

Supporting Information

A transition metal-free tandem process to pyridazinopyrido[3,2-*f*][1,4]thiazepine-diones via Smiles rearrangement

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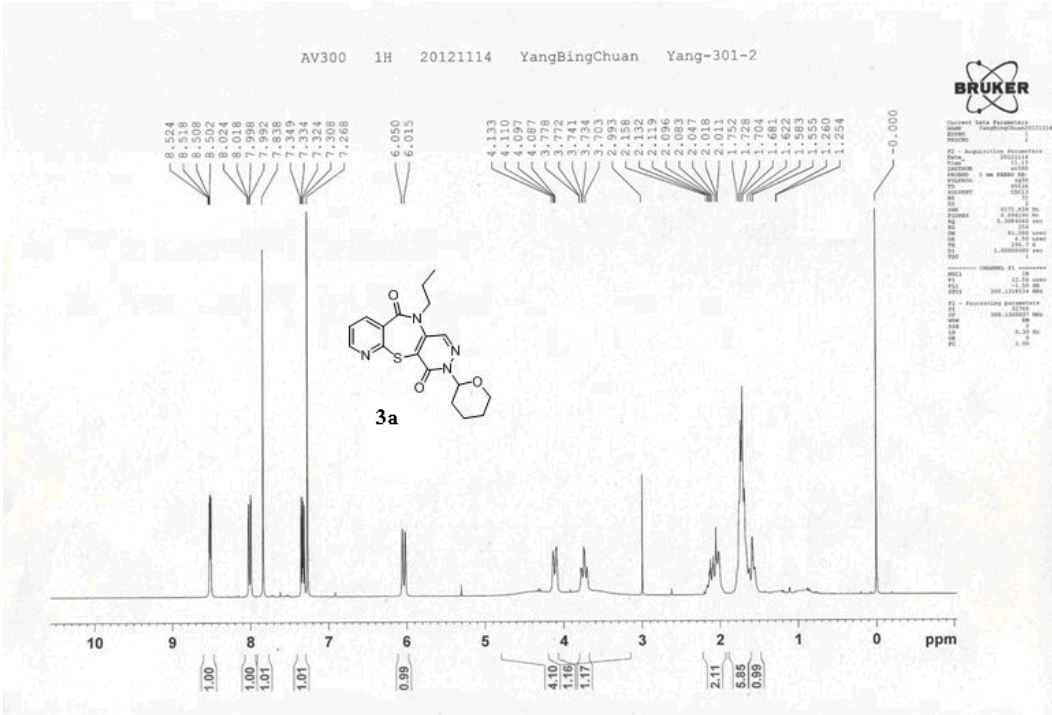
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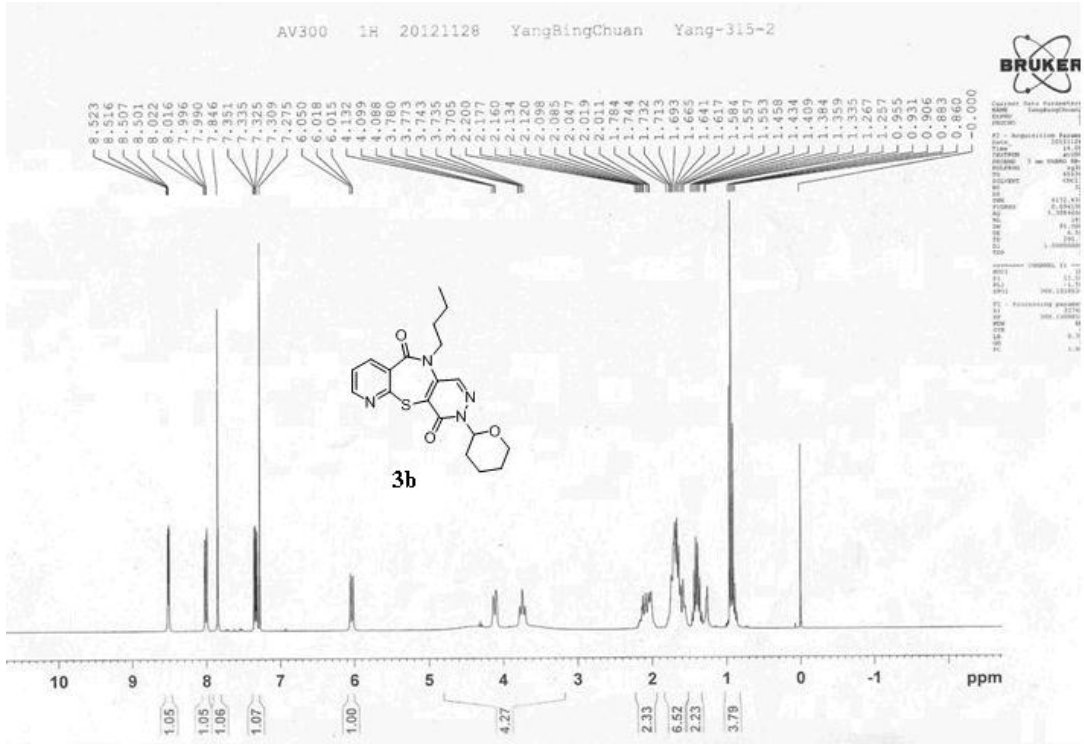
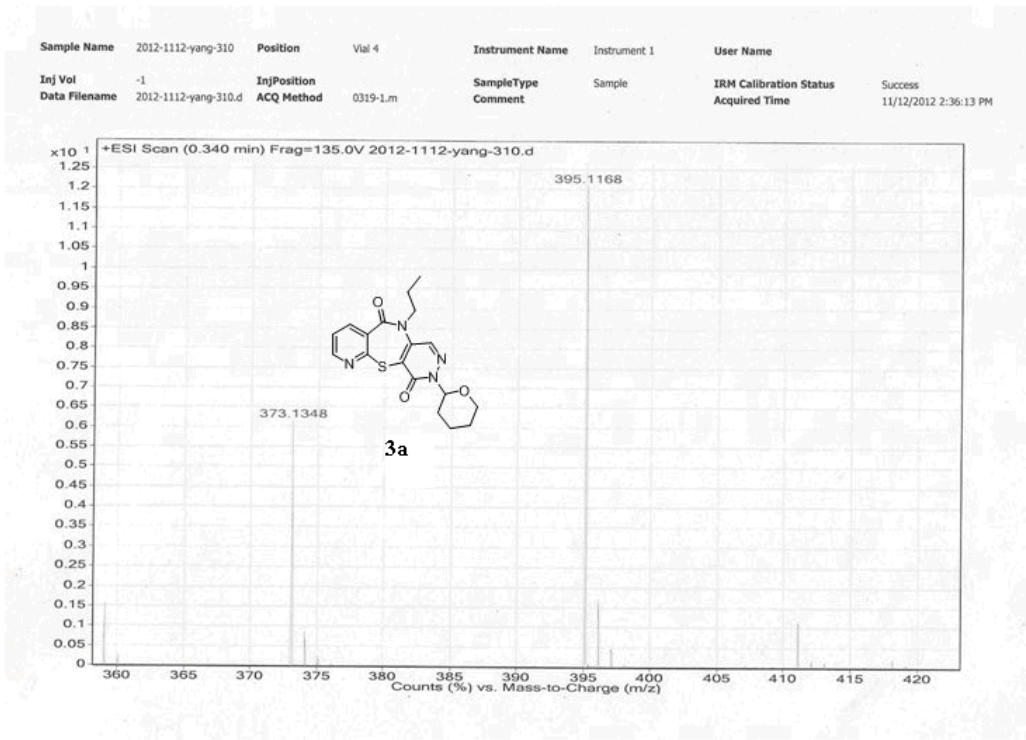
Crystal Structure Determination

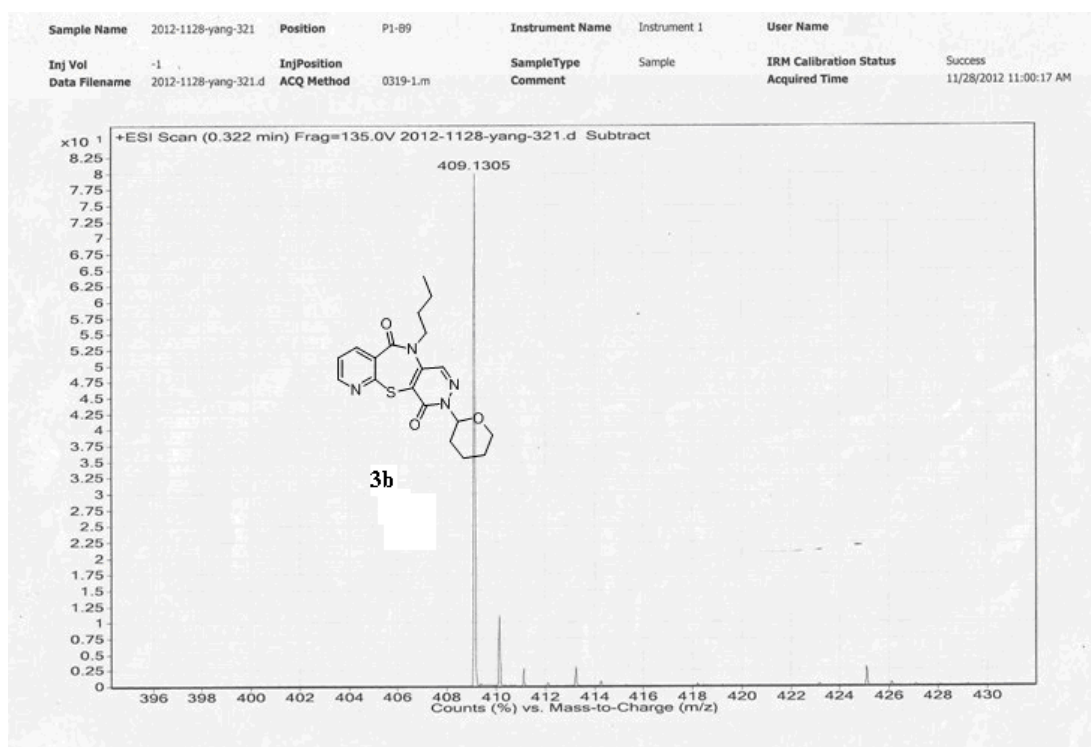
The diffraction data was collected with a Bruker SMART CCD diffractometer using a graphite monochromated Mo K α radiation ($\lambda = 0.71073 \text{ \AA}$) at 273(2) K. The structures were solved by direct methods with SHELXS-97 program and refinements on F² were performed with SHELXL-97 program by full-matrix least-squares techniques with anisotropic thermal parameters for the non-hydrogen atoms.

