

Supporting Information

For

A Novel 5-anilinoquinazoline-8-nitro derivatives as inhibitors of VEGFR-2 tyrosine kinase: synthesis, biological evaluation and molecular docking

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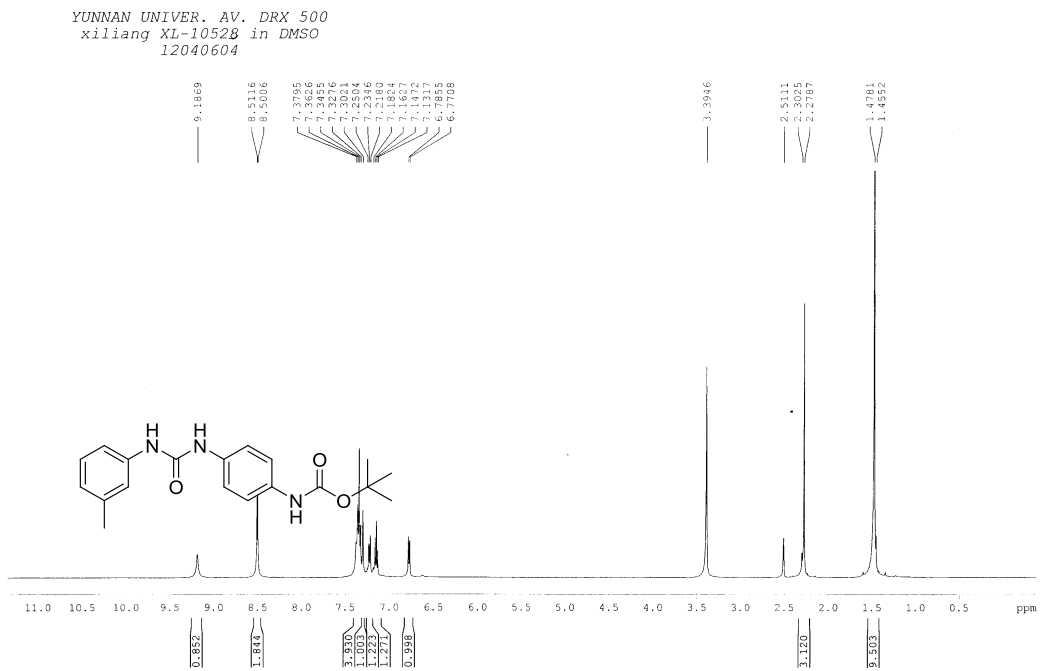
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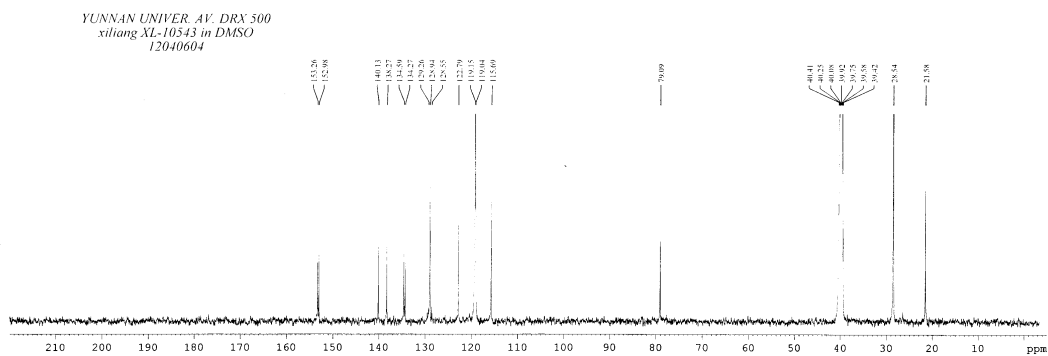
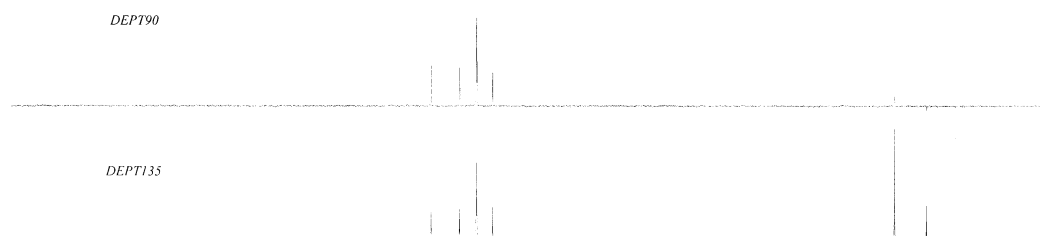
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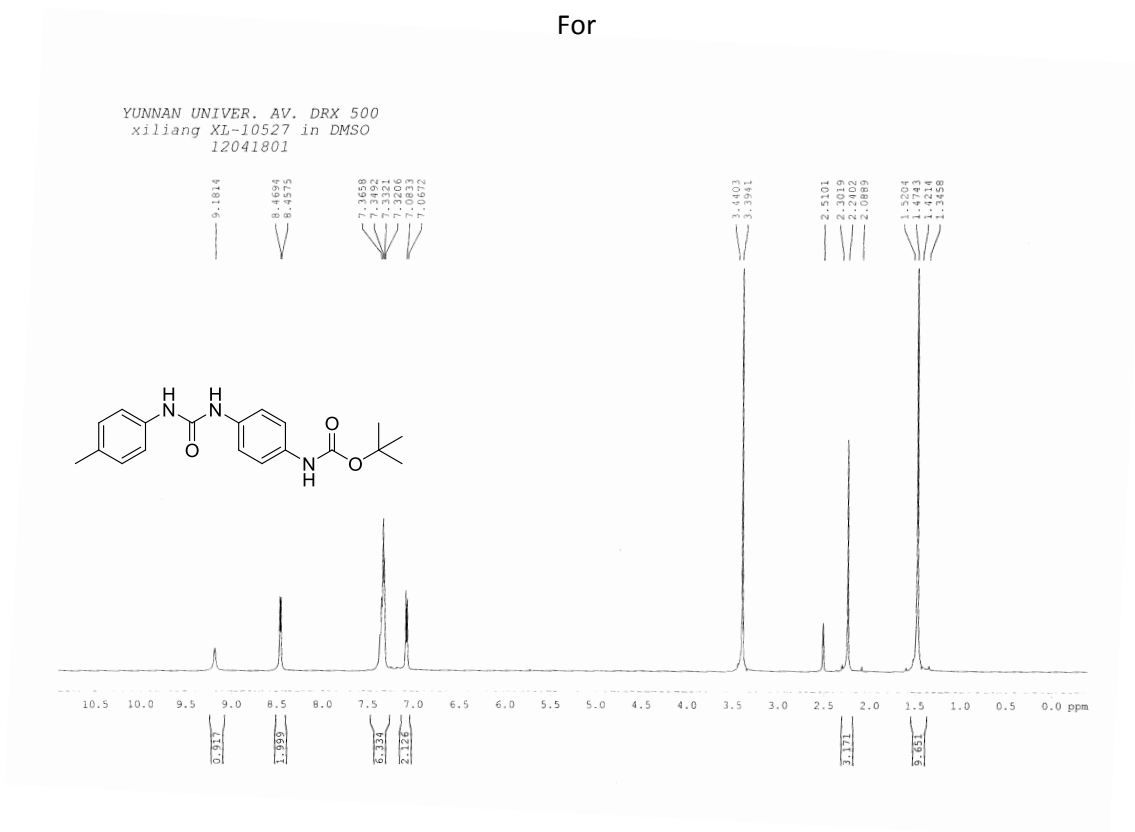
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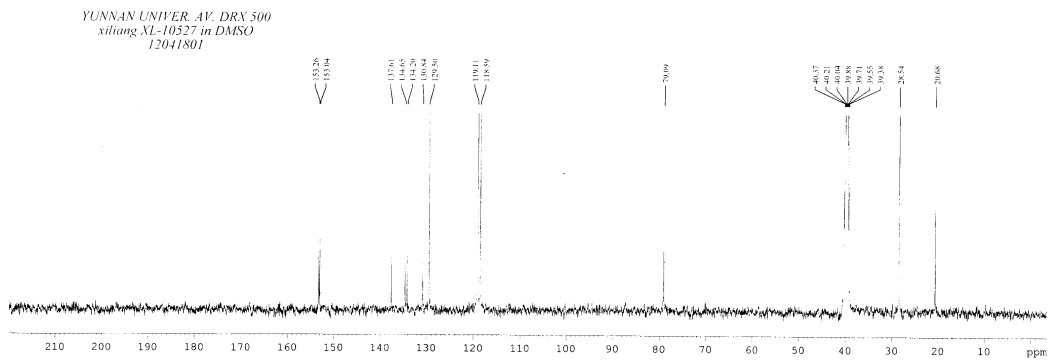
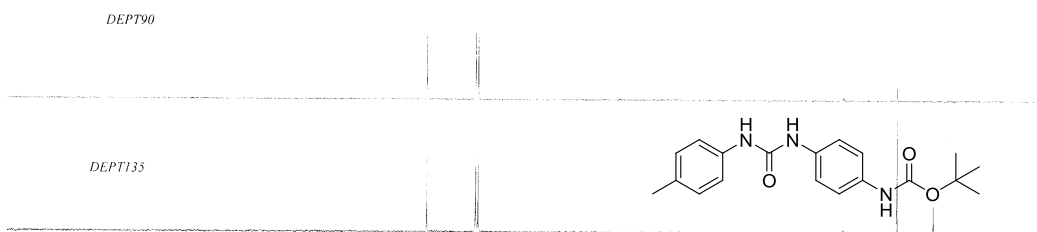
¹³C-NMR spectrum of 4a

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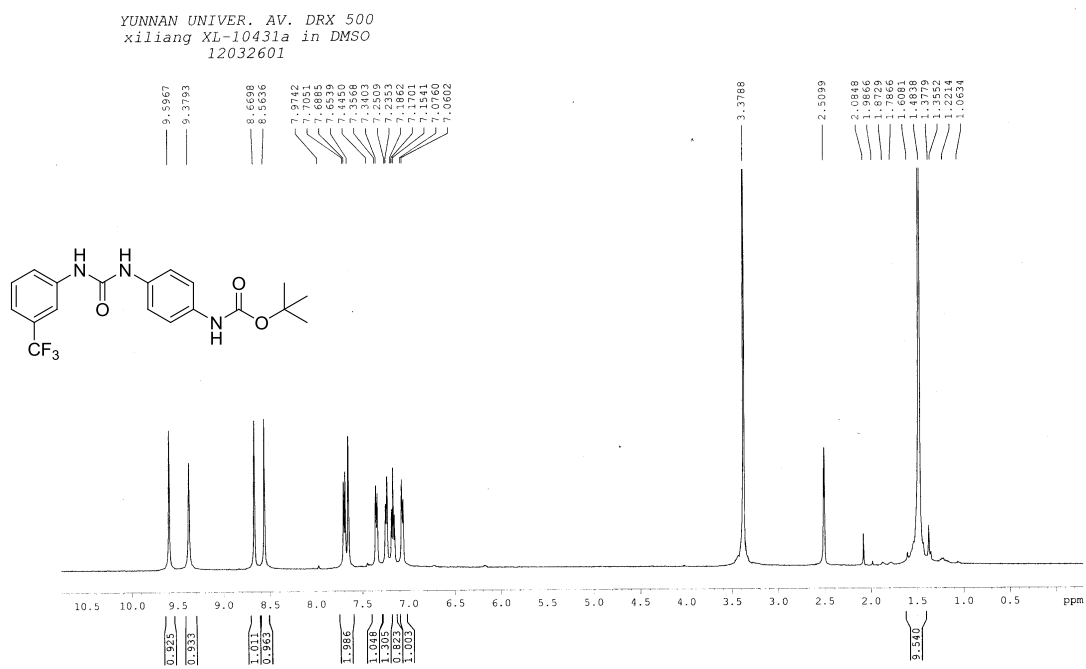
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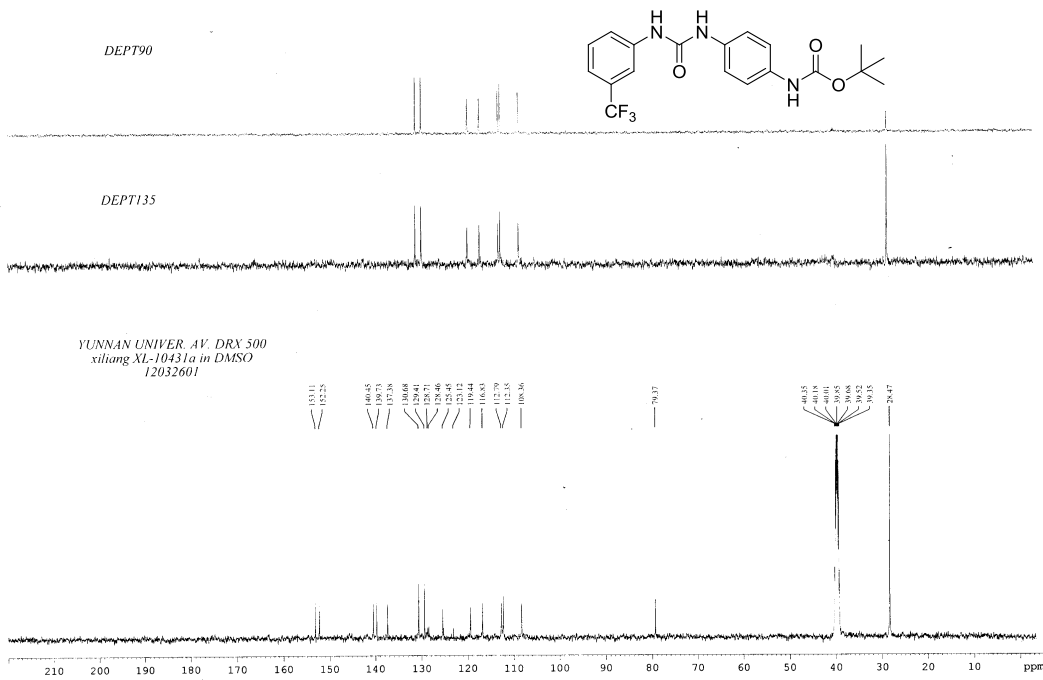
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¹³C-NMR spectrum of 4b



¹H-NMR spectrum of 4d

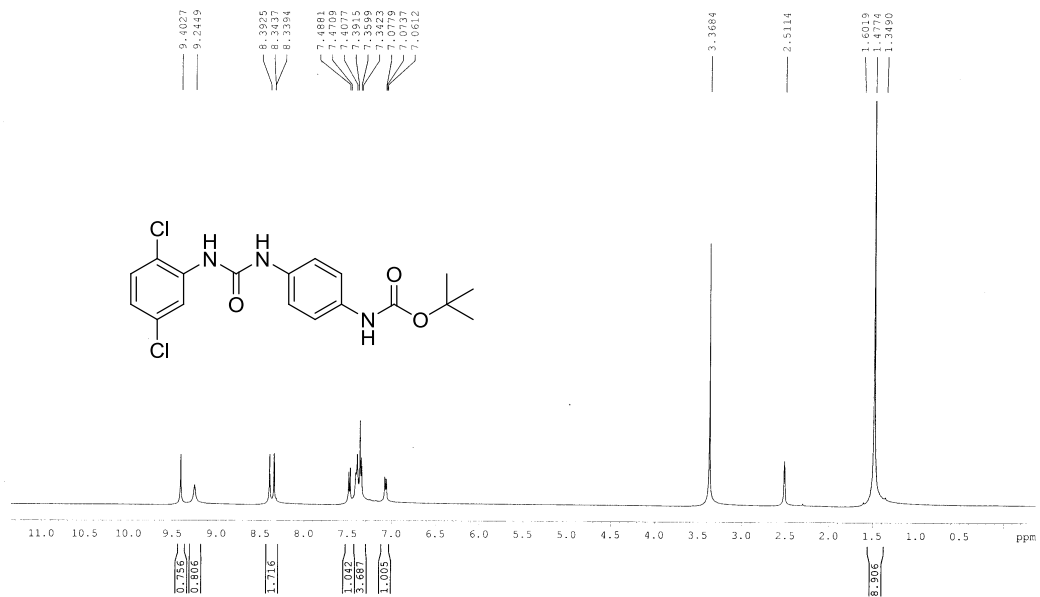


¹³C-NMR spectrum of 4d

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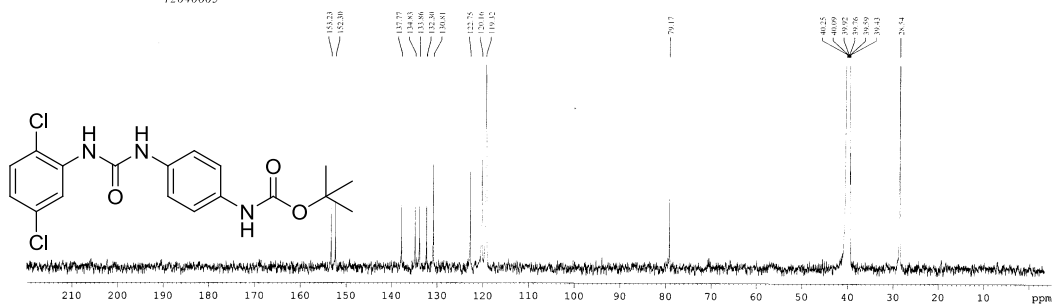
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¹H-NMR spectrum of 4e



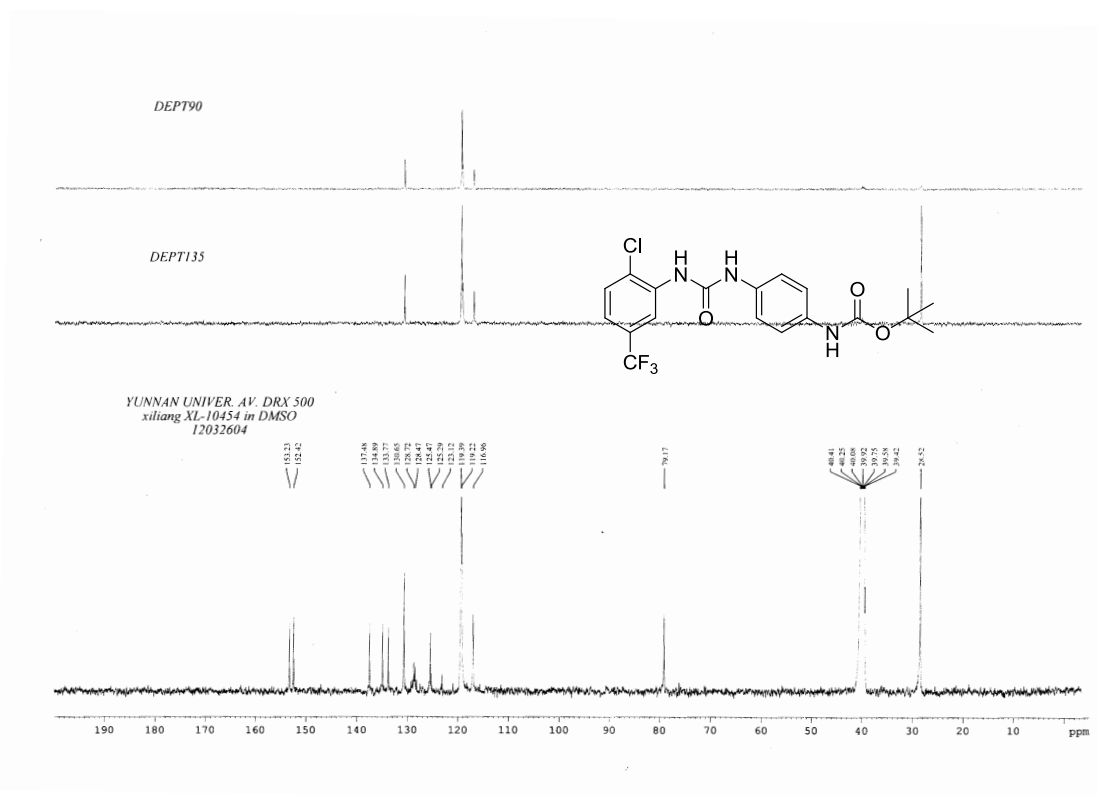
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¹³C-NMR spectrum of 4e



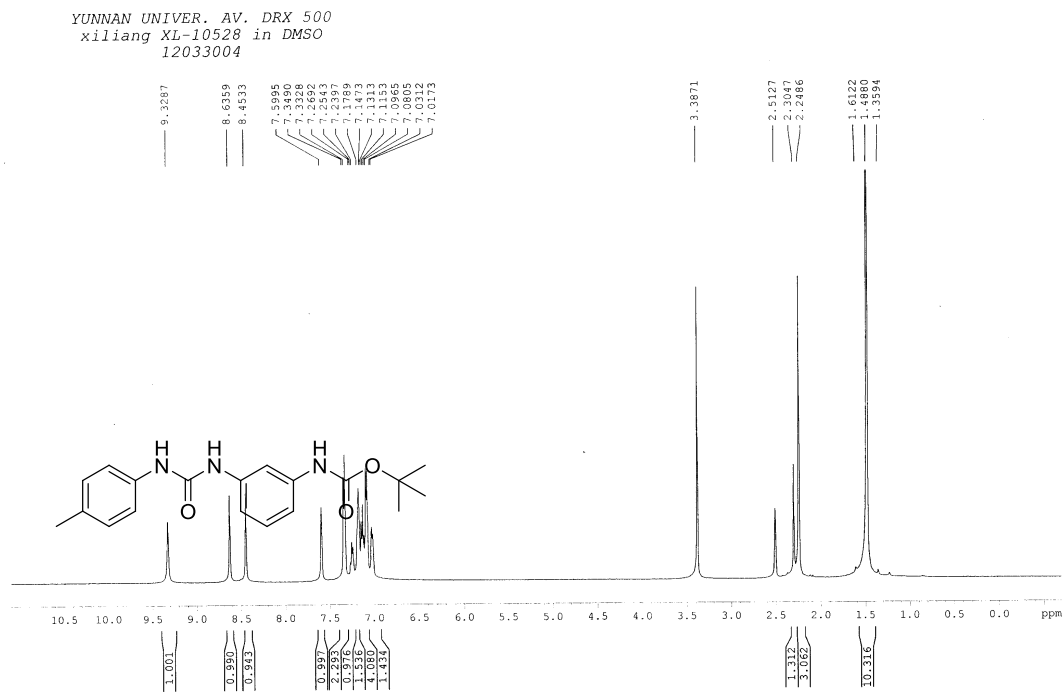
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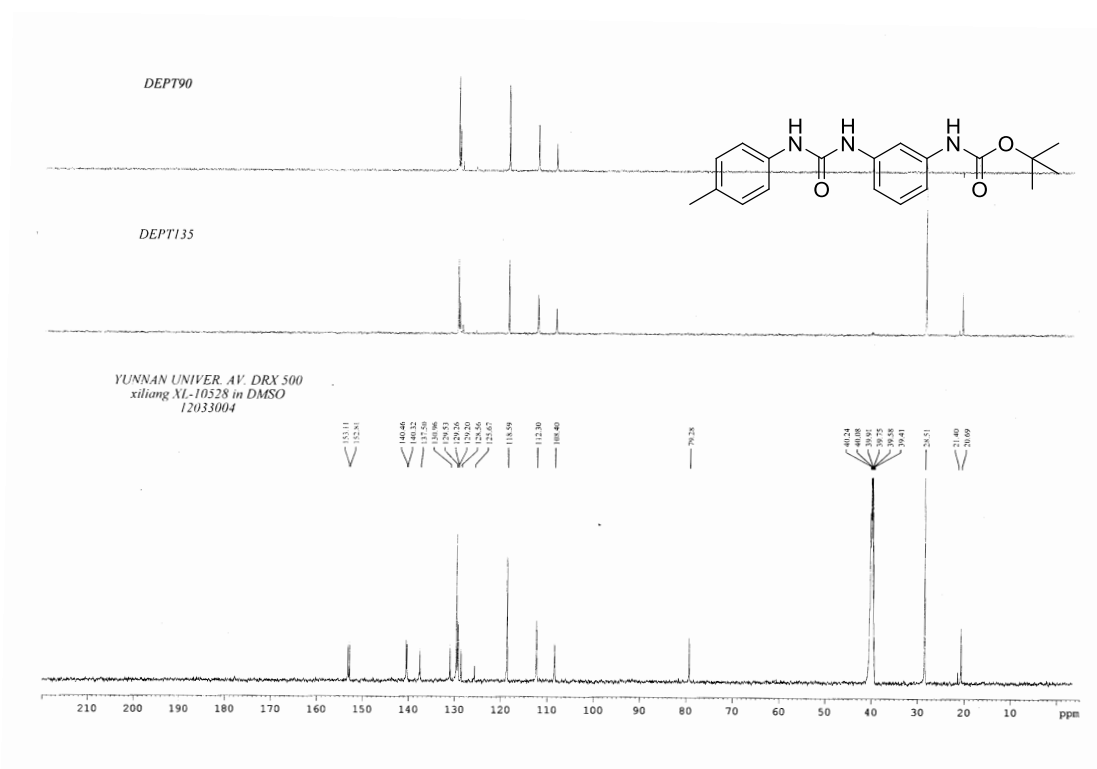
¹³C-NMR spectrum of 4f

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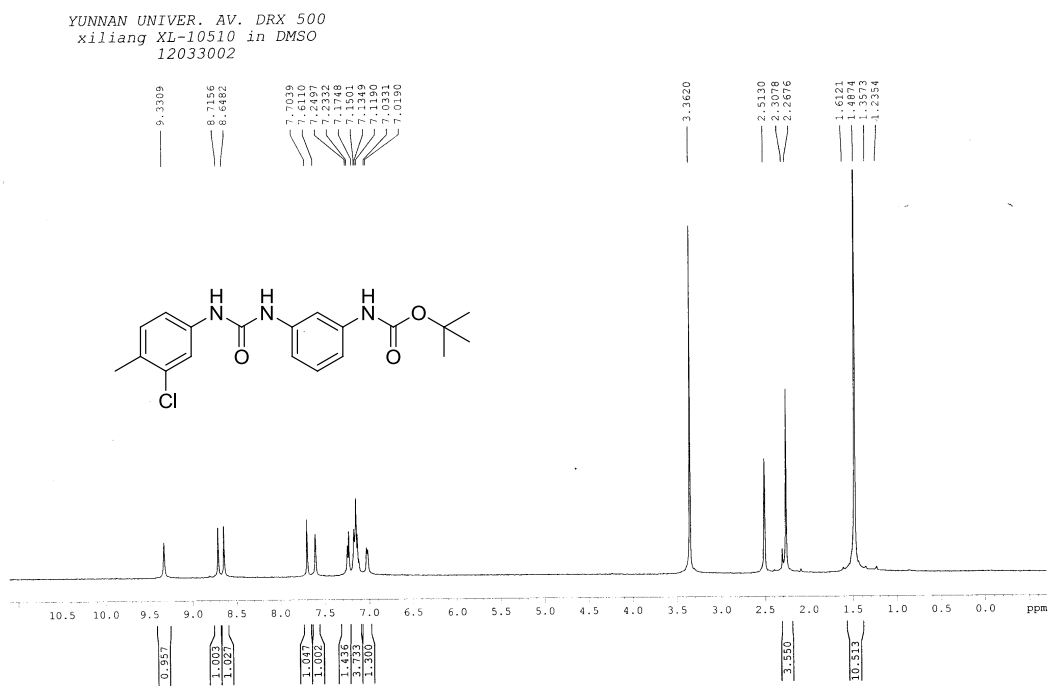


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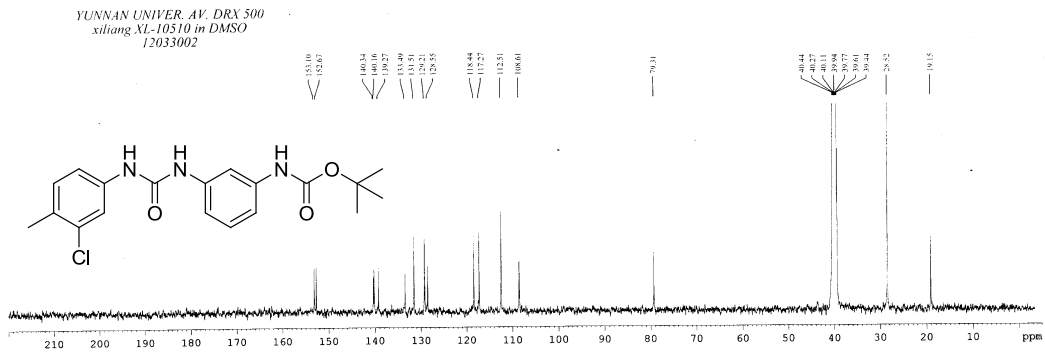
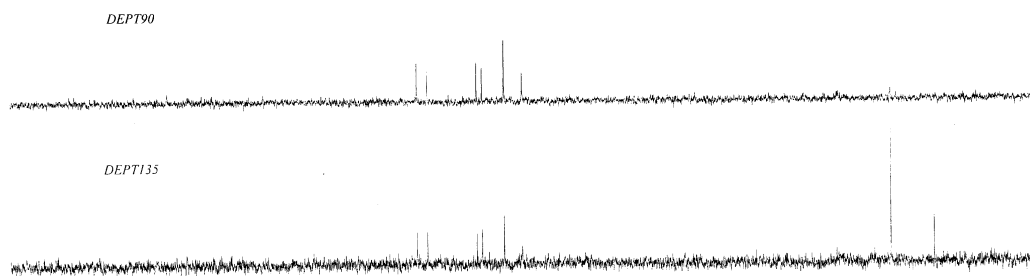


¹³C-NMR spectrum of 4g

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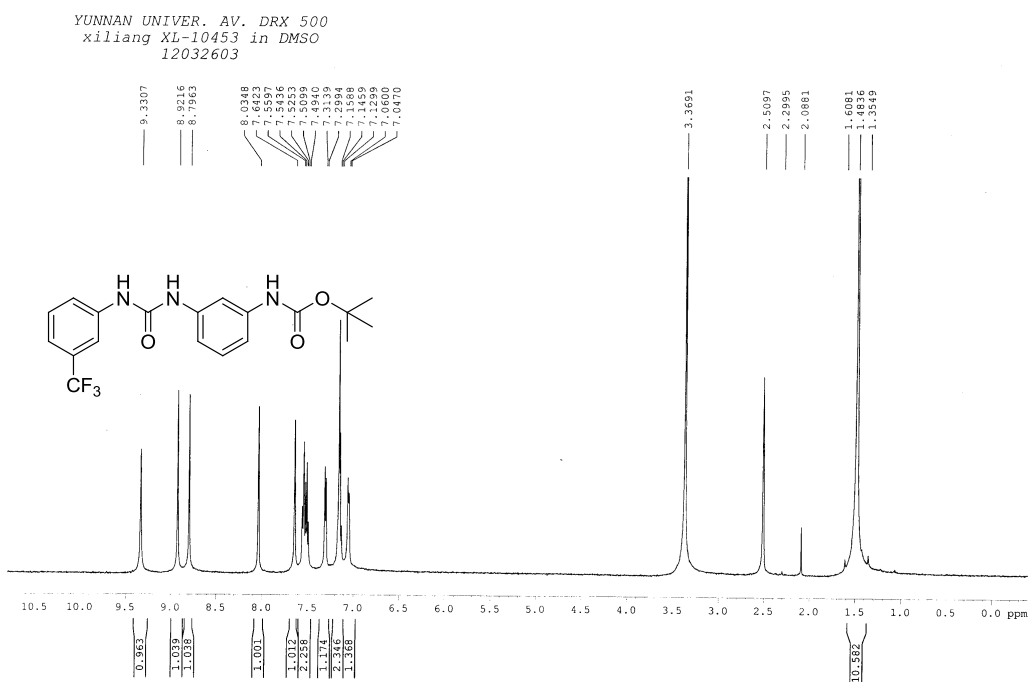
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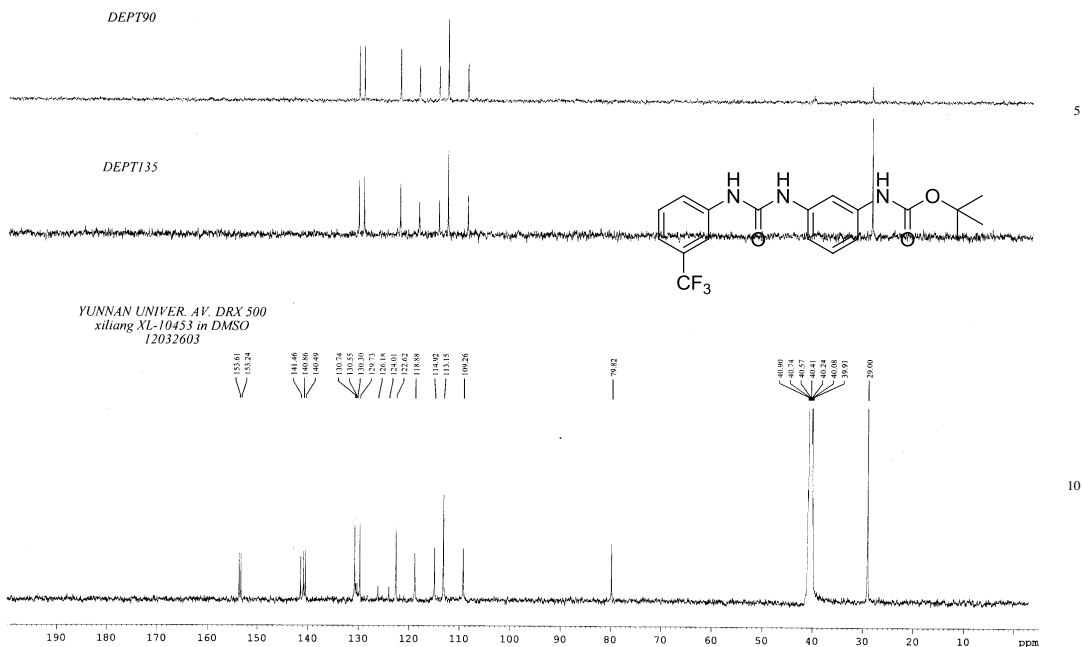
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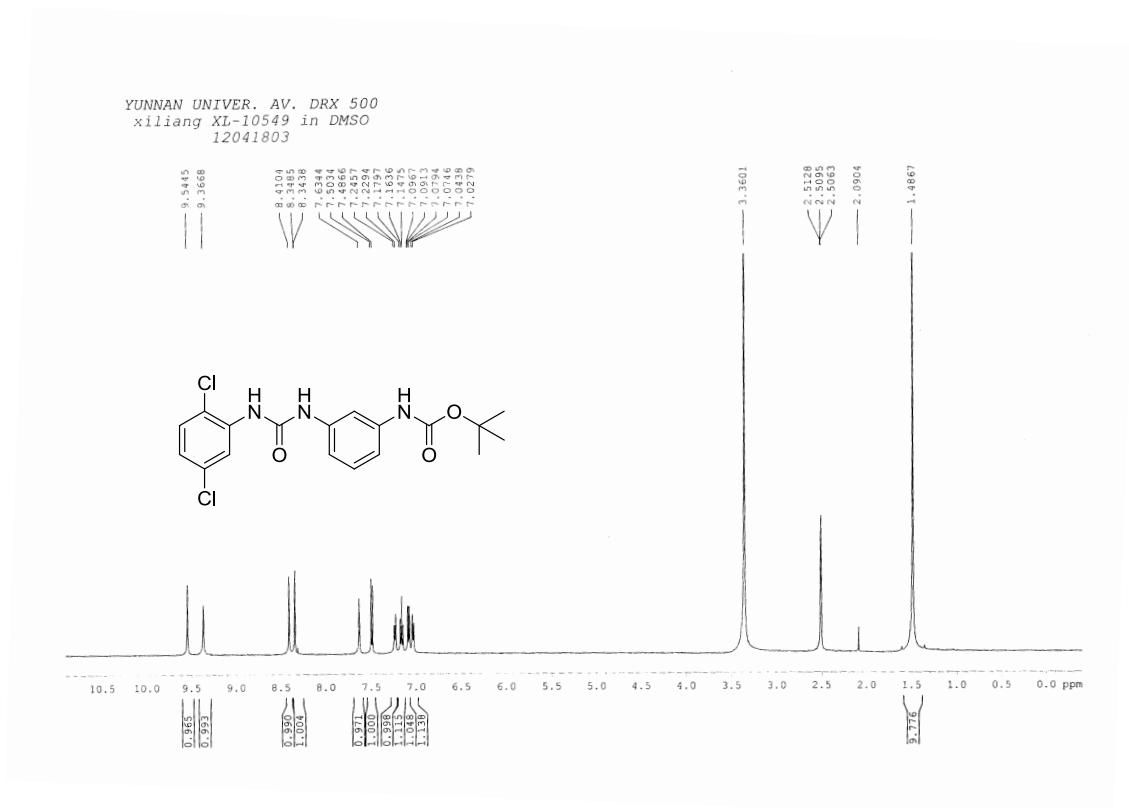
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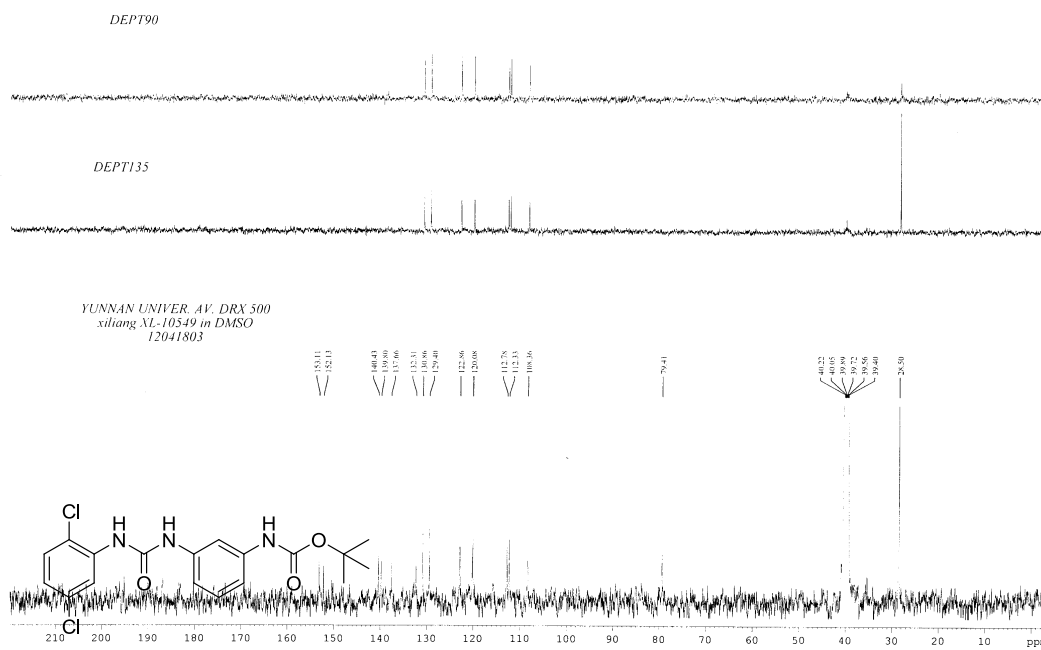
¹H-NMR spectrum of 4i



