Supporting Information for

Gold-carbene assisted formation of tetraarylmethane derivatives: Double X-H activation by gold†

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d Center for X-ray Crystallography and, CSIR-Indian Institute of Chemical Technology, Hyderabad, 500007, India.

Contents:

Electronic Supplementary Material (ESI) for Chemical Communications

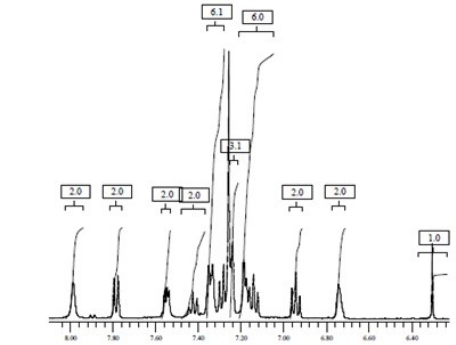
1.1 General

Reactions were carried out in oven dried reaction flasks under nitrogen atmosphere and also solvents and reagents were transferred by oven-dried syringes to ambient temperature. TLC was performed on Merck silica gel aluminium sheets using UV as a visualizing agent and a solvents were removed under reduced pressure. Columns were packed as slurry of silica gel in hexane and ethyl acetate solvent mixture. The elution was assisted by applying pressure with an air pump. ^{13}C NMR spectra were recorded on 75, 100 and 125 MHz spectrometers. ^{1}HNMR spectra were recorded on 300, 400 and 500 MHz spectrometers in appropriate solvents using TMS as internal standard. The following abbreviations were used to explain multiplicities: s = singlet, d = doublet, dd = double doublet, t = triplet, m = multiplet. All reactions were performed under nitrogen atmosphere with freshly distilled and dried solvents. All solvents were distilled using standard procedures. Unless otherwise noted, reagents were obtained from Aldrich, Alfa Aesar, and TCI used without further purification. Synthesis of 6-(2-aminophenyl)-1-alkyl hexa-1,5-diyn-3-ol (**1a-p**) were prepared by following reported procedures.[1]

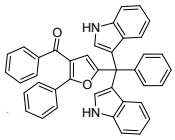
1. (a) R. Vicente, J. González, L. Riesgo, J. González, L. A. López, *Angew. Chem., Int. Ed.,* 2012, **51**, 8063; (b) S. Mata, L. A. López, R. Vicente, *Synlett,* 2015, **26**, 2685; (c) J. González, J. González, C. Pérez-Calleja, L. A. López, R. Vicente, *Angew. Chem., Int. Ed.,* 2013, **52**, 5853; (d) B. Song, L. -H. Li, X. -R. Song, Y. -F. Qiu, M. -J. Zhong, P. -X. Zhou, Y. -M. Liang, *Chem. Eur. J*., 2014, **20**, 5910.

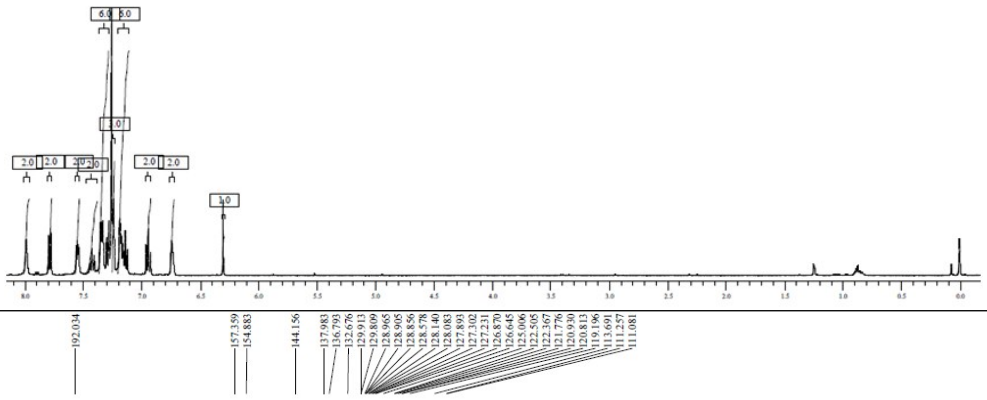
1.2 Copies of ^{1}H and ^{13}C NMR spectra (3a- 3w)

(5-(Di(*1H*-indol-3-yl)(phenyl)methyl)-2-phenylfuran-3-yl)(phenyl)methanone-**3a**

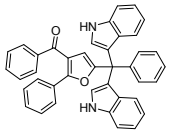


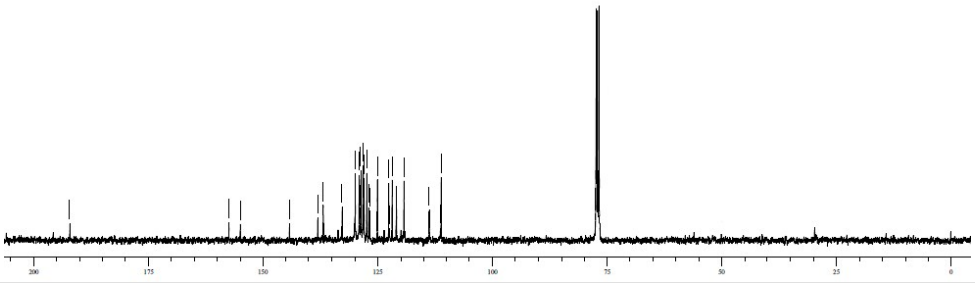
^{1}H NMR : 400 MHz $CDCl_3$
Chemical Formula: $C_{40}H_{28}N_2O_2$
Exact Mass: 568.6



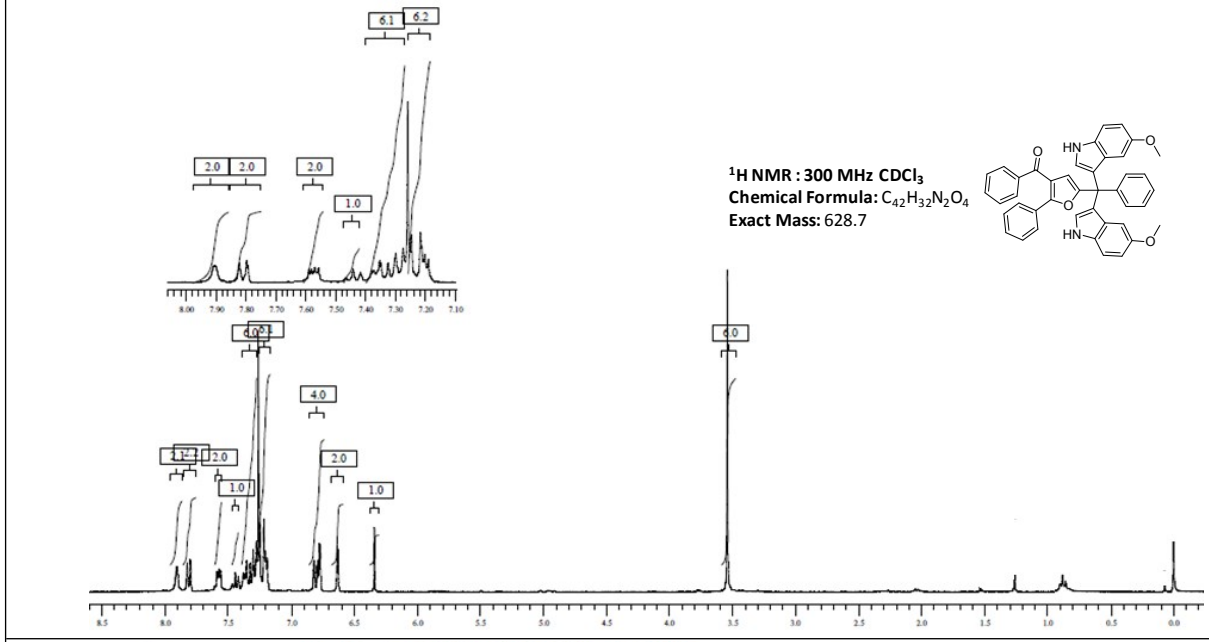


^{13}C NMR : 100 MHz $CDCl_3$
Chemical Formula: $C_{40}H_{28}N_2O_2$
Exact Mass: 568.6

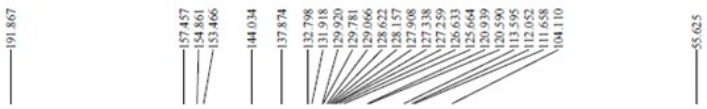




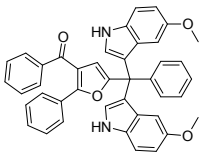
(5-(Bis(5-methoxy-*1H*-indol-3-yl)(phenyl)methyl)-2-phenylfuran-3-yl)(phenyl)methanone- **3b**

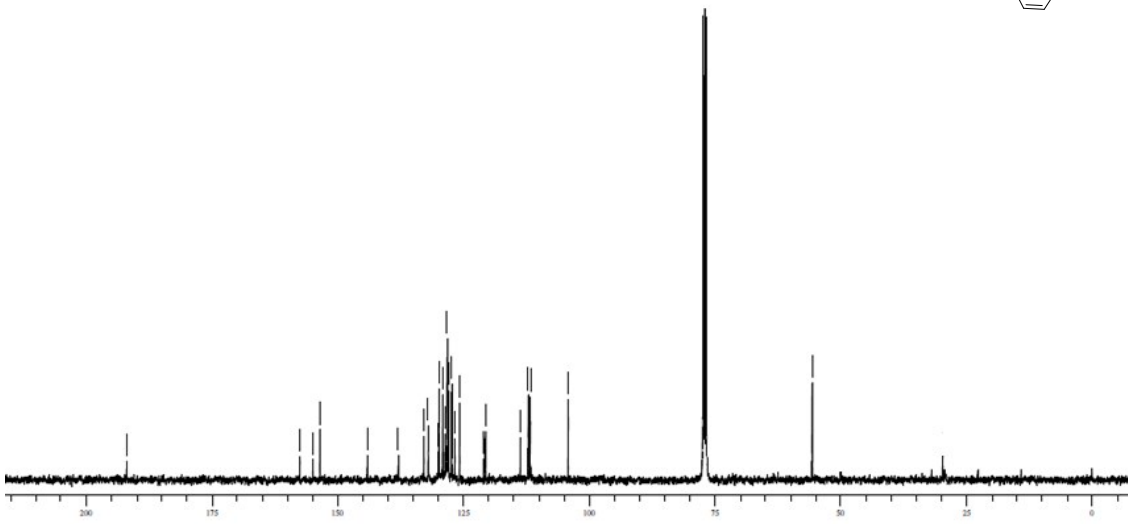


^{1}H NMR : 300 MHz $CDCl_3$
Chemical Formula: $C_{42}H_{32}N_2O_4$
Exact Mass: 628.7

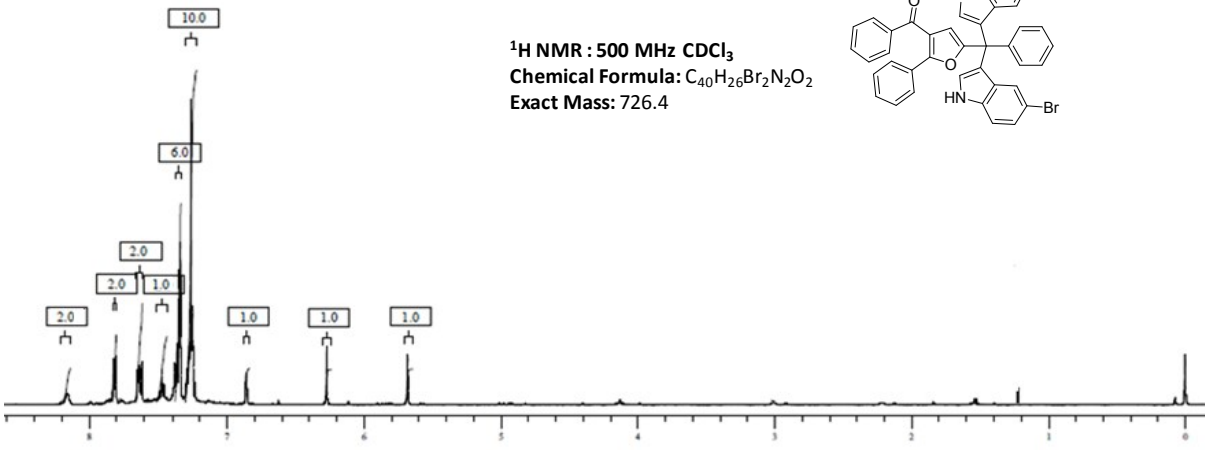


^{13}C NMR : 100 MHz $CDCl_3$
Chemical Formula: $C_{42}H_{32}N_2O_4$
Exact Mass: 628.7

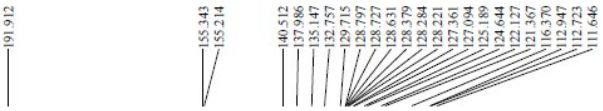




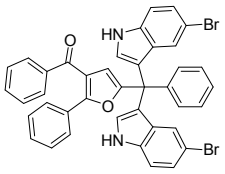
(5-(Bis(5-bromo-*1H*-indol-3-yl)(phenyl)methyl)-2-phenylfuran-3-yl)(phenyl)methanone -**3c**



