

## Supporting Information

*Org. Commun.* 17:2 (2024) 38-55

### Anticancer, antioxidant, DFT calculations, and docking studies of some new peptide-indole conjugates

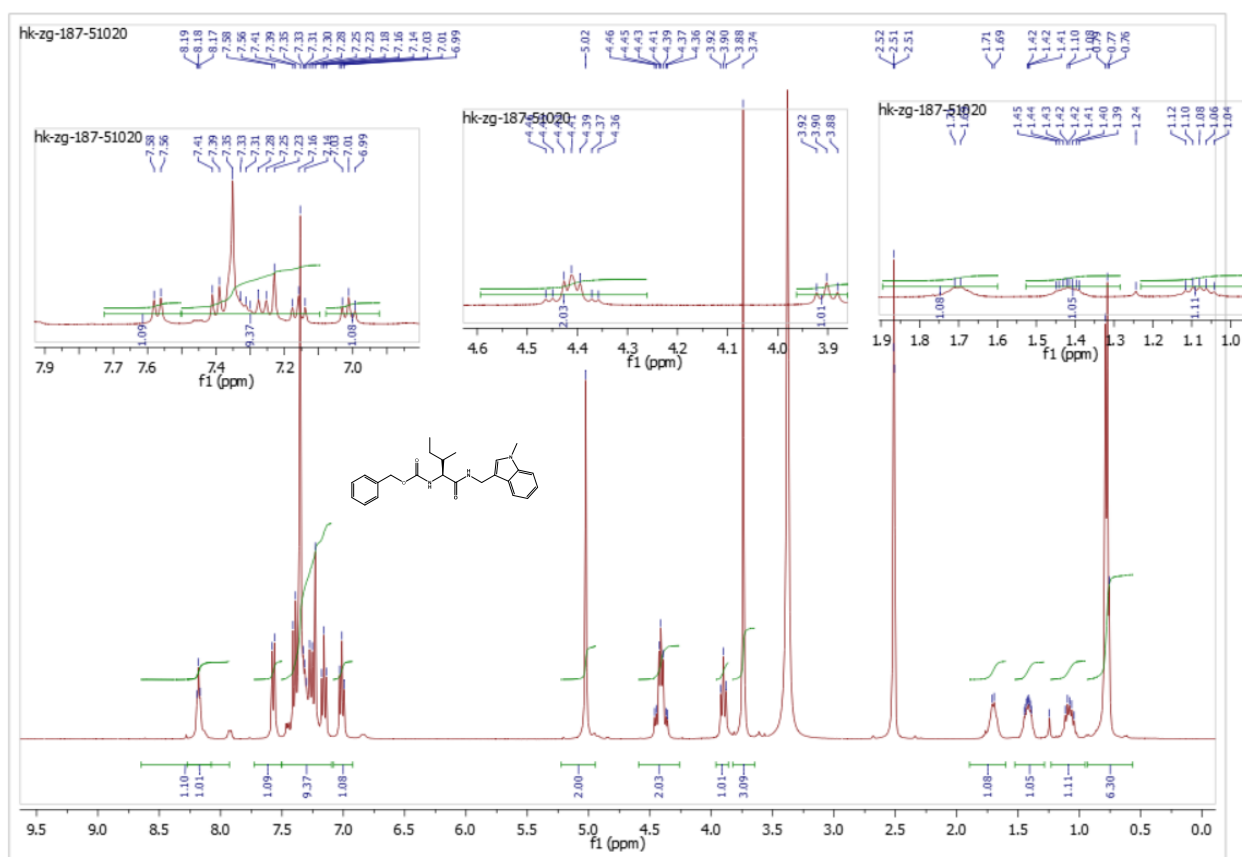
Hasan Küçükbaş\*<sup>1</sup>, Zeynep Gönül<sup>1</sup>, Ali Kuruçay<sup>1</sup>, Burhan Ateş<sup>1</sup>,  
Housseem Boulebd<sup>2</sup>, F. Zehra Küçükbaş<sup>3</sup>

<sup>1</sup> Faculty of Arts and Sciences, Department of Chemistry, İnönü University, 44280 Malatya, Türkiye

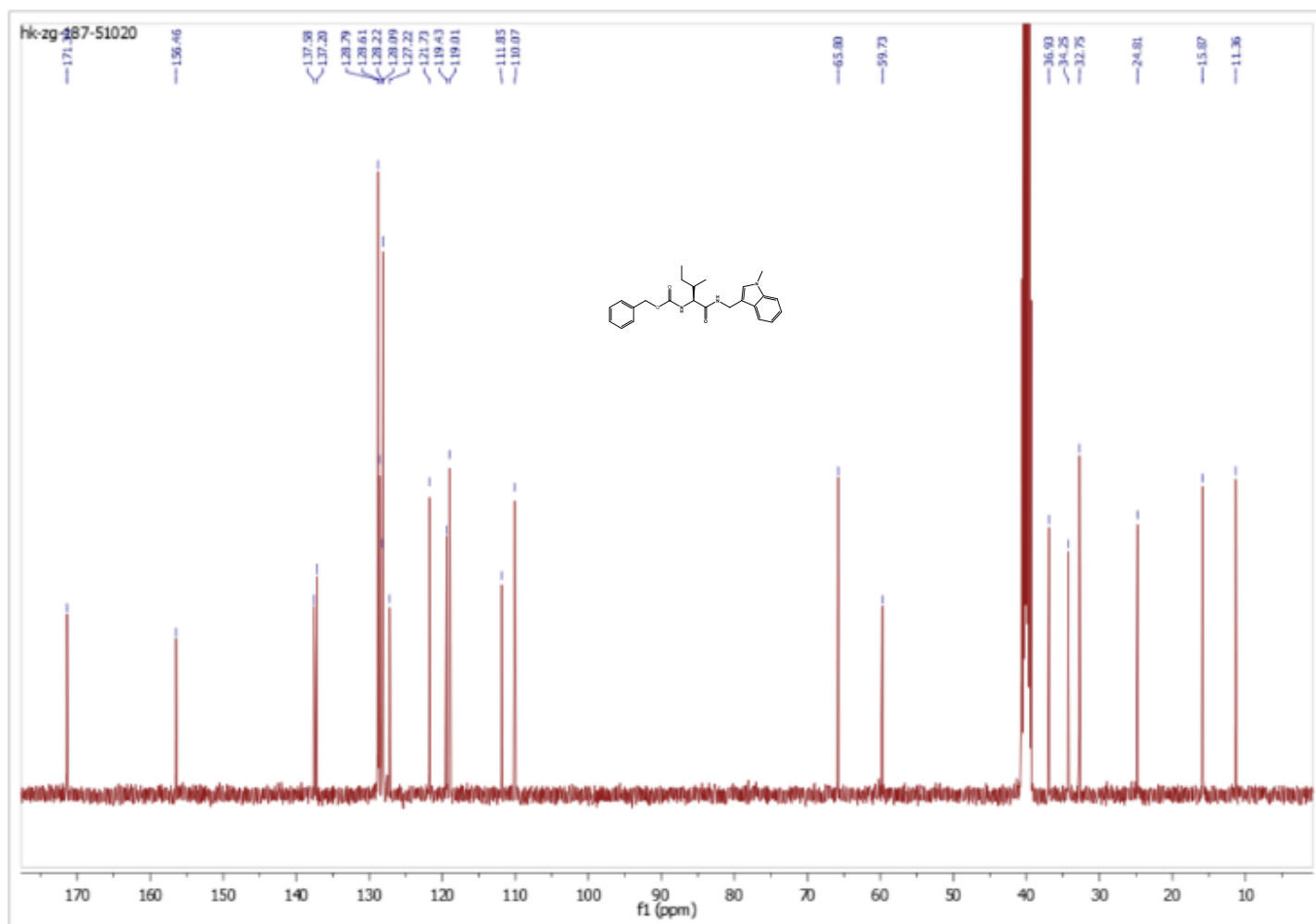
<sup>2</sup> Department of Chemistry, Faculty of Exact Science, University of Constantine 1, Constantine, Algeria

<sup>3</sup> Department of Basic Pharmaceutical Sciences, Faculty of Pharmacy, İnönü University, 44280 Malatya, Türkiye

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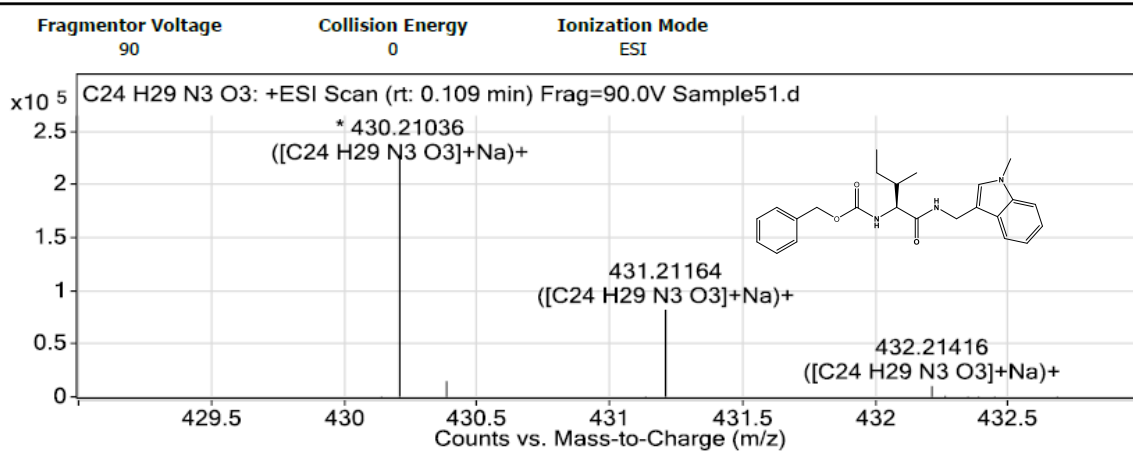