¹³C-NMR spectrum of 4i

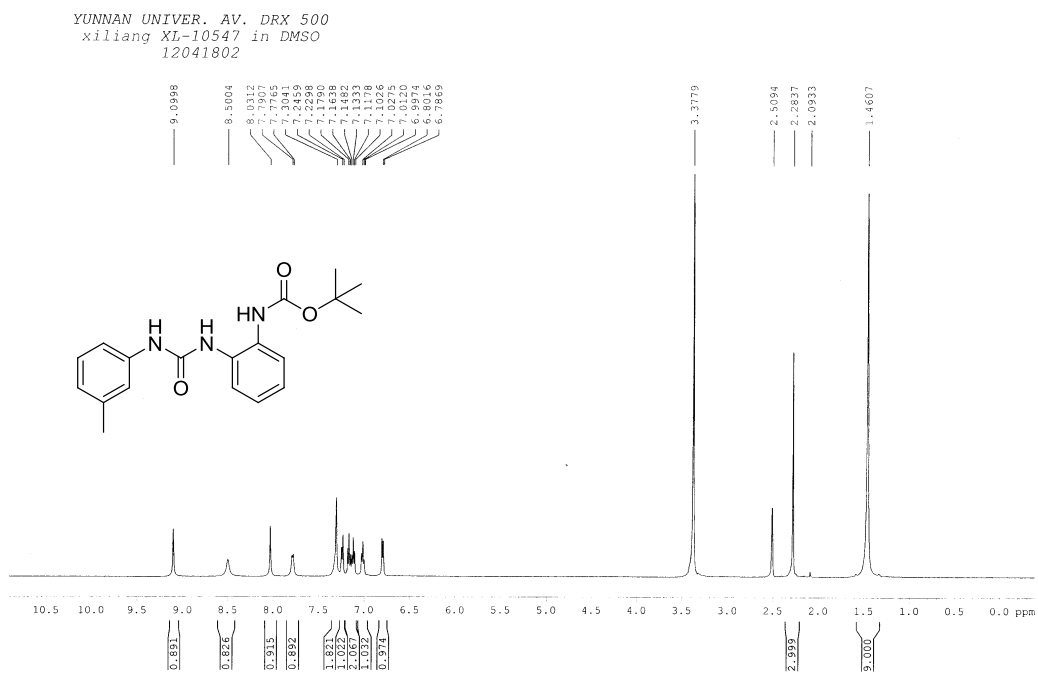


¹H-NMR spectrum of 4j

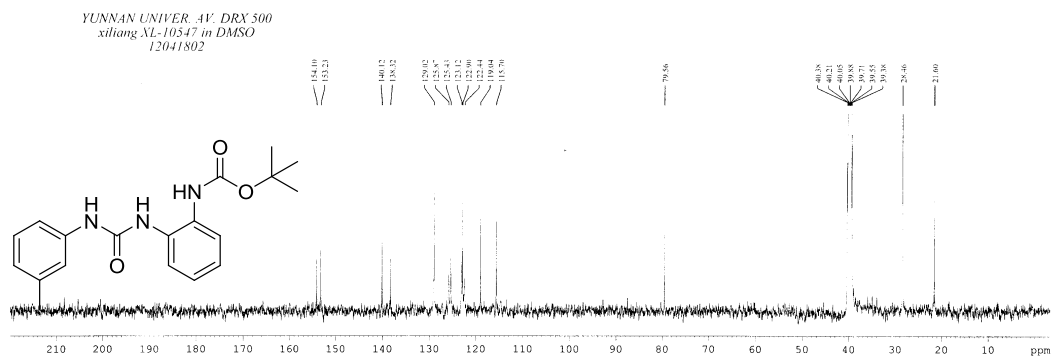
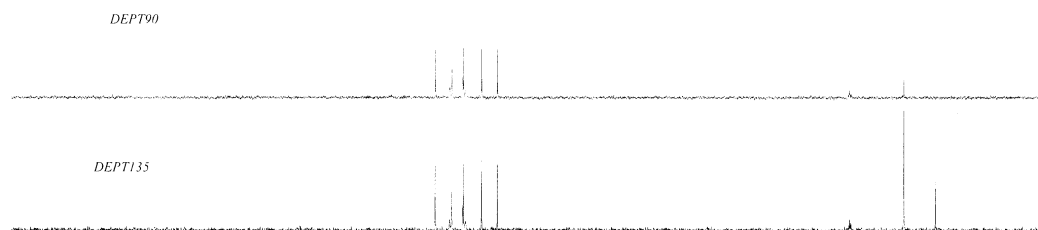


¹³C-NMR spectrum of 4j

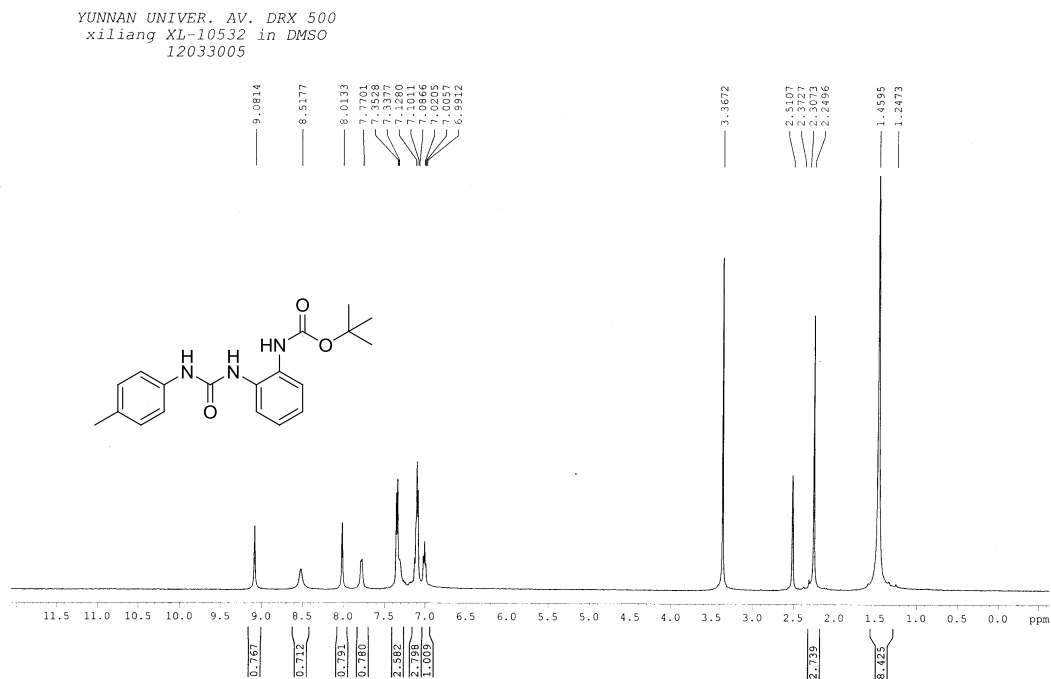
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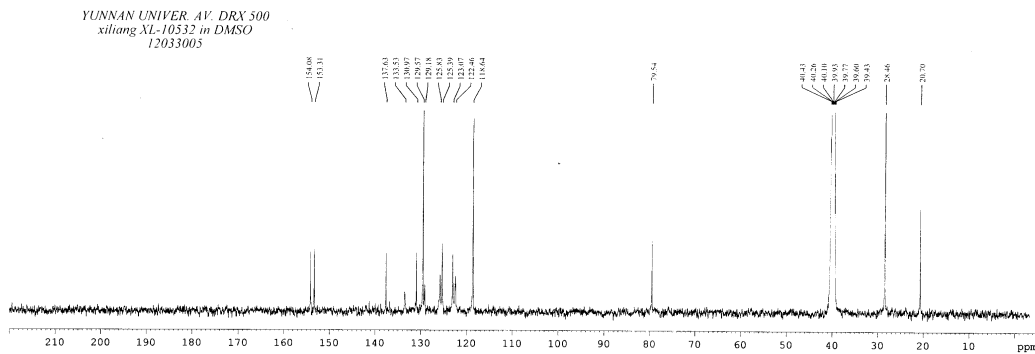
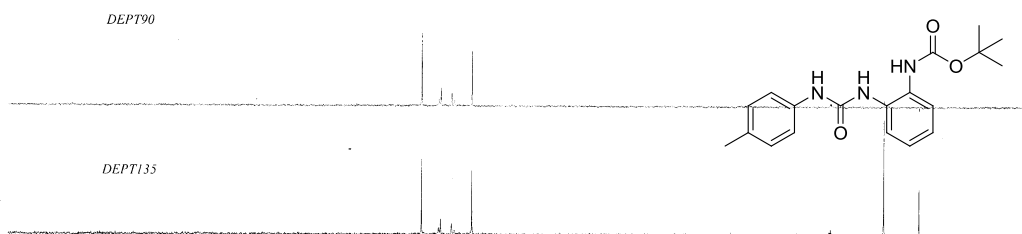
¹H-NMR spectrum of 4I



¹³C-NMR spectrum of 4I



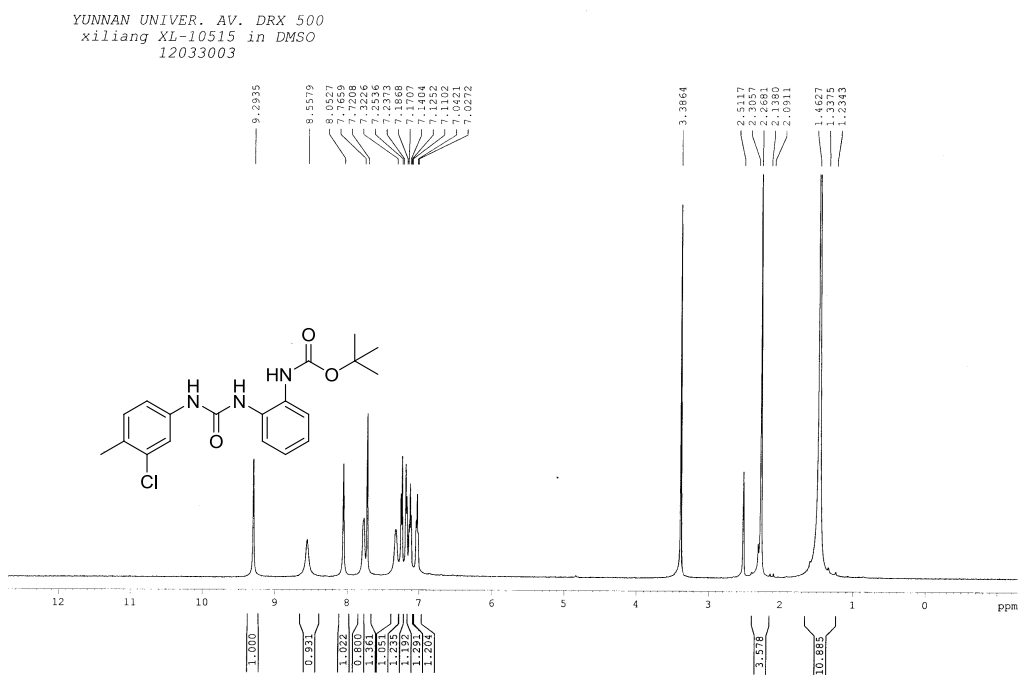
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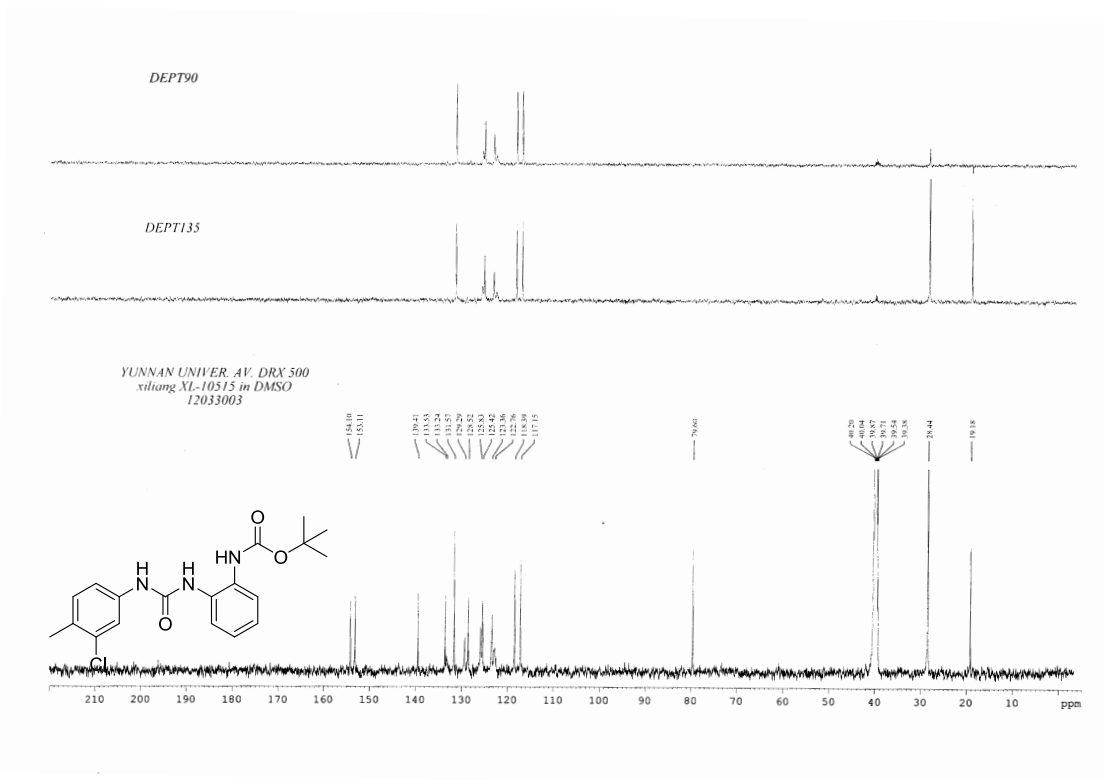
¹³C-NMR spectrum of 4m

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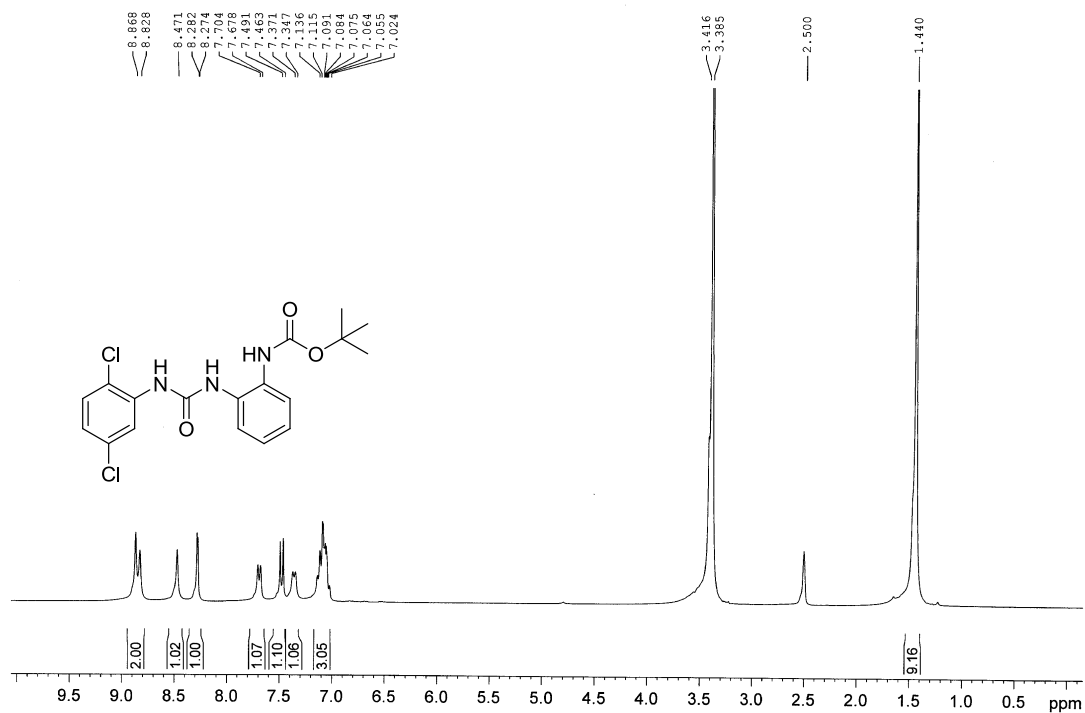


¹H-NMR spectrum of 4n

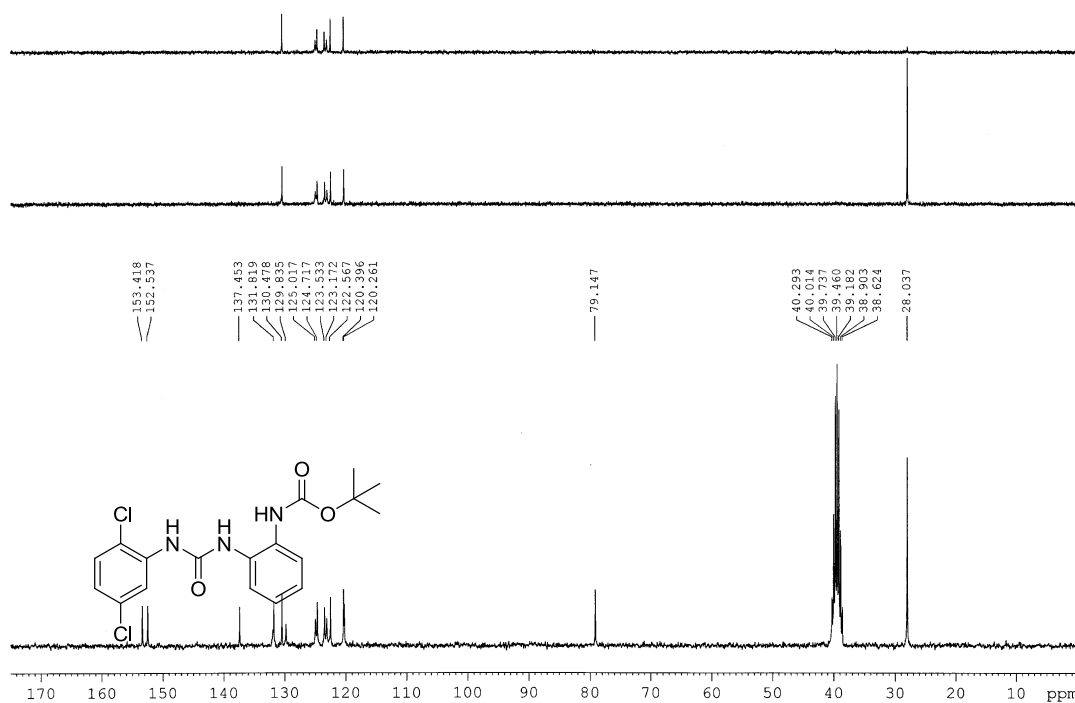


¹³C-NMR spectrum of 4n

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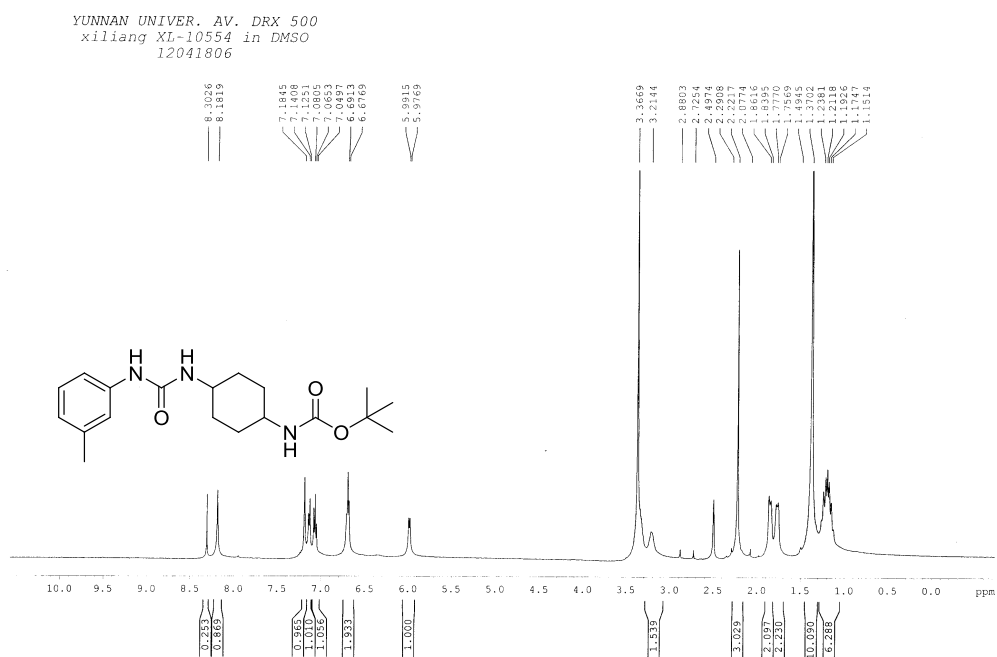
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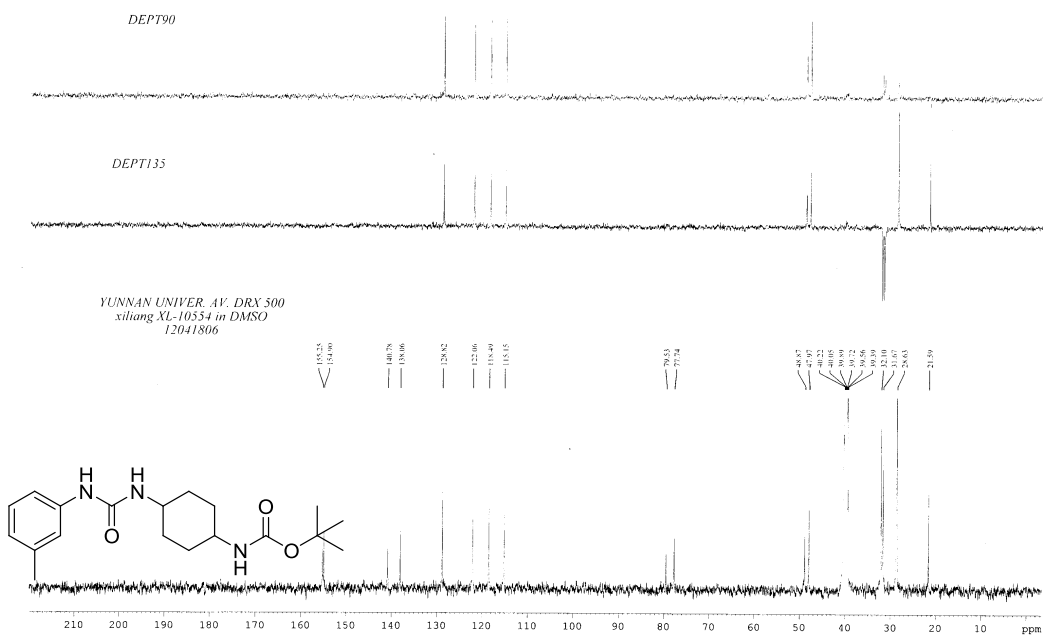
¹³C-NMR spectrum of 4p

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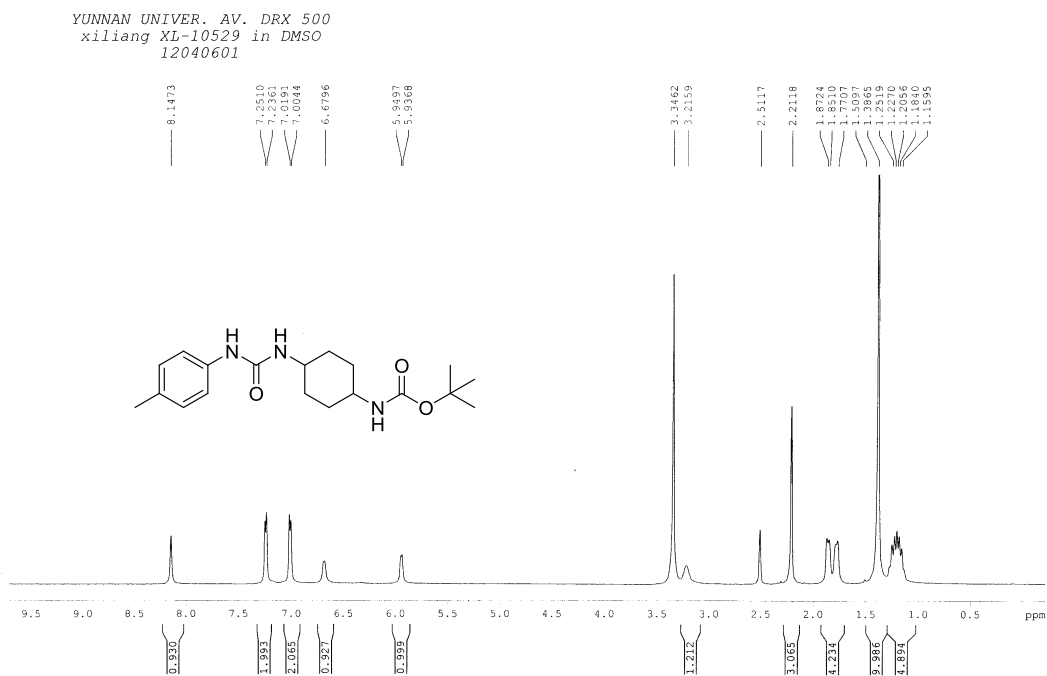
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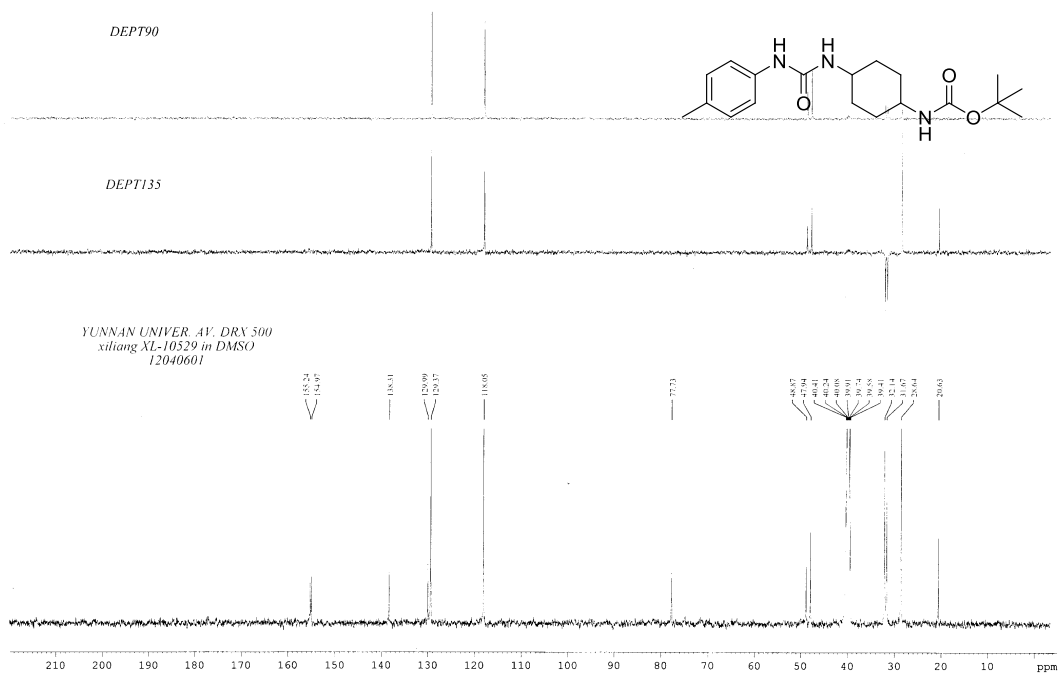
¹H-NMR spectrum of q



¹³C-NMR spectrum of 4q



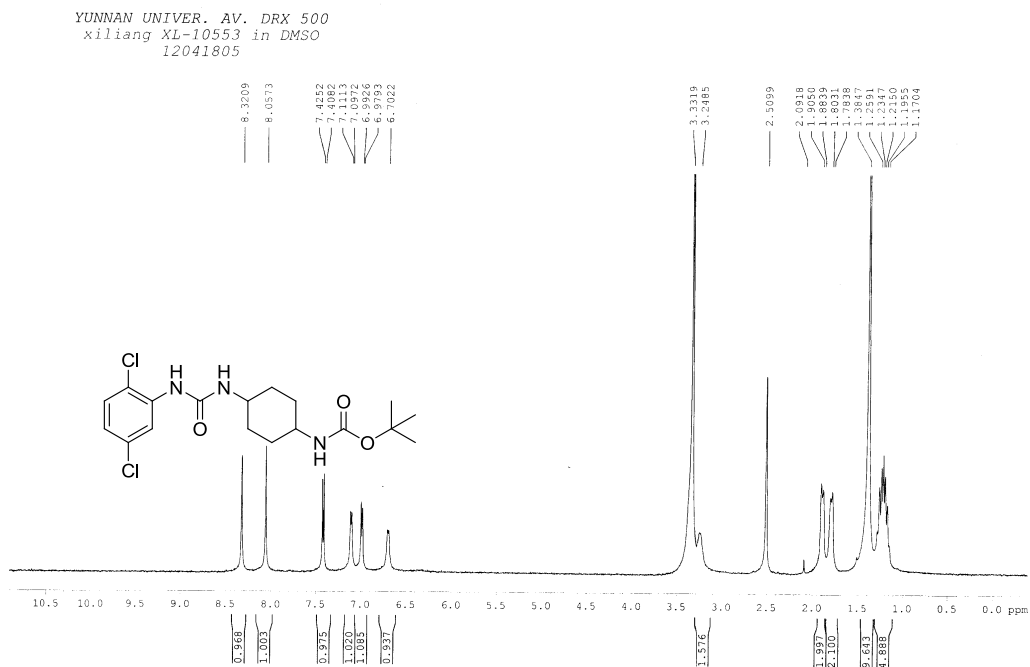
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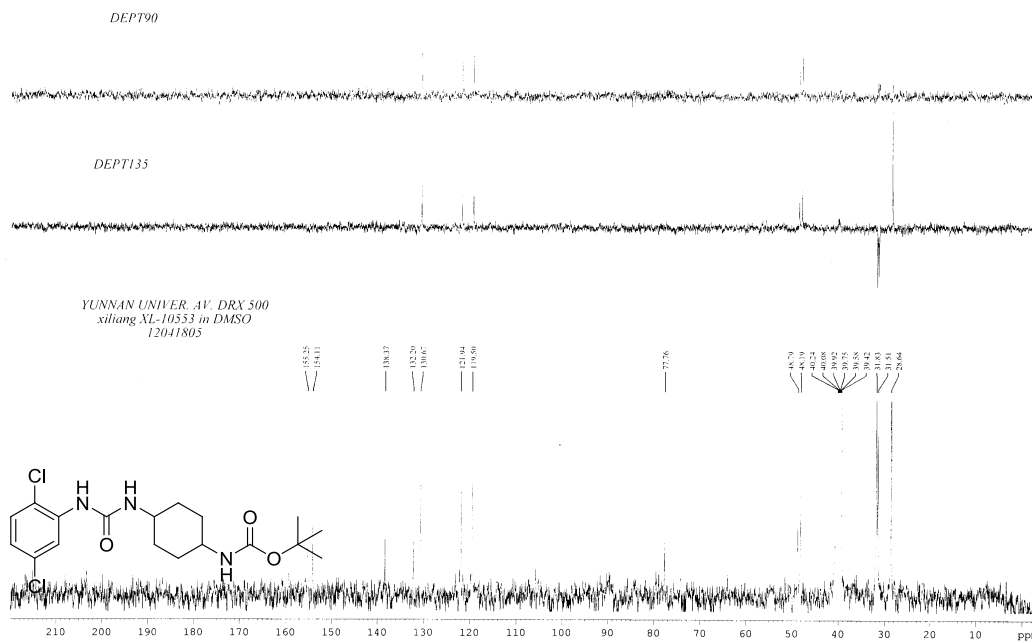
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Supporting Information

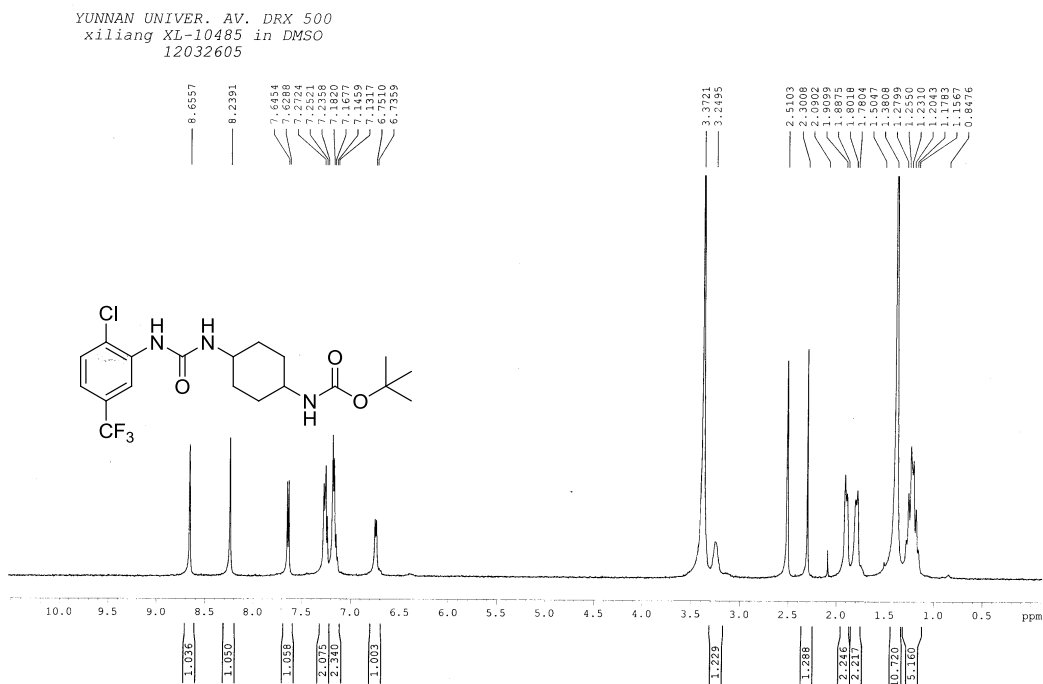
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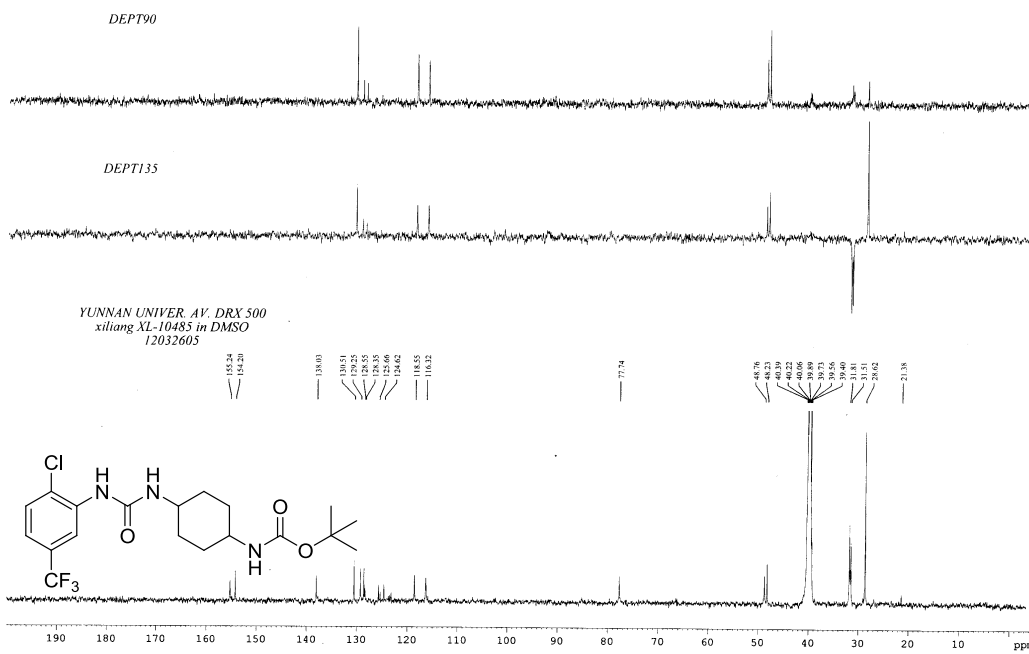
¹H-NMR spectrum of 4s



¹³C-NMR spectrum of 4s



¹H-NMR spectrum of 4t

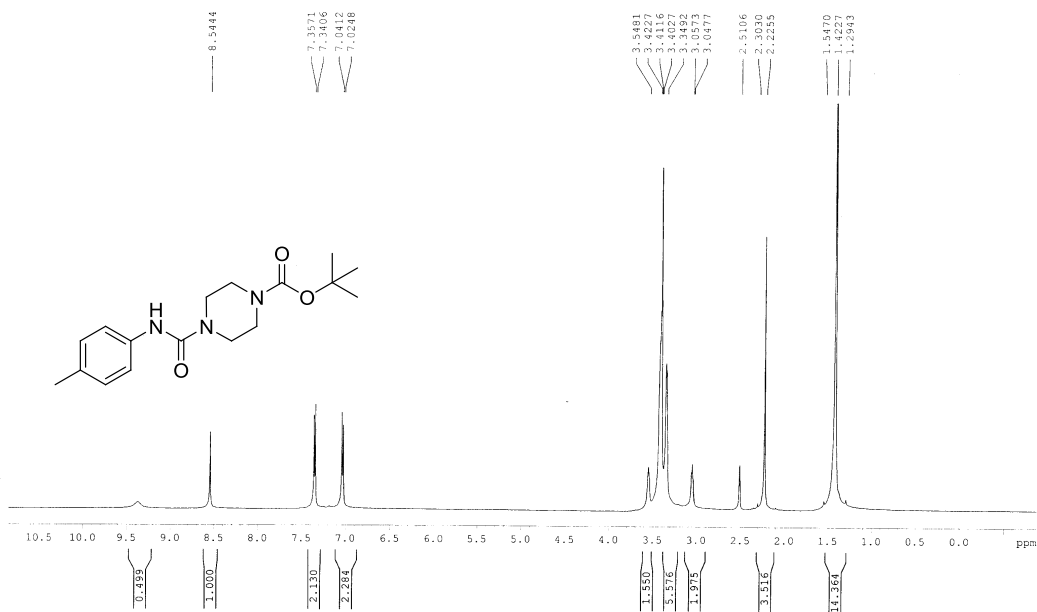


¹³C-NMR spectrum of 4t

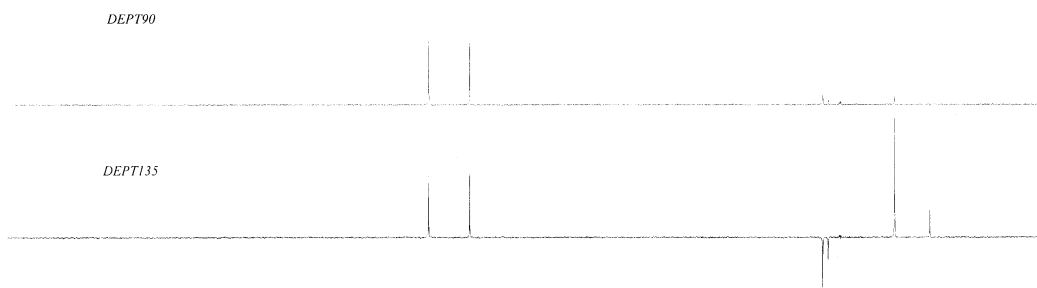
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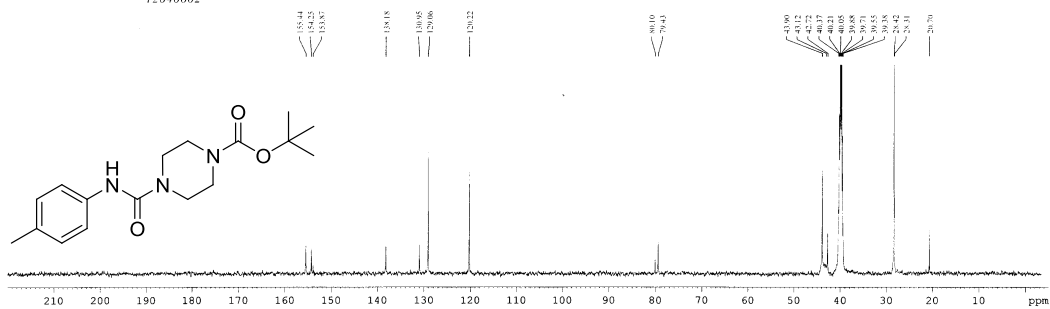
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xiliang XL-10530 in DMSO
12040602



