Electronic Supplementary Information (ESI)

Discovery of Indolyl Acrylamide Derivatives as Human Diacylglycerol Acyltransferase-2 Selective Inhibitors

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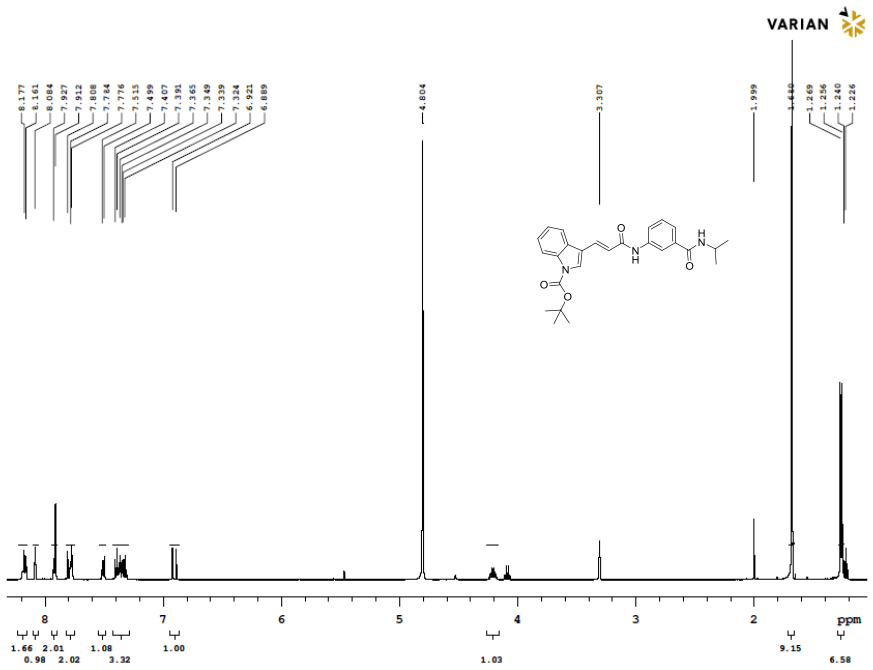
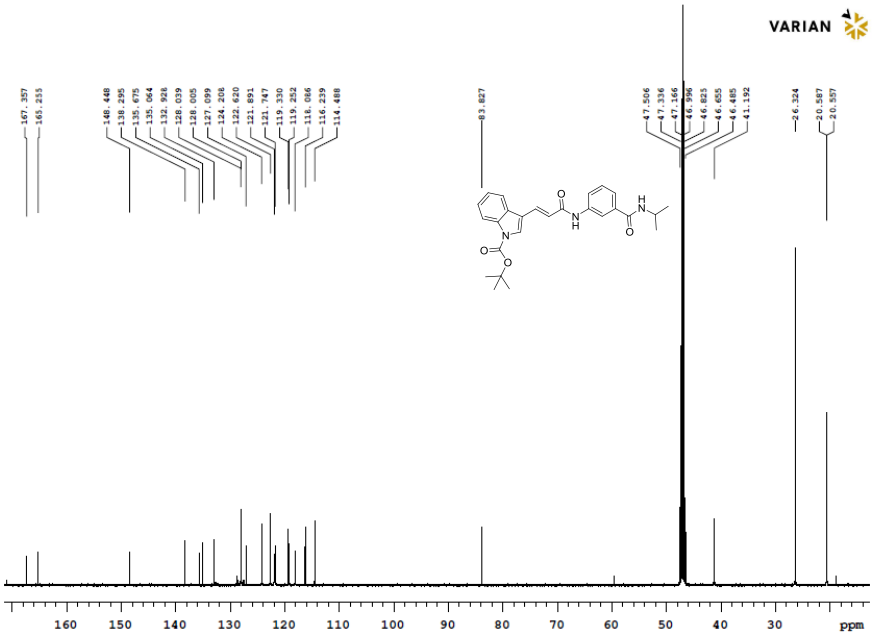
[d]College of Pharmacy, Korea University, Chungnam 339-700, Korea.
[e]College of Pharmacy, Chungnam National University, Daejeong 305-764, Korea.

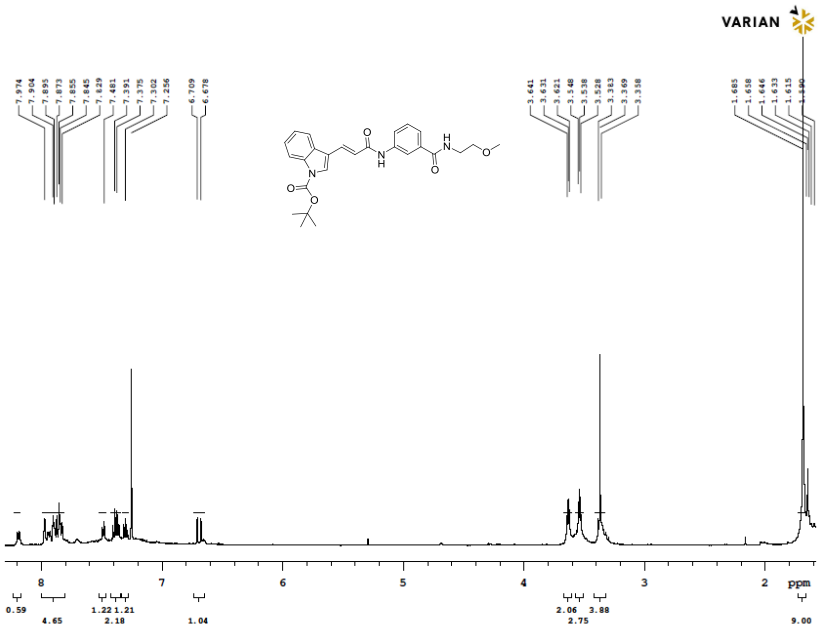
Copies of ^{1}H-NMR and ^{13}H-NMR spectra for compounds



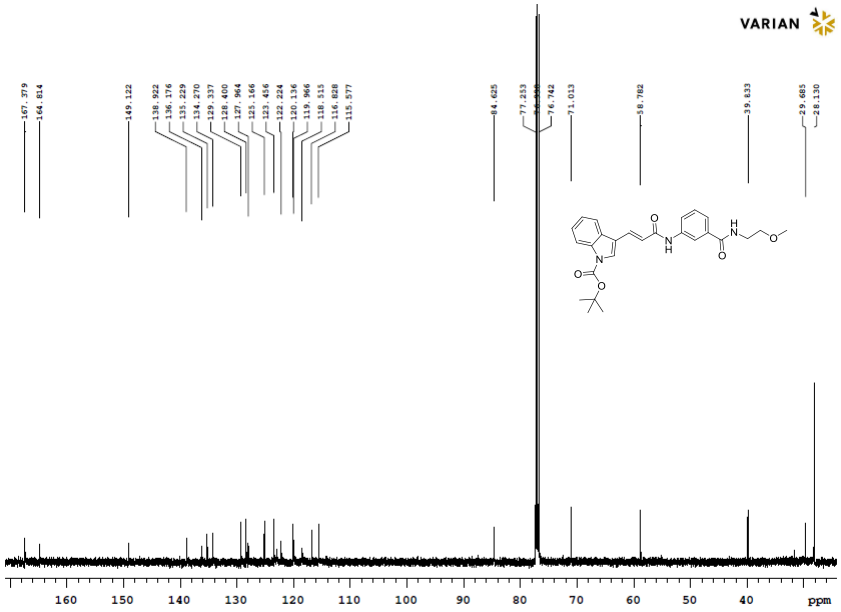
^{1}H-NMR (CD_3OD, 500 MHz):
(*E*)-*tert*-butyl-3-(3-(3-(isopropylcarbamoyl)phenylamino)-3-oxoprop-1-enyl)-1*H*-indole-1-carboxylate (**5a**)



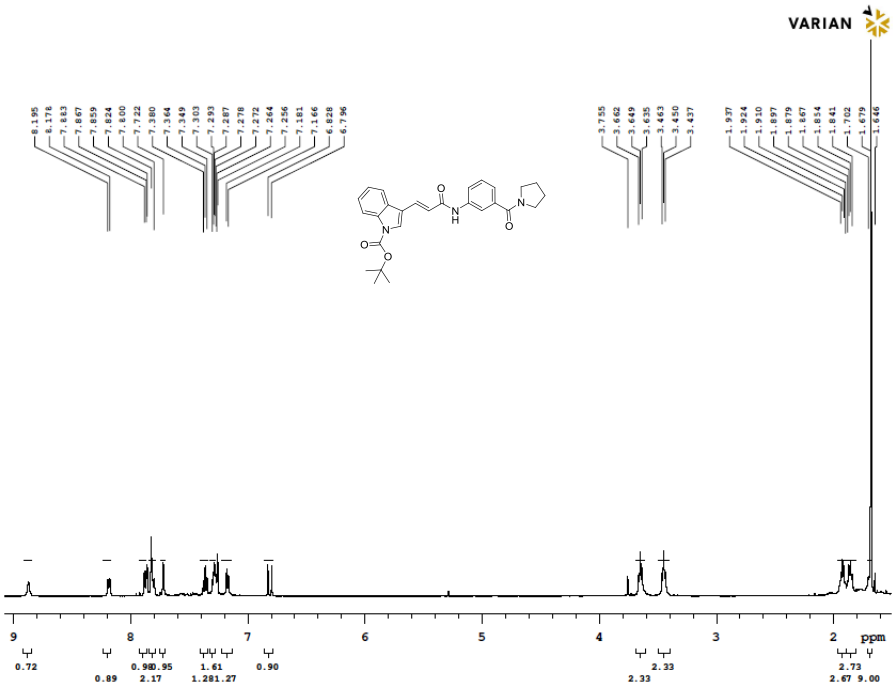
^{13}C-NMR (CD_3OD, 125 MHz):
(*E*)-*tert*-butyl-3-(3-(3-(isopropylcarbamoyl)phenylamino)-3-oxoprop-1-enyl)-1*H*-indole-1-carboxylate (**5a**)



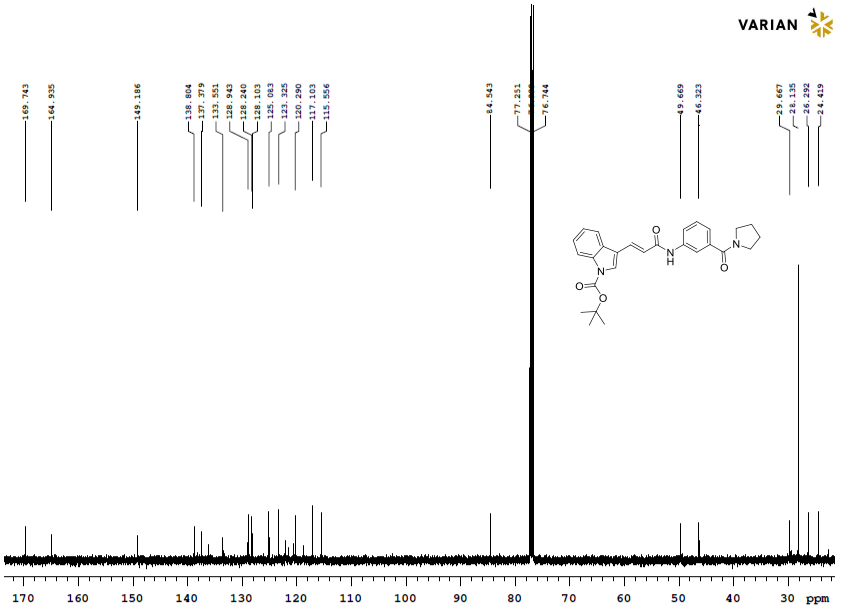
^{1}H-NMR ($CDCl_3$, 500 MHz):
(*E*)-*tert*-butyl-3-(3-(3-(2-methoxyethylcarbamoyl)phenyl amino)-3-oxoprop-1-enyl)-1*H*-indole-1-carboxylate
(**5b**)