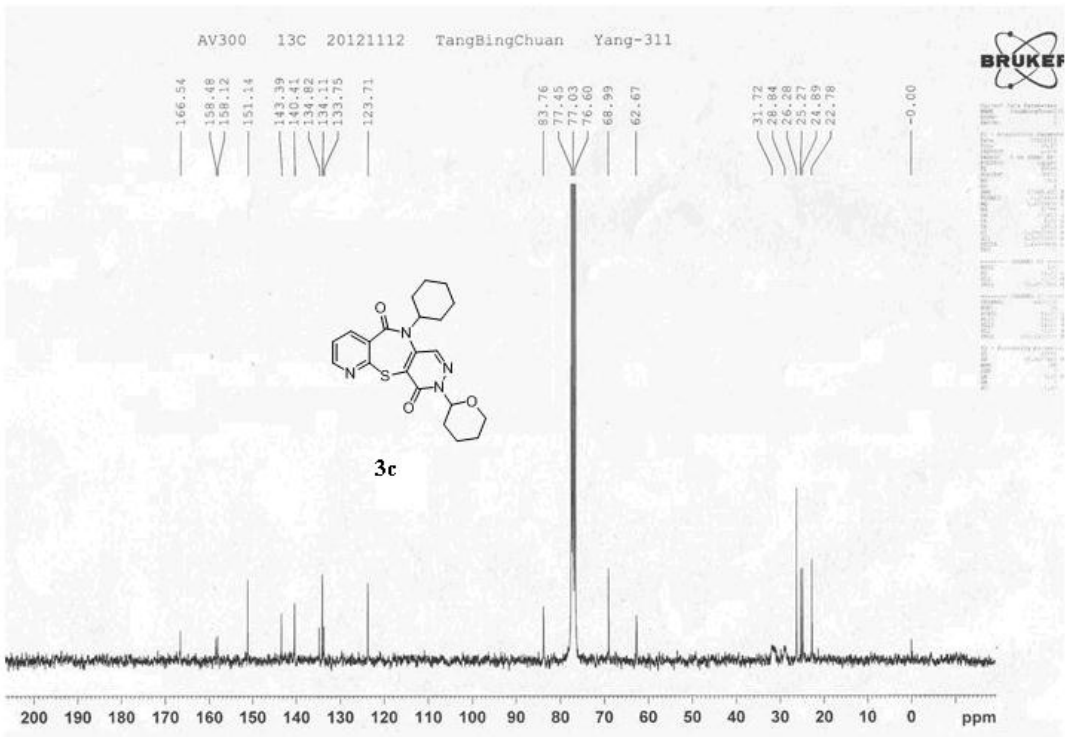
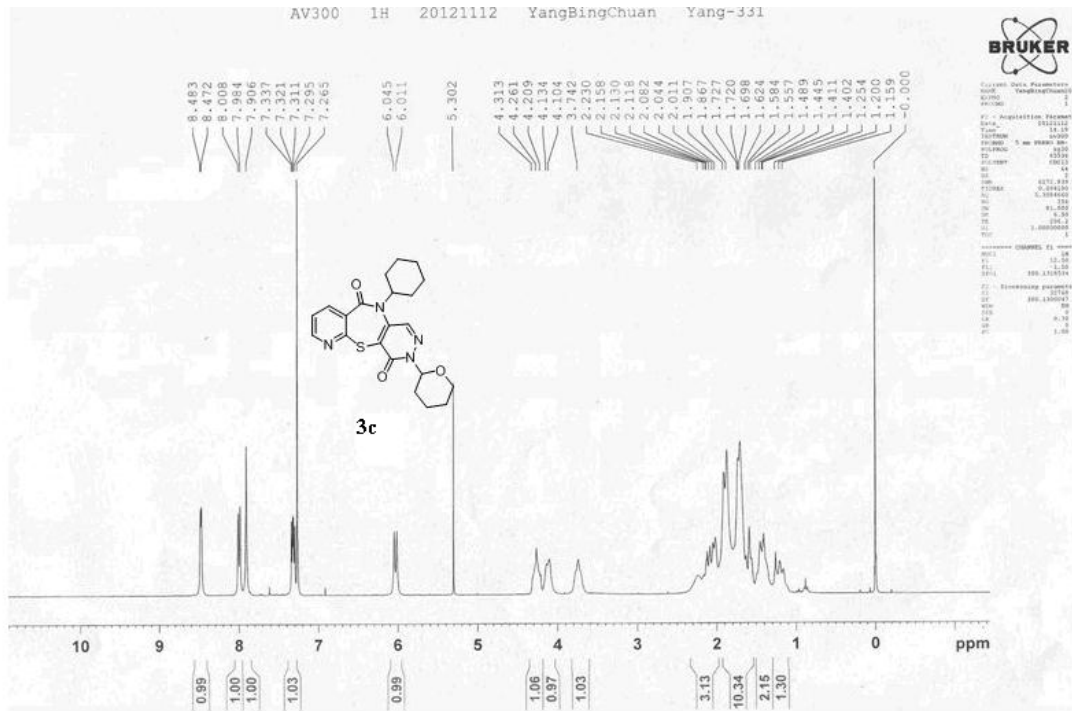
Table S1. Details of Crystal Structure Determination for **3f**.

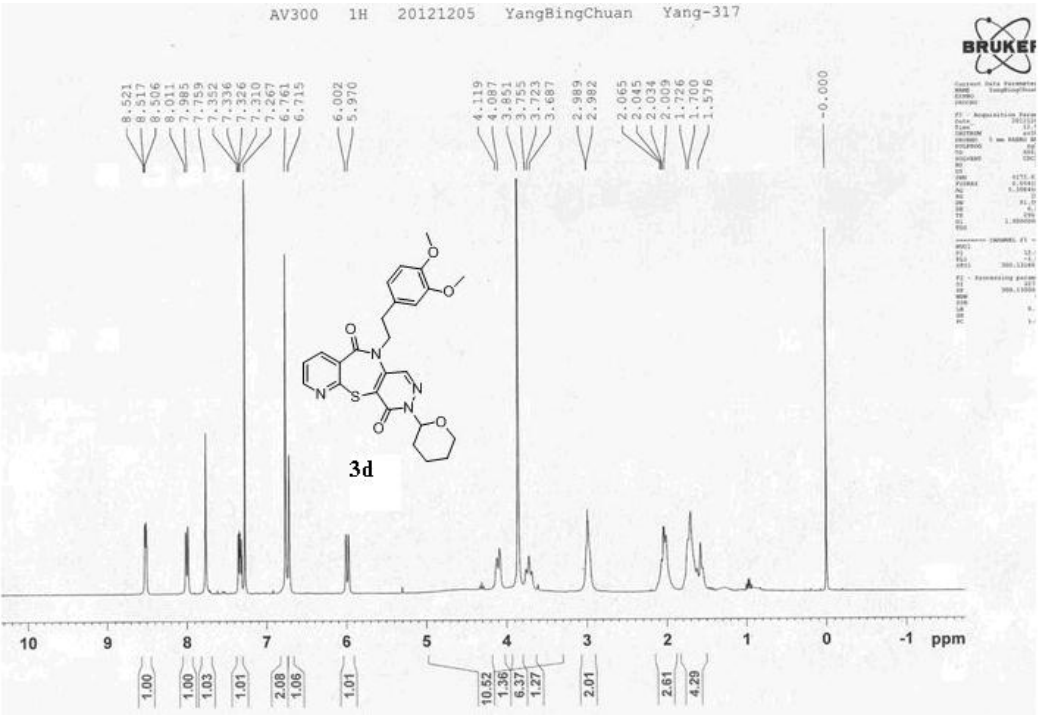
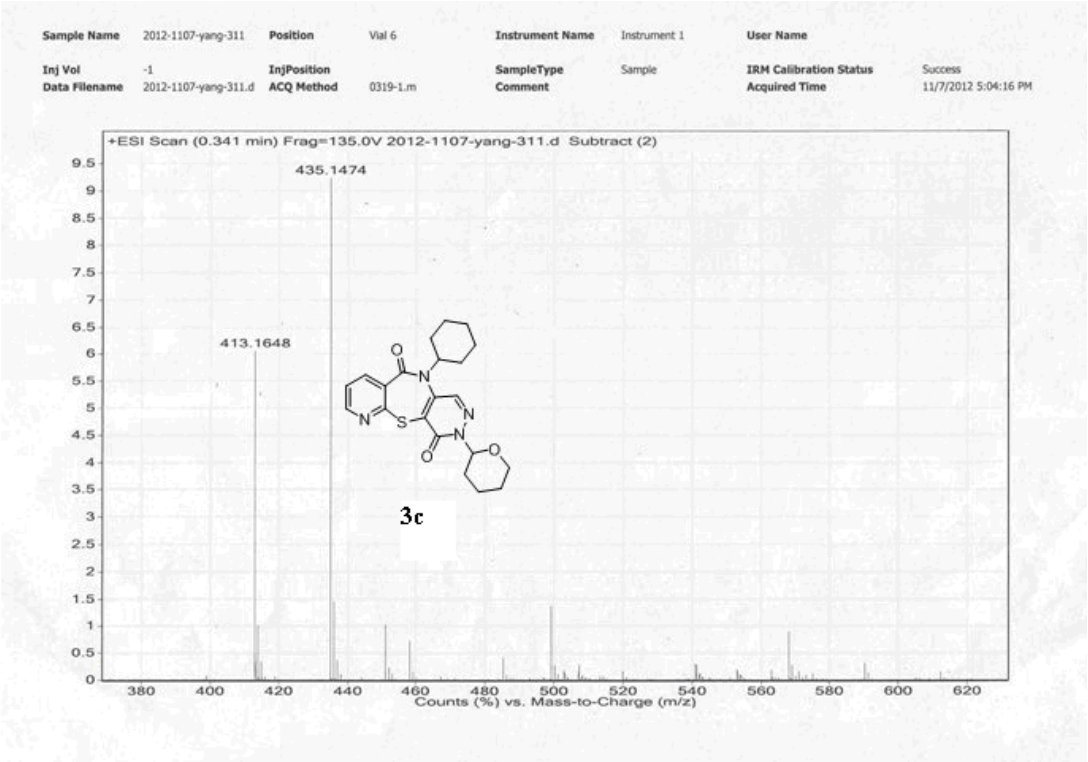
Compound	3f
Chemical formula	C ₂₁ H ₁₇ ClN ₄ O ₃ S
Formula Mass	407.12
Crystal system	monoclinic
<i>a</i> /Å	10.901
<i>b</i> /Å	5.9316
<i>c</i> /Å	30.312
α /°	90.00
β /°	91.762
γ /°	90.00
Unit cell volume/Å ³	1959.1
Temperature/K	293(2)
Space group	<i>P</i> 2 ₁ / <i>n</i>
No. of formula units per unit cell, <i>Z</i>	4
No. of reflections measured	10500
No. of independent reflections	4289
<i>R</i> _{int}	0.0206
Final <i>R</i> _{<i>I</i>} values (<i>I</i> > 2σ(<i>I</i>))	0.0558
Final <i>wR</i> (<i>F</i> ²) values (<i>I</i> > 2σ(<i>I</i>))	0.1595
Final <i>R</i> _{<i>I</i>} values (all data)	0.1240
Final <i>wR</i> (<i>F</i> ²) values (all data)	0.2185