¹H-NMR spectrum of 4u

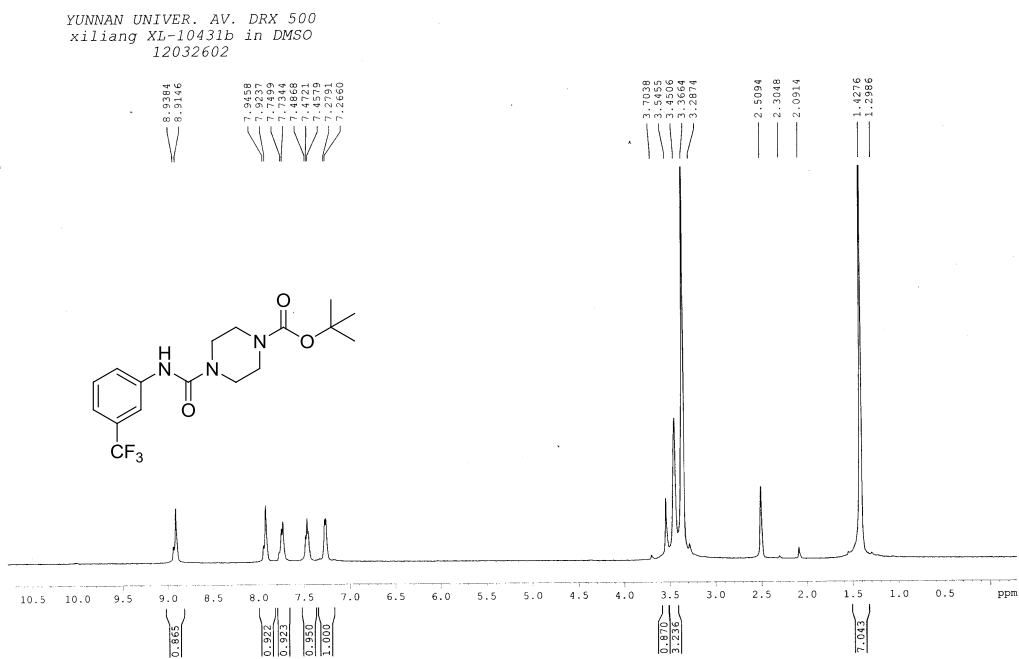


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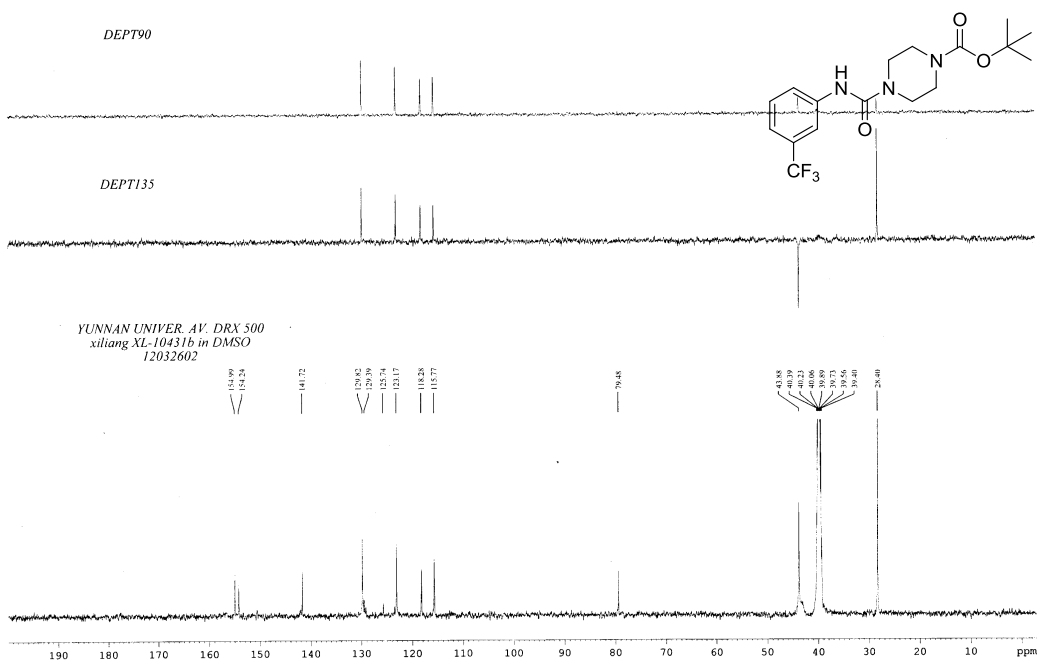


¹³C-NMR spectrum of 4u

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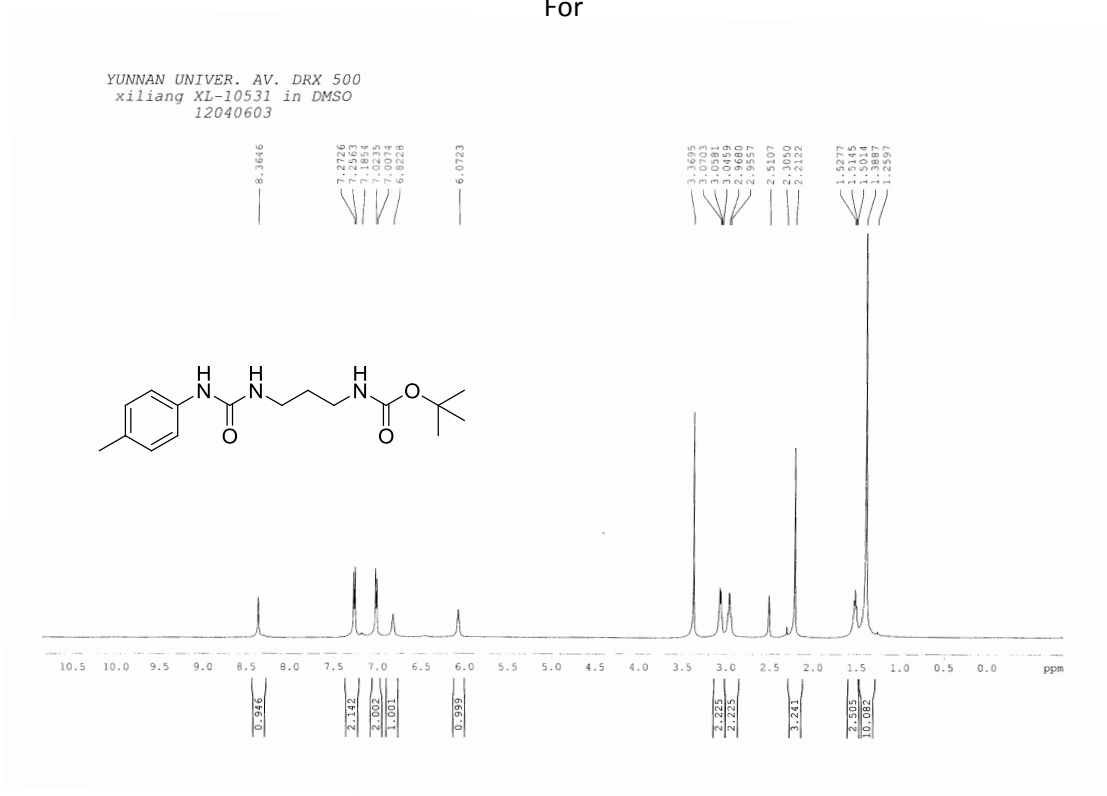
¹H-NMR spectrum of 4v



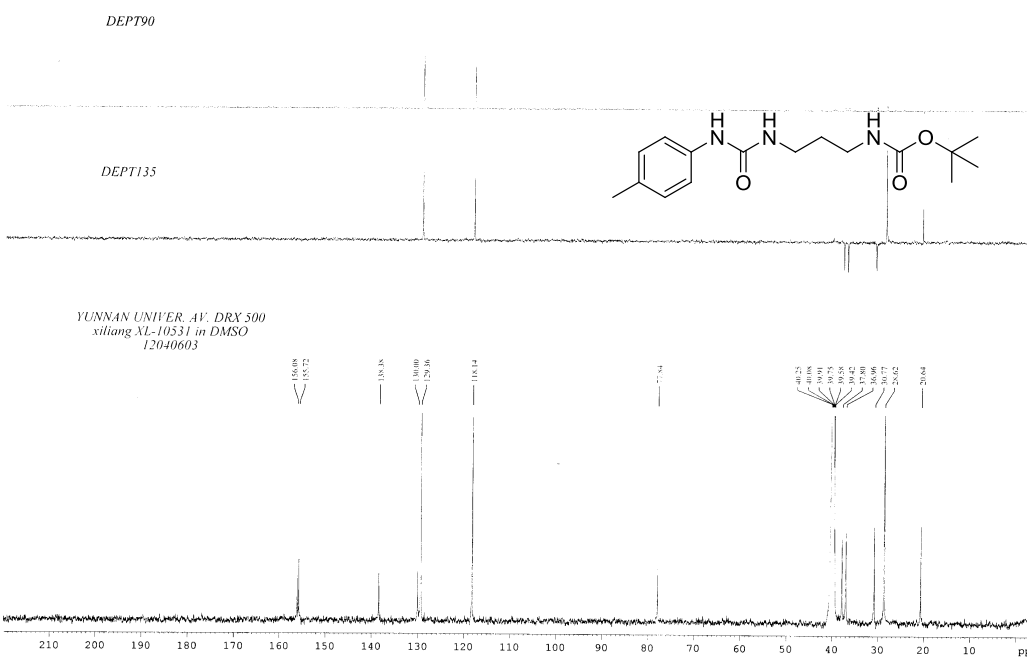
¹³C-NMR spectrum of 4v

Supporting Information

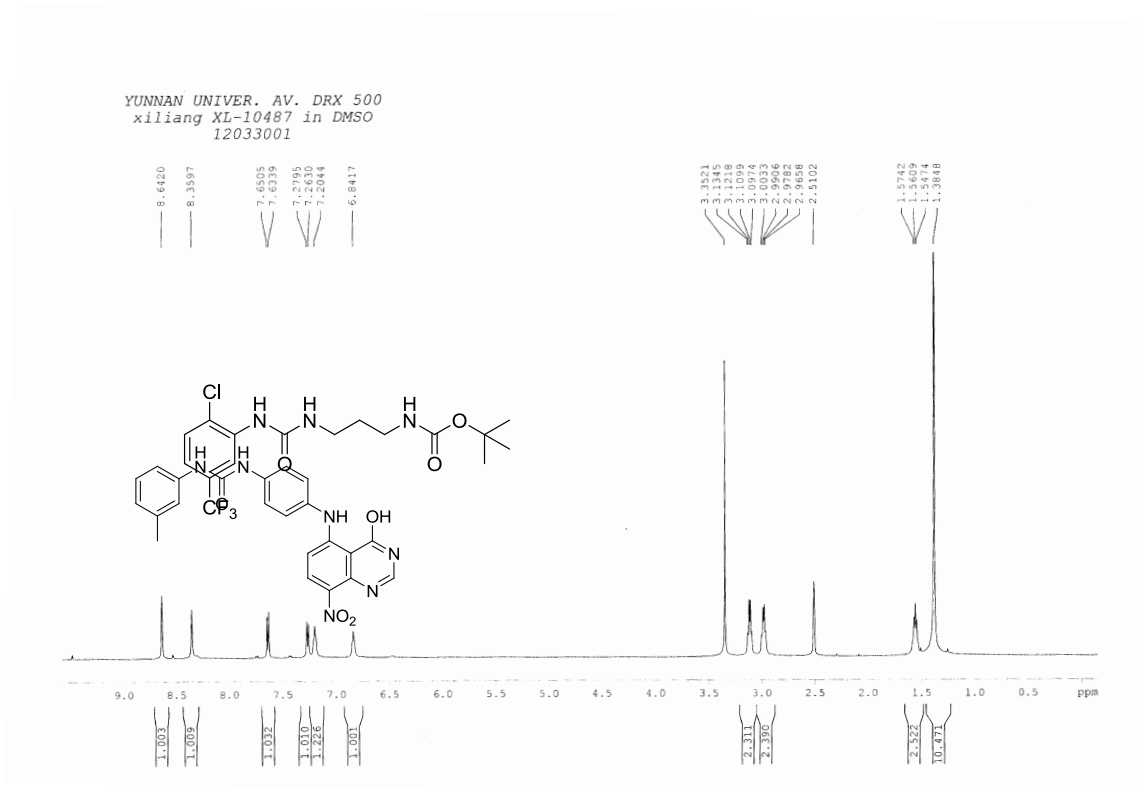
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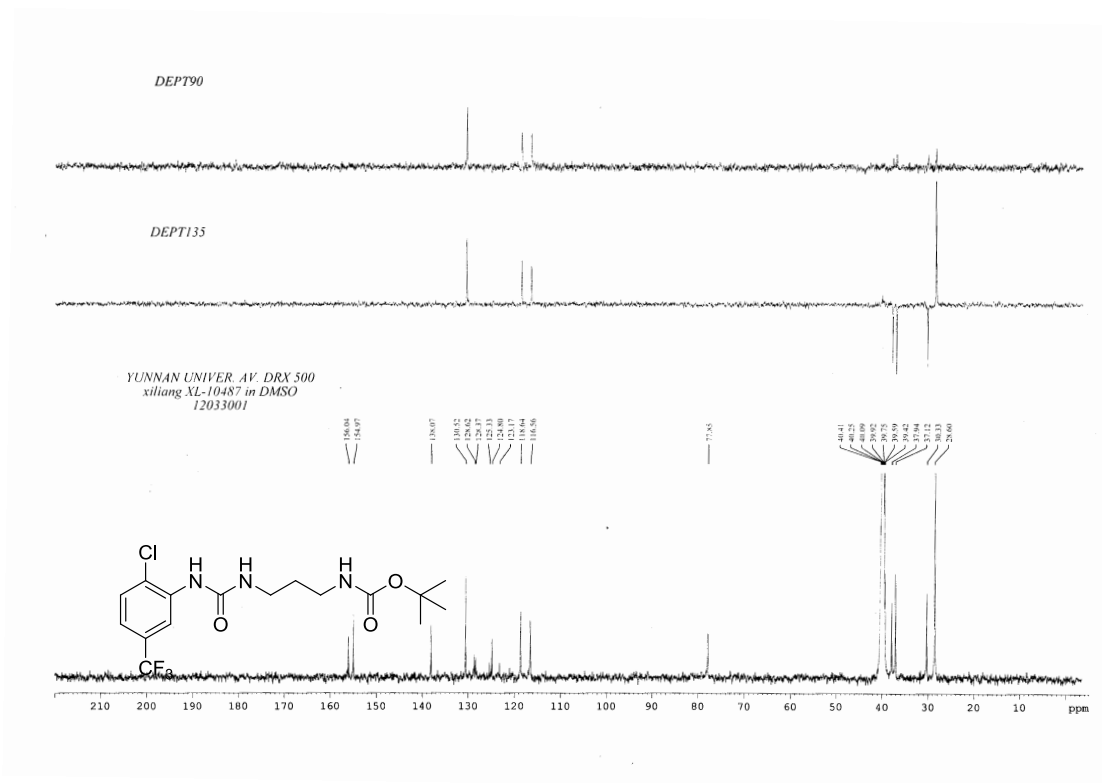
¹H-NMR spectrum of 4x



¹³C-NMR spectrum of 4x



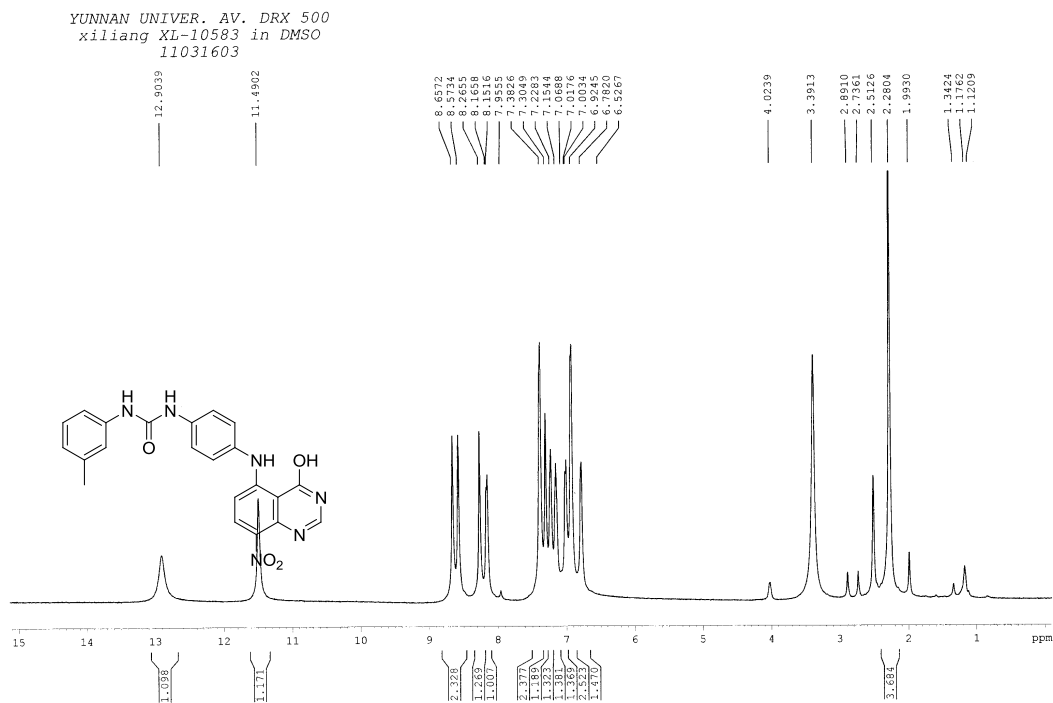
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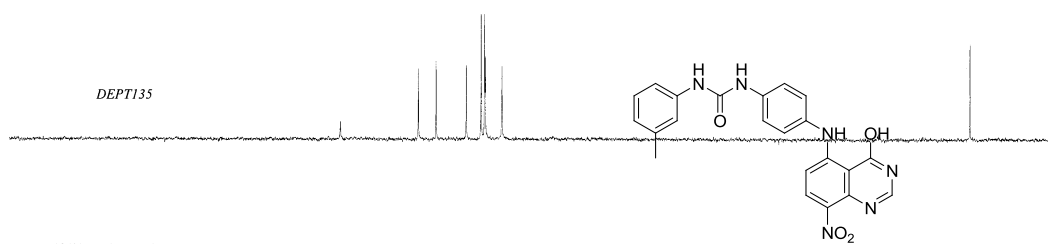
¹³C-NMR spectrum of 4z

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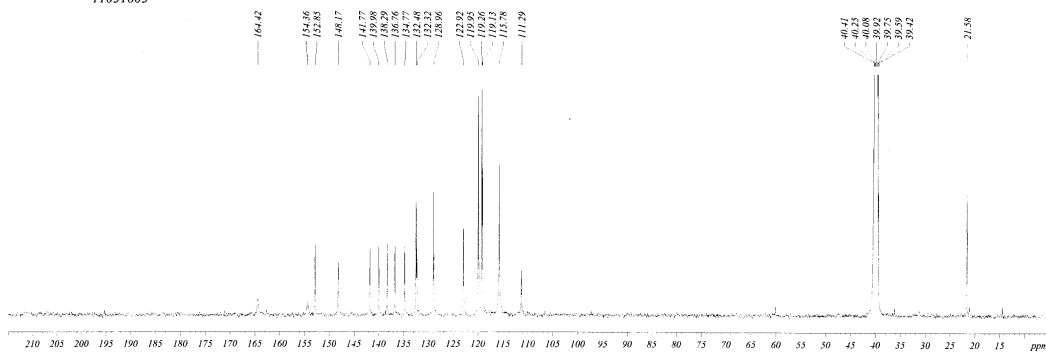
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¹H-NMR spectrum of 6a

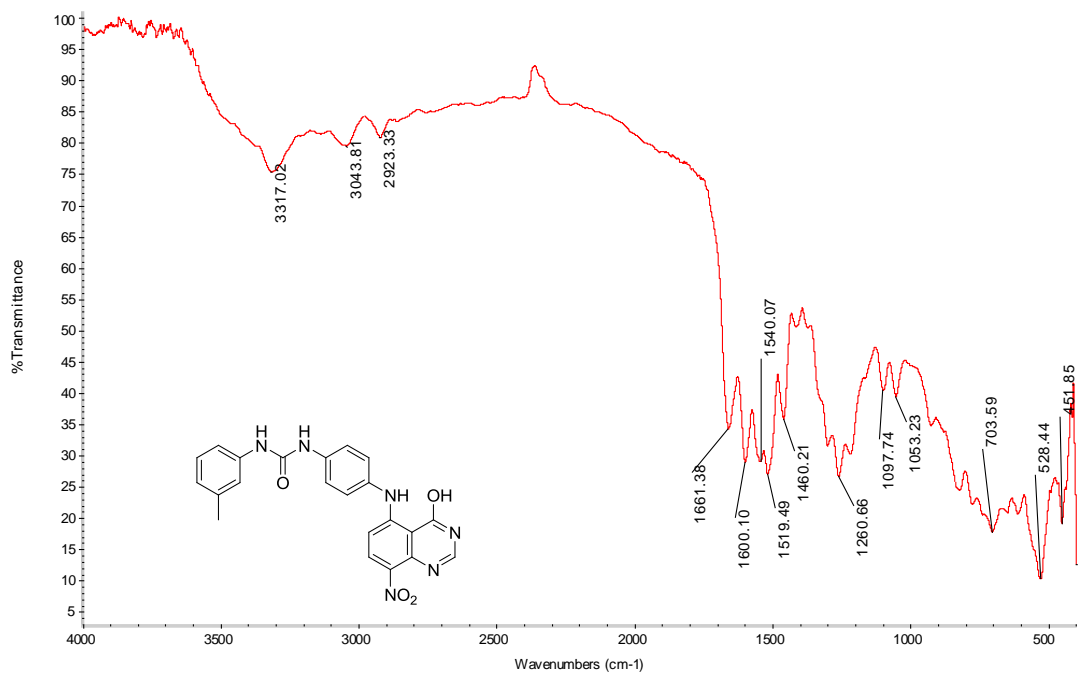


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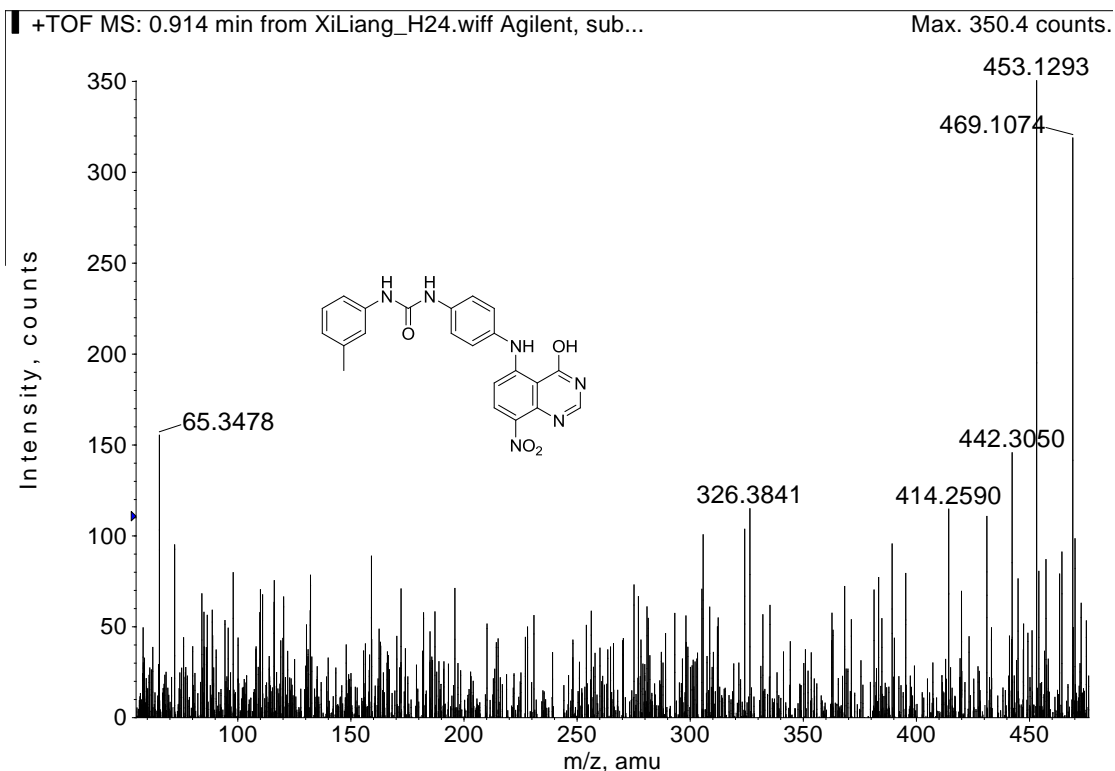


¹³C-NMR spectrum of 6a

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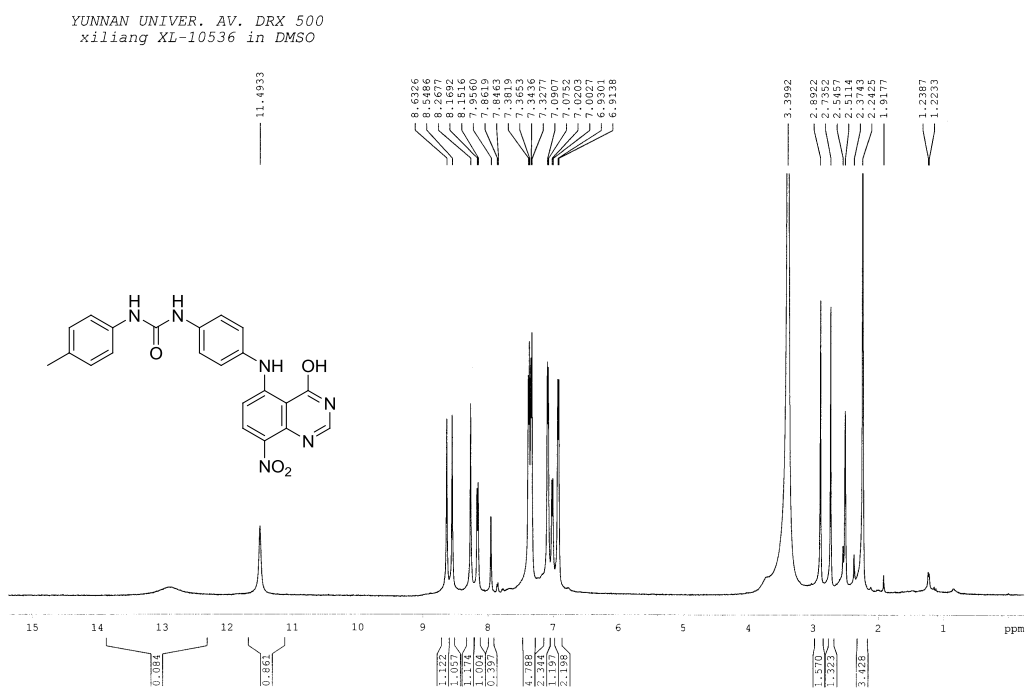


IR spectrum of 6a

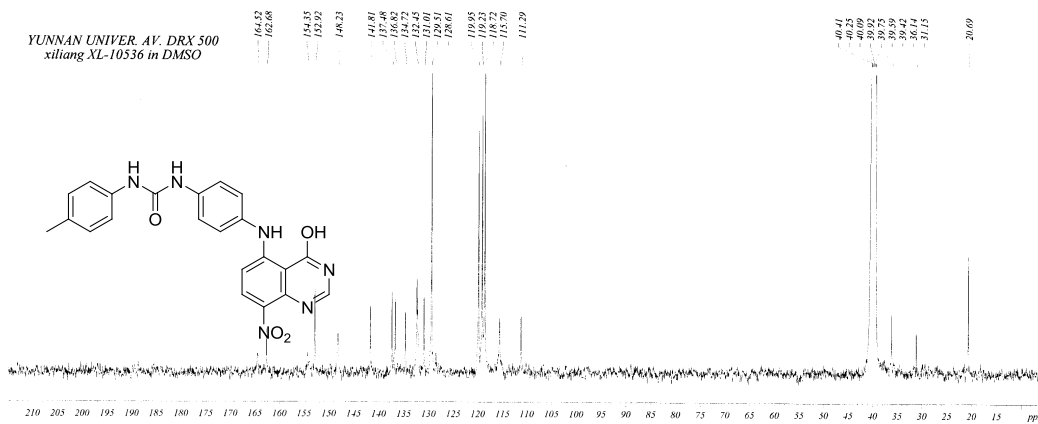
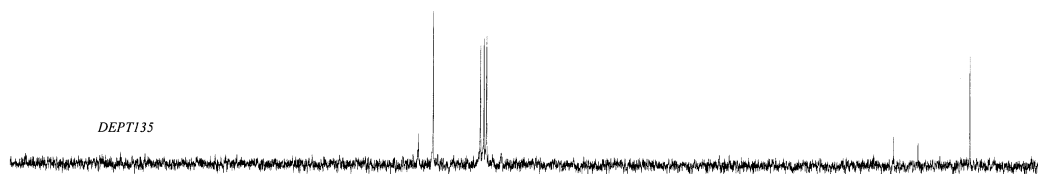


MS spectrum of 6a

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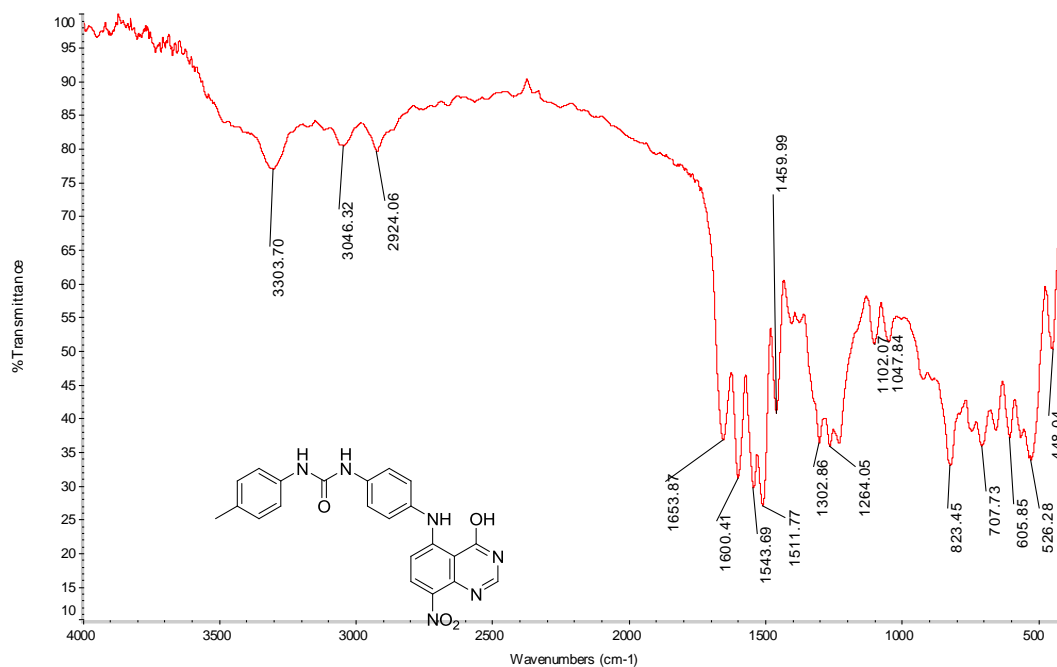


¹H-NMR spectrum of 6b



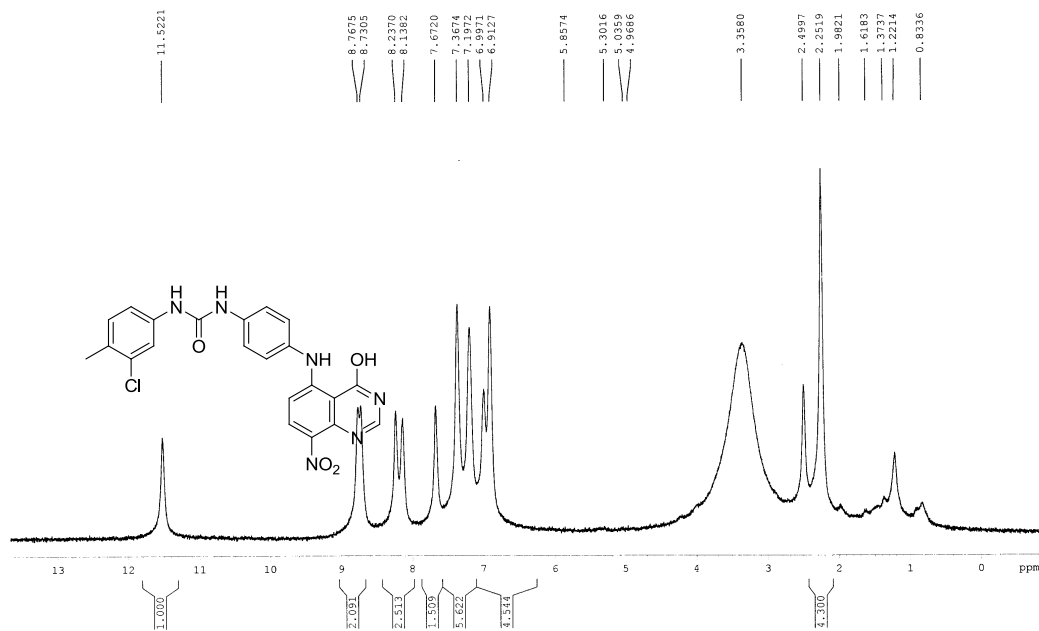
¹³C-NMR spectrum of 6b

For



IR spectrum of 6b

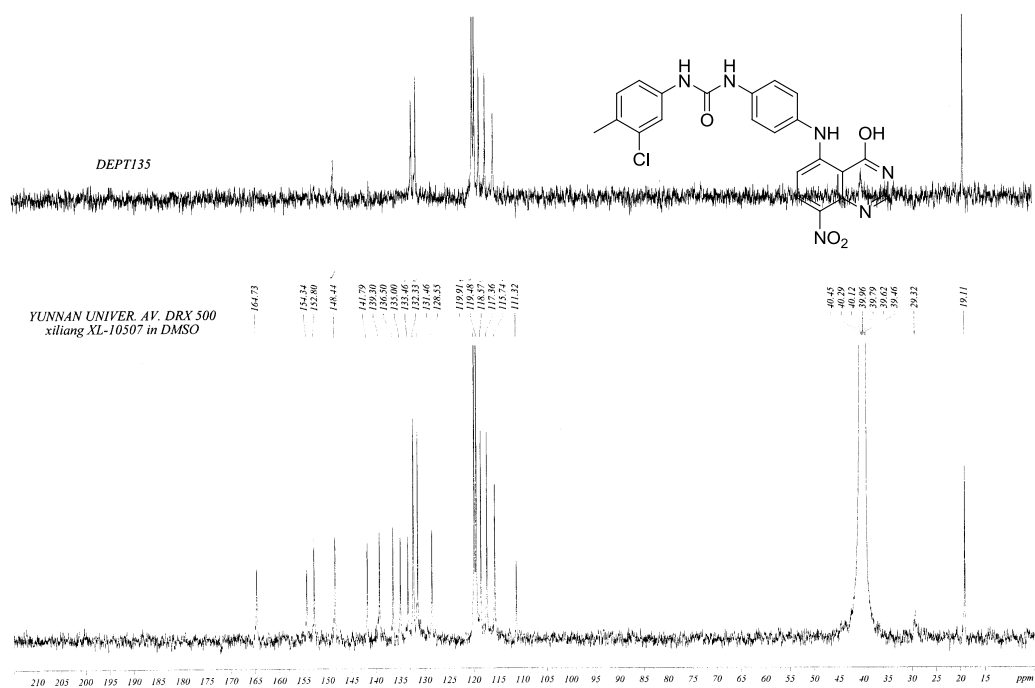
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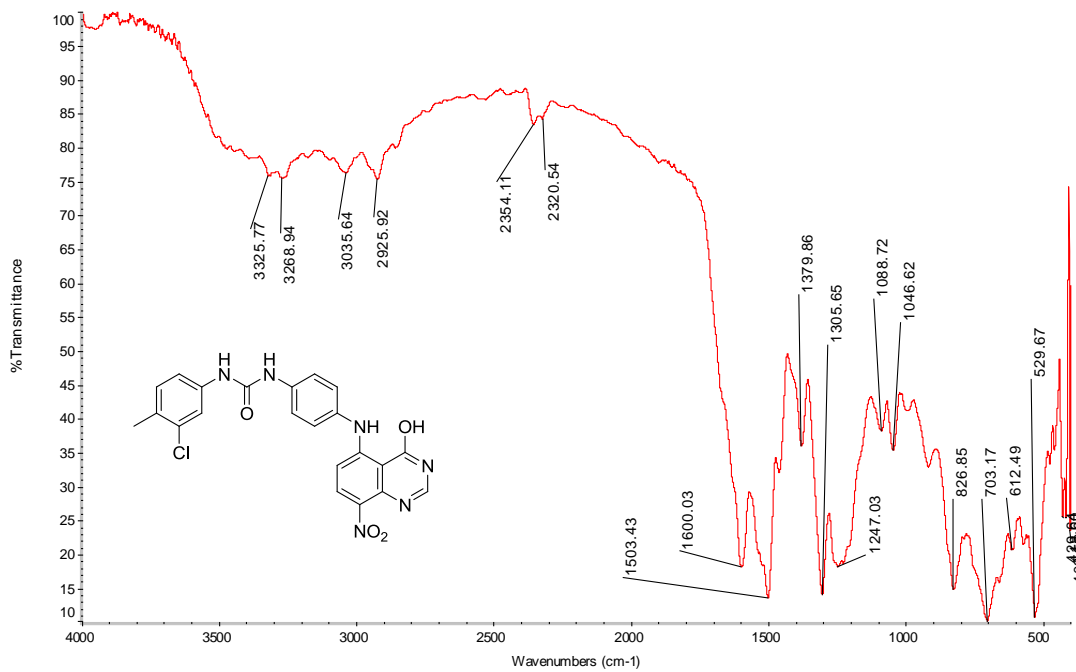
¹H-NMR spectrum of 6c

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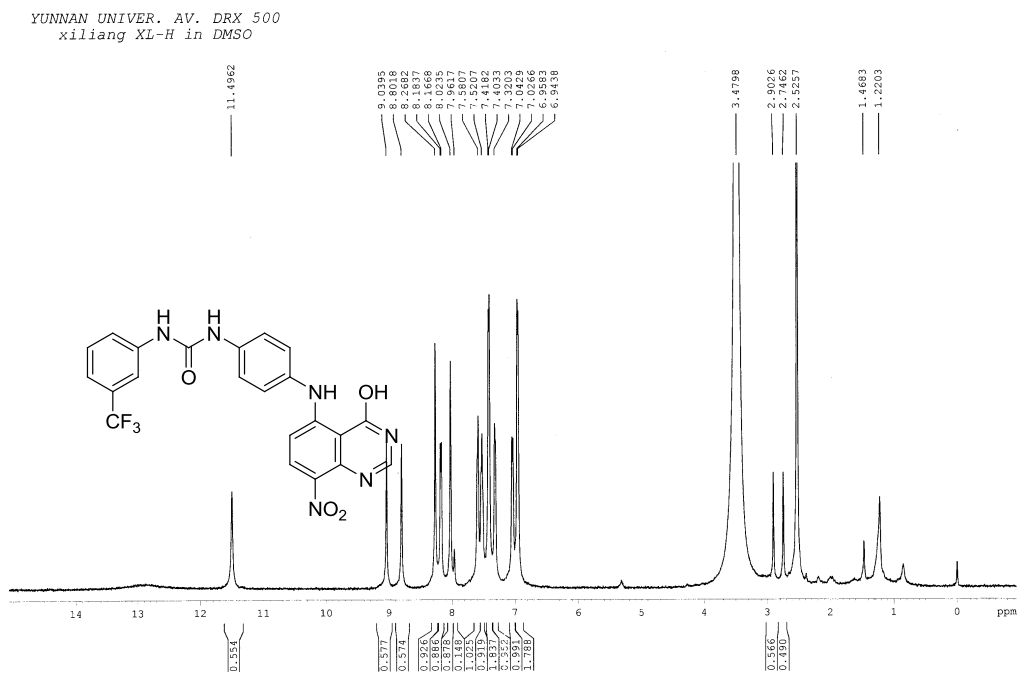
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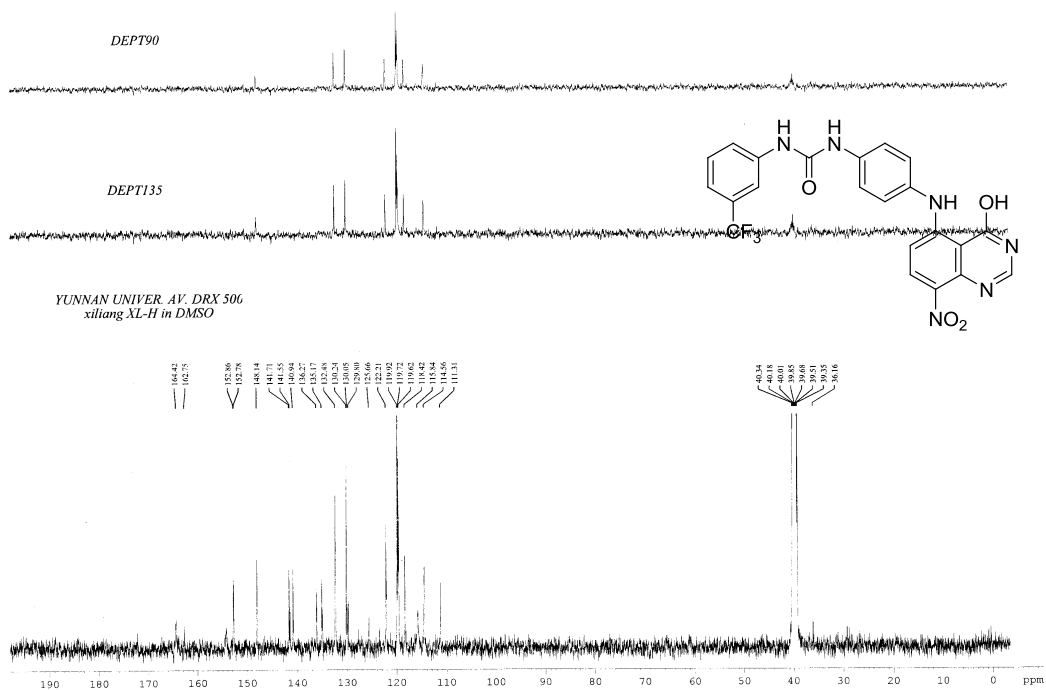
¹³C-NMR spectrum of 6c