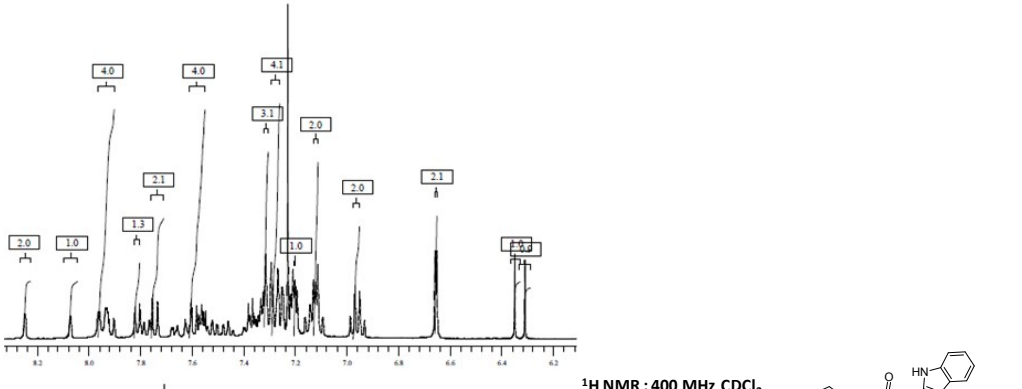
^{1}H NMR : 500 MHz $CDCl_3$
Chemical Formula: $C_{40}H_{26}Br_2N_2O_2$
Exact Mass: 726.4



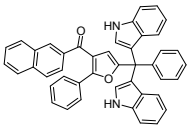
^{13}C NMR : 125 MHz $CDCl_3$
Chemical Formula: $C_{40}H_{26}Br_2N_2O_2$
Exact Mass: 726.4



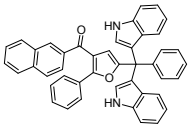
(5-(Di(*1H*-indol-3-yl)(phenyl)methyl)-2-phenylfuran-3-yl)(naphthalen-2-yl)methanone-**3d**

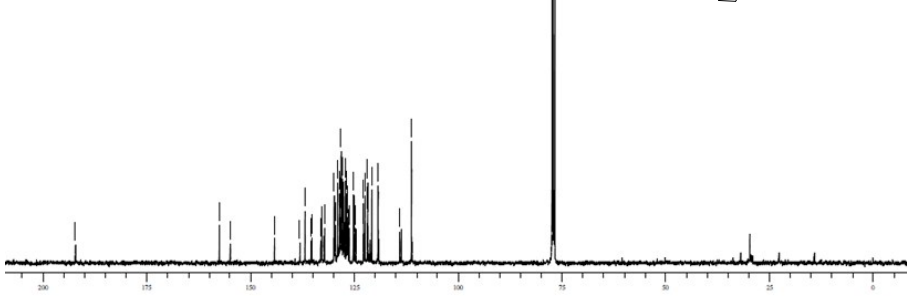


^{1}H NMR : 400 MHz $CDCl_3$
ChemicalFormula:$C_{44}H_{30}N_2O_2$
Exact Mass: 618.7

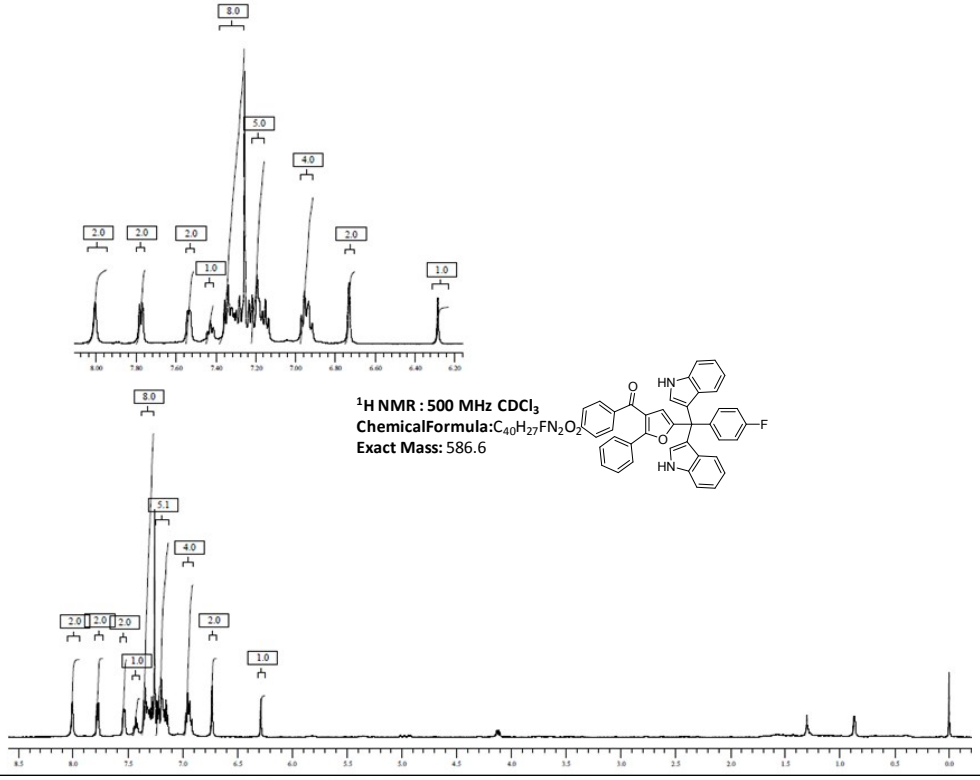


^{13}C NMR : 100 MHz $CDCl_3$
ChemicalFormula:$C_{44}H_{30}N_2O_2$
Exact Mass: 618.7



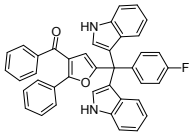


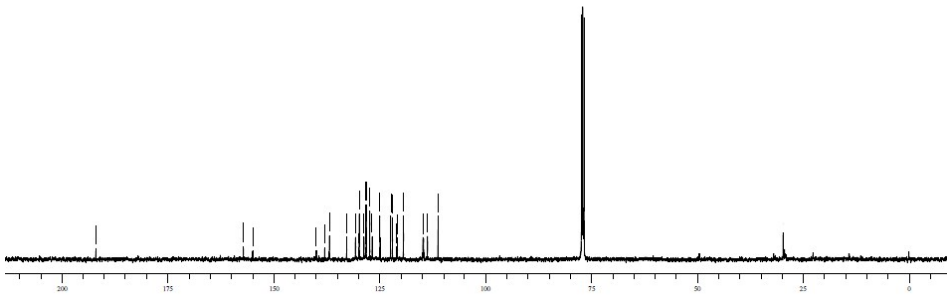
(5-((4-Fluorophenyl)di(*1H*-indol-3-yl)methyl)-2-phenylfuran-3-yl)(phenyl)methanone- **3e**



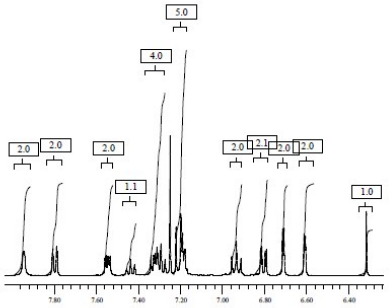
^{1}H NMR : 500 MHz $CDCl_3$
ChemicalFormula:$C_{40}H_{27}FN_2O_2$
Exact Mass: 586.6

^{13}C NMR : 125 MHz $CDCl_3$
ChemicalFormula:$C_{40}H_{27}FN_2O_2$
Exact Mass: 586.6

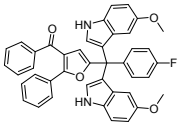


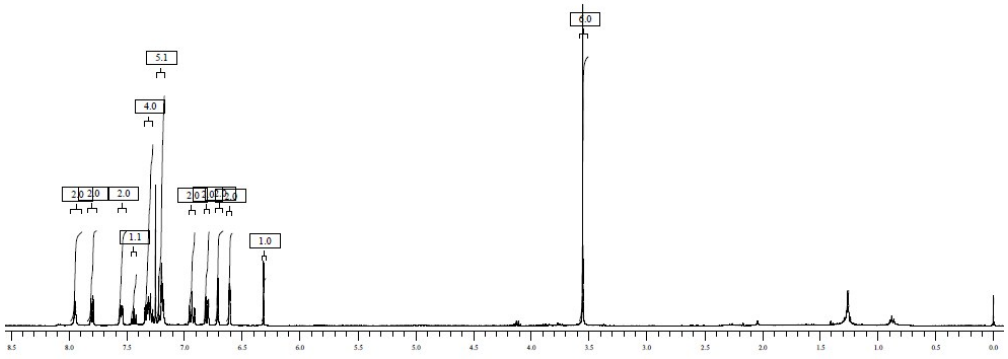


(5-((4-Fluorophenyl)bis(5-methoxy-*1H*-indol-3-yl)methyl)-2-phenylfuran-3-yl)(phenyl)methanone -**3f**

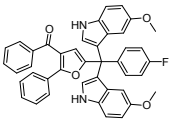


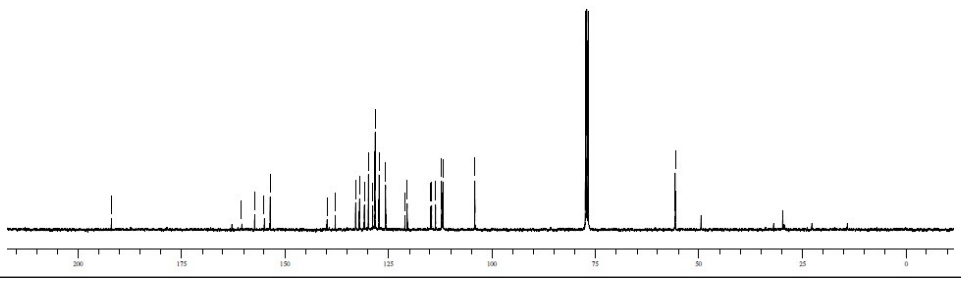
^{1}H NMR : 400 MHz $CDCl_3$
Chemical Formula: $C_{42}H_{31}FN_2O_4$
Exact Mass: 646.7



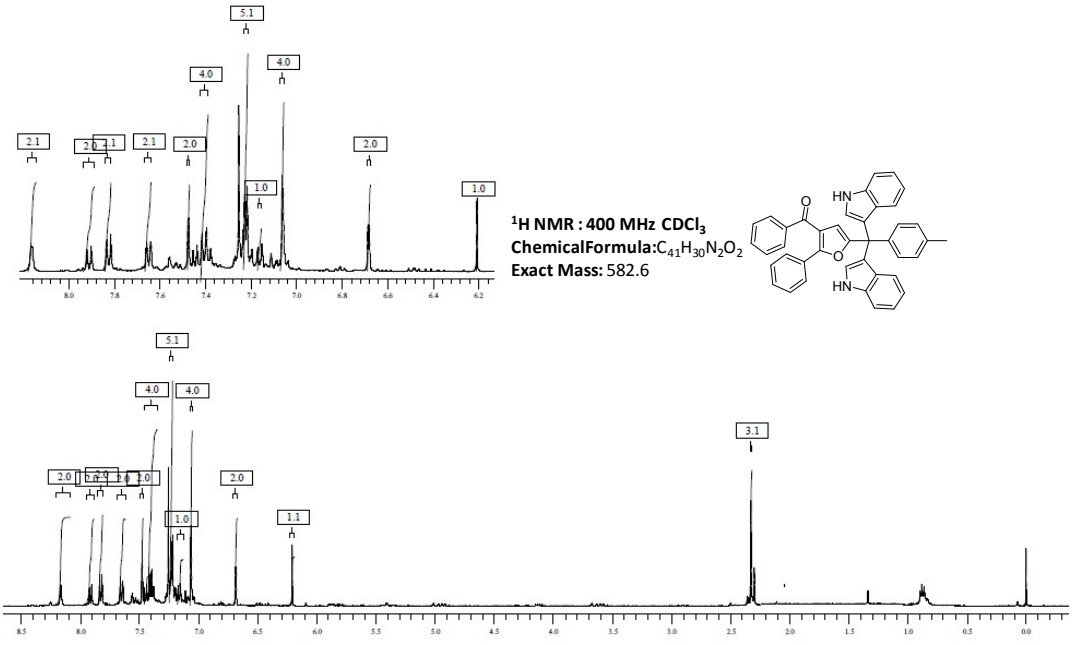


^{13}C NMR : 100 MHz $CDCl_3$
Chemical Formula: $C_{42}H_{31}FN_2O_4$
Exact Mass: 646.7



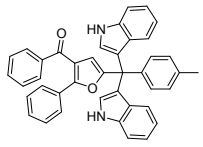


(5-(Di(*1H*-indol-3-yl)(p-tolyl)methyl)-2-phenylfuran-3-yl)(phenyl)methanone -**3g**