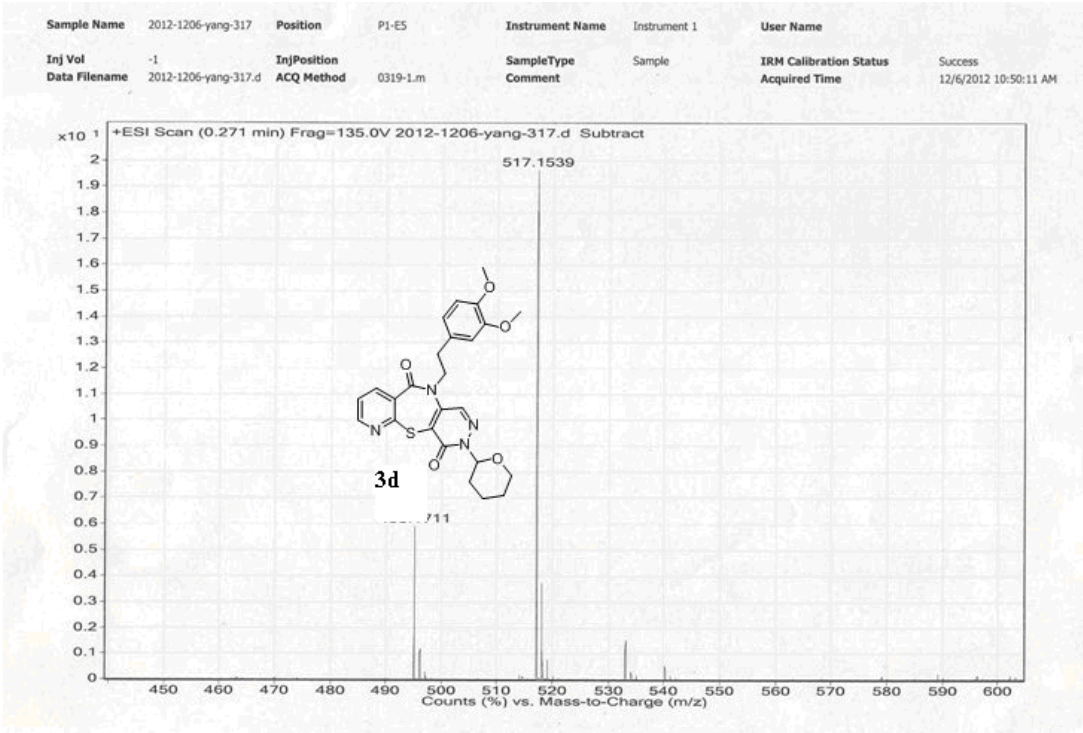
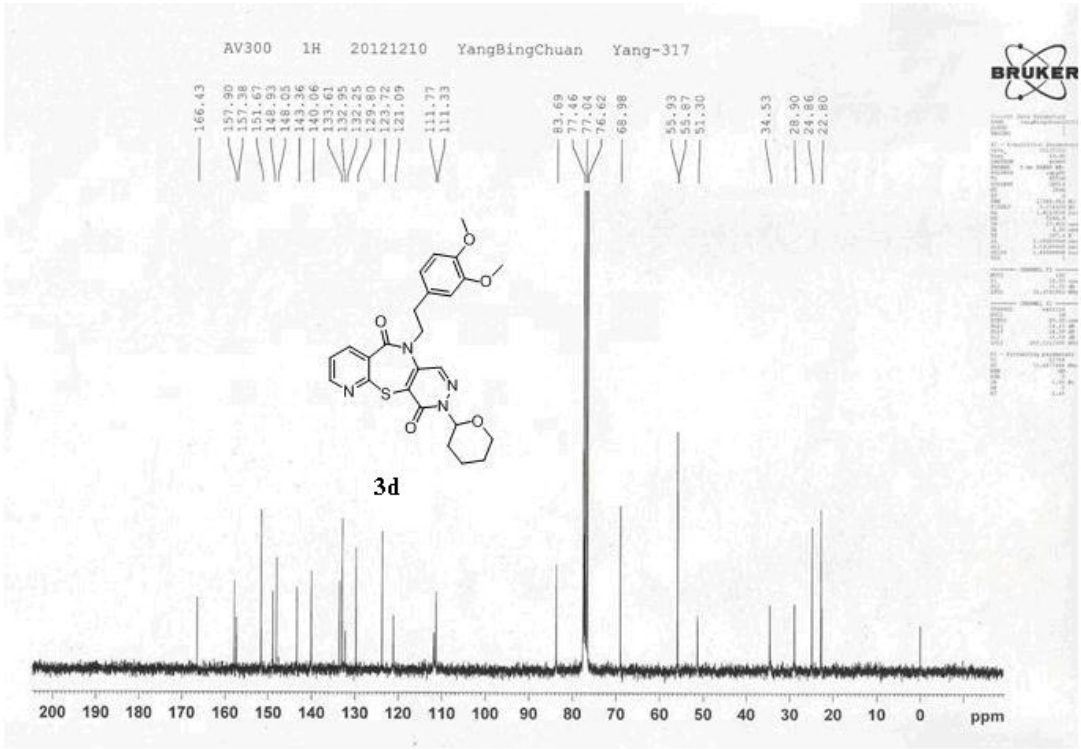


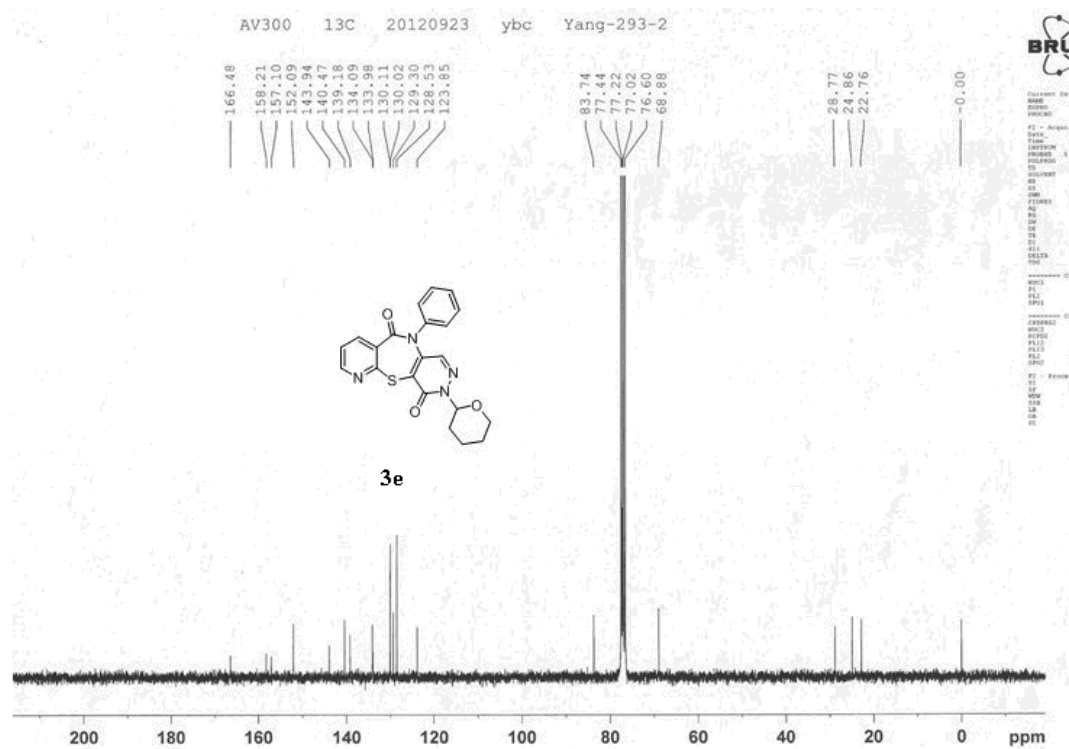
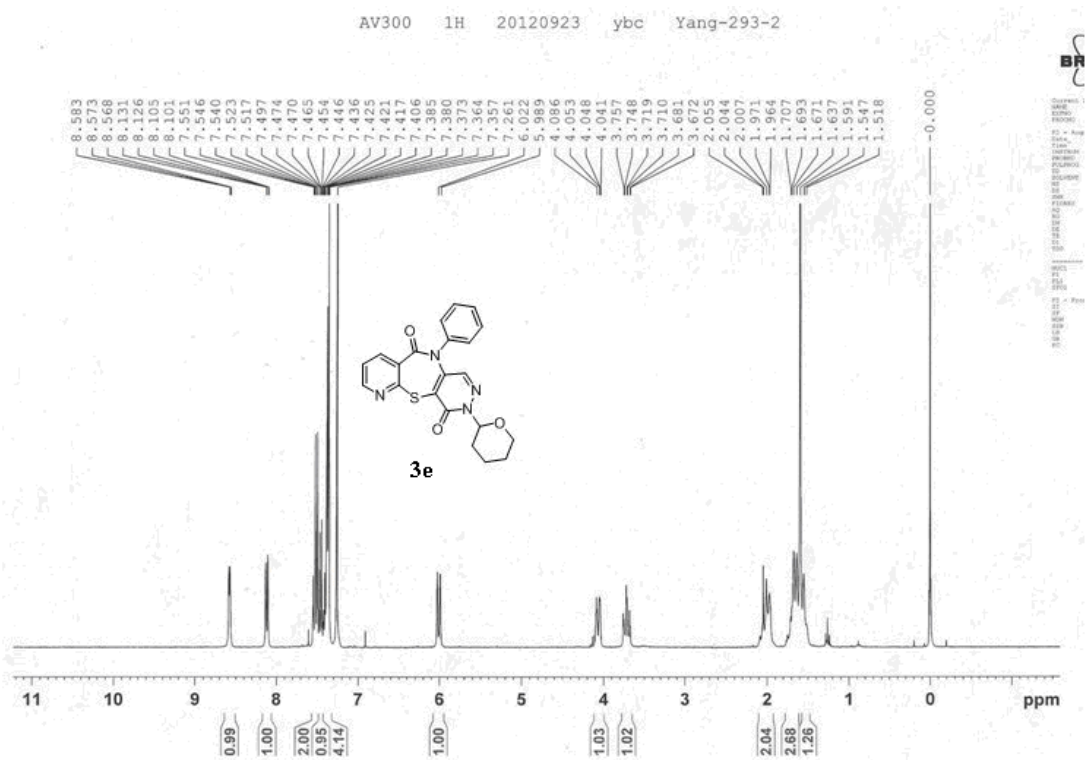




