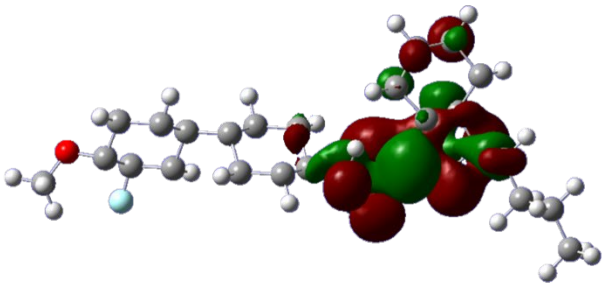

LUMO

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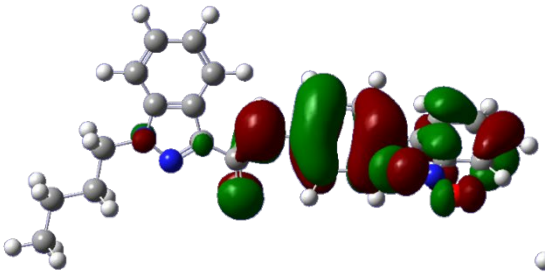

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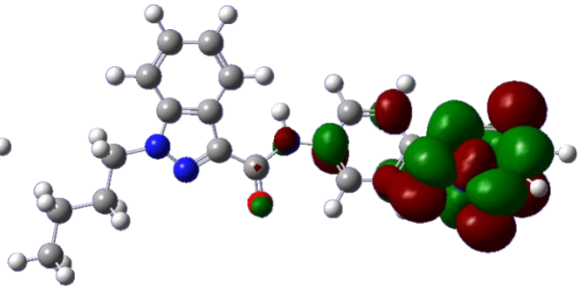

LUMO

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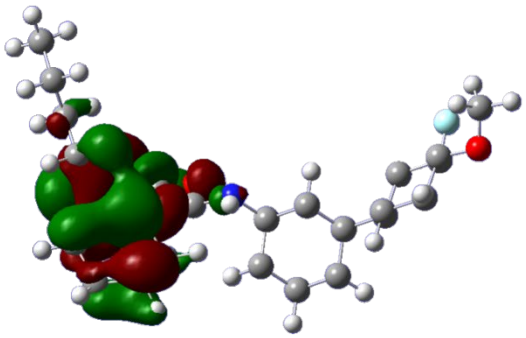

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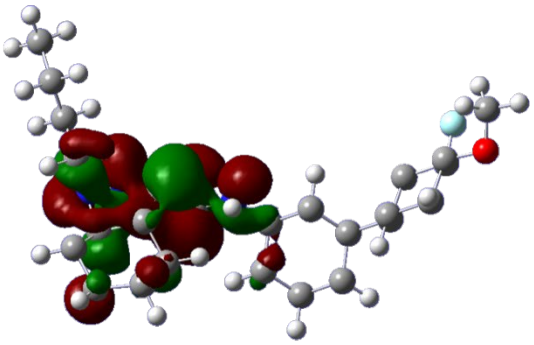

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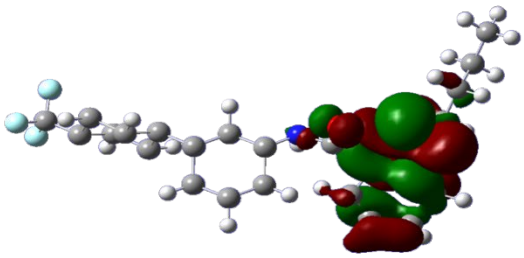

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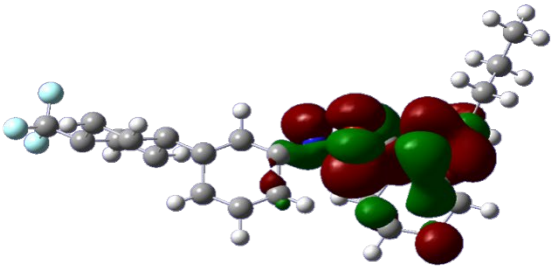

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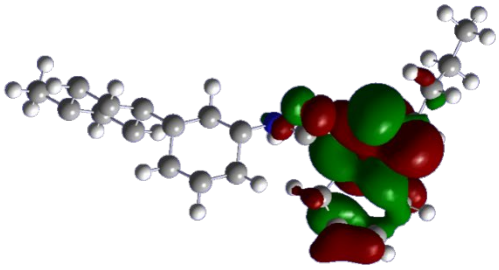

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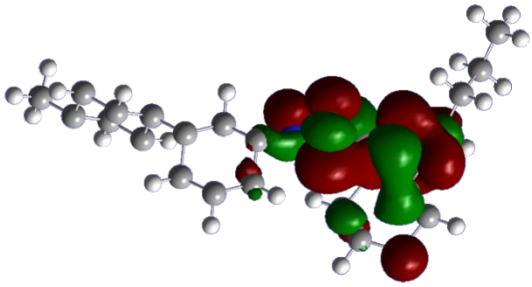

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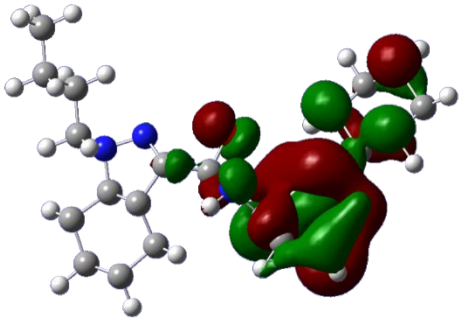

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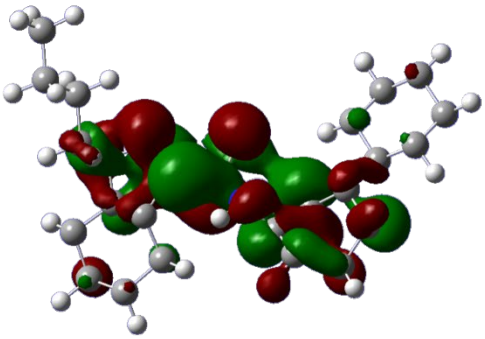

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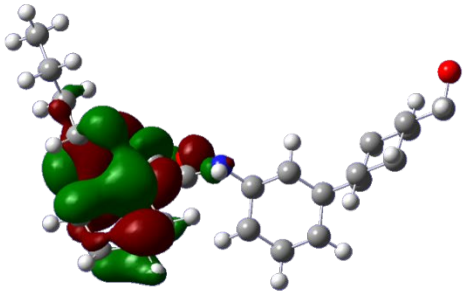

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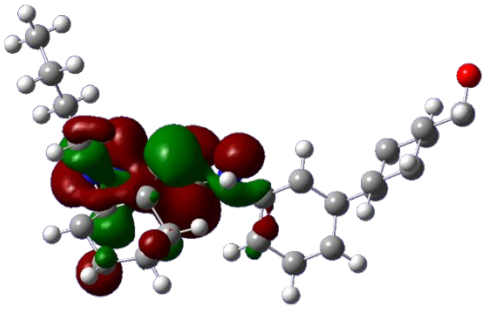

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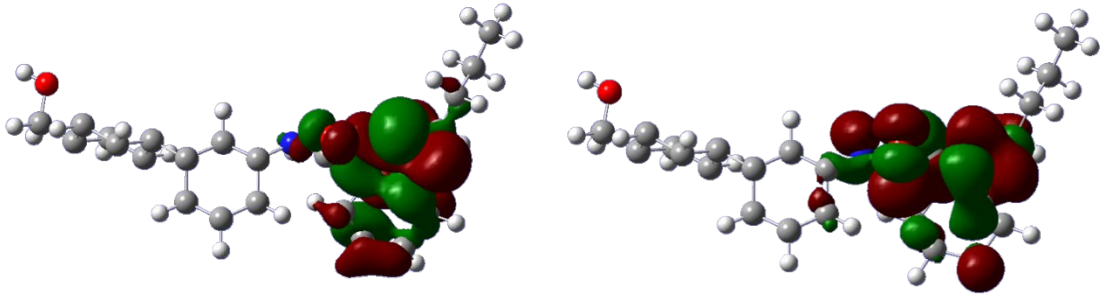
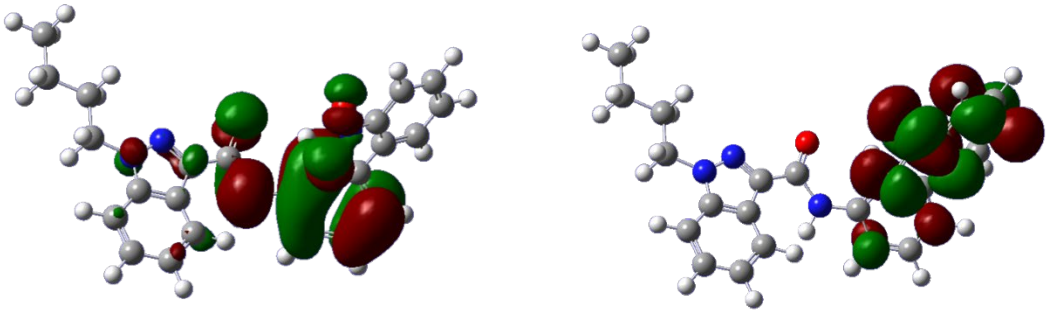