**Figure S1:** <sup>1</sup>H NMR spectrum of compound **1**.

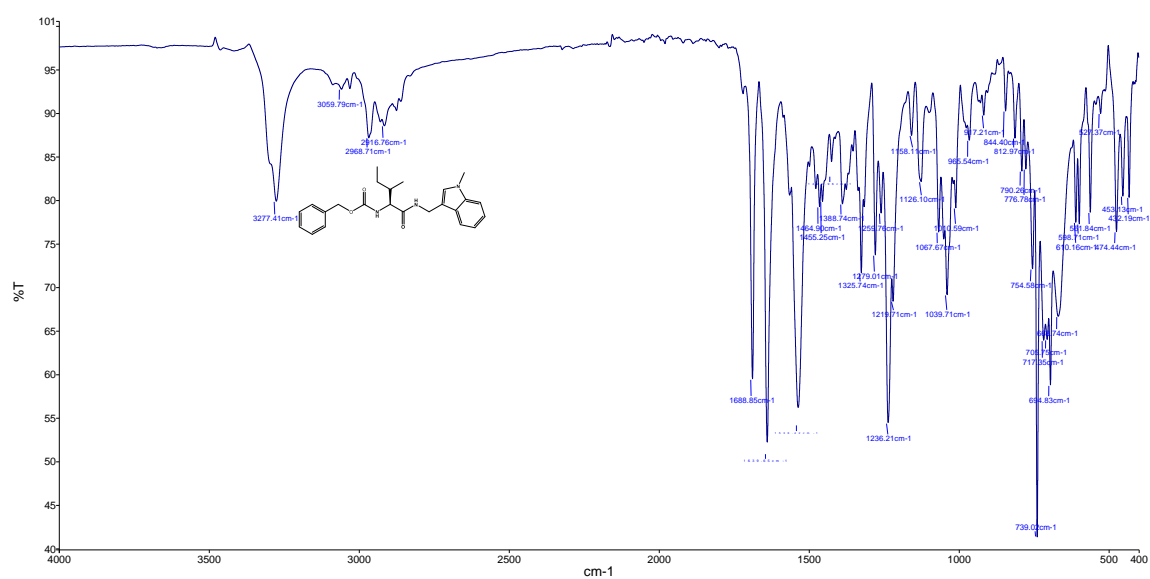


**Figure S2:**  $^{13}\text{C}$  NMR spectrum of compound 1.

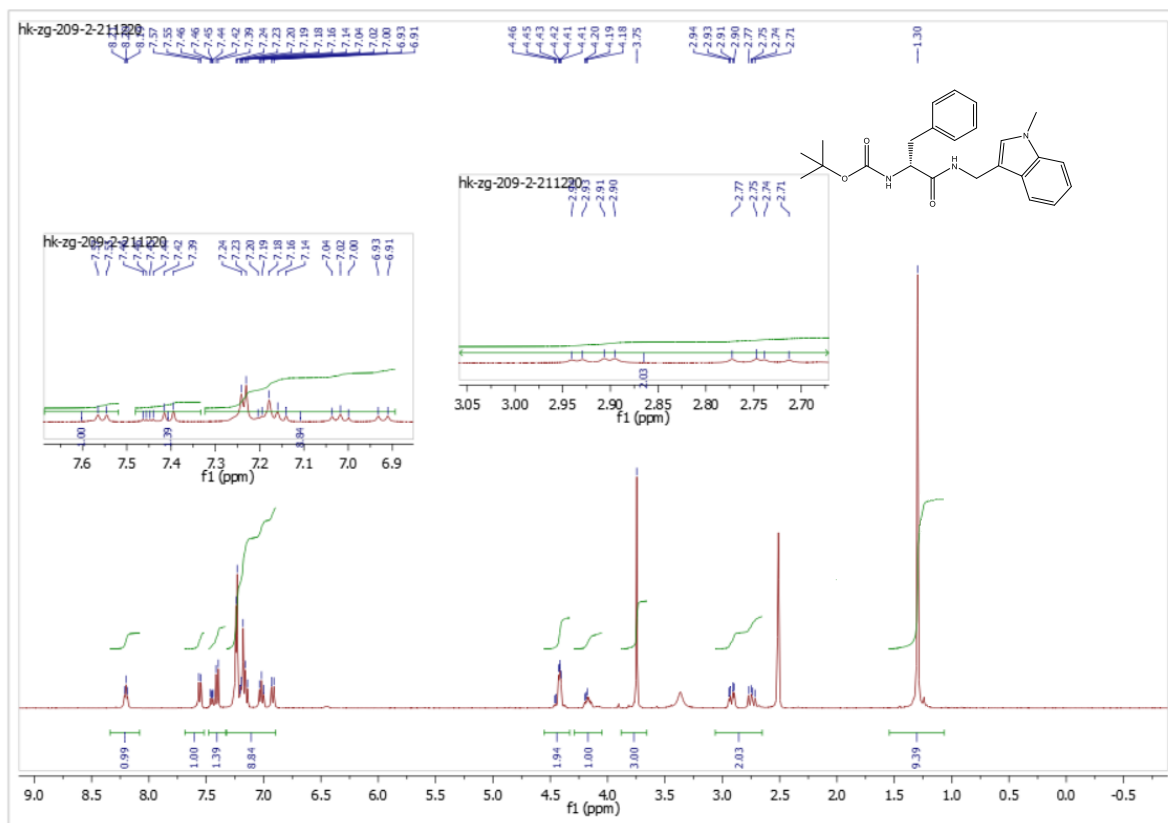
## User Spectra



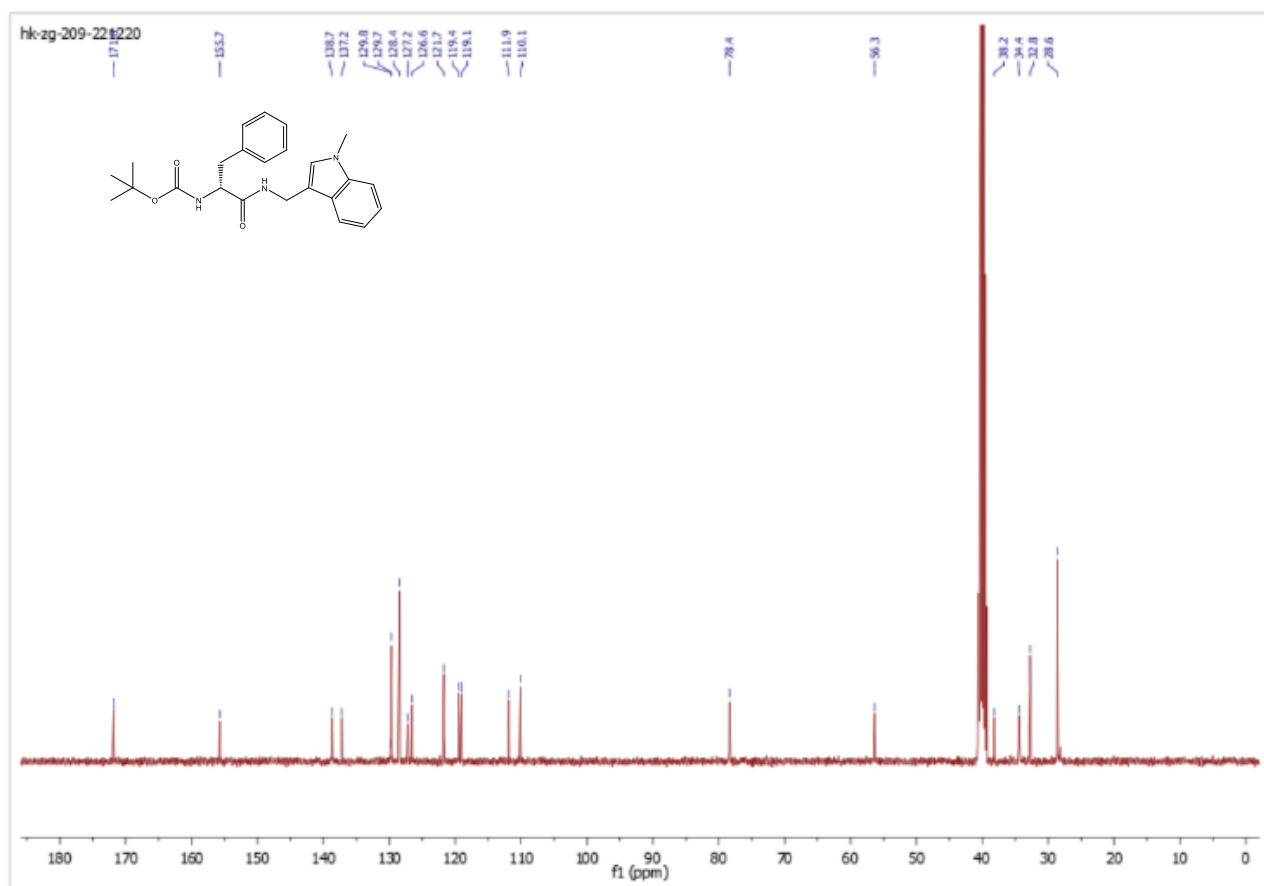
**Figure S3:** Mass spectrum of compound **1**. (M+ Na= 430.211)



**Figure S4:** IR spectrum of compound **1**.

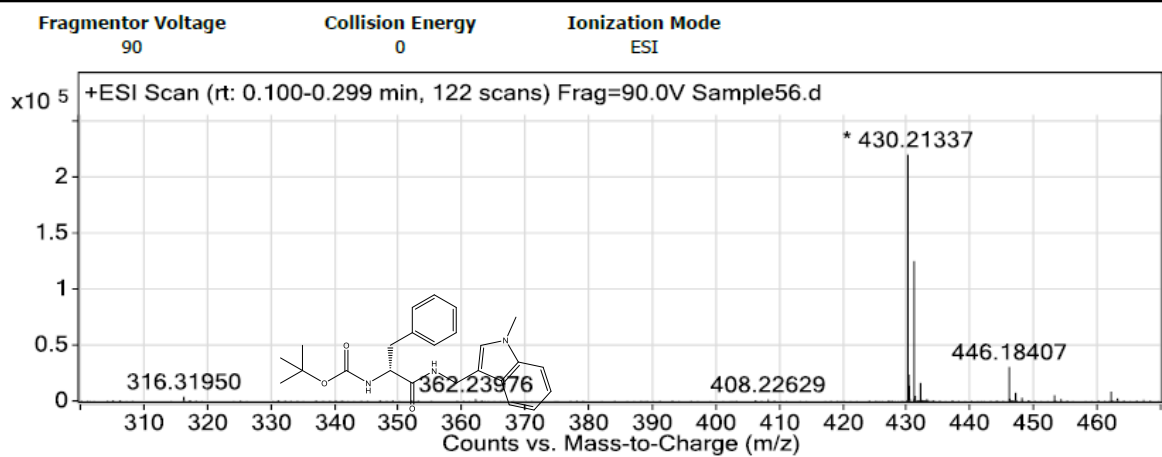


**Figure S5:** <sup>1</sup>H NMR spectrum of compound 2.



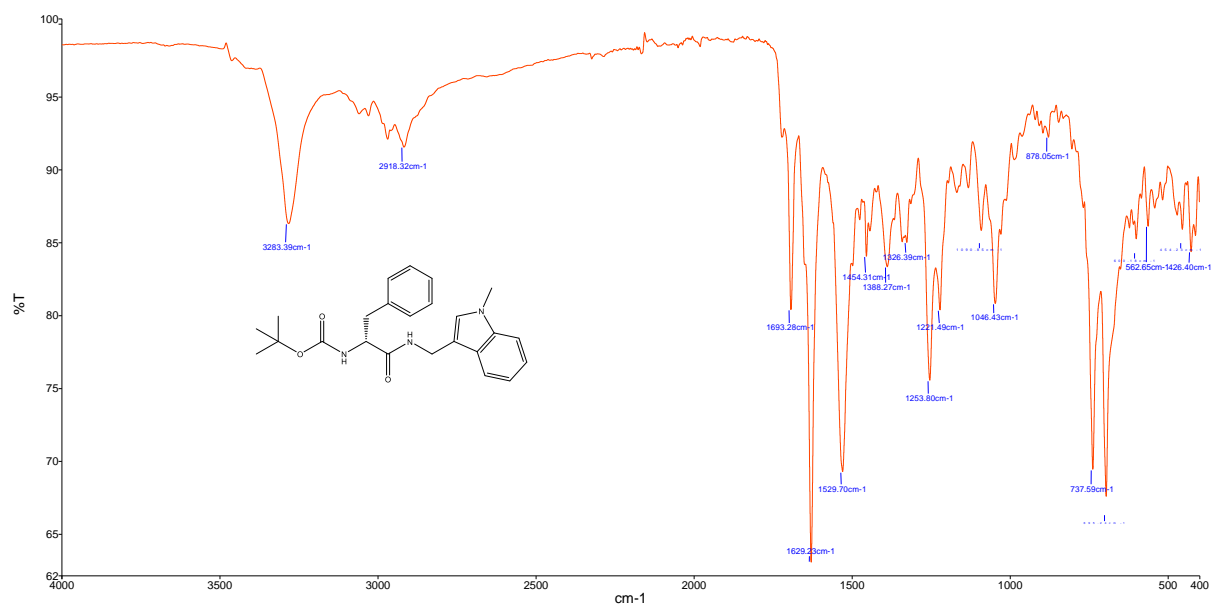
**Figure S6:**  $^{13}\text{C}$  NMR spectrum of compound 2.