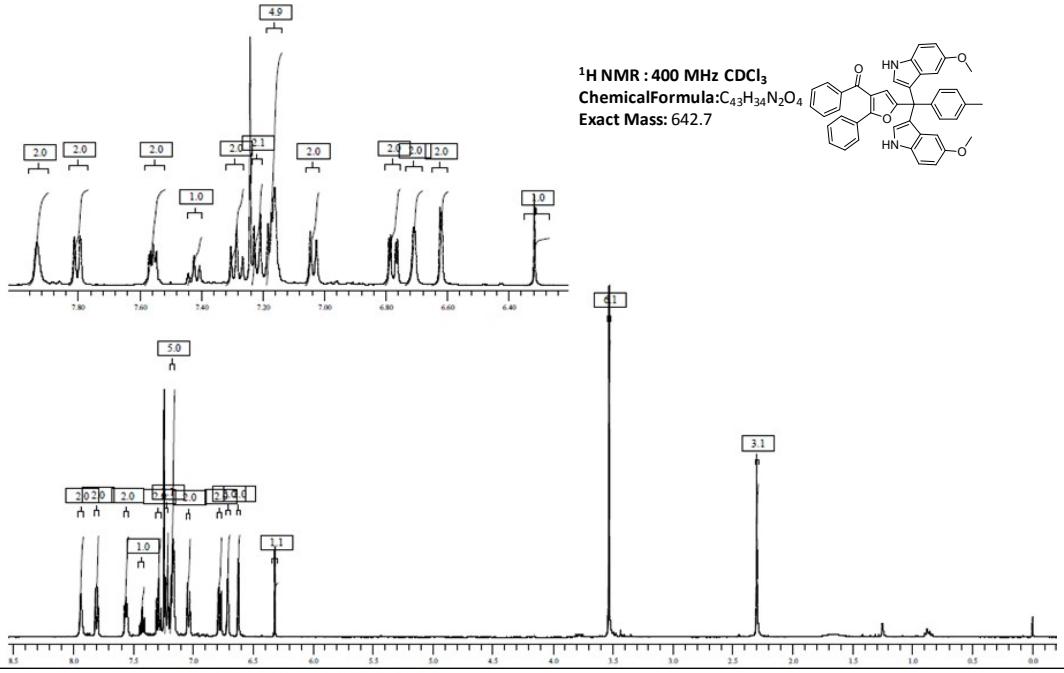


^{1}H NMR : 400 MHz $CDCl_3$
ChemicalFormula:$C_{41}H_{30}N_2O_2$
Exact Mass: 582.6

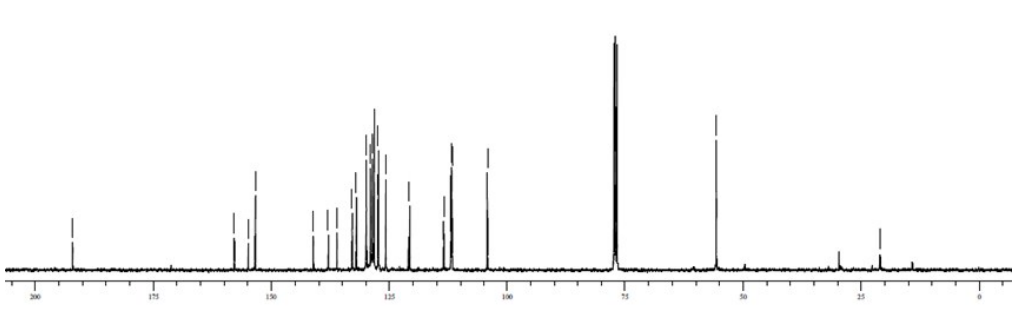
^{13}C NMR : 100 MHz $CDCl_3$
ChemicalFormula:$C_{41}H_{30}N_2O_2$
Exact Mass: 582.6



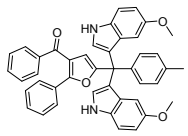
(5-(Bis(5-methoxy-*1H*-indol-3-yl)(p-tolyl)methyl)-2-phenylfuran-3-yl)(phenyl)methanone -**3h**



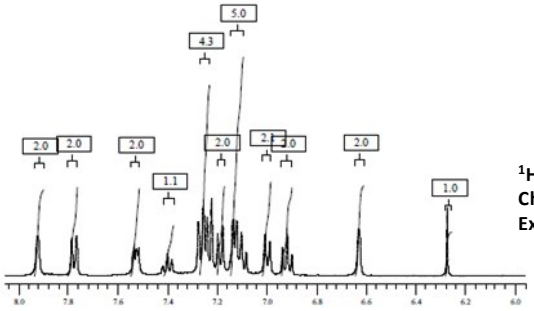
^{1}H NMR : 400 MHz $CDCl_3$
ChemicalFormula: $C_{43}H_{34}N_2O_4$
Exact Mass: 642.7



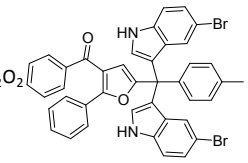
^{13}C NMR : 100 MHz $CDCl_3$
ChemicalFormula: $C_{43}H_{34}N_2O_4$
Exact Mass: 642.7

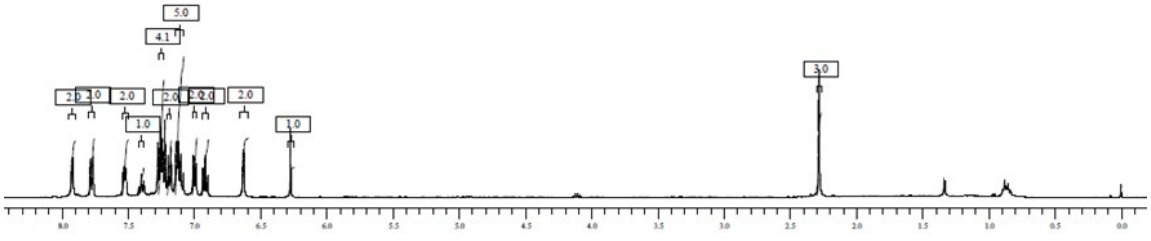


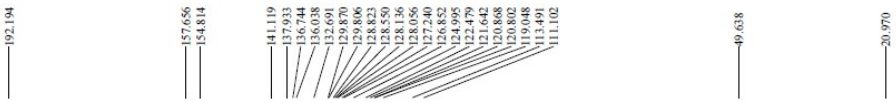
(5-(Bis(5-bromo-*1H*-indol-3-yl)(p-tolyl)methyl)-2-phenylfuran-3-yl)(phenyl)methanone -**3i**



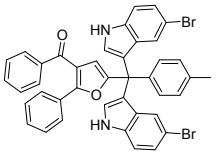
^{1}H NMR : 400 MHz $CDCl_3$
ChemicalFormula: $C_{41}H_{28}Br_2N_2O_2$
Exact Mass: 740.4

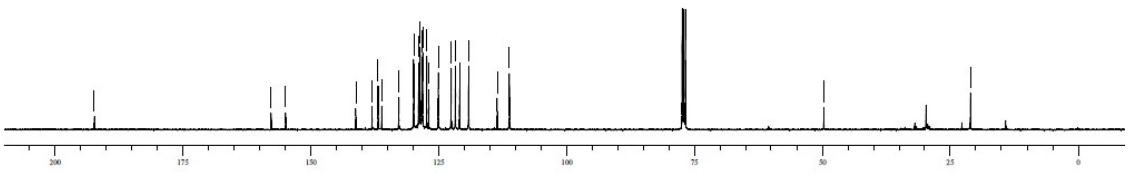




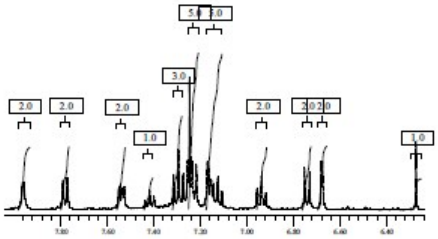


^{13}C NMR : 100 MHz $CDCl_3$
ChemicalFormula: $C_{41}H_{28}Br_2N_2O_2$
Exact Mass: 740.4

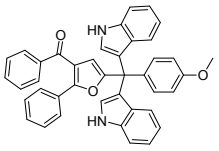


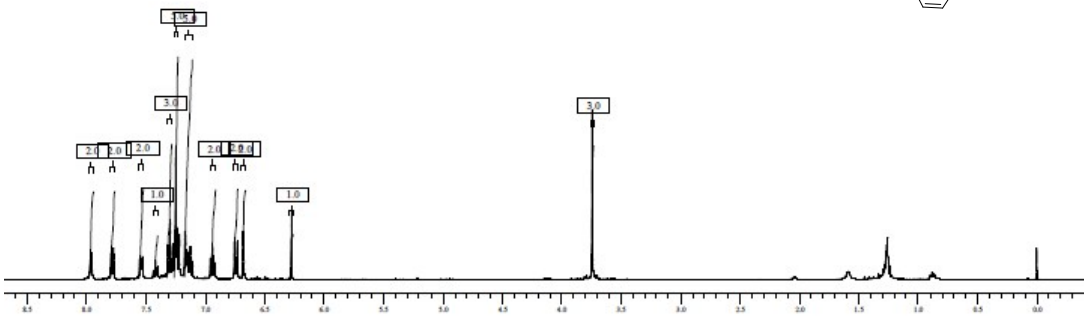


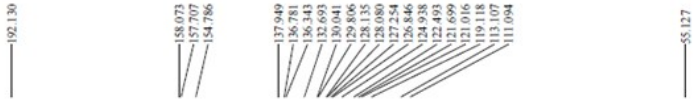
(5-(Di(*1H*-indol-3-yl)(4-methoxyphenyl)methyl)-2-phenylfuran-3-yl)(phenyl)methanone-**3j**



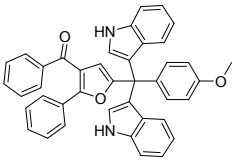
^{1}H NMR : 400 MHz $CDCl_3$
ChemicalFormula:$C_{41}H_{30}N_2O_3$
Exact Mass: 598.6

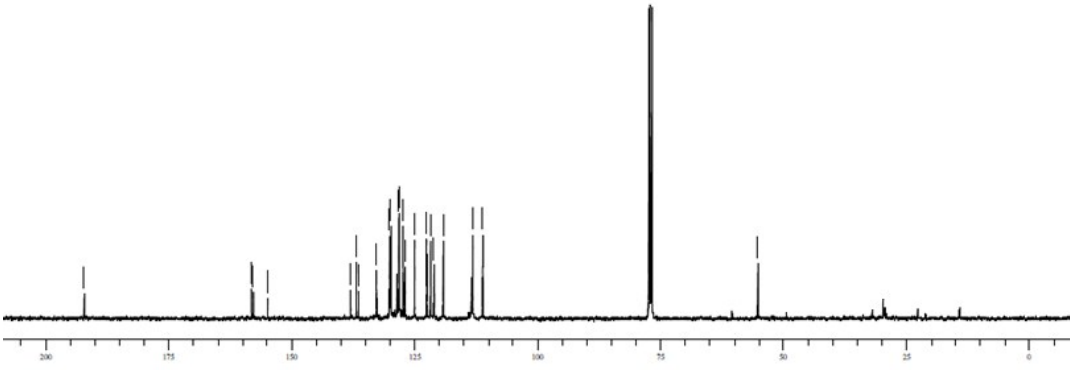




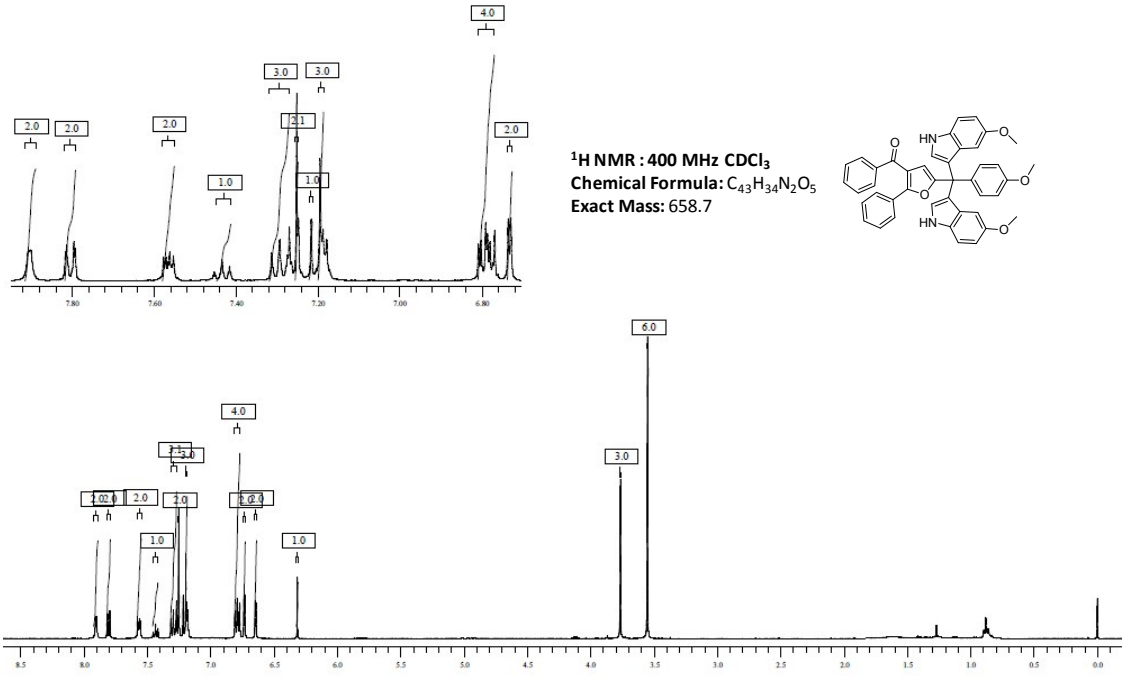


^{13}C NMR : 100 MHz $CDCl_3$
ChemicalFormula:$C_{41}H_{30}N_2O_3$
Exact Mass: 598.6

