

Remote Electronic Effect on the N-Heterocyclic Carbene-catalyzed Asymmetric Intramolecular Stetter Reaction and Structural Revision of Products

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yamak@tokushima-u.ac.jp

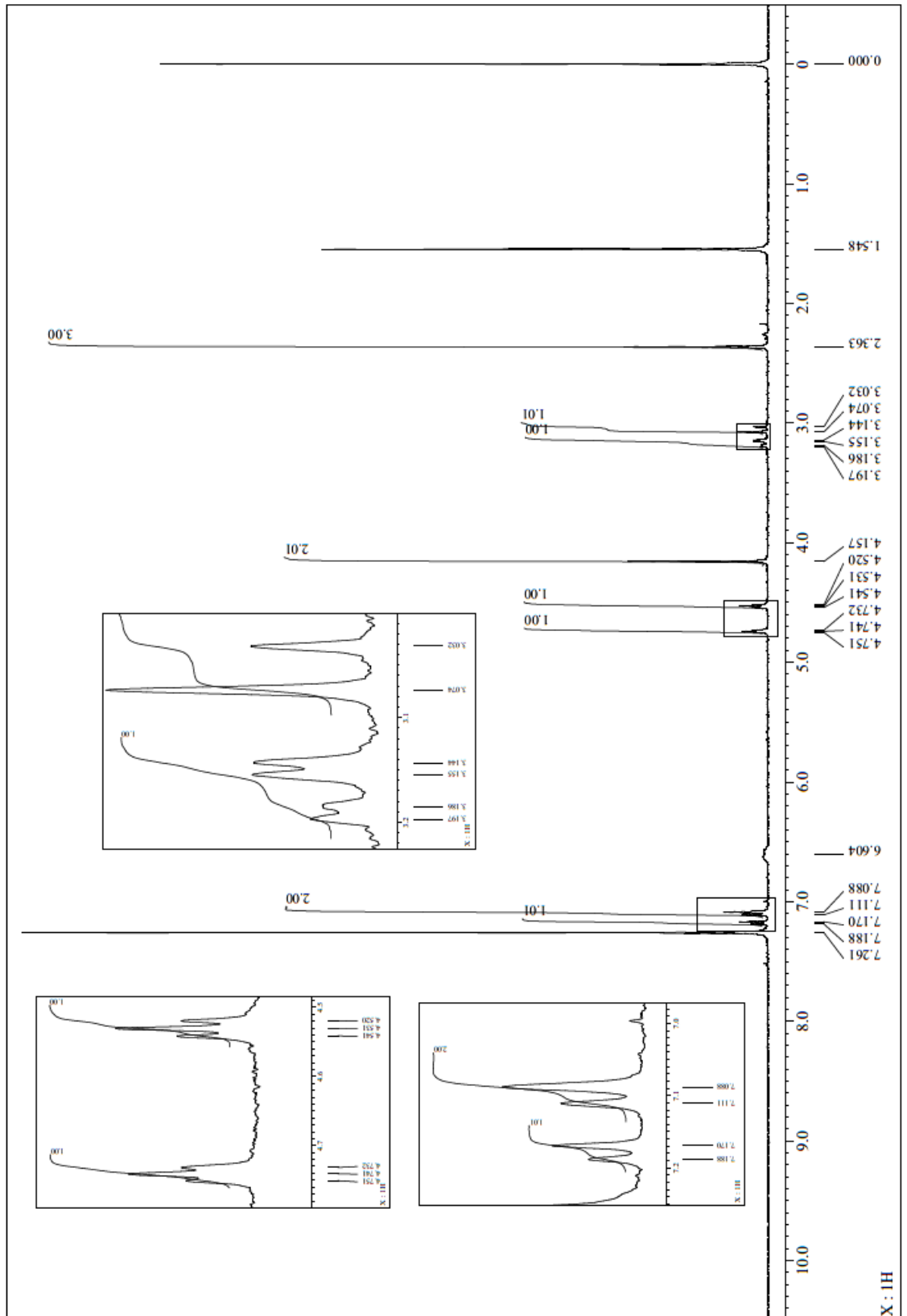
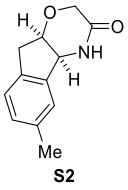
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Supporting Information II