## User Spectra

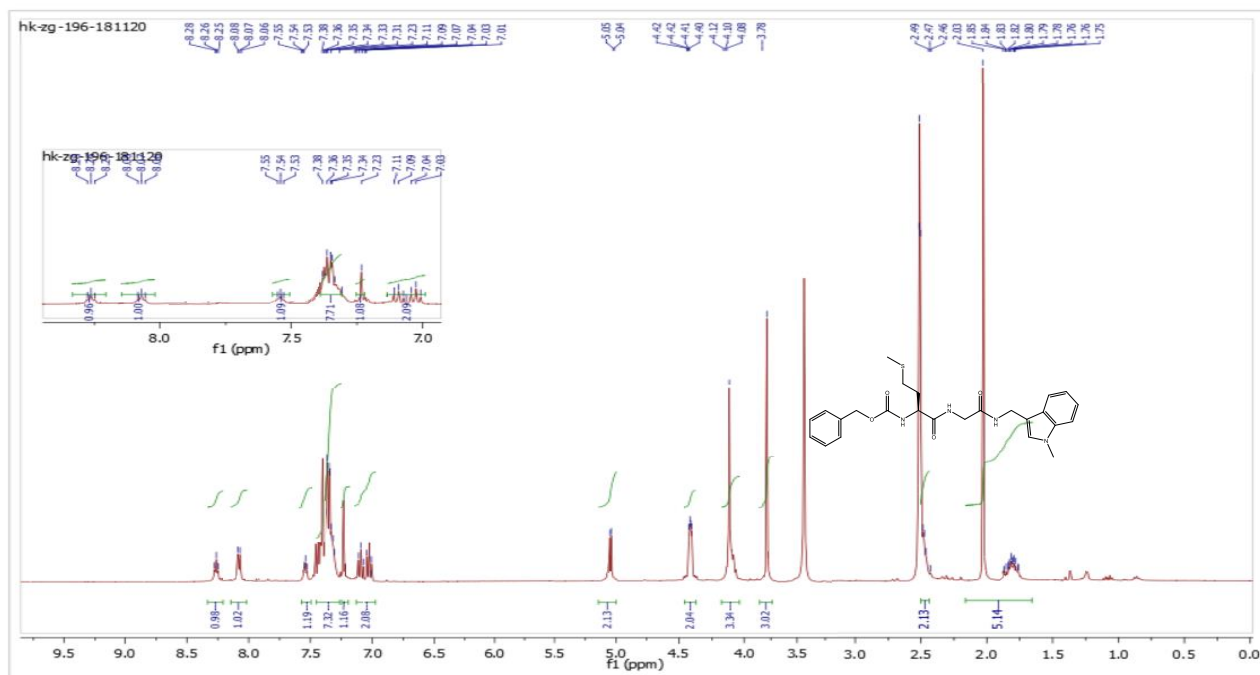


**Figure S7:** Mass spectrum of compound 2. (+ Na= 430.211)

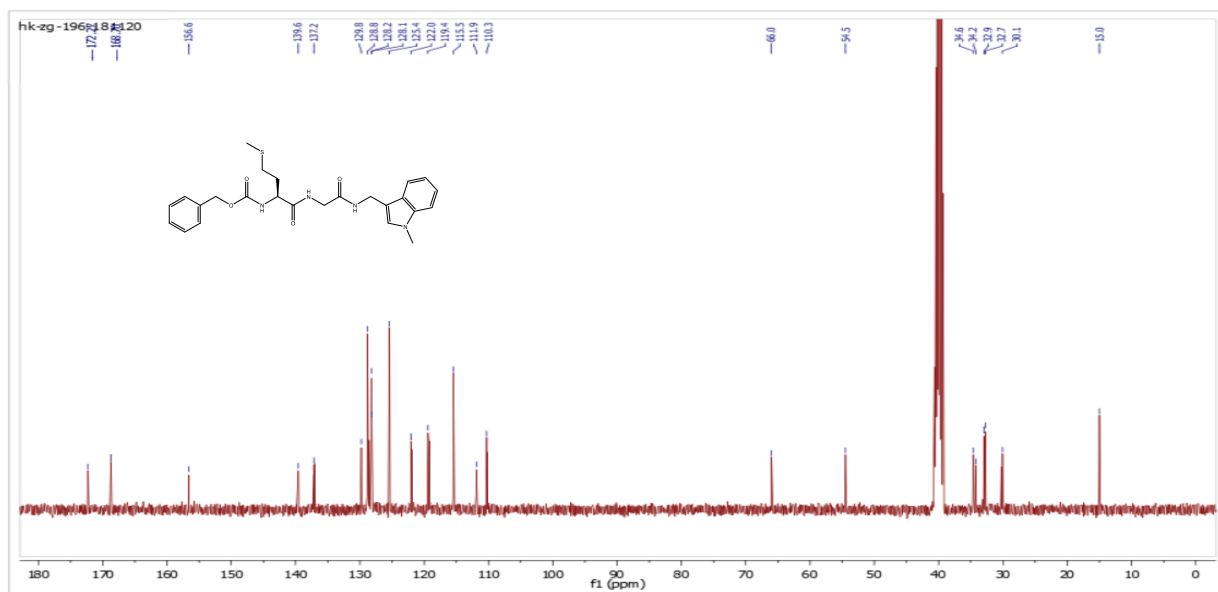




**Figure S8:** IR spectrum of compound 2.

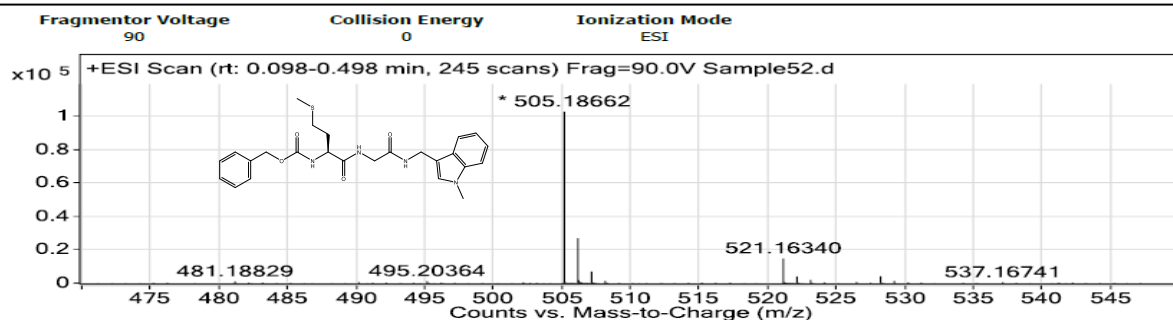


**Figure S9:** <sup>1</sup>H NMR spectrum of compound **3**.



**Figure S10:**  $^{13}\text{C}$  NMR spectrum of compound **3**.

## User Spectra



## User Spectra

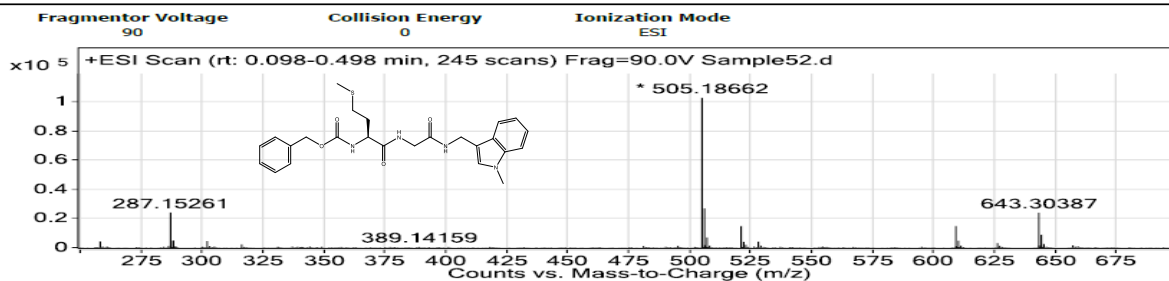
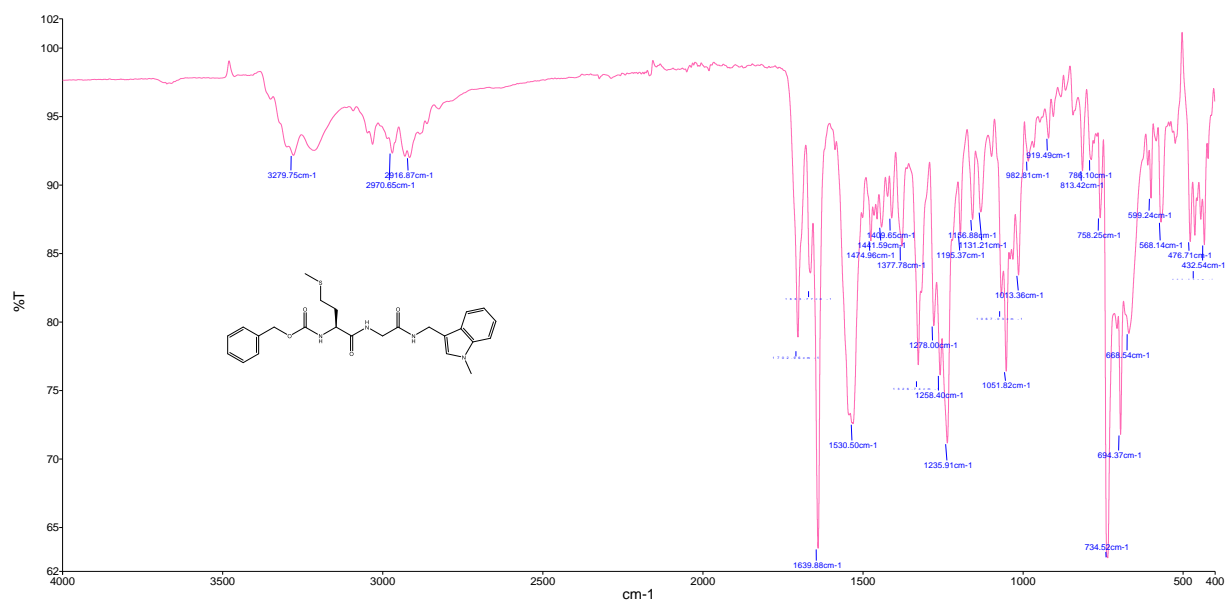
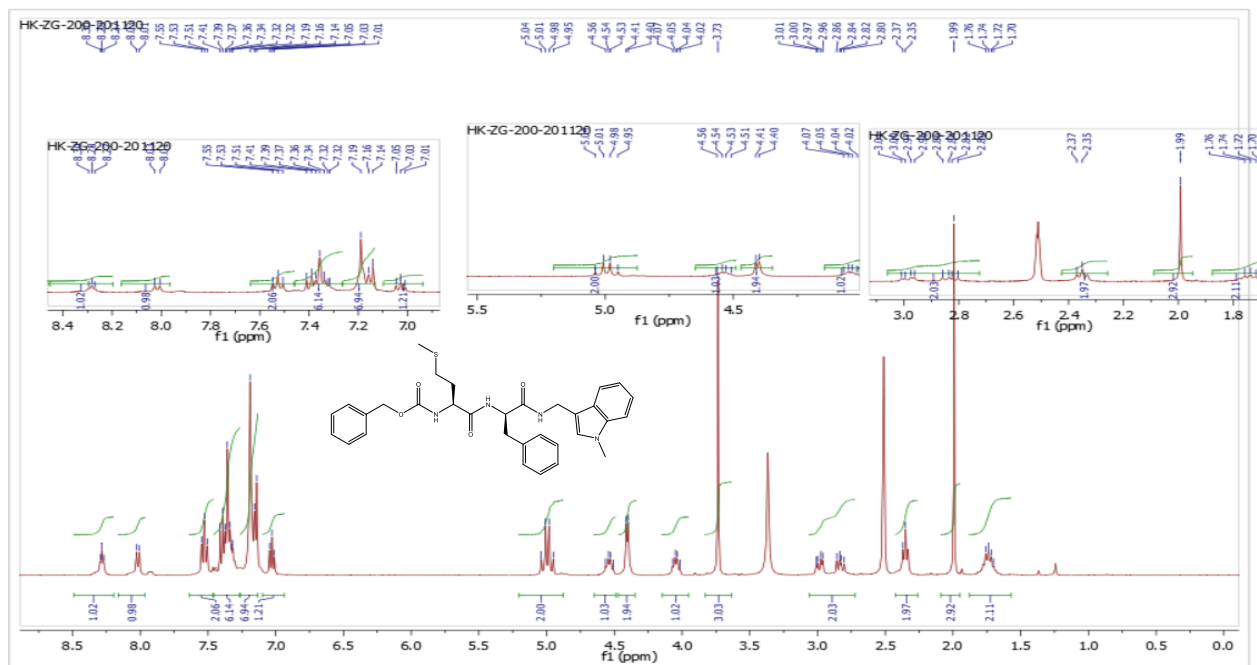