IR spectrum of 6c



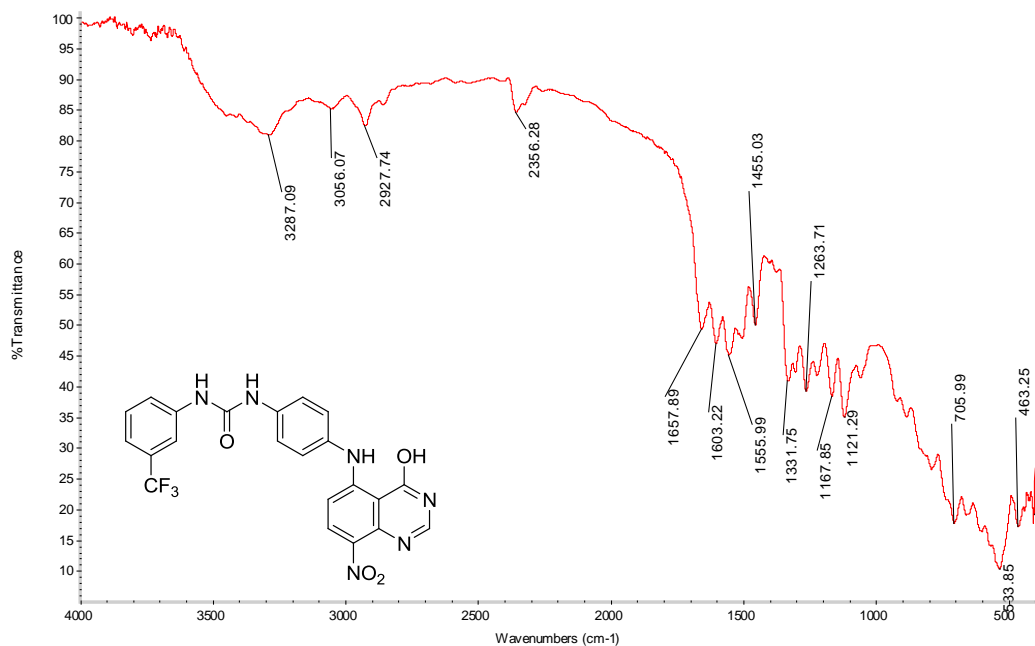
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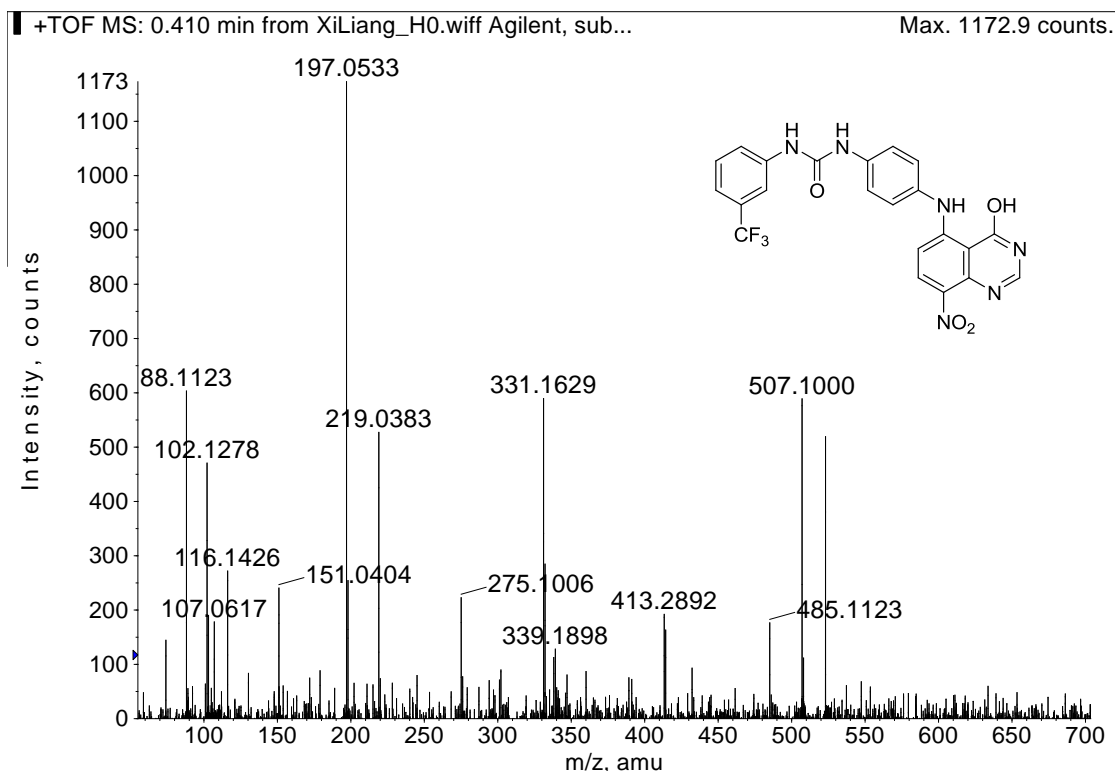
¹³C-NMR spectrum of 6d

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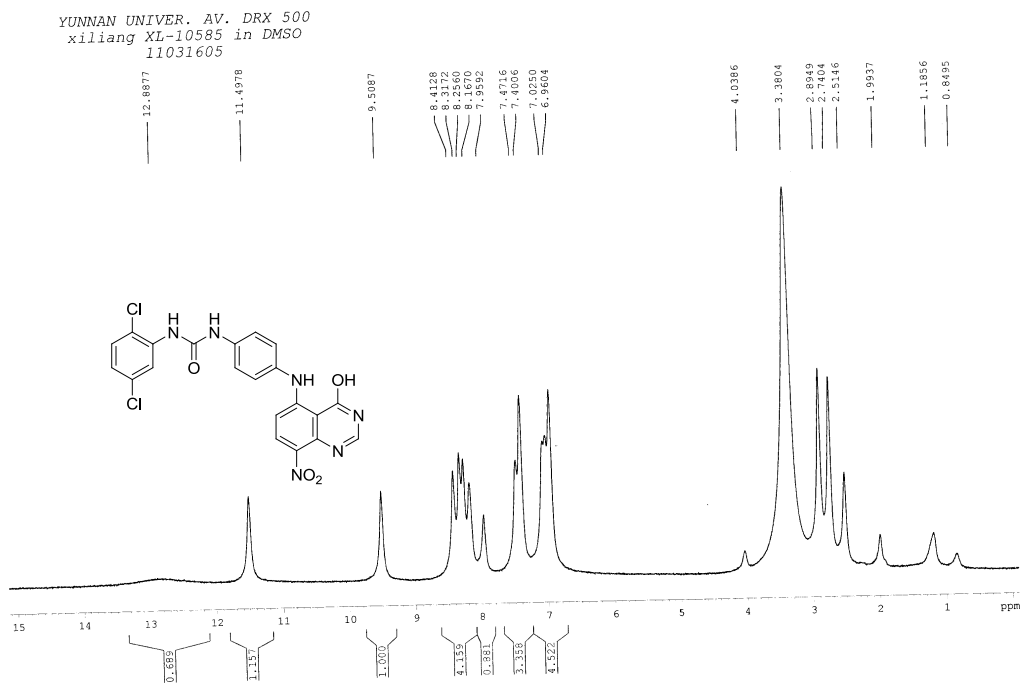


IR spectrum of 6d

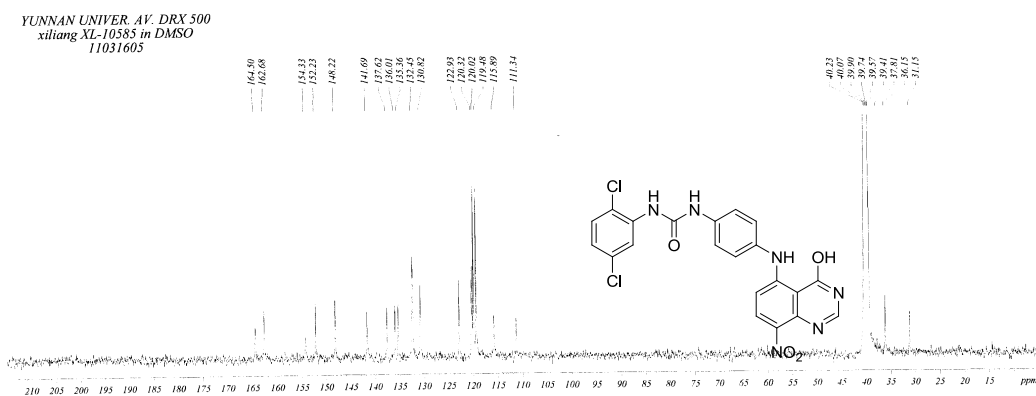
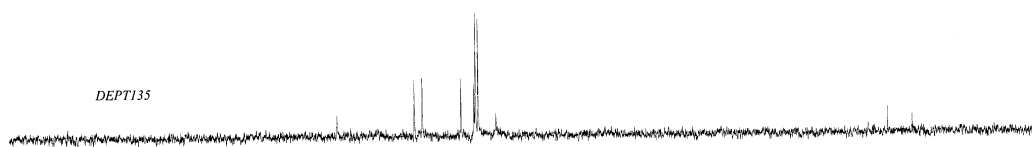


MS spectrum of 6d

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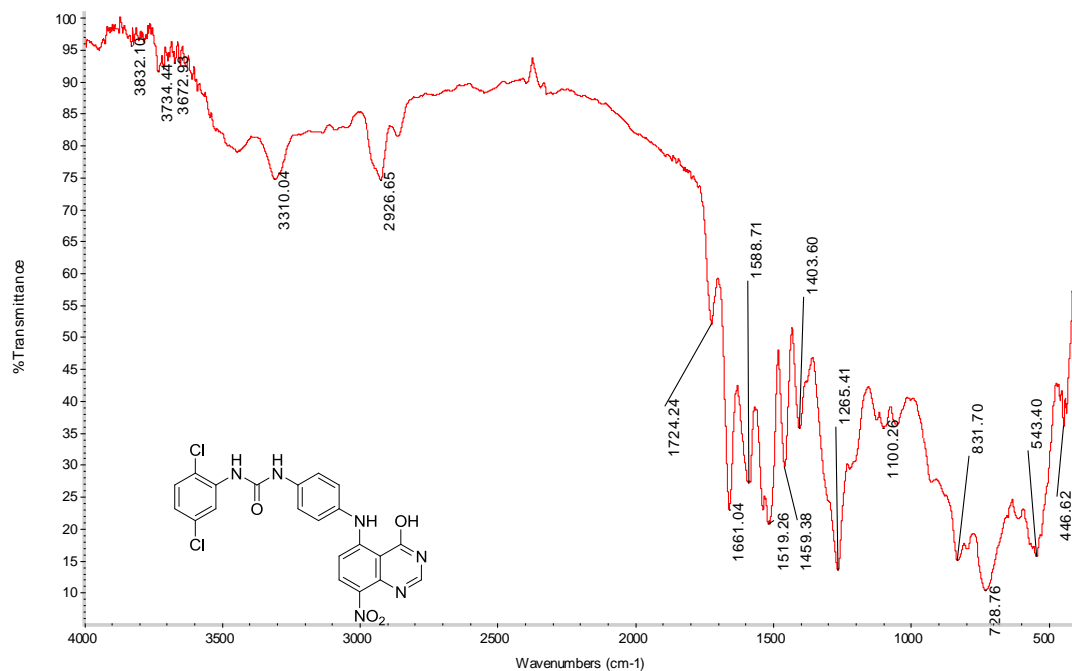
¹H-NMR spectrum of 6e



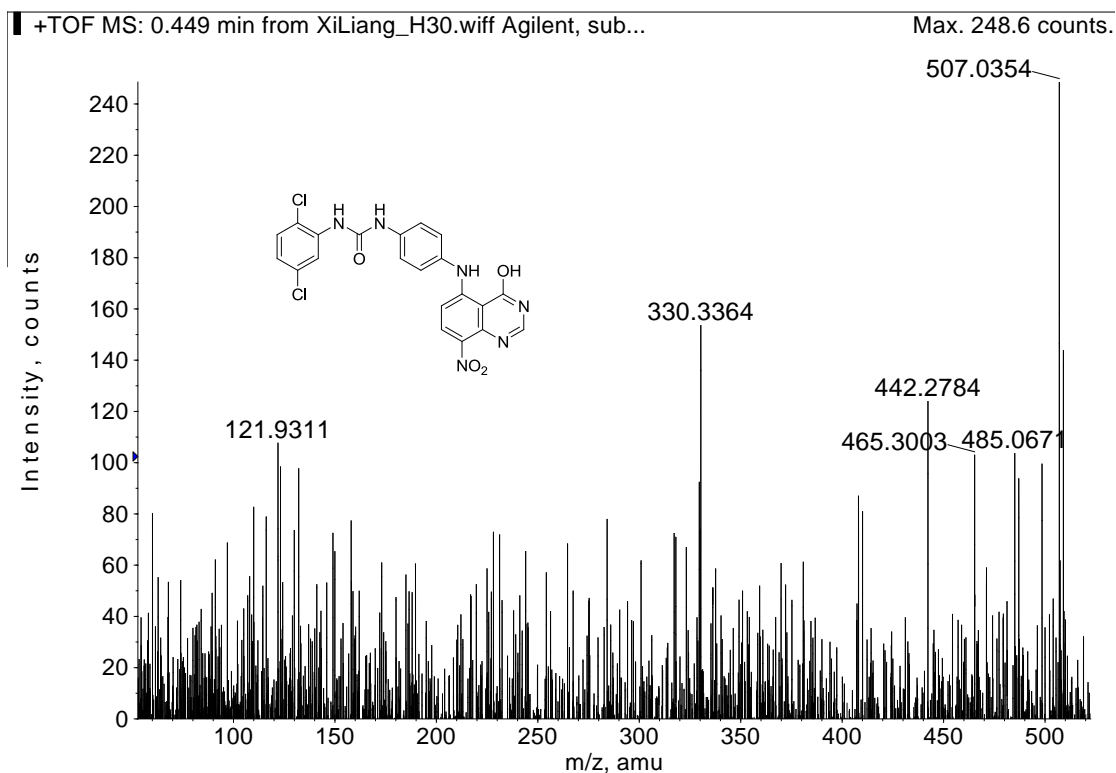
¹³C-NMR spectrum of 6e

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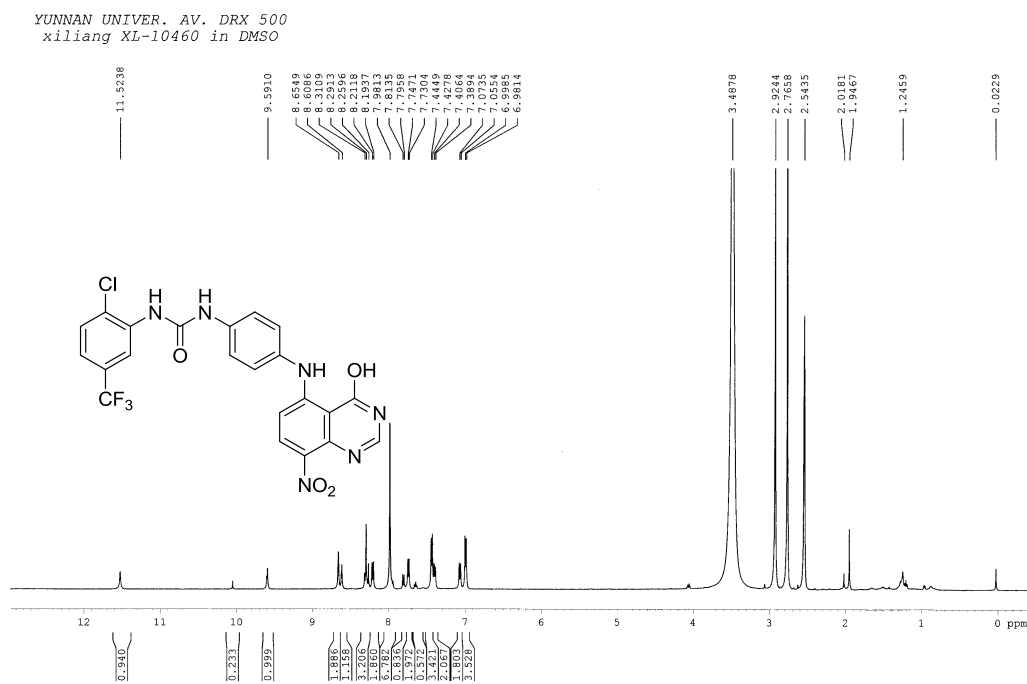
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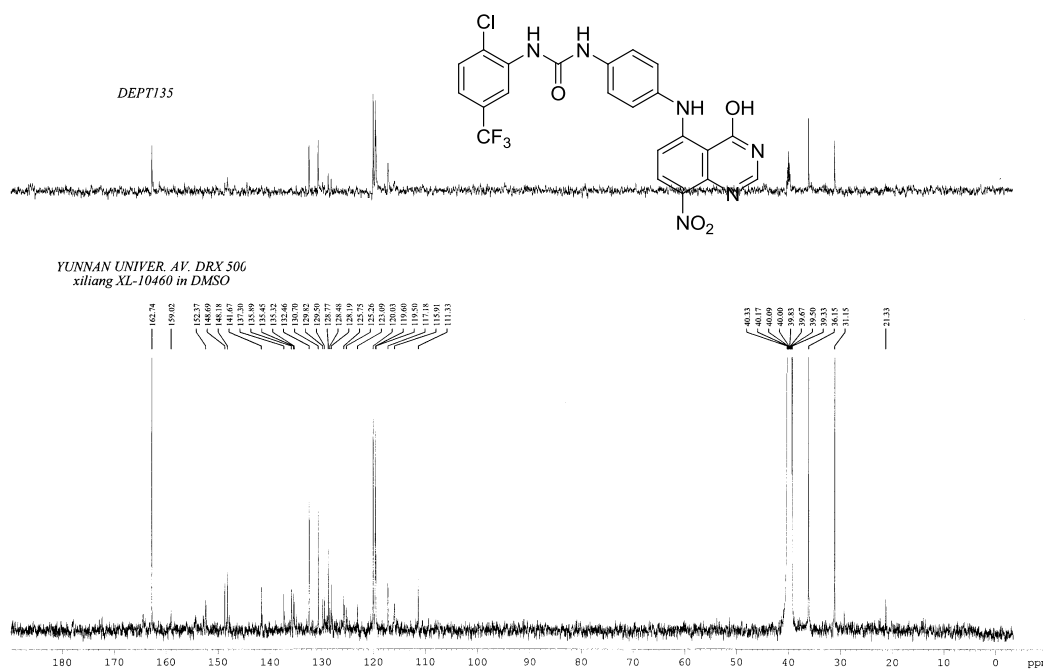
IR spectrum of 6e



MS spectrum of 6e



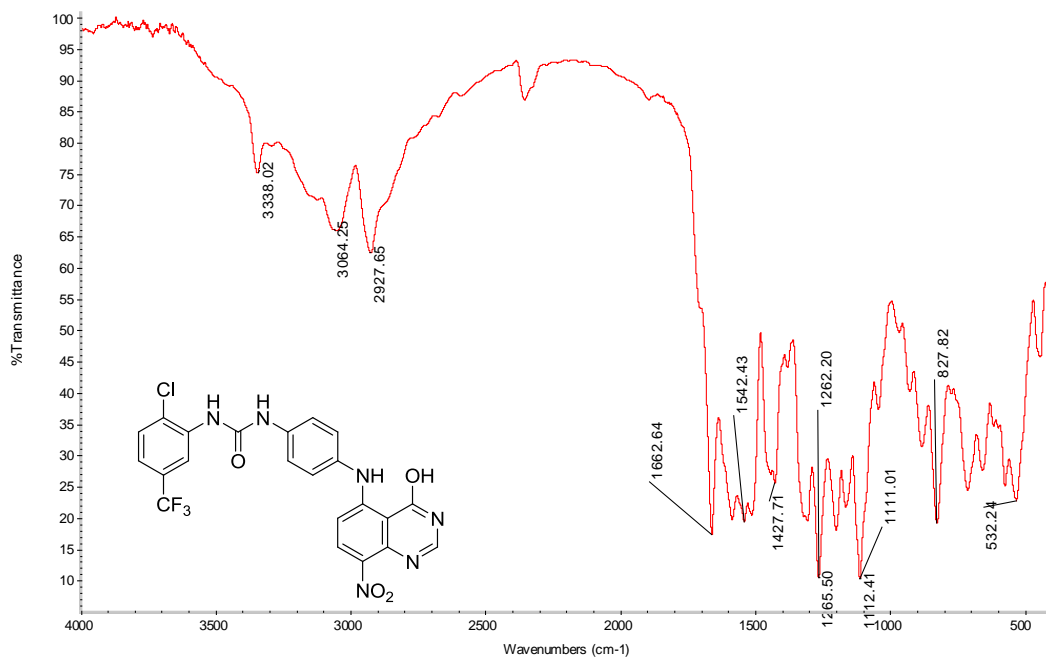
¹H-NMR spectrum of **6f**



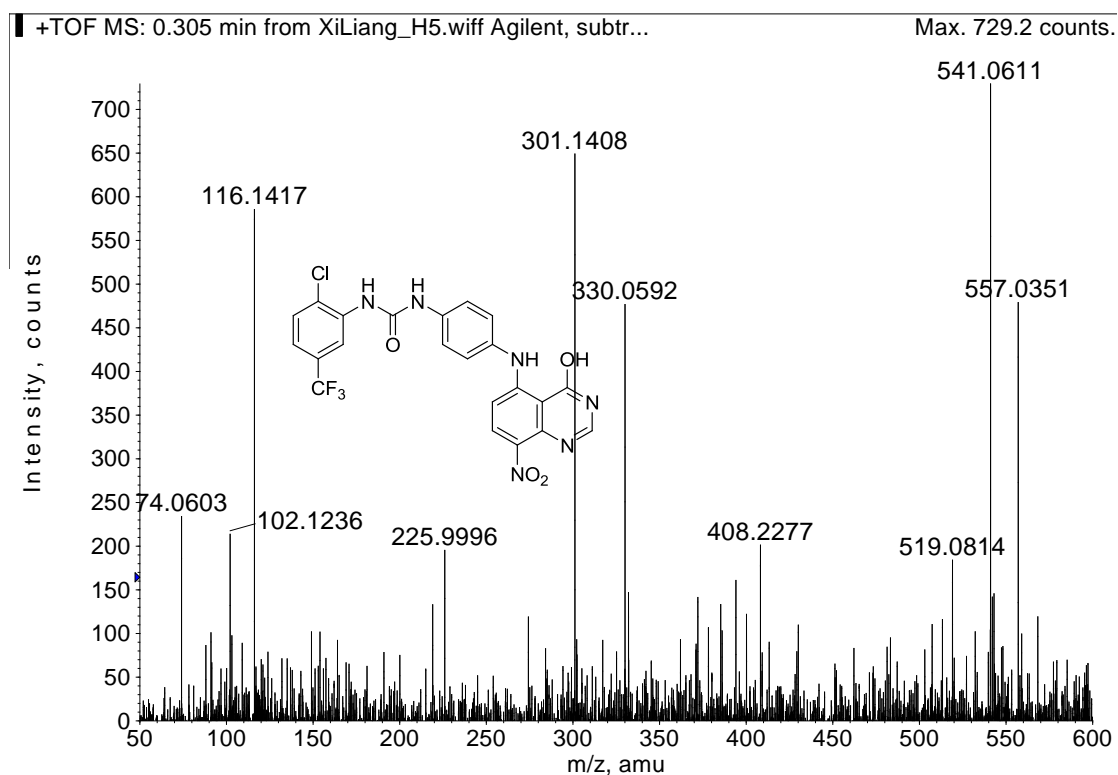
¹³C-NMR spectrum of **6f**

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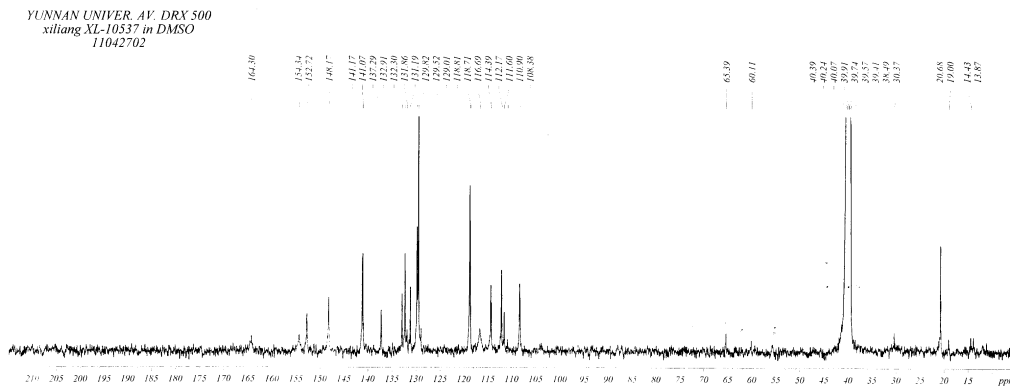
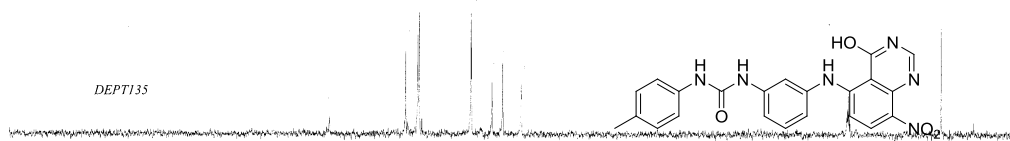
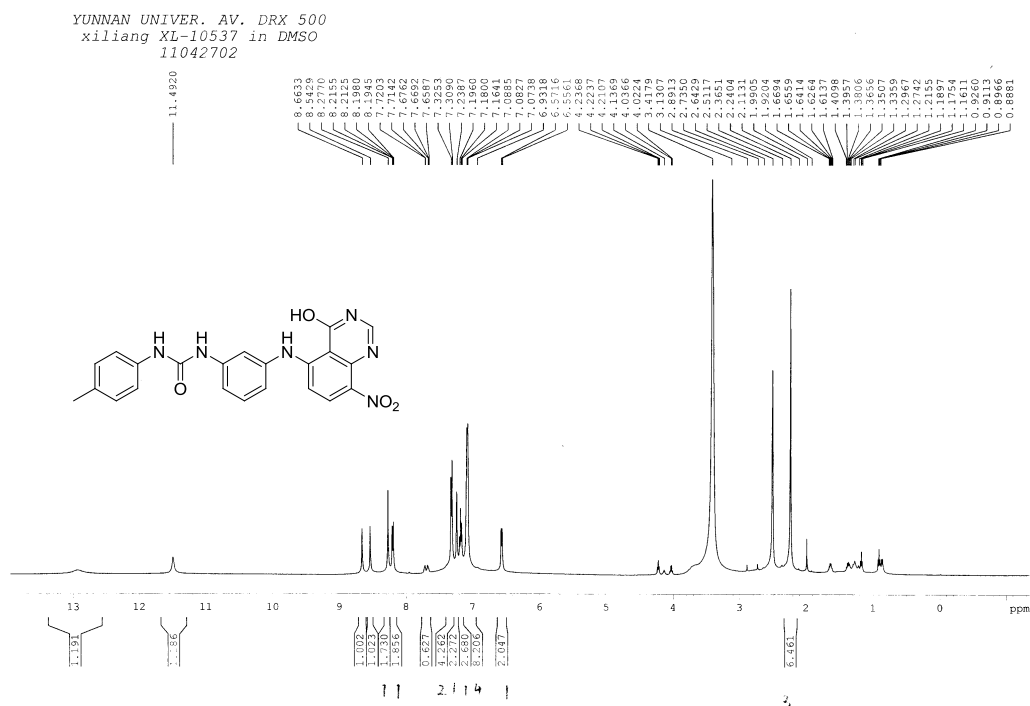
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IR spectrum of 6f

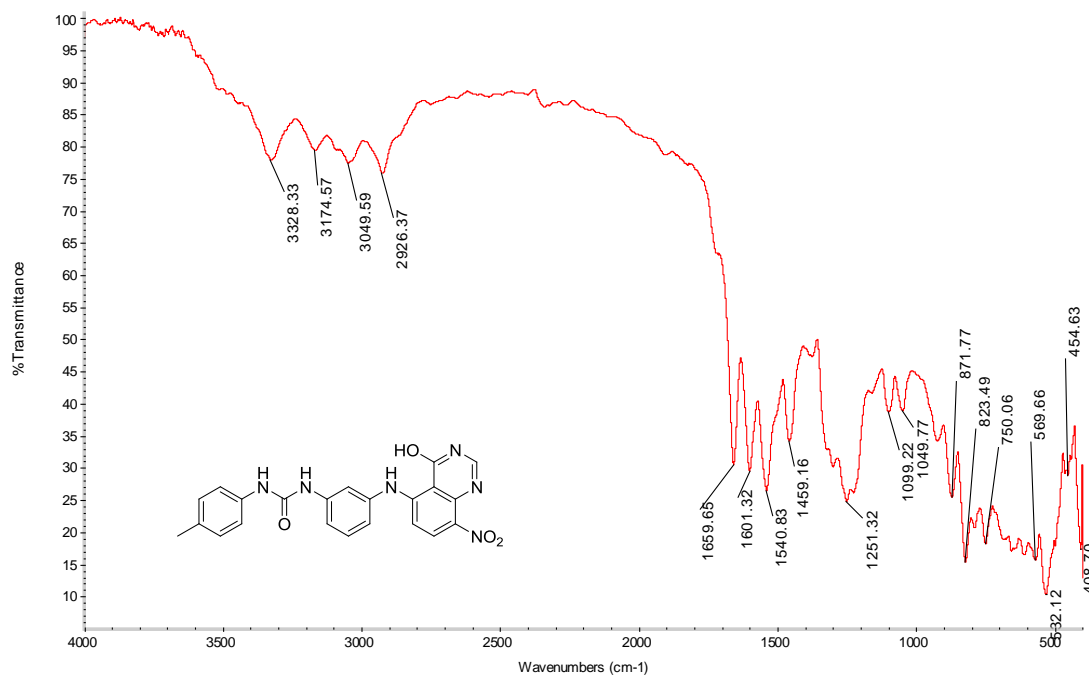


MS spectrum of 6f

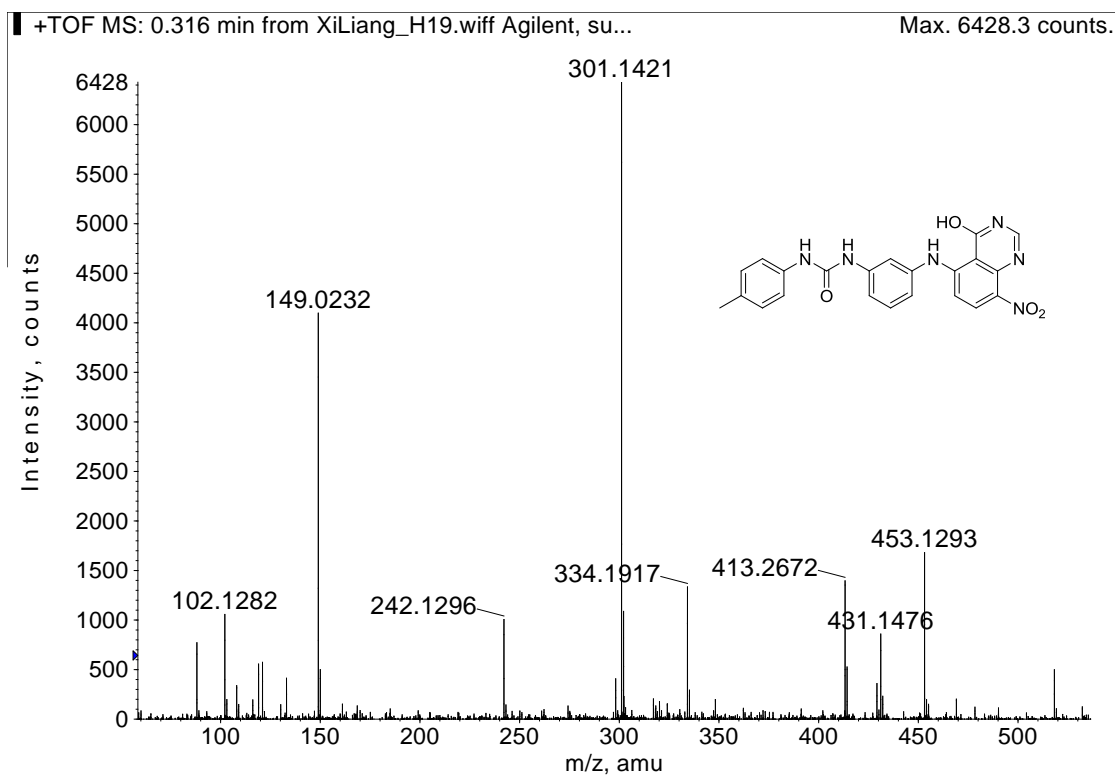


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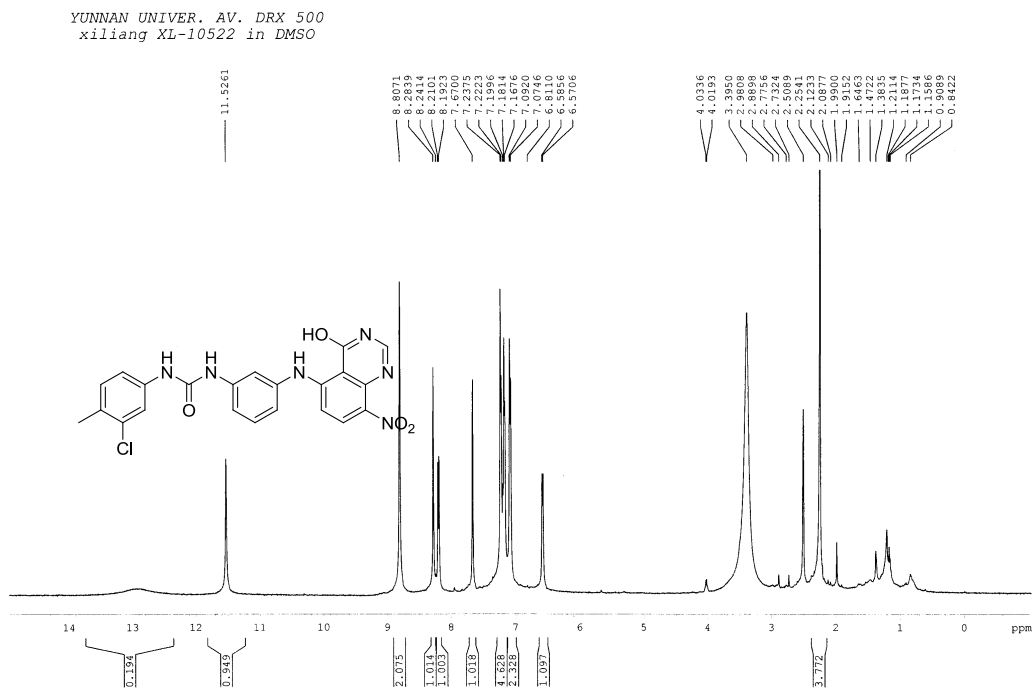


IR spectrum of 6g

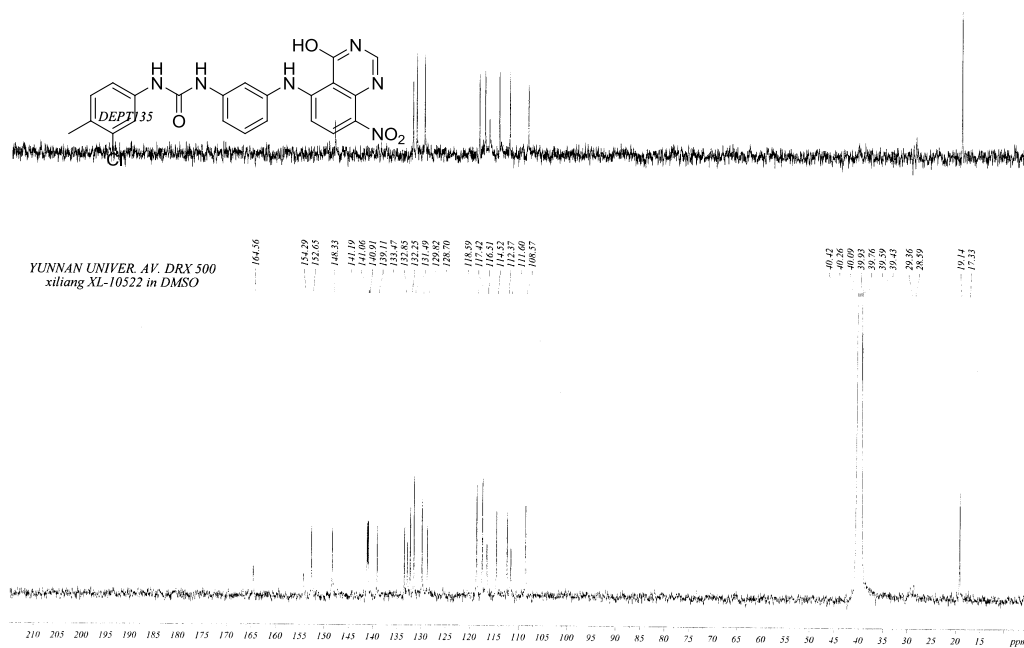


MS spectrum of 6g

For



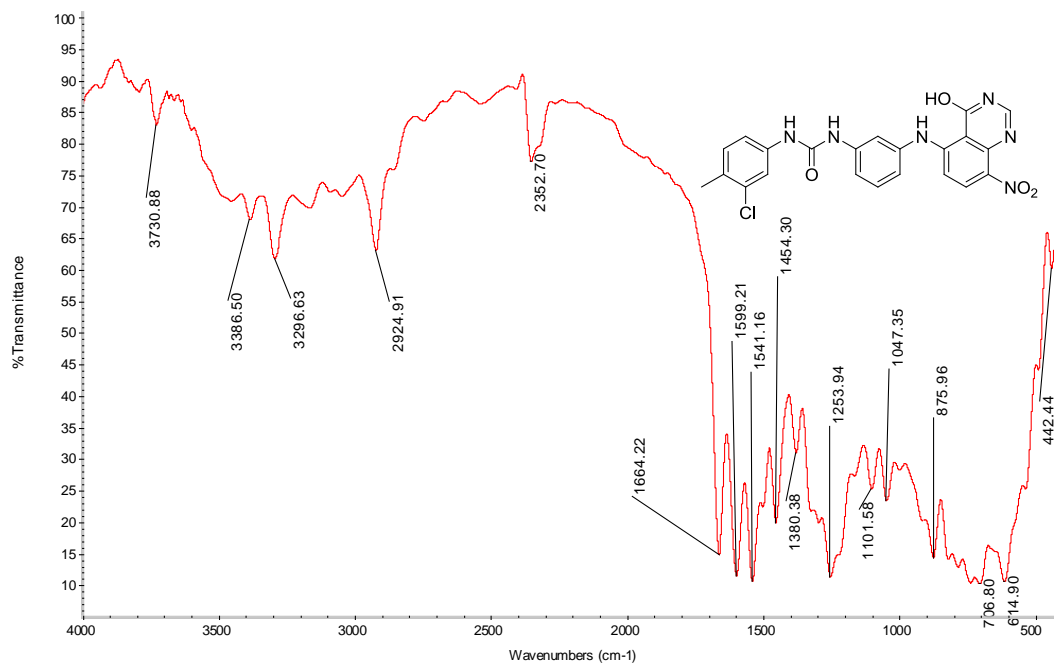
¹H-NMR spectrum of 6h



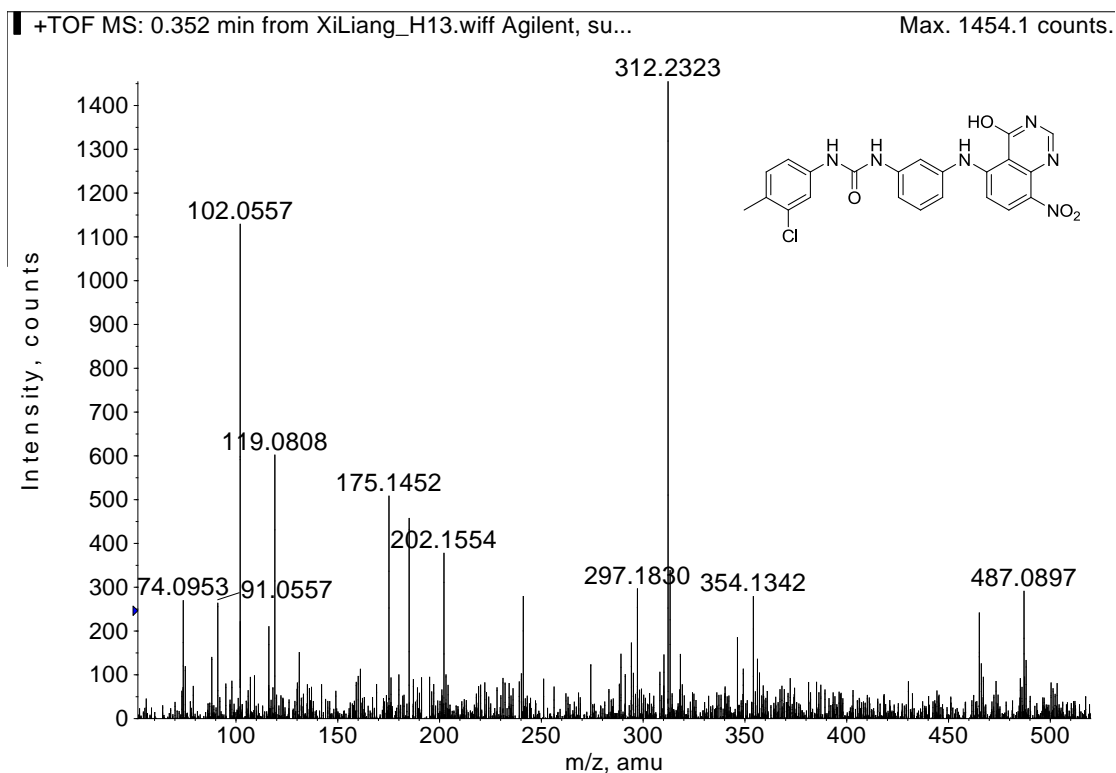
¹³C-NMR spectrum of 6h

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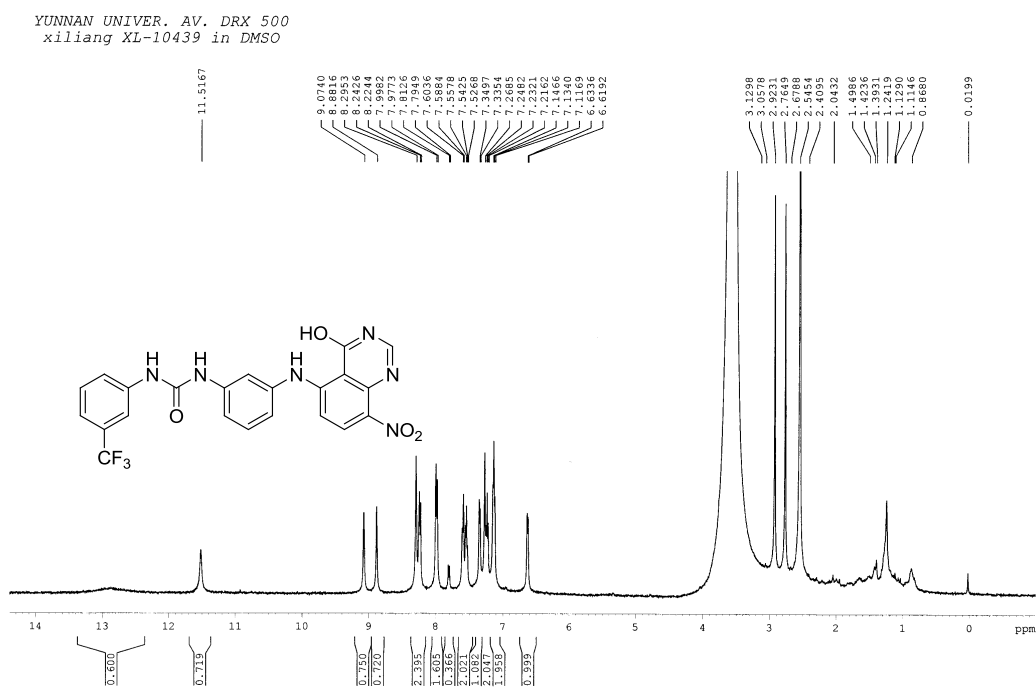
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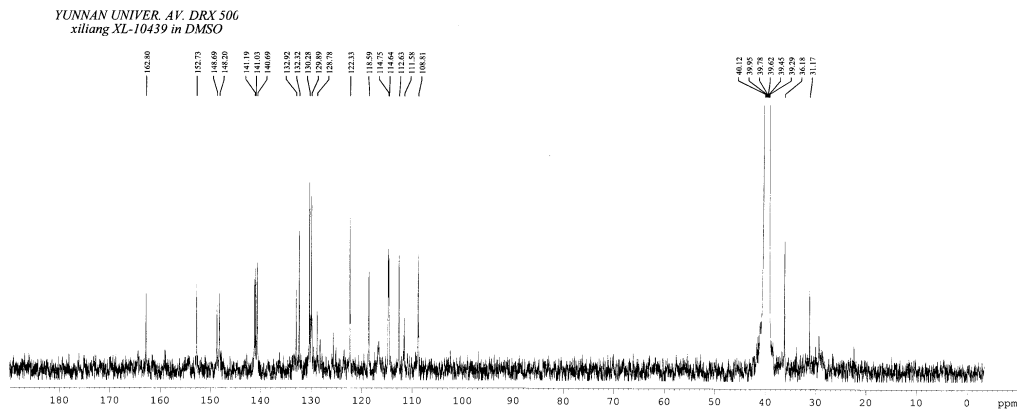
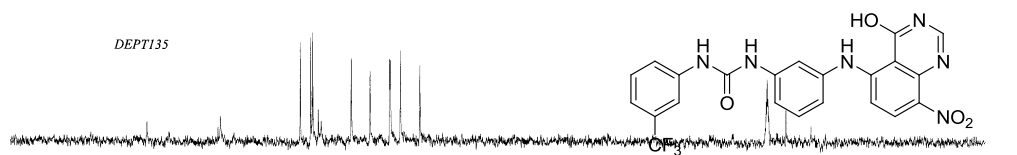
IR spectrum of 6h