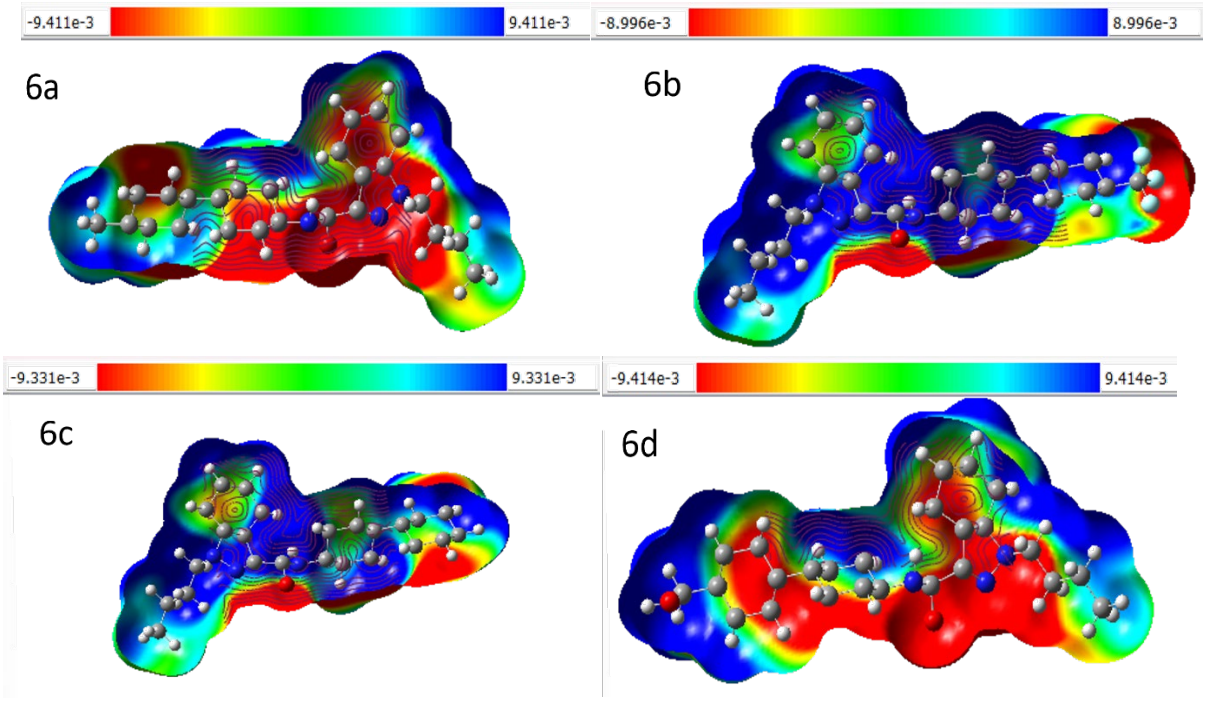
HOMO LUMO

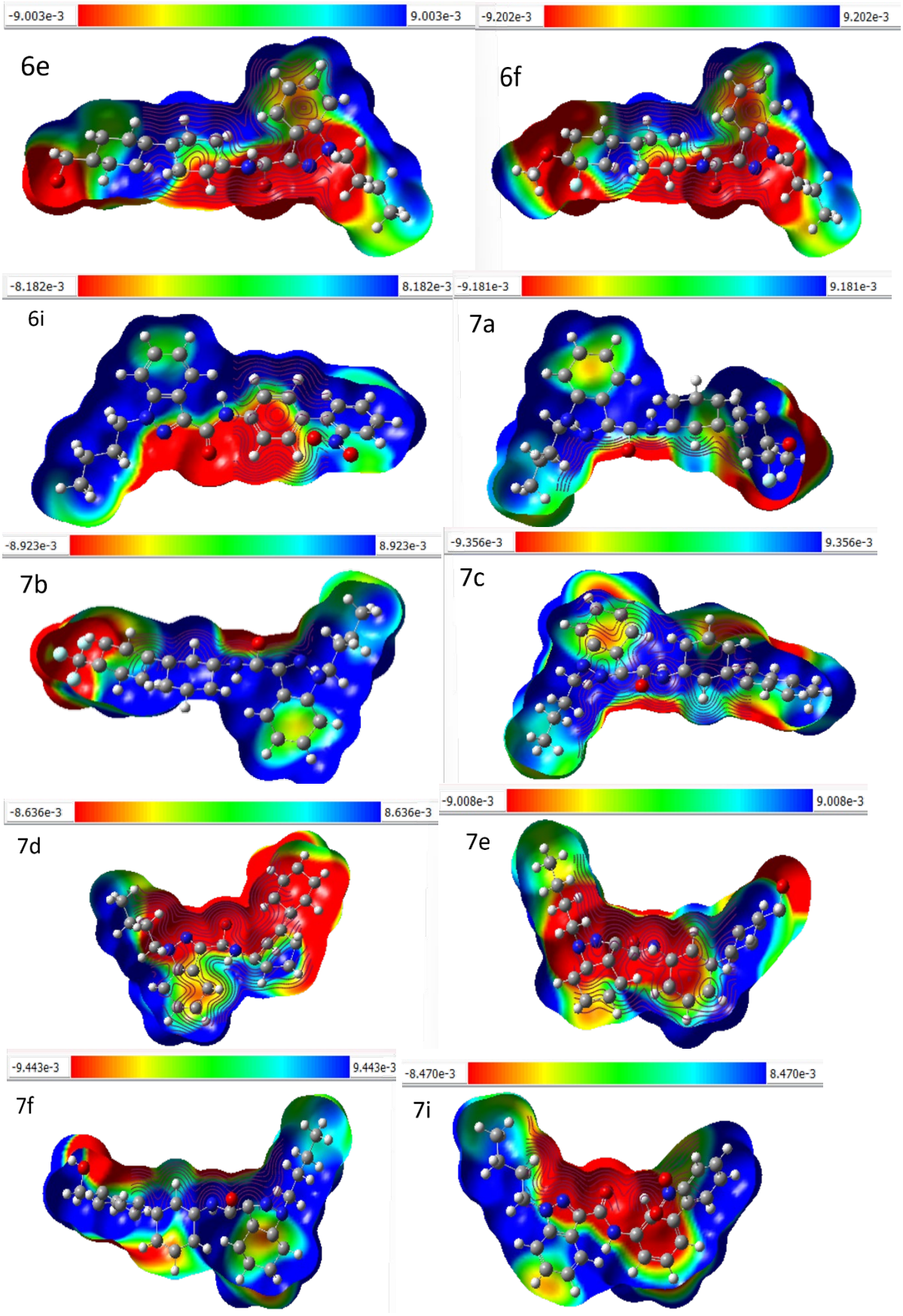
7i



HOMO LUMO

Molecular Electrostatic Potential surface of synthesized indazole derivatives




-9.003e-3
9.003e-3
6e
-9.202e-3
9.202e-3
6f
-8.182e-3
8.182e-3
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-9.181e-3
9.181e-3
7a
-8.923e-3
8.923e-3
7b
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9.356e-3
7c
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8.636e-3
7d
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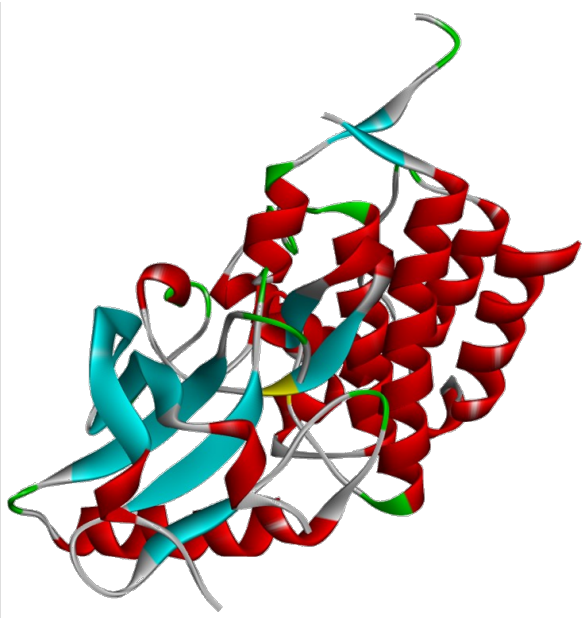
9.008e-3
7e
-9.443e-3
9.443e-3
7f
-8.470e-3
8.470e-3
7i