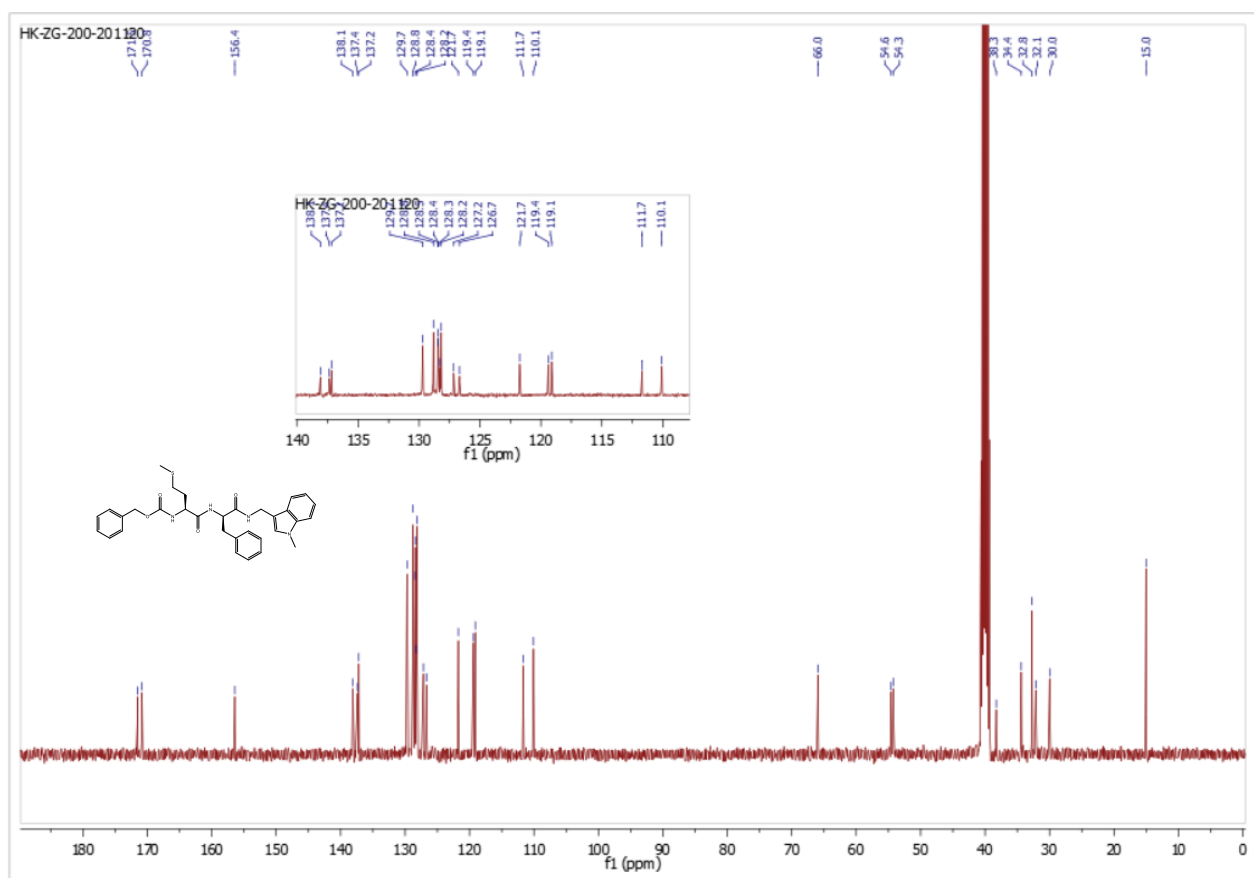
Figure S11: Mass spectrum of compound 3. ( $M+Na=505.189$ )



**Figure S12:** IR spectrum of compound 3.

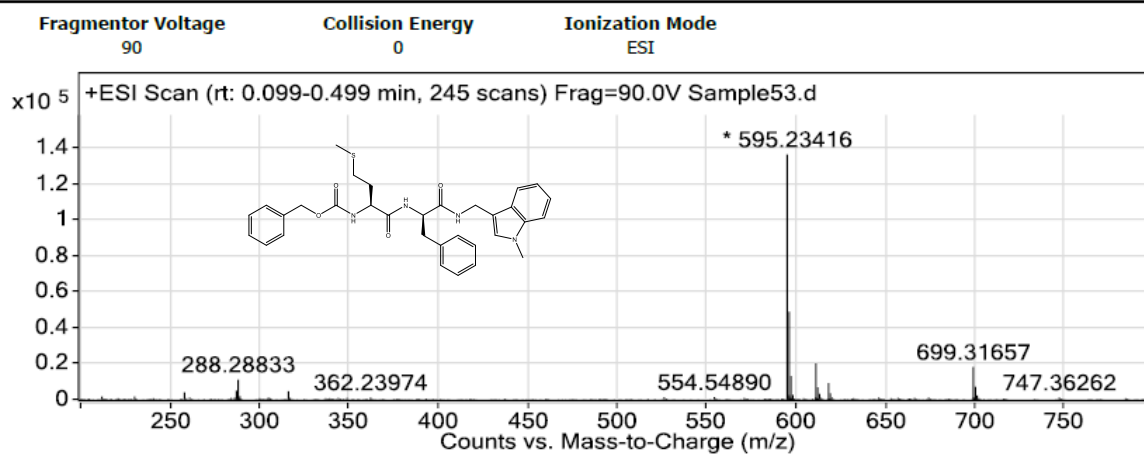


**Figure S13:**  $^1\text{H}$  NMR spectrum of compound 4.



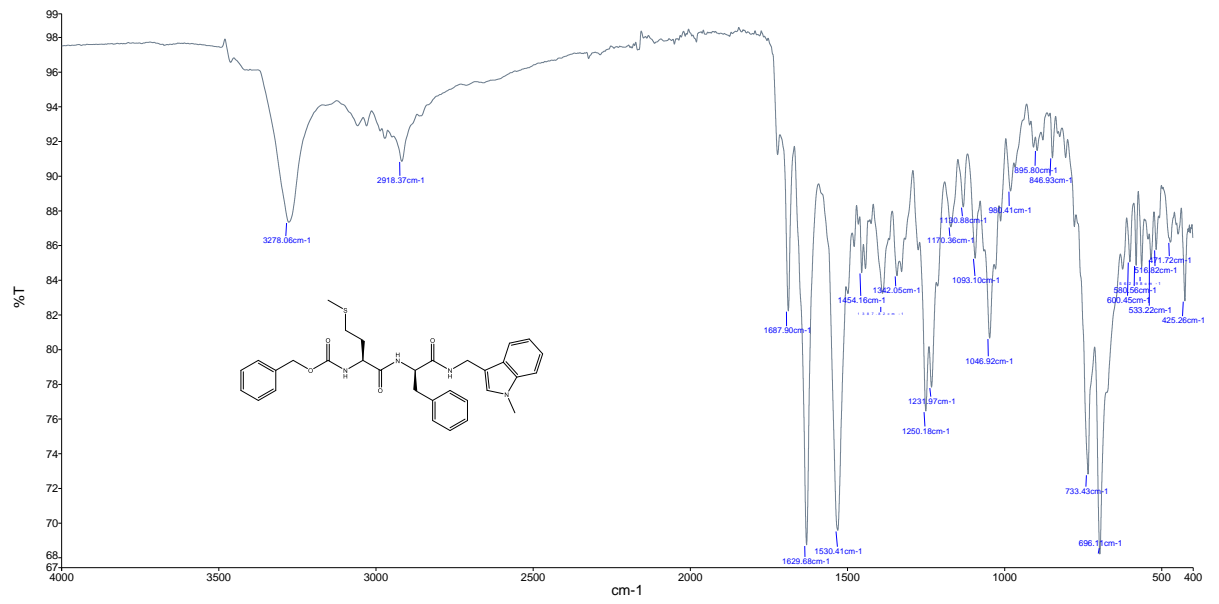
**Figure S14:** <sup>13</sup>C NMR spectrum of compound 4.