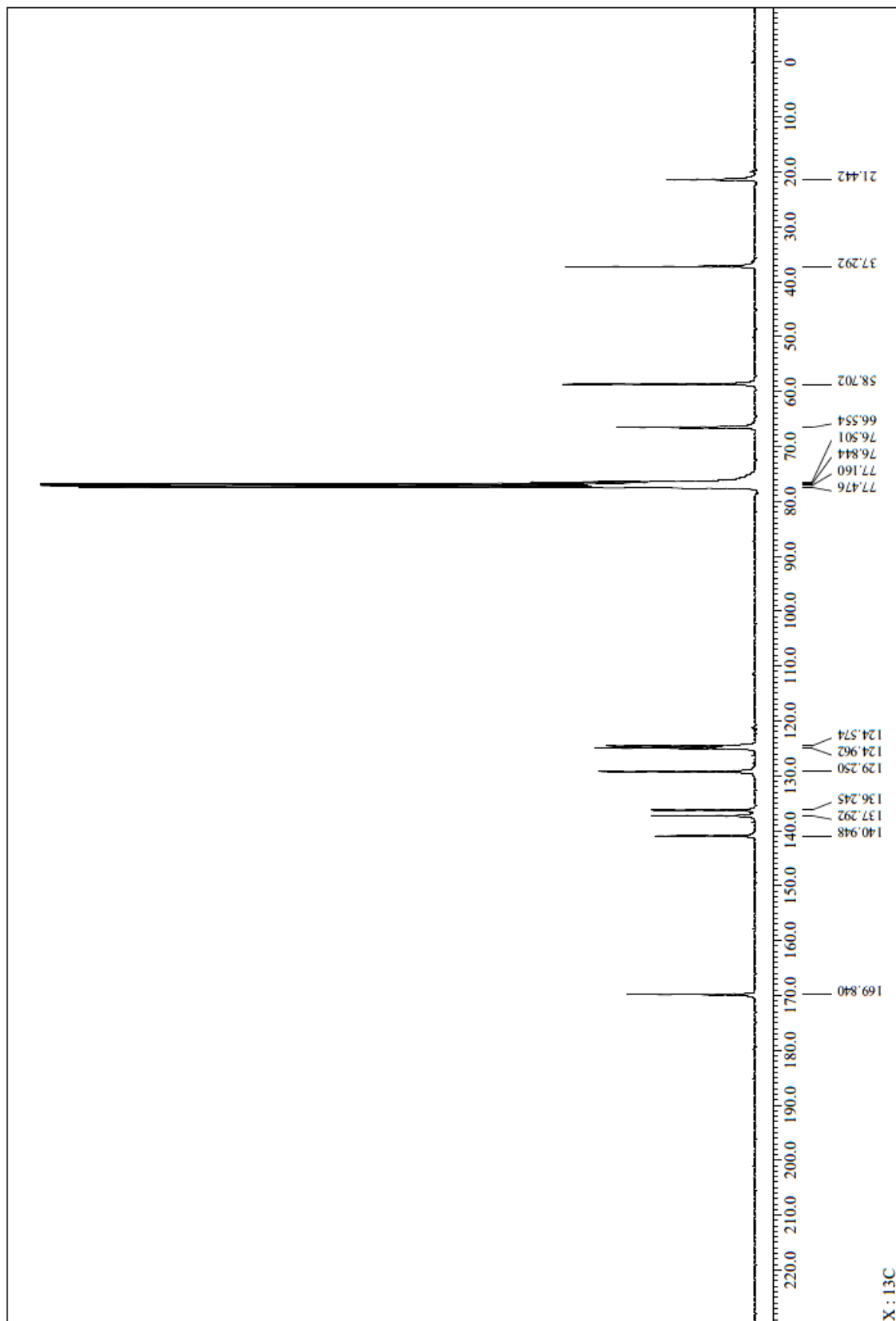
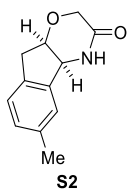
1. Copies of ^1H and ^{13}C NMR spectra