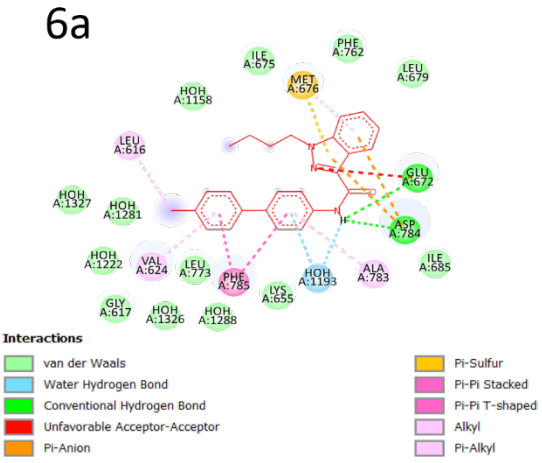
Molecular Docking 2D diagrams of indazole derivatives with Binding energy.

Entry	Receptor	(1) final intermolecular energy + vander Waal + H-bond + desolv energy (Kcal/mol)	2) final total internal energy (Kcal/mol)	(3) torsional free energy (Kcal/mol)	(4) unbound system's energy (Kcal/mol)	Binding energy = [(1)+(2)+(3)-(4)] (Kcal/mol)
6a	6few **4wa9**	-12.77 **-12.21**	-1.62 **-1.64**	+1.79 **+1.79**	-1.62 **-1.89**	-10.98 **-10.42**
6b	6few 4wa9	-12.66 -10.21	-1.75 -1.05	+2.09 +2.09	-1.75 -1.05	-10.57 -8.13
6c	6few **4wa9**	-12.85 **-10.87**	-1.65 **-1.87**	+1.79 **+1.79**	-1.65 **-1.87**	-11.06 **-9.08**
6d	6few 4wa9	-13.48 -11.63	-1.71 -1.77	+2.39 +2.39	-1.71 -1.77	-11.10 -9.24
6e	6few 4wa9	-13.31 -11.06	-1.74 -1.95	+2.09 +2.09	-1.74 -1.95	-11.22 -8.97
6f	6few 4wa9	-13.13 -10.79	-1.77 -1.88	+2.09 +2.09	-1.77 -1.88	-11.04 -8.70
6g	**6few** 4wa9	**-14.40** -11.07	**-1.71** -1.03	**+2.39** +2.39	**-1.71** -1.03	**-12.02** -8.68
6h	**6few** 4wa9	**-13.88** -9.75	**-1.89** -1.16	**+2.09** +2.09	**-1.89** -1.16	**-11.79** -7.66
6i	6few 4wa9	-13.56 -9.05	-1.71 -1.13	+2.09 +2.09	-1.71 -1.31	-11.47 -6.96
7a	6few 4wa9	-13.91 -11.65	-1.53 -1.27	+2.09 +2.09	-1.53 -1.27	-11.82 -9.56
7b	6few 4wa9	-13.53 -11.79	-1.88 -1.12	+2.09 +2.09	-1.88 -1.12	-11.44 -9.70
7c	6few **4wa9**	-13.97 **-12.06**	-1.56 **-0.98**	+1.79 **+1.79**	-1.56 **-0.98**	-12.18 **-10.27**
7d	6few 4wa9	-14.37 -11.63	-1.81 -1.41	+1.79 +1.79	-1.81 -1.41	-12.58 -9.84
7e	6few 4wa9	-14.63 -12.19	-1.63 -0.99	+2.09 +2.09	-1.63 -0.99	-12.54 -10.11
7f	6few 4wa9	-14.56 -12.17	-1.35 -1.07	+2.39 +2.39	-1.35 -1.07	-12.18 -9.78
7g	6few **4wa9**	-15.28 **-12.95**	-1.46 **-1.01**	+2.39 **+2.39**	-1.46 **-1.01**	-12.89 **-10.57**
7h	**6few** 4wa9	**-15.28** -12.76	**-1.48** -1.15	**+2.09** +2.09	**-1.48** -1.15	**-13.19** -10.67
7i	**6few** 4wa9	**-15.08** -10.96	**-2.14** -1.62	**+2.09** +2.09	**-2.14** -1.62	**-12.99** -8.87

PDB: 6few



6a



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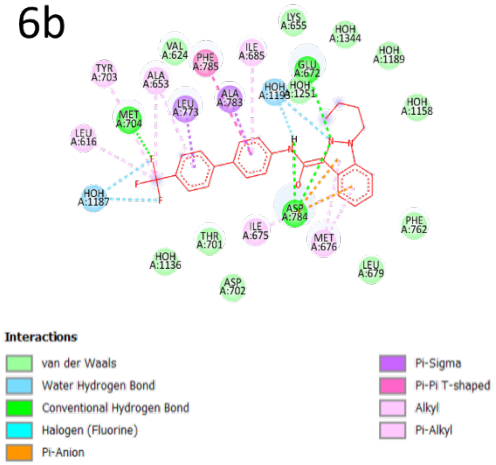

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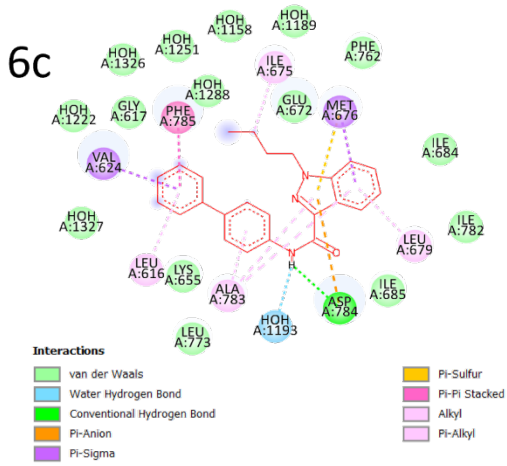