## User Spectra

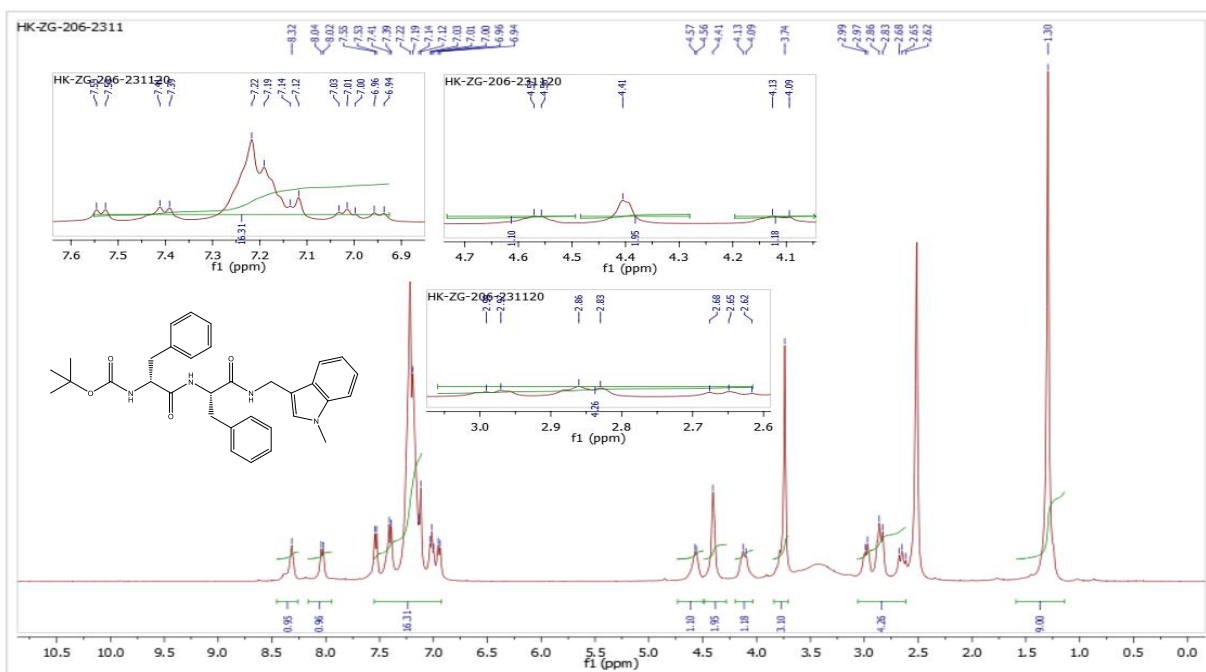


**Figure S15:** Mass spectrum of compound **4**. (M+Na) 595.235 exact mass

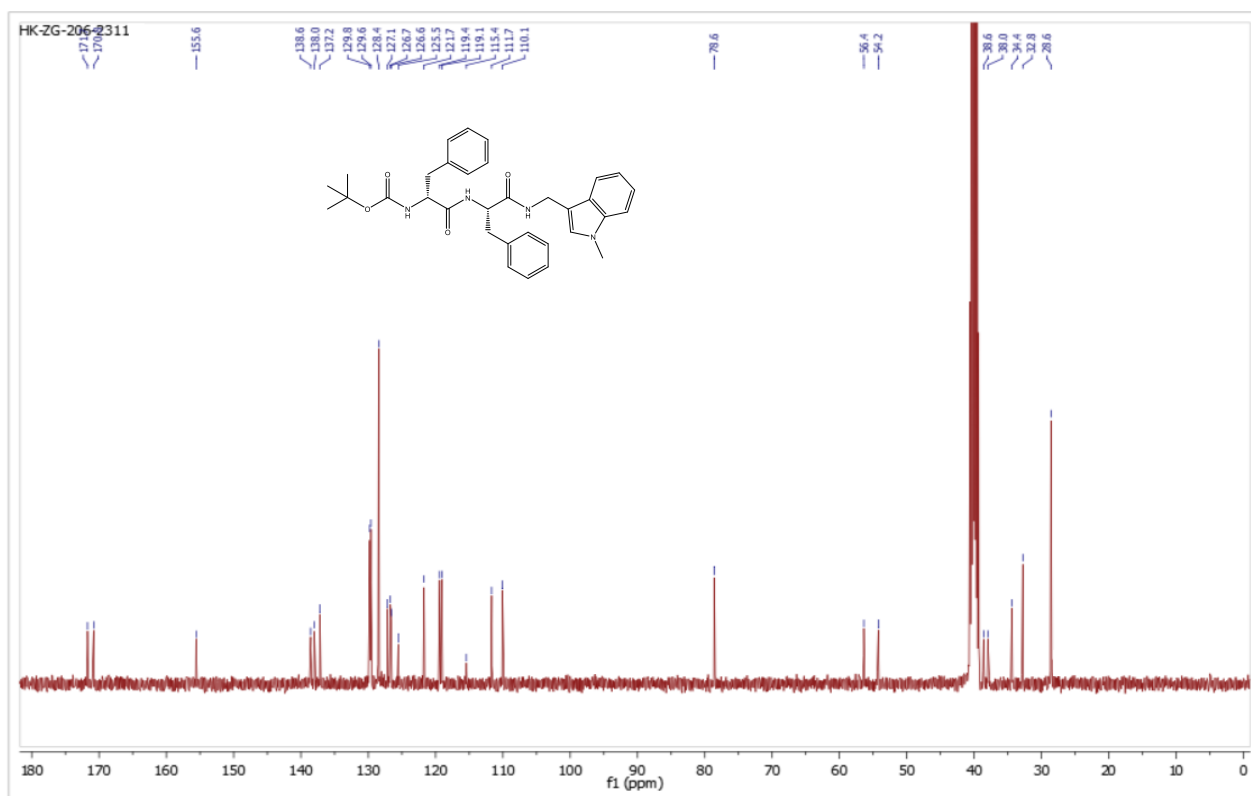




**Figure S16:** IR spectrum of compound **4**.

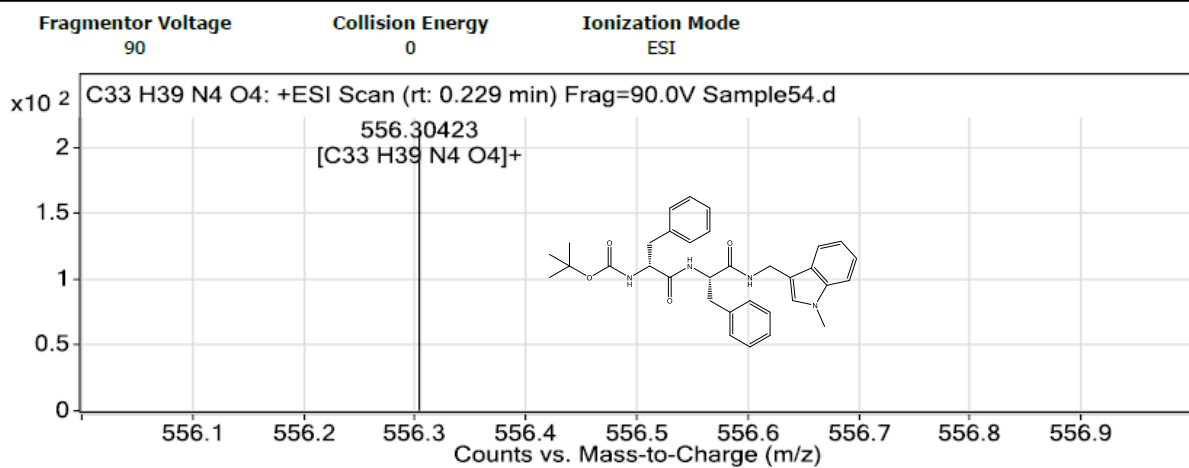


**Figure S17:** <sup>1</sup>H NMR spectrum of compound 5.

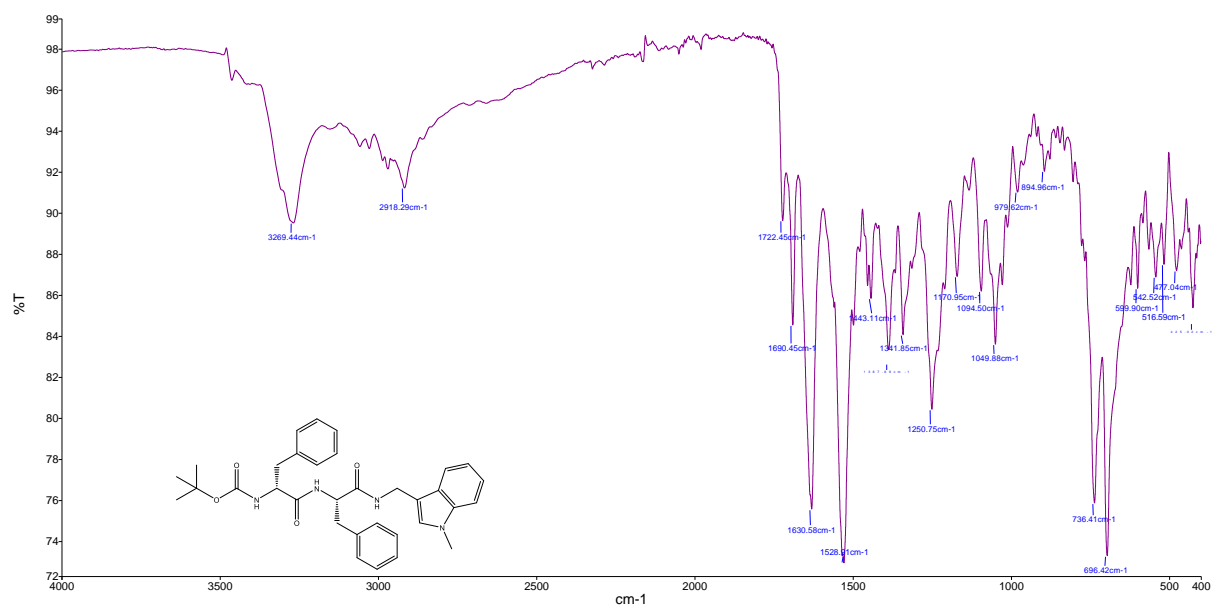


**Figure S18:**  $^{13}\text{C}$  NMR spectrum of compound 5.

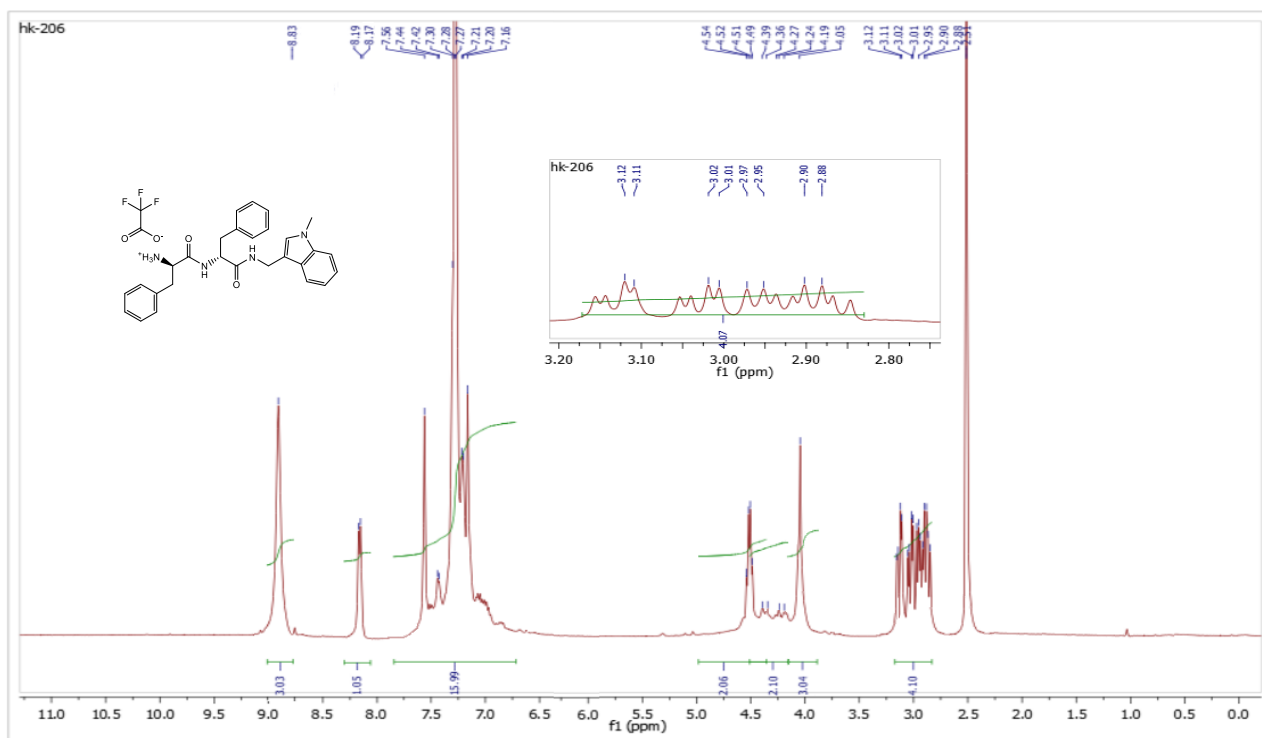
