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SUPPLEMENTARY INFORMATION

for

Synthesis and Iron Coordination Properties of Schizokinen and its Imide Derivative

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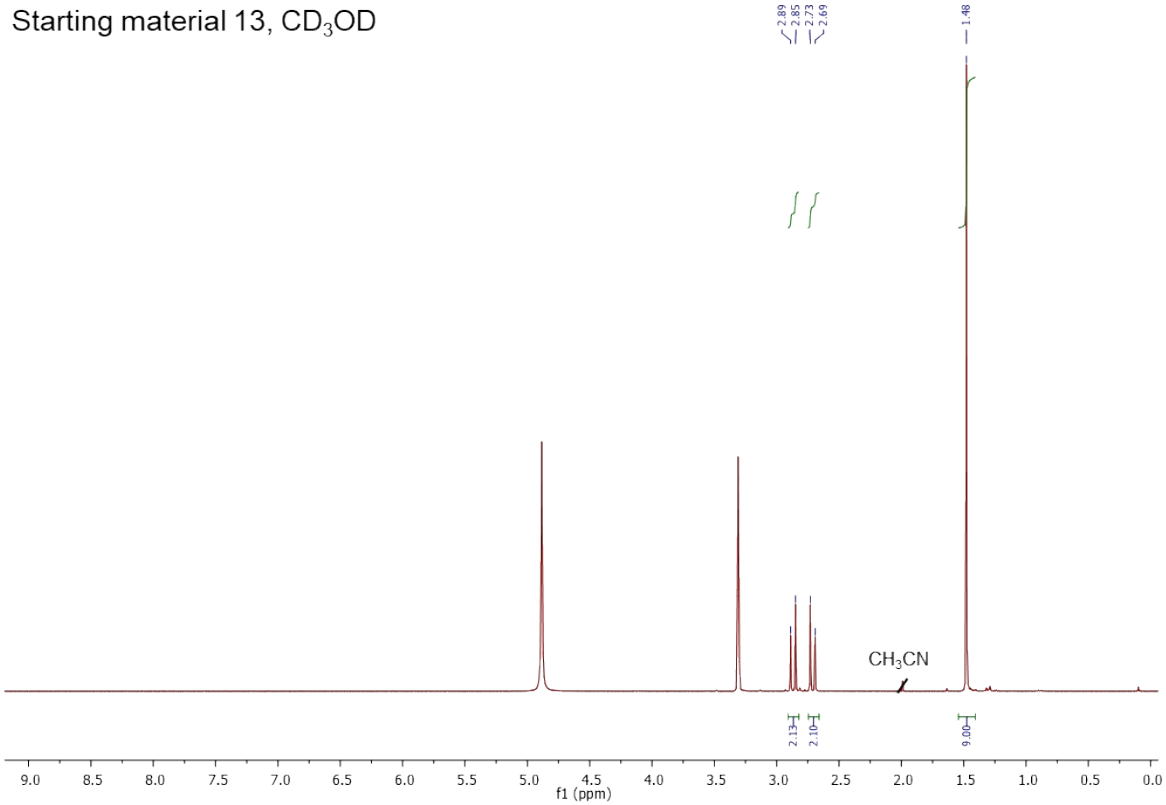
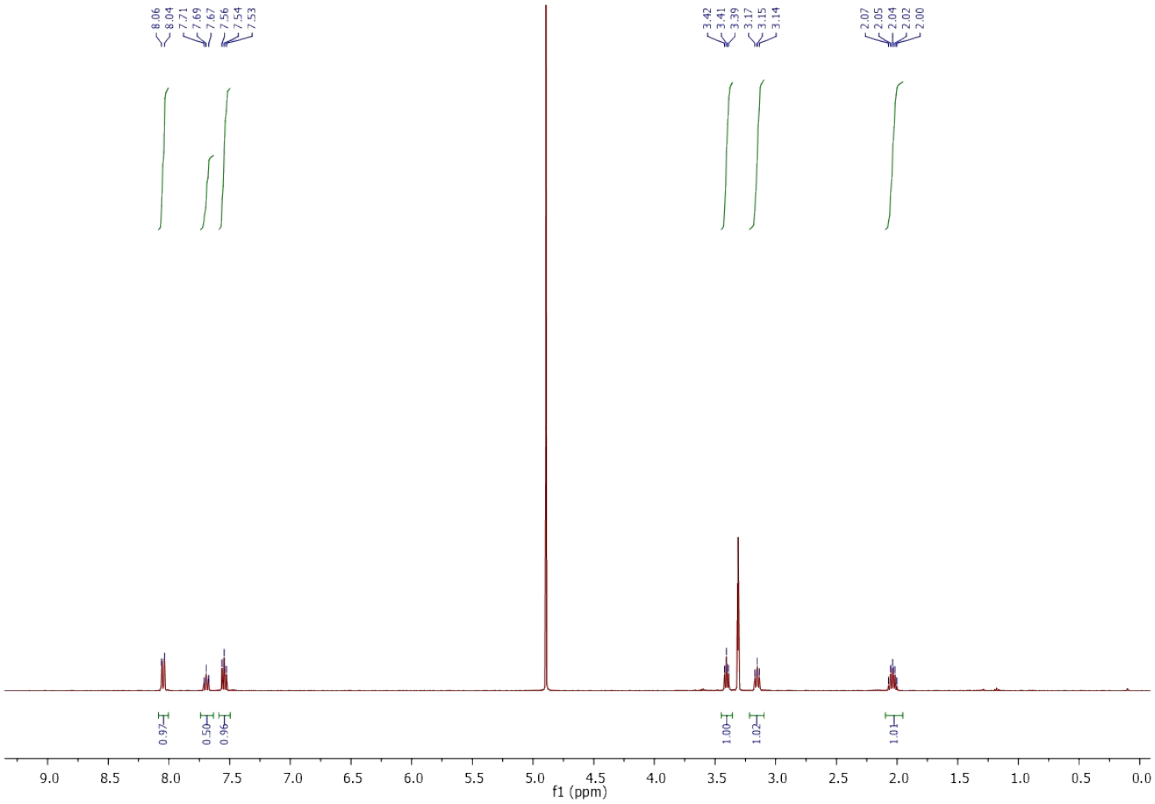
Table S1. Concentration of samples for Job's plots 17