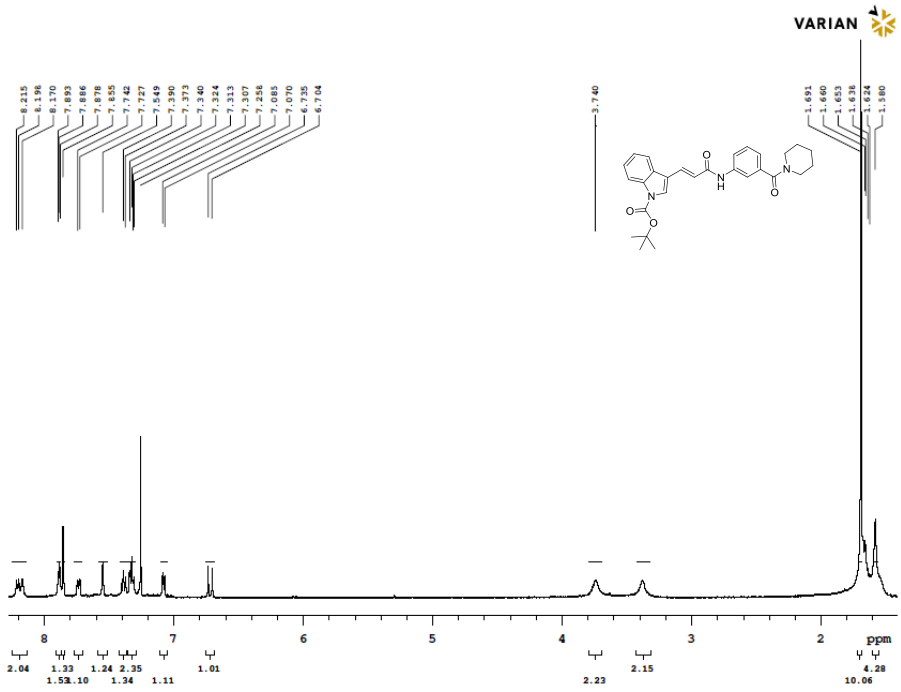
^{13}C-NMR ($CDCl_3$, 125 MHz):
(*E*)-*tert*-butyl-3-(3-(3-(2-methoxyethylcarbamoyl)phenyl amino)-3-oxoprop-1-enyl)-1*H*-indole-1-carboxylate
(**5b**)



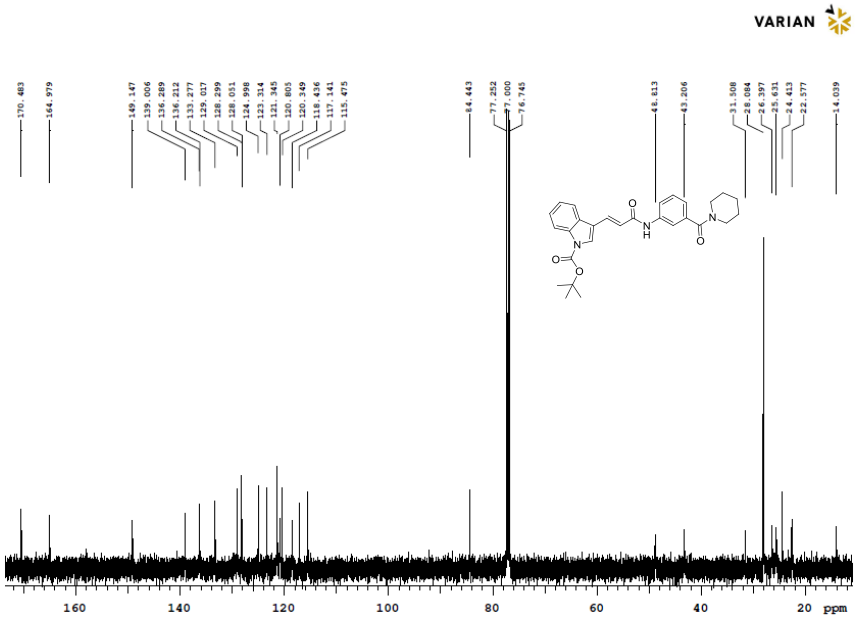
^{1}H-NMR ($CDCl_3$, 500 MHz):
(*E*)-*tert*-butyl-3-(3-oxo-3-(3-(pyrrolidine-1-carbonyl) phenylamino)prop-1-enyl)-1*H*-indole-1-carboxylate (**5c**)



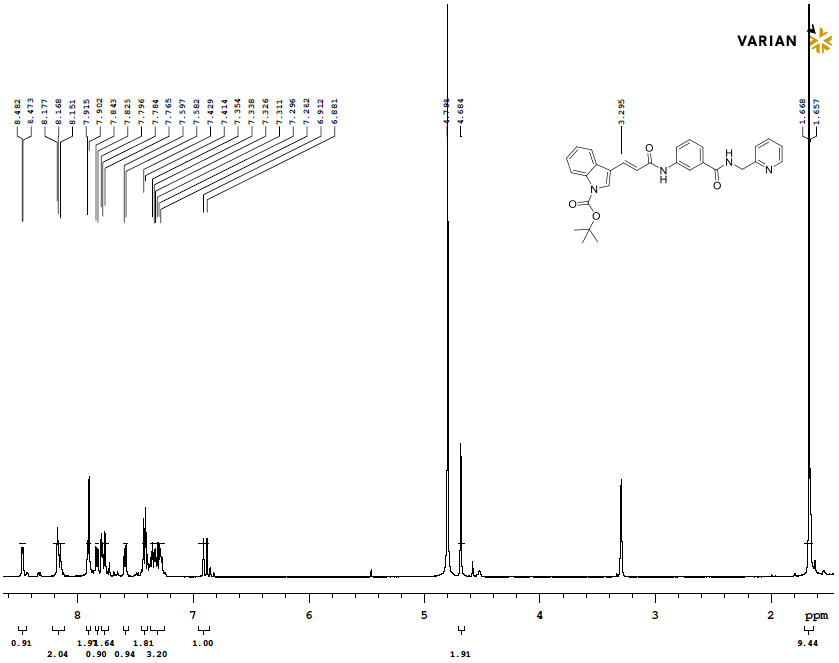
^{13}C-NMR ($CDCl_3$, 125 MHz):
(*E*)-*tert*-butyl-3-(3-oxo-3-(3-(pyrrolidine-1-carbonyl) phenylamino)prop-1-enyl)-1*H*-indole-1-carboxylate (**5c**)



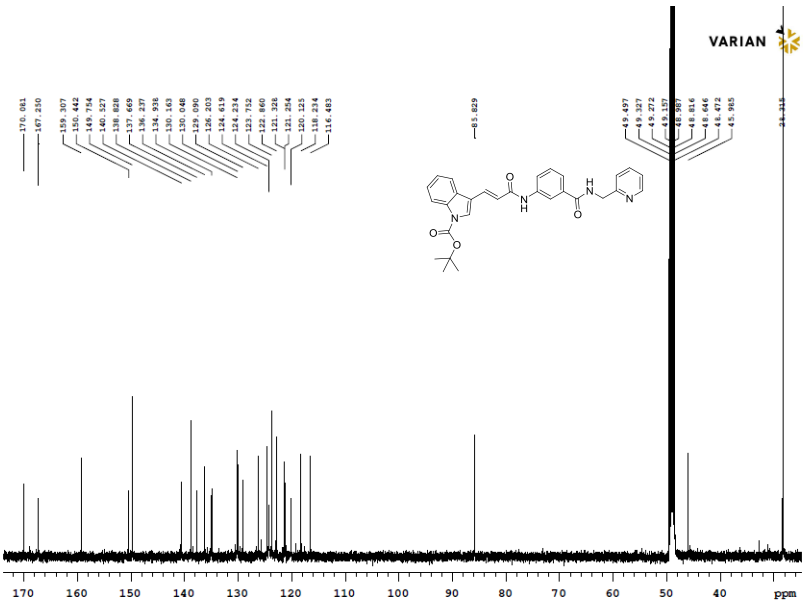
^{1}H-NMR ($CDCl_3$, 500 MHz):
(*E*)-*tert*-butyl-3-(3-oxo-3-(3-(piperidine-1-carbonyl)phenyl amino)prop-1-enyl)-1*H*-indole-1-carboxylate (**5d**)



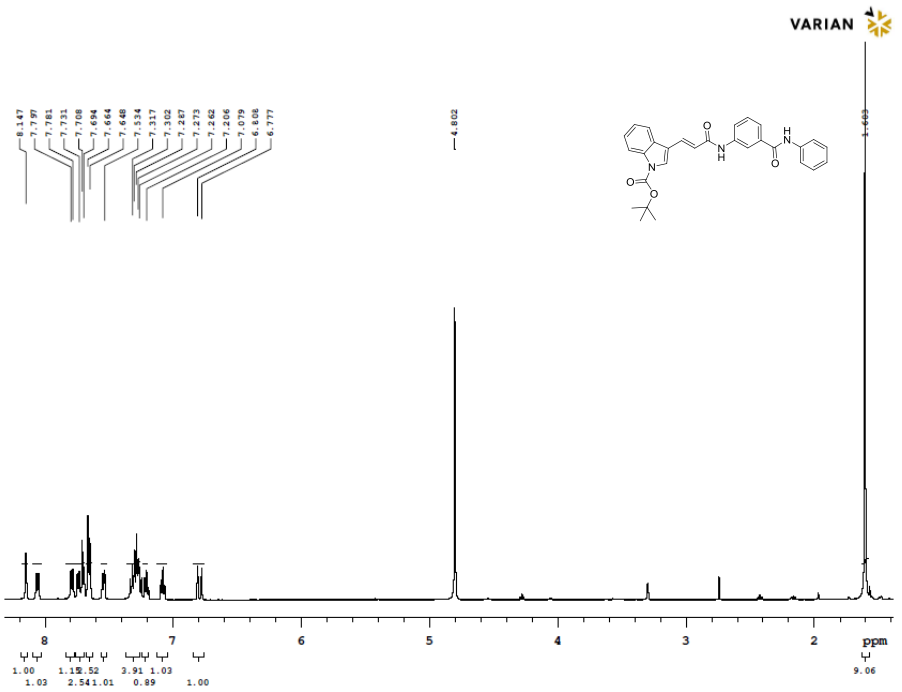
^{13}C-NMR ($CDCl_3$, 125 MHz):
(*E*)-*tert*-butyl-3-(3-oxo-3-(3-(piperidine-1-carbonyl)phenyl amino)prop-1-enyl)-1*H*-indole-1-carboxylate (**5d**)



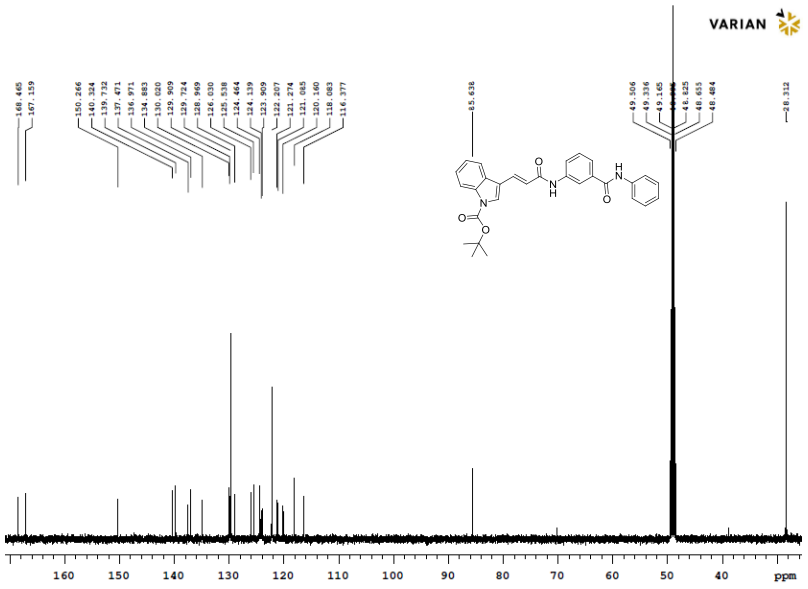
^{1}H-NMR (CD_3OD, 500 MHz):
(*E*)-*tert*-butyl-3-(3-oxo-3-(3-(pyridin-2-ylmethylcarbamoyl) phenylamino)prop-1-enyl)-1*H*-indole-1-carboxylate
(**5e**)