## User Spectra



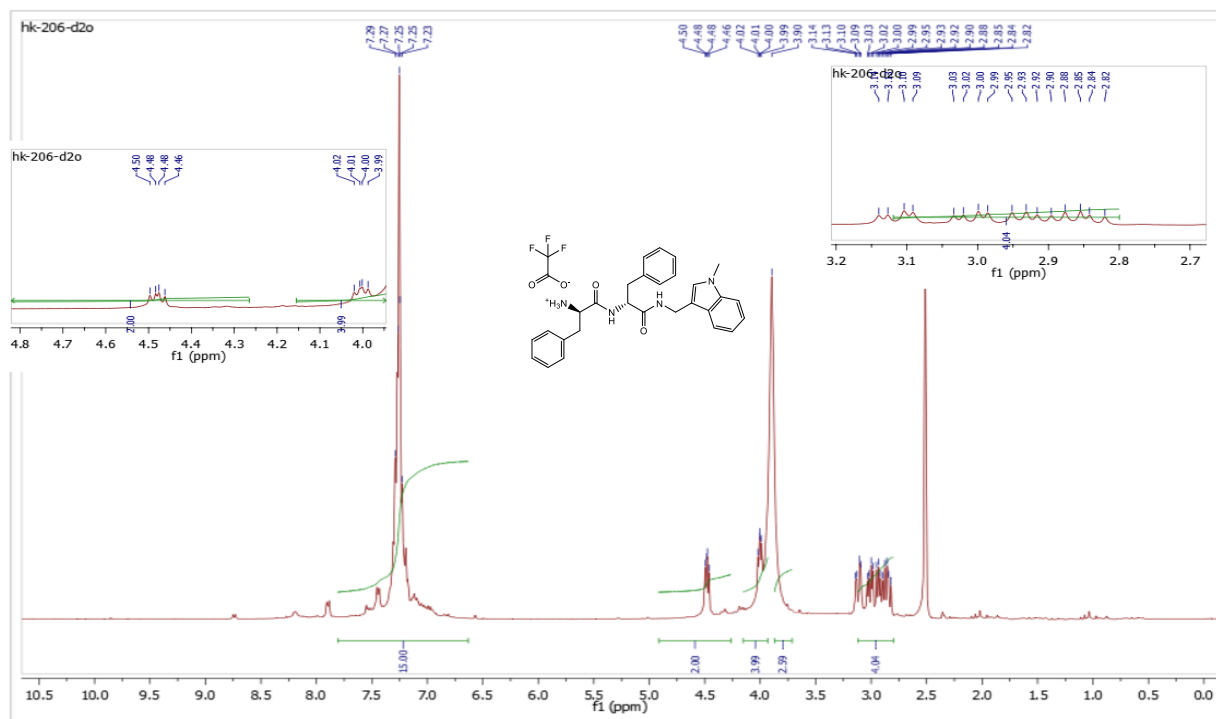
**Figure S19:** Mass spectrum of compound **5**. ( $M+ 2H$ ) 556.305 (555.297 tek H)



**Figure S20:** IR spectrum of compound 5.



**Figure S21:**  $^1\text{H}$  NMR spectrum of compound **6**.



**Figure S22:**  $^1\text{H}$  NMR +  $\text{D}_2\text{O}$  spectrum of compound **6**.

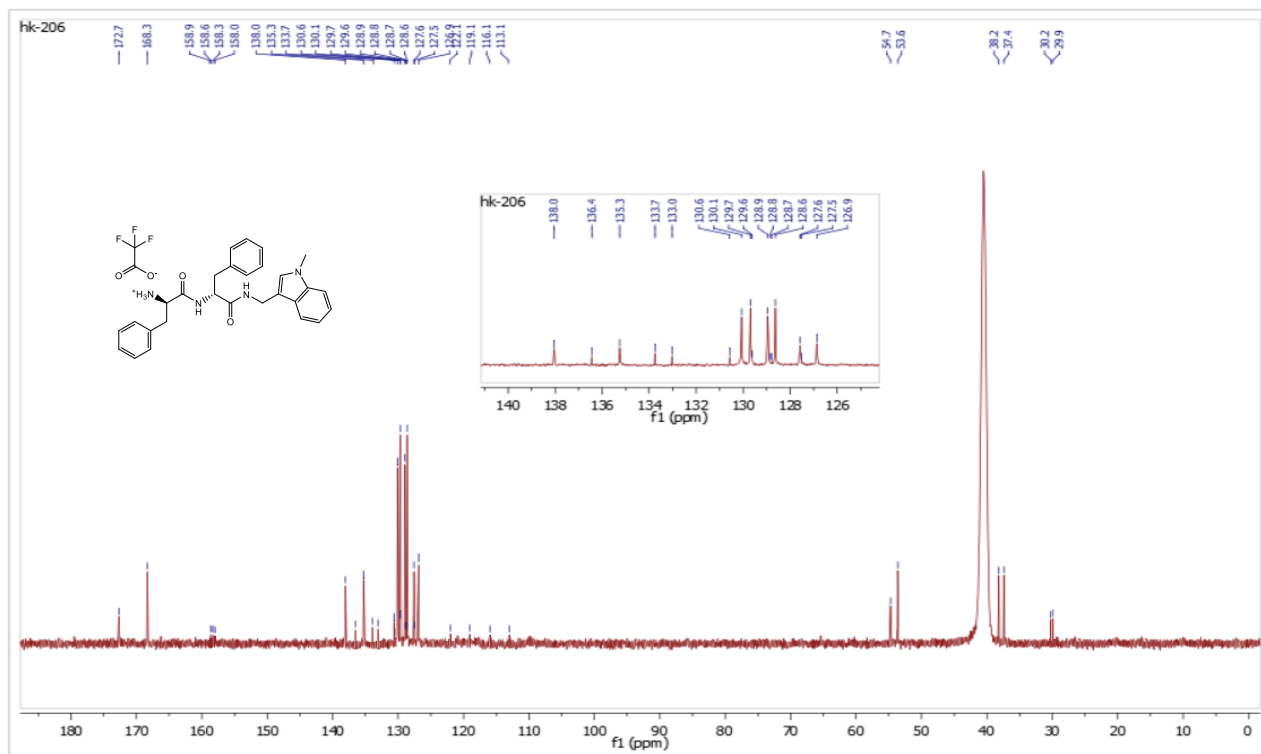
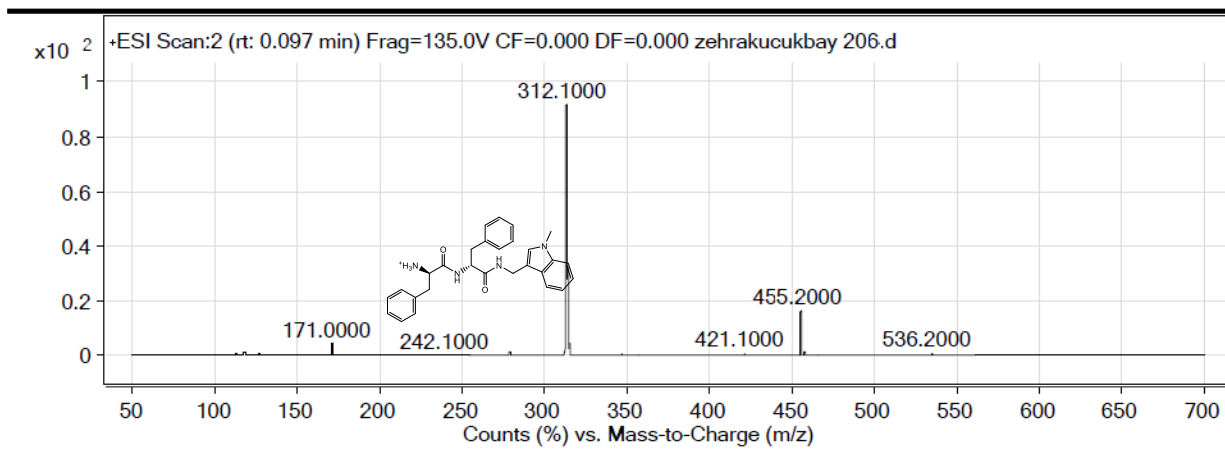
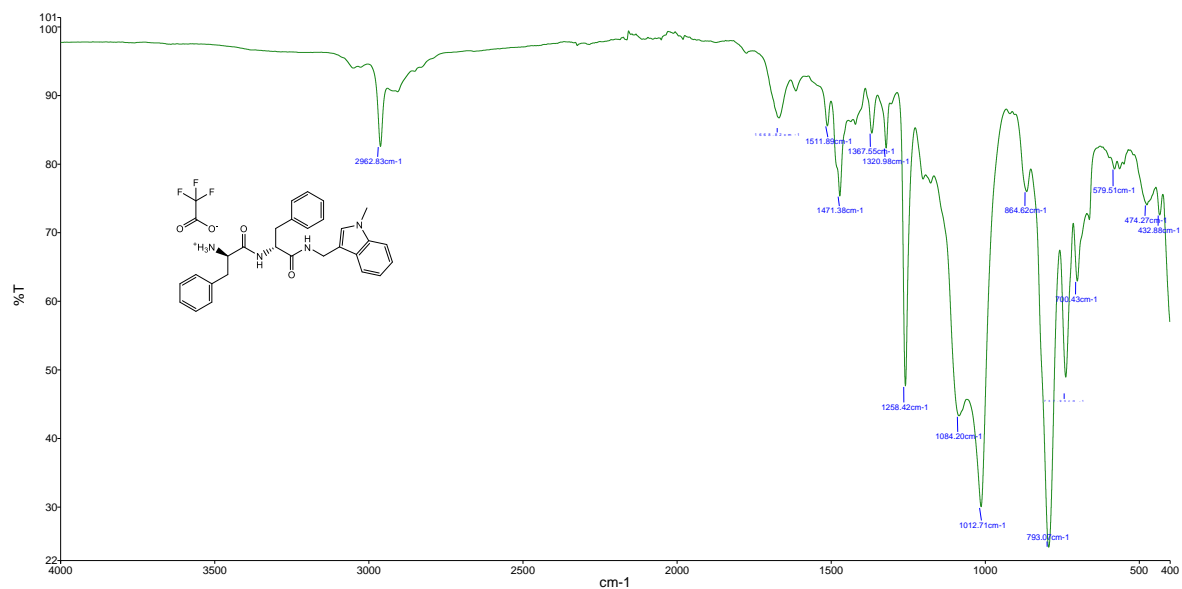


Figure S23:  $^{13}\text{C}$  NMR spectrum of compound 6.