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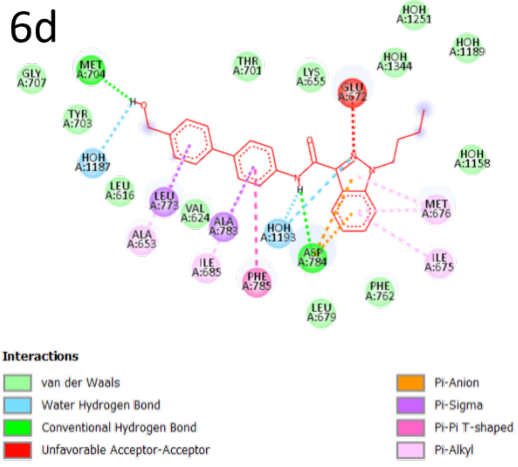
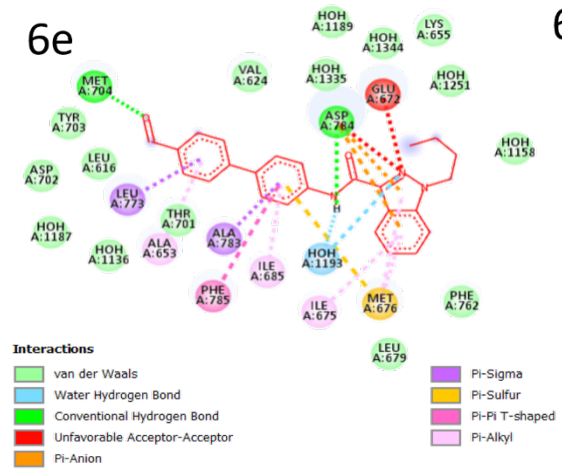
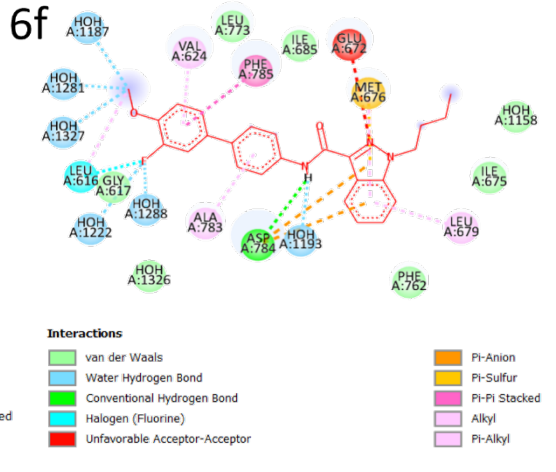
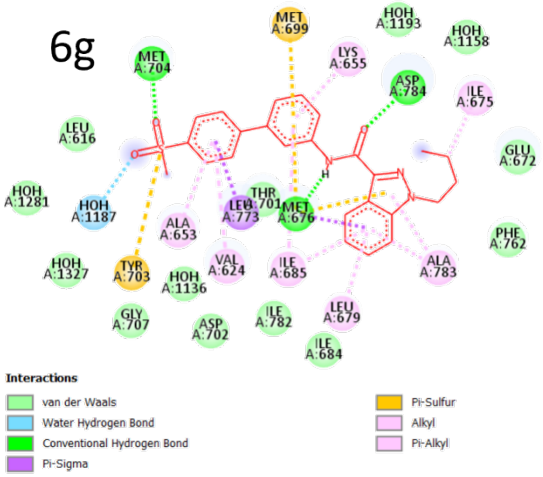
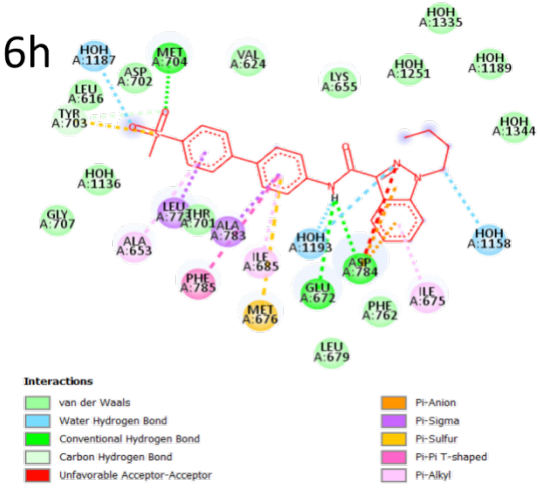
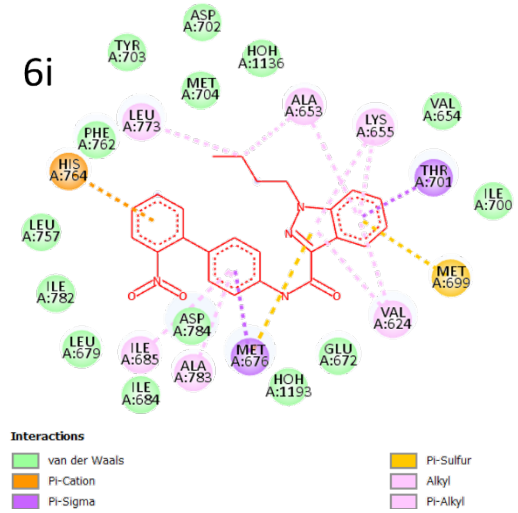


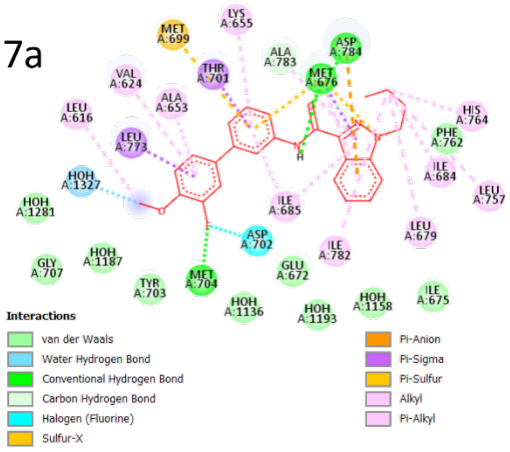

6e
Interactions
van der Waals
Water Hydrogen Bond
Conventional Hydrogen Bond
Unfavorable Acceptor-Acceptor
Pi-Anion
Pi-Sigma
Pi-Sulfur
Pi-Pi T-shaped
Pi-Alkyl


6f
Interactions
van der Waals
Water Hydrogen Bond
Conventional Hydrogen Bond
Halogen (Fluorine)
Unfavorable Acceptor-Acceptor
Pi-Anion
Pi-Sulfur
Pi-Pi Stacked
Alkyl
Pi-Alkyl

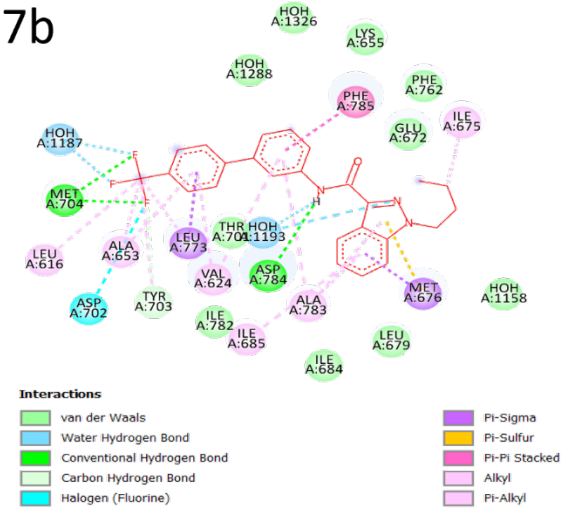

6g
Interactions
van der Waals
Water Hydrogen Bond
Conventional Hydrogen Bond
Pi-Sigma
Pi-Sulfur
Alkyl
Pi-Alkyl


6h
Interactions
van der Waals
Water Hydrogen Bond
Conventional Hydrogen Bond
Carbon Hydrogen Bond
Unfavorable Acceptor-Acceptor
Pi-Anion
Pi-Sigma
Pi-Sulfur
Pi-Pi T-shaped
Pi-Alkyl


6i
Interactions
van der Waals
Pi-Cation
Pi-Sigma
Pi-Sulfur
Alkyl
Pi-Alkyl


7a
Interactions
van der Waals
Water Hydrogen Bond
Conventional Hydrogen Bond
Carbon Hydrogen Bond
Halogen (Fluorine)
Sulfur-X
Pi-Anion
Pi-Sigma
Pi-Sulfur
Alkyl
Pi-Alkyl

7b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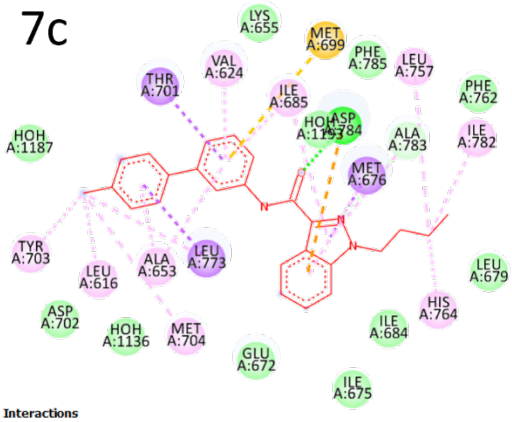
LYS A:655
HOH A:1288
PHE A:762
PHE A:785
ILE A:675
GLU A:672
HOH A:1187
MET A:704
LEU A:773
THR A:701
HOH A:1193
LEU A:616
ALA A:653
VAL A:624
ASP A:784
ASP A:702
TYR A:703
ALA A:783
MET A:676
HOH A:1158
ILE A:782
ILE A:685
LEU A:679
ILE A:684
Interactions
van der Waals
Water Hydrogen Bond
Conventional Hydrogen Bond
Carbon Hydrogen Bond
Halogen (Fluorine)
Pi-Sigma
Pi-Sulfur
Pi-Pi Stacked
Alkyl
Pi-Alkyl