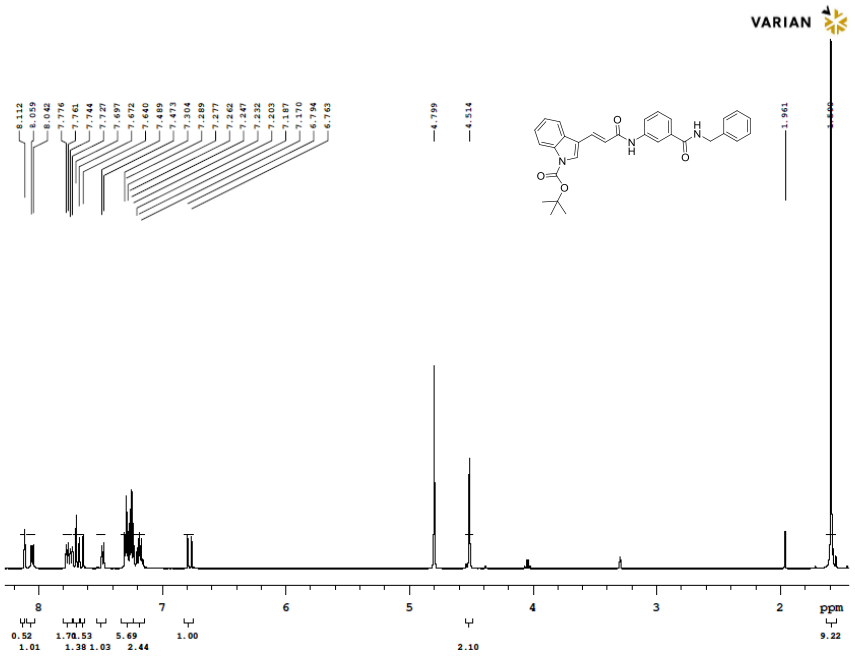
^{1}H-NMR (CD_3OD, 500 MHz):
(*E*)-*tert*-butyl-3-(3-oxo-3-(3-(pyridin-2-ylmethylcarbamoyl) phenylamino)prop-1-enyl)-1*H*-indole-1-carboxylate
(**5e**)



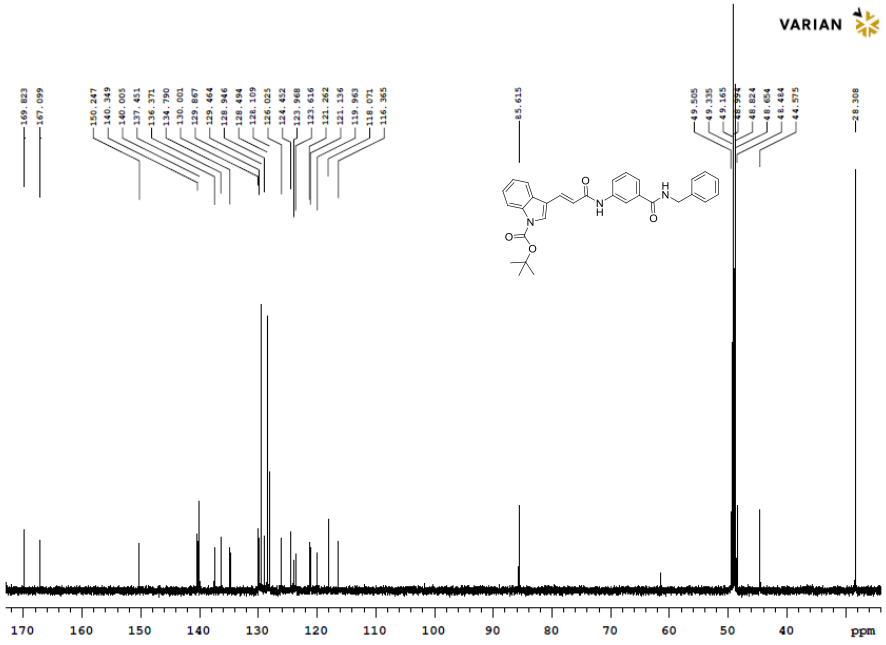
^{1}H-NMR (CD_3OD, 500 MHz):
(*E*)-*tert*-butyl-3-(3-oxo-3-(3-(phenylcarbamoyl)phenylamino) prop-1-enyl)-1*H*-indole-1-carboxylate (**5f**)



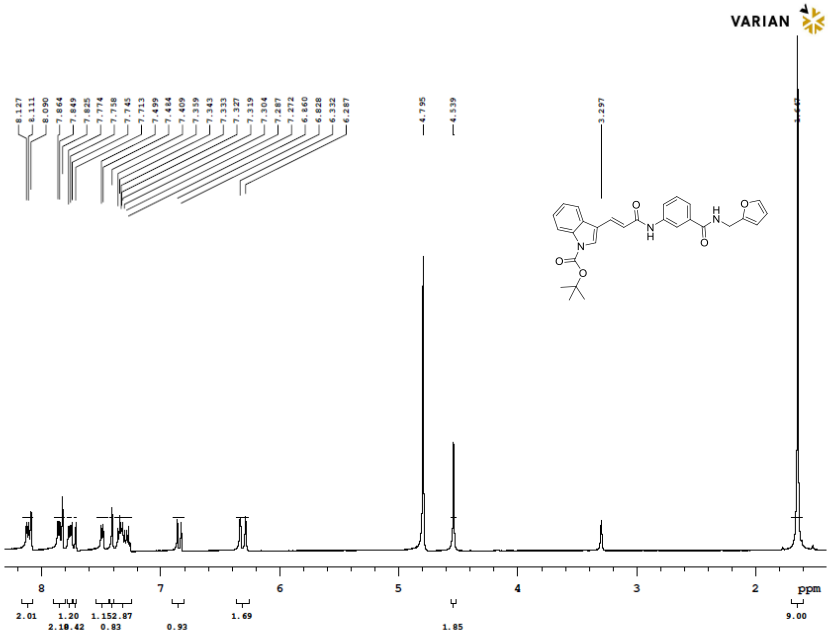
^{13}C-NMR (CD_3OD, 125 MHz):
(*E*)-*tert*-butyl-3-(3-oxo-3-(3-(phenylcarbamoyl)phenylamino) prop-1-enyl)-1*H*-indole-1-carboxylate (**5f**)



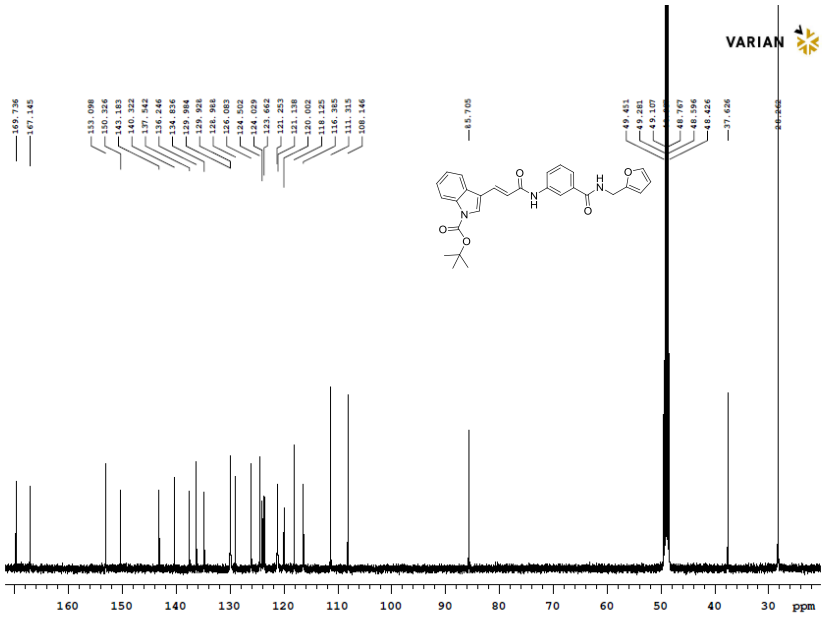
^{1}H-NMR (CD_3OD, 500 MHz):
(*E*)-*tert*-butyl-3-(3-(3-(benzylcarbamoyl)phenylamino)-3-oxoprop-1-enyl)-1*H*-indole-1-carboxylate (**5g**)



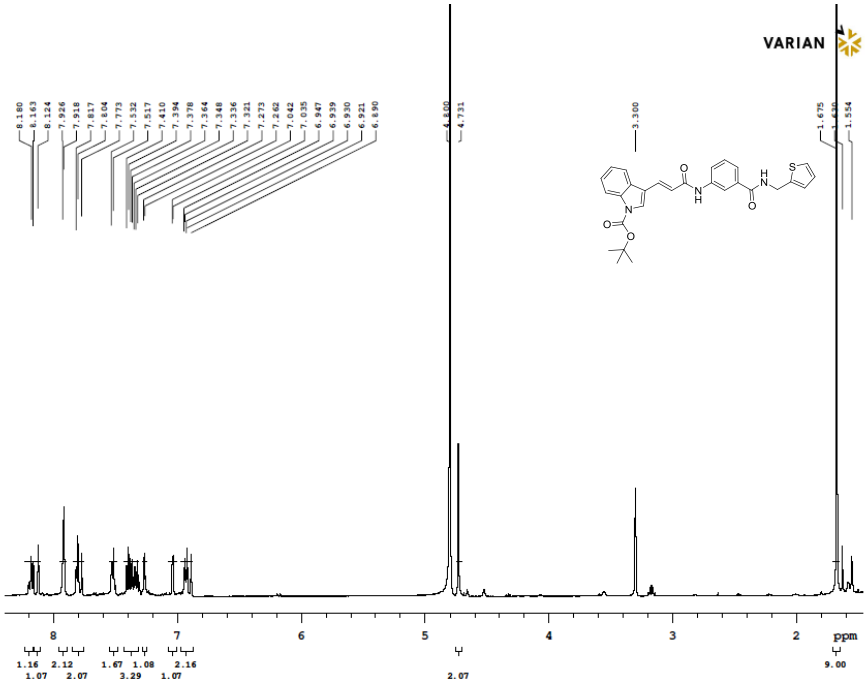
^{13}C-NMR (CD_3OD, 125 MHz):
(*E*)-*tert*-butyl-3-(3-(3-(benzylcarbamoyl)phenylamino)-3-oxoprop-1-enyl)-1*H*-indole-1-carboxylate (**5g**)



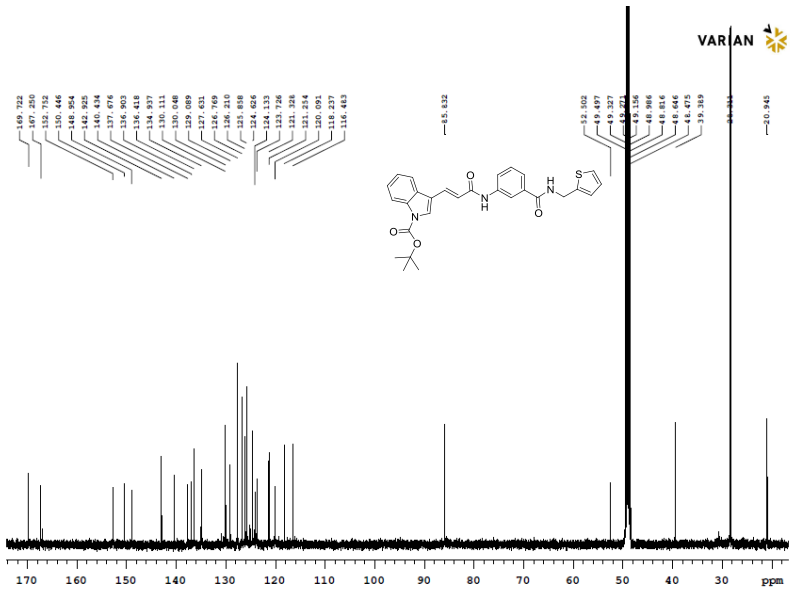
^{1}H-NMR (CD_3OD, 500 MHz):
(*E*)-*tert*-butyl-3-(3-(3-(furan-2-ylmethylcarbamoyl)phenyl amino)-3-oxoprop-1-enyl)-1*H*-indole-1-carboxylate
(**5h**)