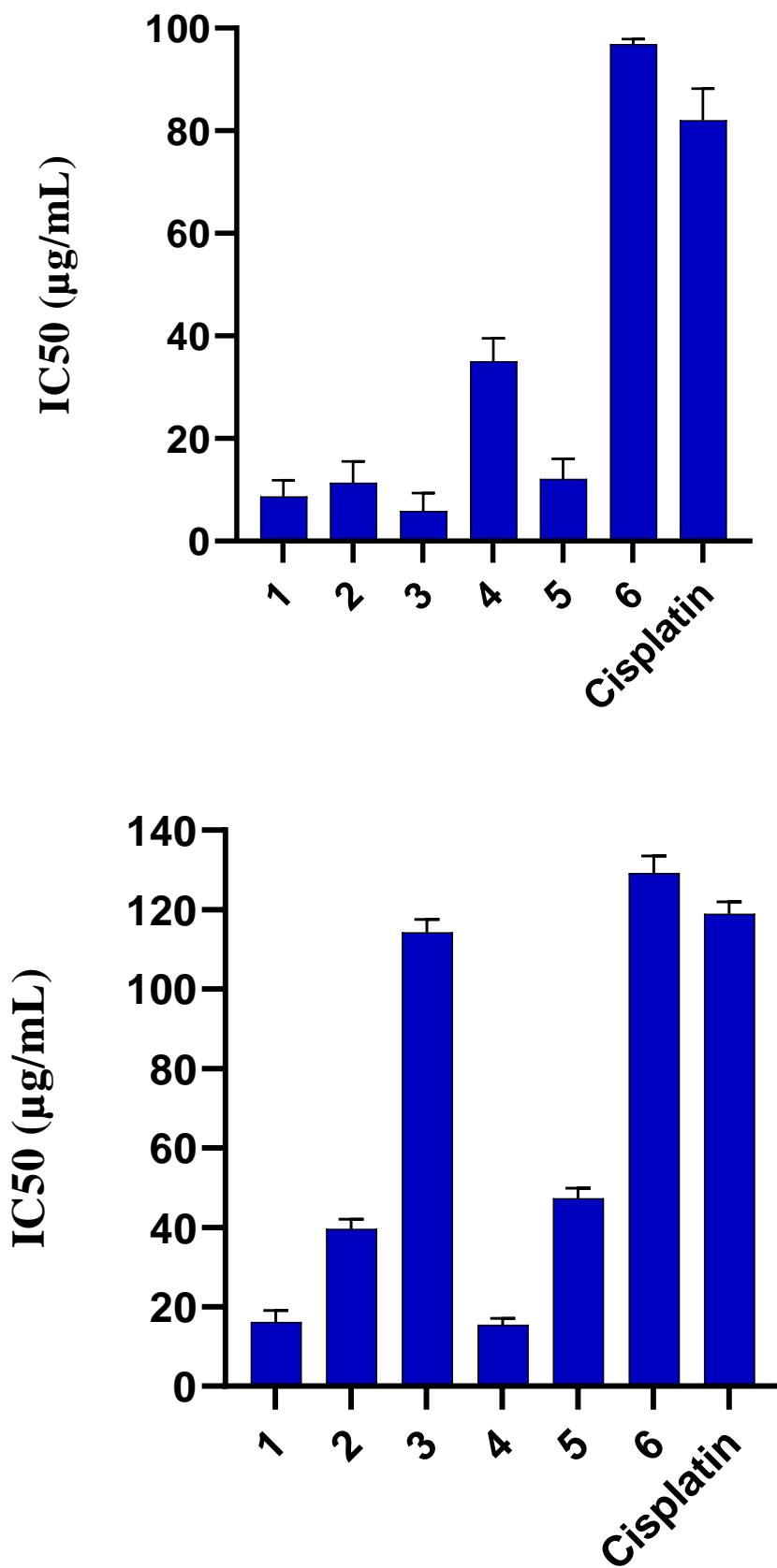




**Figure S24:** Mass spectrum of compound **6**.



**Figure S25:** IR spectrum of compound 6.



**Figure S26:** The IC<sub>50</sub> (μg/mL) values of each peptide-indole conjugate (1-6) against the MCF-7 and A549 cell lines.

**Table S1:** The Cartesian coordinates of compounds **1-6** computed in the gas phase at

B3LYP/6-311G+(d,p) level.

<b>1</b>			
C	-6.91099200	-1.89847900	1.40653900
C	-7.94689000	-1.52049800	0.55282300
C	-7.65855700	-1.11140100	-0.74790600
C	-6.33791600	-1.07925500	-1.19166700
C	-5.29270800	-1.45473300	-0.34340200
C	-5.59265900	-1.86630800	0.95885200
C	-3.86729900	-1.40355500	-0.81707500
O	-3.31183600	-0.12006800	-0.42167700
C	-2.00384300	0.07417100	-0.72093200
N	-1.58824200	1.28620300	-0.28097200
O	-1.30827200	-0.74268300	-1.30524900
C	-0.23234500	1.79216700	-0.51892400
C	0.74411000	1.28724000	0.58017400
N	0.99448200	-0.04359200	0.49495800
O	1.23312200	2.01766800	1.43354600
C	1.83834400	-0.76876800	1.44874900
C	3.08903900	-1.32375300	0.83450300
C	4.25079500	-0.58727500	0.40679300
C	5.17123900	-1.53408400	-0.11815400
N	4.59704900	-2.78641000	-0.01270300
C	3.34687200	-2.64269700	0.56043000
C	4.60331800	0.77131200	0.42579000
C	5.84248300	1.14813500	-0.07358800
C	6.73958500	0.19539700	-0.59336700
C	6.41923400	-1.15612100	-0.62247600
C	5.20575200	-4.03215500	-0.43341500
C	-0.22245700	3.32034400	-0.77101200
C	1.11146900	3.72169100	-1.42337500
C	-0.51584500	4.26040800	0.42199700
C	-1.84107300	4.06625800	1.16901100
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H	-8.46067200	-0.81996300	-1.41660200
H	-6.11590800	-0.76076700	-2.20502000
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H	-3.26401200	-2.19596600	-0.37029300
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H	2.07511300	-0.06195800	2.24556700
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H	3.91804500	1.50995200	0.82734700
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H	-1.01487200	3.47565700	-1.51610900
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C	-3.64699600	-0.16498400	-0.34571900
C	-4.73735500	-0.80807700	0.29954000
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C	-3.34876500	-2.39341800	-0.46047200
C	-3.61889900	1.23729400	-0.40802700
C	-4.66021000	1.95268900	0.16713200
C	-5.73104100	1.29739600	0.80472800
C	-5.78657200	-0.08876300	0.87977700
C	-5.41924900	-3.19003200	0.74579600
H	3.26182500	0.75999900	-0.71364500
H	0.96626600	0.70374900	1.06067600
H	0.00957400	-1.08094000	-0.02191300
H	-1.60106500	-0.33360300	-2.40005800
H	-1.15796600	-1.98946500	-1.98217400
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H	-4.65236200	3.03599000	0.12563400
H	-6.52881800	1.88542100	1.24449400
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C	2.86357100	-1.11509300	0.59574500
C	4.00203500	-1.87328000	-0.11861000
N	2.85015600	0.27735800	0.16288200
C	-0.81454000	-1.64461800	-0.31235000
C	-1.72006600	-0.55372700	-0.89090700
N	-3.01164000	-0.92092500	-1.06574600
O	-1.29075600	0.56005600	-1.16431000
C	-4.03813300	-0.01423400	-1.59988100
C	-5.40128100	-0.37295200	-1.10077500
C	-5.90422200	-0.24238400	0.24342900
C	-7.24888000	-0.70060300	0.22683100
N	-7.54816100	-1.09036500	-1.06505400
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C	3.01657700	4.87935100	0.33984600
C	4.23613200	5.55302300	0.23677200
C	4.36790700	6.65861000	-0.60205900
C	3.27766100	7.09929300	-1.34939000
C	2.05603200	6.43246900	-1.25381100
C	1.92715200	5.33058400	-0.41272100
O	5.50244300	-3.70757200	-0.21351700
C	5.89997400	-4.98815100	0.21735600
S	7.36805300	-5.54955200	-0.70093000
H	0.64916000	-0.14065000	-0.40886800
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H	3.76153300	-2.00081000	-1.18010200
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H	3.16582500	0.50632000	-0.76855200
H	-0.81037600	-2.51507200	-0.97834600
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H	-3.75216700	0.99680000	-1.30076300
H	-4.02058900	-0.03670900	-2.69497200
H	-6.45736500	-1.12463100	-2.90291200
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H	-5.73781300	0.57597000	3.52839600
H	-8.06920900	-0.23353200	3.46188500
H	-9.07193300	-1.05787600	1.35307200
H	-9.62135300	-0.86732100	-1.36095400
H	-8.76556800	-1.82755400	-2.58034800
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H	4.56746600	-3.13070600	1.55216800
H	3.51447000	-3.93595200	0.37559200
H	1.90927800	3.66313300	1.74161000
H	3.65930800	3.65506600	1.99751900
H	5.08663700	5.21106600	0.81756100
H	5.31900100	7.17459600	-0.67077600
H	3.37743500	7.96023100	-2.00090900
H	1.20415800	6.77361000	-1.83128500
H	0.97581300	4.81389100	-0.33985000
H	6.20485400	-4.98020700	1.27184800
H	5.08629600	-5.71195700	0.09547300
H	6.74656800	-5.70284300	-1.88826500
<b>4</b>			
N	0.90183500	-0.40133700	-0.94110400
C	1.28746400	-0.63741900	0.33908300
O	1.39519900	-1.75273400	0.82915300
C	1.64155700	0.60635100	1.18030700
C	3.16507100	0.77352700	1.32989500
N	1.08267700	1.84566300	0.64821900
C	0.39517800	-1.45052400	-1.81509500
C	-1.08033100	-1.12619300	-2.11180800
N	-1.98443200	-2.04186800	-1.69245700
O	-1.38118100	-0.08363100	-2.68257100
C	-3.43650100	-1.83742800	-1.80868200
C	-4.18037700	-2.48011200	-0.68211000
C	-4.15259500	-2.11246500	0.71252400
C	-5.04035900	-2.99365700	1.38629300
N	-5.57968100	-3.85431900	0.44764300
C	-5.05271700	-3.53479400	-0.78745700
C	-3.47153400	-1.13129800	1.45144200
C	-3.69203900	-1.05216400	2.81912100
C	-4.57686100	-1.93387700	3.46825200
C	-5.26267500	-2.91569600	2.76433700
C	-6.54563500	-4.89993000	0.72024600
C	-0.21645300	2.20410000	0.89094300
O	-0.44308900	3.46293900	0.44900800
O	-1.04819300	1.48769800	1.40745500
C	3.86790500	-0.39441000	2.01024900
C	-1.81454300	3.93664400	0.57383100
C	-1.89629400	5.28828000	-0.07691200
C	-1.70947600	6.45179200	0.67457800
C	-1.76912500	7.70503100	0.06844000
C	-2.01755000	7.80579500	-1.29944800
C	-2.20725100	6.65055800	-2.05718900
C	-2.14724600	5.39938800	-1.44813600