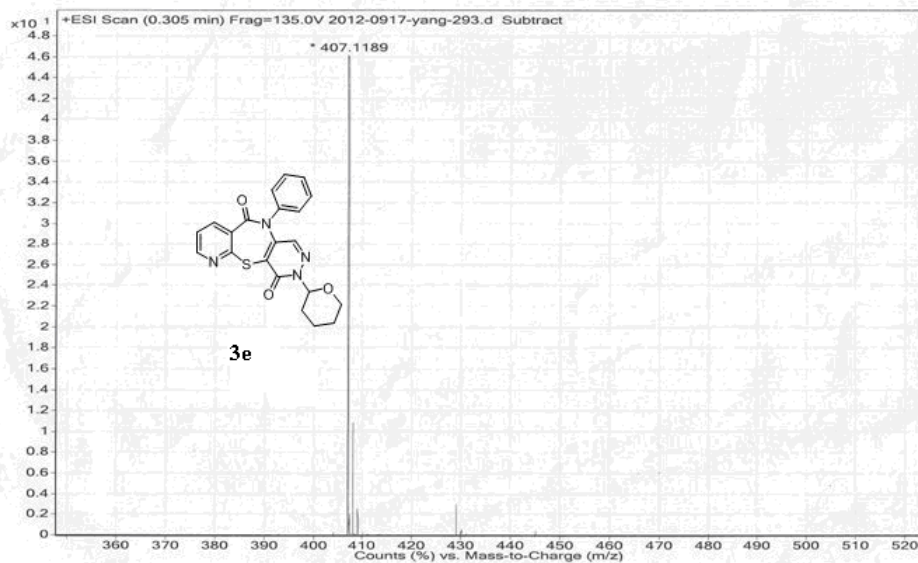




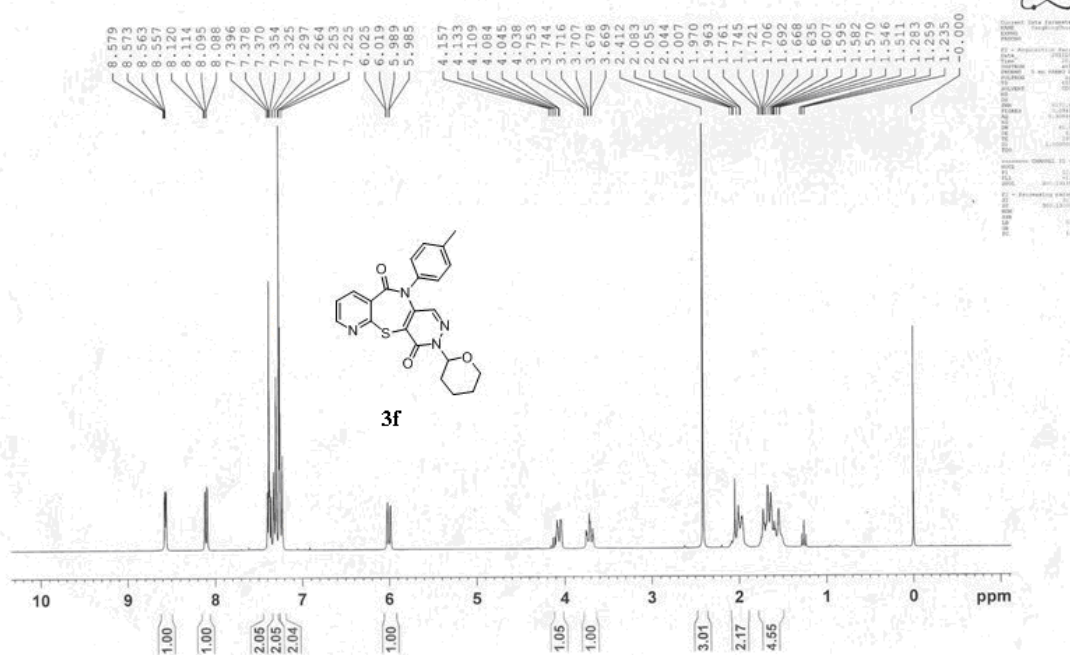


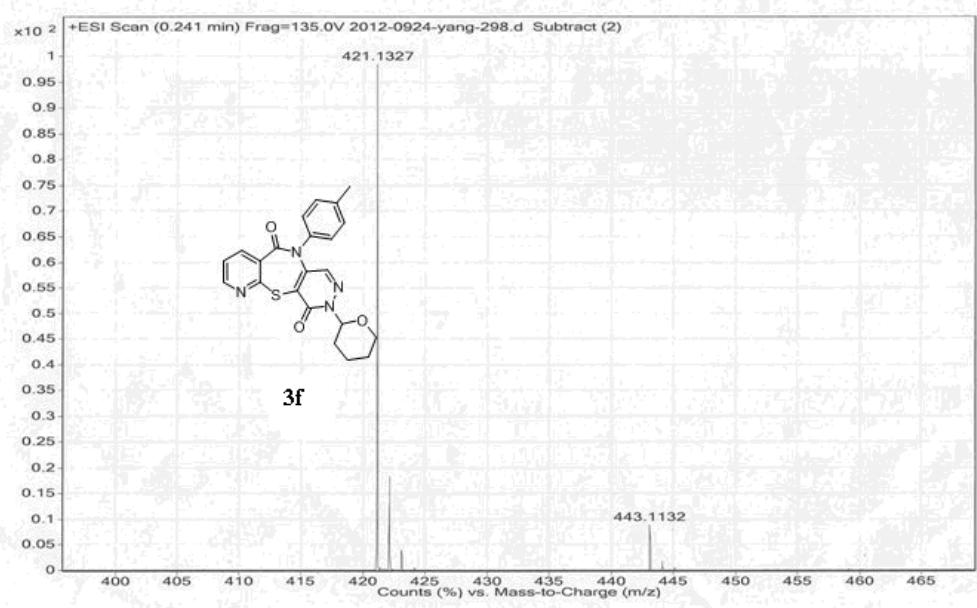
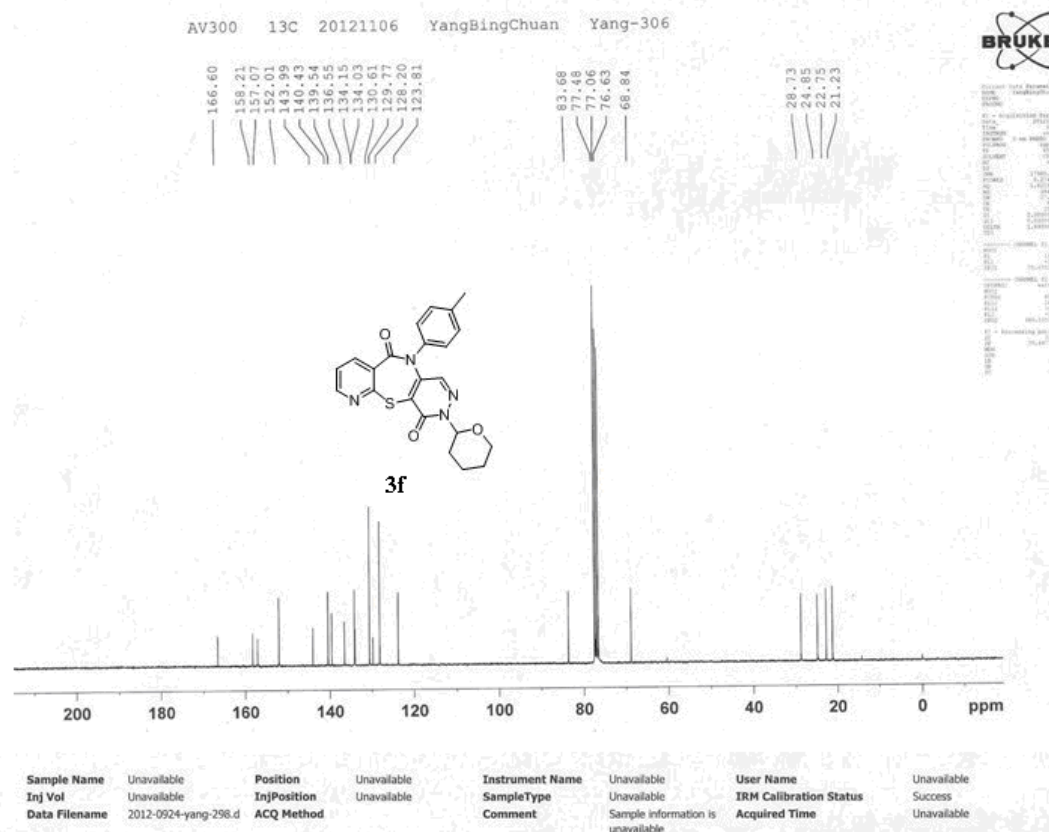


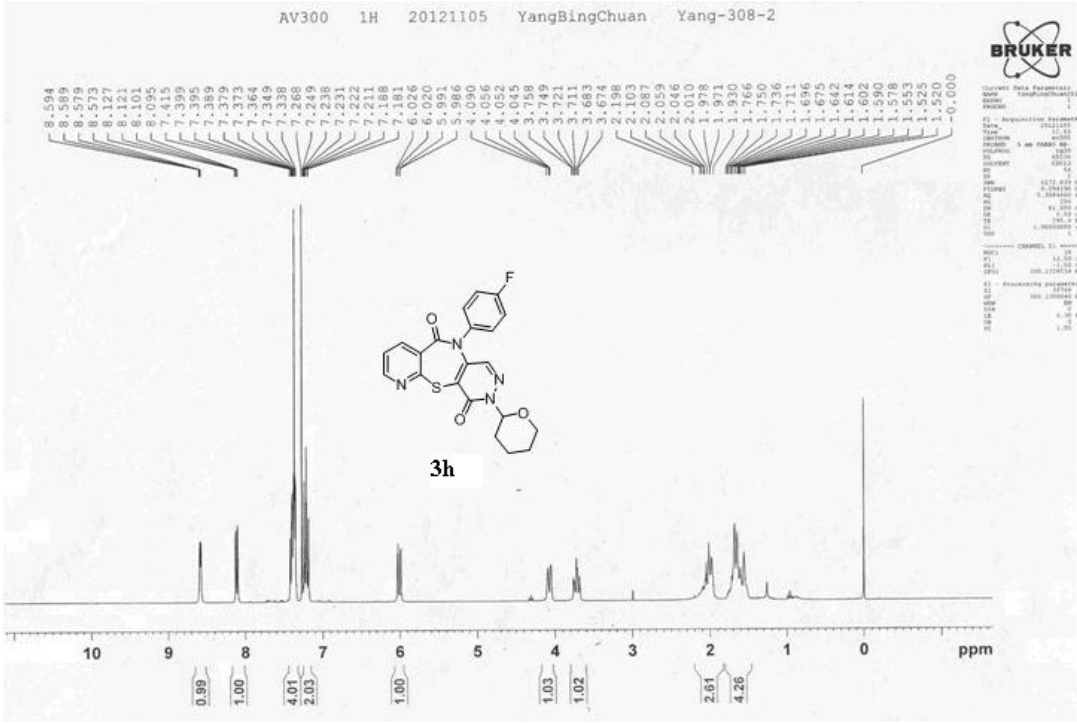
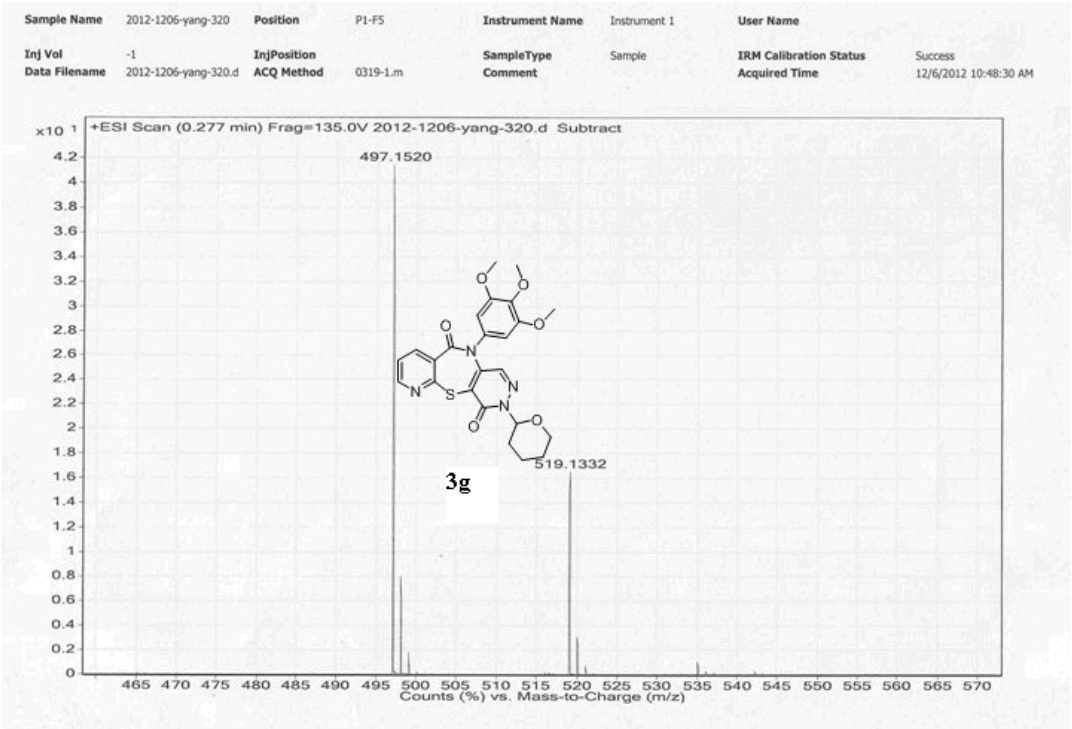
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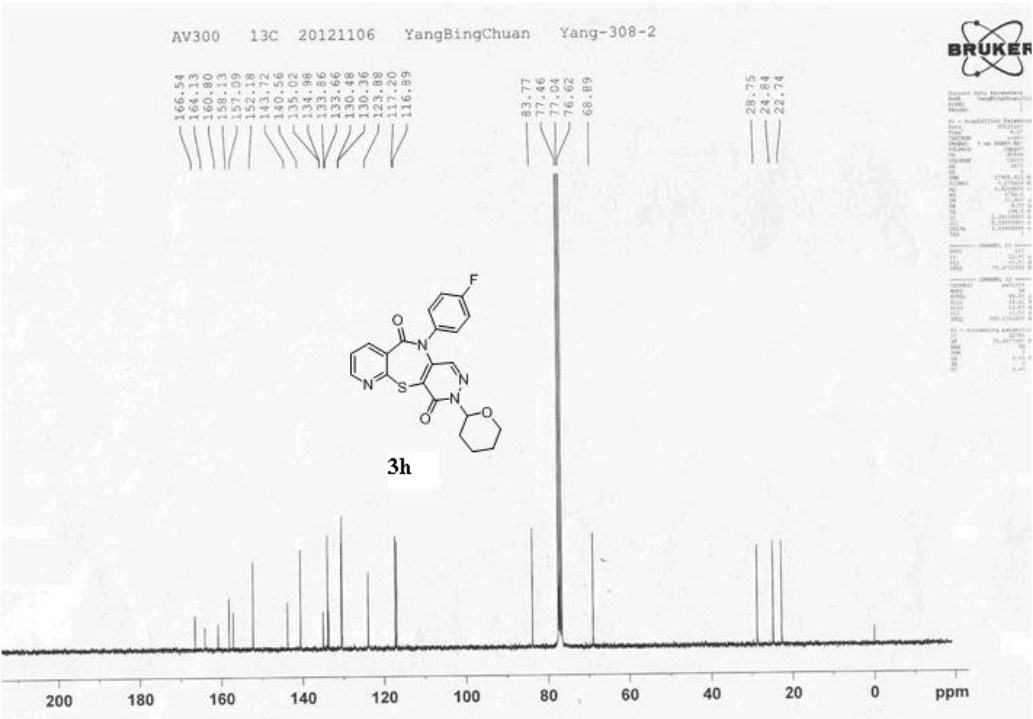