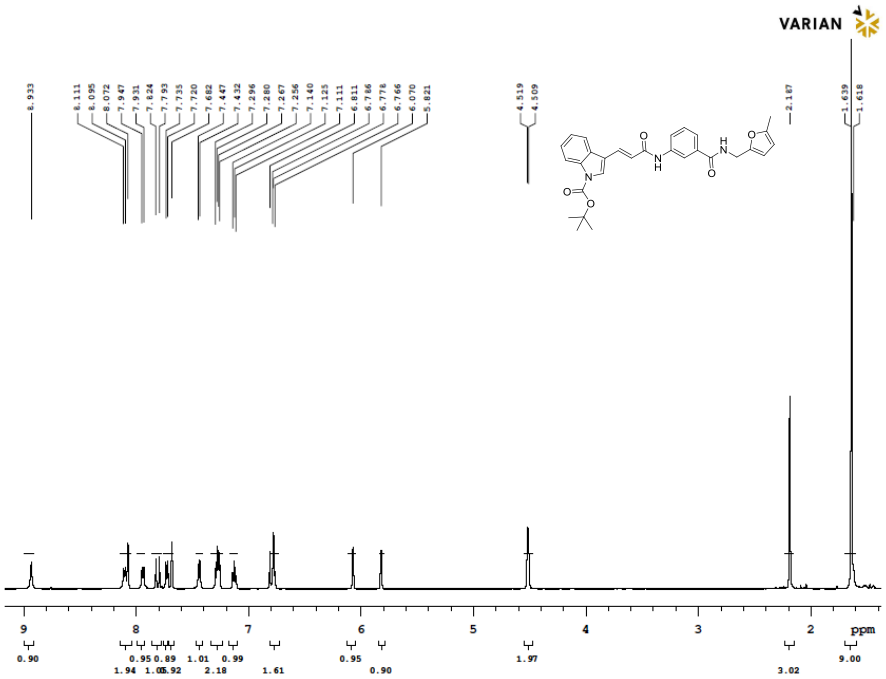
^{13}C-NMR (CD_3OD, 125 MHz):
(*E*)-*tert*-butyl-3-(3-(3-(furan-2-ylmethylcarbamoyl)phenyl amino)-3-oxoprop-1-enyl)-1*H*-indole-1-carboxylate
(**5h**)



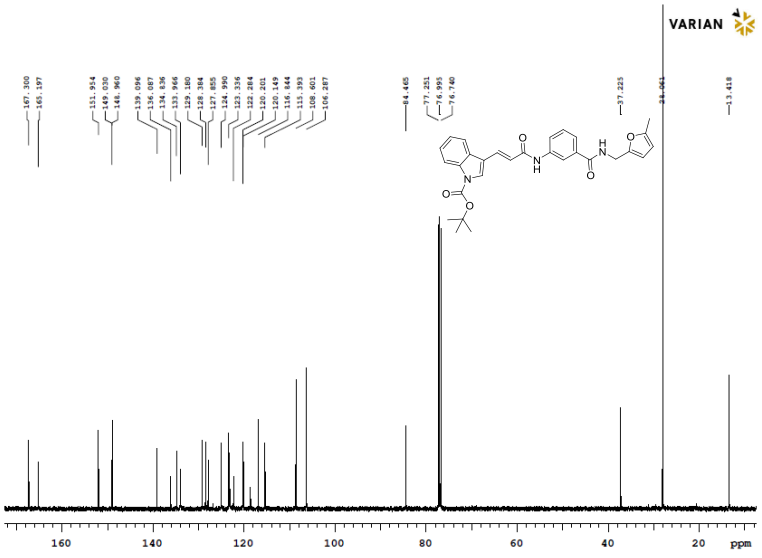
^{1}H-NMR (CD_3OD, 500 MHz):
(*E*)-*tert*-butyl-3-(3-oxo-3-(3-(thiophen-2-ylmethylcarbamoyl) phenylamino)prop-1-enyl)-1*H*-indole-1-carboxylate (**5i**)



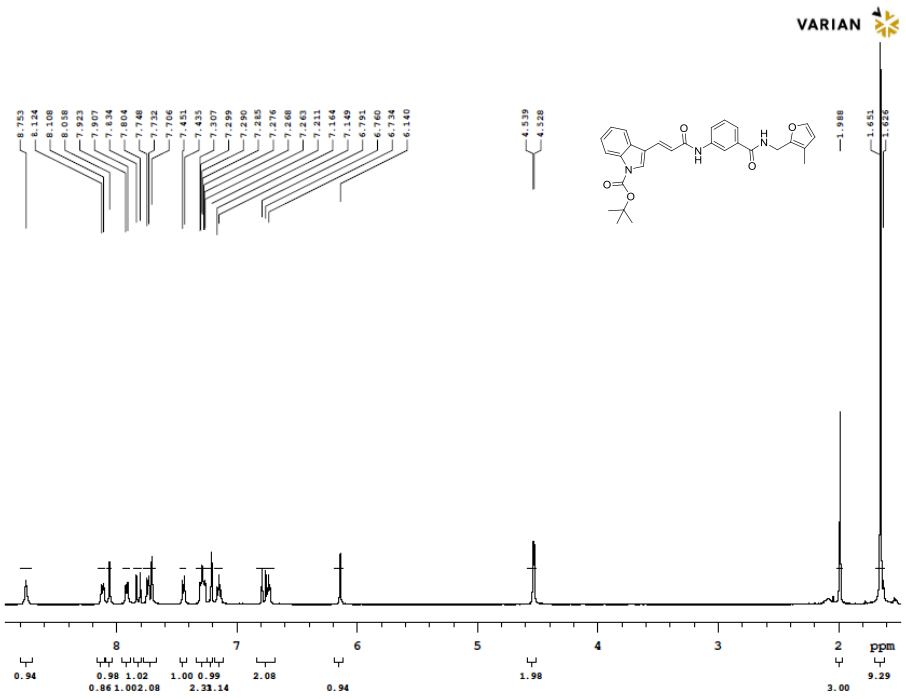
^{13}C-NMR (CD_3OD, 125 MHz):
(*E*)-*tert*-butyl-3-(3-oxo-3-(3-(thiophen-2-ylmethylcarbamoyl) phenylamino)prop-1-enyl)-1*H*-indole-1-carboxylate (**5i**)



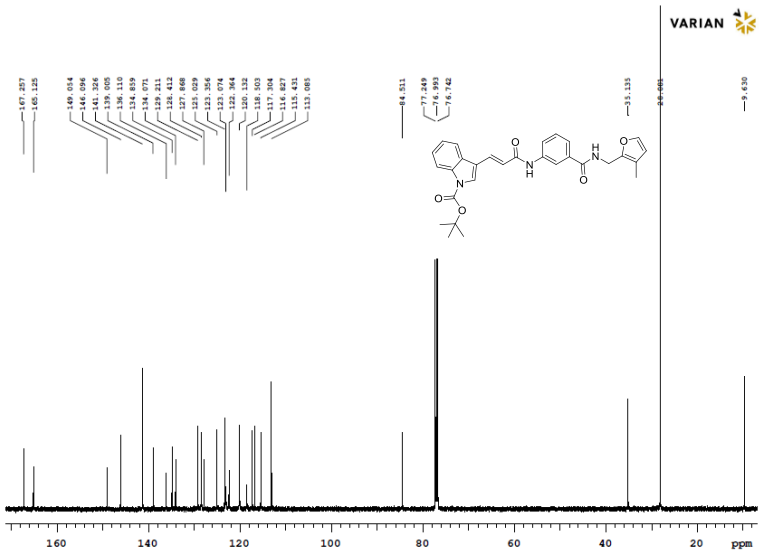
^{1}H-NMR ($CDCl_3$, 500 MHz):
(*E*)-*tert*-butyl-3-(3-(3-(5-methylfuran-2-ylmethylcarbamoyl)phenyl amino)-3-oxoprop-1-enyl)-1*H*-indole-1-carboxylate (**5j**)



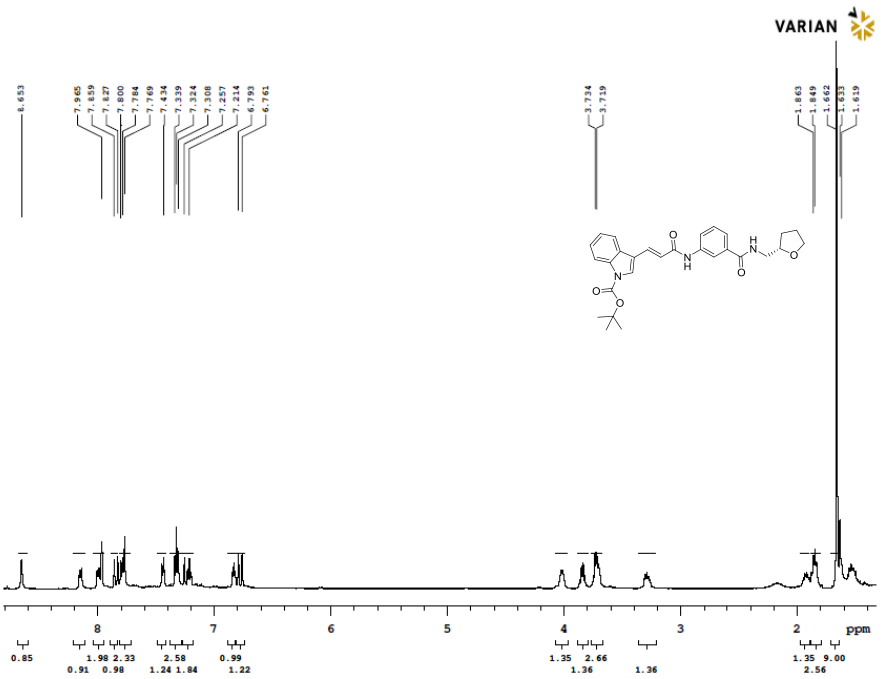
^{13}C-NMR ($CDCl_3$, 125 MHz):
(*E*)-*tert*-butyl-3-(3-(3-(5-methylfuran-2-ylmethylcarbamoyl)phenyl amino)-3-oxoprop-1-enyl)-1*H*-indole-1-carboxylate (**5j**)



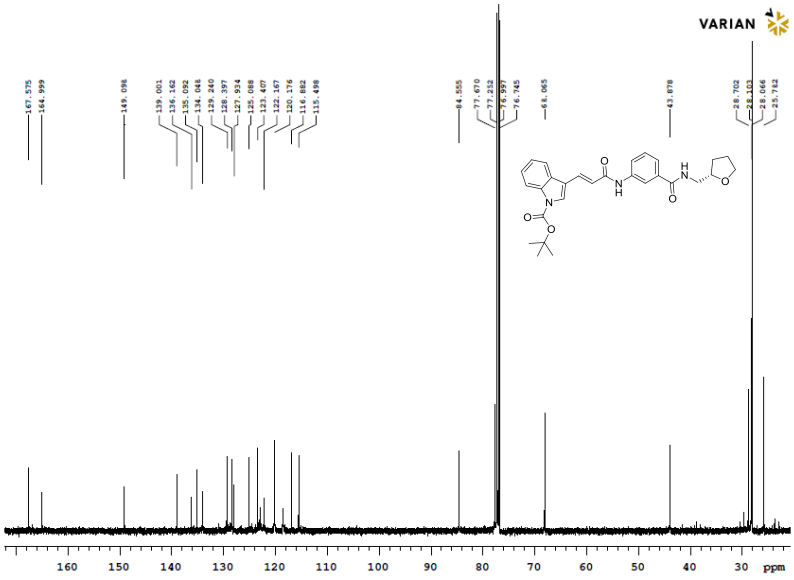
^{1}H-NMR ($CDCl_3$, 500 MHz):
(*E*)-*tert*-butyl-3-(3-(3-(3-methylfuran-2-ylmethylcarbamoyl)phenyl amino)-3-oxoprop-1-enyl)-1*H*-indole-1-carboxylate (**5k**)