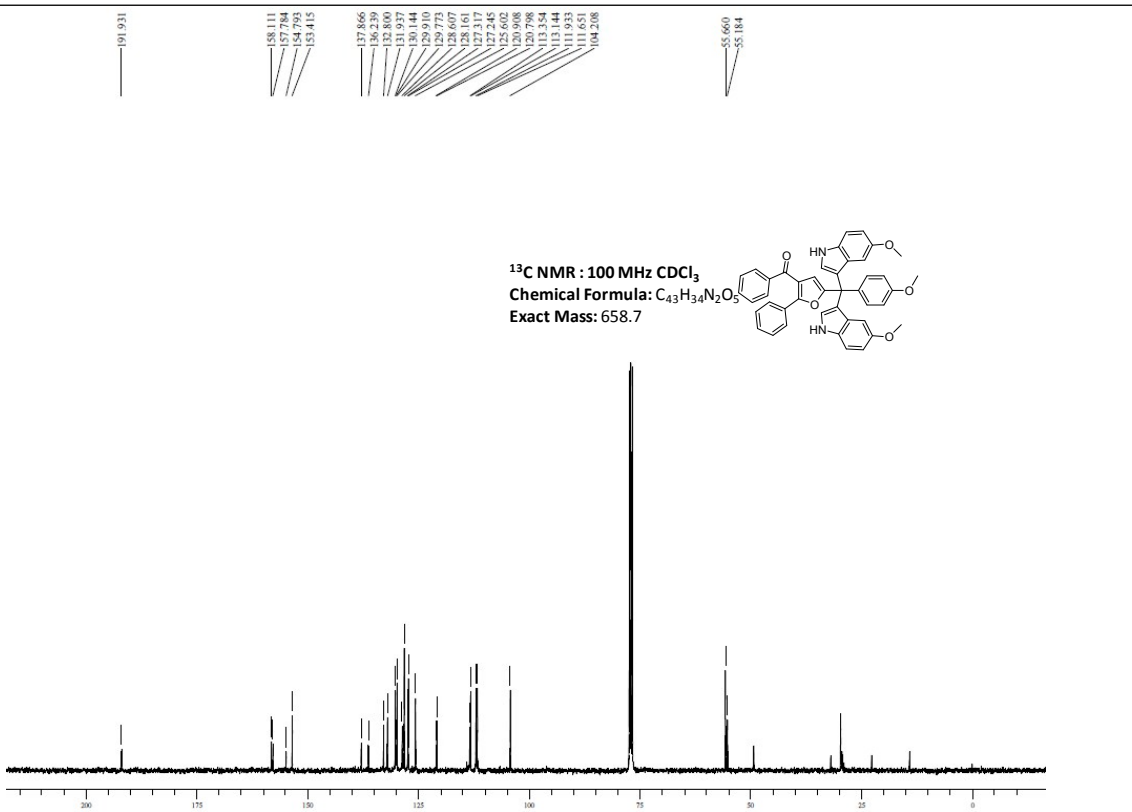




(5-(Bis(5-methoxy-*1H*-indol-3-yl)(4-methoxyphenyl)methyl)-2-phenylfuran-3-yl)(phenyl)methanone -**3k**

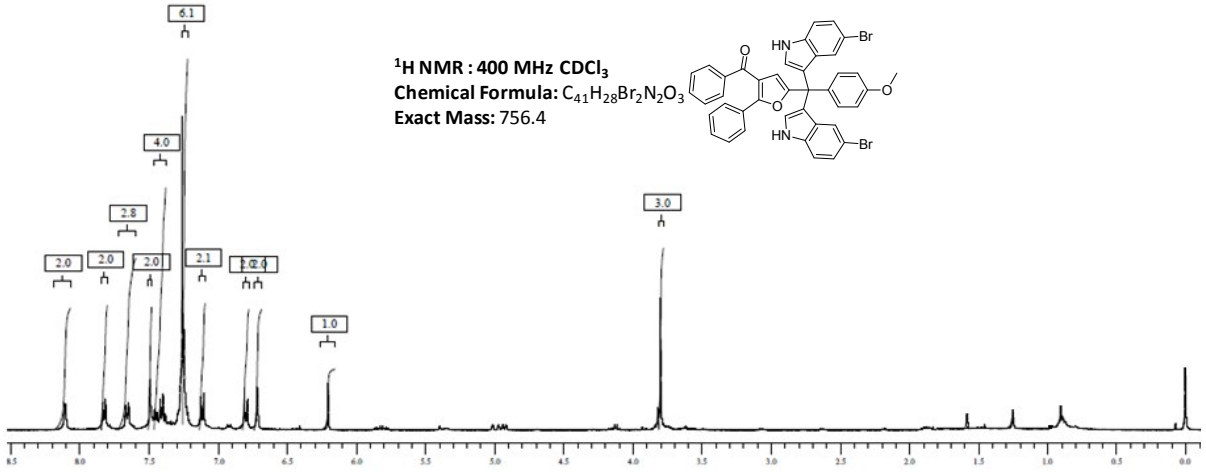


^{1}H NMR : 400 MHz $CDCl_3$
Chemical Formula: $C_{43}H_{34}N_2O_5$
Exact Mass: 658.7



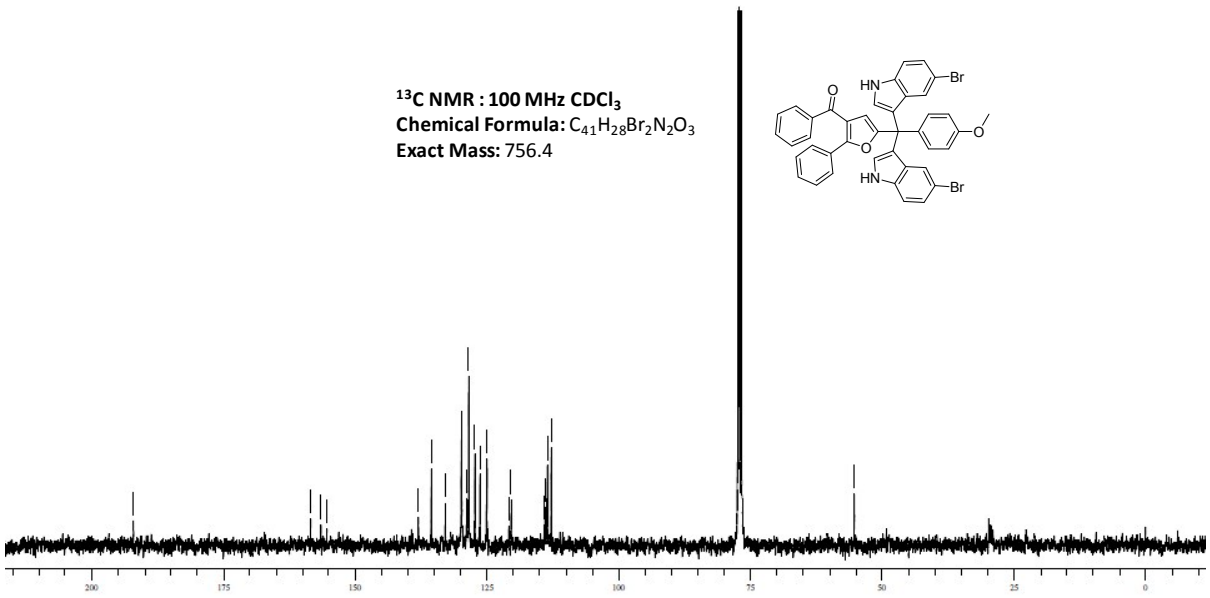
^{13}C NMR : 100 MHz $CDCl_3$
Chemical Formula: $C_{43}H_{34}N_2O_5$
Exact Mass: 658.7

(5-(Bis(5-bromo-*1H*-indol-3-yl)(4-methoxyphenyl)methyl)-2-phenylfuran-3-yl)(phenyl)methanone -**3l**

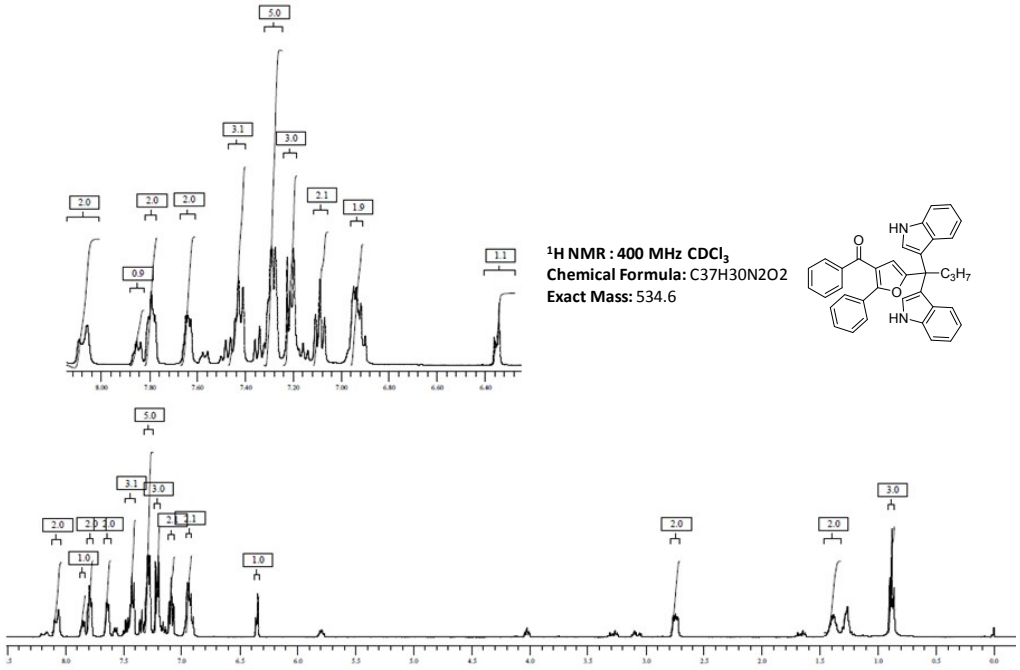


^{1}H NMR : 400 MHz $CDCl_3$
Chemical Formula: $C_{41}H_{28}Br_2N_2O_3$
Exact Mass: 756.4

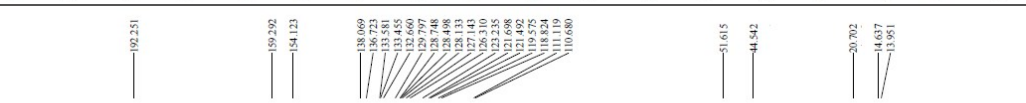
^{13}C NMR : 100 MHz $CDCl_3$
Chemical Formula: $C_{41}H_{28}Br_2N_2O_3$
Exact Mass: 756.4



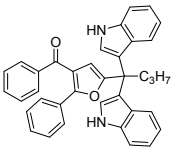
(5-(1,1-Di(*1H*-indol-3-yl)butyl)-2-phenylfuran-3-yl)(phenyl)methanone -**3m**

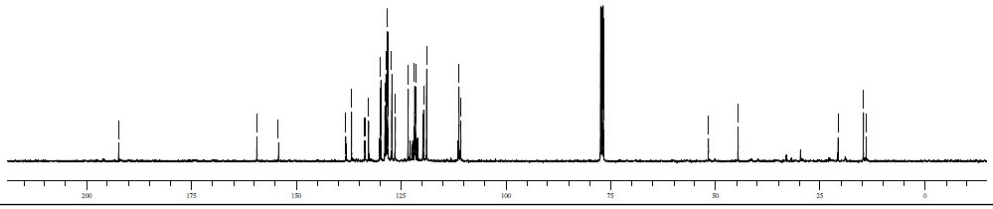


^{1}H NMR : 400 MHz $CDCl_3$
Chemical Formula: C37H30N2O2
Exact Mass: 534.6

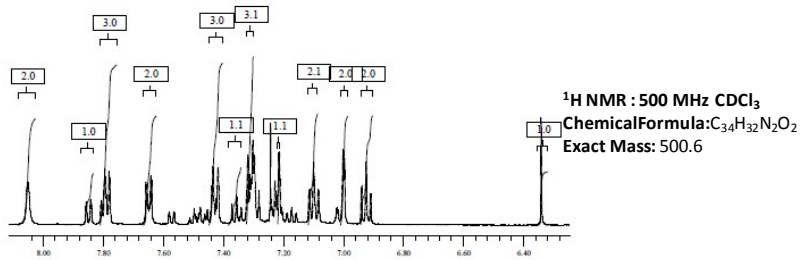


^{13}C NMR : 100 MHz $CDCl_3$
Chemical Formula: C37H30N2O2
Exact Mass: 534.6

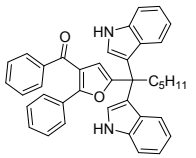


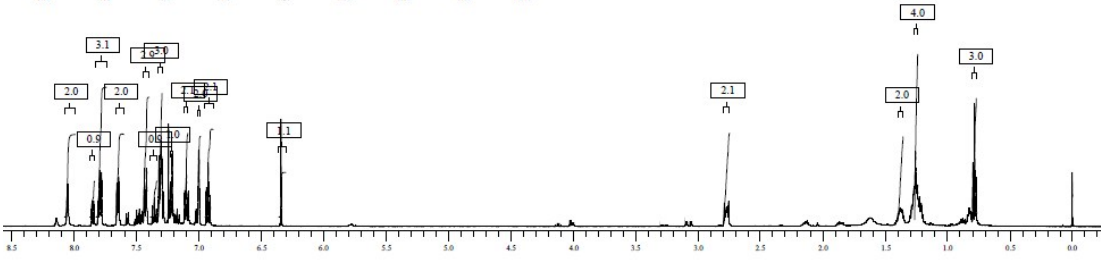


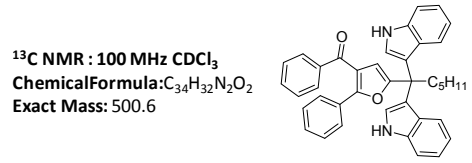
(5-(1,1-Di(*1H*-indol-3-yl)hexyl)-2-phenylfuran-3-yl)(phenyl)methanone-**3n**