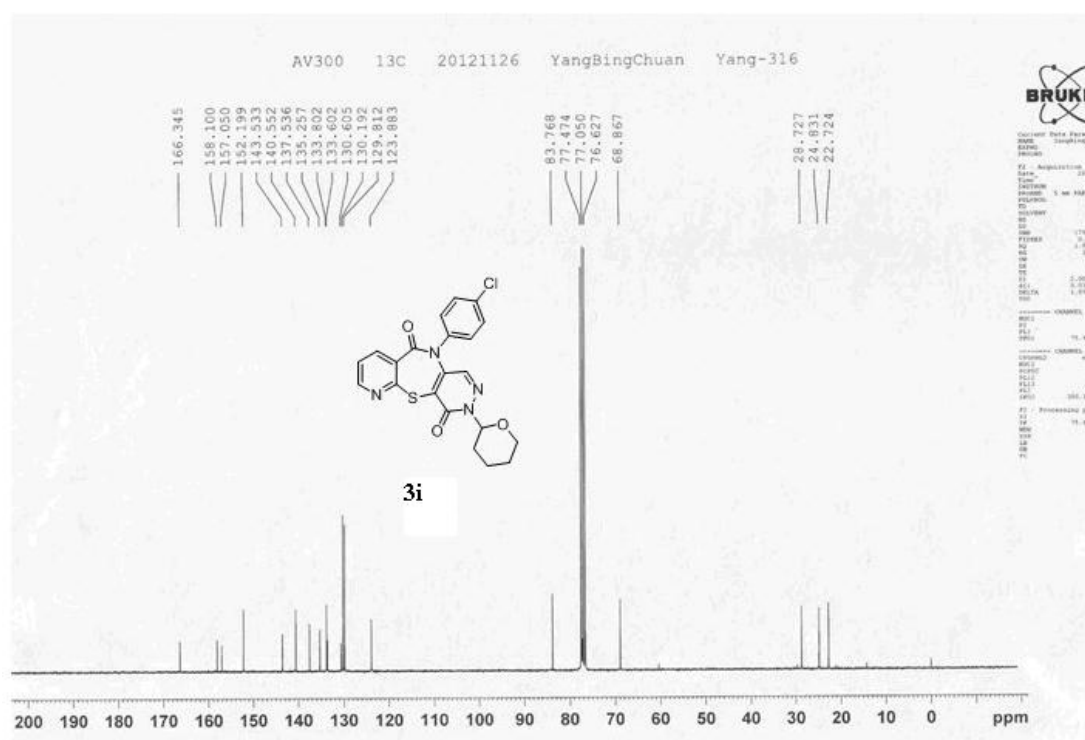
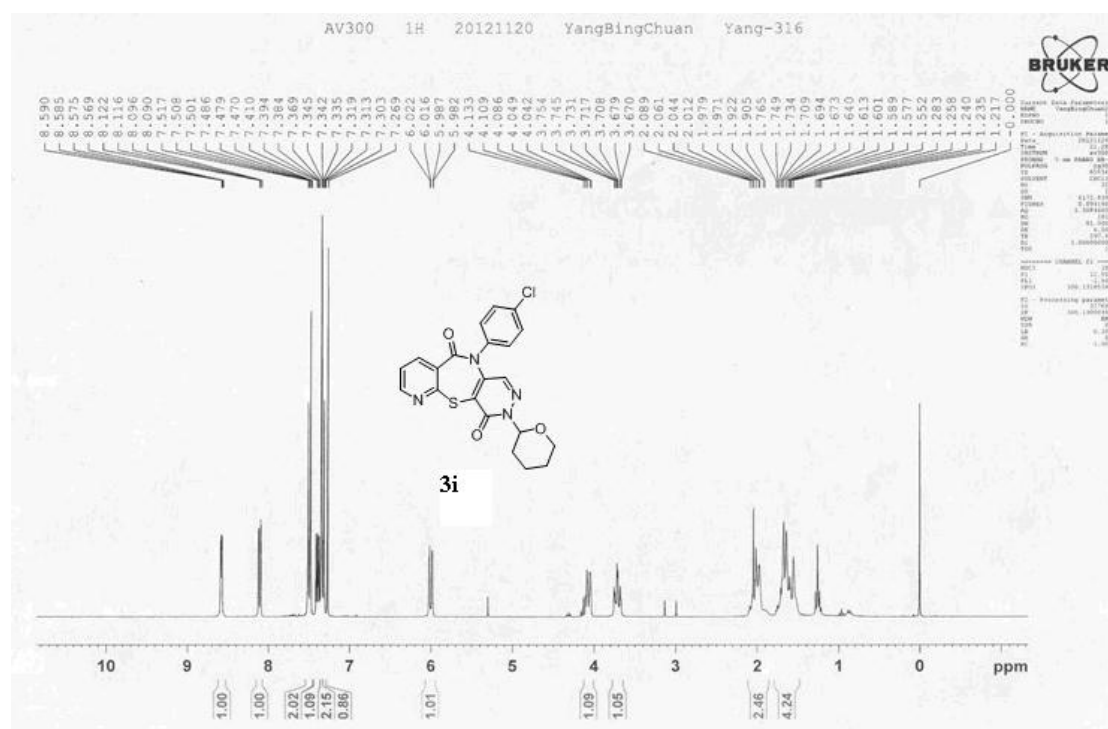
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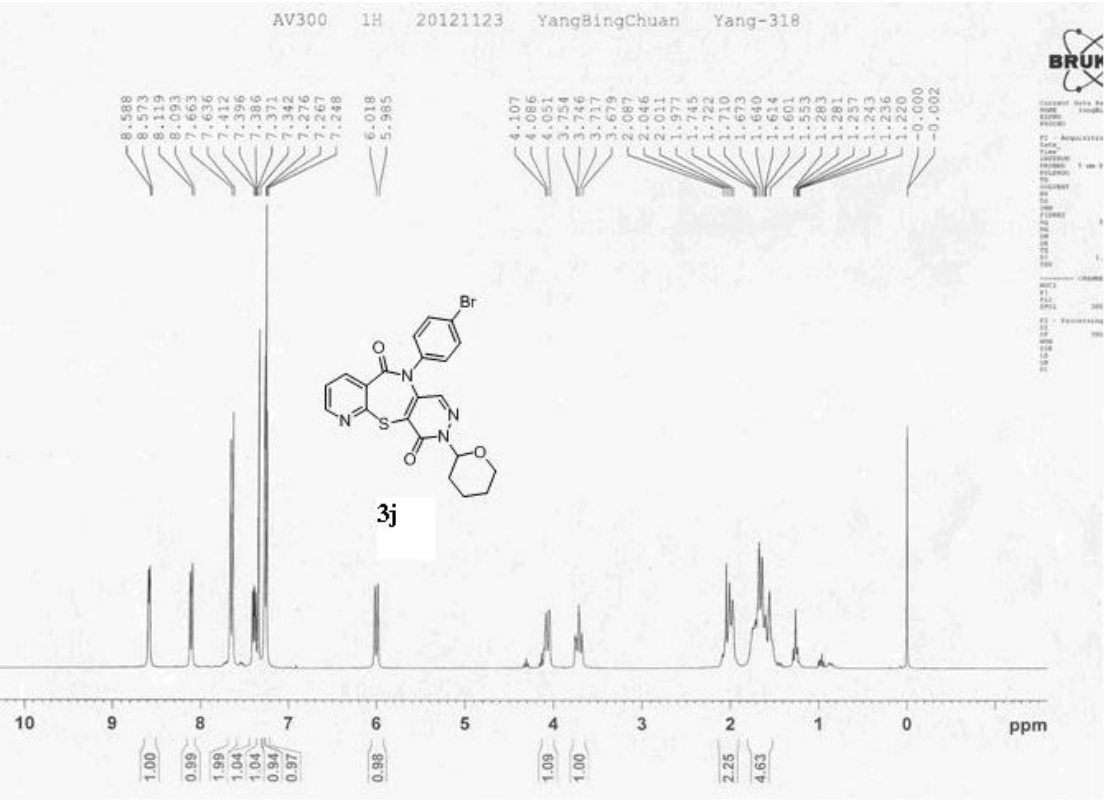
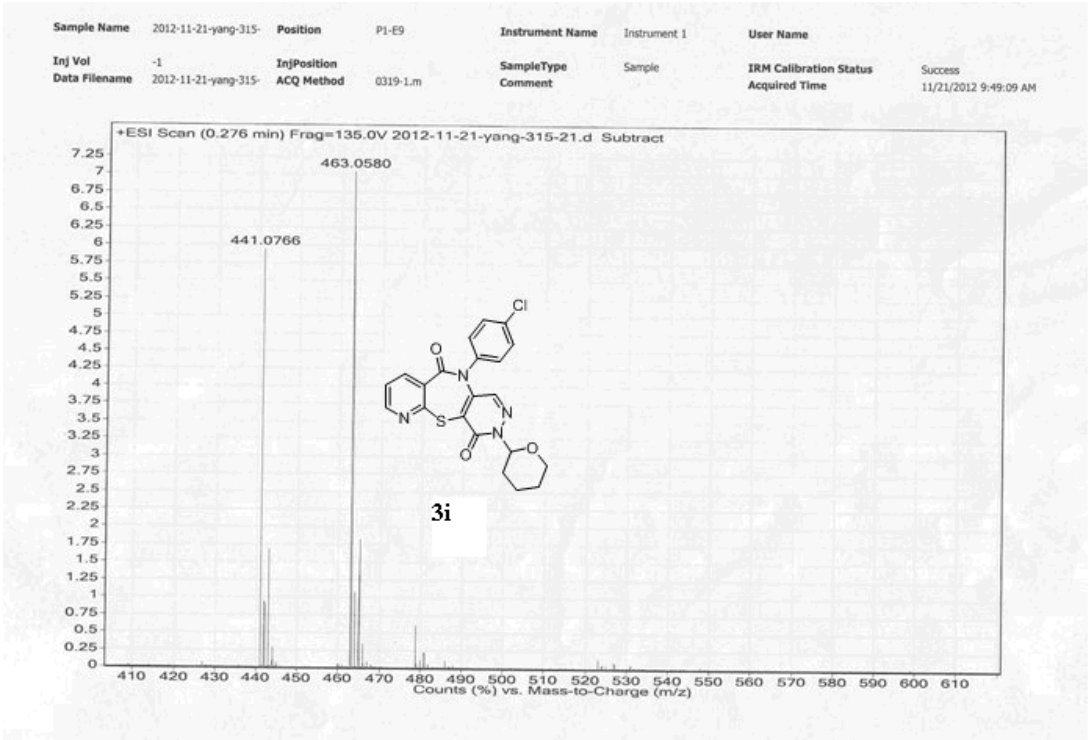