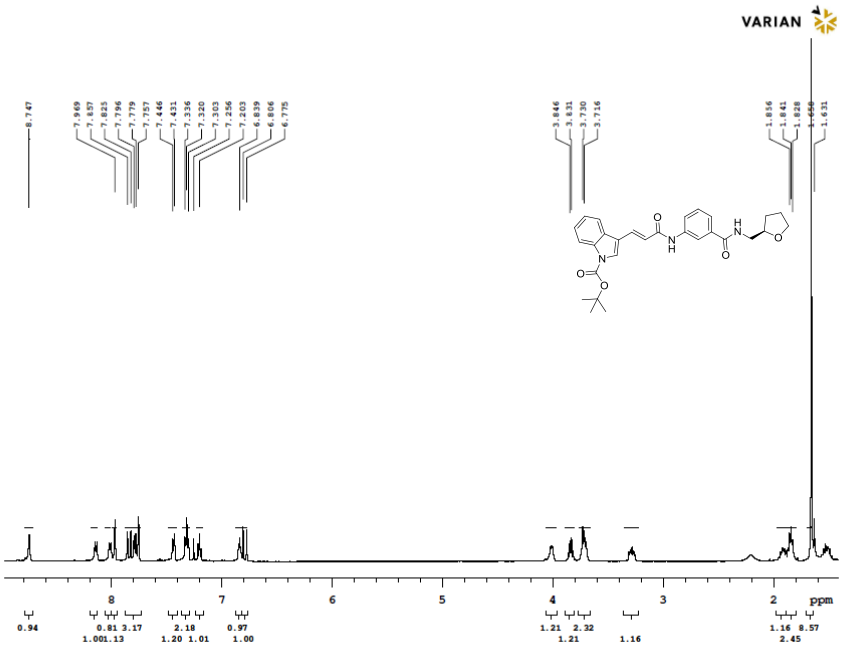
^{13}C-NMR ($CDCl_3$, 125 MHz):
(*E*)-*tert*-butyl-3-(3-(3-(3-methylfuran-2-ylmethylcarbamoyl)phenyl amino)-3-oxoprop-1-enyl)-1*H*-indole-1-carboxylate (**5k**)



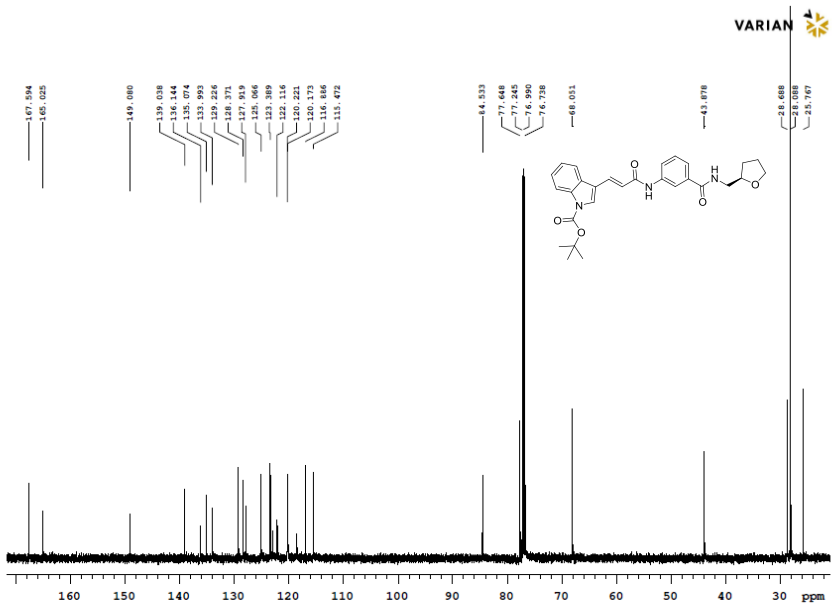
^{1}H-NMR ($CDCl_3$, 500 MHz):
(*S*,*E*)-*tert*-butyl-3-(3-oxo-3-(3-((tetrahydrofuran-2-yl)methyl carbamoyl)phenylamino)prop-1-enyl)-1*H*-indole-1-carboxylate (**5l**)



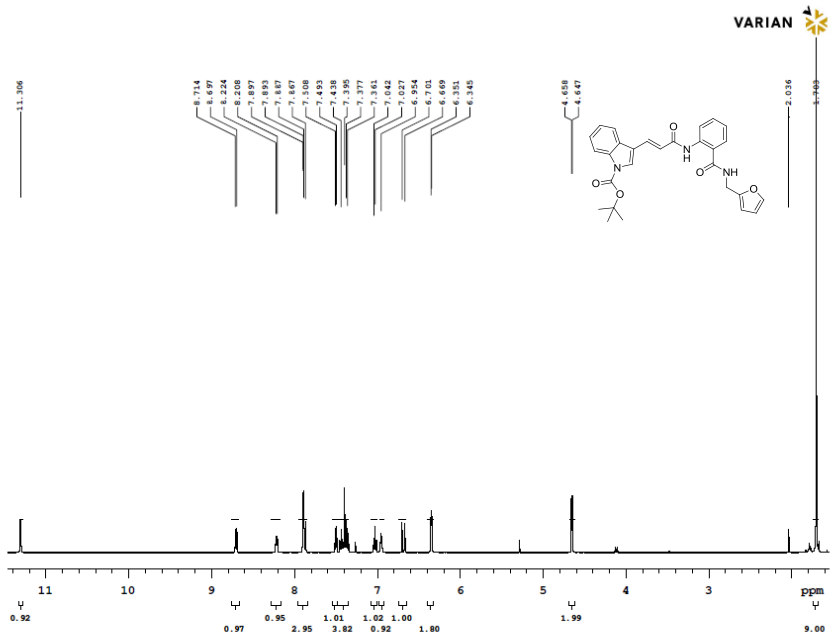
^{13}C-NMR ($CDCl_3$, 125 MHz):
(*S*,*E*)-*tert*-butyl-3-(3-oxo-3-(3-((tetrahydrofuran-2-yl)methyl carbamoyl)phenylamino)prop-1-enyl)-1*H*-indole-1-carboxylate (**5l**)



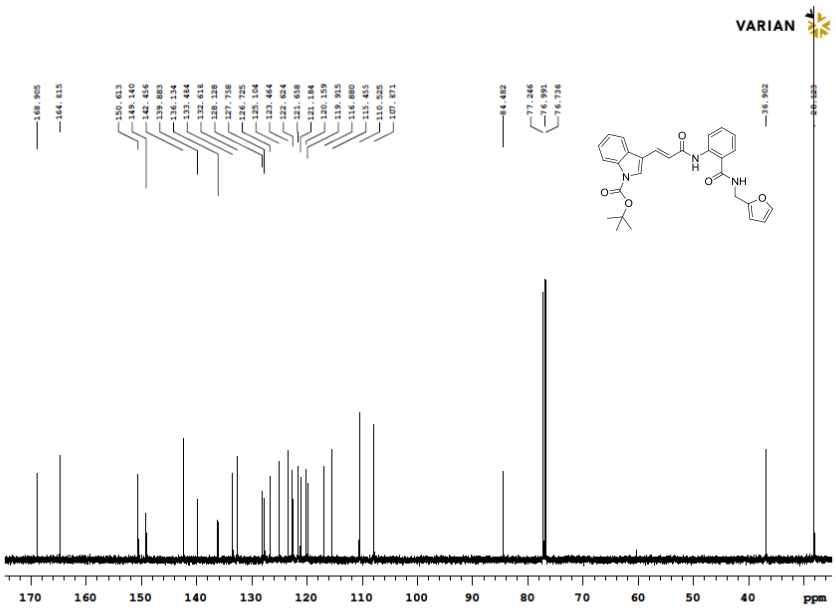
^{1}H-NMR ($CDCl_3$, 500 MHz):
(*R*,*E*)-*tert*-butyl-3-(3-oxo-3-(3-((tetrahydrofuran-2-yl)methyl carbamoyl)phenylamino)prop-1-enyl)-1*H*-indole-1-carboxylate (**5m**)



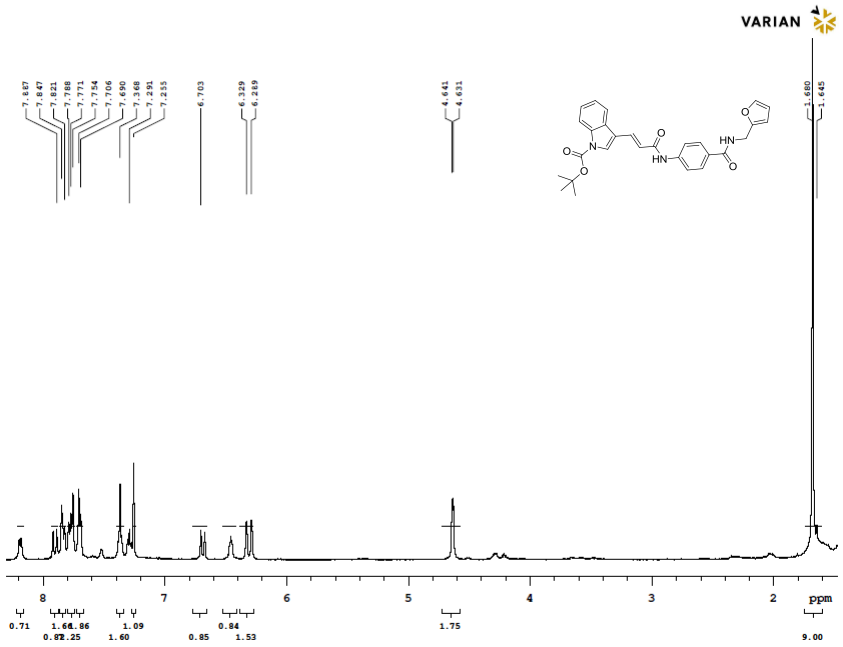
^{13}C-NMR ($CDCl_3$, 125 MHz):
(*R*,*E*)-*tert*-butyl-3-(3-oxo-3-(3-((tetrahydrofuran-2-yl)methyl carbamoyl)phenylamino)prop-1-enyl)-1*H*-indole-1-carboxylate (**5m**)



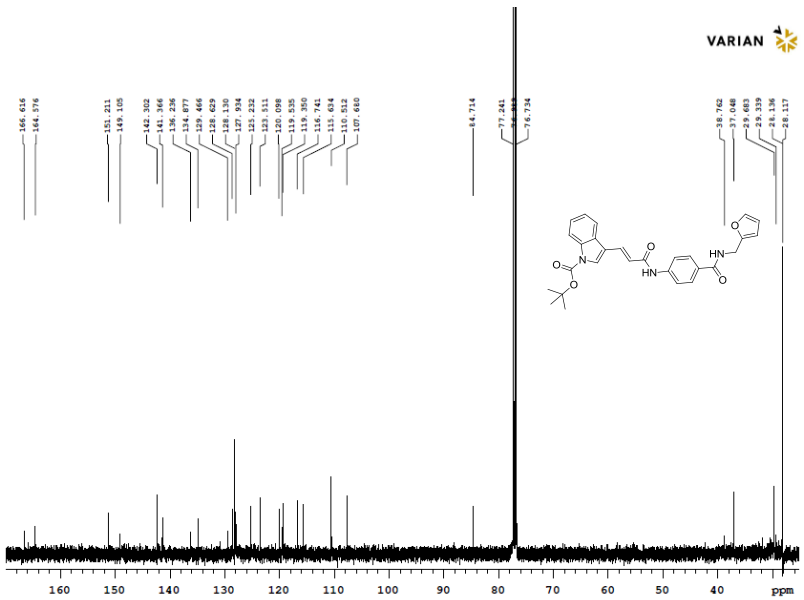
^{1}H-NMR ($CDCl_3$, 500 MHz):
(*E*)-*tert*-butyl-3-(3-(2-(furan-2-ylmethylcarbamoyl)phenylamino)-3-oxoprop-1-enyl)-1*H*-indole-1-carboxylate
(**5n**)