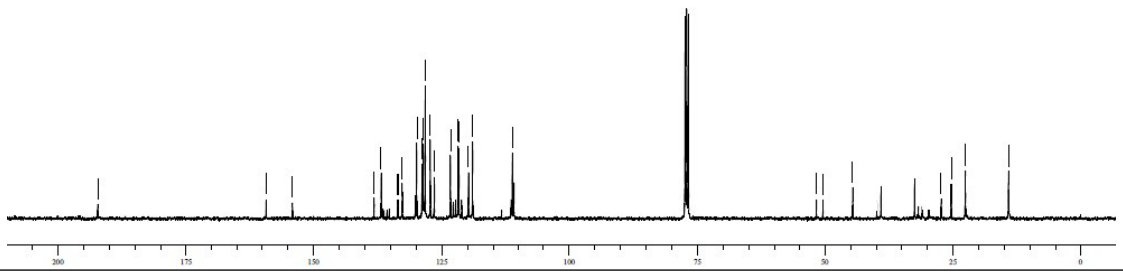
^{1}H NMR : 500 MHz $CDCl_3$
ChemicalFormula: $C_{34}H_{32}N_2O_2$
Exact Mass: 500.6



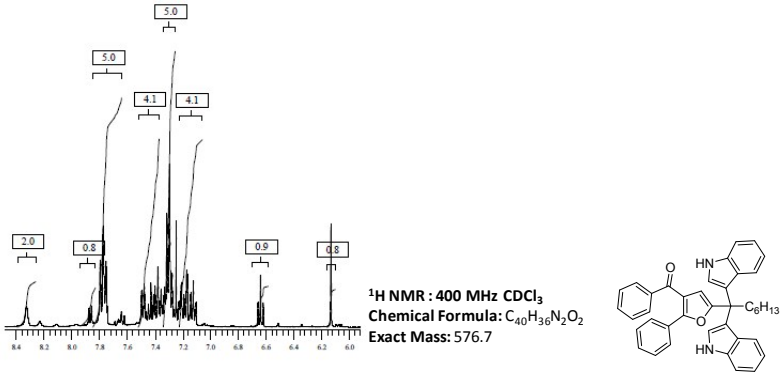




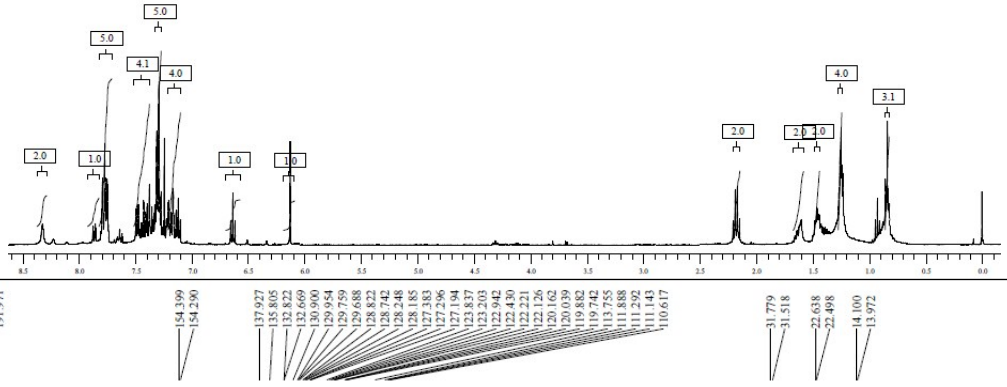
^{13}C NMR : 100 MHz $CDCl_3$
ChemicalFormula: $C_{34}H_{32}N_2O_2$
Exact Mass: 500.6



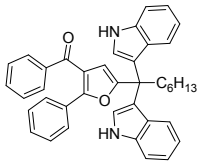
(5-(1,1-Di(*1H*-indol-3-yl)heptyl)-2-phenylfuran-3-yl)(phenyl)methanone -**3o**

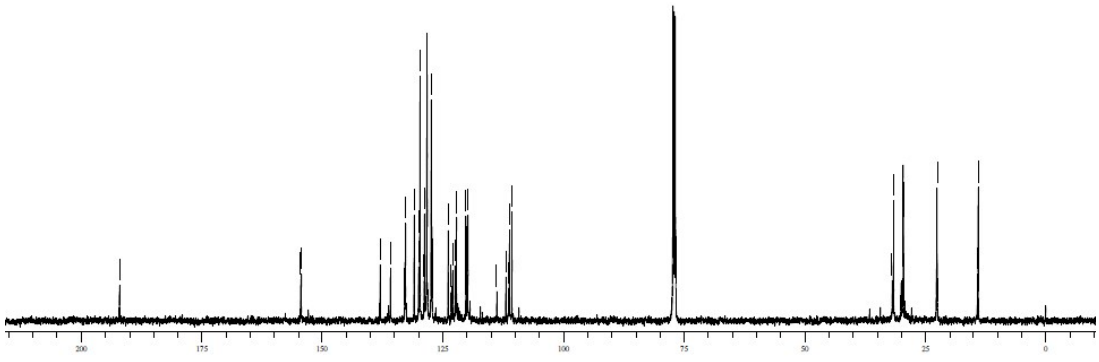


^{1}H NMR : 400 MHz $CDCl_3$
Chemical Formula: $C_{40}H_{36}N_2O_2$
Exact Mass: 576.7

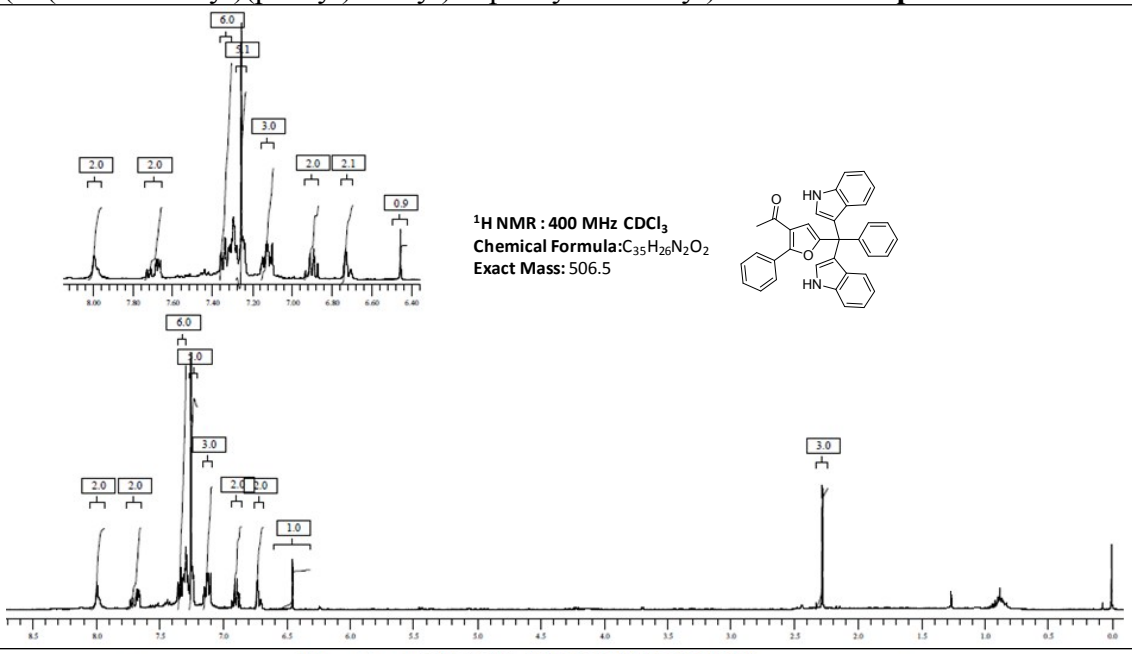


^{13}C NMR : 125 MHz $CDCl_3$
Chemical Formula: $C_{40}H_{36}N_2O_2$
Exact Mass: 576.7

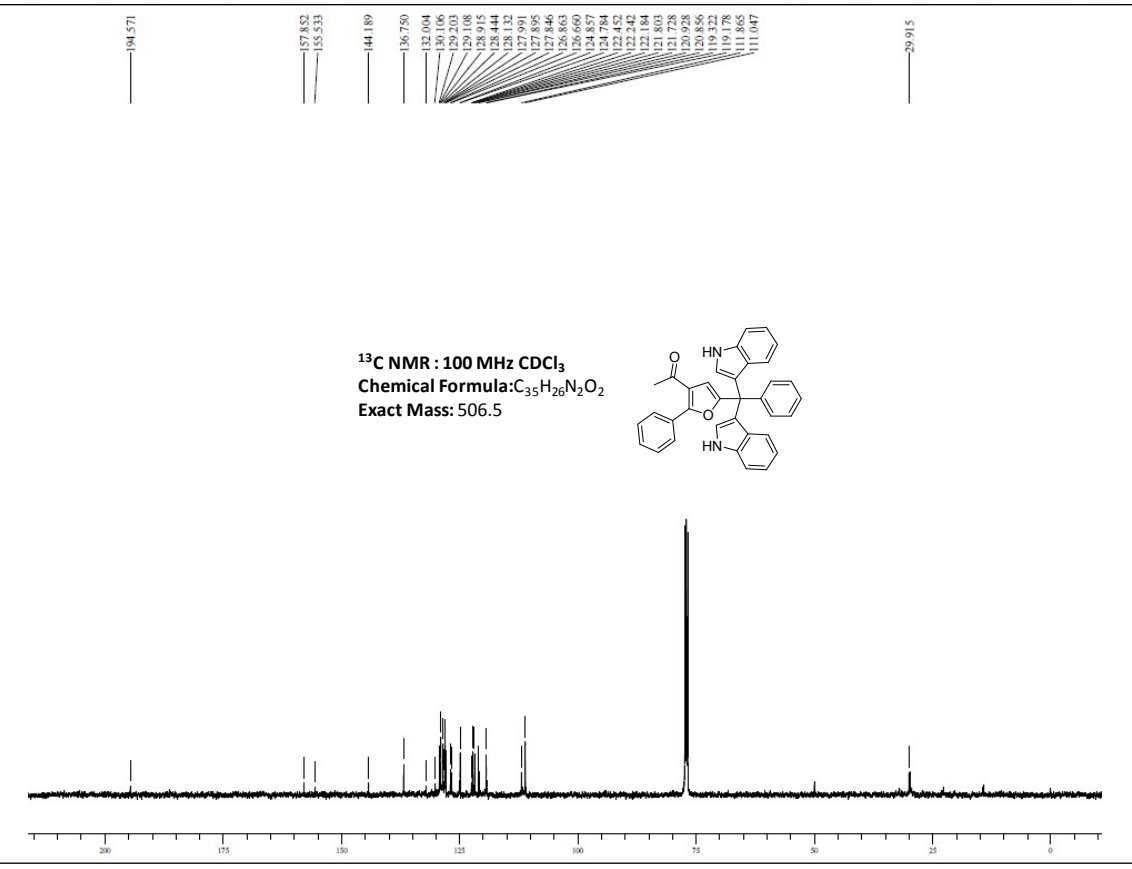




1-(5-(Di(*1H*-indol-3-yl)(phenyl)methyl)-2-phenylfuran-3-yl)ethan-1-one-**3p**

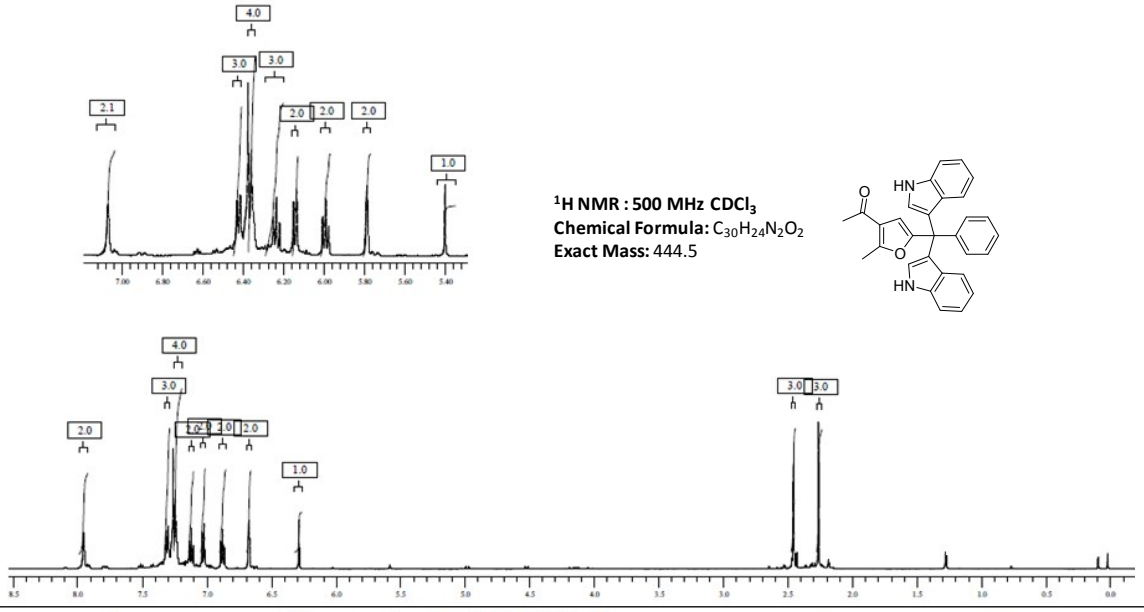


^{1}H NMR : 400 MHz $CDCl_3$
Chemical Formula: $C_{35}H_{26}N_2O_2$
Exact Mass: 506.5