^1H NMR of S2



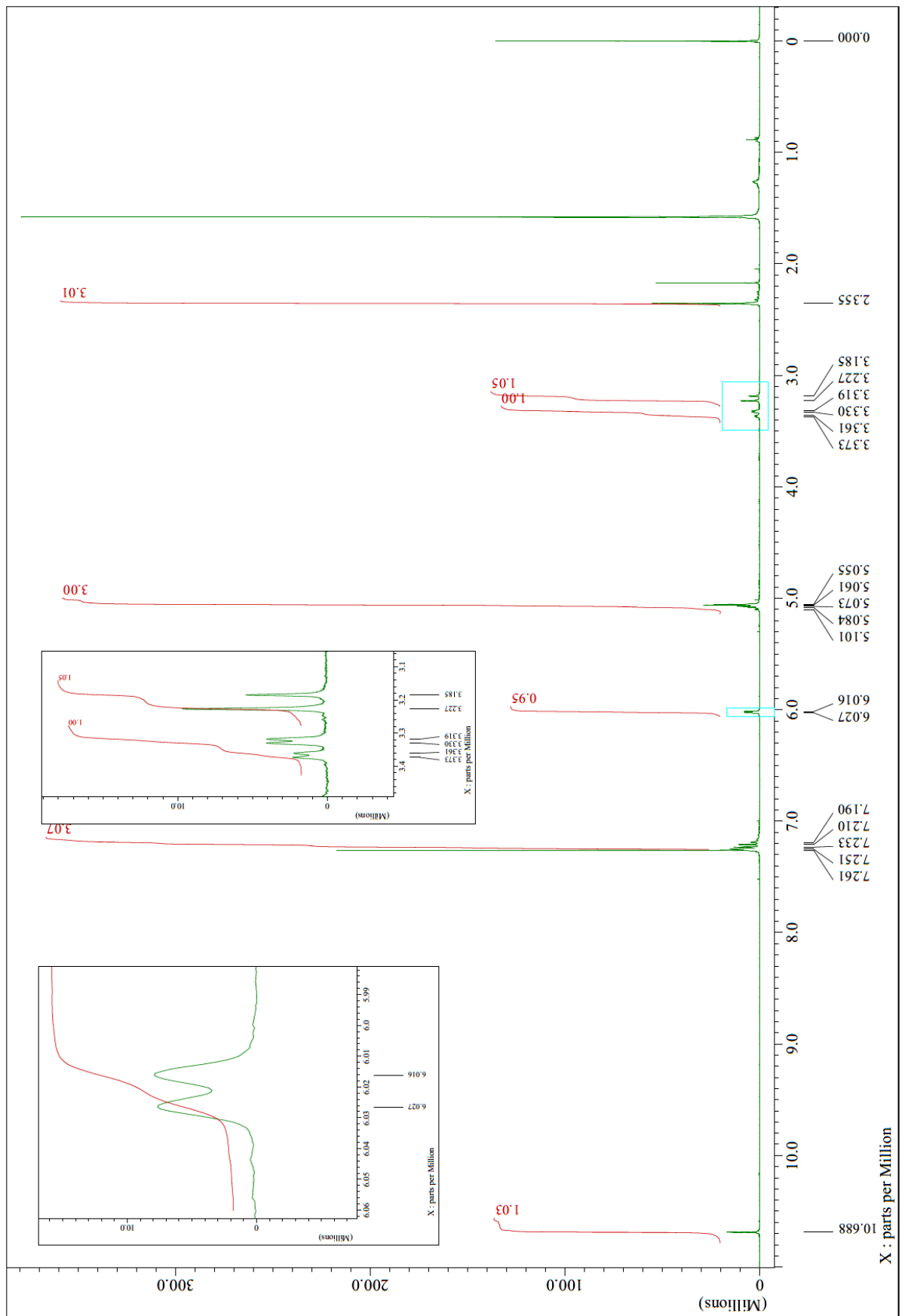
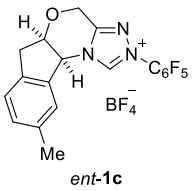
Supporting Information II