1. ^{1}H NMR of starting materials 13 and 14

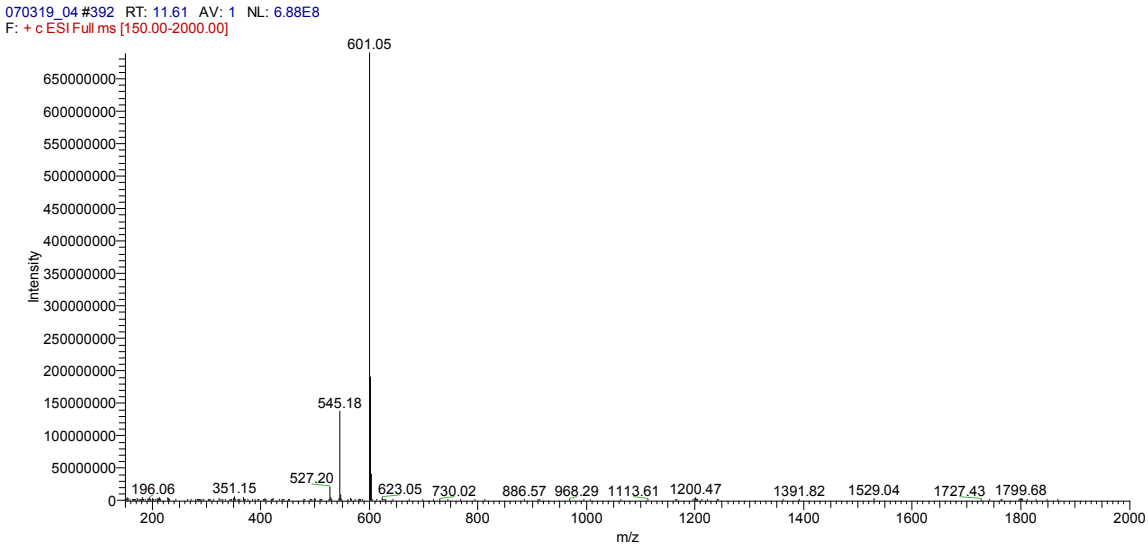
Starting material 13, CD_3OD



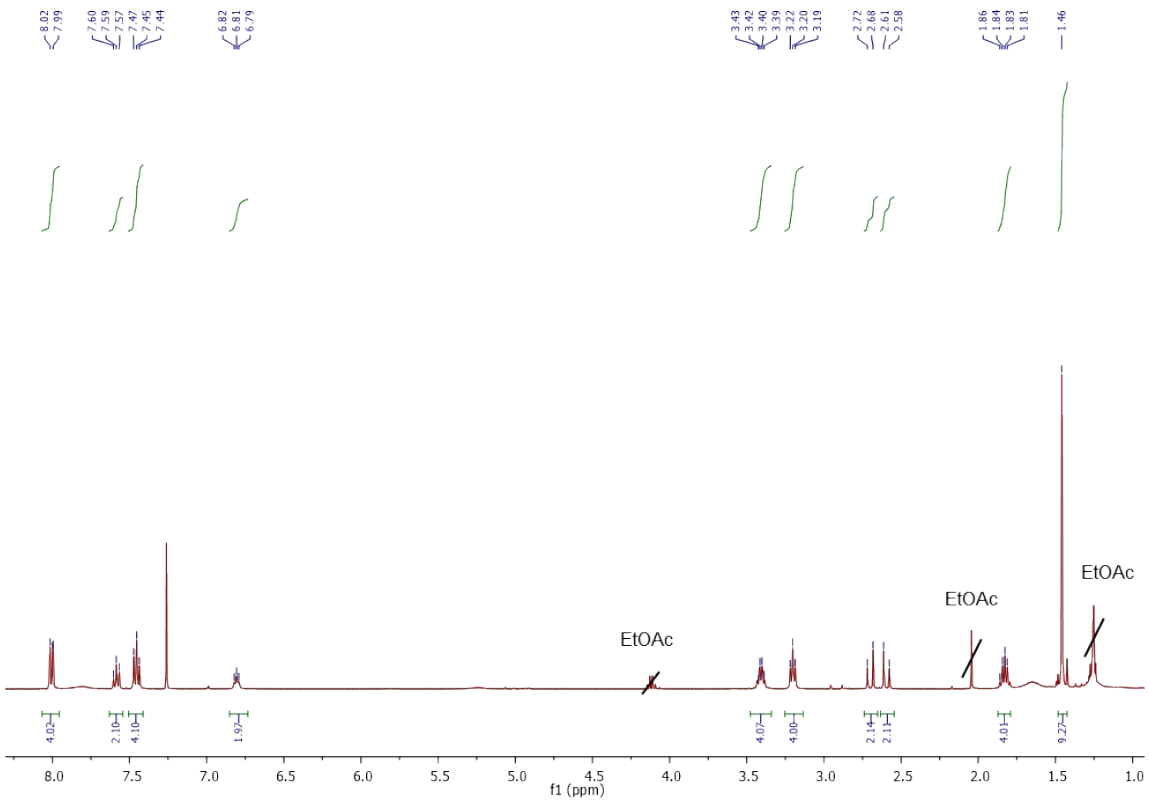
Starting material 14, CD_3OD



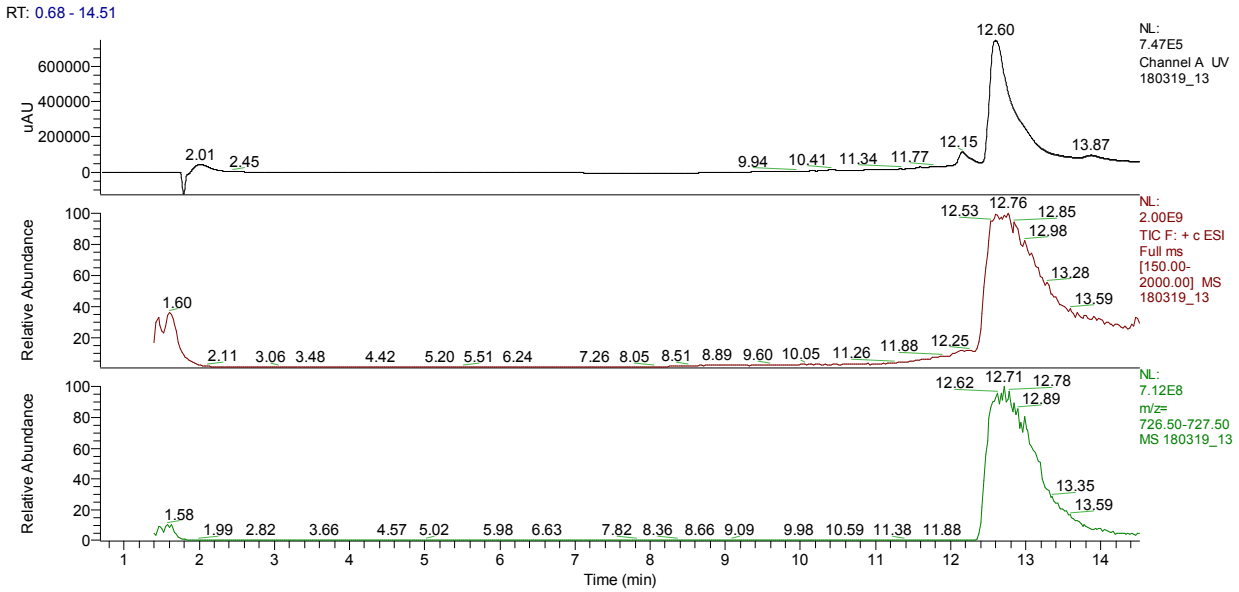
2. MS and ^{1}H NMR spectra of intermediate 15