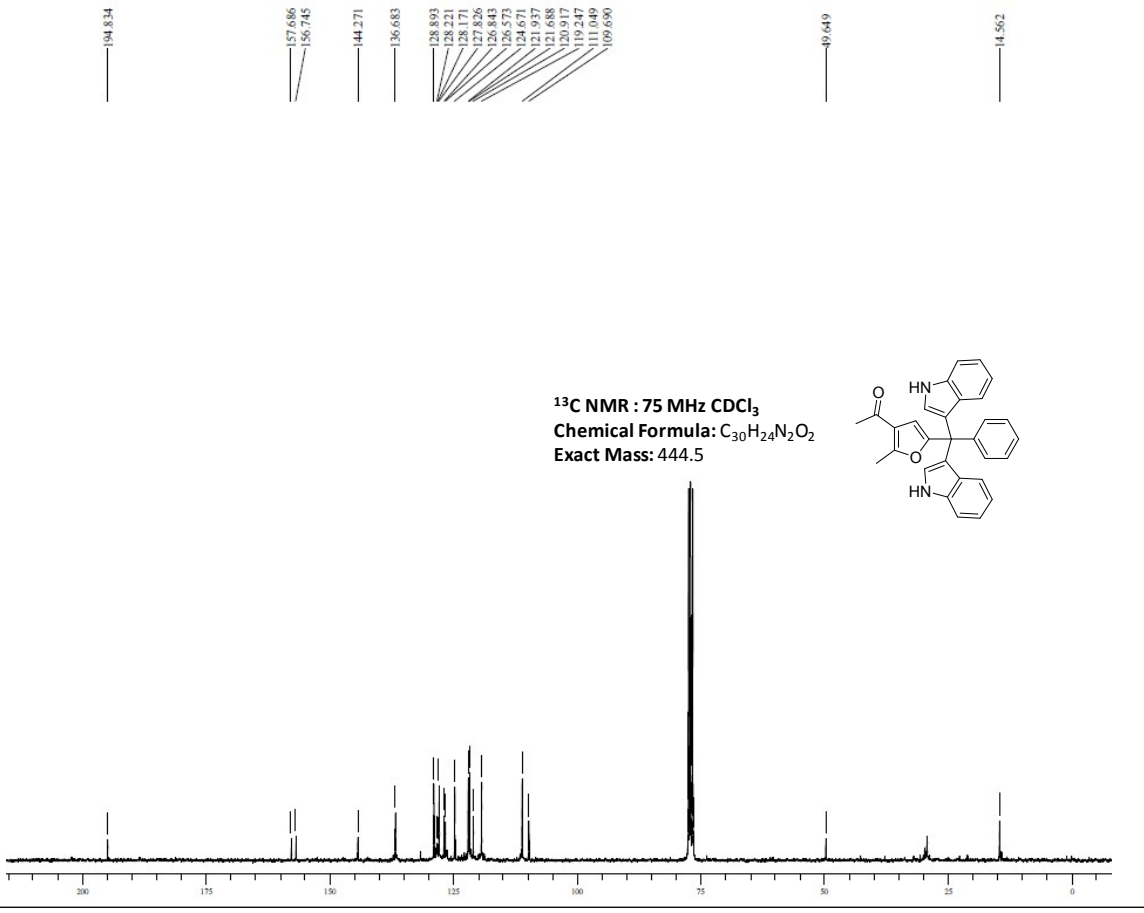


^{13}C NMR : 100 MHz $CDCl_3$
Chemical Formula: $C_{35}H_{26}N_2O_2$
Exact Mass: 506.5

1-(5-(Di(*1H*-indol-3-yl)(phenyl)methyl)-2-methylfuran-3-yl)ethanone-**3q**

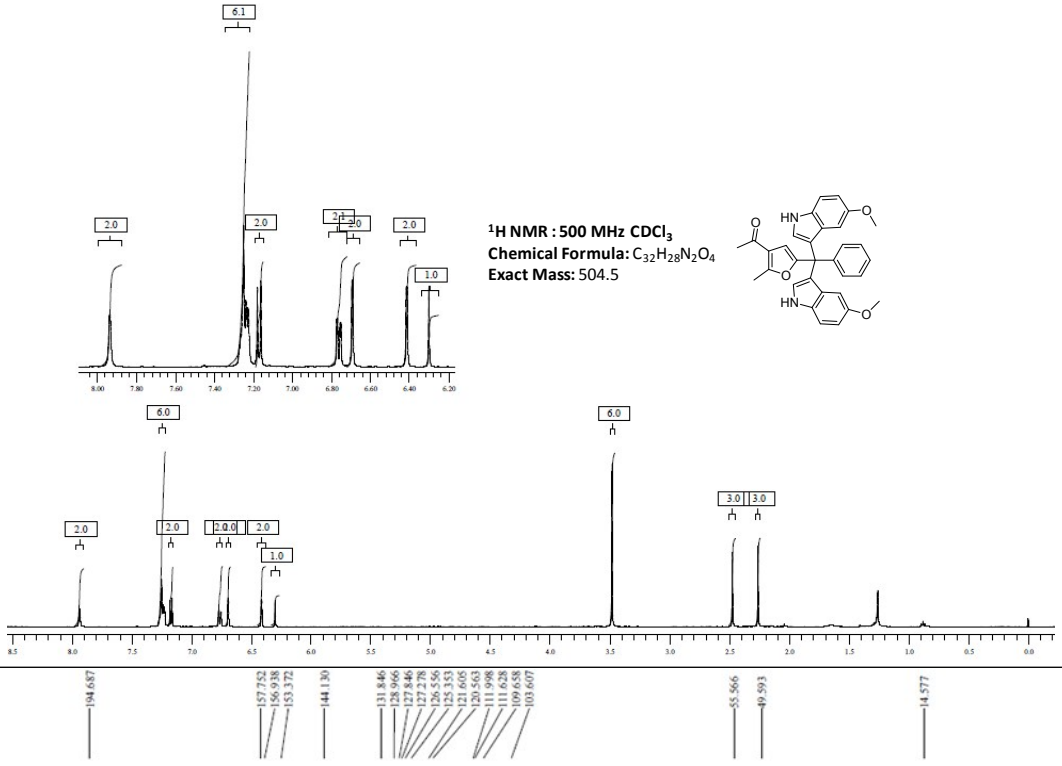


^{1}H NMR : 500 MHz $CDCl_3$
Chemical Formula: $C_{30}H_{24}N_2O_2$
Exact Mass: 444.5



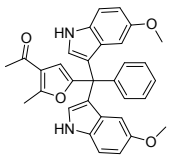
^{13}C NMR : 75 MHz $CDCl_3$
Chemical Formula: $C_{30}H_{24}N_2O_2$
Exact Mass: 444.5

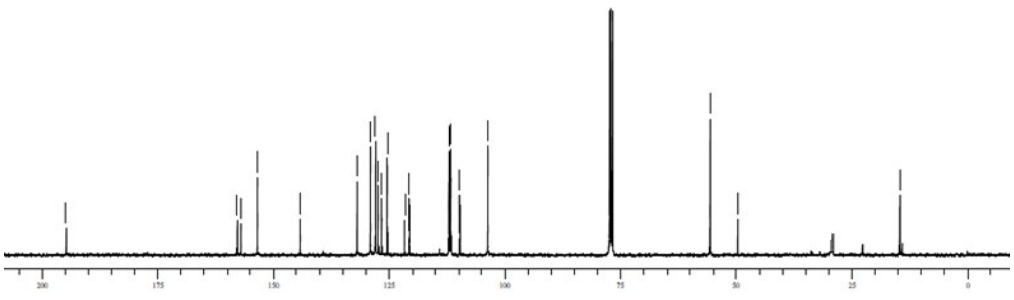
1-(5-(Bis(5-methoxy-*1H*-indol-3-yl)(phenyl)methyl)-2-methylfuran-3-yl)ethanone-**3r**



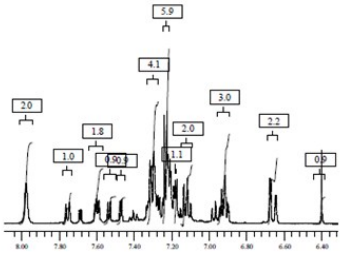
^{1}H NMR : 500 MHz $CDCl_3$
Chemical Formula: $C_{32}H_{28}N_2O_4$
Exact Mass: 504.5

^{13}C NMR : 100 MHz $CDCl_3$
Chemical Formula: $C_{32}H_{28}N_2O_4$
Exact Mass: 504.5

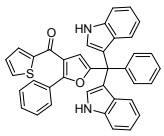


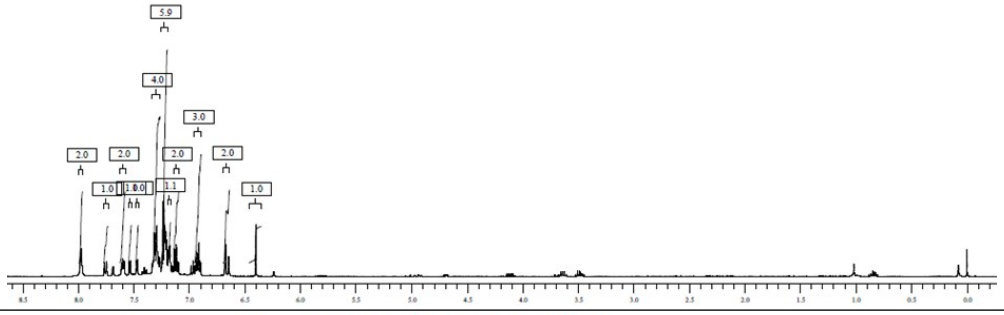


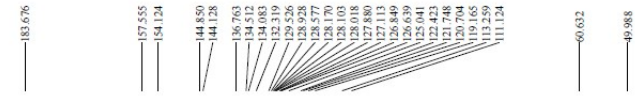
(5-(Di(*1H*-indol-3-yl)(phenyl)methyl)-2-phenylfuran-3-yl)(thiophen-2-yl)methanone -**3s**



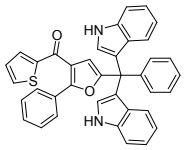
^{1}H NMR : 400 MHz $CDCl_3$
ChemicalFormula:$C_{38}H_{26}N_2O_2S$
Exact Mass: 574.6