MS spectrum of 6h



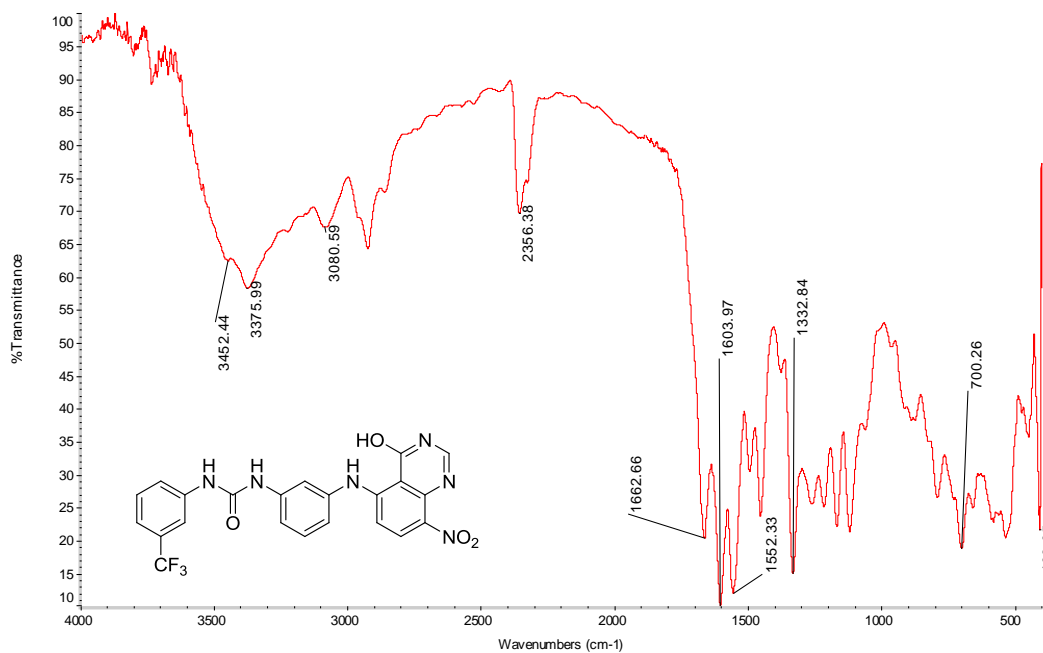
¹H-NMR spectrum of 6i



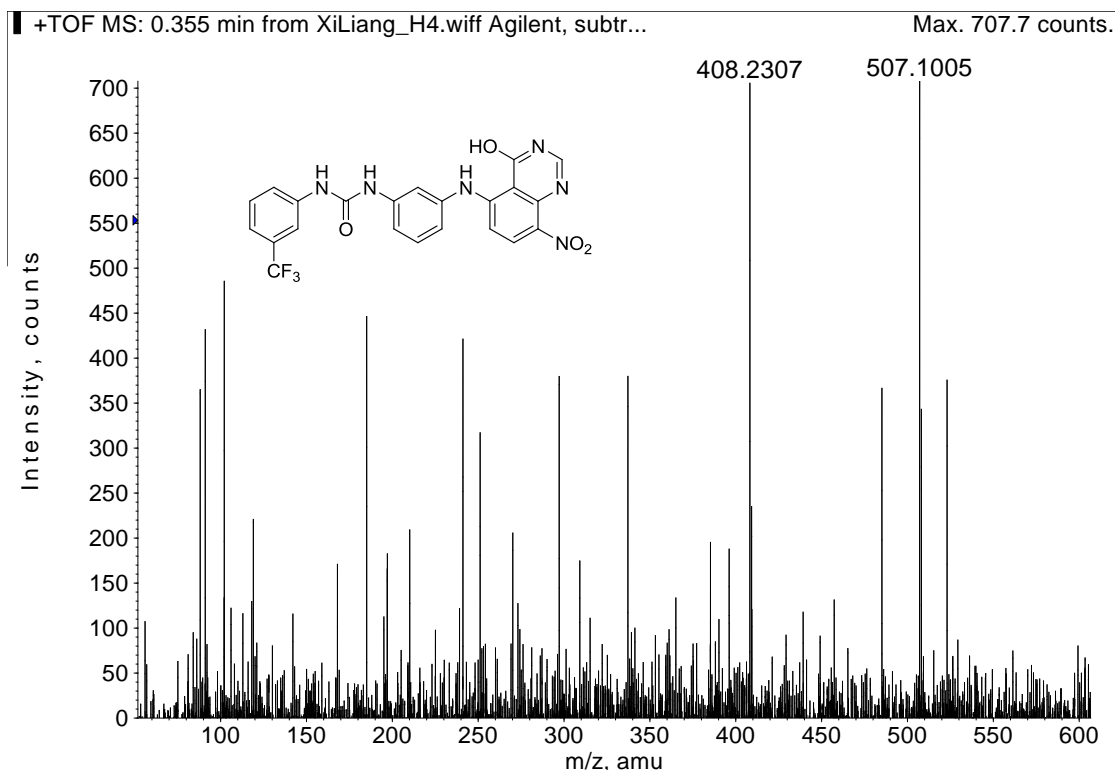
¹³C-NMR spectrum of 6i

Supporting Information

For

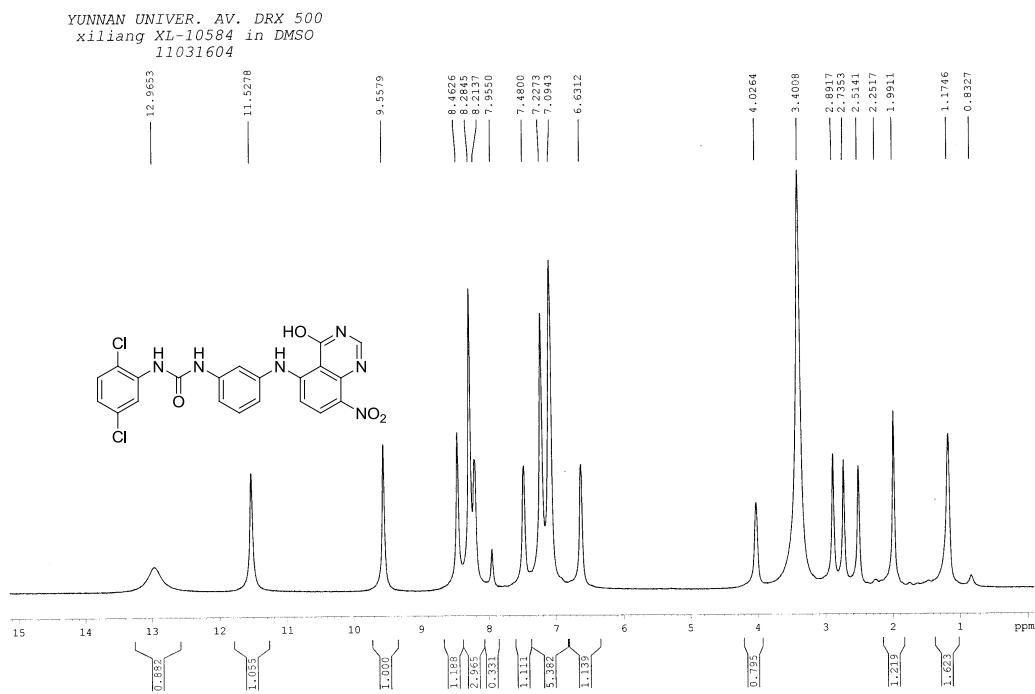


IR spectrum of 6i

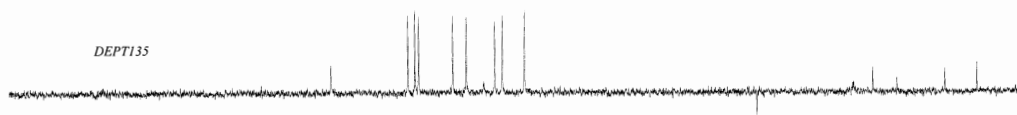


MS spectrum of 6i

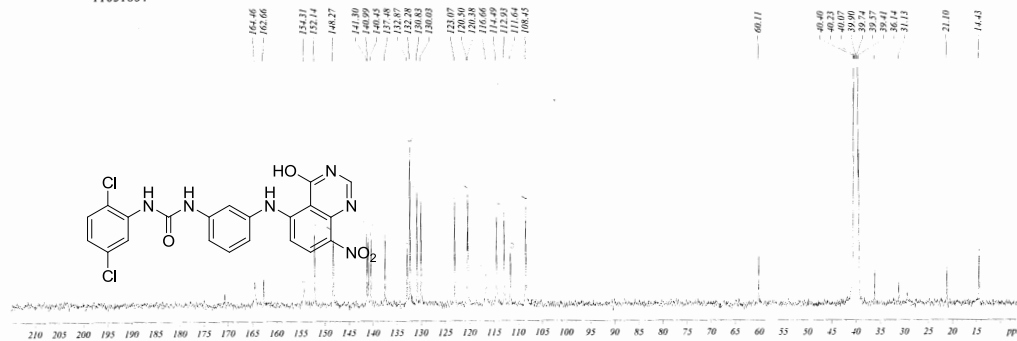
For



¹H-NMR spectrum of 6j



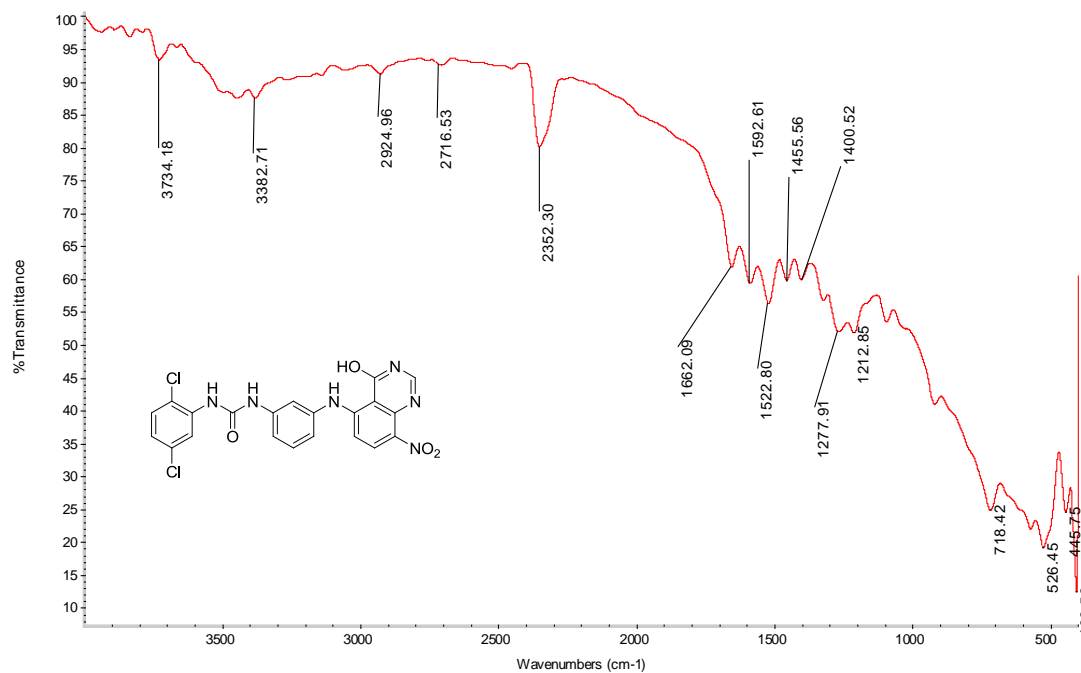
YUNNAN UNIVER. AV. DRX 500
 xiliang XL-10584 in DMSO
 11031604



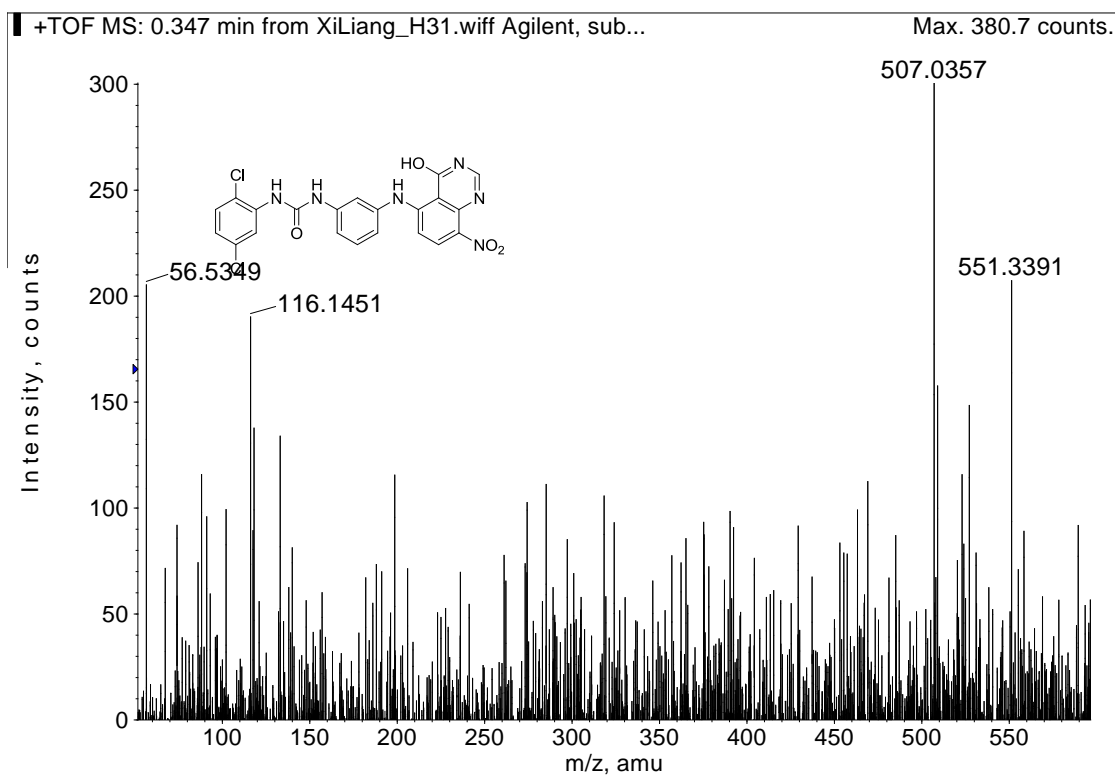
¹³C-NMR spectrum of 6j

Supporting Information

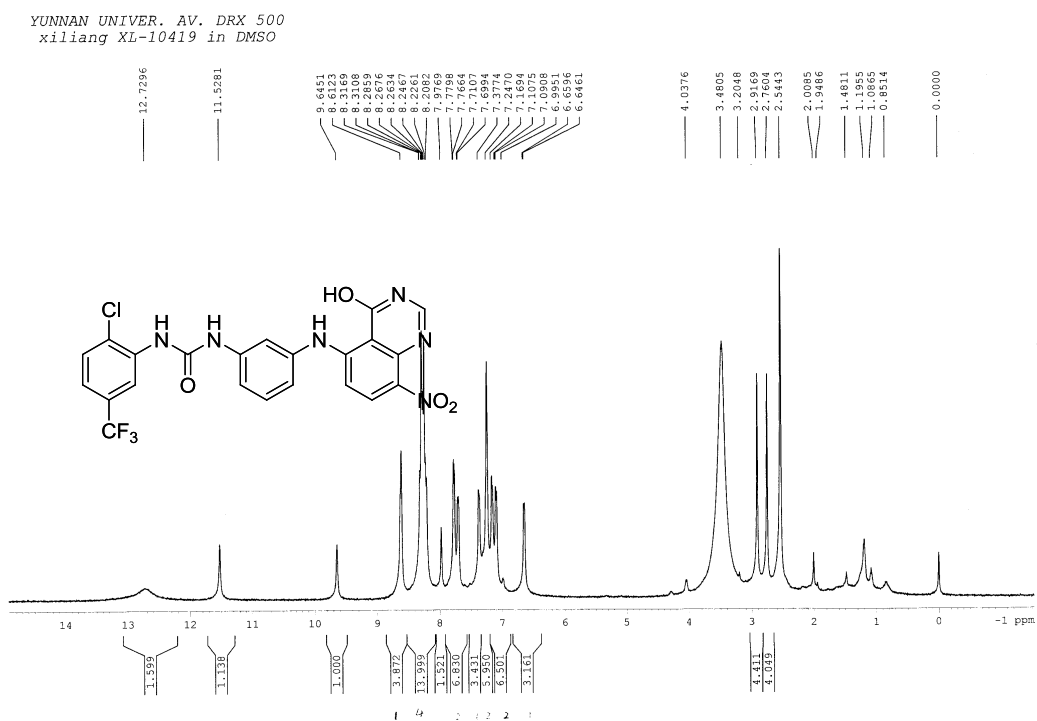
For



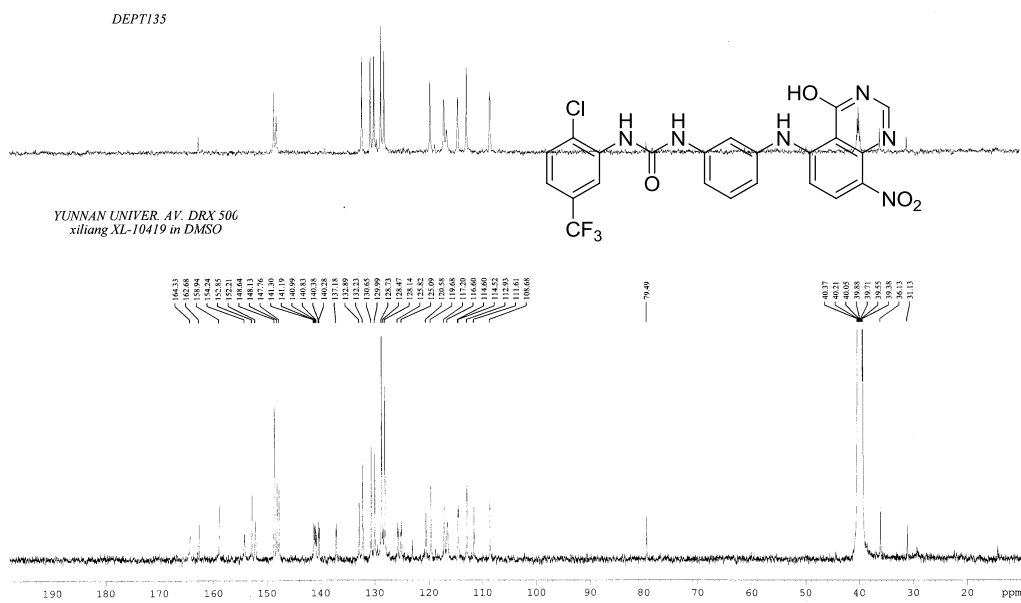
IR spectrum of 6j



MS spectrum of 6j



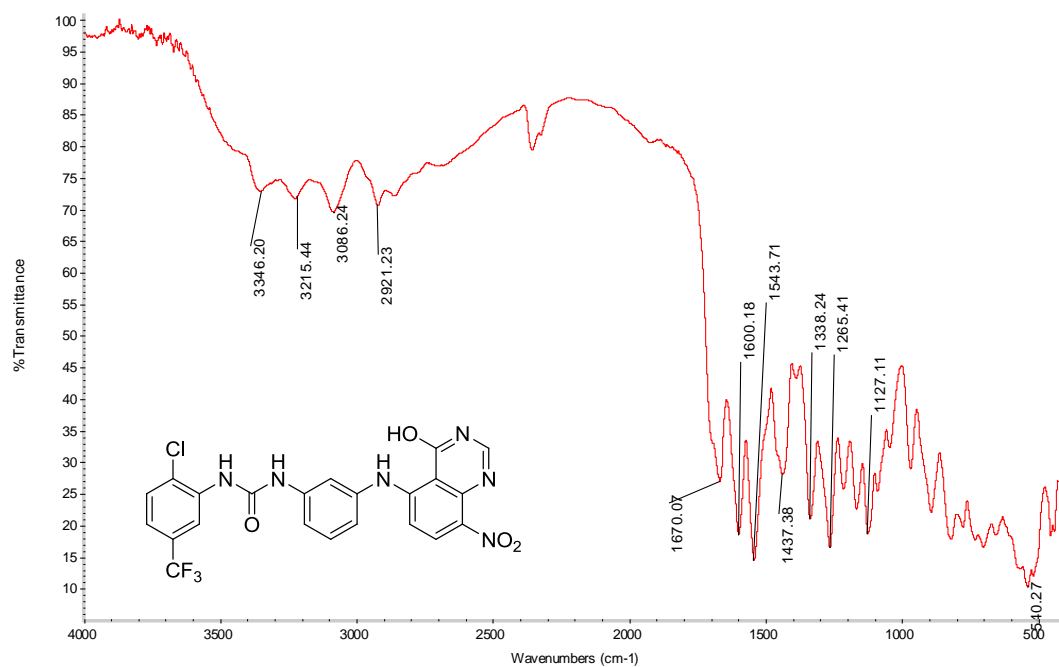
¹H-NMR spectrum of 6k



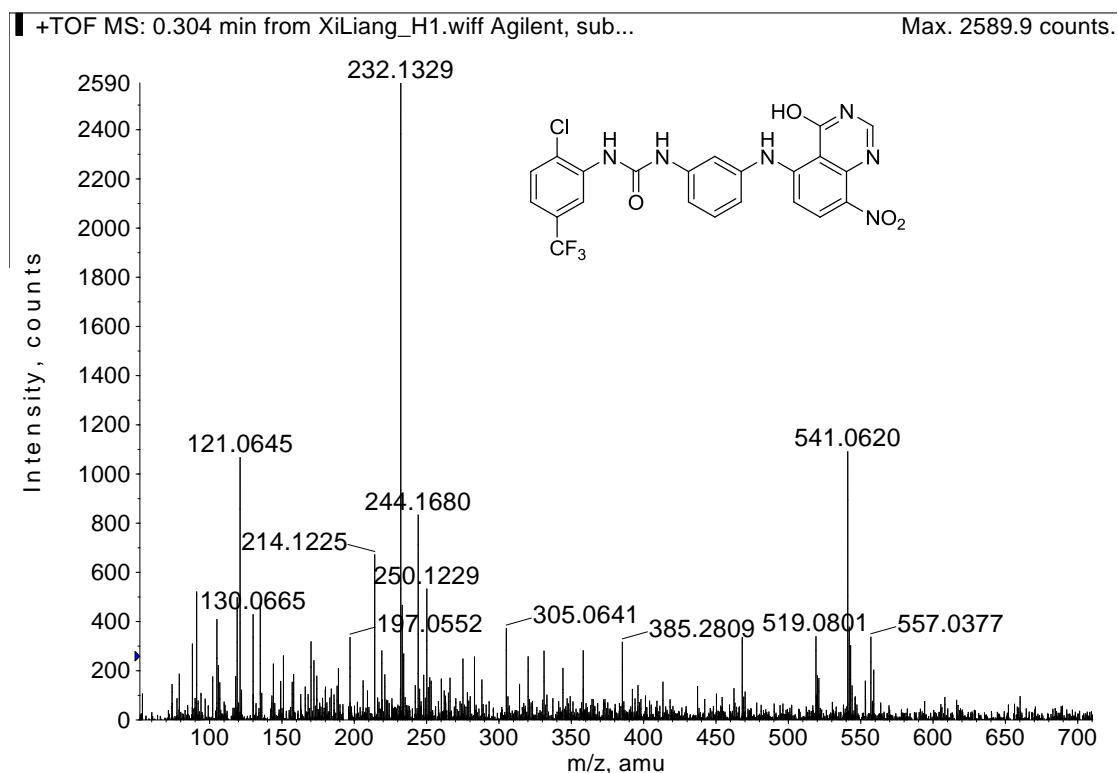
¹³C-NMR spectrum of 6k

Supporting Information

For

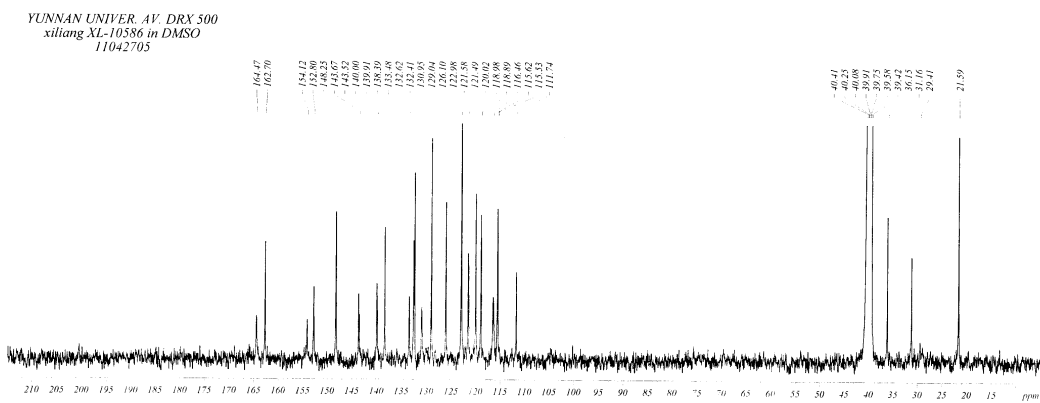
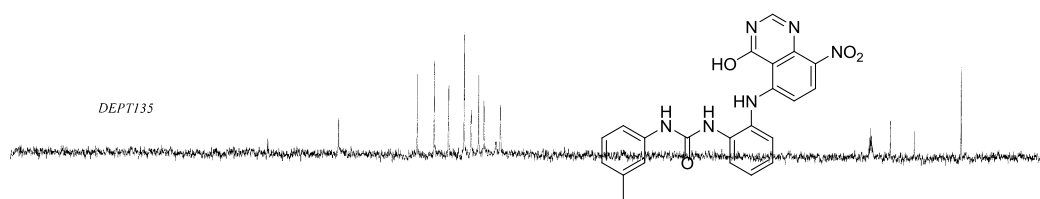
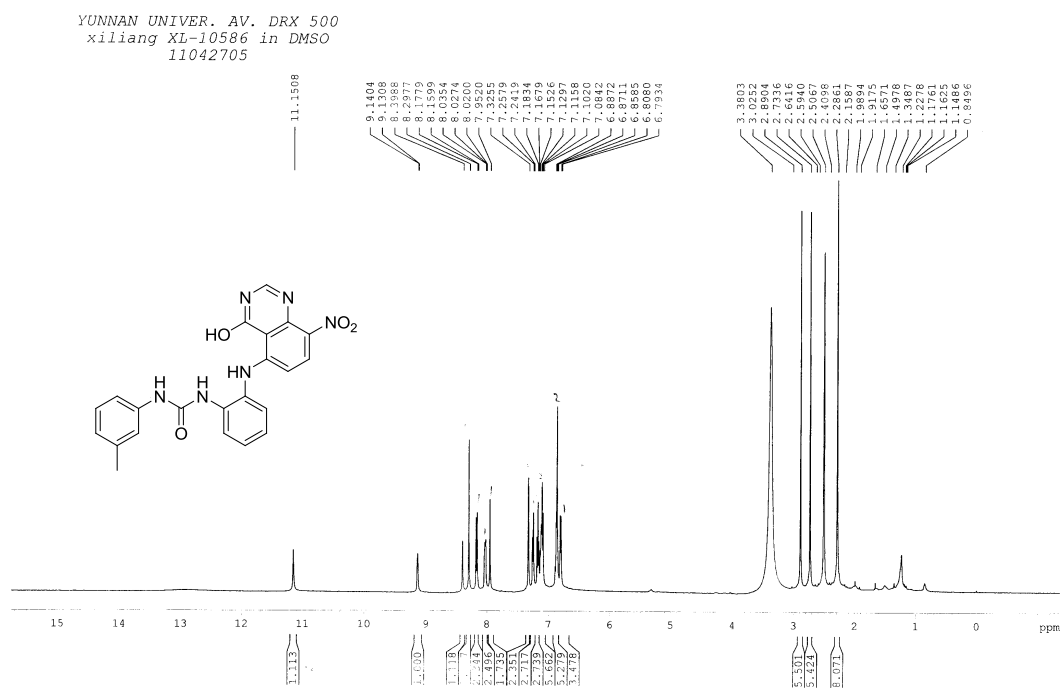