^{13}C NMR of S2



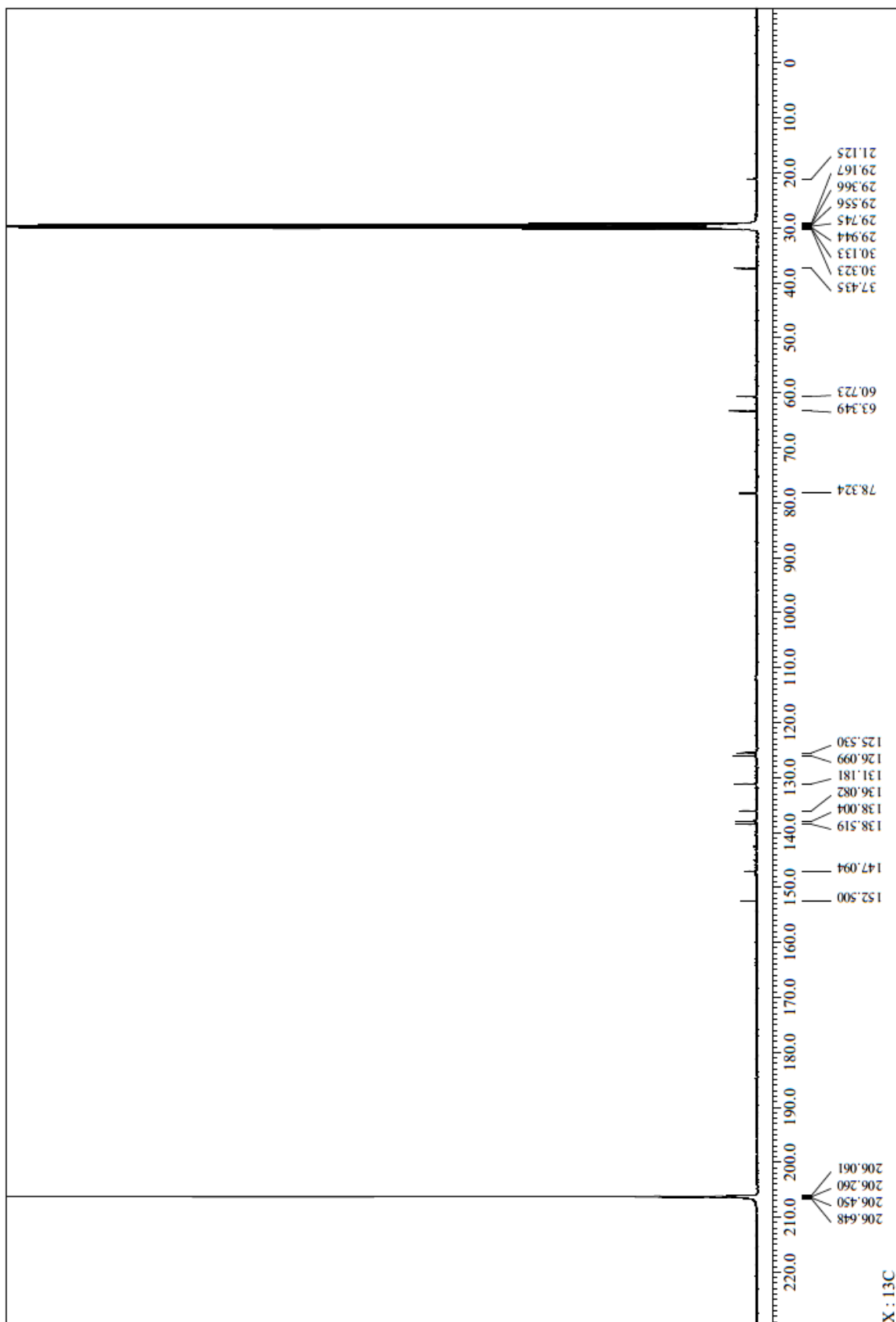
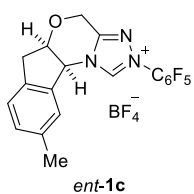
Supporting Information II