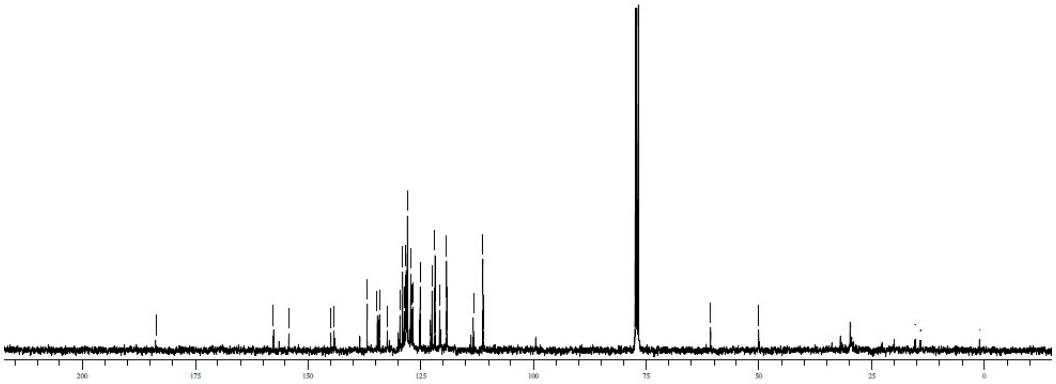




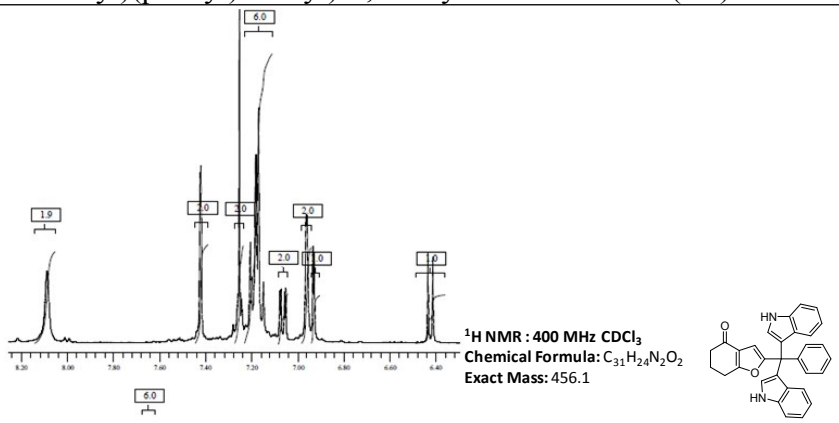


^{13}C NMR : 100 MHz $CDCl_3$
ChemicalFormula:$C_{38}H_{26}N_2O_2S$
Exact Mass: 574.6

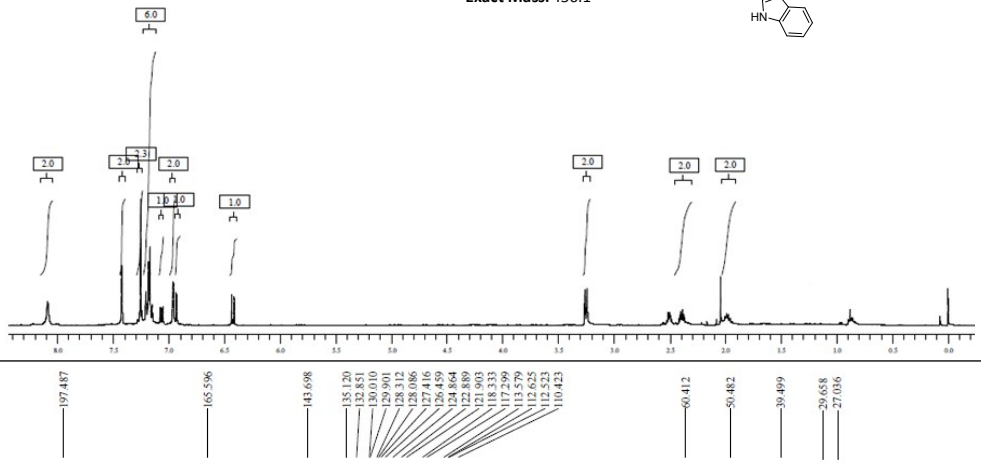




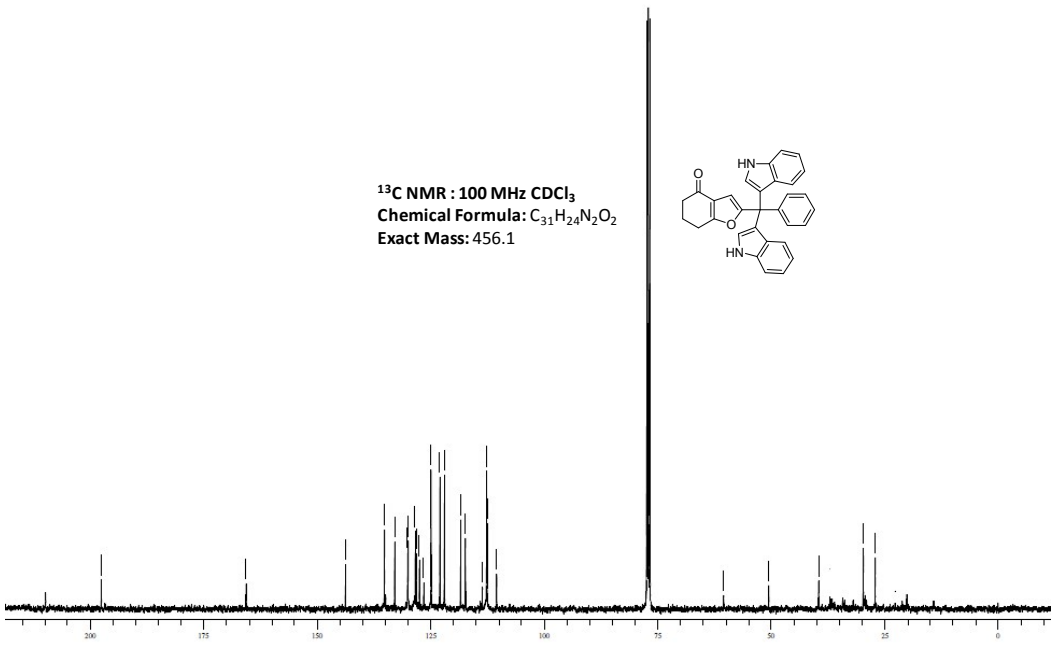
2-(Di(*1H*-indol-3-yl)(phenyl)methyl)-6,7-dihydrobenzofuran-4(5H)-one -**3t**



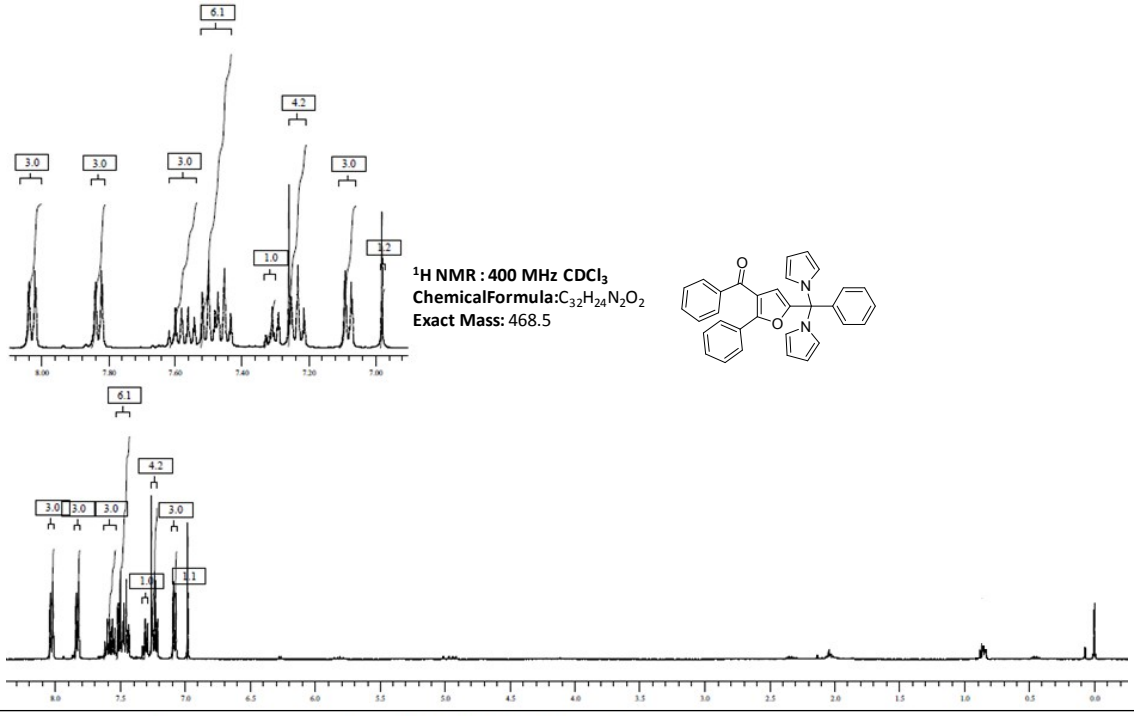
^{1}H NMR : 400 MHz $CDCl_3$
Chemical Formula: $C_{31}H_{24}N_2O_2$
Exact Mass: 456.1



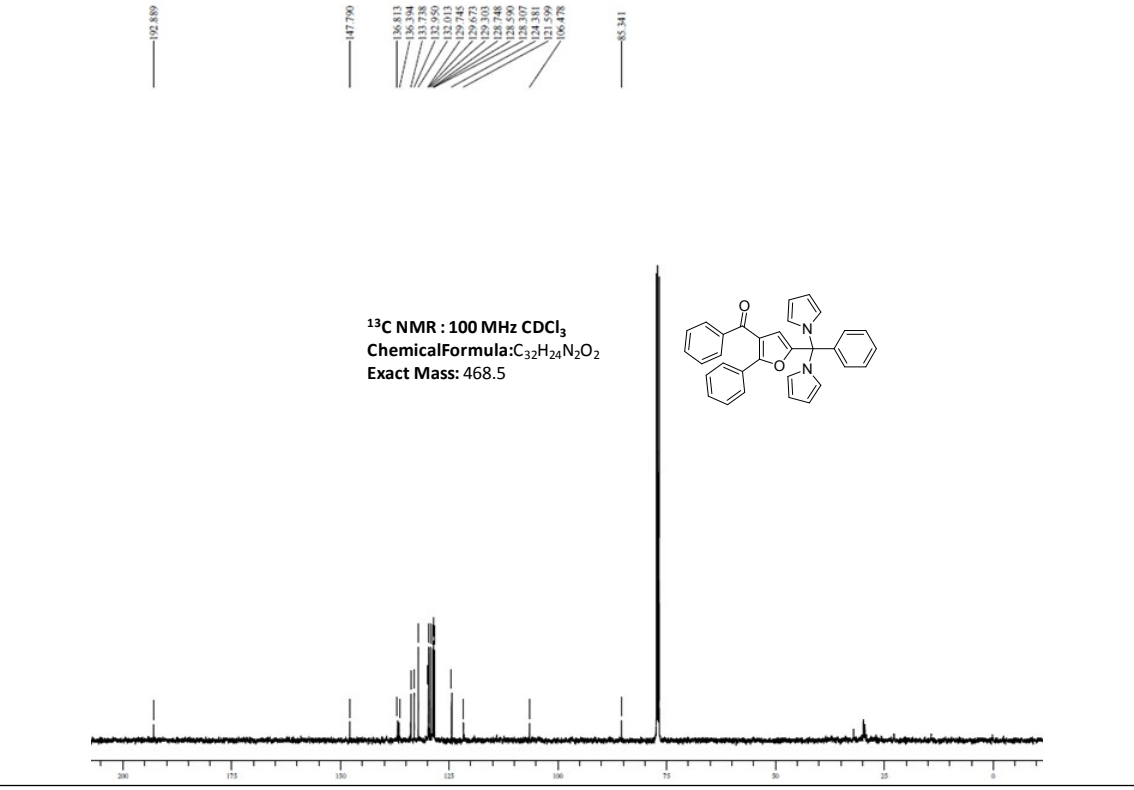
^{13}C NMR : 100 MHz $CDCl_3$
Chemical Formula: $C_{31}H_{24}N_2O_2$
Exact Mass: 456.1



Phenyl(2-phenyl-5-(phenyldi(*1H*-pyrrol-1-yl)methyl)furan-3-yl)methanone -**3u**

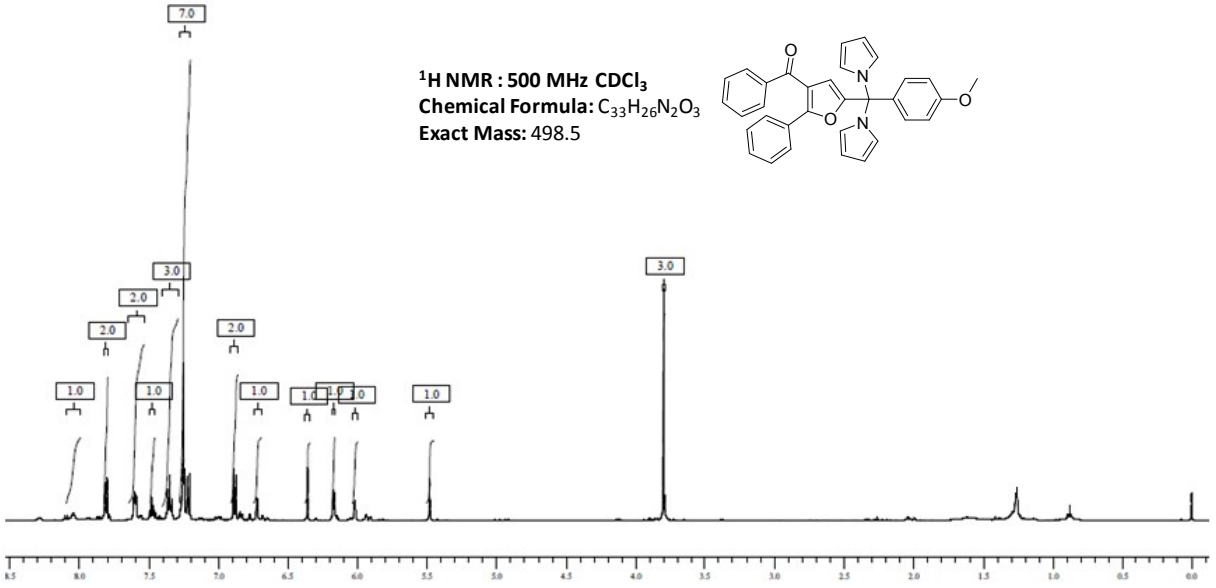


^{1}H NMR : 400 MHz $CDCl_3$
ChemicalFormula:$C_{32}H_{24}N_2O_2$
Exact Mass: 468.5