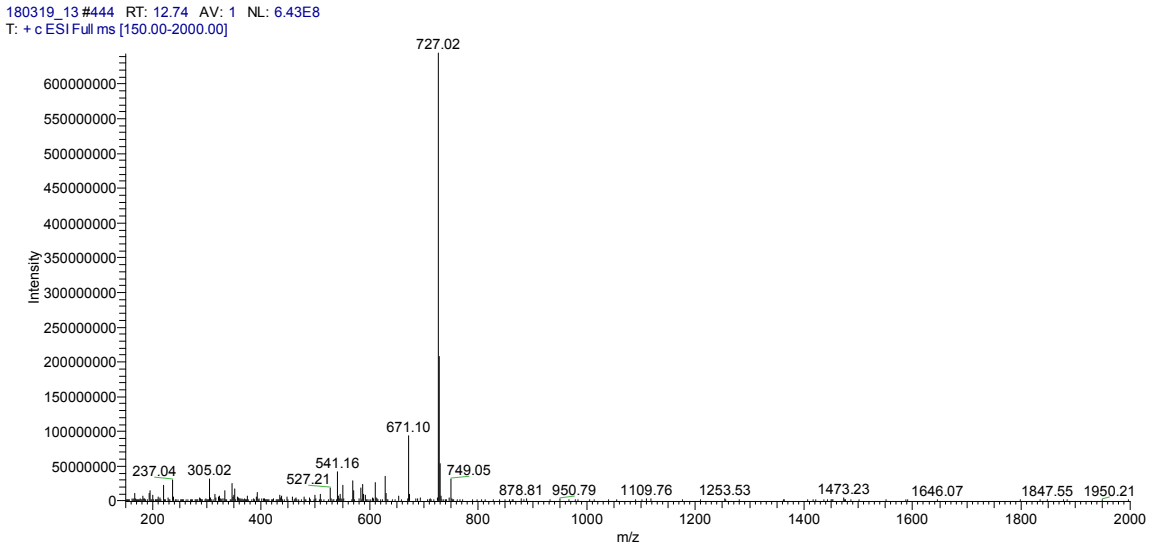


Intermediate 15, $CDCl_3$

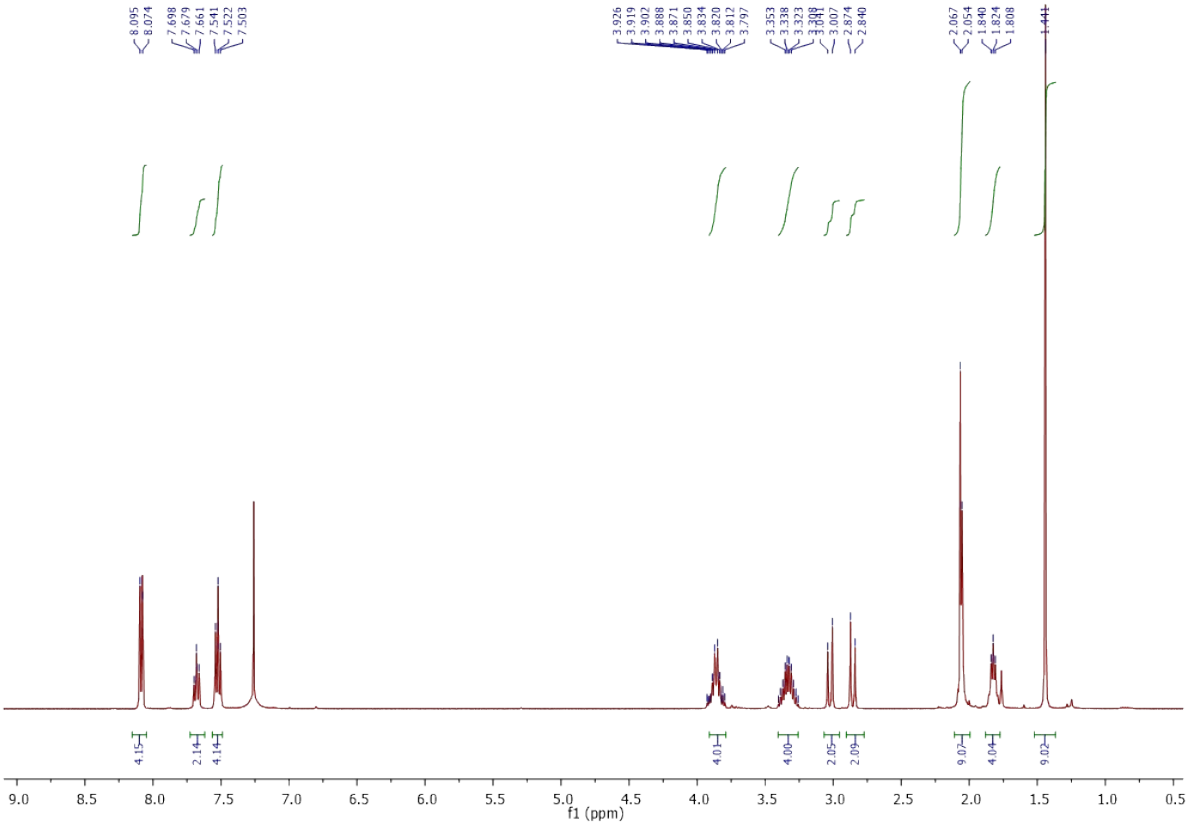


3. HPLC-UV/MS, ^{1}H and DEPT NMR of intermediate 16b

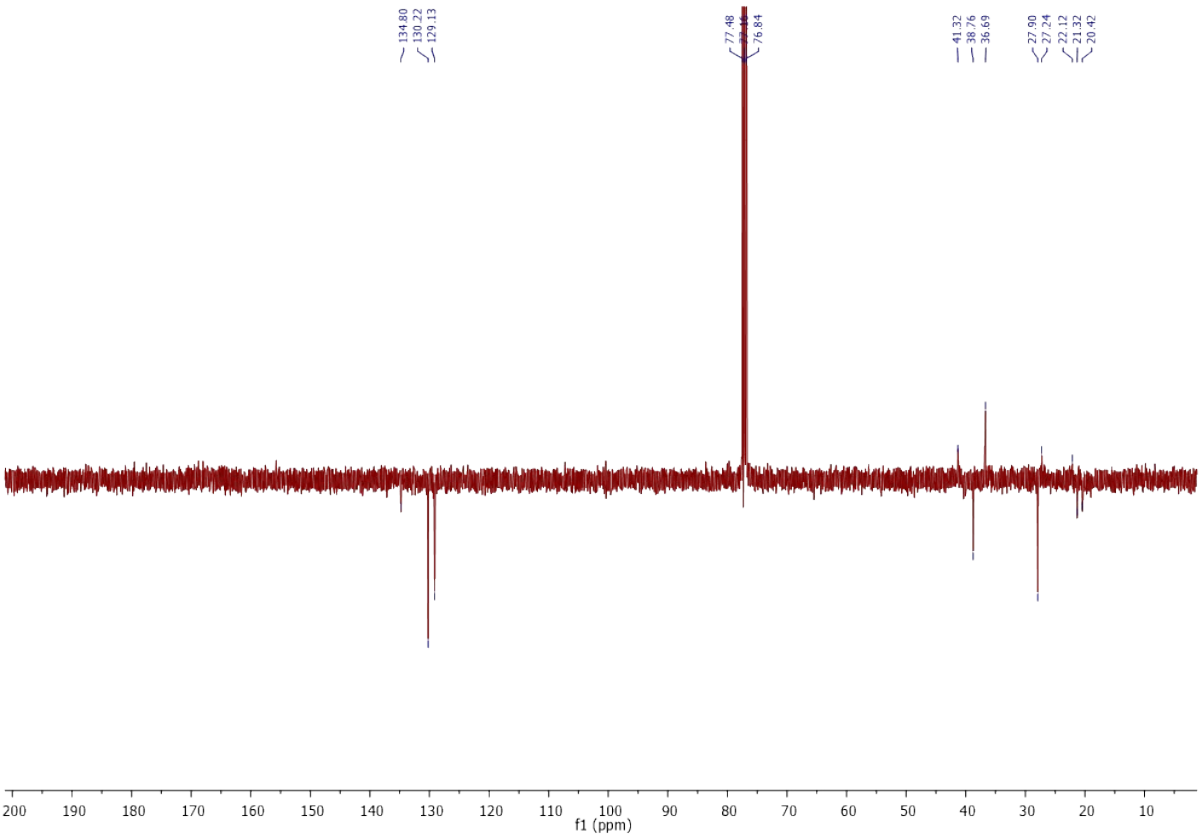




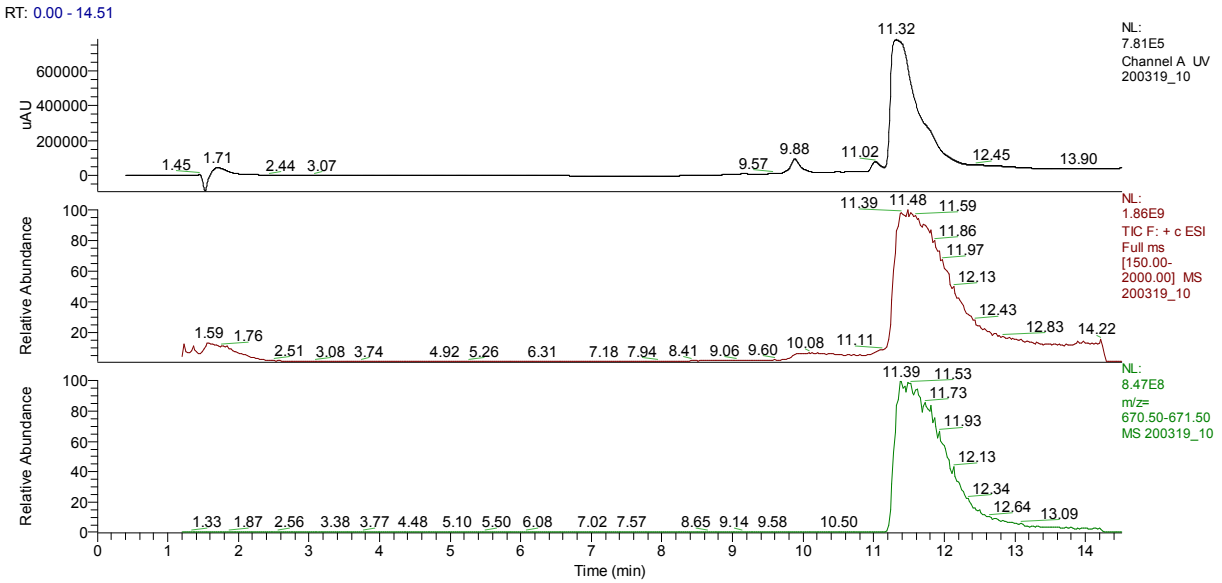
Intermediate 16b, $CDCl_3$

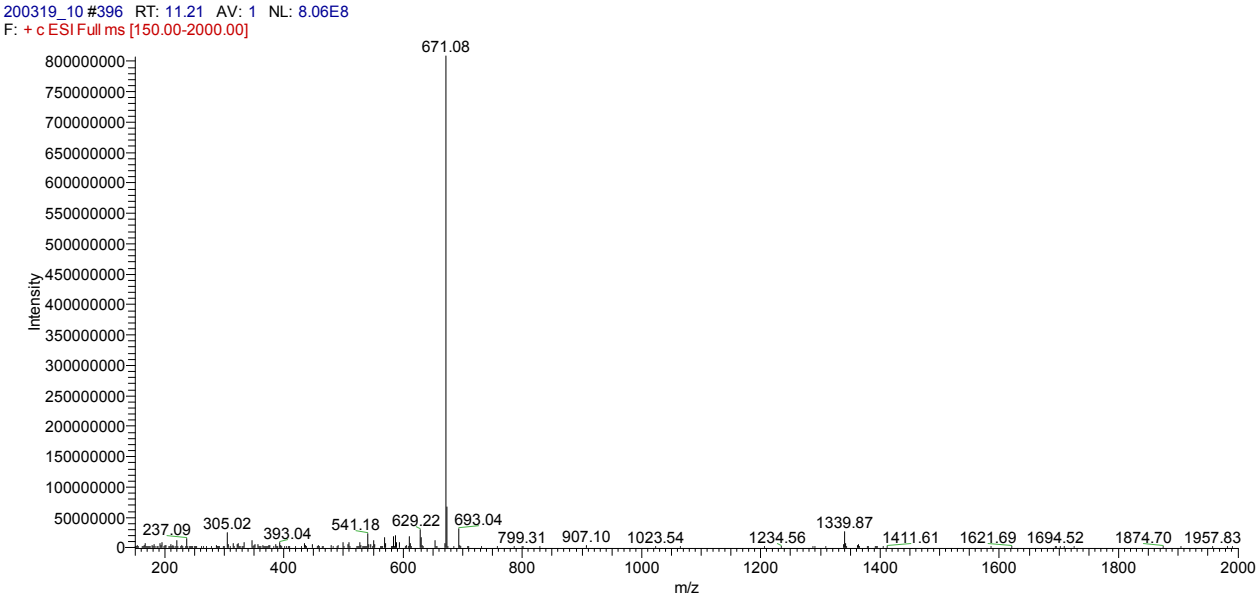