7c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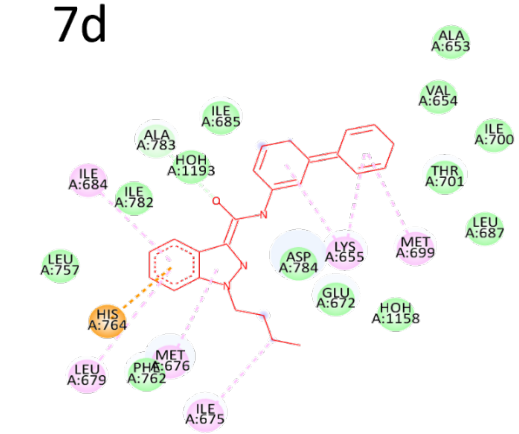
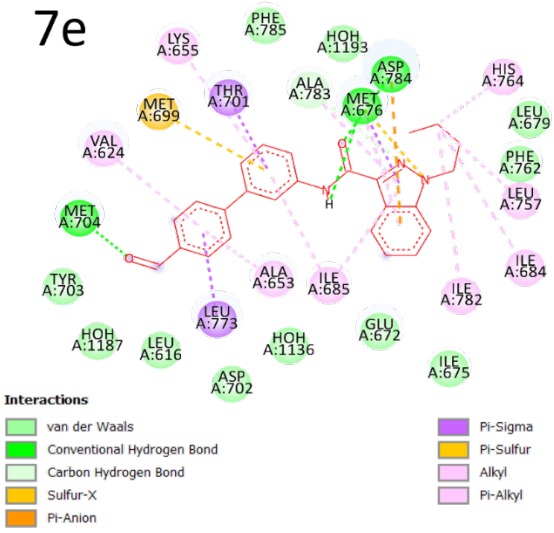
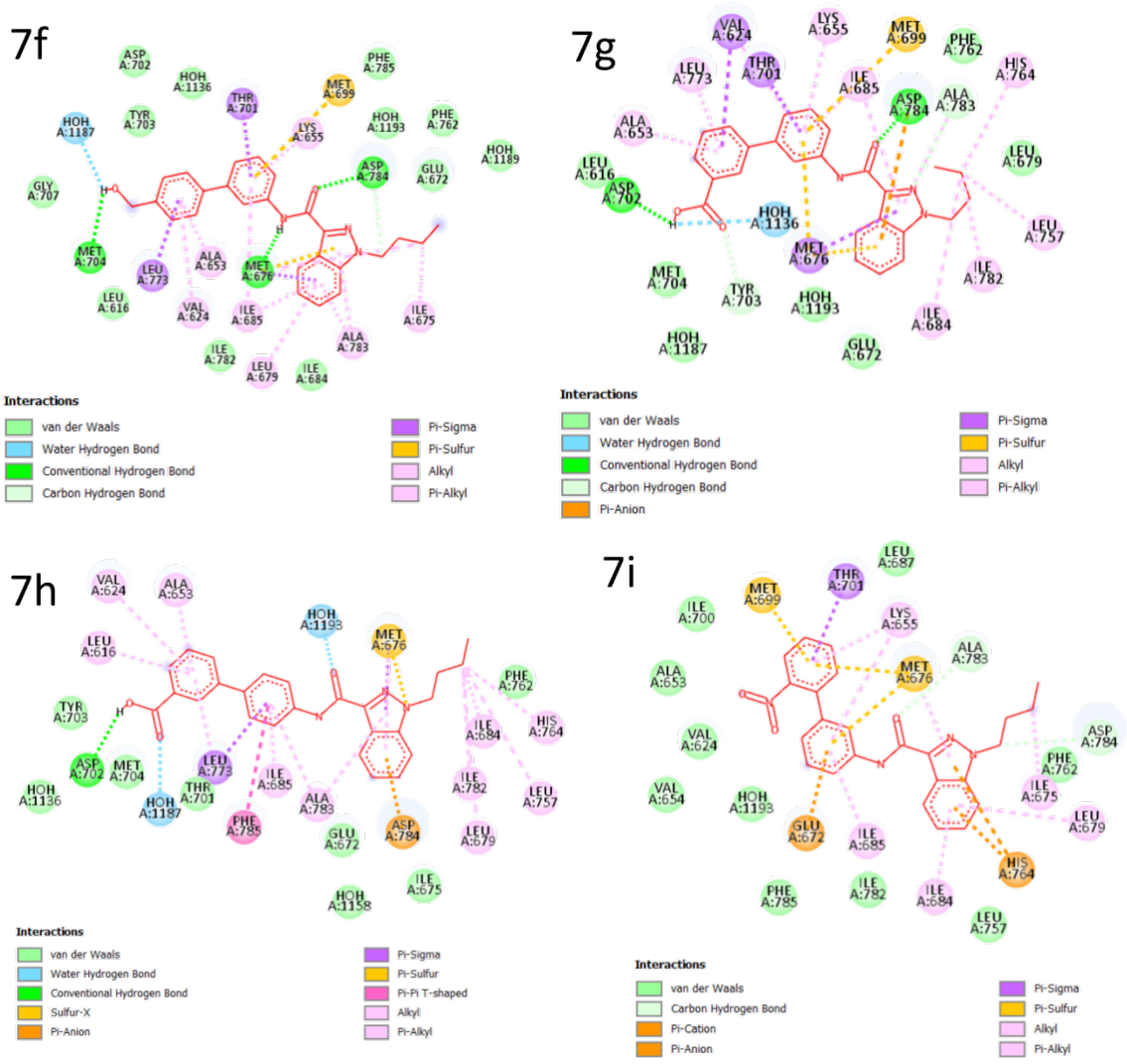
MET A:699
PHE A:785
LEU A:757
VAL A:624
THR A:701
ILE A:685
PHE A:762
HOH A:1187
HOH A:1193
ASP A:784
ALA A:783
ILE A:782
MET A:676
TYR A:703
LEU A:616
ALA A:653
LEU A:773
LEU A:679
ASP A:702
HOH A:1136
MET A:704
HIS A:764
ILE A:684
GLU A:672
ILE A:675
Interactions
van der Waals
Conventional Hydrogen Bond
Carbon Hydrogen Bond
Pi-Anion
Pi-Sigma
Pi-Sulfur
Alkyl
Pi-Alkyl

7d


ALA A:653
VAL A:654
ILE A:685
ILE A:700
ALA A:783
HOH A:1193
THR A:701
ILE A:684
ILE A:782
LEU A:687
MET A:699
LEU A:757
ASP A:784
LYS A:655
GLU A:672
HOH A:1158
HIS A:764
MET A:676
LEU A:679
PHE A:762
ILE A:675
Interactions
van der Waals
Carbon Hydrogen Bond
Pi-Cation
Alkyl
Pi-Alkyl

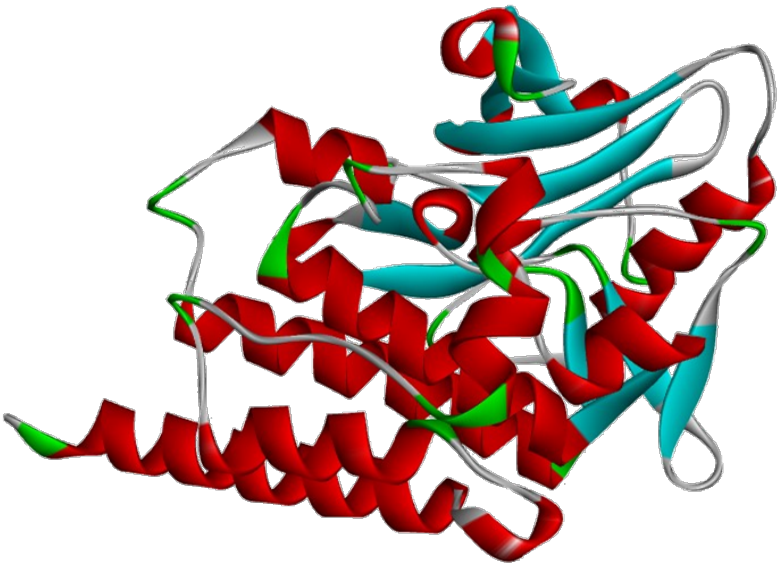
7e


PHE A:785
LYS A:655
HOH A:1193
ASP A:784
HIS A:764
ALA A:783
THR A:701
MET A:676
LEU A:679
MET A:699
VAL A:624
PHE A:762
LEU A:757
MET A:704
ILE A:684
TYR A:703
ALA A:653
ILE A:685
ILE A:782
LEU A:773
HOH A:1187
GLU A:672
LEU A:616
HOH A:1136
ILE A:675
ASP A:702
Interactions
van der Waals
Conventional Hydrogen Bond
Carbon Hydrogen Bond
Sulfur-X
Pi-Anion
Pi-Sigma
Pi-Sulfur
Alkyl
Pi-Alkyl