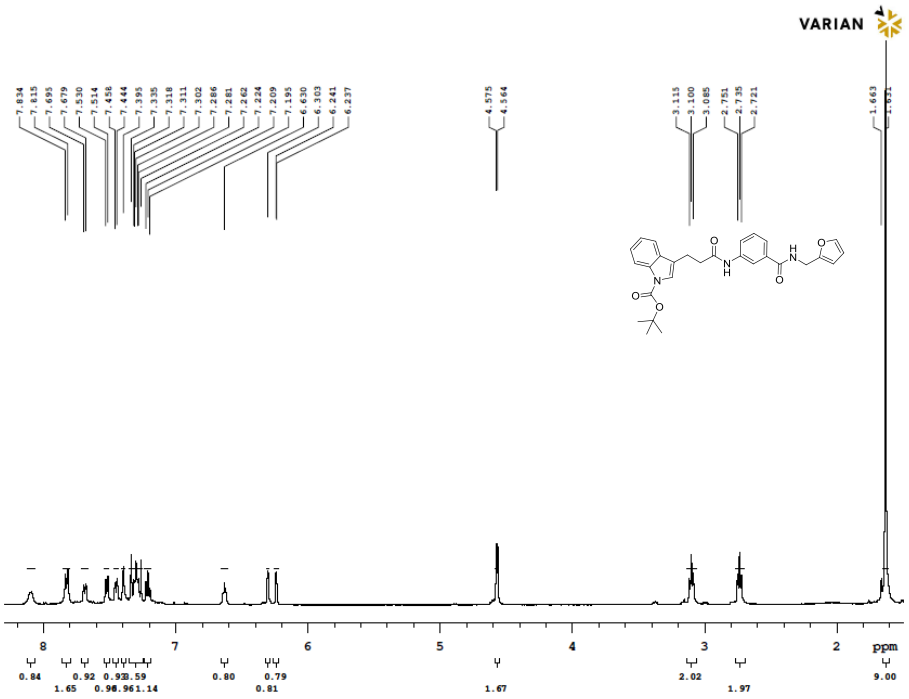
^{13}C-NMR ($CDCl_3$, 125 MHz):
(*E*)-*tert*-butyl-3-(3-(2-(furan-2-ylmethylcarbamoyl)phenylamino)-3-oxoprop-1-enyl)-1*H*-indole-1-carboxylate
(**5n**)



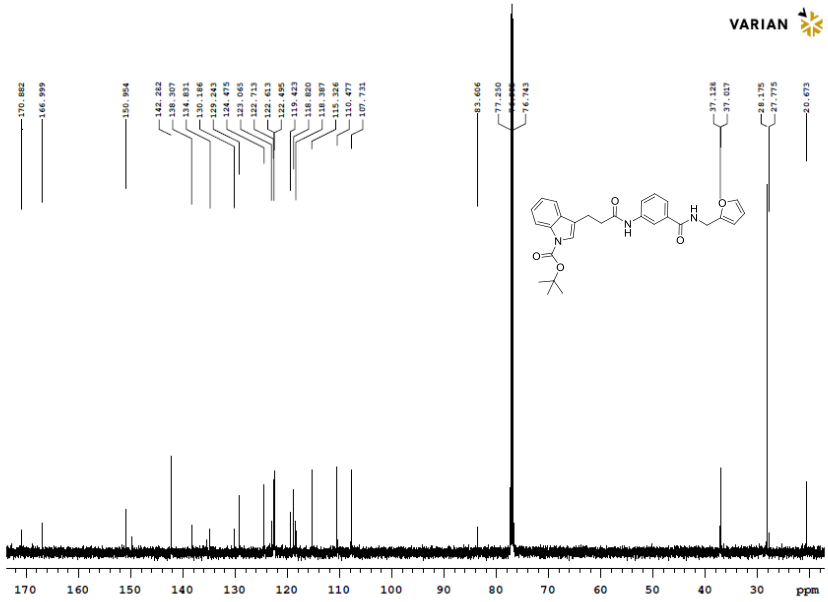
^{1}H-NMR ($CDCl_3$, 500 MHz):
(*E*)-*tert*-butyl-3-(3-(4-(furan-2-ylmethylcarbamoyl)phenyl amino)-3-oxoprop-1-enyl)-1*H*-indole-1-carboxylate
(**5o**)



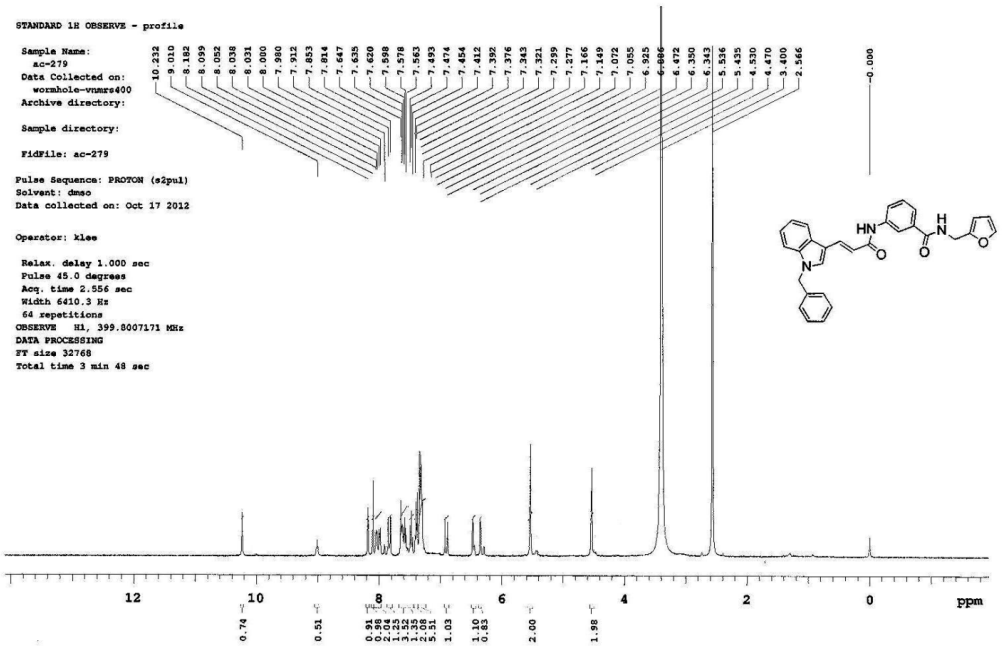
^{13}C-NMR ($CDCl_3$, 125 MHz):
(*E*)-*tert*-butyl-3-(3-(4-(furan-2-ylmethylcarbamoyl)phenyl amino)-3-oxoprop-1-enyl)-1*H*-indole-1-carboxylate
(**5o**)



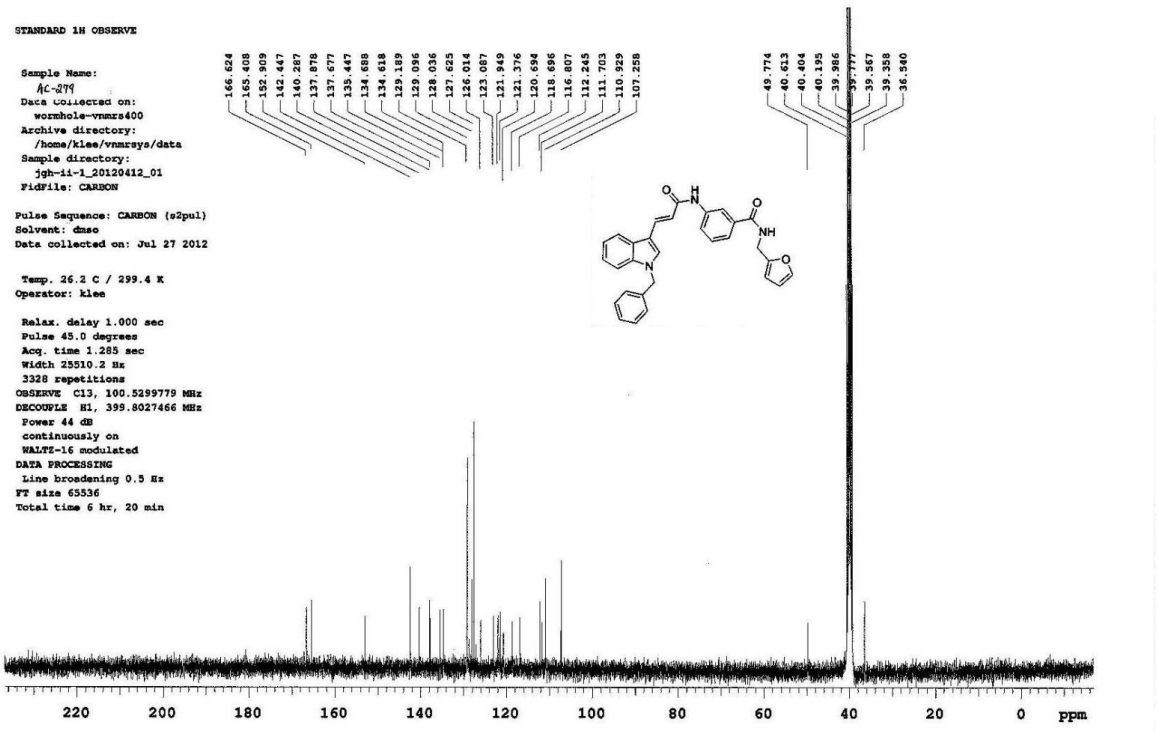
^{1}H-NMR ($CDCl_3$, 500 MHz):
tert-Butyl 3-(3-(3-(furan-2-ylmethylcarbamoyl)phenylamino)-3-oxopropyl)-1*H*-indole-1-carboxylate (**5p**)



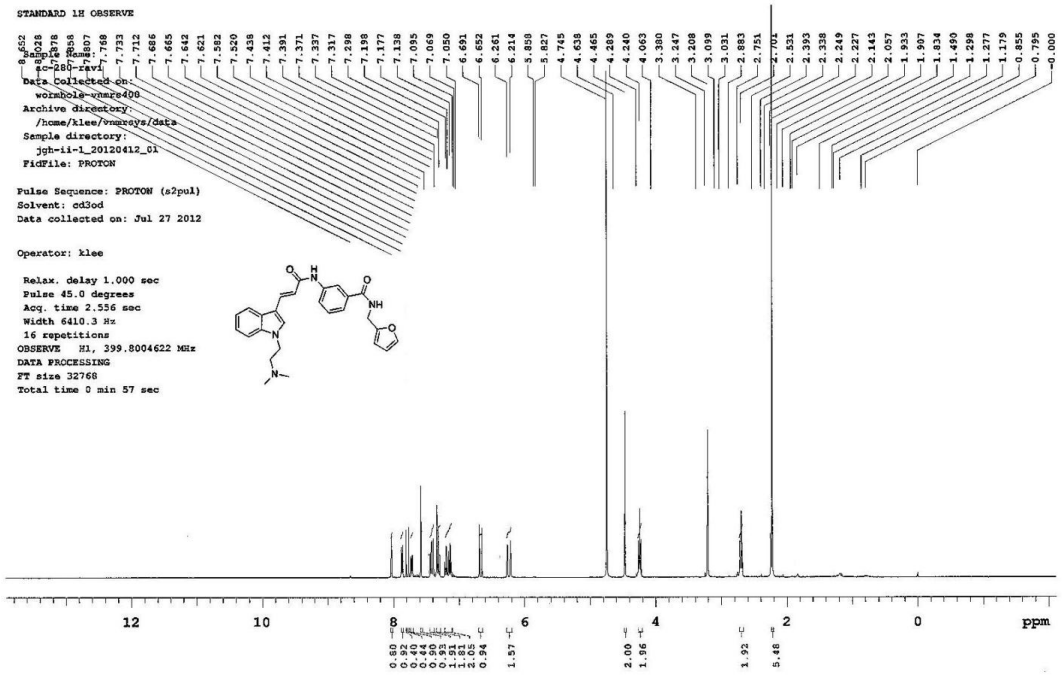
^{13}C-NMR ($CDCl_3$, 125 MHz):
tert-Butyl 3-(3-(3-(furan-2-ylmethylcarbamoyl)phenylamino)-3-oxopropyl)-1*H*-indole-1-carboxylate (**5p**)