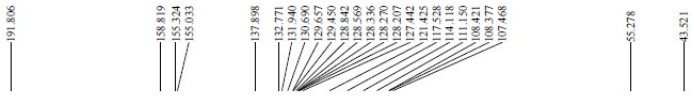


^{13}C NMR : 100 MHz $CDCl_3$
ChemicalFormula:$C_{32}H_{24}N_2O_2$
Exact Mass: 468.5

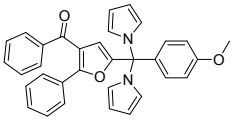
(5-((4-Methoxyphenyl)di(*1H*-pyrrol-1-yl)methyl)-2-phenylfuran-3-yl)(phenyl)methanone-**3v**

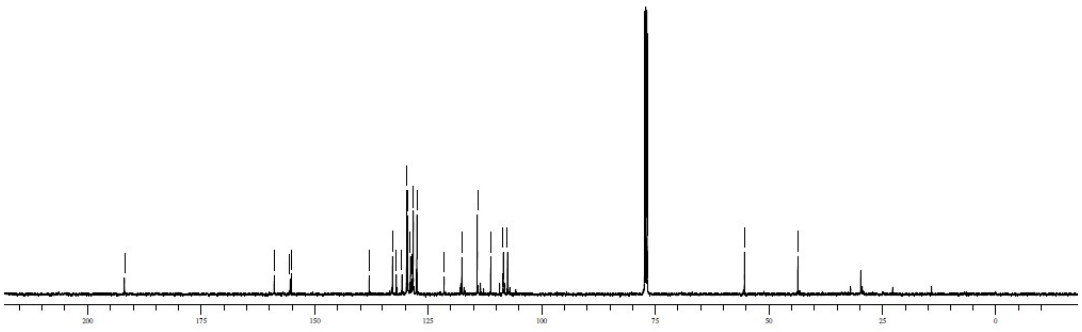


^{1}H NMR : 500 MHz $CDCl_3$
Chemical Formula: $C_{33}H_{26}N_2O_3$
Exact Mass: 498.5

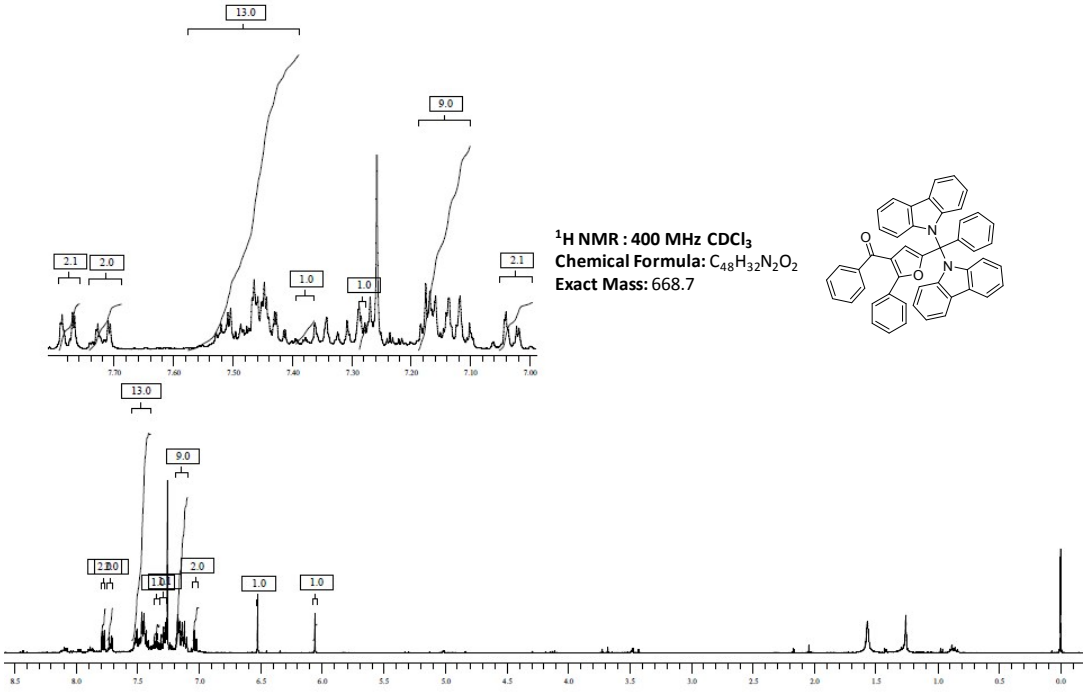


^{13}C NMR : 125 MHz $CDCl_3$
Chemical Formula: $C_{33}H_{26}N_2O_3$
Exact Mass: 498.5

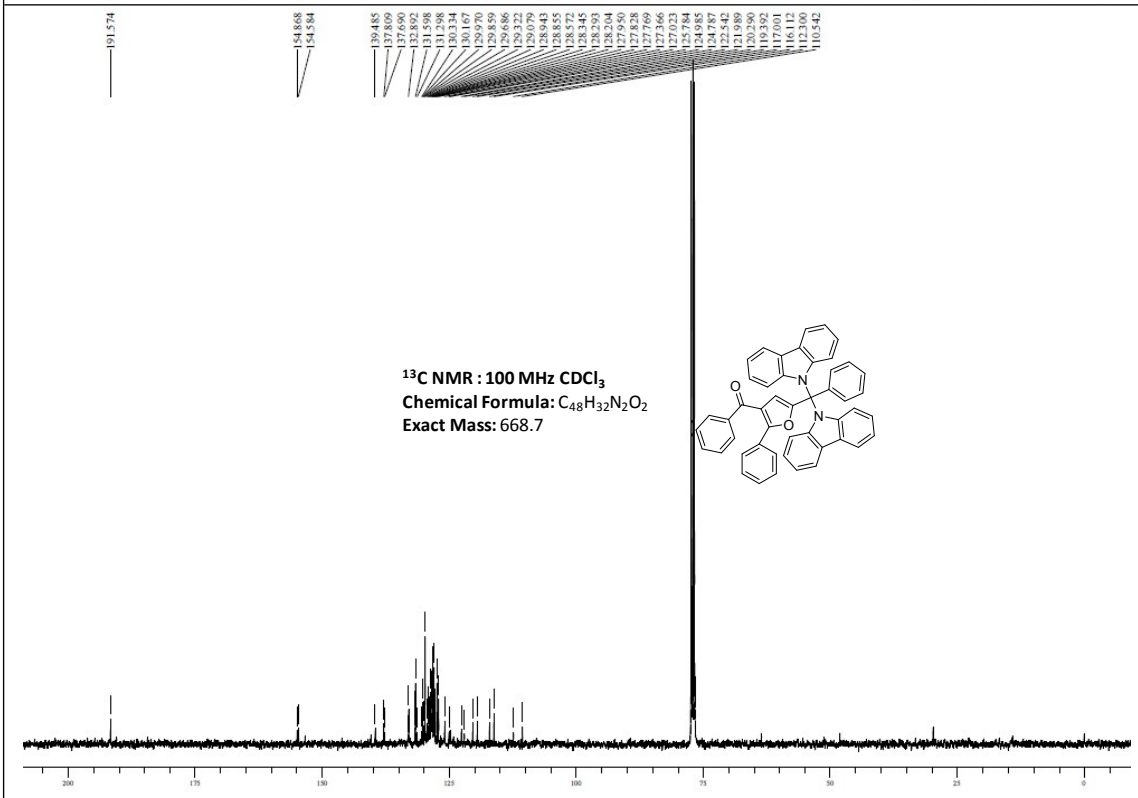




(5-(Di(*9H*-carbazol-9-yl)(phenyl)methyl)-2-phenylfuran-3-yl)(phenyl)methanone-**3w**



^{1}H NMR : 400 MHz $CDCl_3$
Chemical Formula: $C_{48}H_{32}N_2O_2$
Exact Mass: 668.7



^{13}C NMR : 100 MHz $CDCl_3$
Chemical Formula: $C_{48}H_{32}N_2O_2$
Exact Mass: 668.7

1.3 X-ray crystallography data of 3a

X-ray data for the compounds were collected at room temperature using a Bruker Smart Apex CCD diffractometer with graphite monochromatedMoKα radiation (λ=0.71073Å) with ω-scan method.[2] Preliminary lattice parameters and orientation matrices were obtained from four sets of frames. Integration and scaling of intensity data were accomplished using SAINT program [1]. The structure was solved by direct methods using SHELXS and refinement was carried out by full-matrix least-squares technique using SHELXL.[3] Anisotropic displacement parameters were included for all non-hydrogen atoms.The N-bound H atom was located in difference Fourier maps, and their positions and isotropic displacement parameters were refined. All C bound H atoms and O bound H atom were positioned geometrically and treated as riding on their parent C atoms [C-H = 0.93-0.97 Å, andU_{iso}(H) = 1.2U_{eq}(C)]. One of methanol label suffix B is partially disordered.

Crystal Data for BB84: $C_{41}H_{32}NO_3$ (*M* =586.67 g/mol): monoclinic, space group C2/c (no. 15), *a* = 42.209(4) Å, *b* = 10.8705(9) Å, *c* = 32.818(3) Å, *β* = 124.056(3)°, *V* = 12475.3(19) Å^3, *Z* = 16, *T* = 294.15 K, μ(MoKα) = 0.078 mm^{-1}, *Dcalc* = 1.249 g/cm^3, 71086 reflections measured (2.996° ≤ 2Θ ≤ 56.882°), 15149 unique (R_{int} = 0.0446, R_{sigma} = 0.0413) which were used in all calculations. The final R_1 was 0.0615 (I >2σ(I)) and wR_2 was 0.1735 (all data). CCDC1852196 contains supplementary Crystallographic data for the structure. These data can be obtained free of charge at www.ccdc.cam.ac.uk/conts/retrieving.html [or from the Cambridge Crystallographic Data Centre (CCDC), 12 Union Road, Cambridge CB2 1EZ, UK; fax: +44(0) 1223 336 033; email: deposit@ccdc.cam.ac.uk].

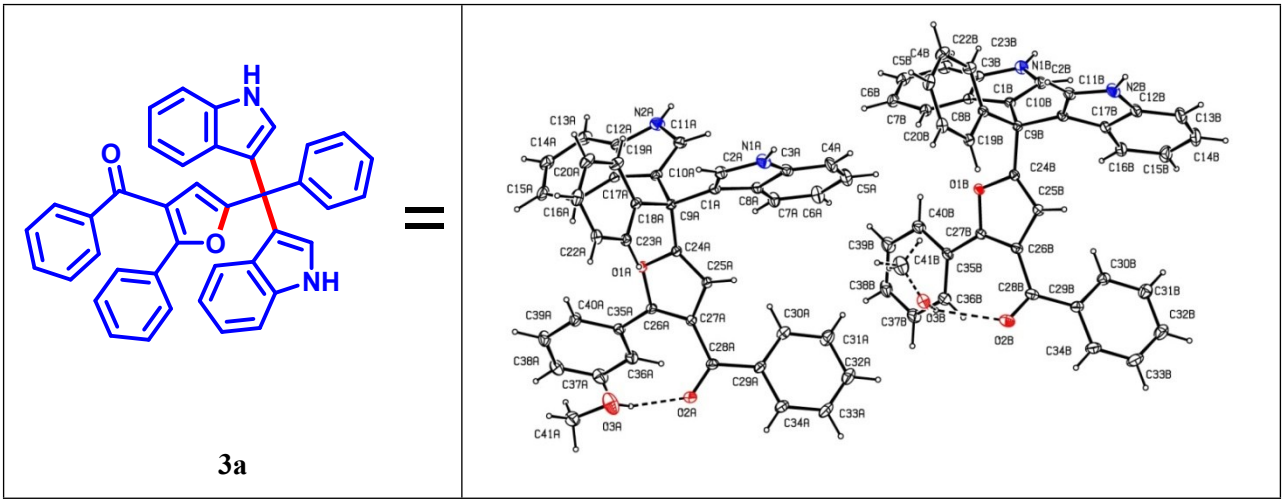


Fig.1 A view of BB84, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are represented by circles of arbitrary radii. Hydrogen bonds are shown as dashed lines. One of methanol label suffix B is partially disordered and shown as dashed bonds.

2. Bruker (2001). SAINT (Version 6.28a) & SMART (Version 5.625). Bruker AXS Inc., Madison, Wisconsin, USA.

3. Sheldrick G. M. (2015) Acta Crystallogr C71: 3-8.