¹H NMR of *ent-1c*



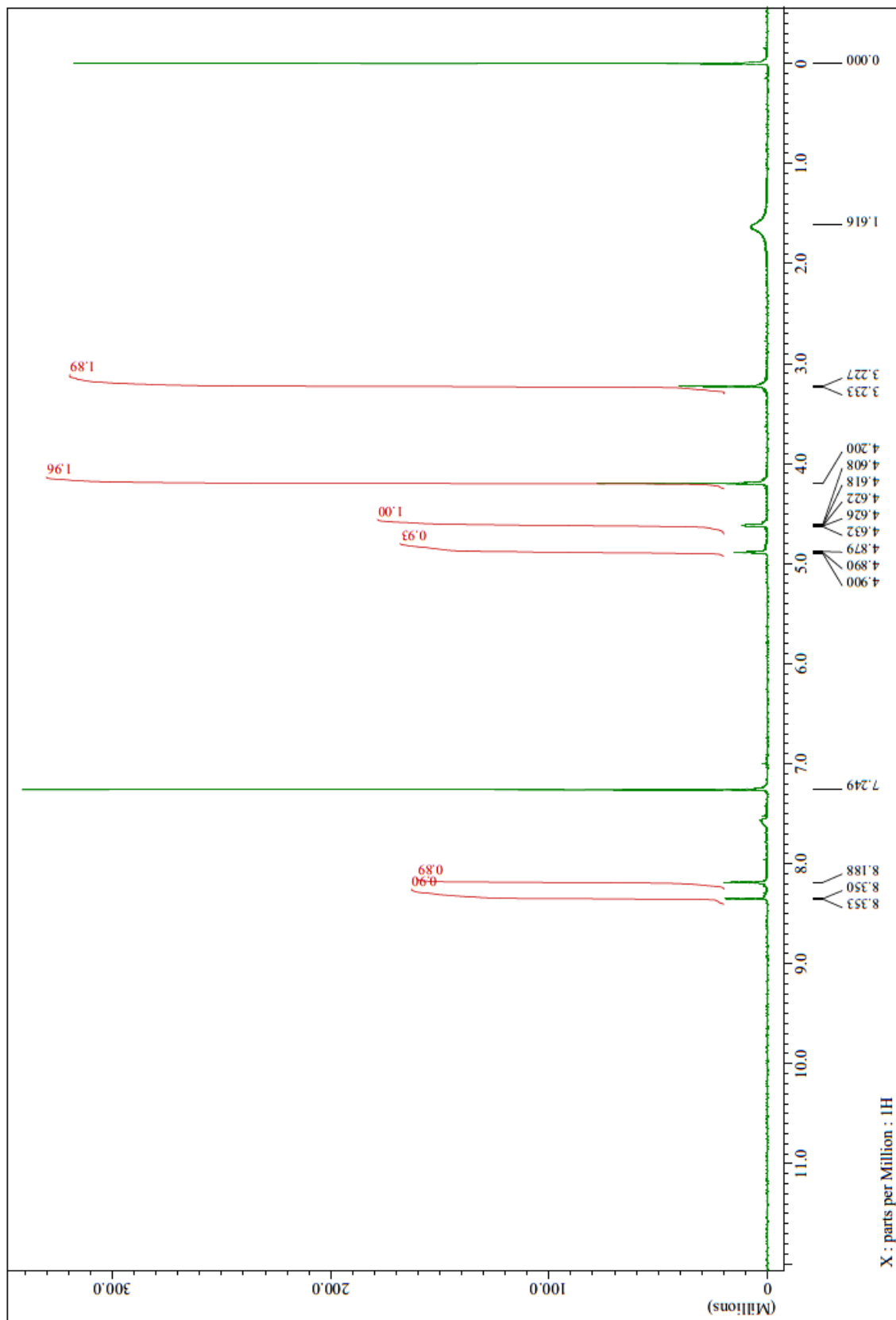
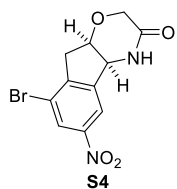
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^{13}C NMR of *ent-1c*