Intermediate 16b, $CDCl_3$

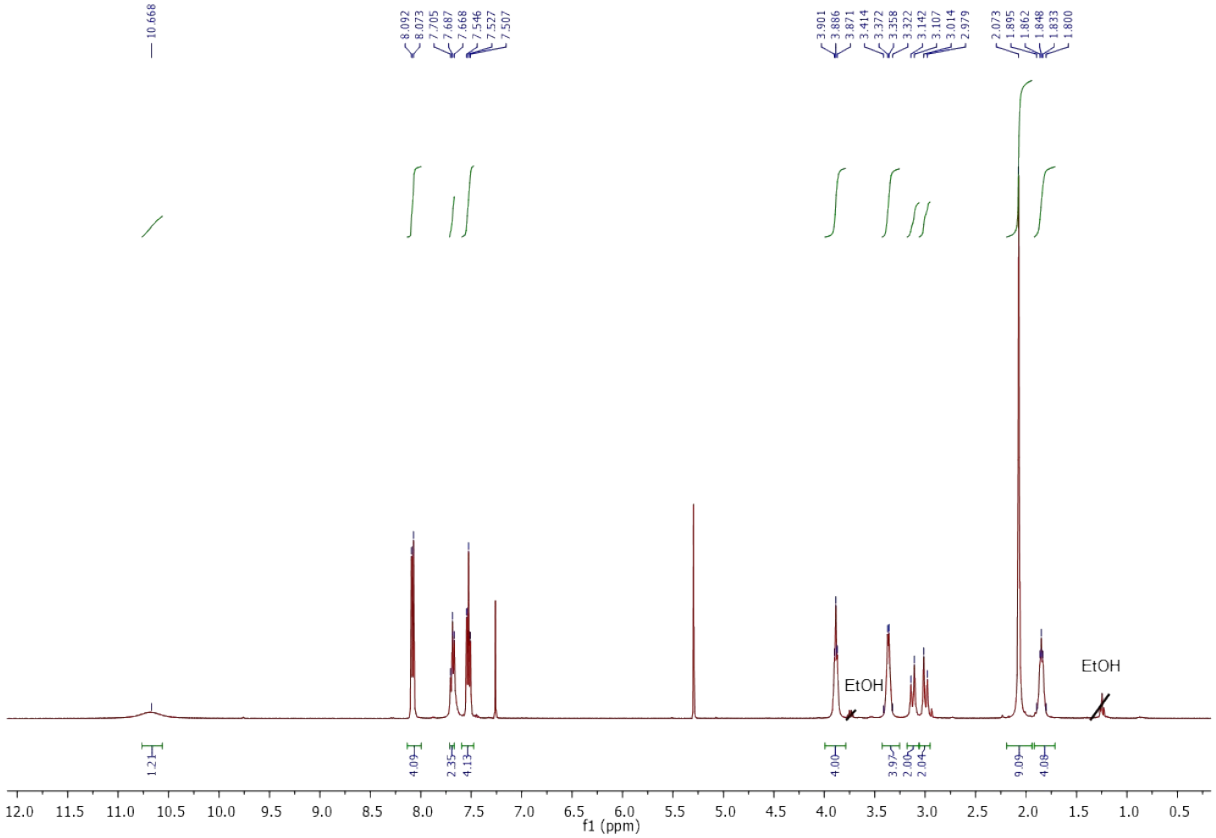


4. HPLC-UV/MS and ^{1}H NMR of intermediate 17

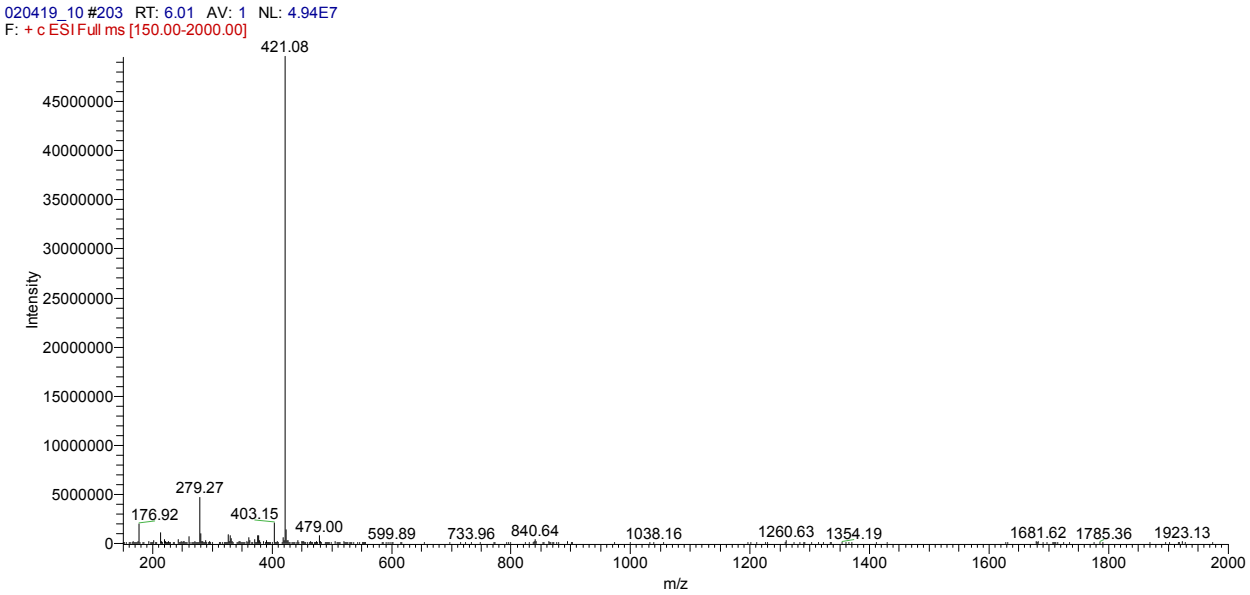




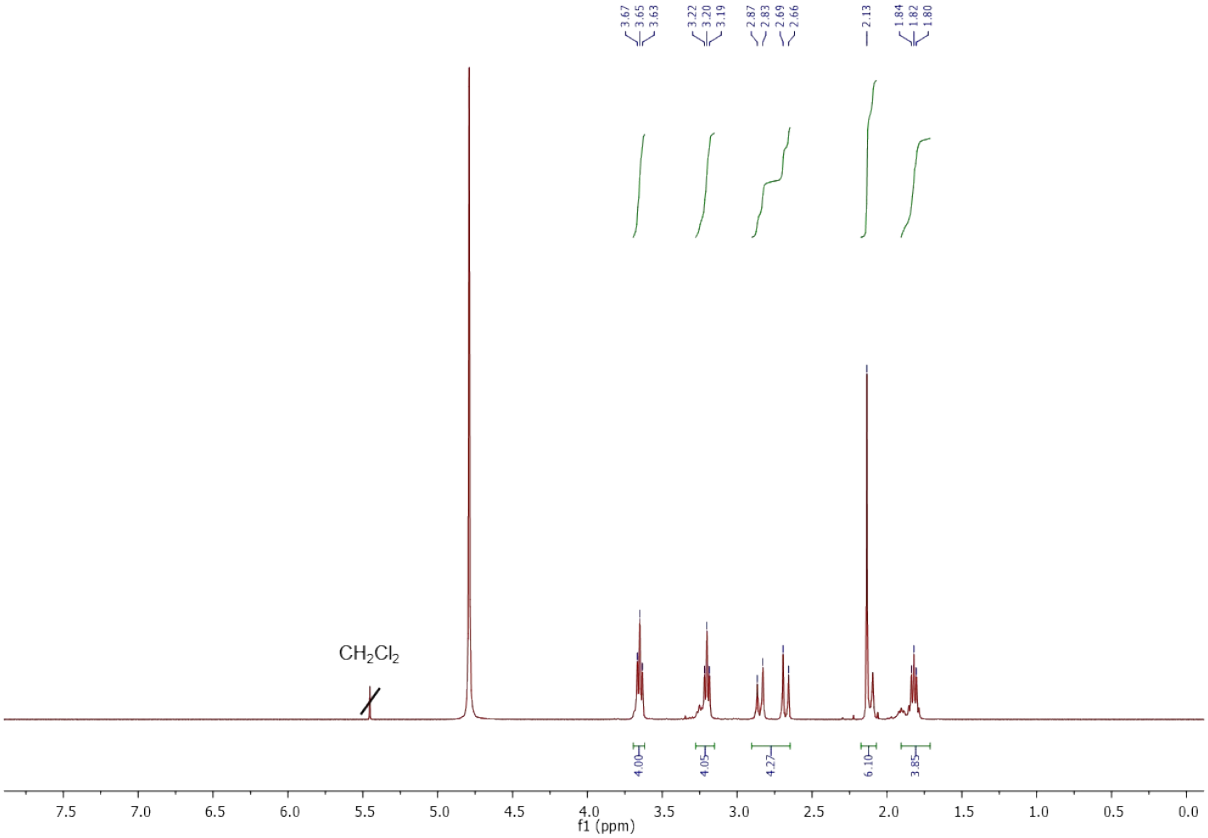
Intermediate 17, $CDCl_3$ and CD_2Cl_2



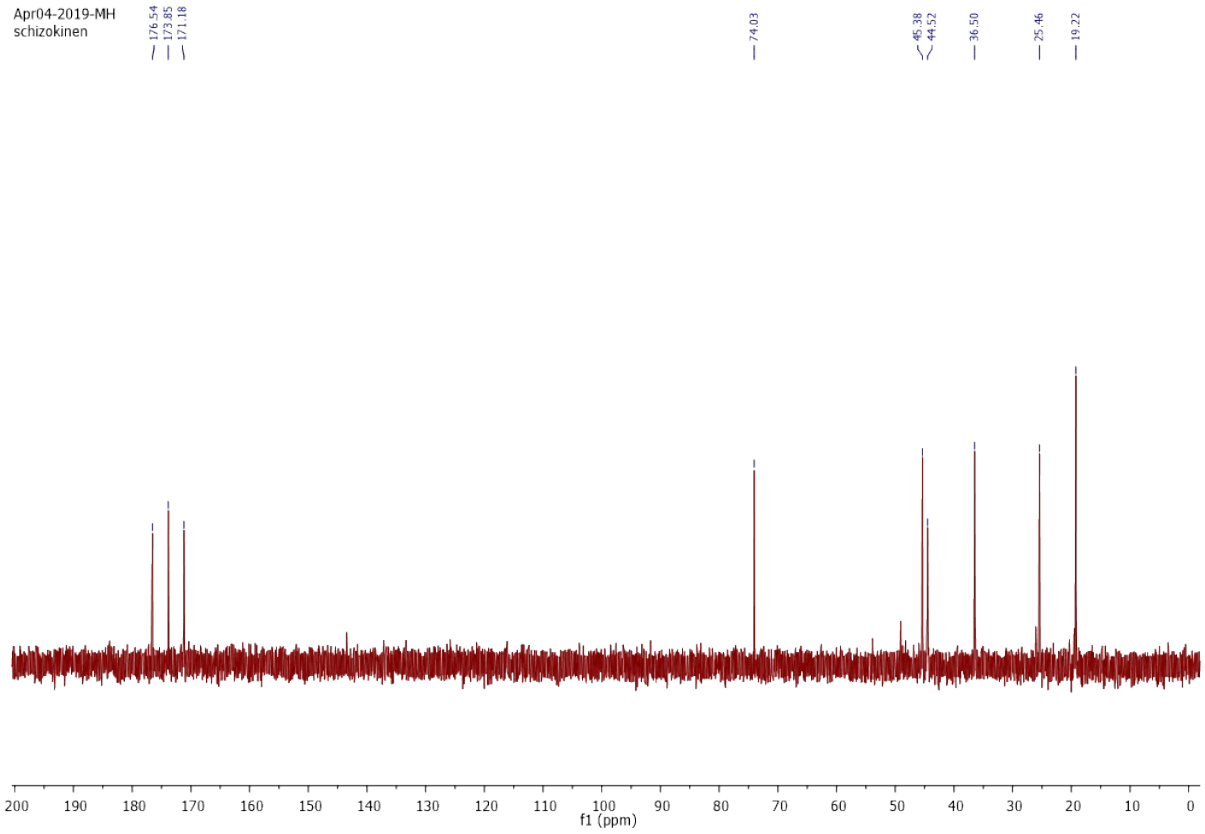
5. MS, ^{1}H, ^{13}C and DEPT NMR of schizokinen 1