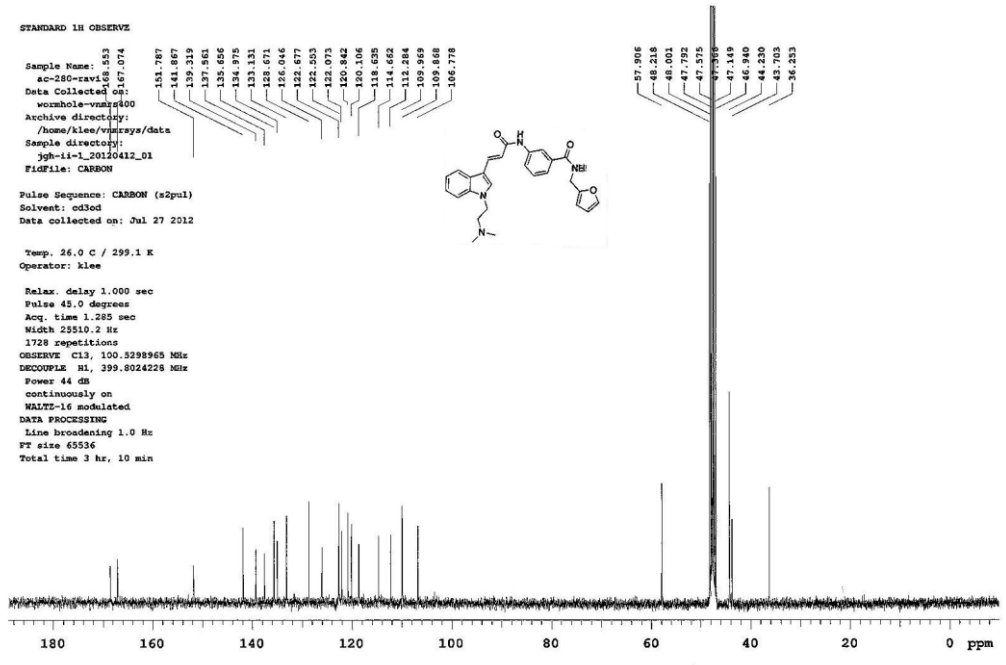
^{1}H-NMR (DMSO, 400 MHz):
(*E*)-3-(3-(1-benzyl-1*H*-indol-3-yl)acrylamido)-*N*-(furan-2-ylmethyl)benzamide (**6**)



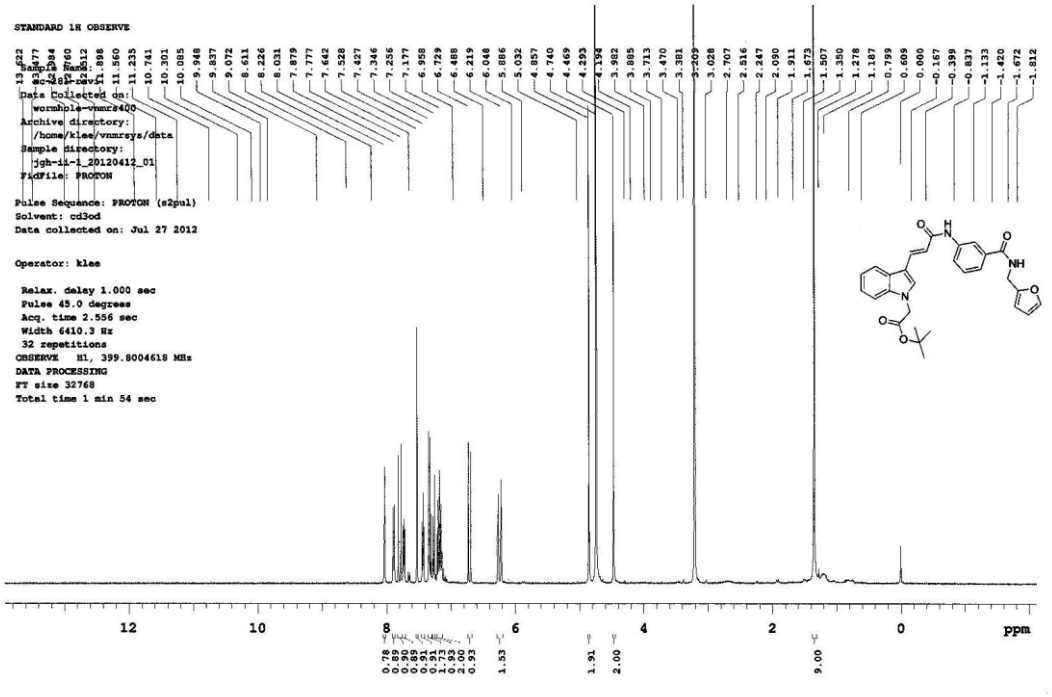
^{13}C-NMR (DMSO, 100 MHz):
(*E*)-3-(3-(1-benzyl-1*H*-indol-3-yl)acrylamido)-*N*-(furan-2-ylmethyl)benzamide (**6**)



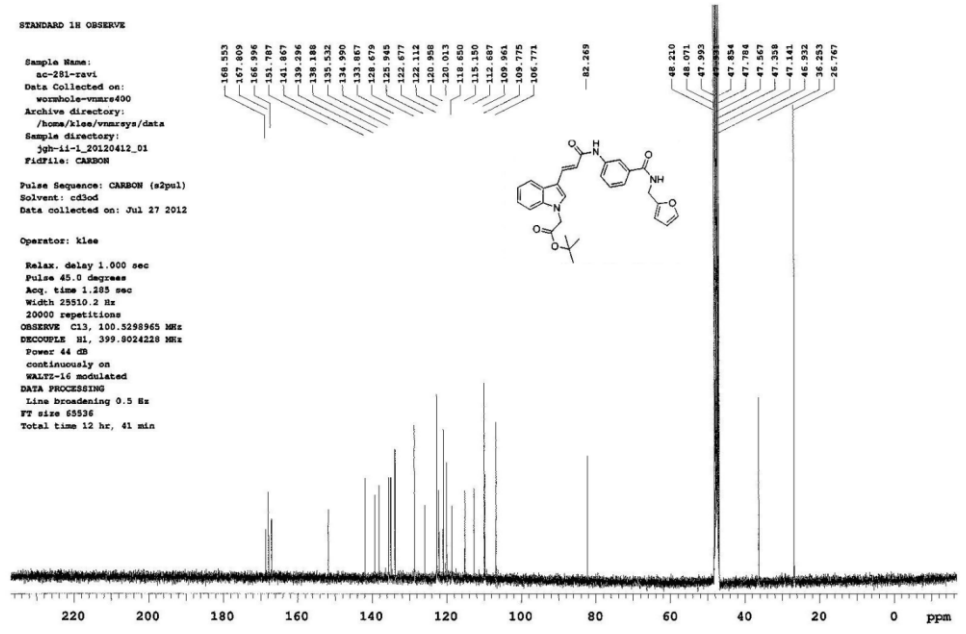
^{1}H-NMR (CD_3OD, 400 MHz)
(*E*)-3-(3-(1-(2-(dimethylamino) ethyl)-1*H*-indol-3-yl) acrylamido)-*N*-(furan-2-ylmethyl) benzamide (**7**)



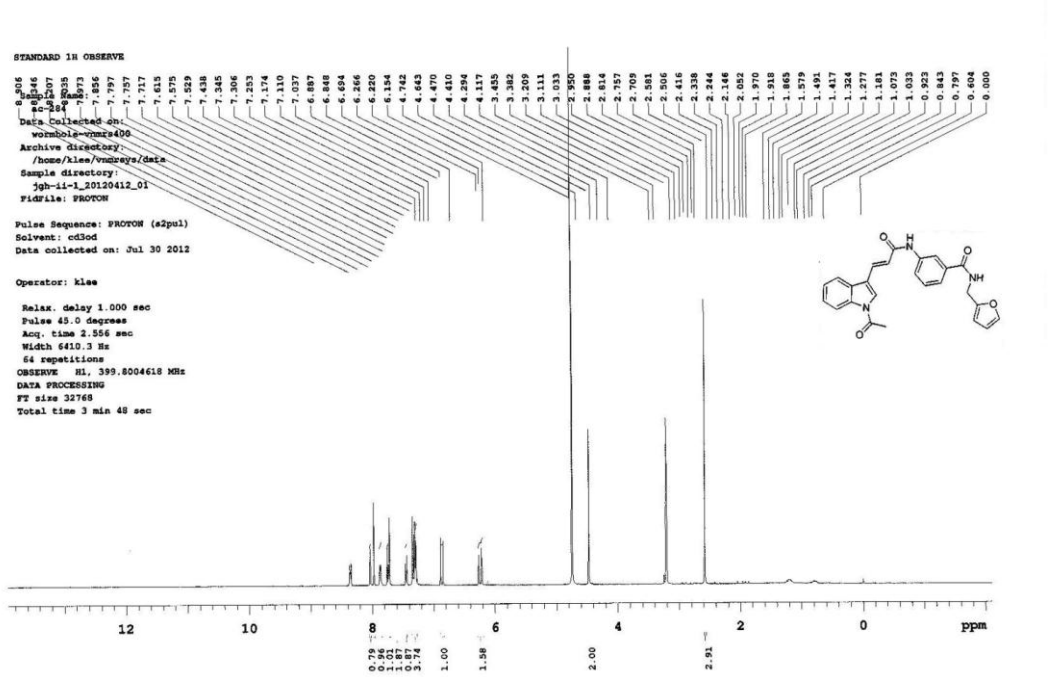
^{13}C-NMR (CD_3OD, 100 MHz)
(*E*)-3-(3-(1-(2-(dimethylamino) ethyl)-1*H*-indol-3-yl) acrylamido)-*N*-(furan-2-ylmethyl) benzamide (**7**)



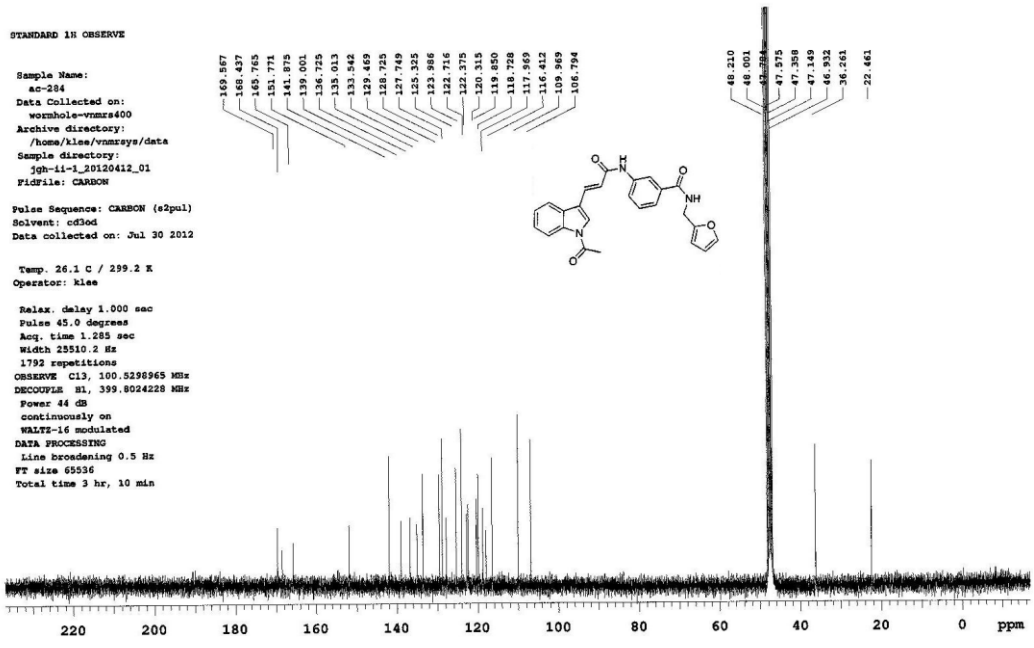
^{1}H-NMR (CD_3OD, 400 MHz)
(*E*)-*tert*-butyl-2-(3-(3-(3-(furan-2-ylmethylcarbamoyl) phenyl-amino)-3-oxoprop-1-enyl)-1*H*-indol-1-yl) acetate
(**8**)