IR spectrum of 6k



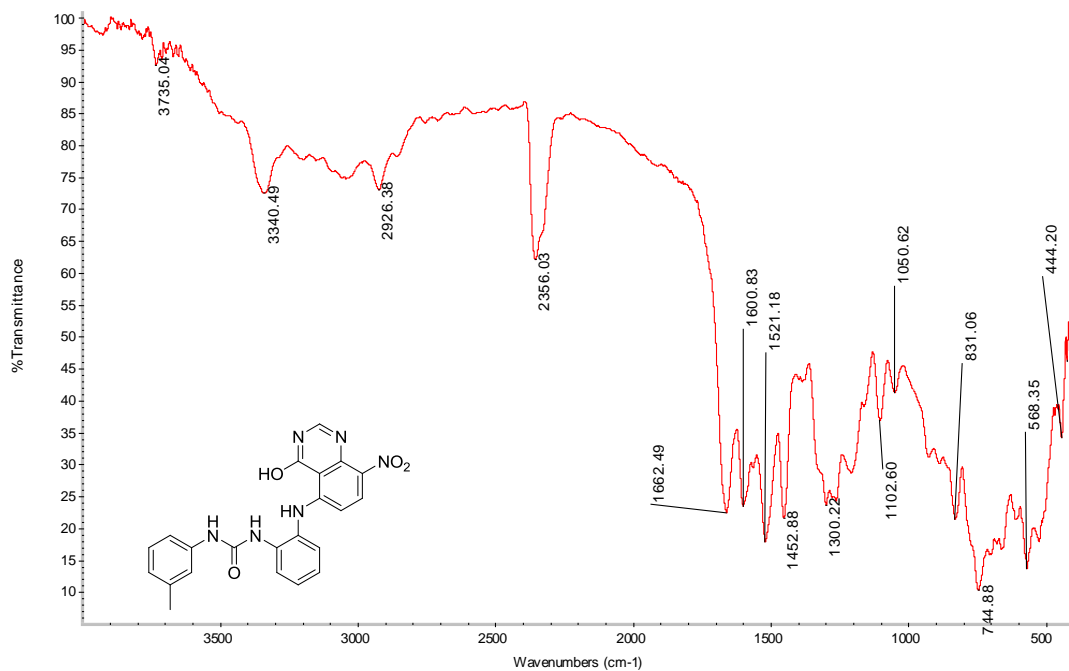
MS spectrum of 6k

For

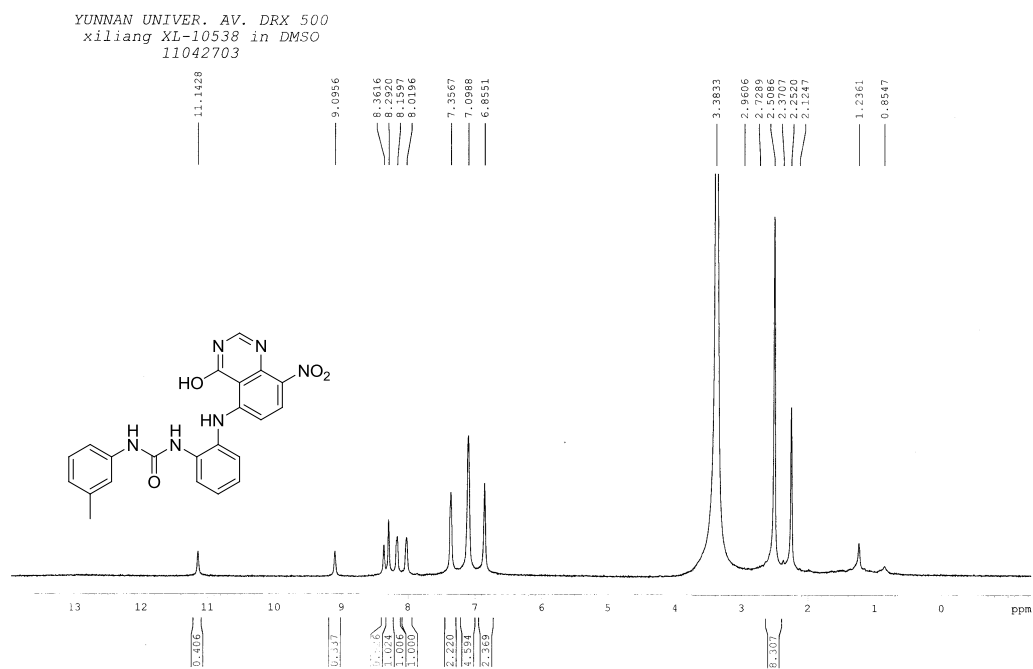


Supporting Information

For

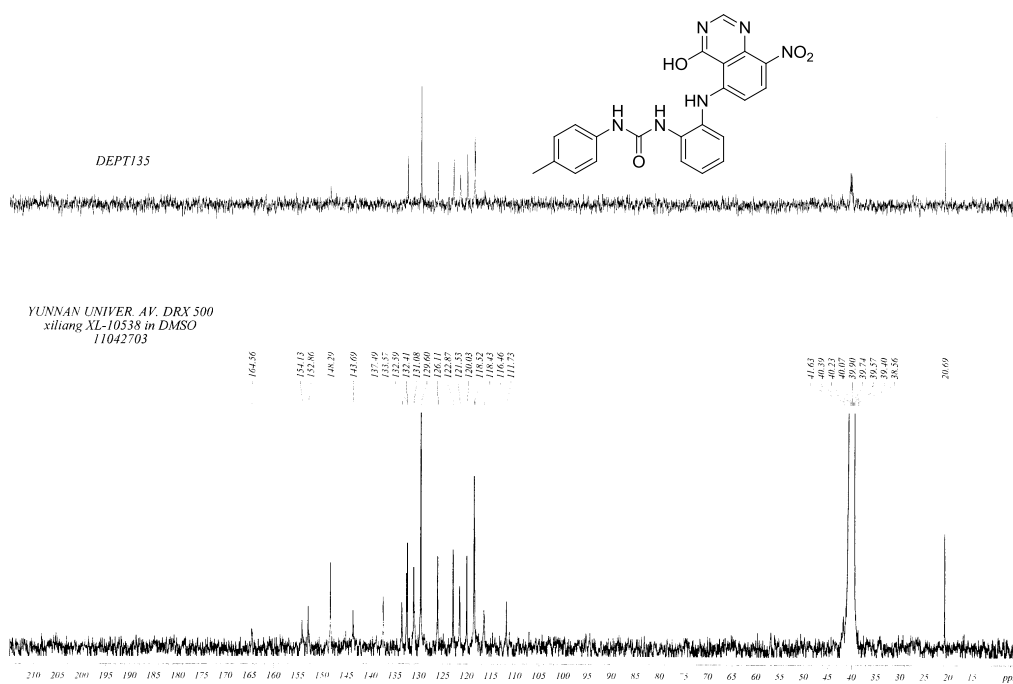


IR spectrum of 6l

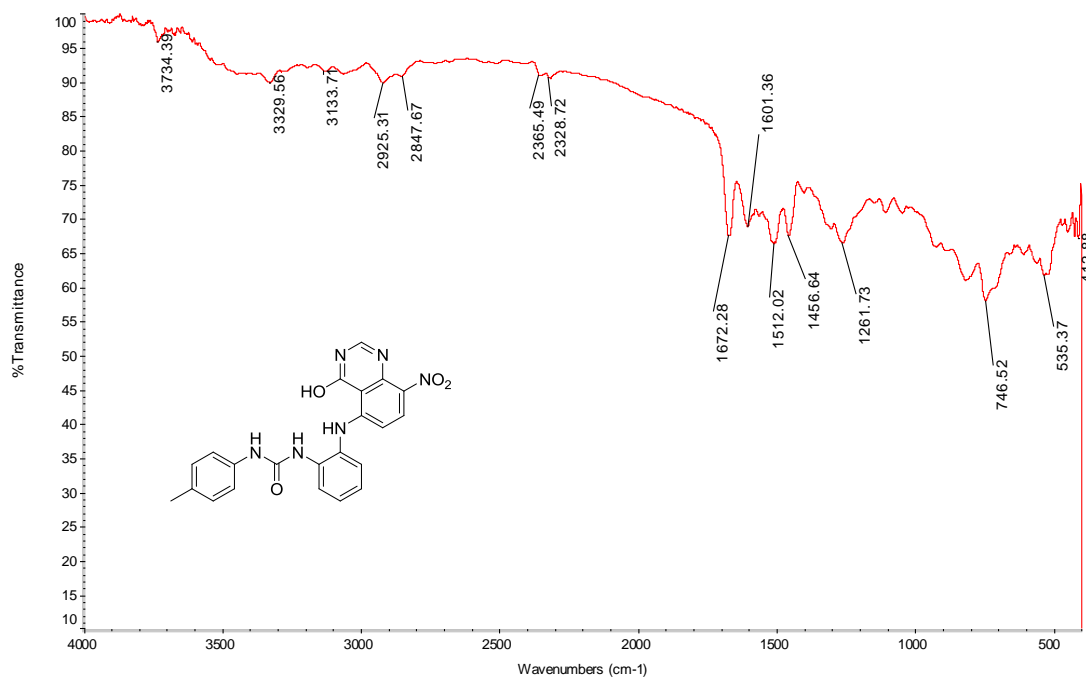


¹H-NMR spectrum of 6m

For



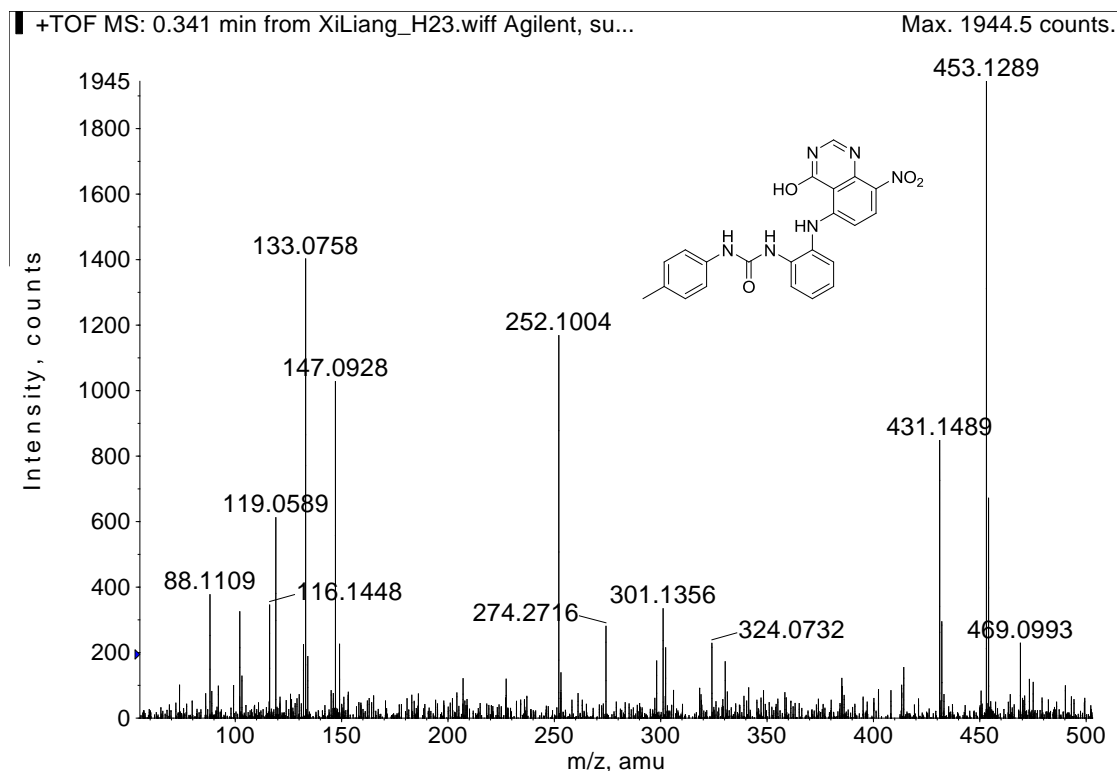
¹³C-NMR spectrum of 6m



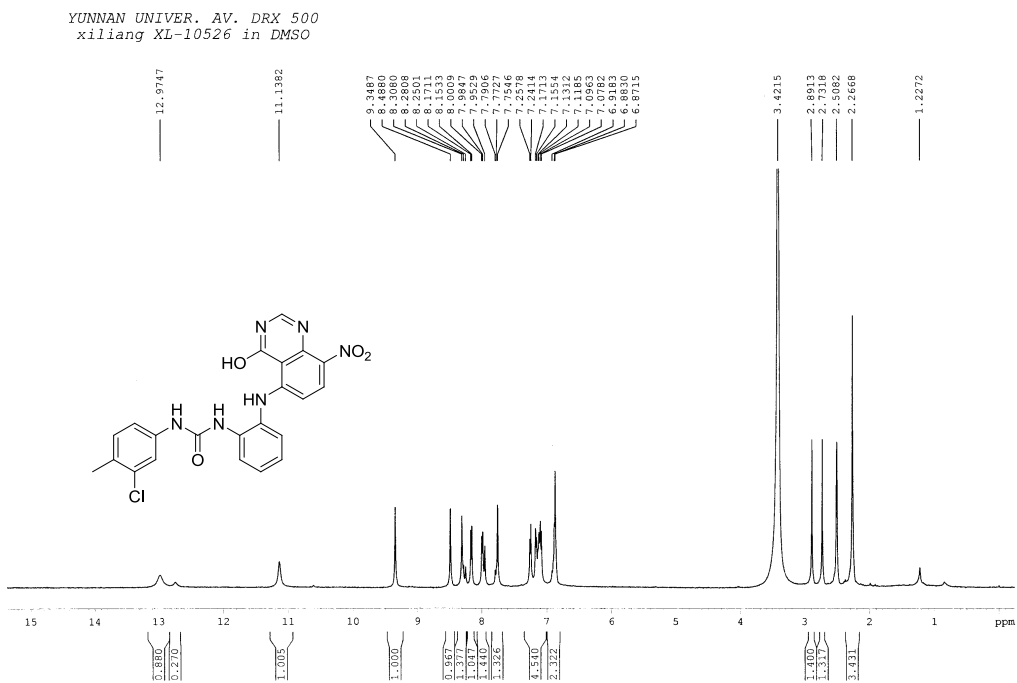
IR spectrum of 6m

Supporting Information

For

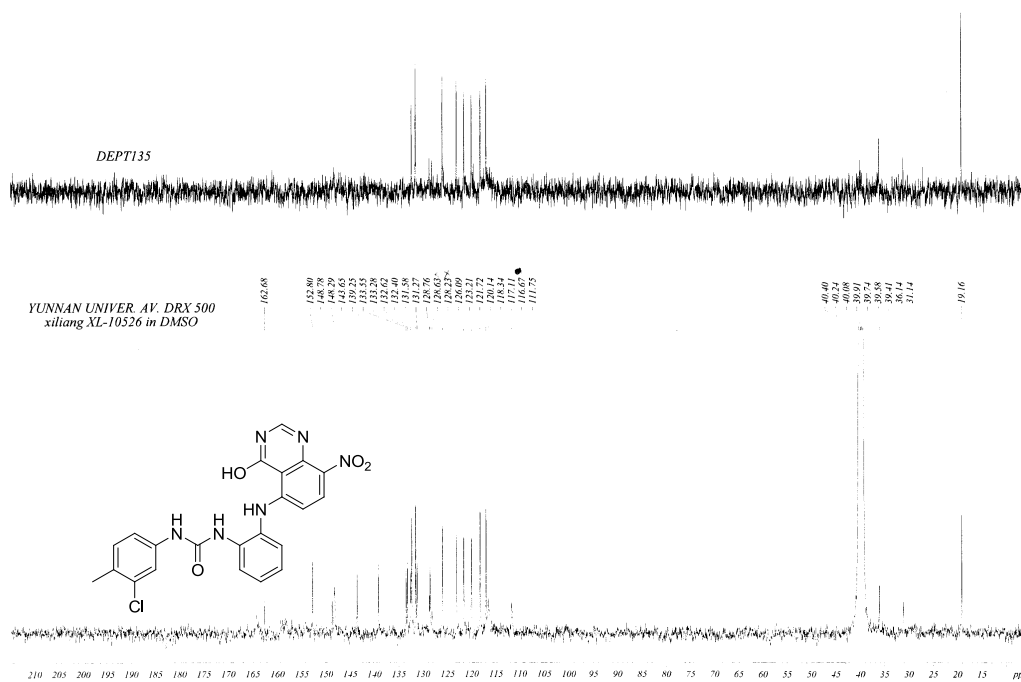


MS spectrum of 6m

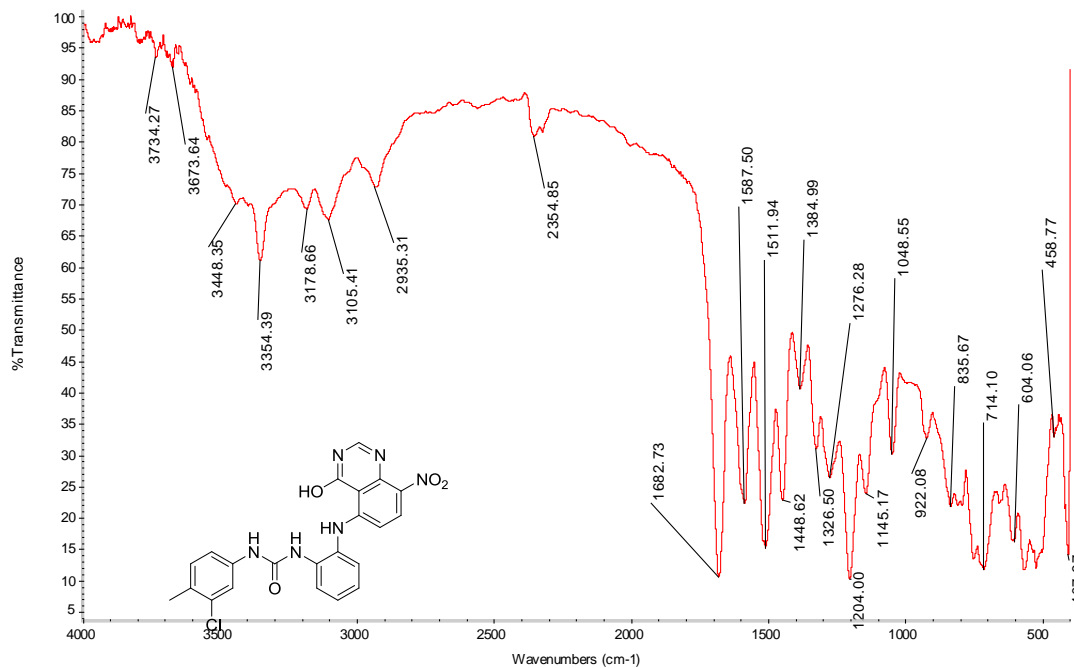


¹H-NMR spectrum of 6n

For



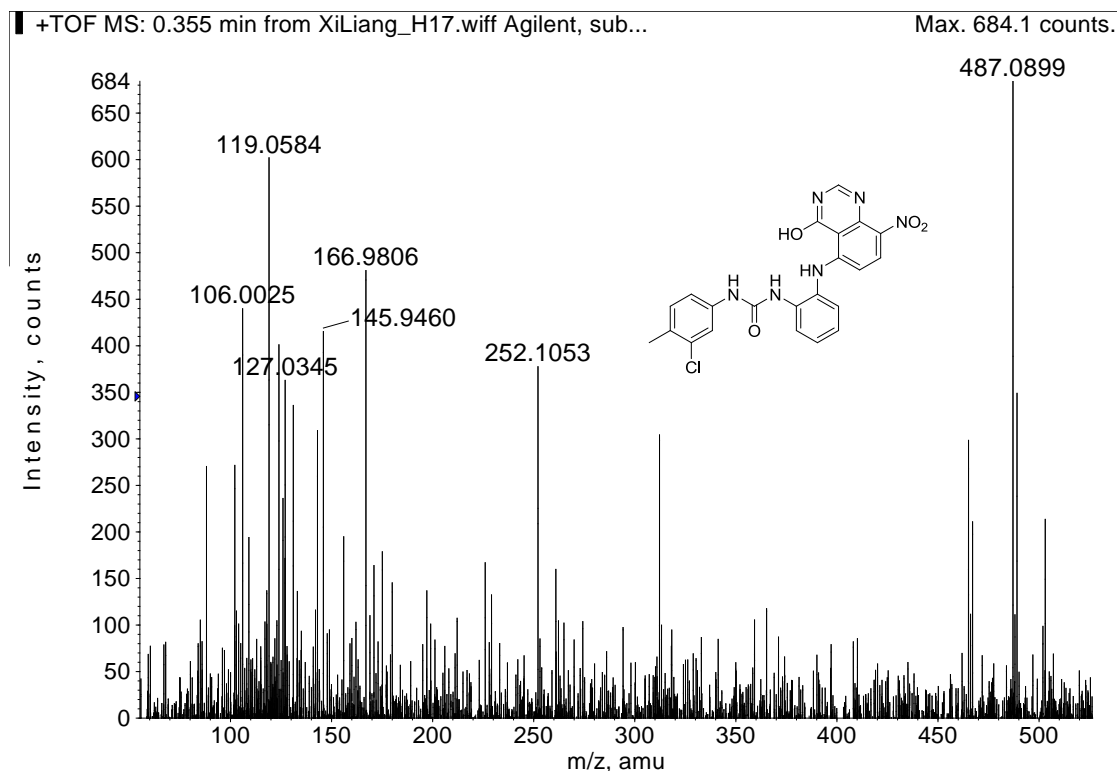
¹³C-NMR spectrum of 6n



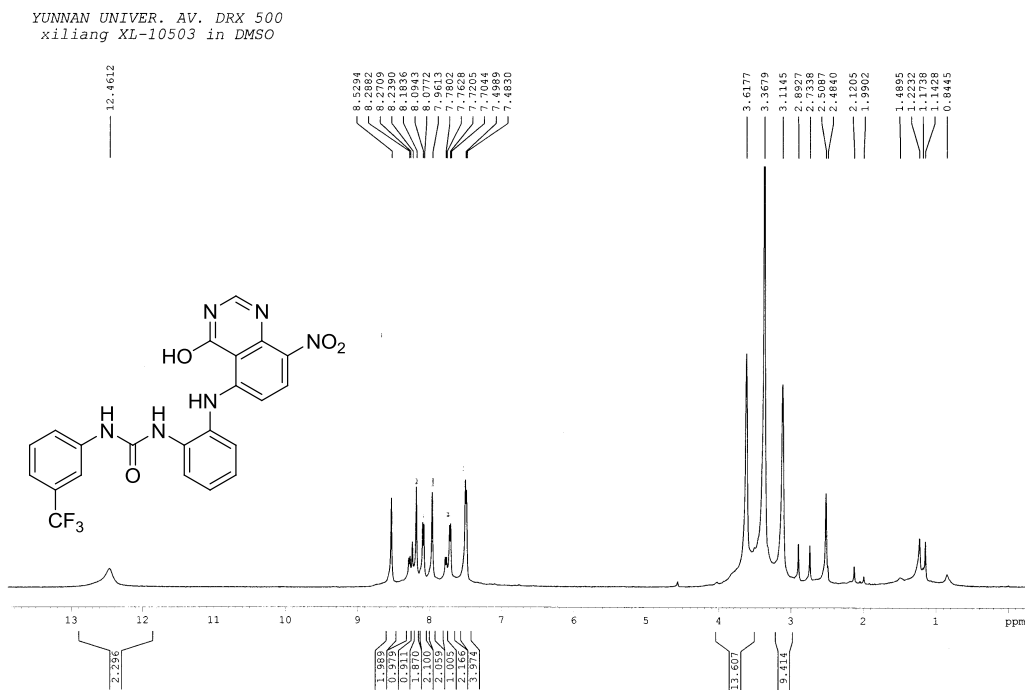
IR spectrum of 6n

Supporting Information

For

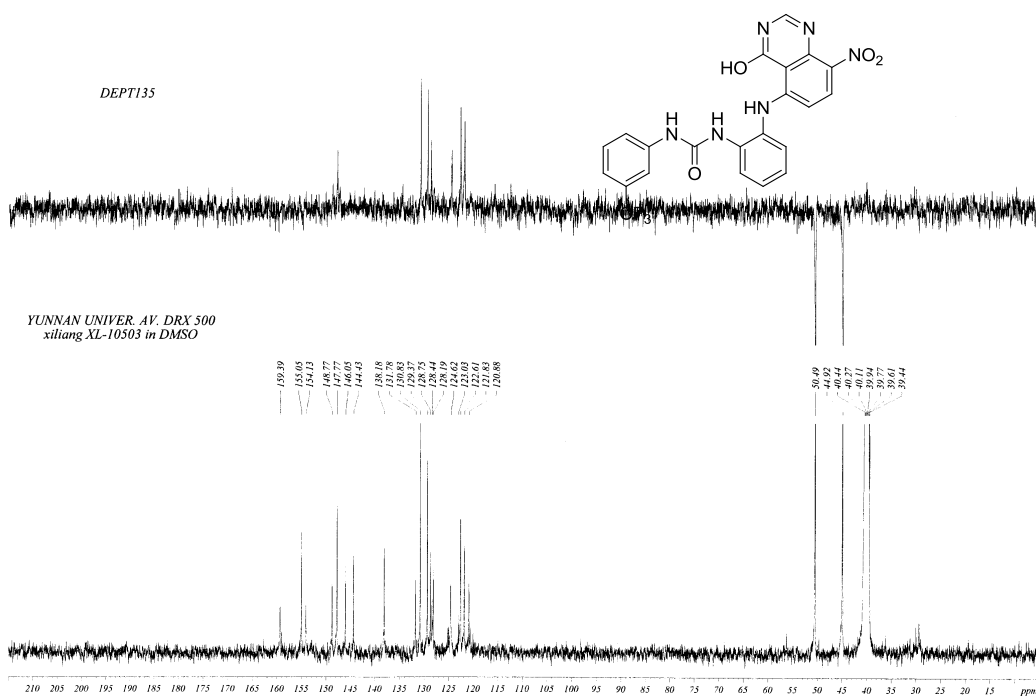


MS spectrum of 6n

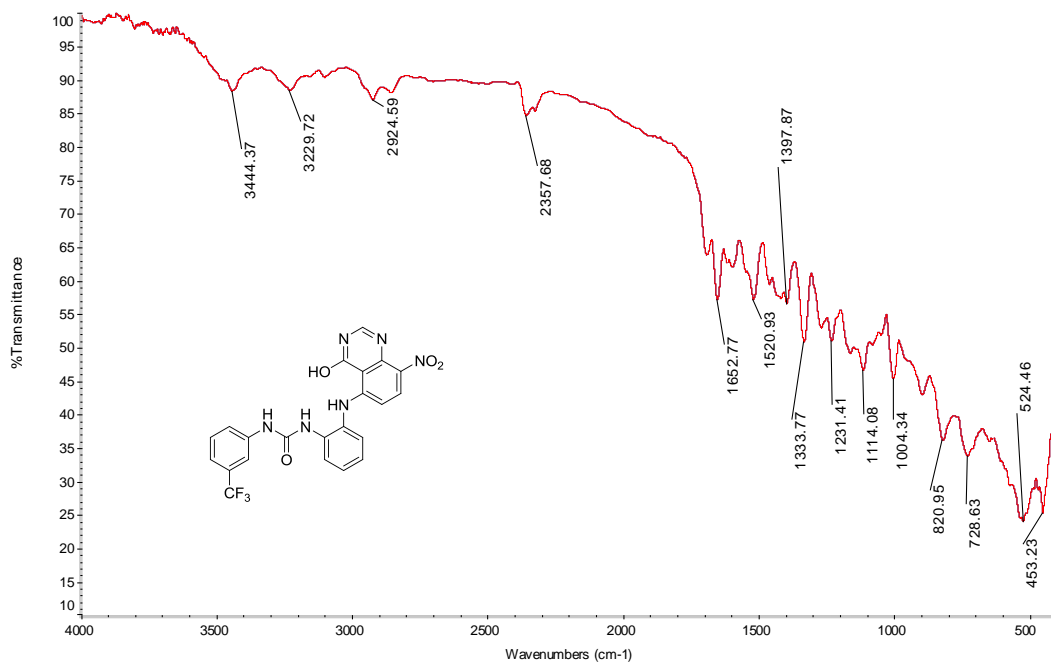


¹H-NMR spectrum of 6o

For



¹³C-NMR spectrum of 60

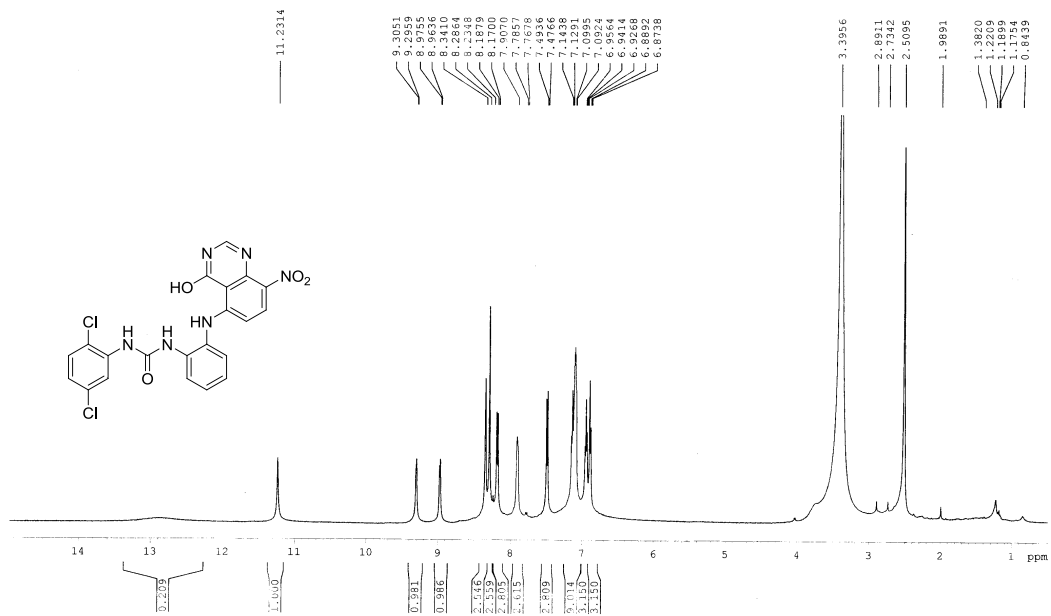


IR spectrum of 60

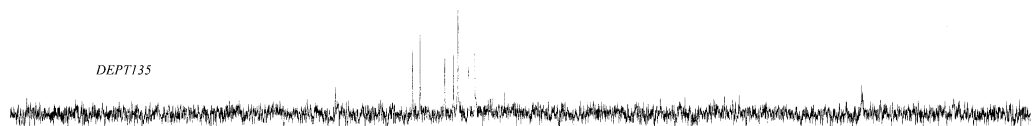
Supporting Information

For

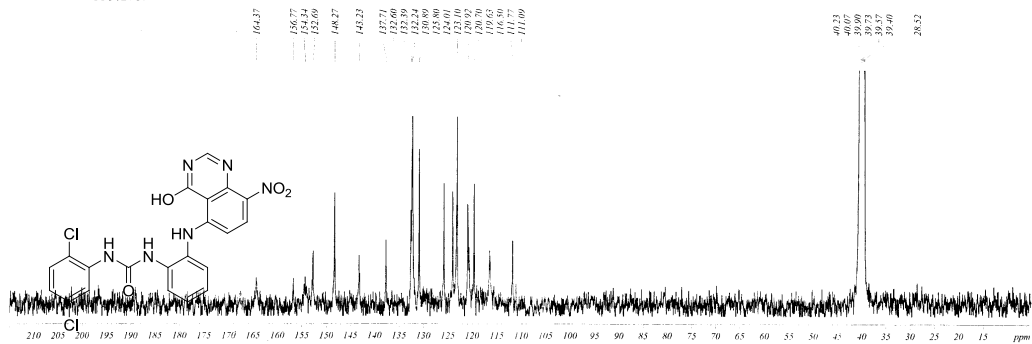
YUNNAN UNIVER. AV. DRX 500
xiliang XL-105101 in DMSO
11042707