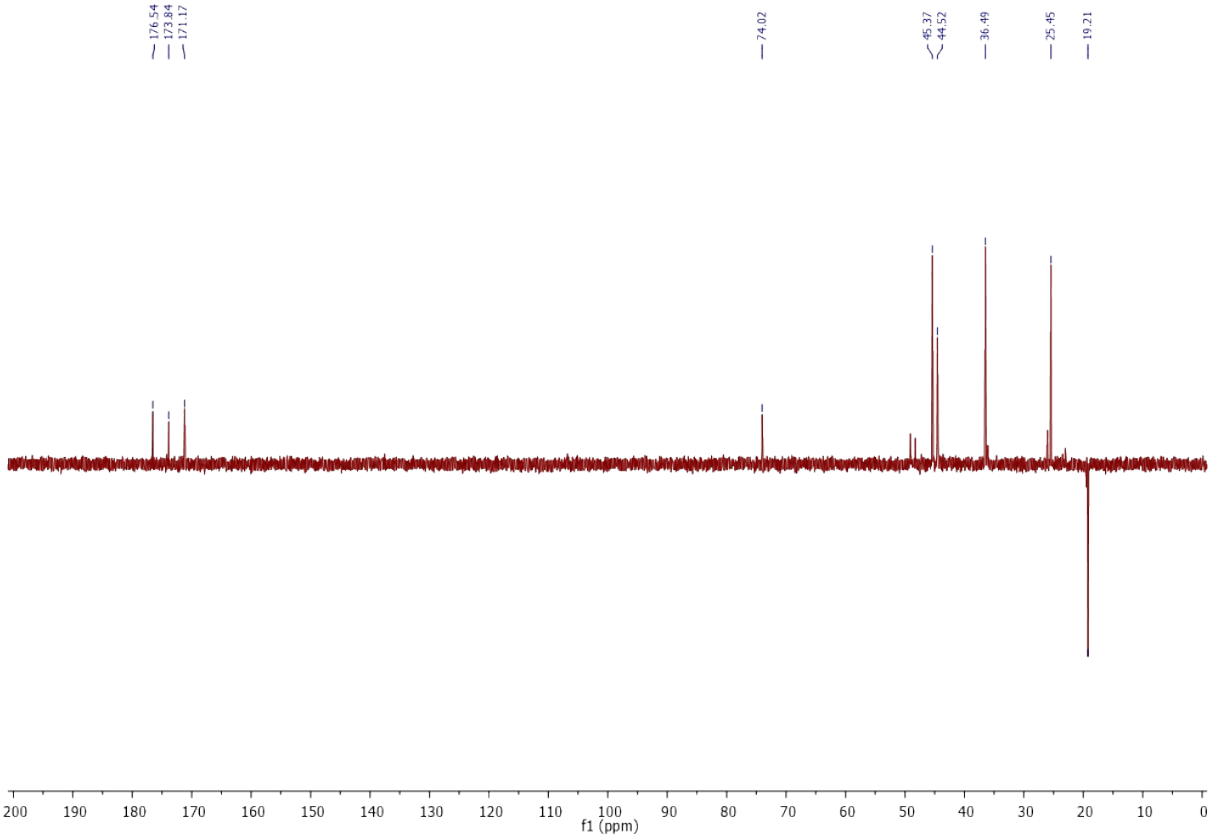
Schizokinen 1, D_2O



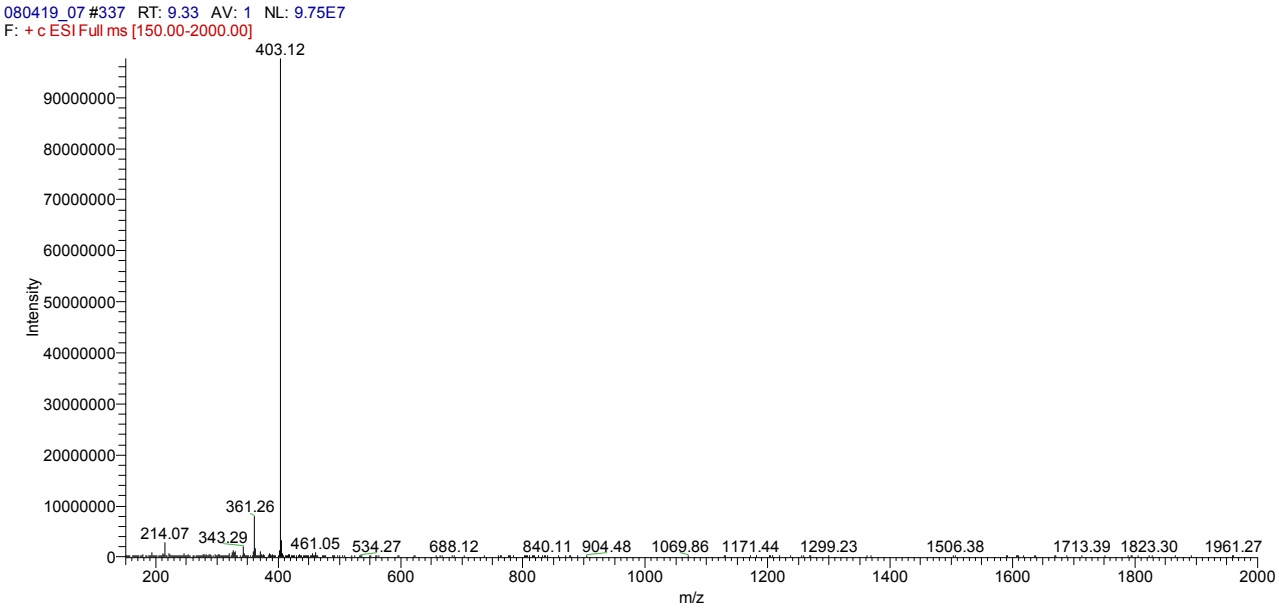
Schizokinen 1, D_2O



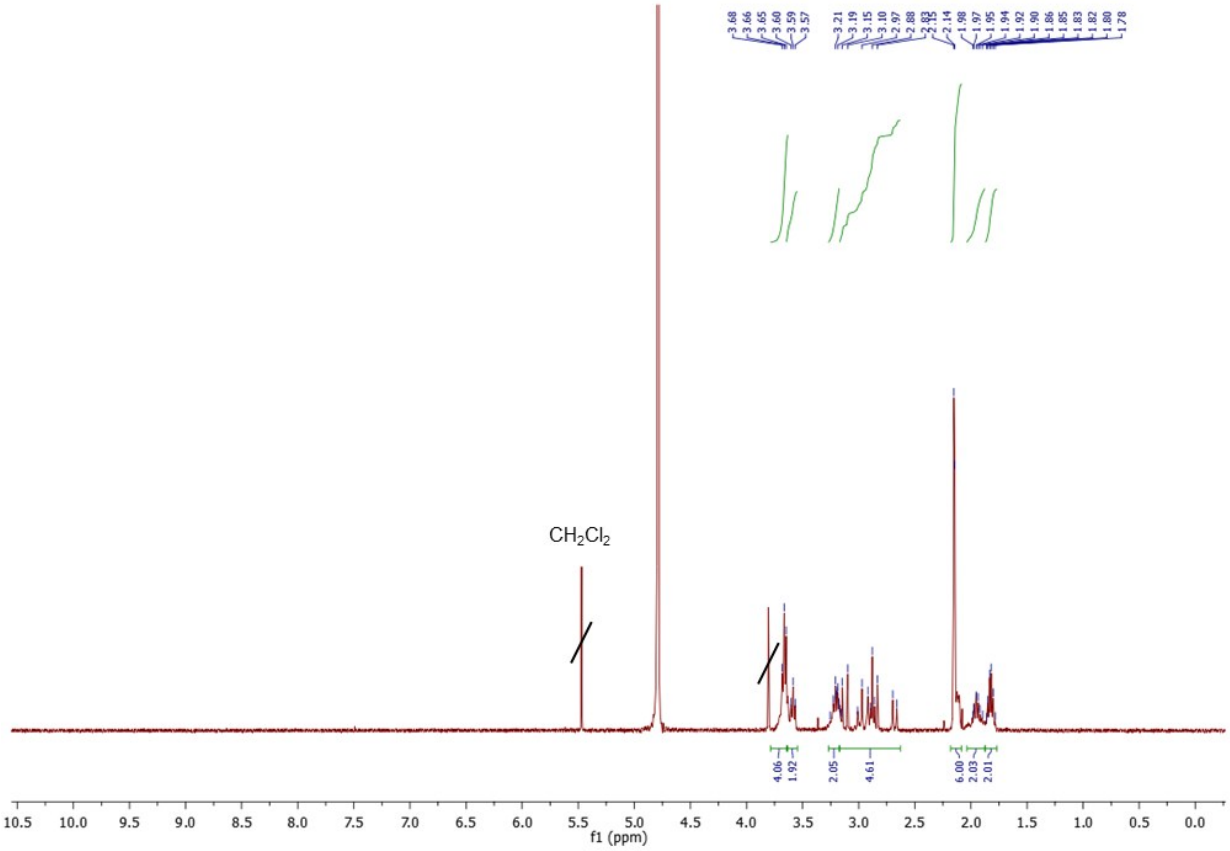
Schizokinen 1, D_2O



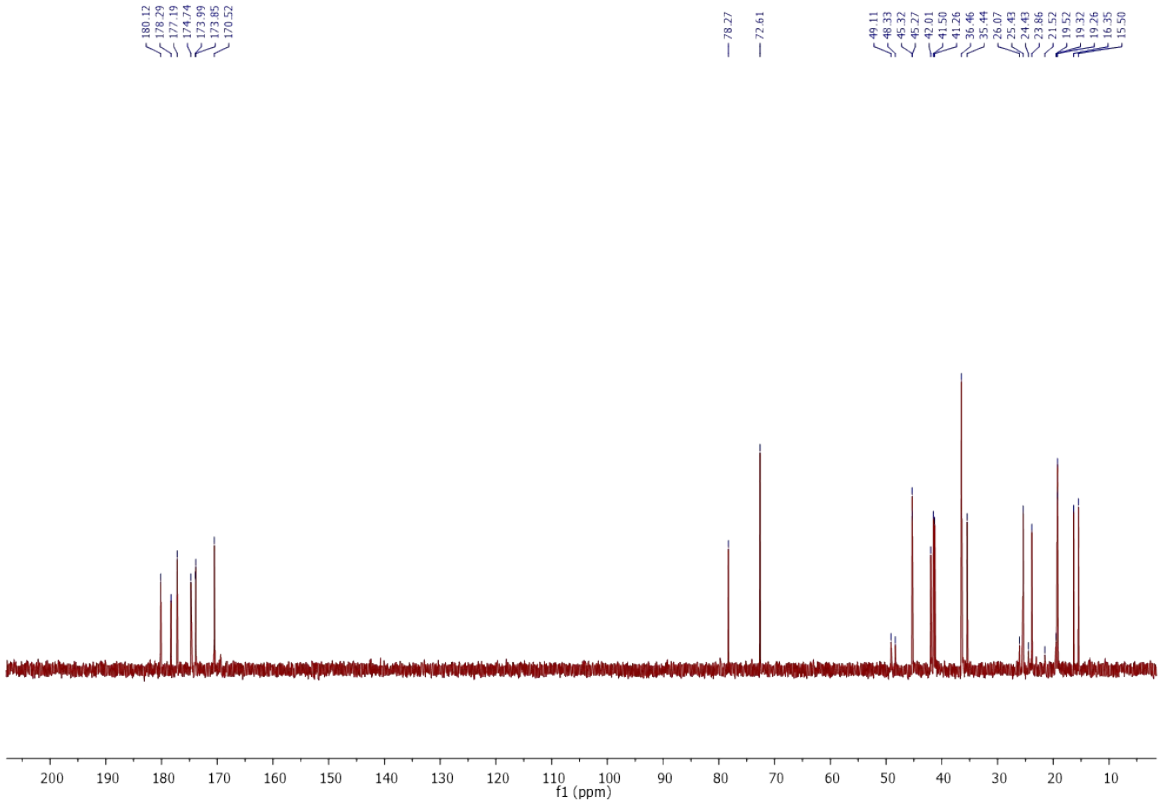
6. MS, ^{1}H and ^{13}C NMR of cyclic imide derivative 9