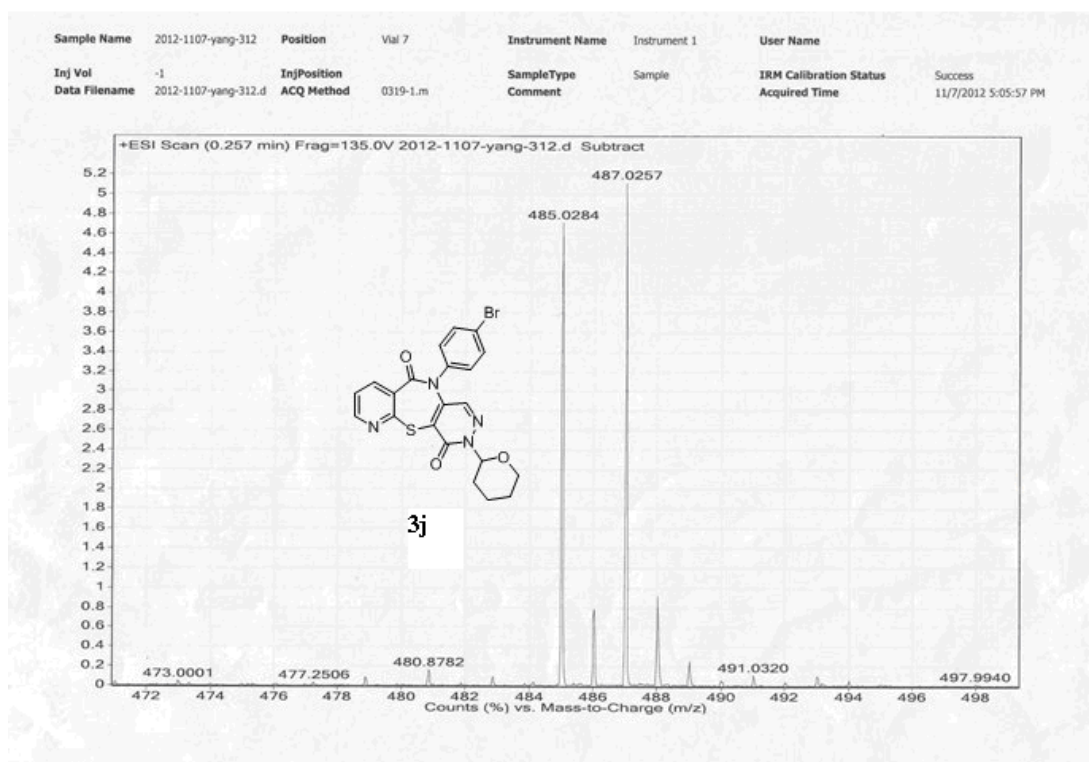
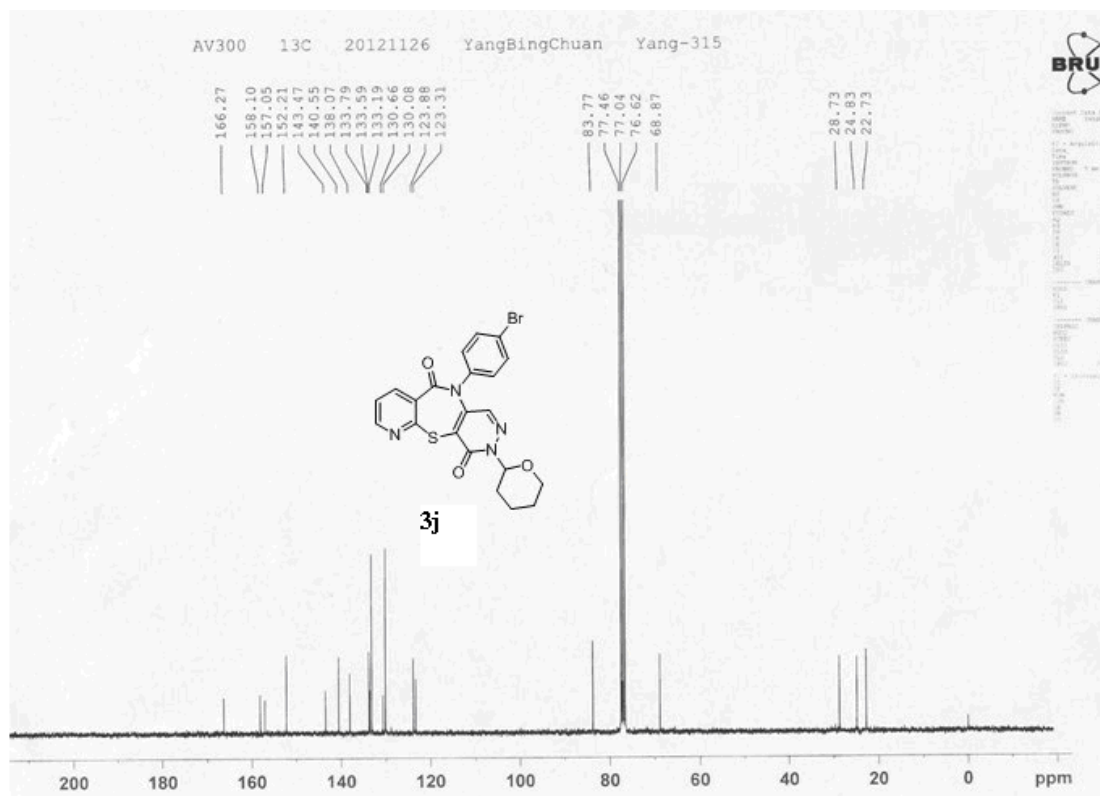


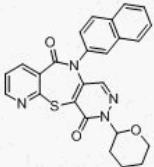
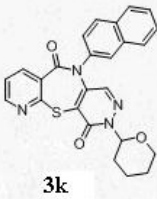