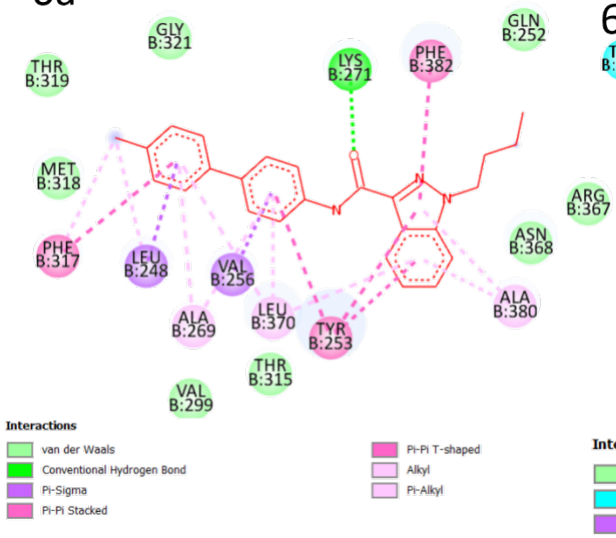


Molecular Docking 2D diagrams of indazole derivatives

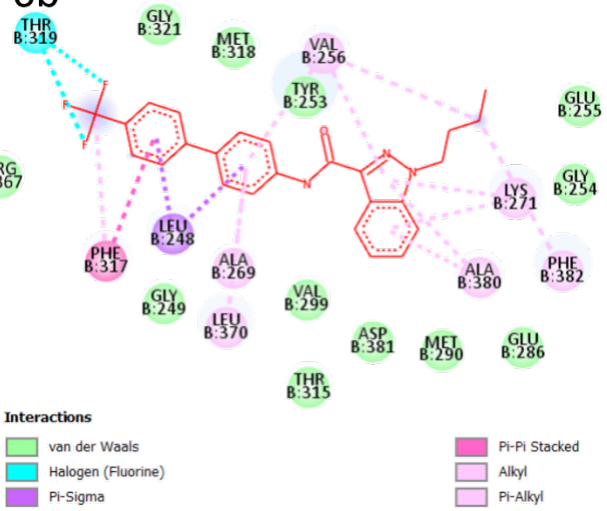
PDB: 4WA9



6a


GLY B:321
GLN B:252
THR B:319
LYS B:271
PHE B:382
MET B:318
ARG B:367
PHE B:317
LEU B:248
VAL B:256
ASN B:368
ALA B:269
LEU B:370
TYR B:253
ALA B:380
THR B:315
VAL B:299
Interactions
van der Waals
Conventional Hydrogen Bond
Pi-Sigma
Pi-Pi Stacked
Pi-Pi T-shaped
Alkyl
Pi-Alkyl

6b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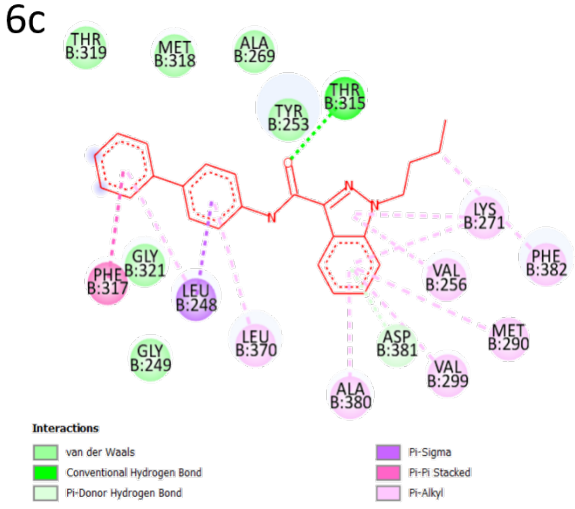
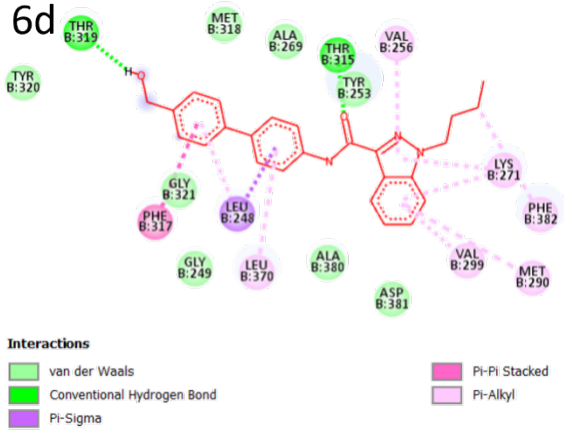
GLY B:321
MET B:318
VAL B:256
TYR B:253
GLU B:255
GLY B:254
LYS B:271
LEU B:248
PHE B:317
ALA B:269
ALA B:380
PHE B:382
GLY B:249
VAL B:299
LEU B:370
ASP B:381
MET B:290
GLU B:286
THR B:315
Interactions
van der Waals
Halogen (Fluorine)
Pi-Sigma
Pi-Pi Stacked
Alkyl
Pi-Alkyl

6c


THR B:319
MET B:318
ALA B:269
TYR B:253
THR B:315
LYS B:271
PHE B:317
GLY B:321
PHE B:382
VAL B:256
LEU B:248
MET B:290
ASP B:381
LEU B:370
GLY B:249
VAL B:299
ALA B:380
Interactions
van der Waals
Conventional Hydrogen Bond
Pi-Donor Hydrogen Bond
Pi-Sigma
Pi-Pi Stacked
Pi-Alkyl

6d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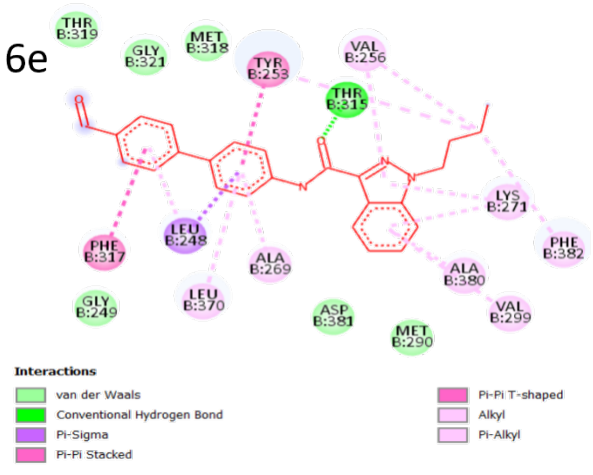
MET B:318
ALA B:269
VAL B:256
TYR B:320
THR B:315
TYR B:253
LYS B:271
GLY B:321
PHE B:317
LEU B:248
PHE B:382
GLY B:249
LEU B:370
ALA B:380
VAL B:299
MET B:290
ASP B:381
Interactions
van der Waals
Conventional Hydrogen Bond
Pi-Sigma
Pi-Pi Stacked
Pi-Alkyl