Cyclic imide derivative 9, D_2O



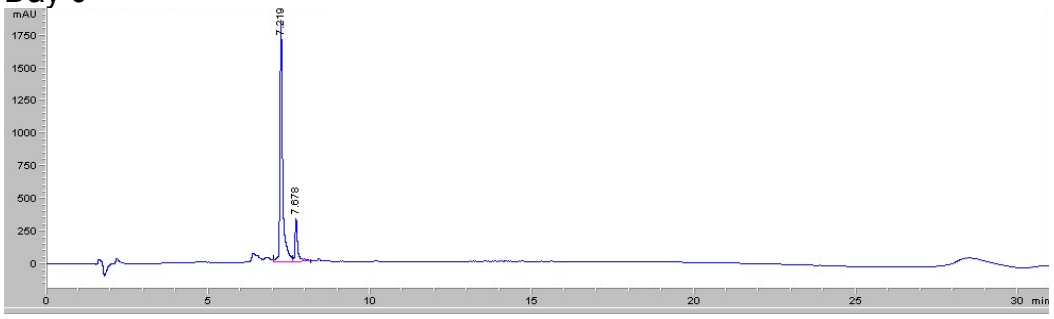
Cyclic imide derivative 9, D_2O



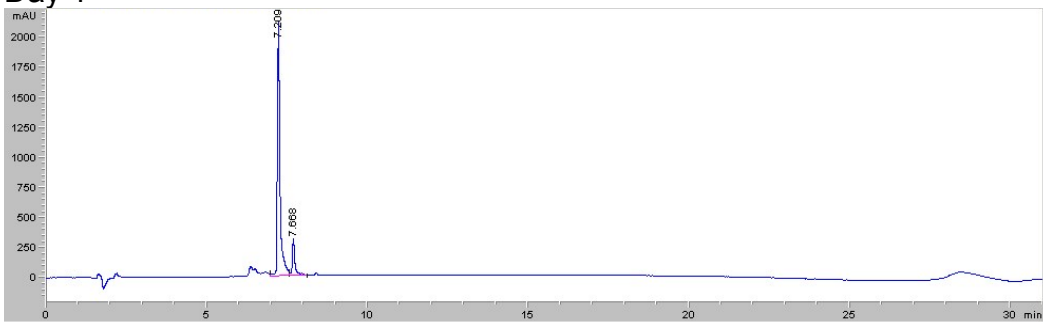
7. UV-HPLC analysis for the stability of 1 and 9 over 1 week

*Sample of schizokinen **1**, pH= 7.4, room temperature*

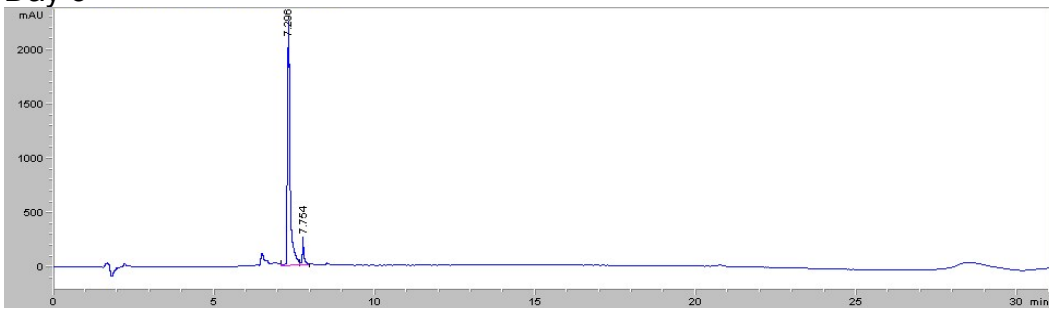
Day 0



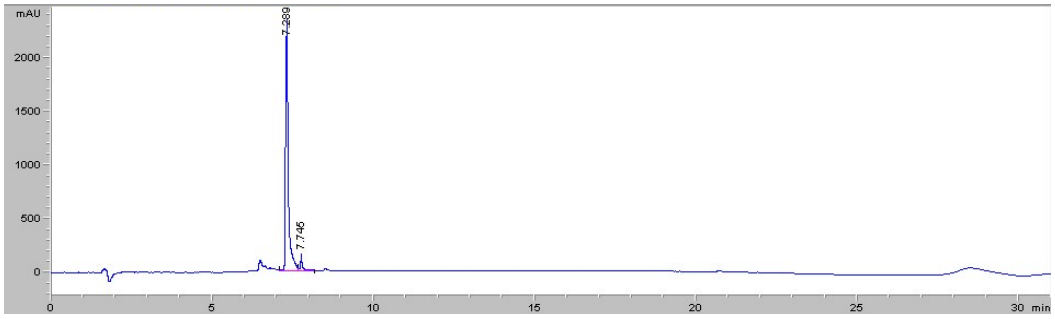
Day 1



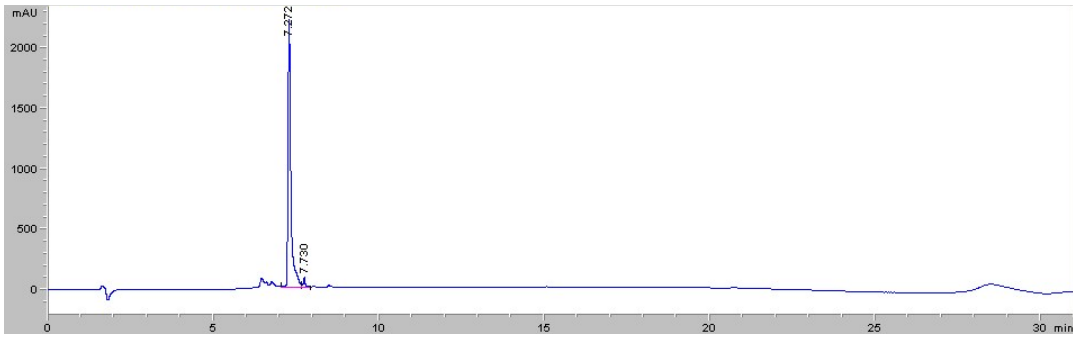
Day 3



Day 5

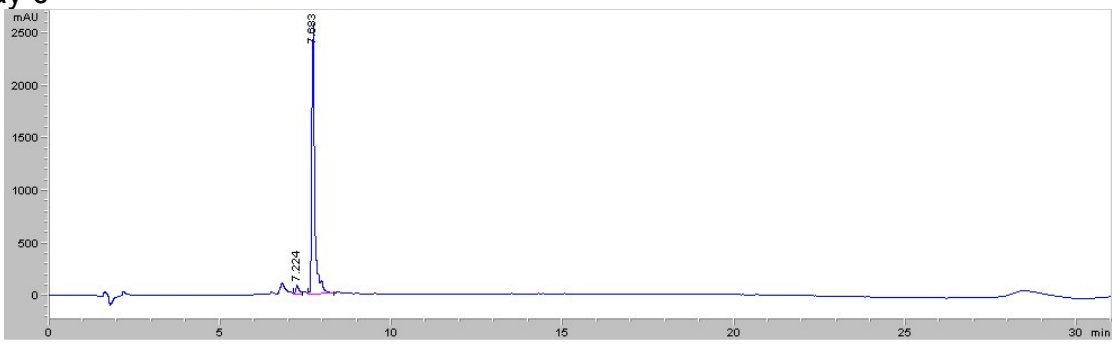


Day 7

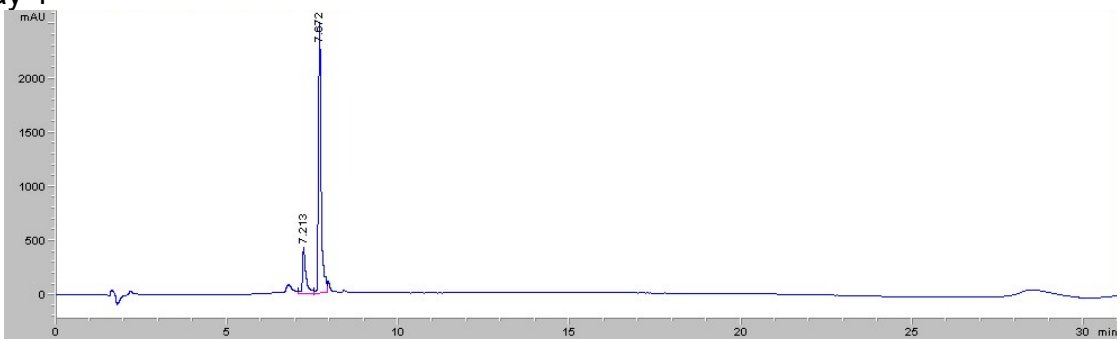


*<u>Sample of schizokinen imide **9**, pH= 7.4, room temperature</u>*

Day 0



Day 1



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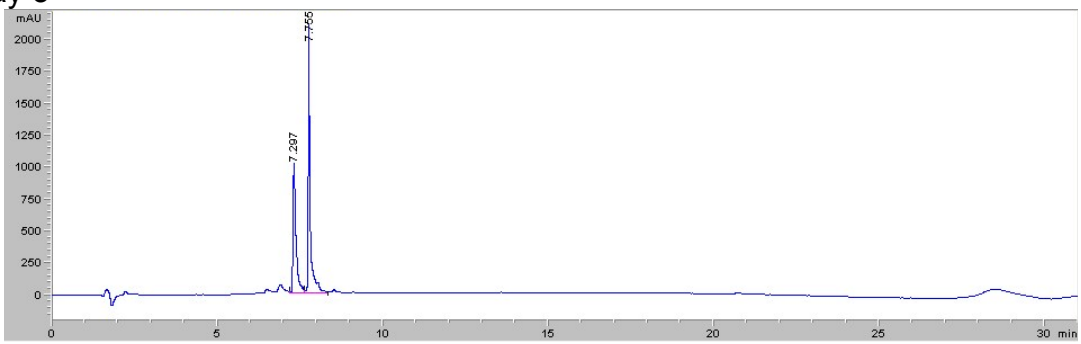