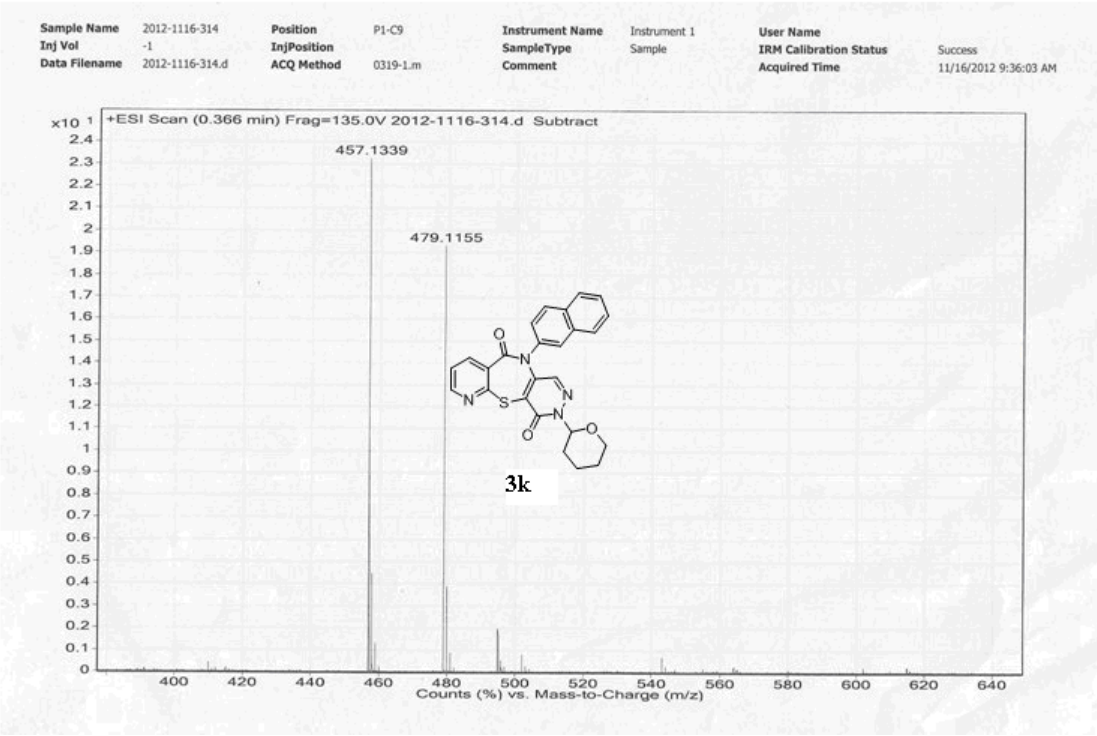


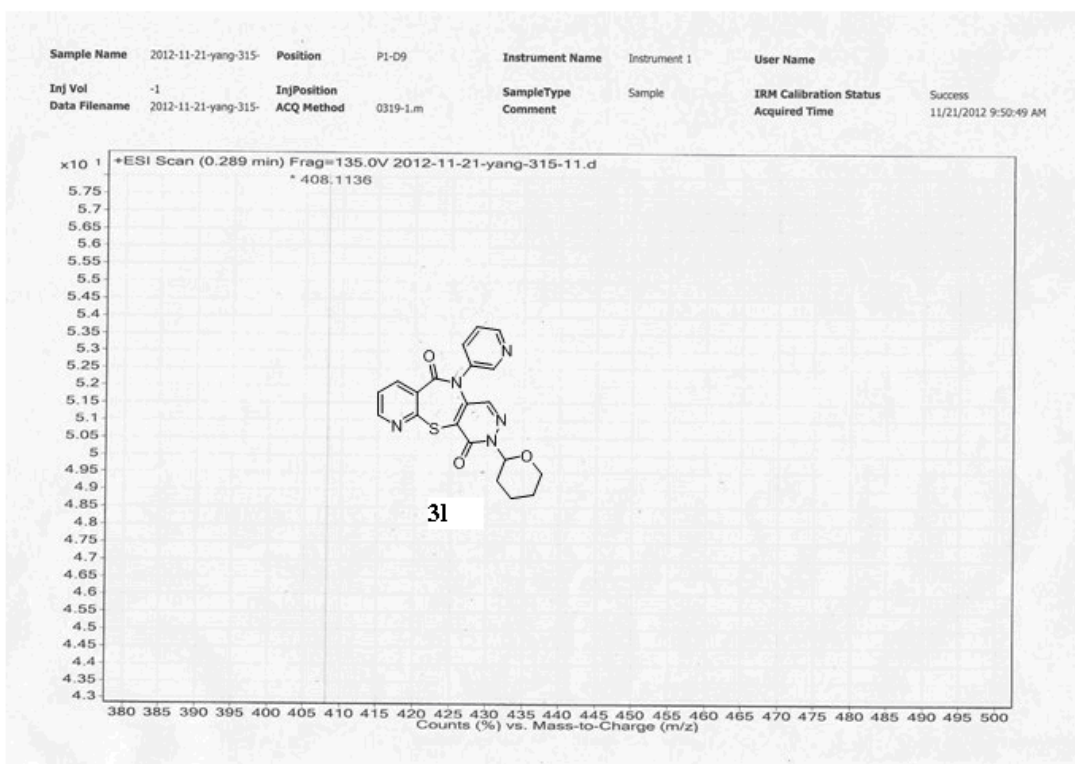


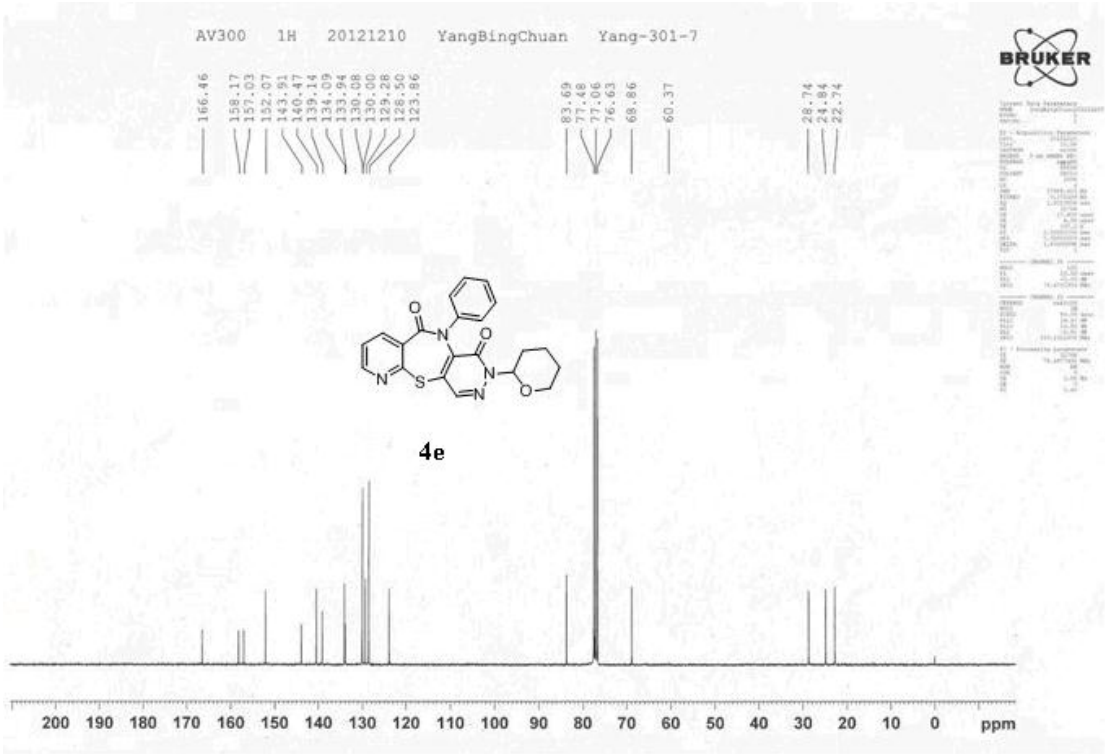
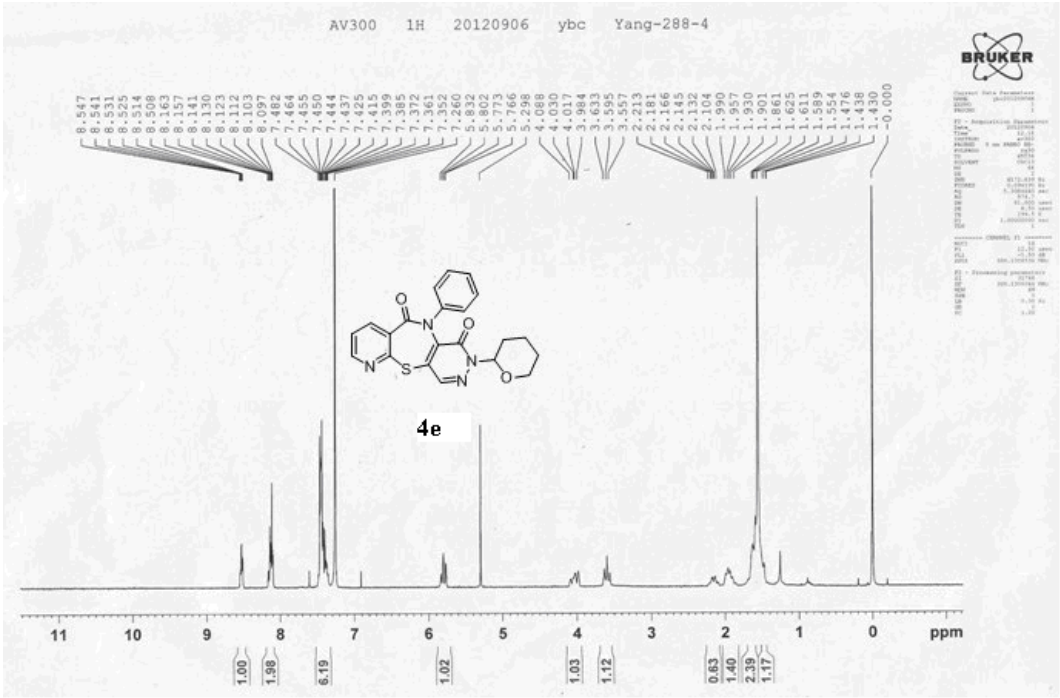


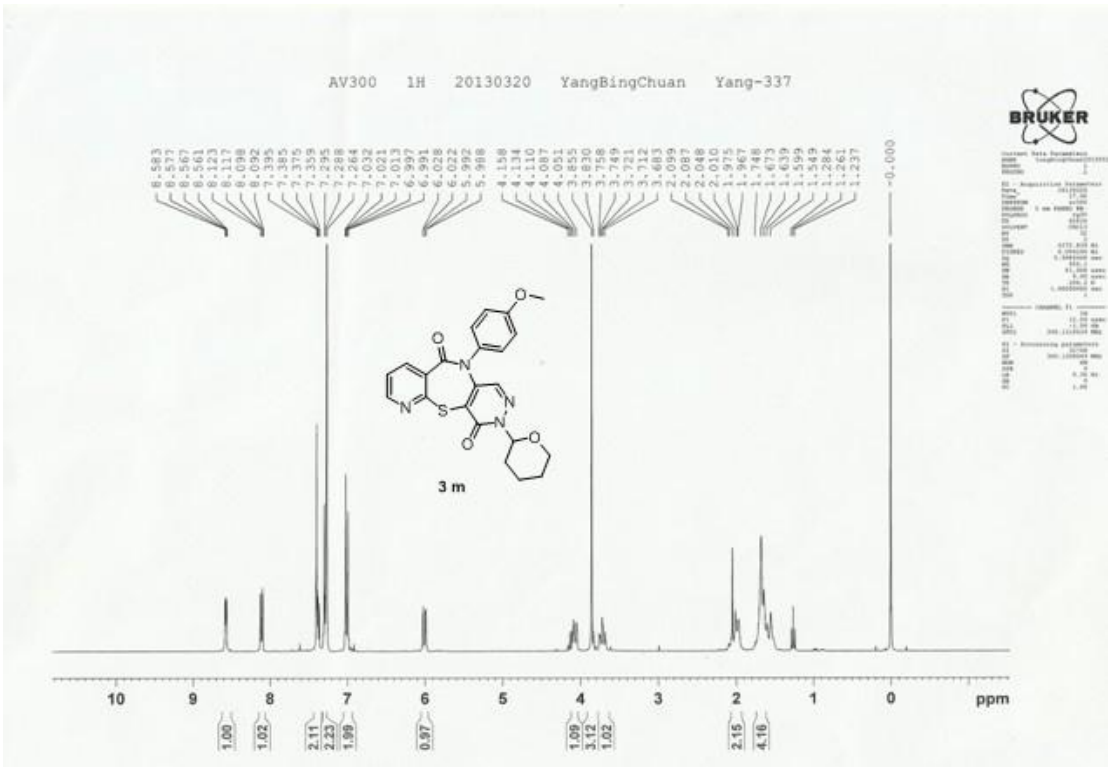
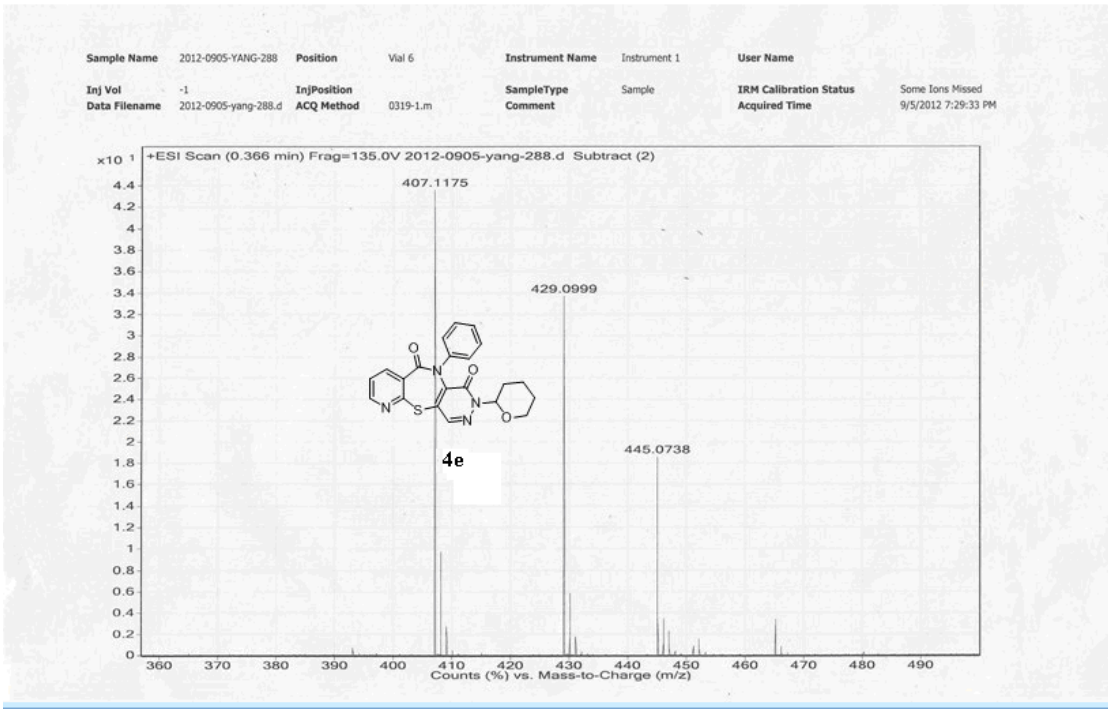