6e



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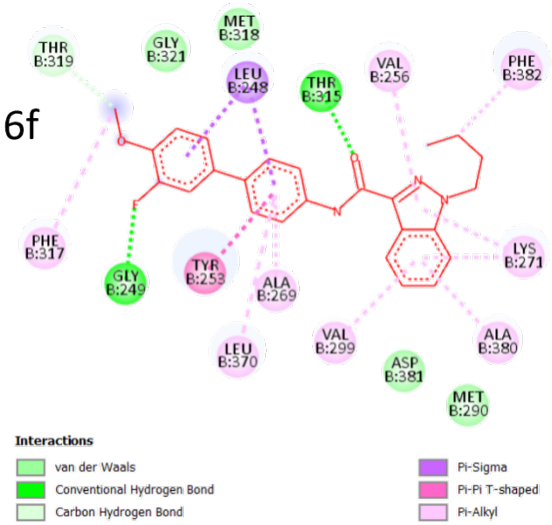
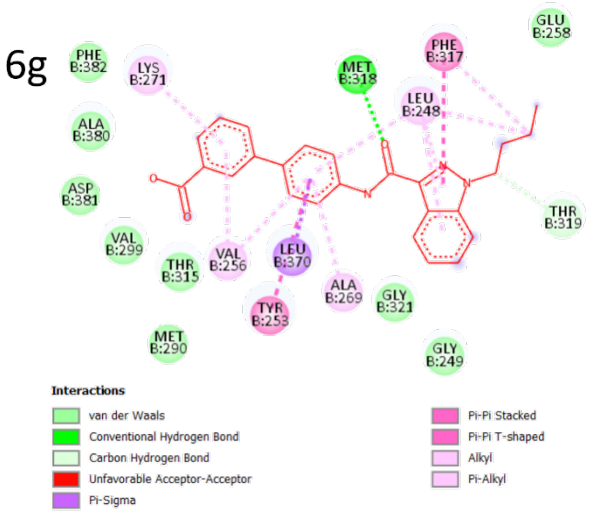
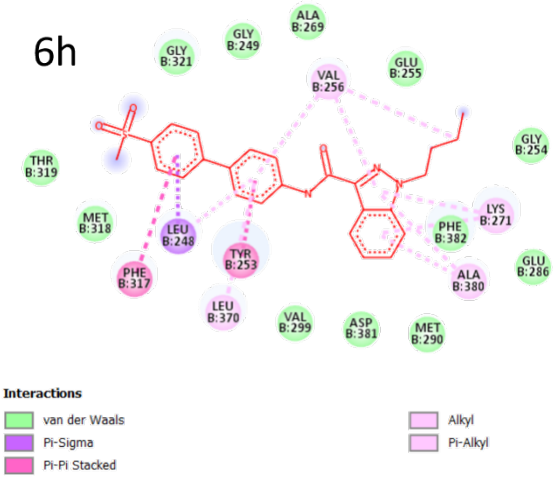


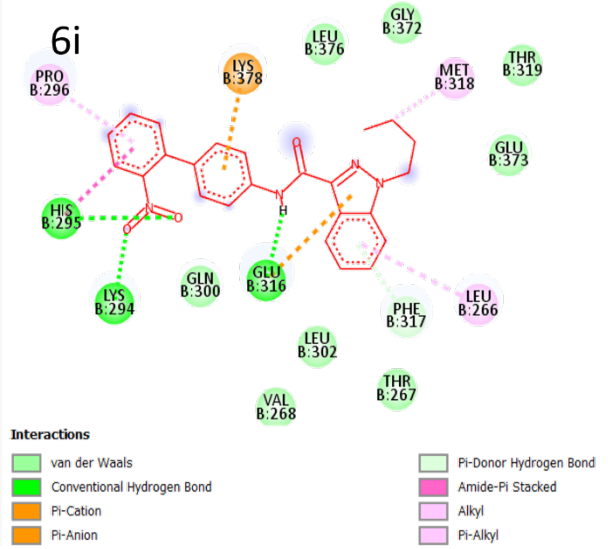
6g



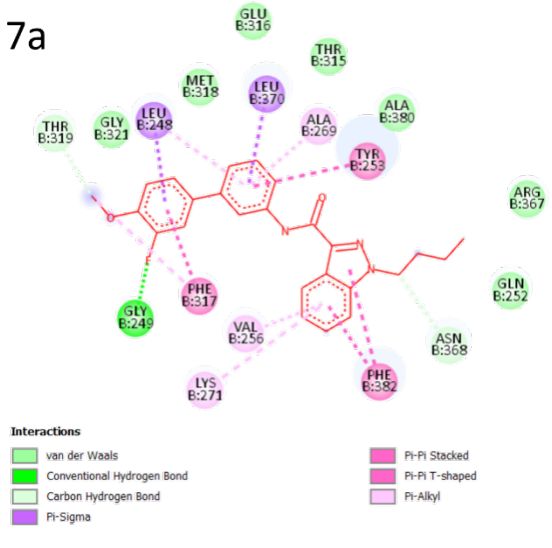
6h



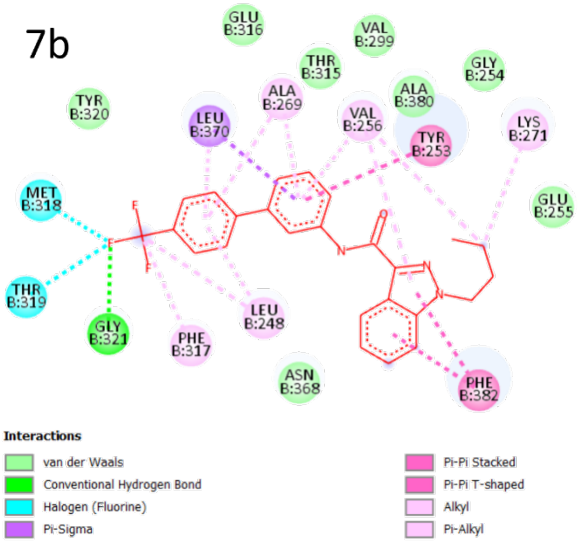
6i



7a



7b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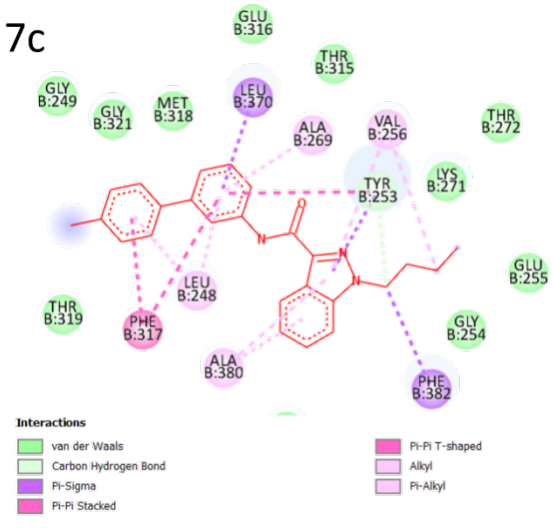
THR B:315
GLY B:254
TYR B:320
ALA B:269
ALA B:380
LEU B:370
VAL B:256
LYS B:271
TYR B:253
MET B:318
GLU B:255
THR B:319
GLY B:321
LEU B:248
PHE B:317
ASN B:368
PHE B:382
Interactions
van der Waals
Conventional Hydrogen Bond
Halogen (Fluorine)
Pi-Sigma
Pi-Pi Stacked
Pi-Pi T-shaped
Alkyl
Pi-Alkyl

7c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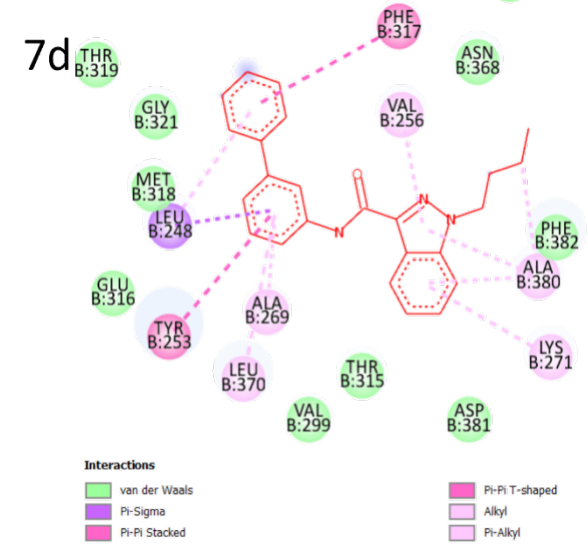
THR B:315
GLY B:249
GLY B:321
MET B:318
LEU B:370
ALA B:269
VAL B:256
THR B:272
TYR B:253
LYS B:271
GLU B:255
LEU B:248
THR B:319
PHE B:317
GLY B:254
ALA B:380
PHE B:382
Interactions
van der Waals
Carbon Hydrogen Bond
Pi-Sigma
Pi-Pi Stacked
Pi-Pi T-shaped
Alkyl
Pi-Alkyl