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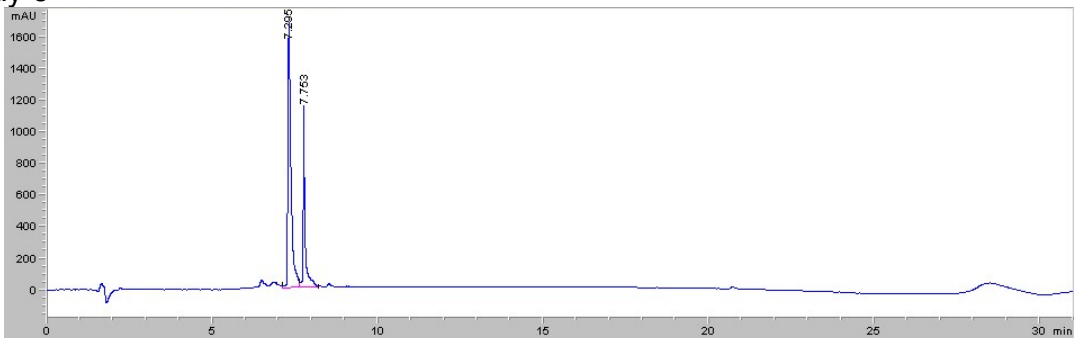
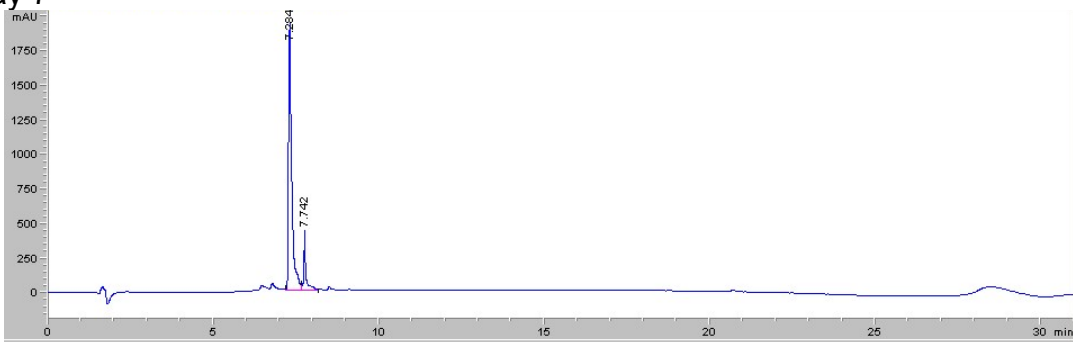
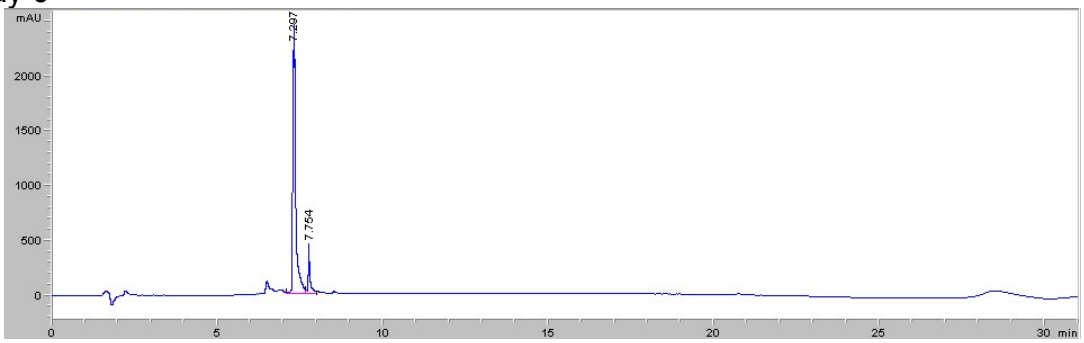


Day 7

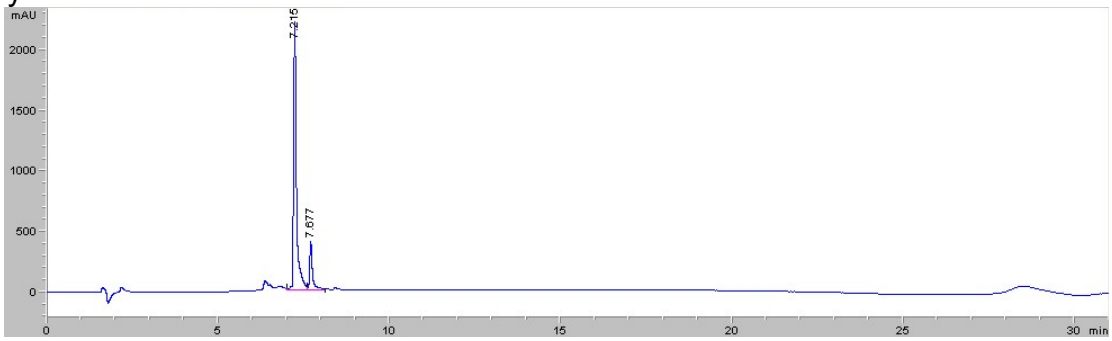


*<u>Sample of schizokinen **1**, pH= 7.4, -20 °C</u>*

Day 0



Day 1



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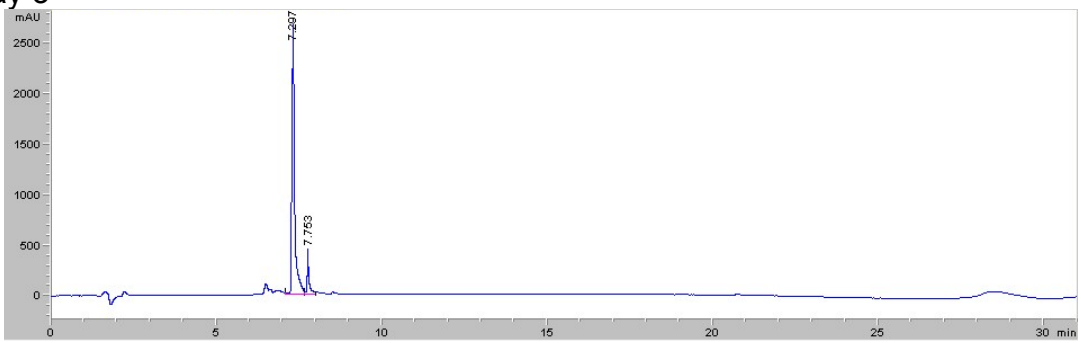

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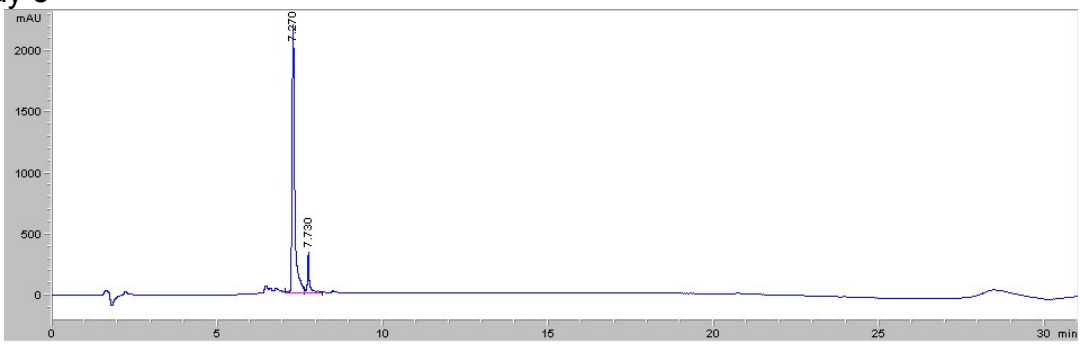
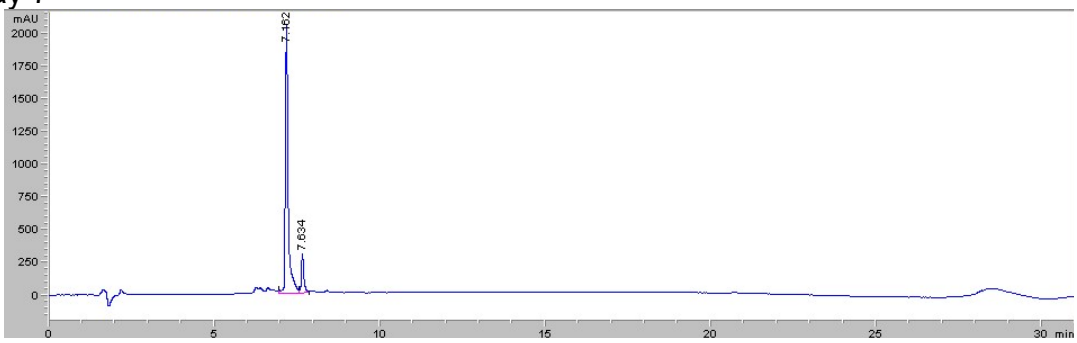
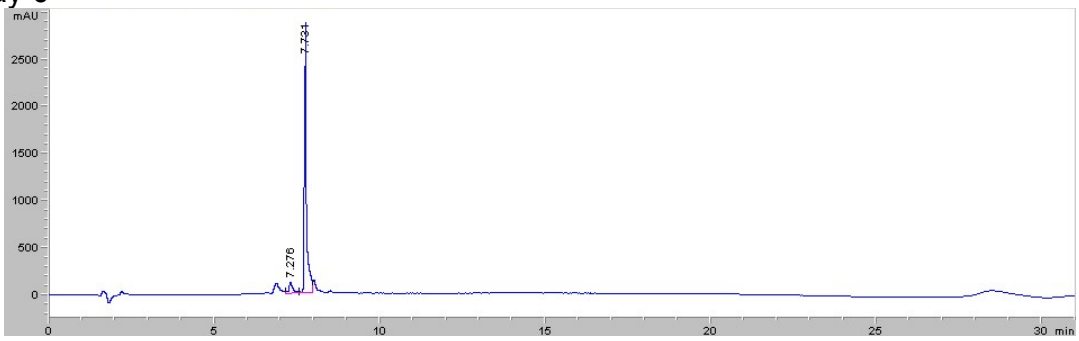