O	5.23081400	-0.00228400	2.19061400
C	6.01721500	-1.02823700	2.75144100
S	7.73368200	-0.46922400	2.98308800
H	0.70967300	0.55427200	-1.20977700
H	1.19442000	0.41231900	2.15879400
H	3.62096500	0.93672900	0.34744300
H	3.34897600	1.67094400	1.92901300
H	1.70696900	2.57777800	0.34316500
H	0.49357800	-2.38343200	-1.25803900
H	-1.66685400	-2.82929400	-1.14705200
H	-3.59780800	-0.75698000	-1.83543000
H	-3.78926300	-2.23488200	-2.76639600
H	-5.35382400	-4.08721300	-1.66559400
H	-2.77877300	-0.44478300	0.97841900
H	-3.16823200	-0.29936500	3.39628200
H	-4.72520500	-1.84687400	4.53877400
H	-5.94240300	-3.59170000	3.27039300
H	-7.47046700	-4.48226900	1.12961300
H	-6.78133100	-5.41759400	-0.20926300
H	-6.14414800	-5.62825200	1.43110400
H	3.40690100	-0.60947900	2.98451800
H	3.80677400	-1.30491900	1.40607800
H	-2.47303600	3.21316900	0.09107300
H	-2.07015600	3.98173200	1.63396500
H	-1.51800700	6.37537000	1.74005300
H	-1.62515100	8.60047800	0.66253100
H	-2.06766500	8.78017700	-1.77241800
H	-2.40561100	6.72452500	-3.12052300
H	-2.29709800	4.50170000	-2.03905400
H	5.66446000	-1.30120500	3.75430400
H	5.99945400	-1.92307400	2.11947600
H	8.04135600	-0.39915900	1.67166000
C	1.18523700	-1.54103100	-3.14160900
H	1.04576800	-0.60262000	-3.68399600
H	0.72341800	-2.32651700	-3.74976600
C	2.65705300	-1.83164100	-2.95482700
C	3.60996200	-0.81572800	-3.07885600
C	3.09981900	-3.12217900	-2.64200500
C	4.96699000	-1.07747200	-2.89237800
H	3.28706200	0.18884300	-3.33273200
C	4.45354700	-3.38921600	-2.45358200
H	2.37878700	-3.92815700	-2.54542500
C	5.39303200	-2.36594600	-2.57741600
H	5.69009200	-0.27608600	-2.99784500
H	4.77567500	-4.39644800	-2.21335400
H	6.44777800	-2.57334100	-2.43558500
<b>5</b>			
N	-0.84084500	1.28085400	0.41316500
C	-1.53433300	0.12171000	0.33851600
O	-1.03635500	-0.97005600	0.61214900
C	-2.99866600	0.23951100	-0.11549700
C	-3.12286500	0.61949600	-1.62560900
N	-3.63479100	-1.02878600	0.16902900
C	0.57285000	1.32995000	0.80925100
C	1.47209300	1.04359000	-0.42276200



N	1.56258800	-0.26898100	-0.73833800
O	2.00892500	1.94306000	-1.05841900
C	2.32785800	-0.75450900	-1.89341300
C	3.70377200	-1.24748900	-1.55342800
C	4.07103800	-2.54197200	-1.04121200
C	5.48094100	-2.52795000	-0.85447000
N	5.94375700	-1.28286400	-1.23208600
C	4.86648400	-0.52647600	-1.65038900
C	3.35842400	-3.71013800	-0.72784600
C	4.04839900	-4.81483400	-0.24815900
C	5.44454200	-4.77917000	-0.07169500
C	6.17885600	-3.63878400	-0.37226300
C	7.32820400	-0.85435400	-1.20581000
C	-4.97770200	-1.11436900	0.37432700
O	-5.30643500	-2.37199500	0.74771100
O	-5.75016700	-0.18268900	0.22800900
C	-6.70603500	-2.75941600	1.01356900
H	-1.26475800	2.12626700	0.05500100
H	-3.49408900	1.02068900	0.46852800
H	-2.44226100	-0.00636300	-2.20943200
H	-4.14120300	0.34870800	-1.91233800
H	-3.03207900	-1.79997200	0.42359400
H	0.71395100	0.53099100	1.53975700
H	1.02134300	-0.92355400	-0.18665300
H	1.74465700	-1.55020700	-2.36547500
H	2.39247600	0.07374500	-2.59962600
H	5.00925400	0.49180800	-1.97983700
H	2.28197500	-3.75452100	-0.85619000
H	3.50642600	-5.72107700	-0.00283400
H	5.95598900	-5.65731200	0.30574500
H	7.25398400	-3.61859600	-0.23489500
H	7.94400800	-1.47366400	-1.86520900
H	7.38579100	0.17880100	-1.54706300
H	7.73440200	-0.90765900	-0.19144200
C	0.89087600	2.68745300	1.45624500
H	0.06783800	2.92688300	2.13614400
H	0.91527800	3.45033700	0.67437300
C	2.19335200	2.69649500	2.23104500
C	2.22344900	2.26154100	3.56146200
C	3.38518800	3.13493400	1.64450000
C	3.41152600	2.26175400	4.28911600
H	1.30580200	1.92696600	4.03636500
C	4.57443600	3.14049900	2.37190100
H	3.37582300	3.45883600	0.61053900
C	4.59272600	2.70360000	3.69514300
H	3.41321700	1.92361400	5.31949300
H	5.48850600	3.48865000	1.90308100
H	5.51810500	2.70995100	4.26027800
C	-7.26064900	-1.95237100	2.19049700
H	-6.60604400	-2.05135600	3.06037300
H	-7.35600100	-0.89753600	1.93743300
H	-8.24678600	-2.33852600	2.46317400
C	-6.57261600	-4.23672700	1.38537800
H	-7.55638700	-4.65602100	1.60975500
H	-6.13371000	-4.80285100	0.56082400

H	-5.93516700	-4.35623200	2.26423000
C	-7.54704400	-2.59332200	-0.25472300
H	-7.09781000	-3.14688000	-1.08350200
H	-8.54863700	-2.99683000	-0.08179000
H	-7.63643200	-1.54498300	-0.53554300
C	-2.89722700	2.08485800	-1.92733800
C	-1.75296500	2.52914600	-2.59928500
C	-3.84828100	3.03530400	-1.52719300
C	-1.55811900	3.88542400	-2.86266400
H	-1.00418100	1.81106900	-2.91684500
C	-3.65636400	4.38959000	-1.78953600
H	-4.74876200	2.70493800	-1.01876600
C	-2.50881400	4.81924200	-2.45735200
H	-0.66225300	4.20774700	-3.38099700
H	-4.40514600	5.10935900	-1.47774300
H	-2.35982700	5.87337000	-2.66233900
<b>6</b>			
N	0.47587200	-1.62413000	0.41964200
C	1.13292500	-0.44086000	0.42891500
O	0.61199200	0.60886300	0.79403200
C	2.61484500	-0.47549800	-0.01122100
C	2.81405300	-0.89358700	-1.49345500
N	3.21452900	0.85091400	0.23670700
C	-0.95502900	-1.72039400	0.72024900
C	-1.76449900	-1.31619200	-0.53406100
N	-2.36617400	-0.11078200	-0.46921200
O	-1.82678800	-2.05443200	-1.51230400
C	-3.13602000	0.44121700	-1.59287900
C	-3.90841500	1.65592000	-1.18867600
C	-3.38301700	2.94937000	-0.83068600
C	-4.49828700	3.77933300	-0.53351700
N	-5.64348400	3.02506200	-0.70104500
C	-5.27343800	1.75484300	-1.09447300
C	-2.08949100	3.48778300	-0.73268900
C	-1.94013300	4.81444100	-0.35420500
C	-3.05847600	5.61985000	-0.06748000
C	-4.34997300	5.11592400	-0.15222600
C	-7.00139000	3.50254300	-0.52453000
H	0.91189000	-2.41822200	-0.03071400
H	3.12942700	-1.20709200	0.62073000
H	2.11469200	-0.33354300	-2.12196700
H	3.82274400	-0.56978100	-1.77177400
H	2.53377700	1.41160800	0.75359100
H	-1.15678000	-1.02490900	1.53648900
H	-2.17282400	0.49088600	0.31807400
H	-2.44934500	0.67140700	-2.41662400
H	-3.80605900	-0.34048000	-1.95596300
H	-6.02629000	1.00343300	-1.28148000
H	-1.21727500	2.87767100	-0.94074100
H	-0.94665300	5.24028200	-0.27348900
H	-2.90887300	6.65231300	0.22684300
H	-5.20628400	5.74206900	0.07046400
H	-7.24056700	4.28791000	-1.24799900
H	-7.69143000	2.67225700	-0.67174800
H	-7.14538600	3.89722900	0.48506800

C	-1.29080600	-3.15641000	1.16158800
H	-0.58621900	-3.43158700	1.95180700
H	-1.11915600	-3.82355000	0.31248600
C	-2.71044000	-3.31355300	1.66418100
C	-3.02096400	-3.06048400	3.00542200
C	-3.74017200	-3.70582500	0.80173300
C	-4.32623500	-3.19241700	3.47480400
H	-2.23225400	-2.76690000	3.69172000
C	-5.04650700	-3.84073200	1.26920000
H	-3.51365500	-3.90080800	-0.24065300
C	-5.34416100	-3.58350100	2.60625400
H	-4.54633400	-2.99689800	4.51847000
H	-5.83136300	-4.15161200	0.58831100
H	-6.35953500	-3.69260900	2.97056000
C	2.69785900	-2.37840000	-1.77325500
C	1.58997600	-2.91066200	-2.44236400
C	3.71872400	-3.24962900	-1.36733800
C	1.50247000	-4.28030900	-2.69659800
H	0.78030100	-2.26059500	-2.75594700
C	3.63315000	-4.61567500	-1.62142200
H	4.59241800	-2.85449900	-0.85793200
C	2.52264100	-5.13531600	-2.28767500
H	0.63363100	-4.67219700	-3.21270200
H	4.43482400	-5.27318200	-1.30451000
H	2.45647000	-6.19867700	-2.48797000
H	4.58698400	0.70030700	1.00841300
H	3.36611100	1.33775700	-0.64230800
O	5.54764000	0.47264700	1.45199900
C	6.53621500	1.33953700	1.43154600
O	7.61990800	1.17780000	1.91882000
C	6.21498300	2.67294500	0.68366200
F	7.21574500	3.54225300	0.75549000
F	5.96303800	2.43026500	-0.63047500
F	5.10604800	3.26303400	1.19116900