7d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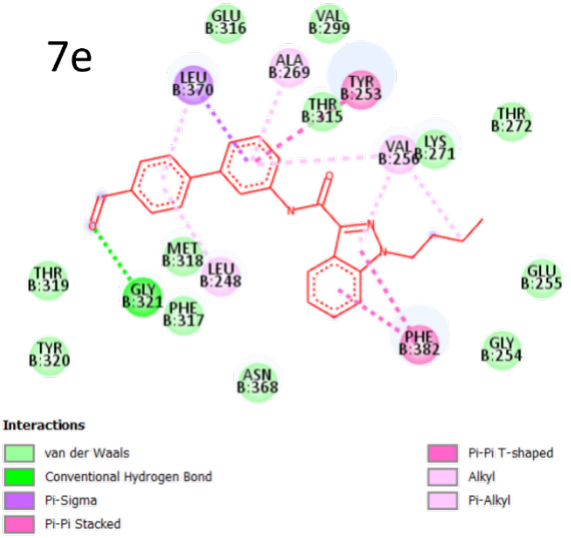
ASN B:368
GLY B:321
VAL B:256
MET B:318
LEU B:248
PHE B:382
ALA B:380
GLU B:316
ALA B:269
TYR B:253
LYS B:271
LEU B:370
THR B:315
VAL B:299
ASP B:381
Interactions
van der Waals
Pi-Sigma
Pi-Pi Stacked
Pi-Pi T-shaped
Alkyl
Pi-Alkyl

7e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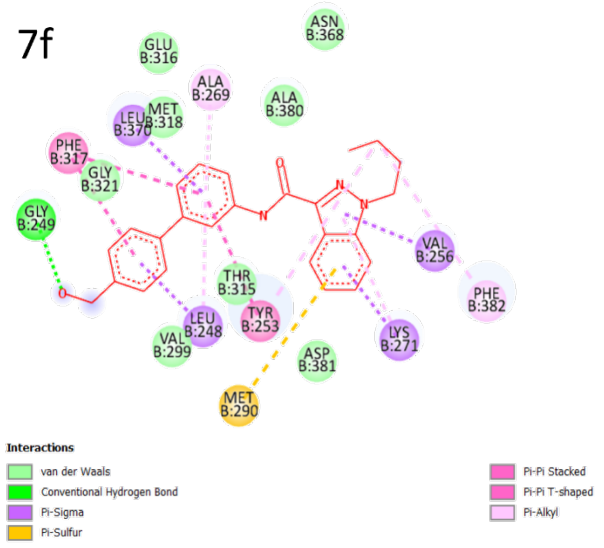
VAL B:299
ALA B:269
LEU B:370
TYR B:253
THR B:315
THR B:272
VAL B:256
LYS B:271
MET B:318
LEU B:248
THR B:319
GLY B:321
PHE B:317
GLU B:255
PHE B:382
GLY B:254
TYR B:320
ASN B:368
Interactions
van der Waals
Conventional Hydrogen Bond
Pi-Sigma
Pi-Pi Stacked
Pi-Pi T-shaped
Alkyl
Pi-Alkyl

7f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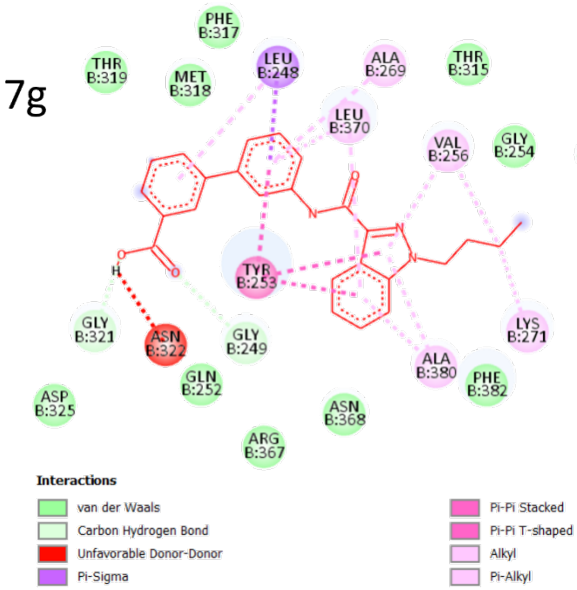
GLY B:321
GLY B:249
VAL B:256
PHE B:382
THR B:315
LEU B:248
TYR B:253
VAL B:299
LYS B:271
ASP B:381
MET B:290
Interactions
van der Waals
Conventional Hydrogen Bond
Pi-Sigma
Pi-Sulfur
Pi-Pi Stacked
Pi-Pi T-shaped
Pi-Alkyl

7g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MET B:318
LEU B:248
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THR B:315
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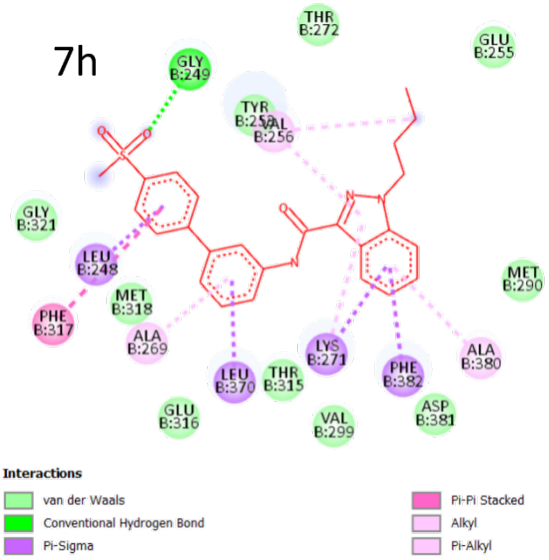
VAL B:256
GLY B:254
TYR B:253
GLY B:321
ASN B:322
GLY B:249
LYS B:271
ALA B:380
PHE B:382
GLN B:252
ASP B:325
ASN B:368
ARG B:367
Interactions
van der Waals
Carbon Hydrogen Bond
Unfavorable Donor-Donor
Pi-Sigma
Pi-Pi Stacked
Pi-Pi T-shaped
Alkyl
Pi-Alkyl

7h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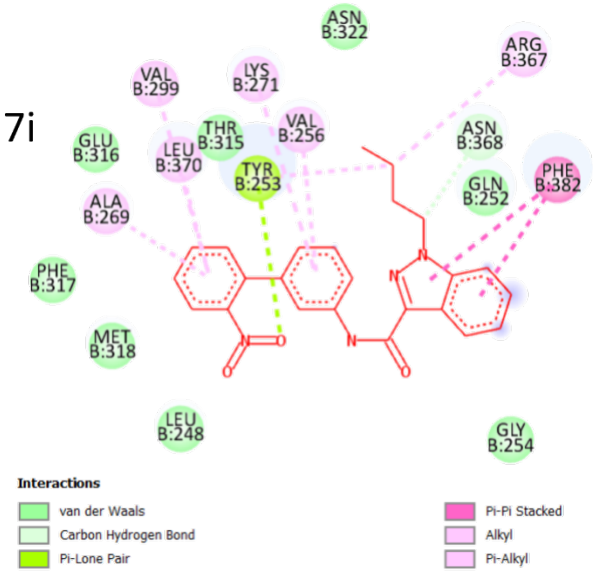
VAL B:256
GLY B:321
LEU B:248
MET B:290
MET B:318
PHE B:317
ALA B:269
LYS B:271
ALA B:380
LEU B:370
THR B:315
PHE B:382
GLU B:316
VAL B:299
ASP B:381
Interactions
van der Waals
Conventional Hydrogen Bond
Pi-Sigma
Pi-Pi Stacked
Alkyl
Pi-Alkyl

7i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ARG B:367
VAL B:299
LYS B:271
GLU B:316
THR B:315
VAL B:256
ASN B:368
LEU B:370
TYR B:253
PHE B:382
GLN B:252
ALA B:269
PHE B:317
MET B:318
LEU B:248
GLY B:254
Interactions
van der Waals
Carbon Hydrogen Bond
Pi-Lone Pair
Pi-Pi Stacked
Alkyl
Pi-Alkyl