Day 7

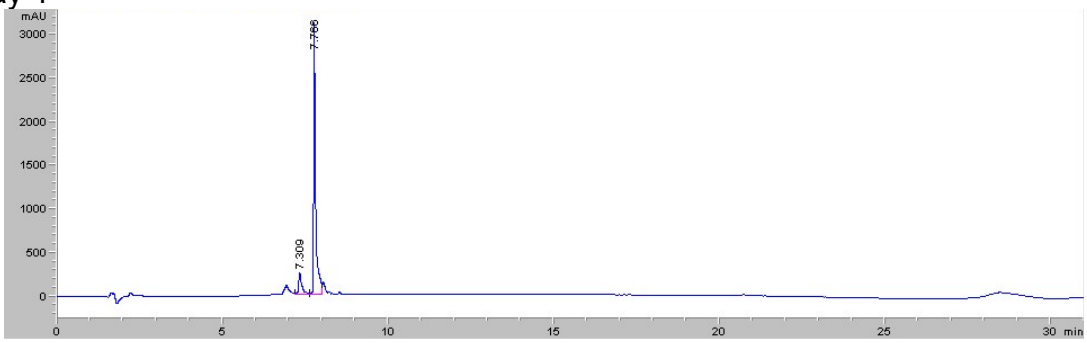


*<u>Sample of schizokinen imide **9**, pH= 7.4, -20 °C</u>*

Day 0



Day 1



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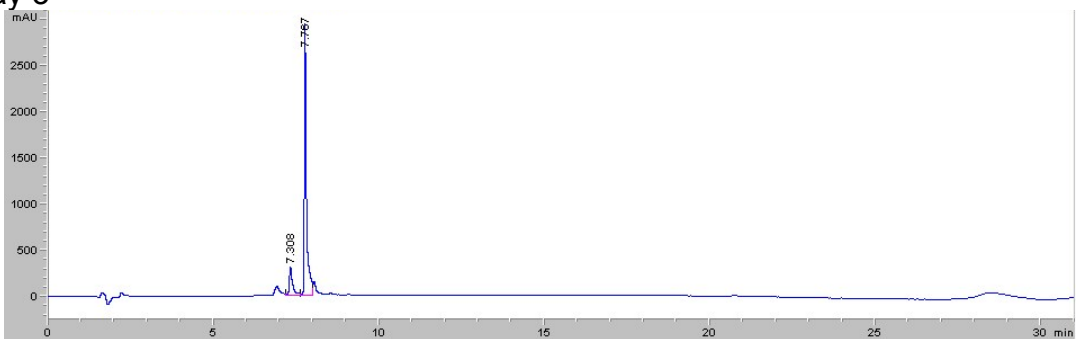
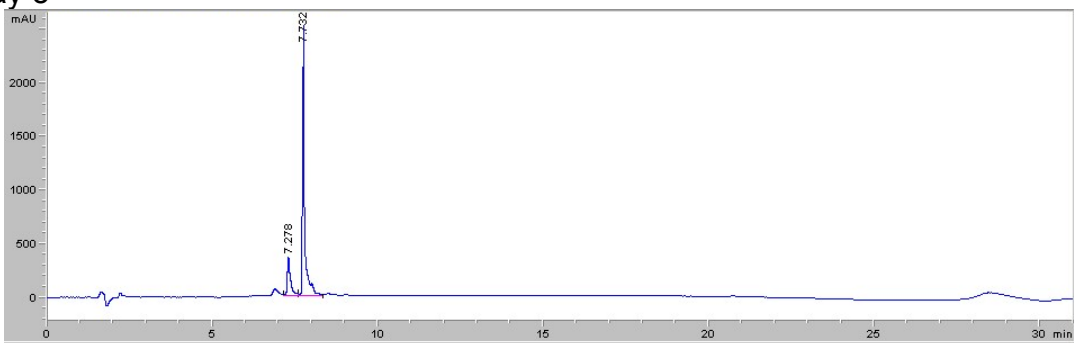
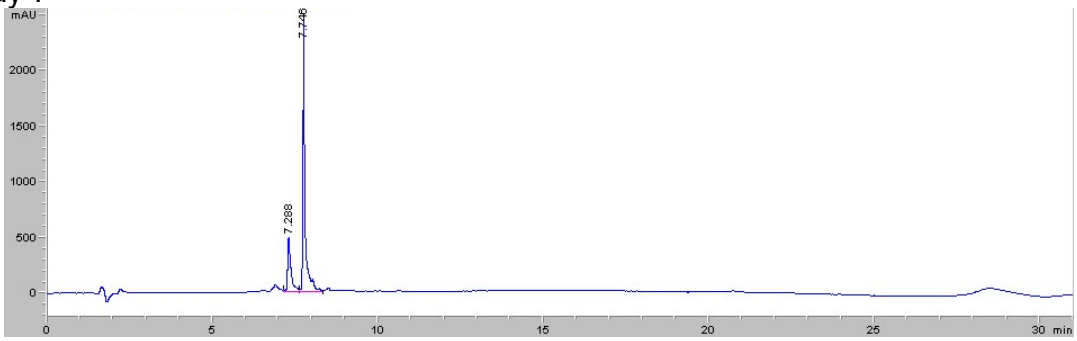


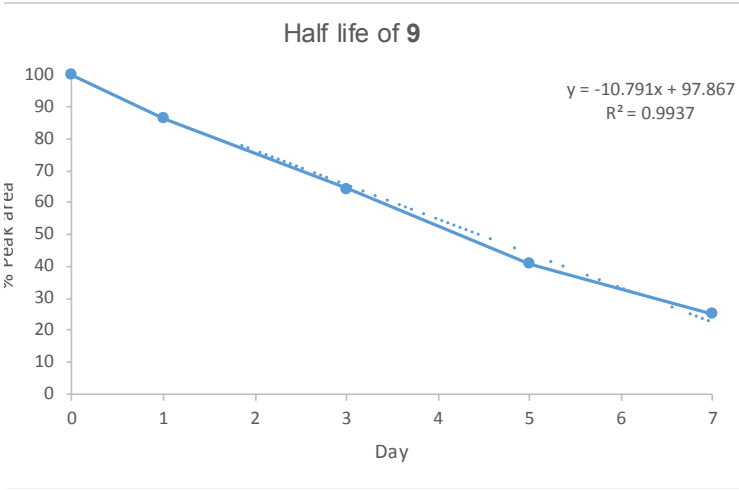
Day 5



Day 7



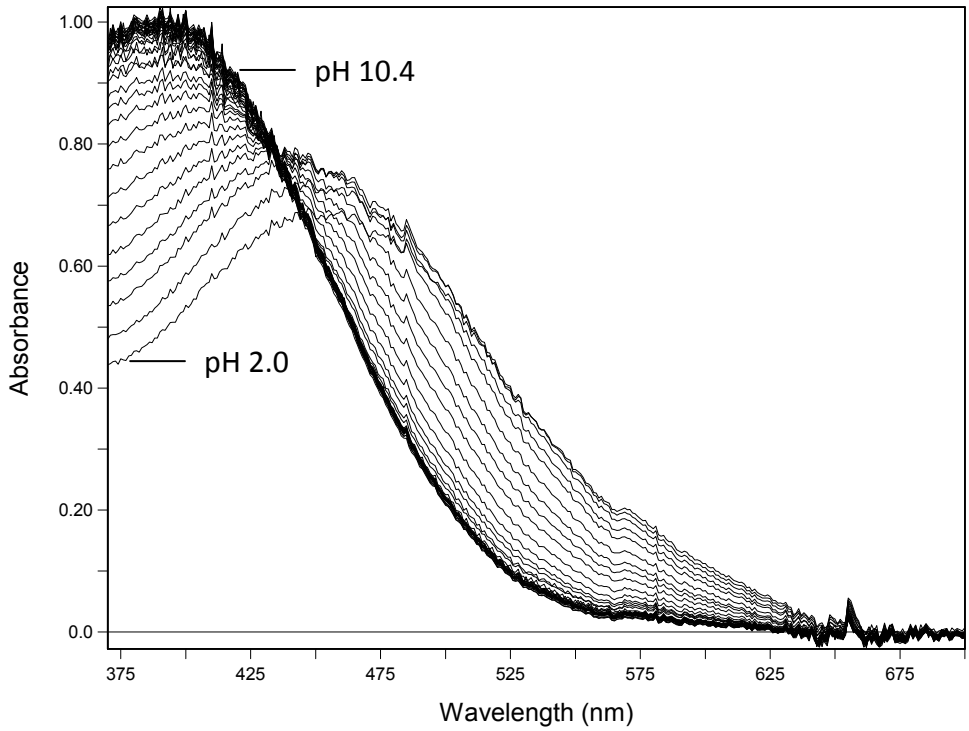
8. Half-life ($t_{1/2}$) calculation for cyclic imide derivative 9



Day	Peak area	% unit
0	15680	100
1	13557	86.46045918
3	10073	64.24107143
5	6397	40.79719388
7	3948	25.17857143
	day	hour
Half life of cyclic imide	4.435826	106.4598276

9. Spectrophotometric titration of 1 and 9

Schizokinen (**1**) iron complex spectra



Schizokinen Imide (**9**) iron complex spectra

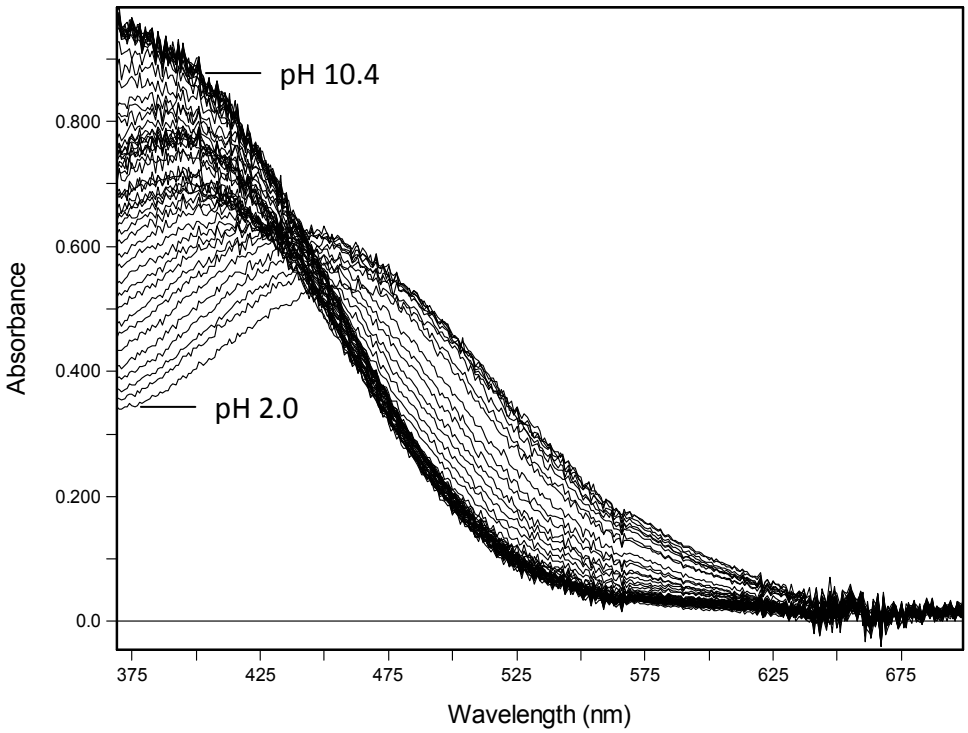


Table S1. Concentration of samples for the Job's plots

	Molar L	Molar Fe	C_L	$C_{Fe\text{-}NTA}$
1	1	9	0.2mM	1.8mM
2	2	8	0.4mM	1.6mM
3	3	7	0.6mM	1.4mM
4	4	6	0.8mM	1.2mM
5	5	5	1.0mM	1.0mM
6	6	4	1.2mM	0.8mM
7	7	3	1.4mM	0.6mM
8	8	2	1.6mM	0.4mM
9	9	1	1.8mM	0.2mM

L: ligand; C_L: concentration of ligand; $C_{Fe\text{-}NTA}$: concentration of Fe-NTA