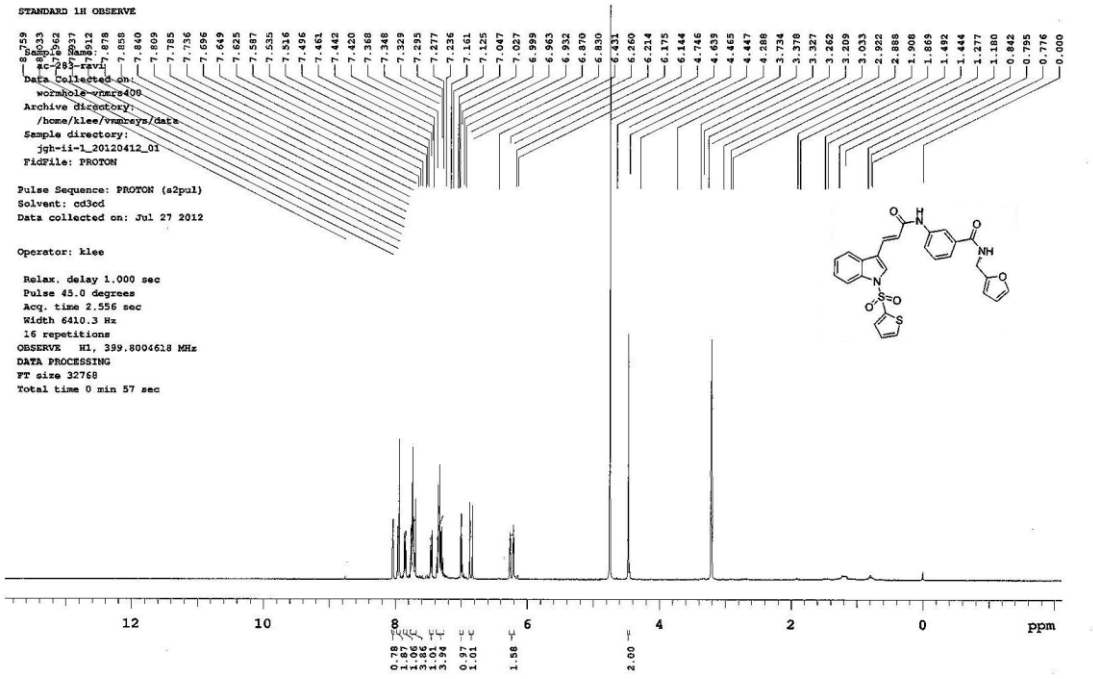
^{13}C-NMR (CD_3OD, 100 MHz)
(*E*)-*tert*-butyl-2-(3-(3-(3-(furan-2-ylmethylcarbamoyl) phenyl-amino)-3-oxoprop-1-enyl)-1*H*-indol-1-yl) acetate
(**8**)



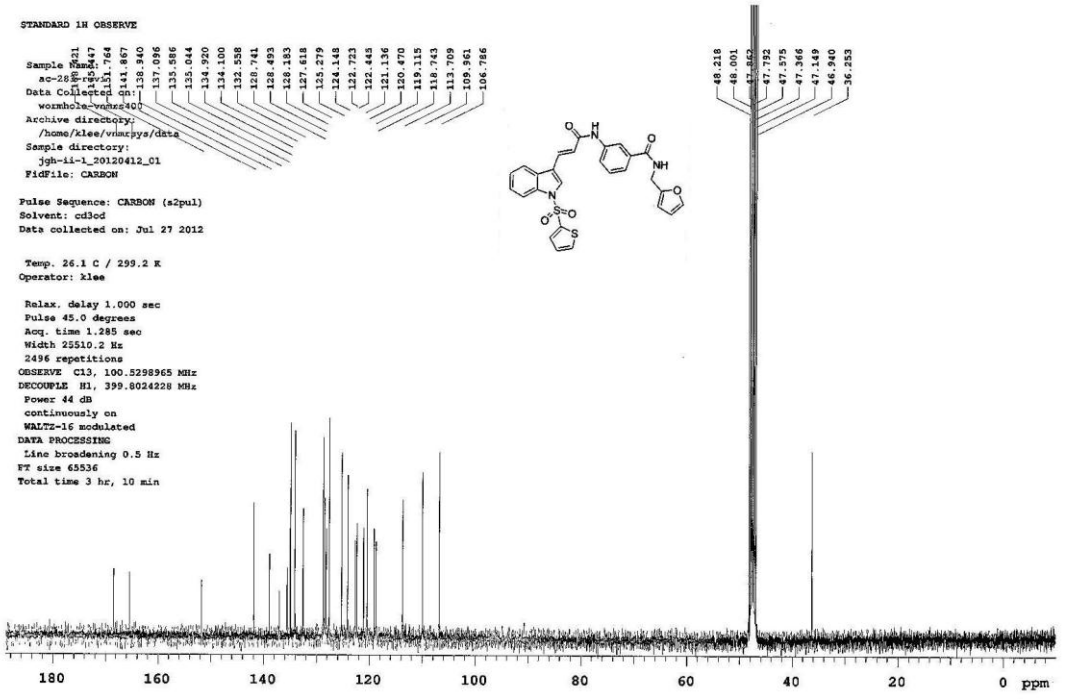
^{1}H-NMR (CD_3OD, 400 MHz)
(*E*)-3-(3-(1-acetyl-1*H*-indol-3-yl) acrylamido)-*N*-(furan-2-ylmethyl) benzamide (**9**)



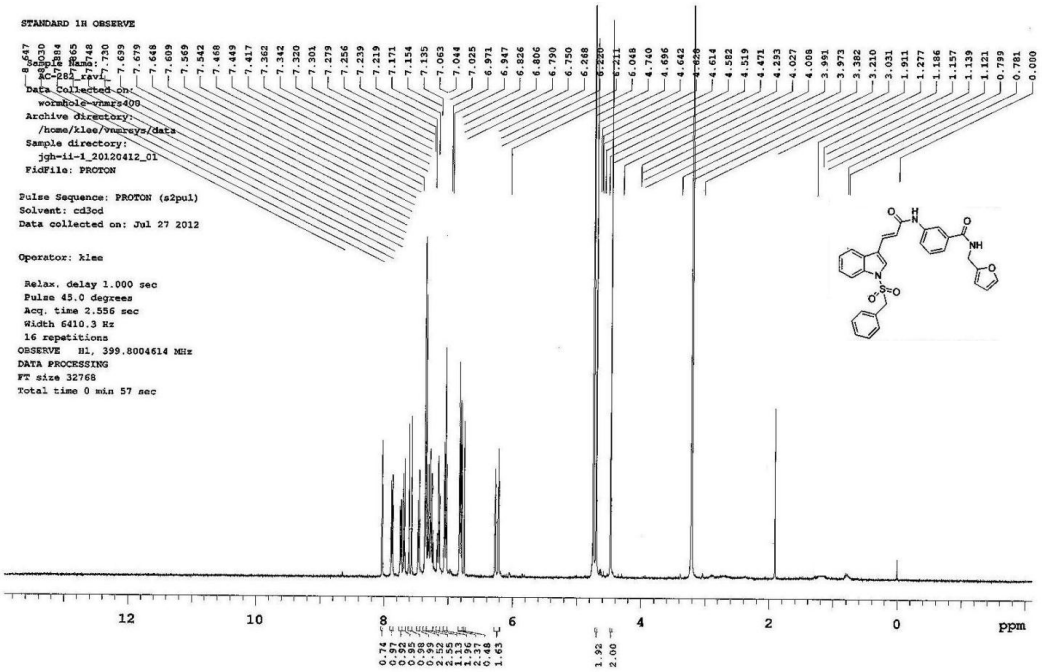
^{13}C-NMR (CD_3OD, 100 MHz)
(*E*)-3-(3-(1-acetyl-1*H*-indol-3-yl) acrylamido)-*N*-(furan-2-ylmethyl) benzamide (**9**)



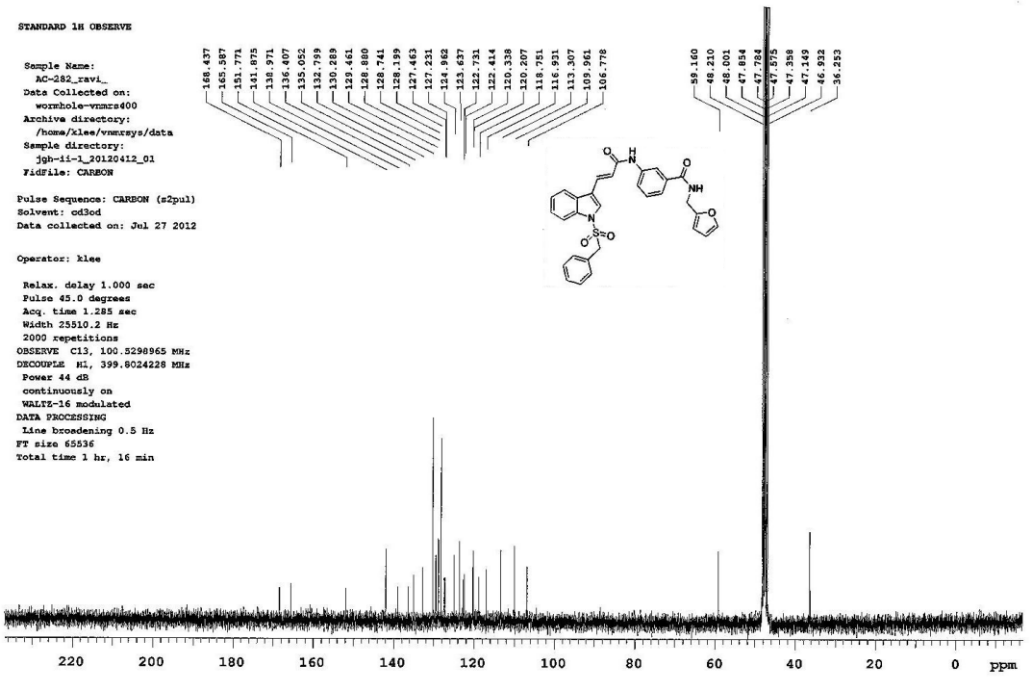
^{1}H-NMR (CD_3OD, 400 MHz)
(*E*)-*N*-(furan-2-ylmethyl)-3-(3-(1-(thiophen-2-ylsulfonyl)-1*H*-indol-3-yl) acrylamido) benzamide (**10**)



^{13}C-NMR (CD_3OD, 100 MHz)
(*E*)-*N*-(furan-2-ylmethyl)-3-(3-(1-(thiophen-2-ylsulfonyl)-1*H*-indol-3-yl) acrylamido) benzamide (**10**)



^{1}H-NMR (CD_3OD, 400 MHz)
(*E*)-3-(3-(1-(benzylsulfonyl)-1*H*-indol-3-yl) acrylamido)-*N*-(furan-2-ylmethyl) benzamide (**11**)



^{13}C-NMR (CD_3OD, 100 MHz)
(*E*)-3-(3-(1-(benzylsulfonyl)-1*H*-indol-3-yl) acrylamido)-*N*-(furan-2-ylmethyl) benzamide (**11**)