¹H-NMR spectrum of 6p

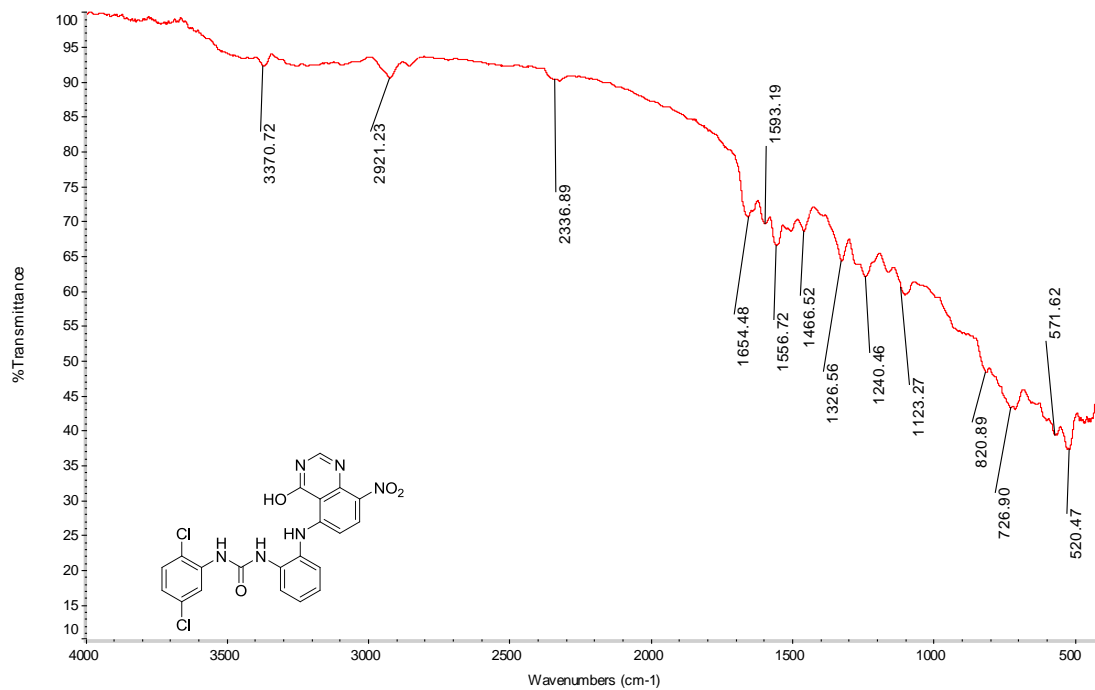


YUNNAN UNIVER. AV. DRX 500
xiliang XL-105101 in DMSO
11042707

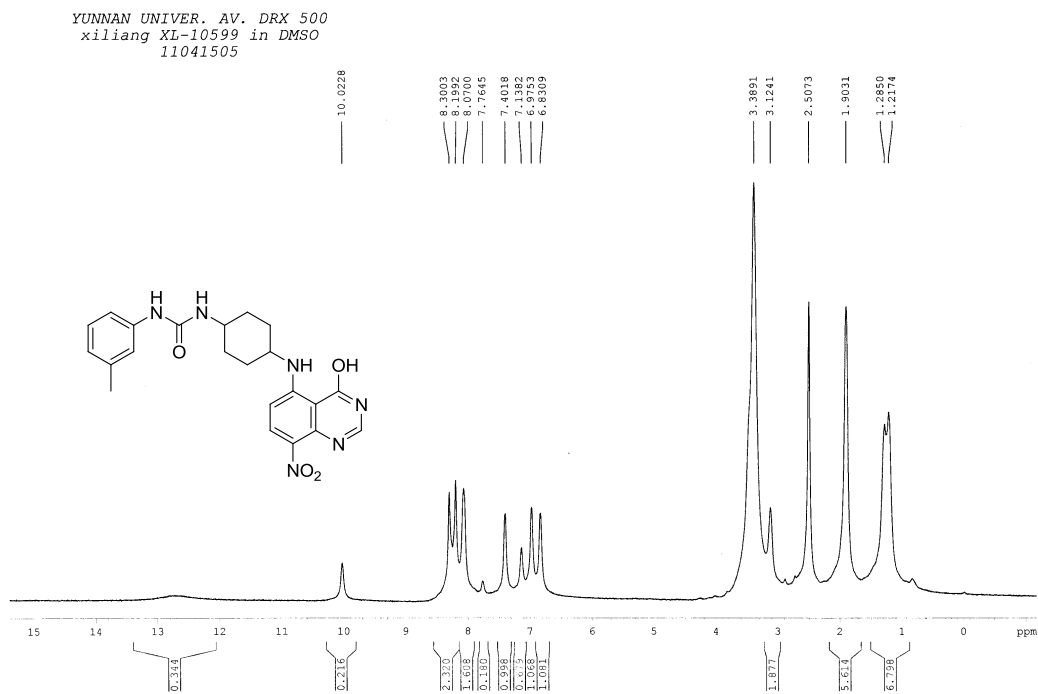


¹³C-NMR spectrum of 6p

For



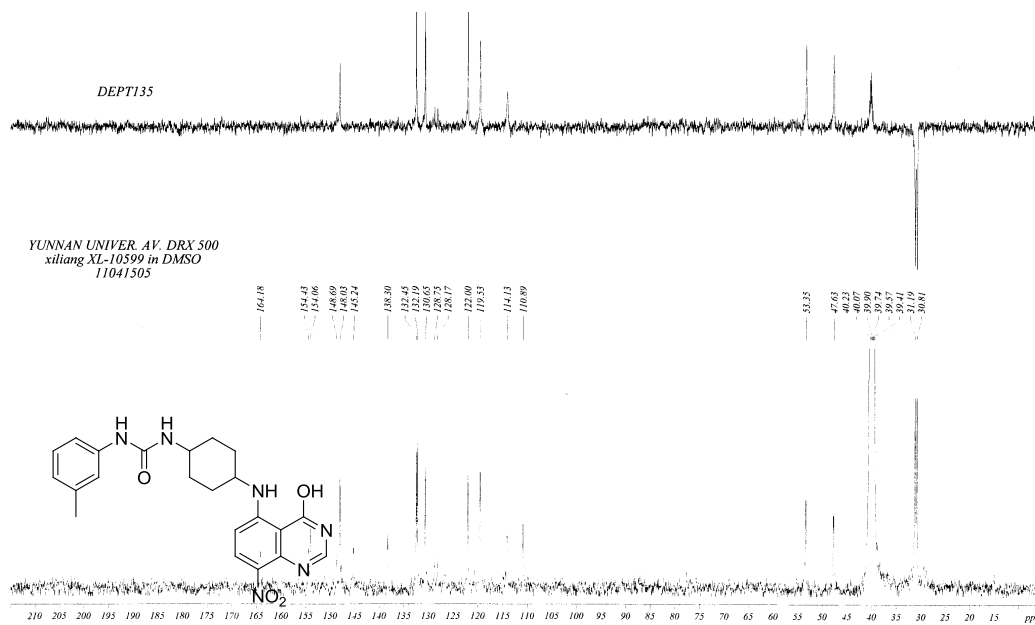
IR spectrum of 6p



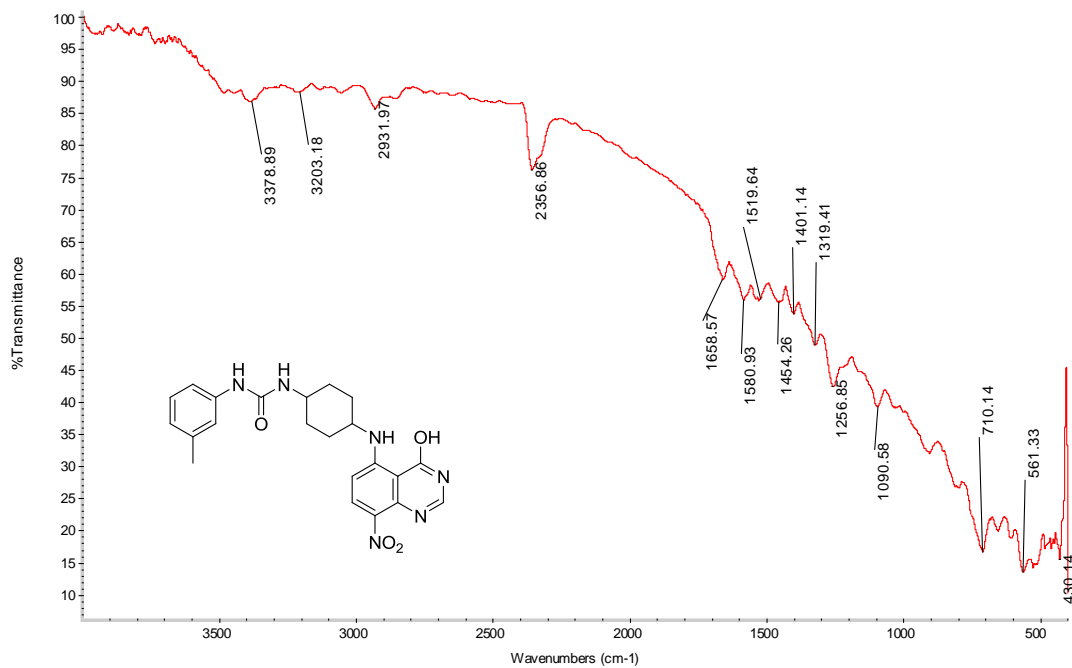
¹H-NMR spectrum of 6q

Supporting Information

For

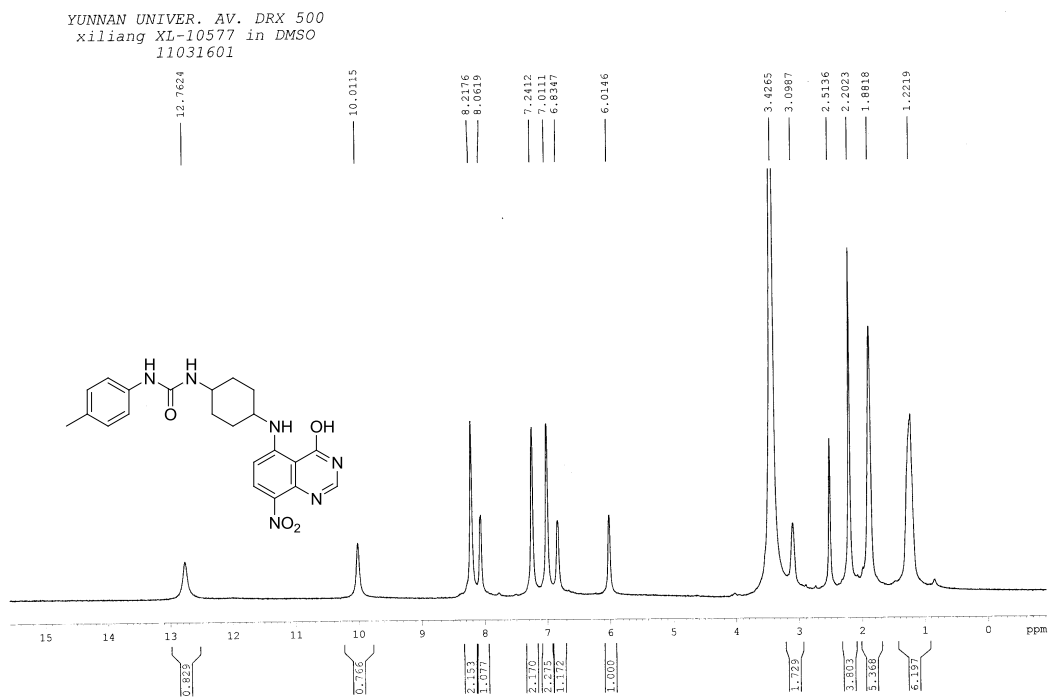


¹³C-NMR spectrum of 6q

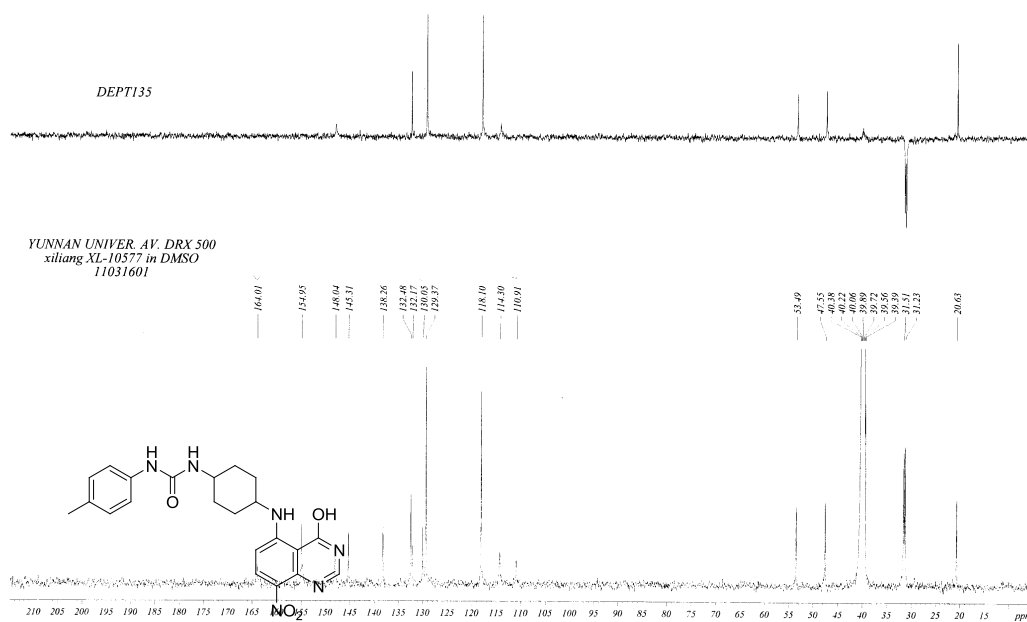


IR spectrum of 6q

For



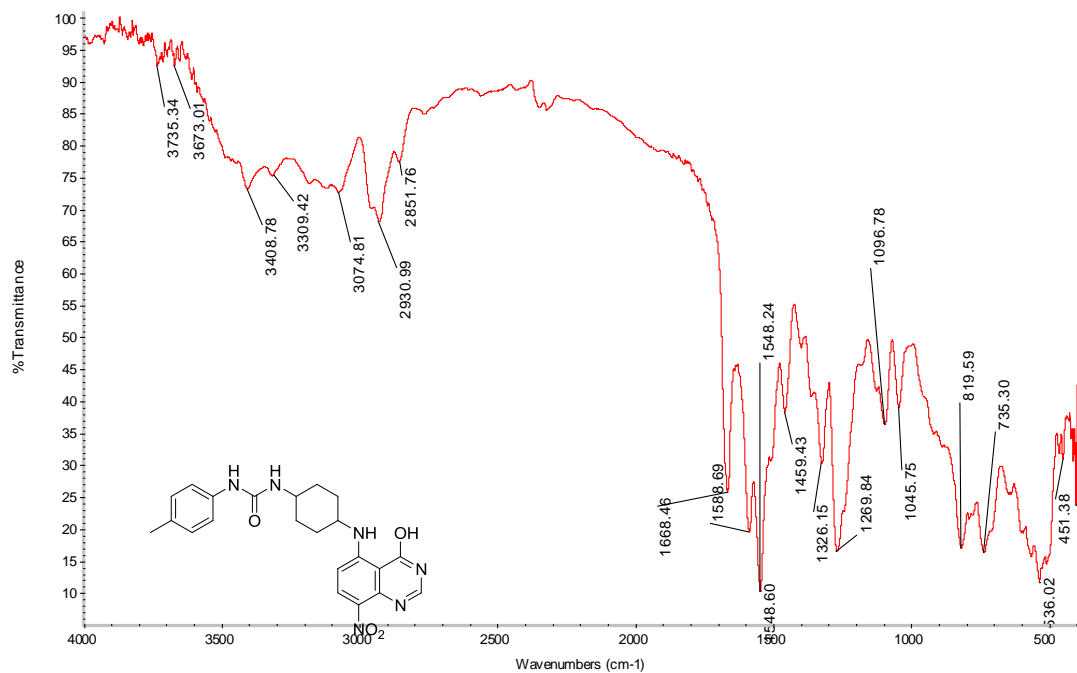
¹H-NMR spectrum of 6r



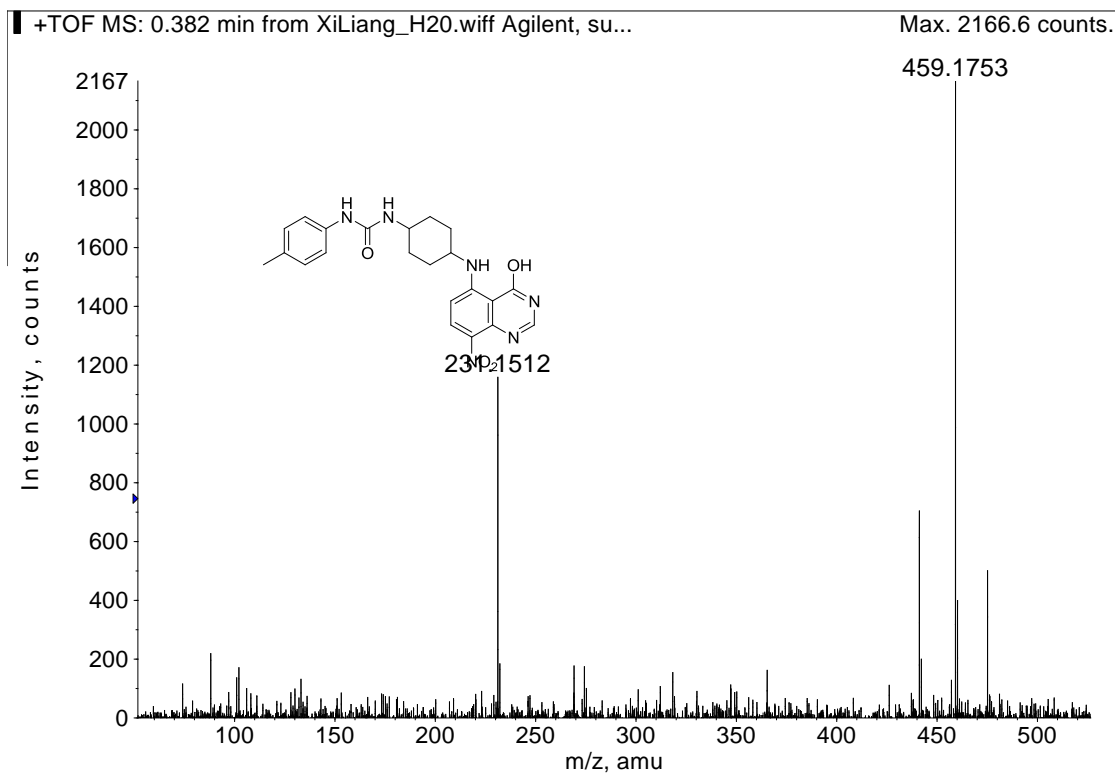
¹³C-NMR spectrum of 6r

Supporting Information

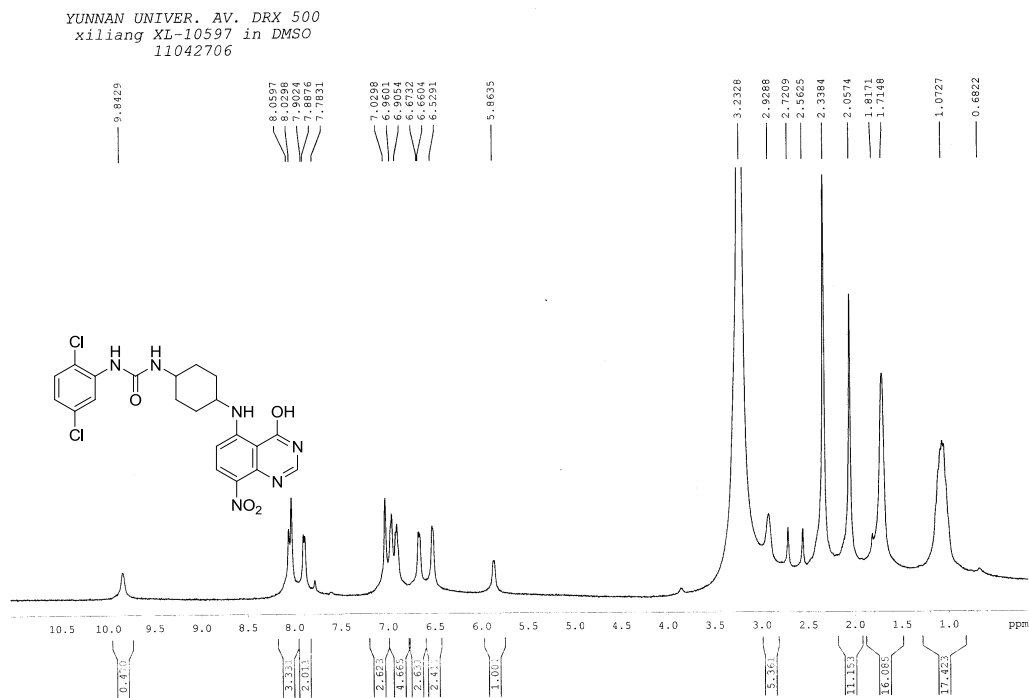
For



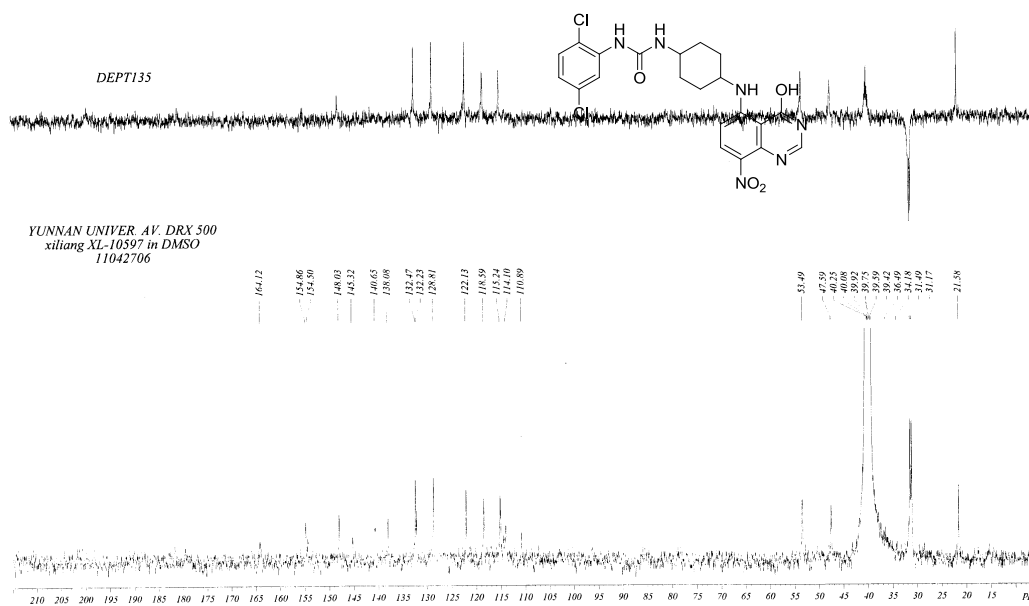
IR spectrum of 6r



MS spectrum of 6r



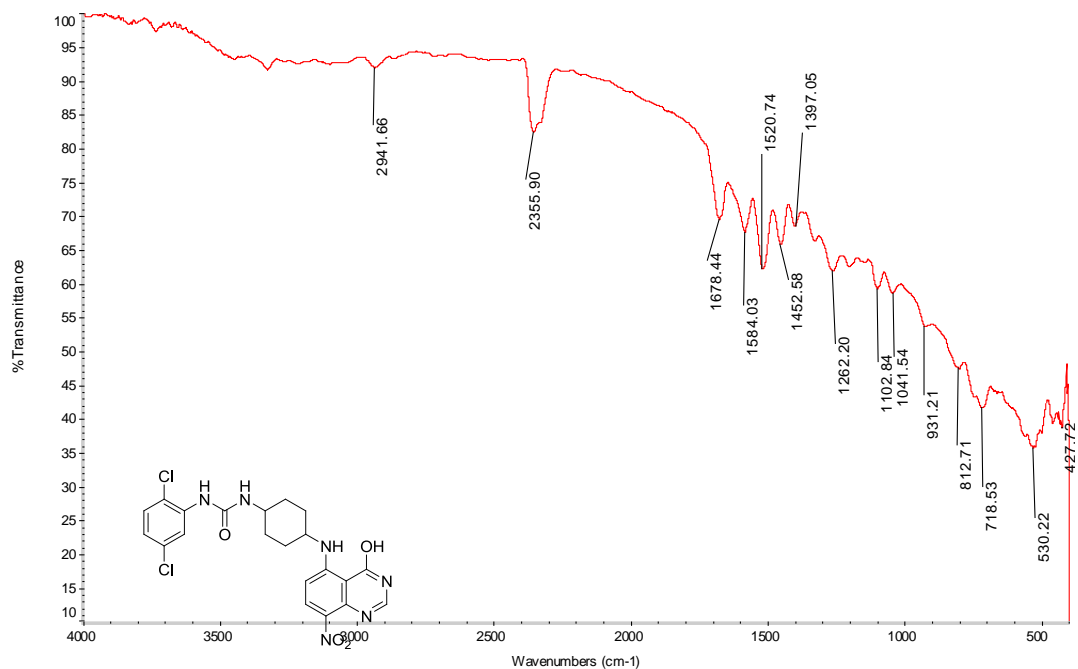
¹H-NMR spectrum of 6s



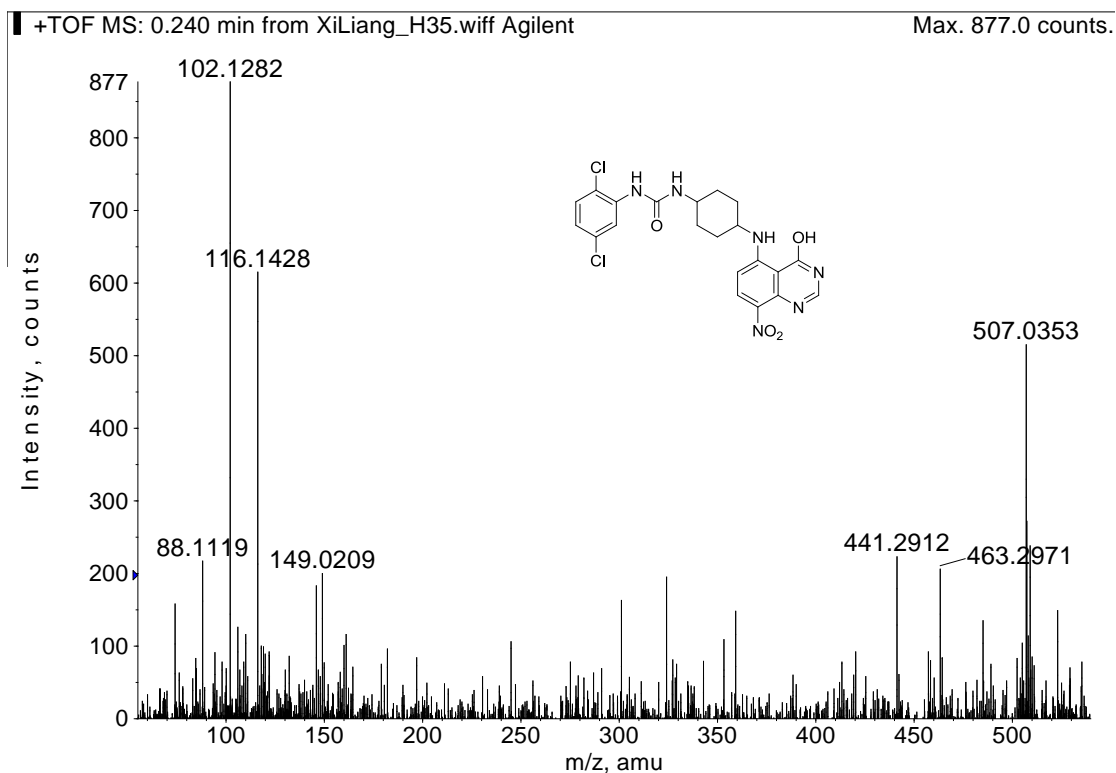
¹³C-NMR spectrum of 6s

Supporting Information

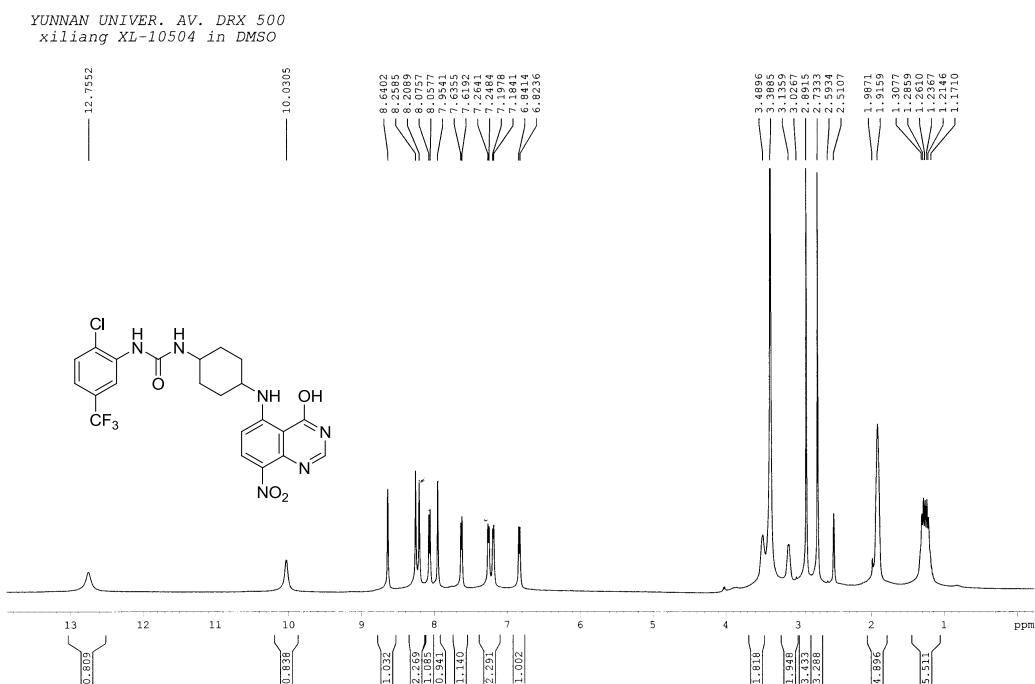
For



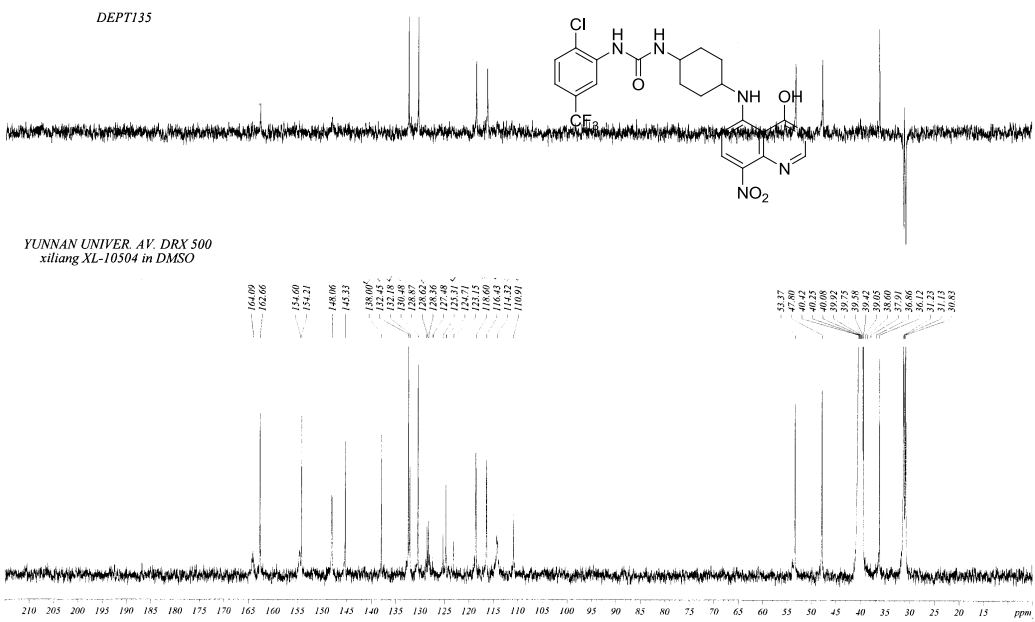
IR spectrum of 6s



MS spectrum of 6s



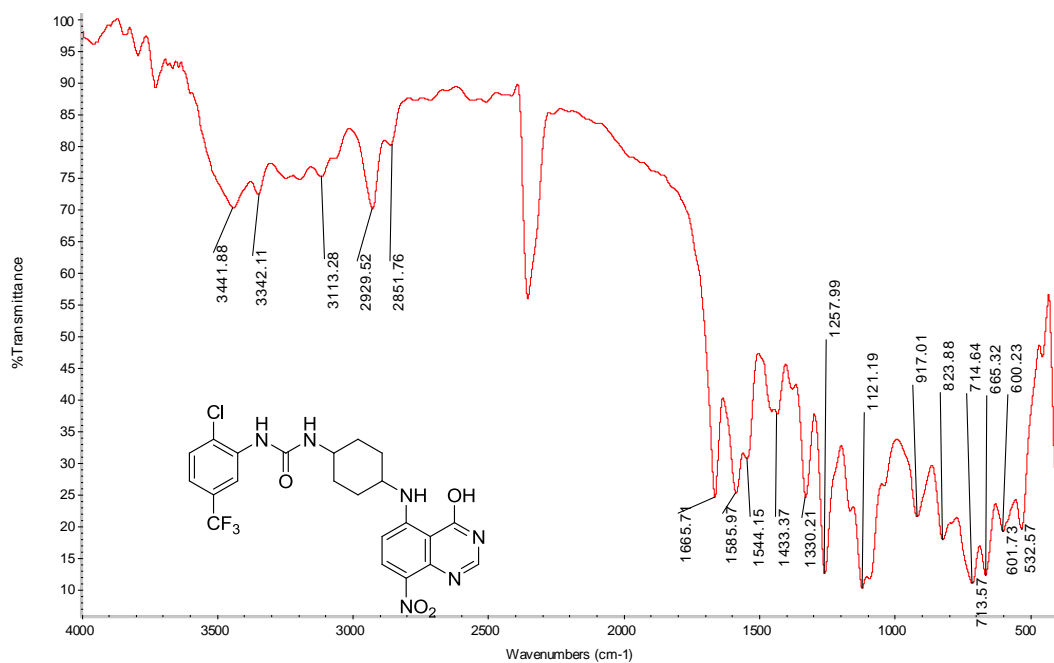
¹H-NMR spectrum of 6t



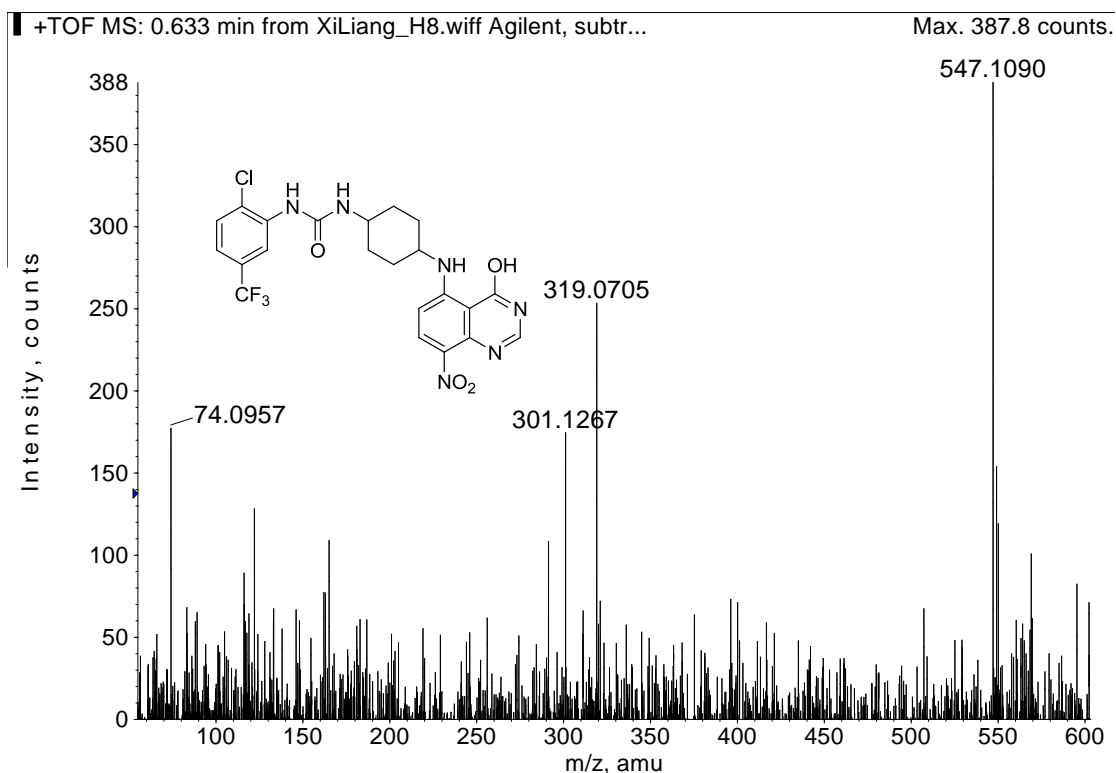
¹³C-NMR spectrum of 6t

Supporting Information

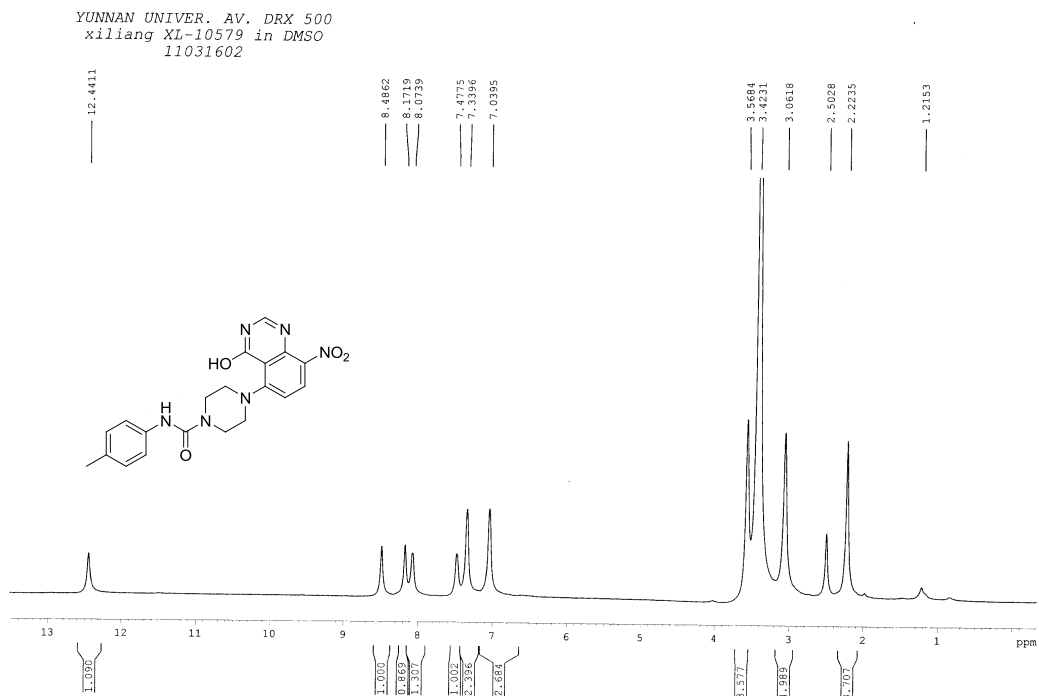
For



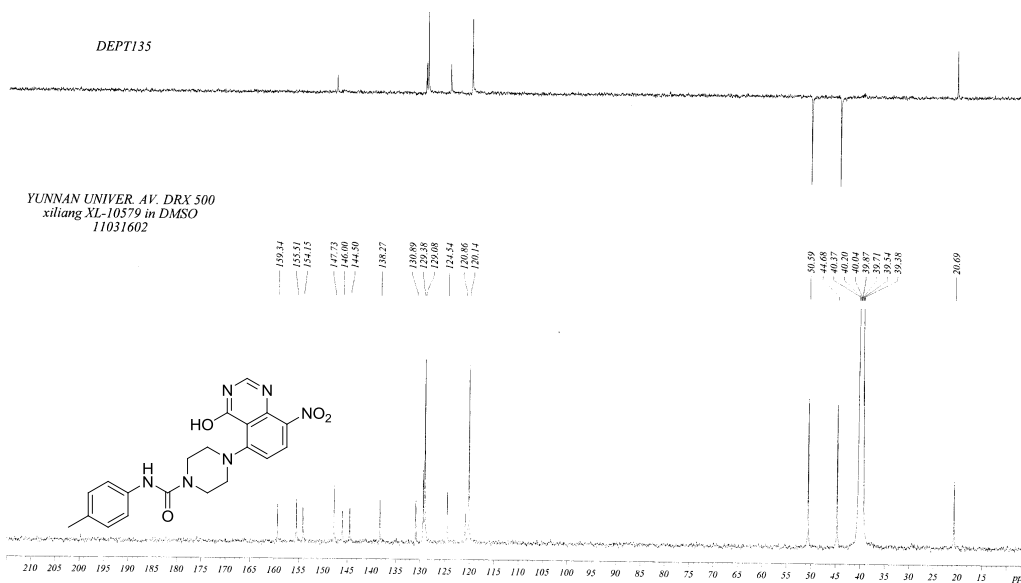
IR spectrum of 6t



MS spectrum of 6t



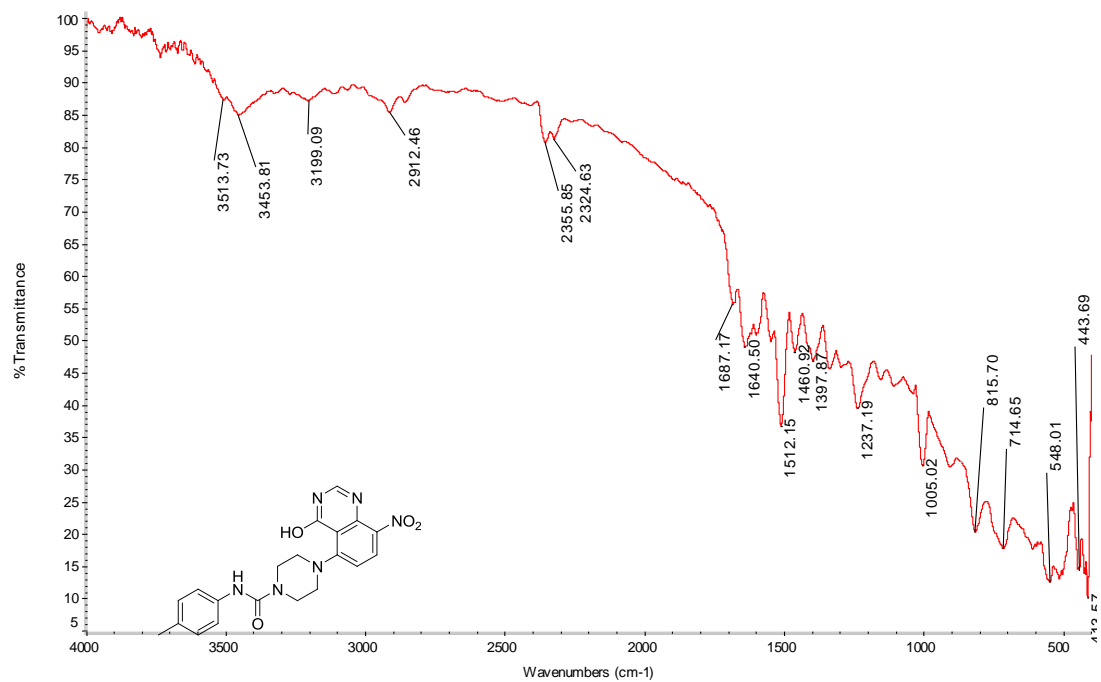
¹H-NMR spectrum of 6u



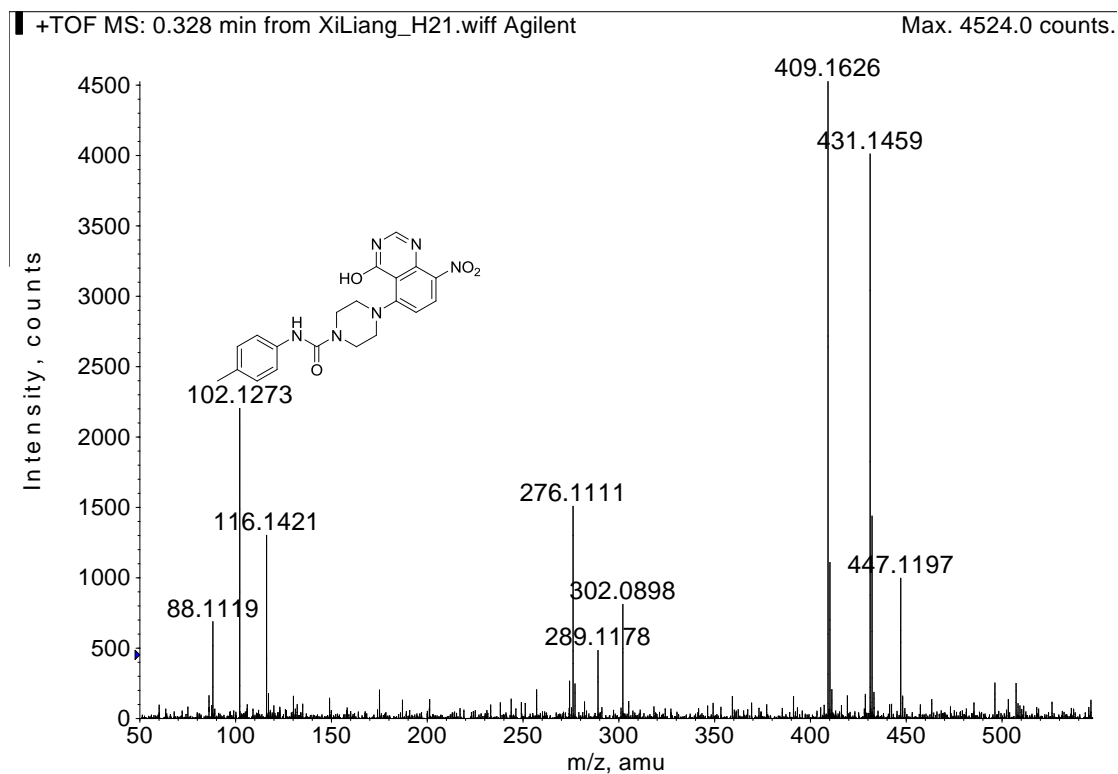
¹³C-NMR spectrum of 6u

Supporting Information

For

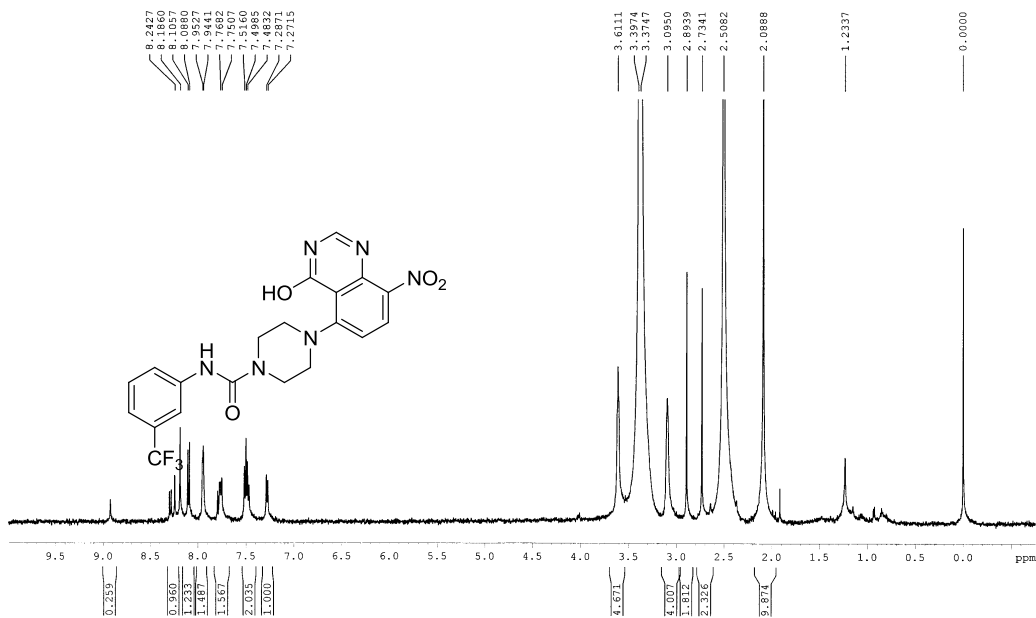


IR spectrum of 6u

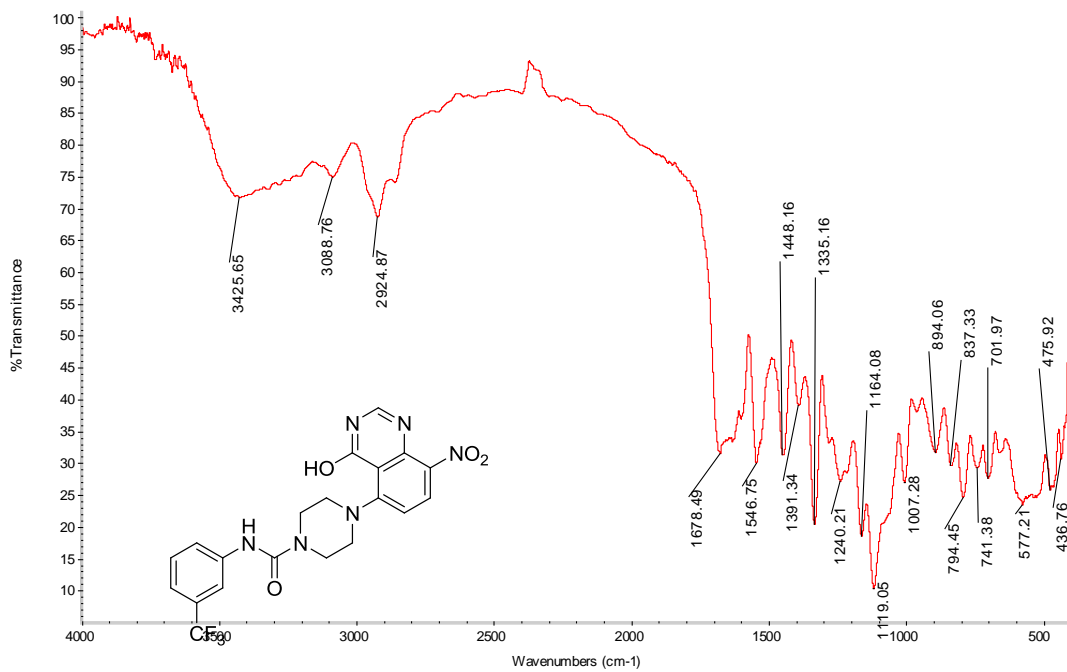


MS spectrum of 6u

YUNNAN UNIVER. AV. DRX 500
 xiliang XL-10478 in DMSO

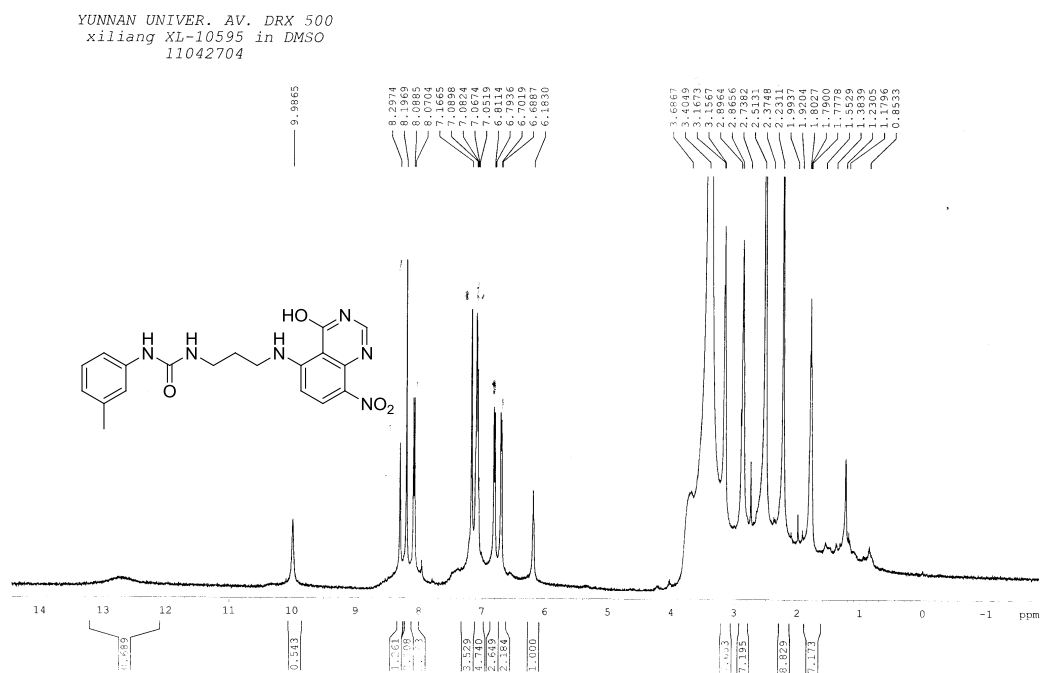


¹H-NMR spectrum of 6v

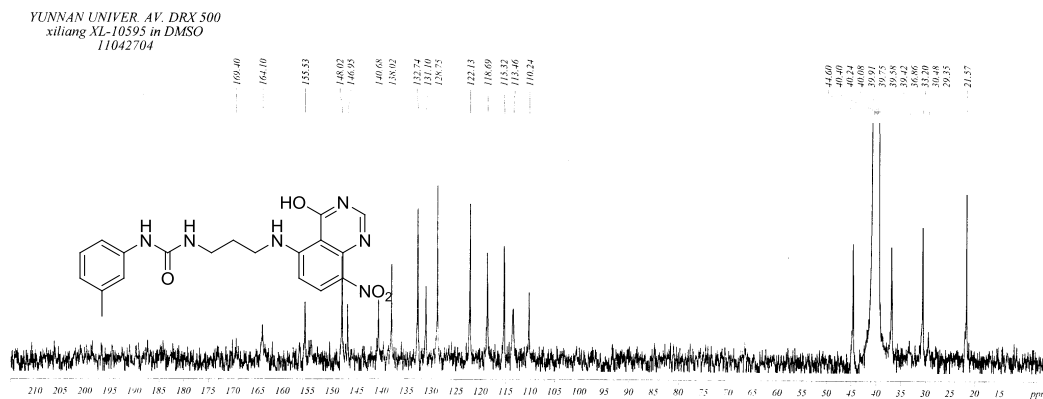
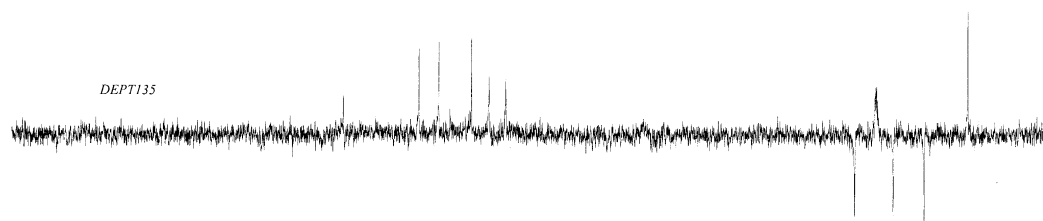