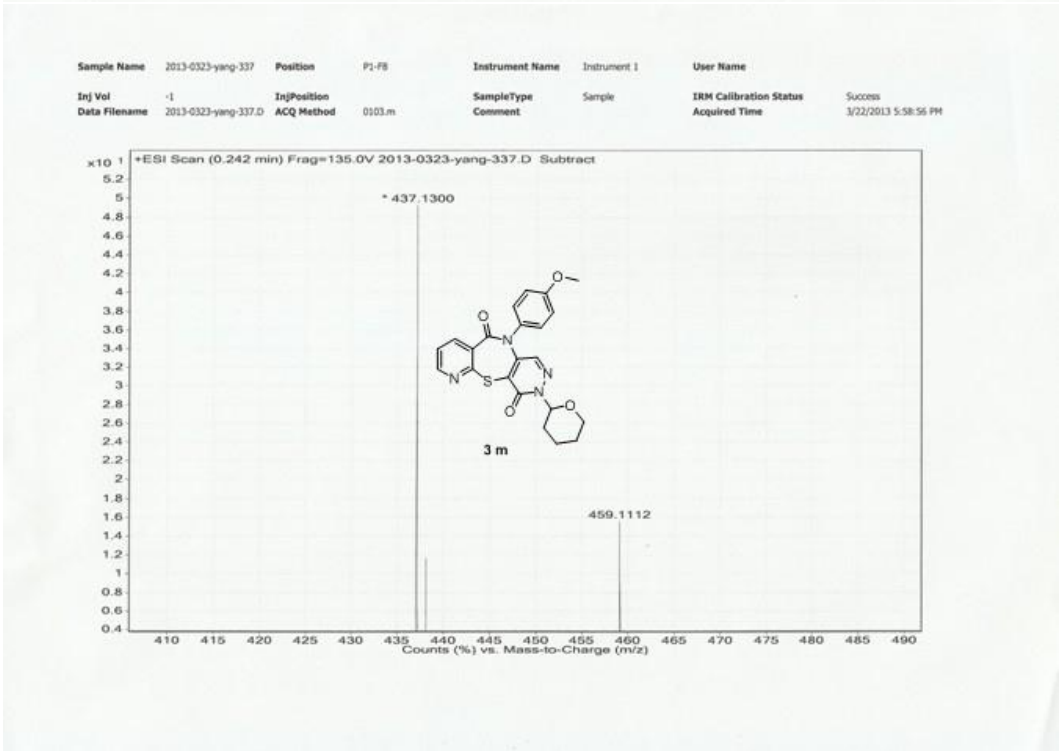
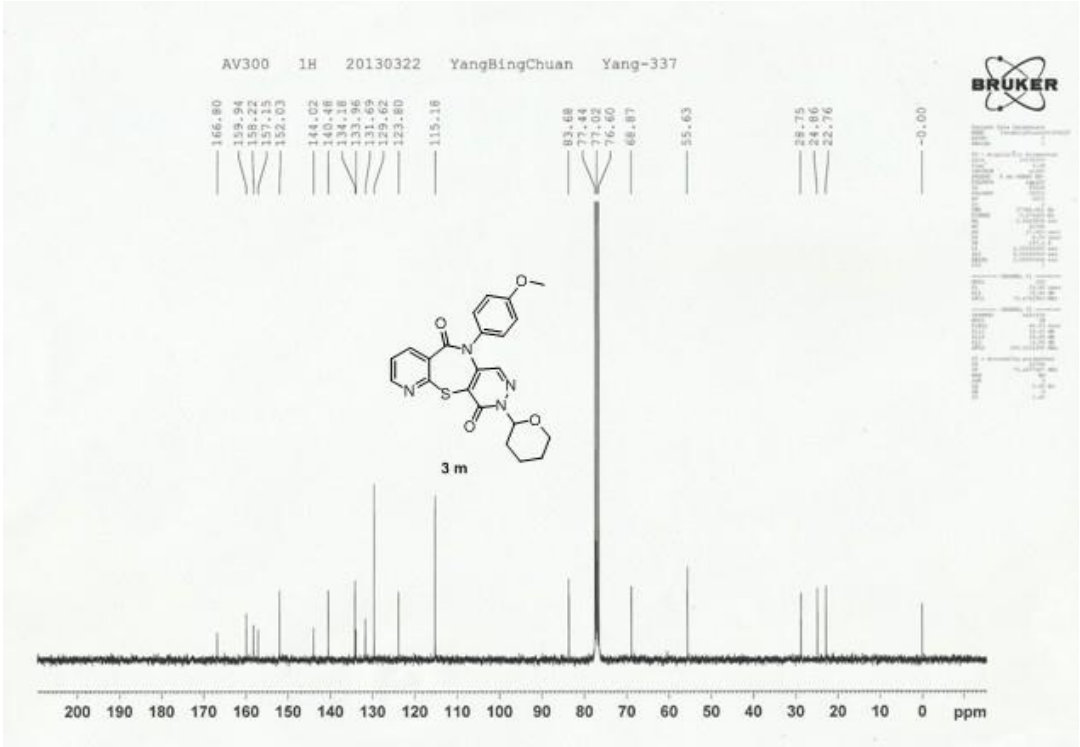


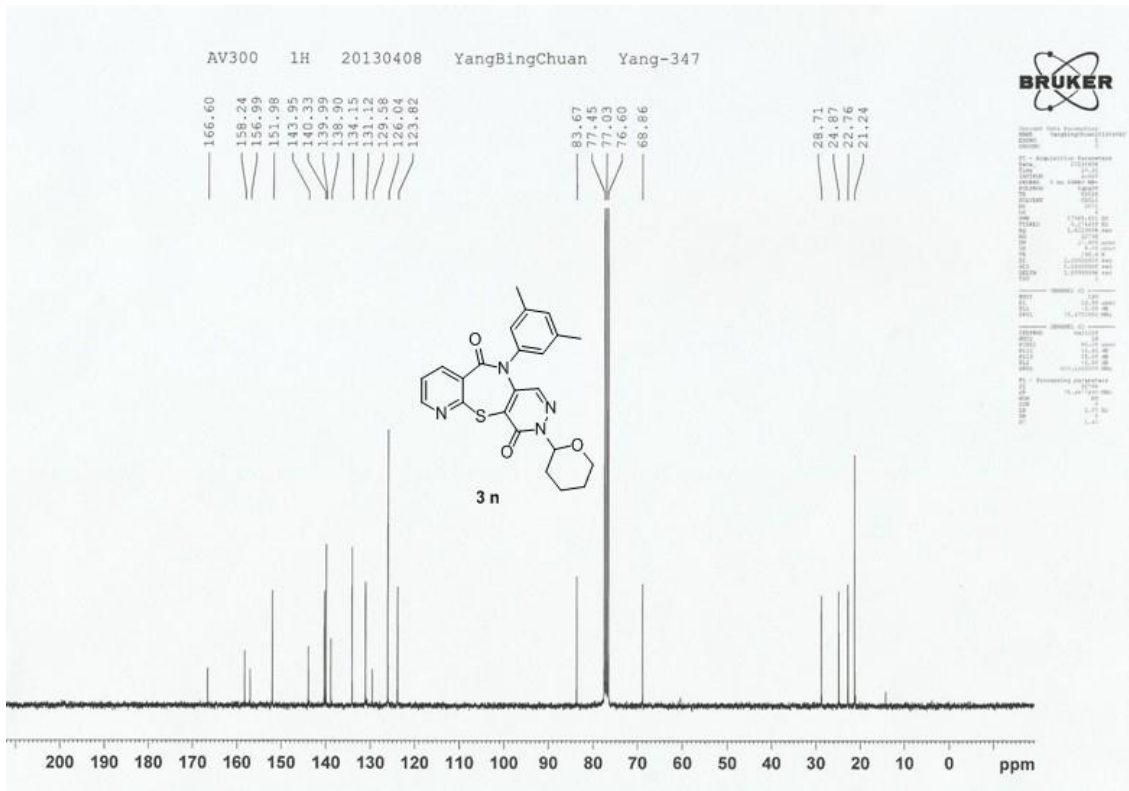
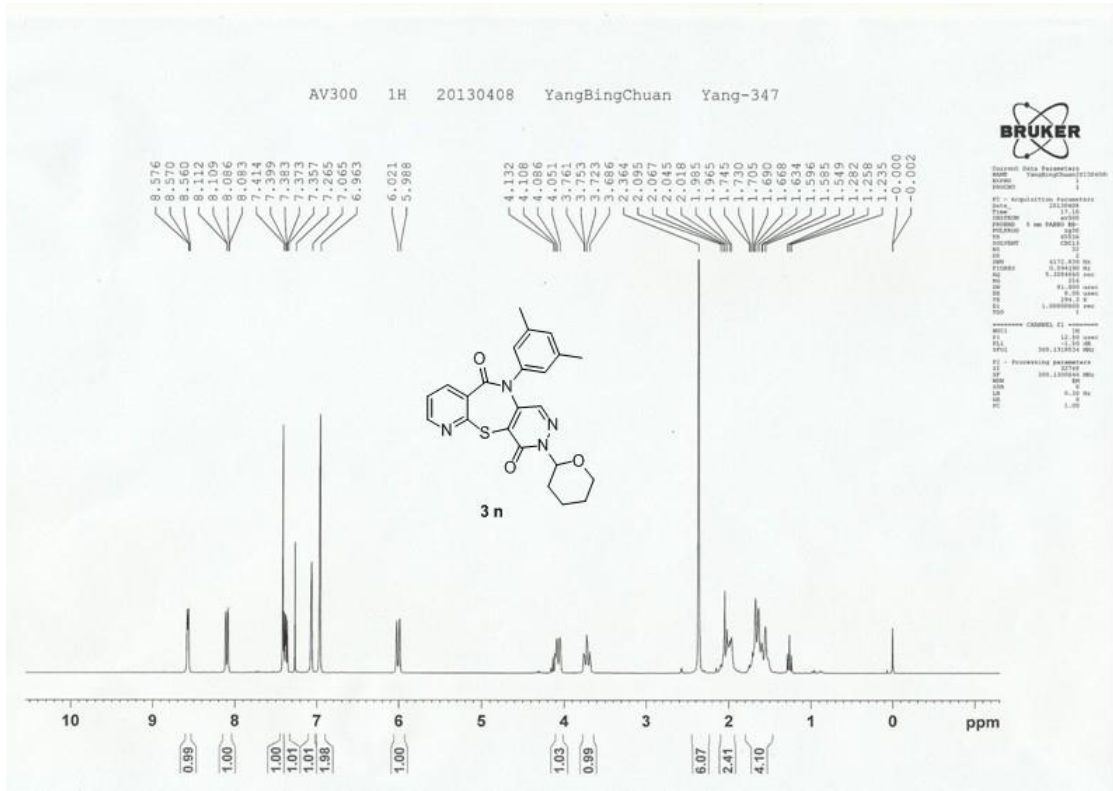












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