IR spectrum of 6v

Supporting Information
For

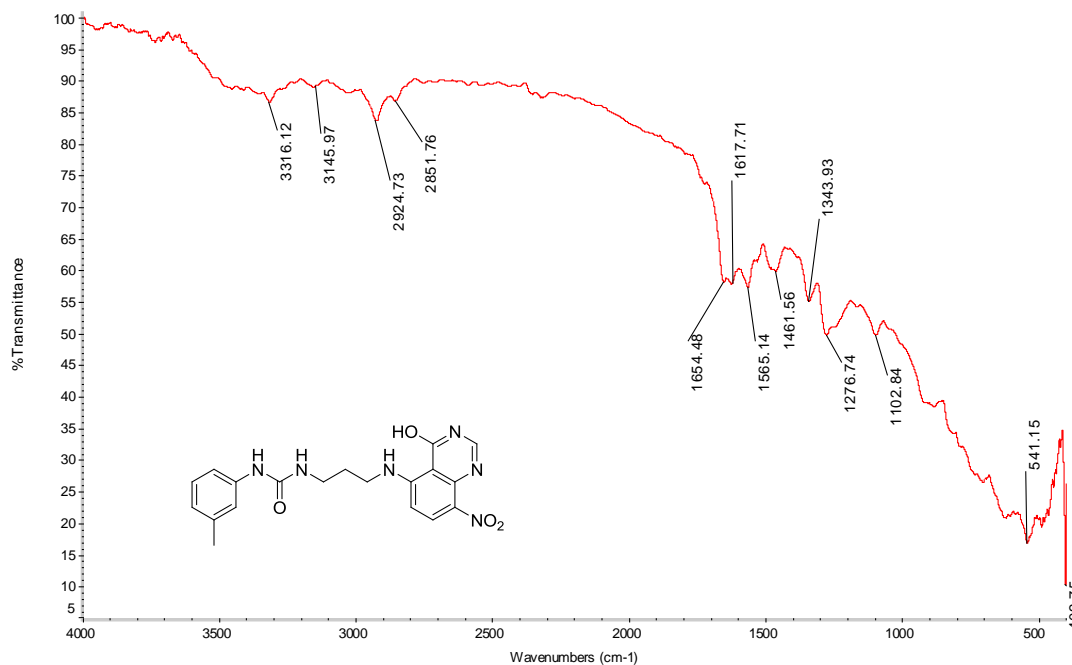


¹H-NMR spectrum of 6w

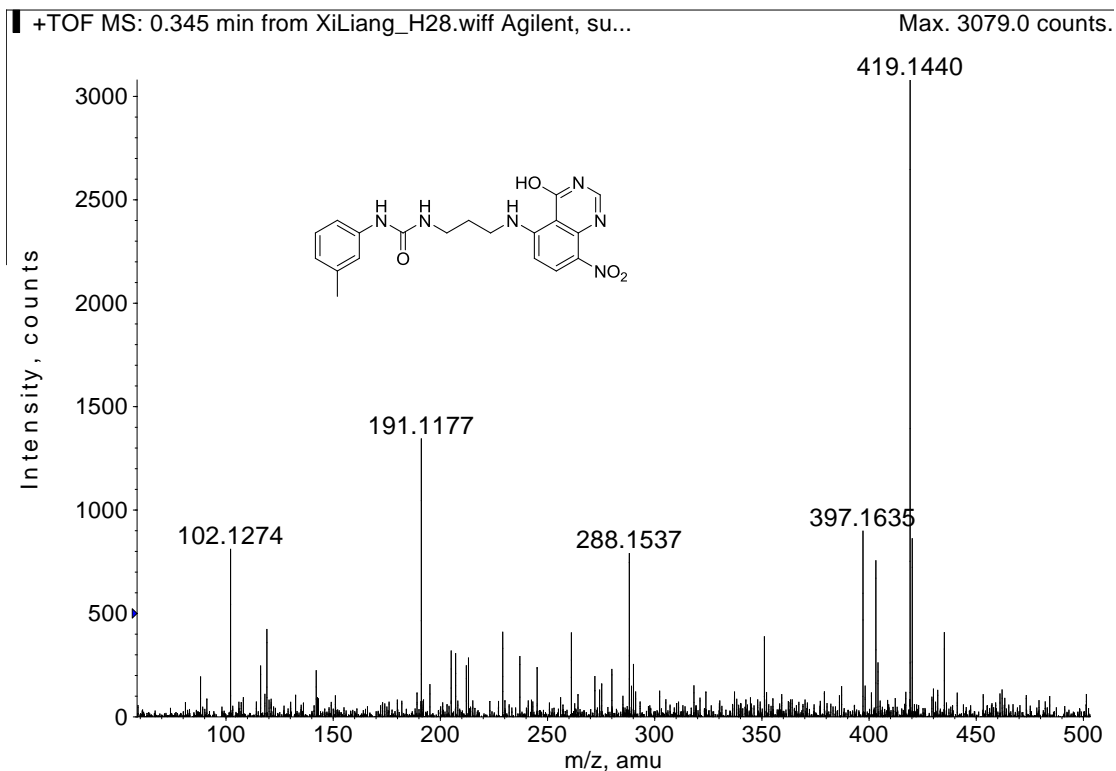


¹³C-NMR spectrum of 6w

For



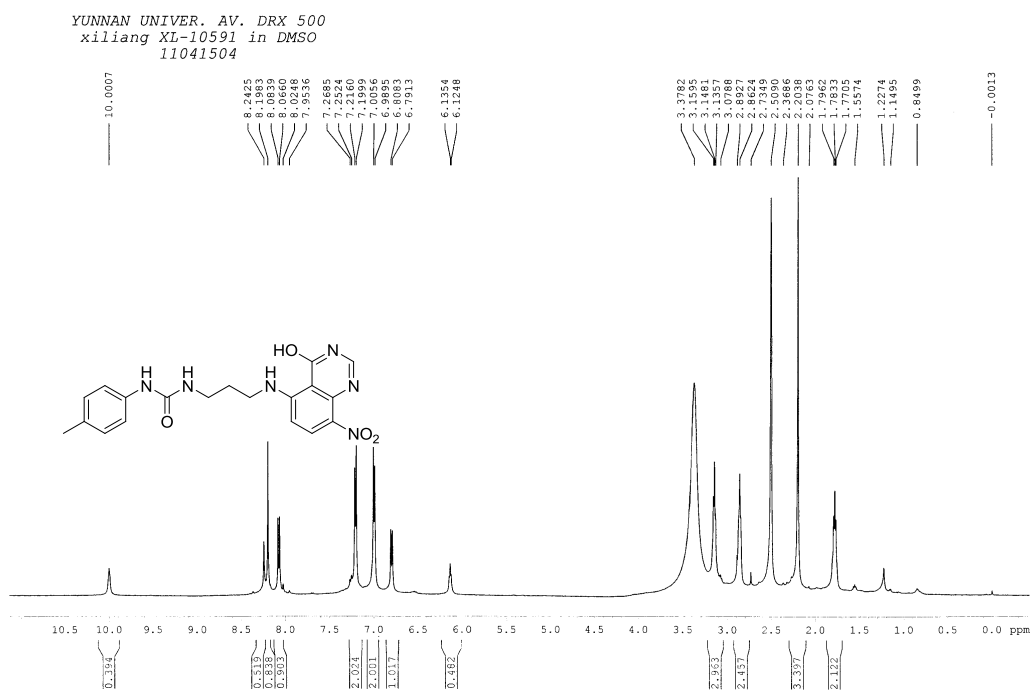
IR spectrum of 6w



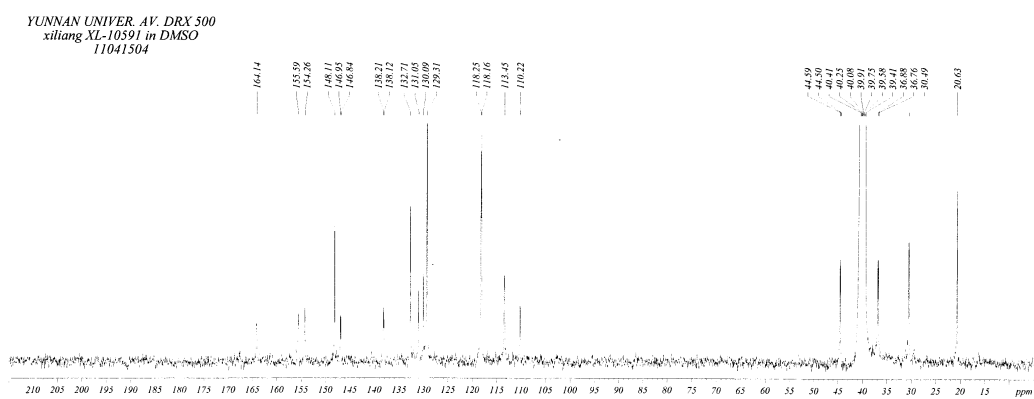
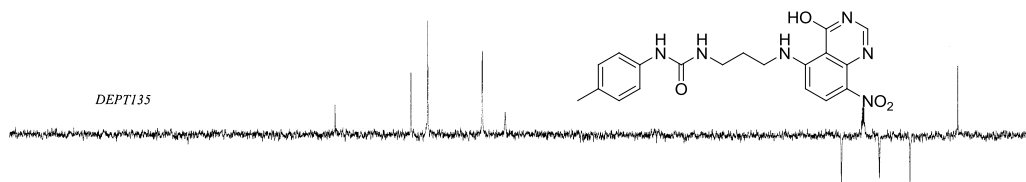
MS spectrum of 6w

Supporting Information

For

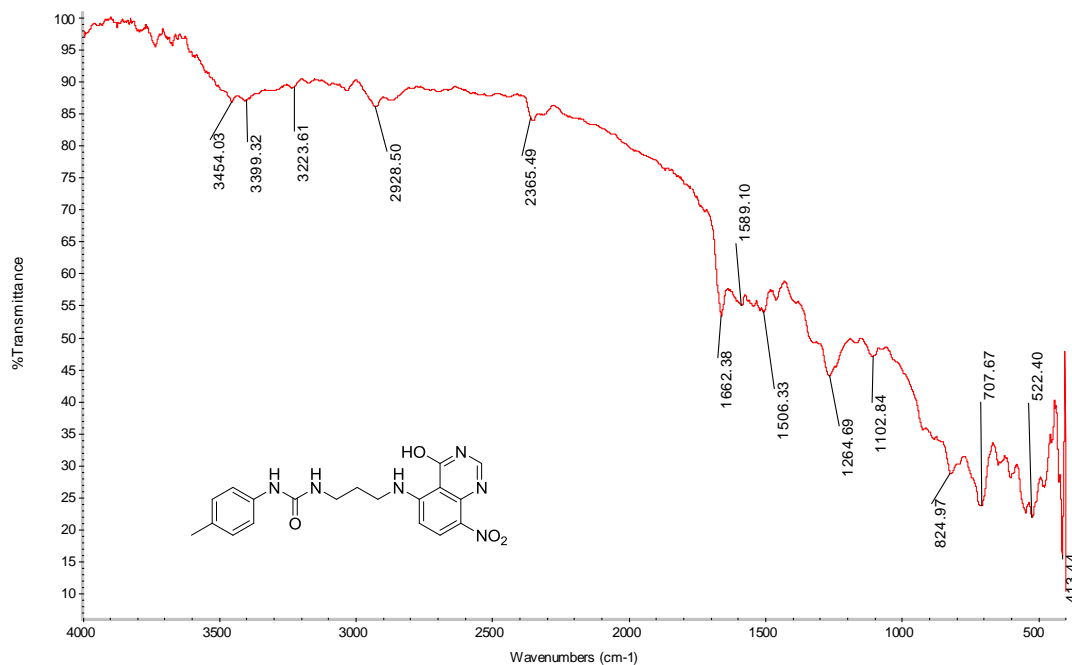


¹H-NMR spectrum of 6x

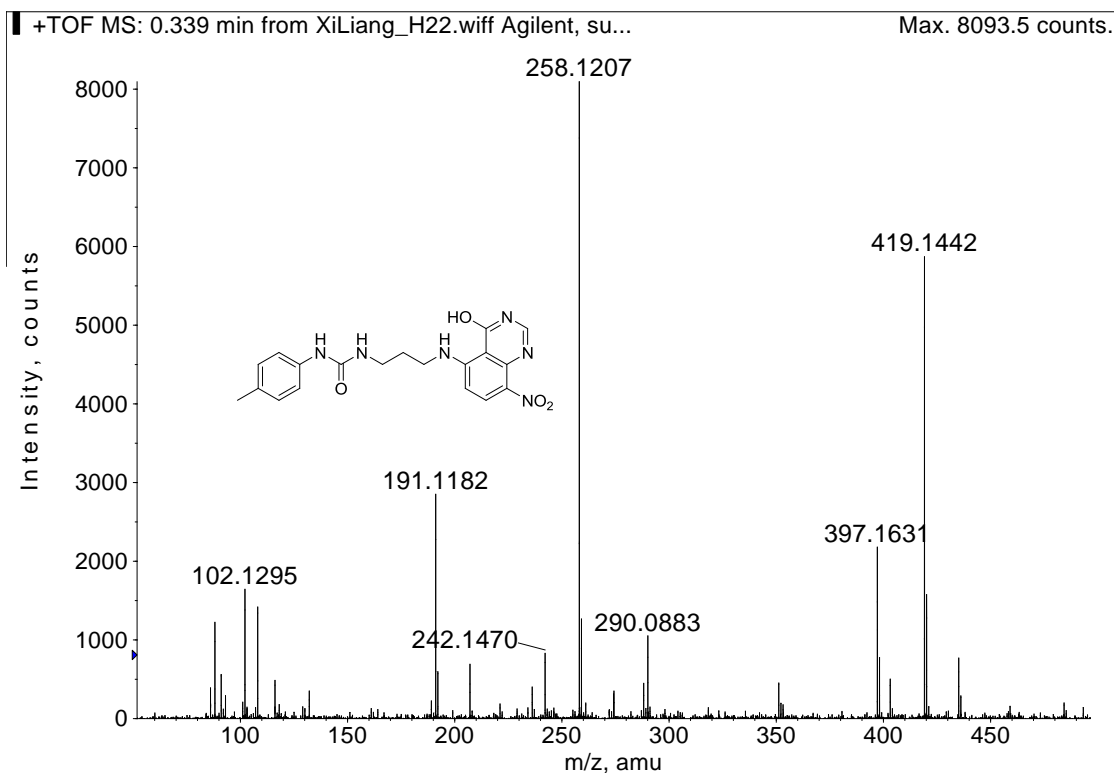


¹³C-NMR spectrum of 6x

For



IR spectrum of 6x

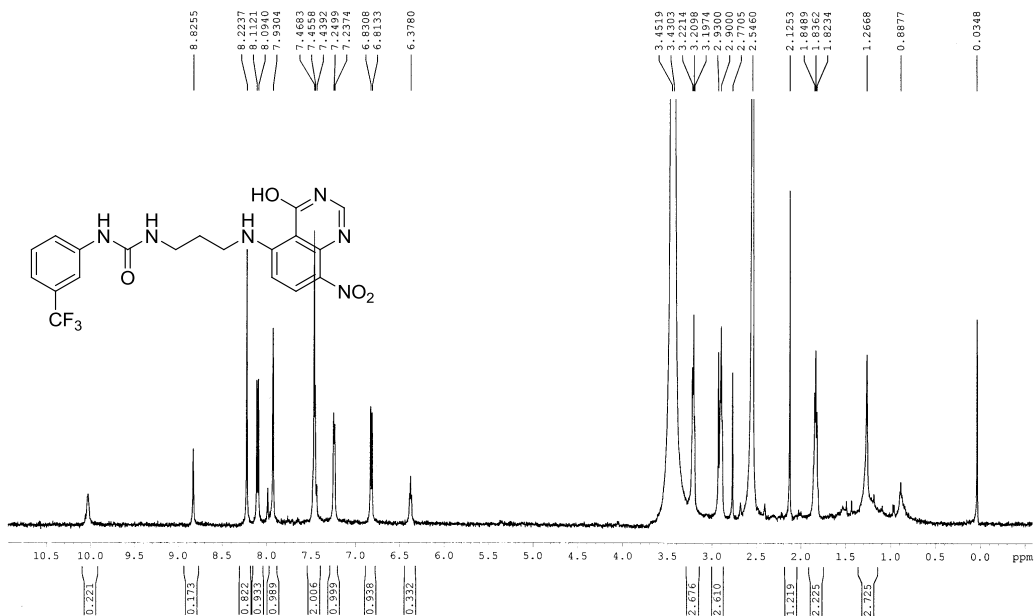


MS spectrum of 6x

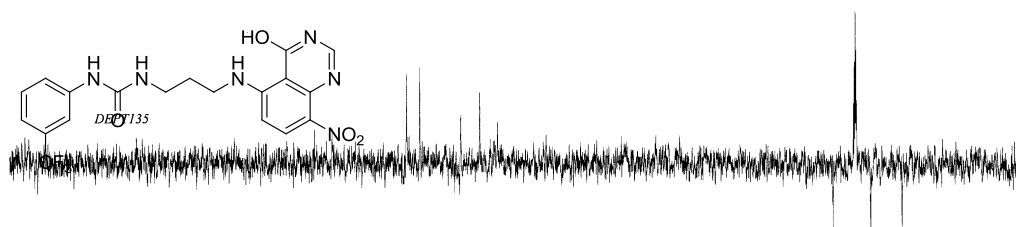
Supporting Information

For

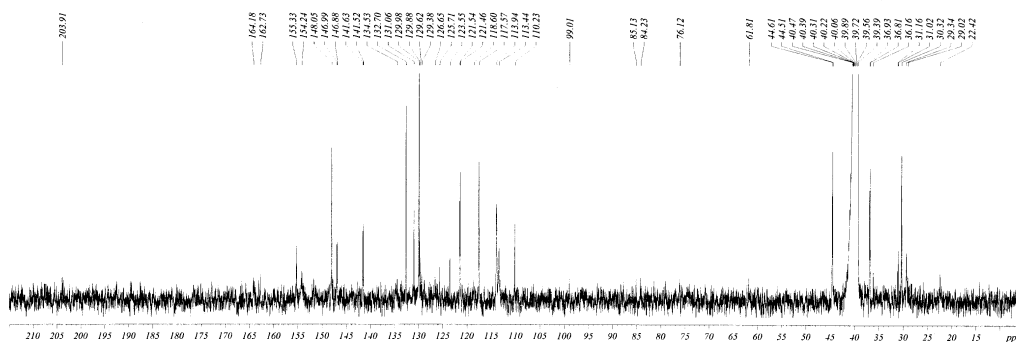
YUNNAN UNIVER. AV. DRX 500
xiliang XL-10480 in DMSO



¹H-NMR spectrum of 6y

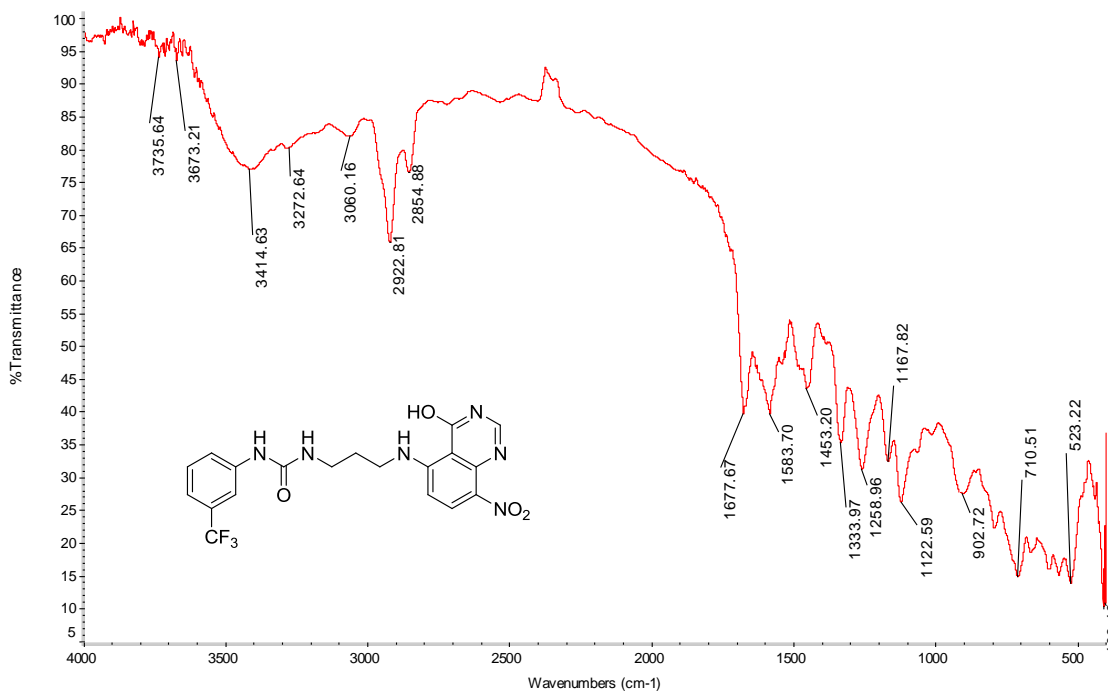


YUNNAN UNIVER. AV. DRX 500
xiliang XL-10480 in DMSO

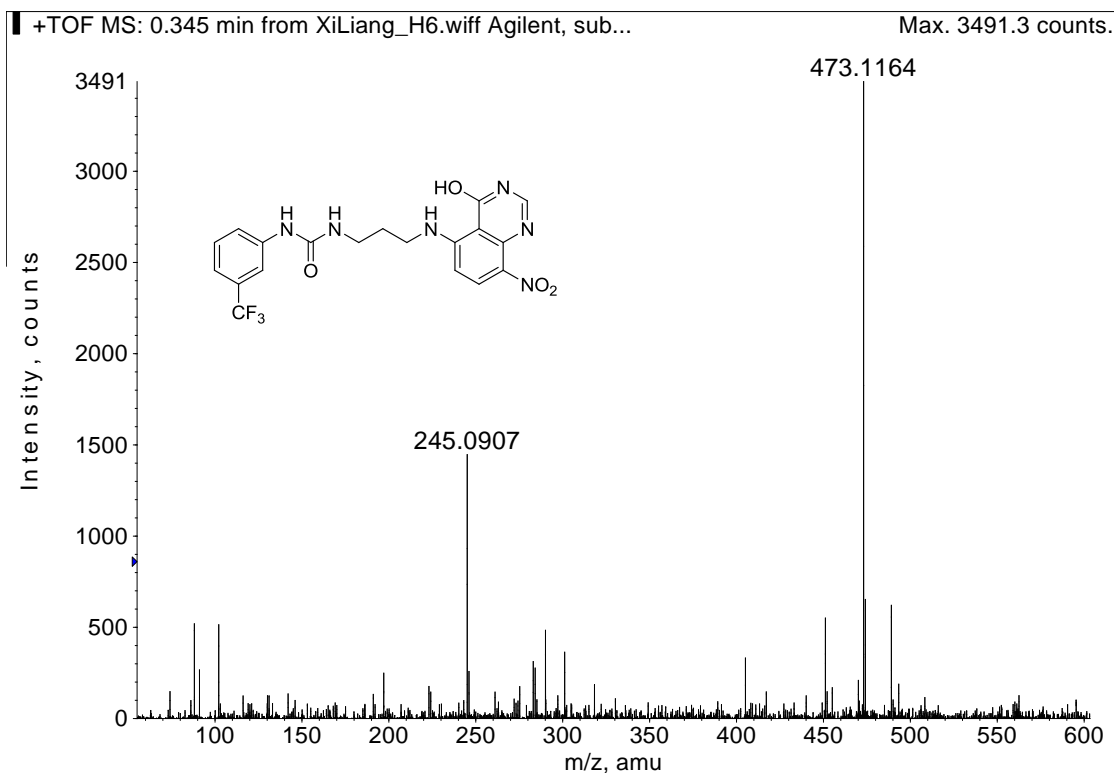


¹³C-NMR spectrum of 6y

For



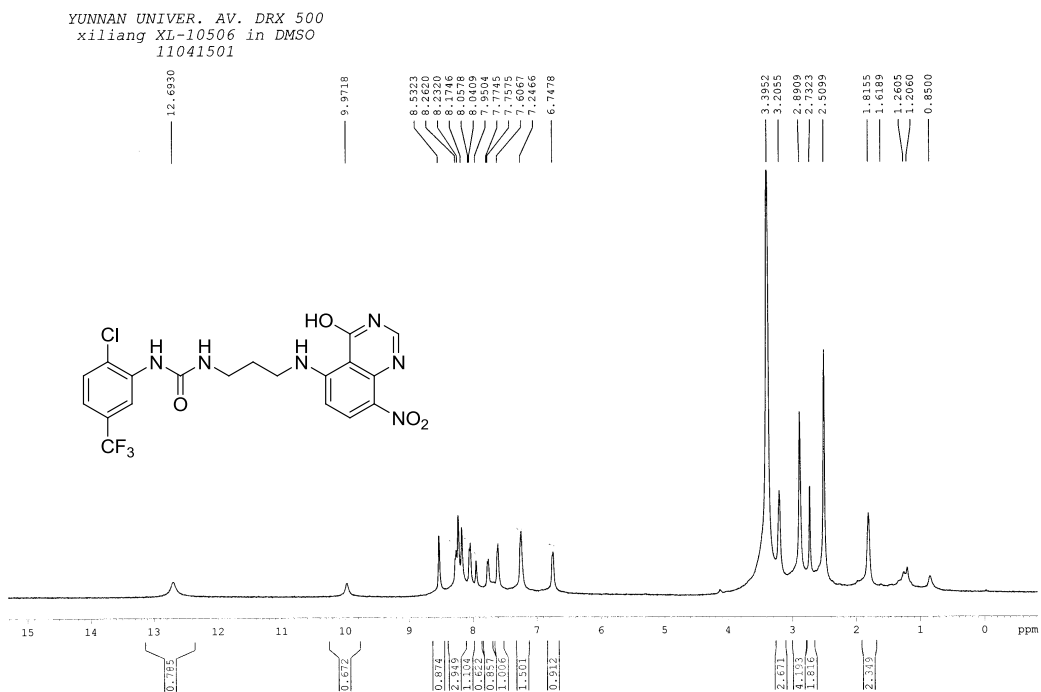
IR spectrum of 6y



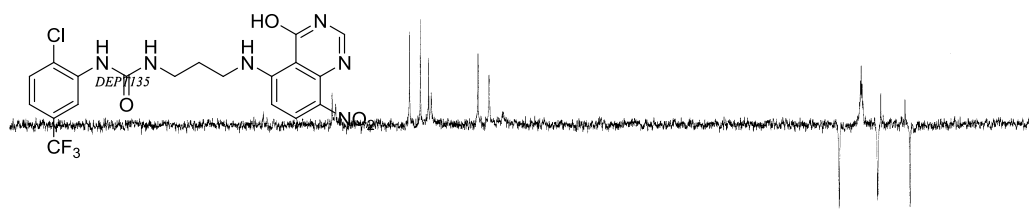
MS spectrum of 6y

Supporting Information

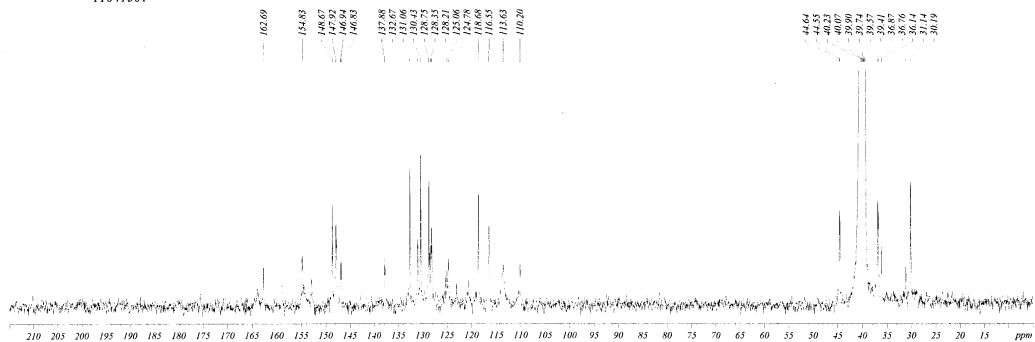
For



¹H-NMR spectrum of 6z

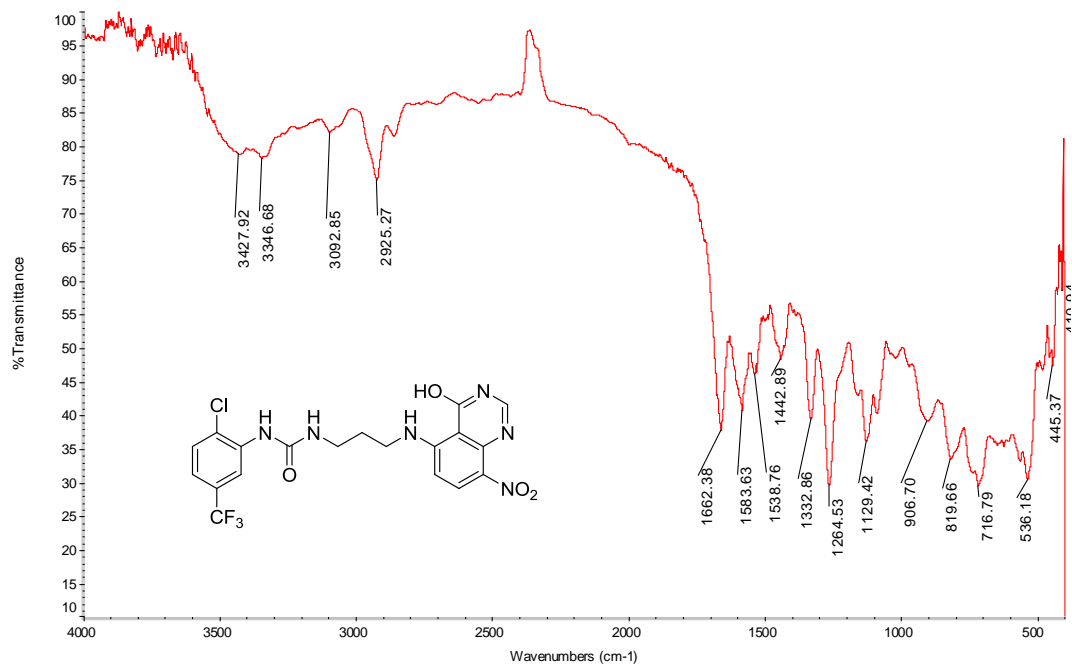


YUNNAN UNIVER. AV. DRX 500
xiliang XL-10506 in DMSO
11041501

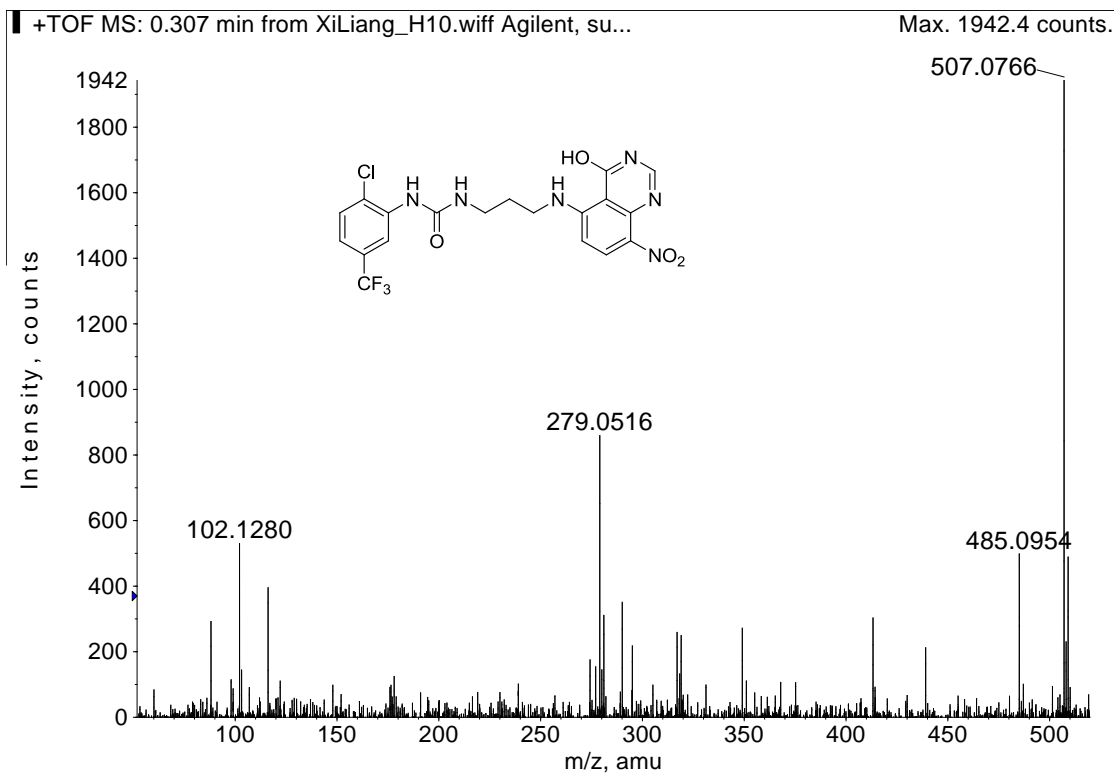


¹³C-NMR spectrum of 6z

For



IR spectrum of 6z

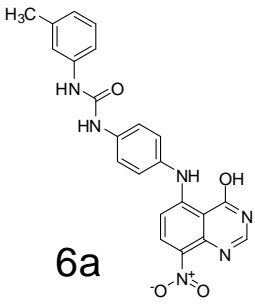
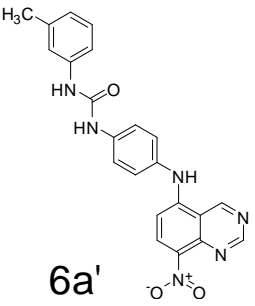
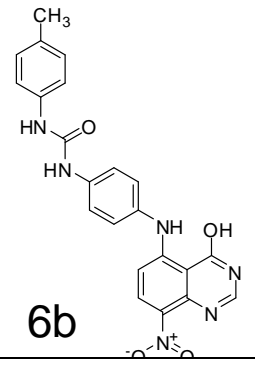
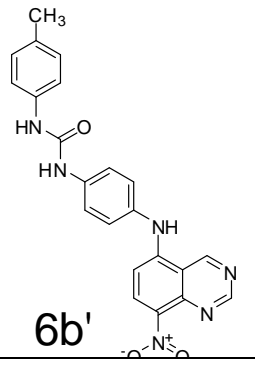
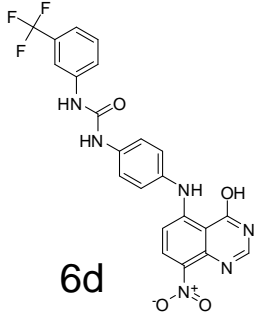
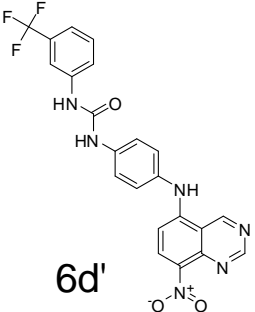
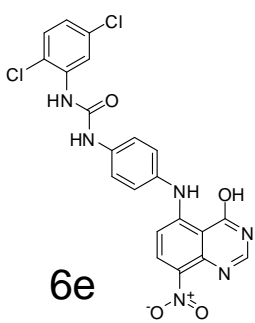
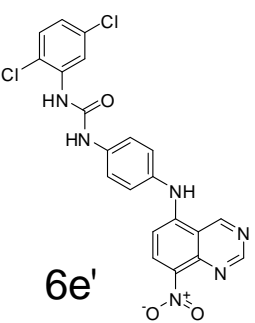


MS spectrum of 6z

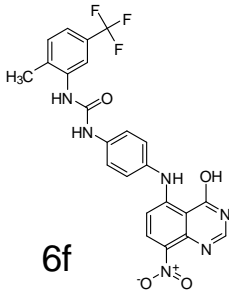
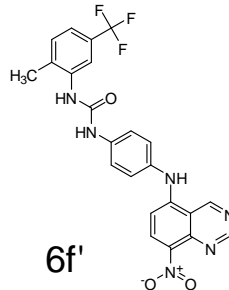
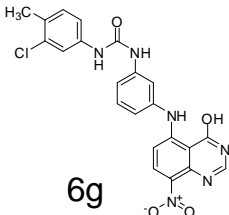
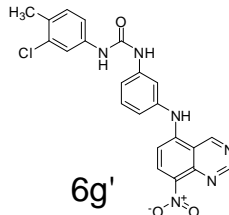
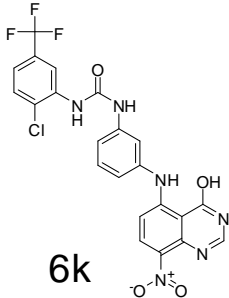
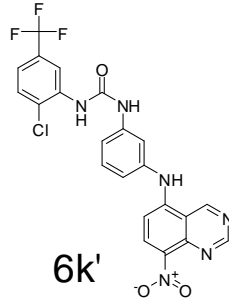
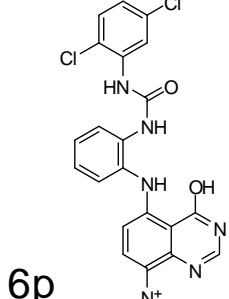
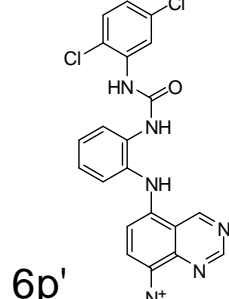
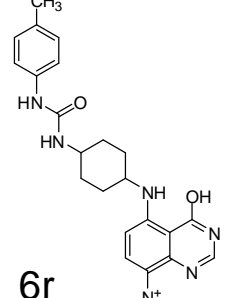
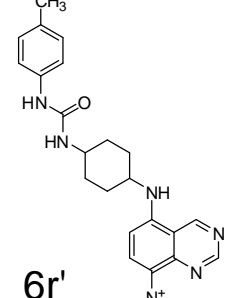
Supporting Information

For

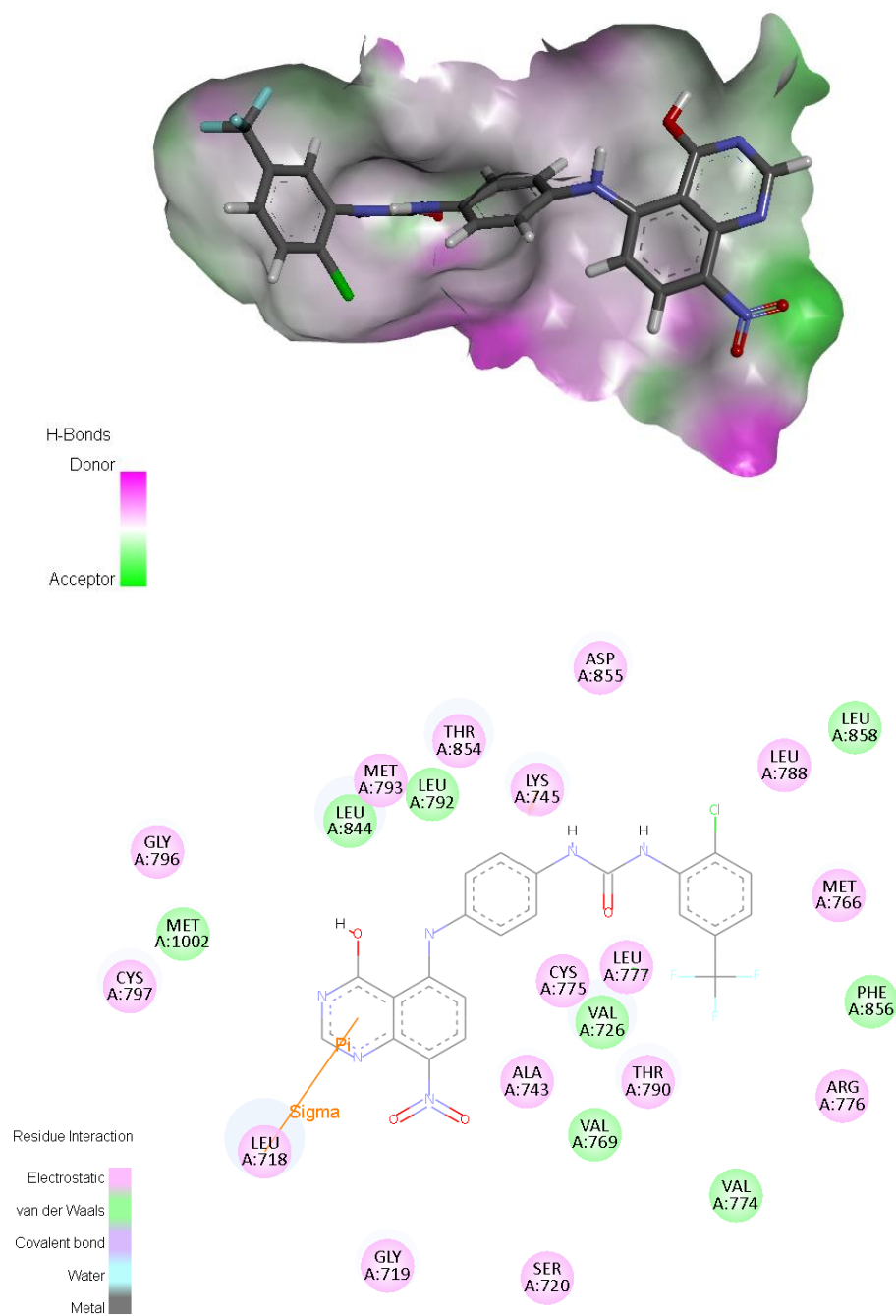
The calculated logP and logD(PH = 7.4) of
 4-hydroxy quinazolines and none 4-hydroxy quinazolines

4-hydroxy quinazolines	logP	logD(7.4)	none 4-hydroxy quinazolines	logP	logD(7.4)
 <p>6a</p>	2.52	0.024	 <p>6a'</p>	3.11	3.11
 <p>6b</p>	2.52	0.024	 <p>6b'</p>	3.11	3.11
 <p>6d</p>	3.42	0.92	 <p>6d'</p>	4.00	4.00
 <p>6e</p>	3.53	1.03	 <p>6e'</p>	4.12	4.12

For

 <p>6f</p>	3.88	1.38	 <p>6f'</p>	4.46	4.46
 <p>6g</p>	4.50	2.00	 <p>6g'</p>	5.09	5.09
 <p>6k</p>	4.95	2.45	 <p>6k'</p>	5.53	5.53
 <p>6p</p>	2.48	1.78	 <p>6p'</p>	4.87	4.87
 <p>6r</p>	2.64	0.14	 <p>6r'</p>	3.23	3.23

Supporting Information
For
The Binding mode of Compound **6f** in EGFR Kinase activity pocket area



5

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The Binding mode of Compound **6f** in VEGFR-2 Kinase activity pocket area