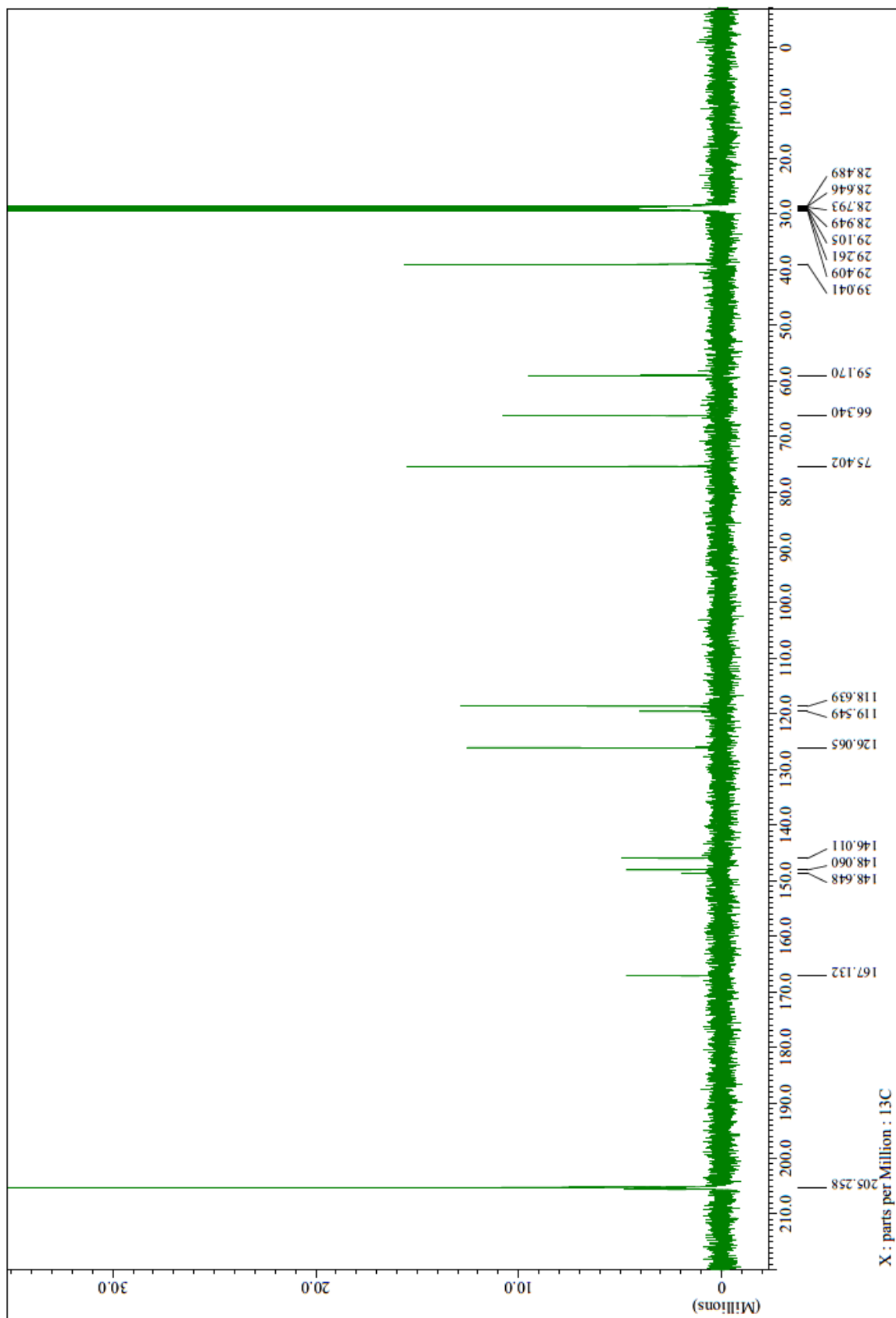
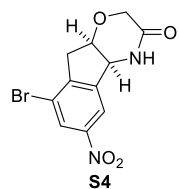
Supporting Information II

¹H NMR of S4



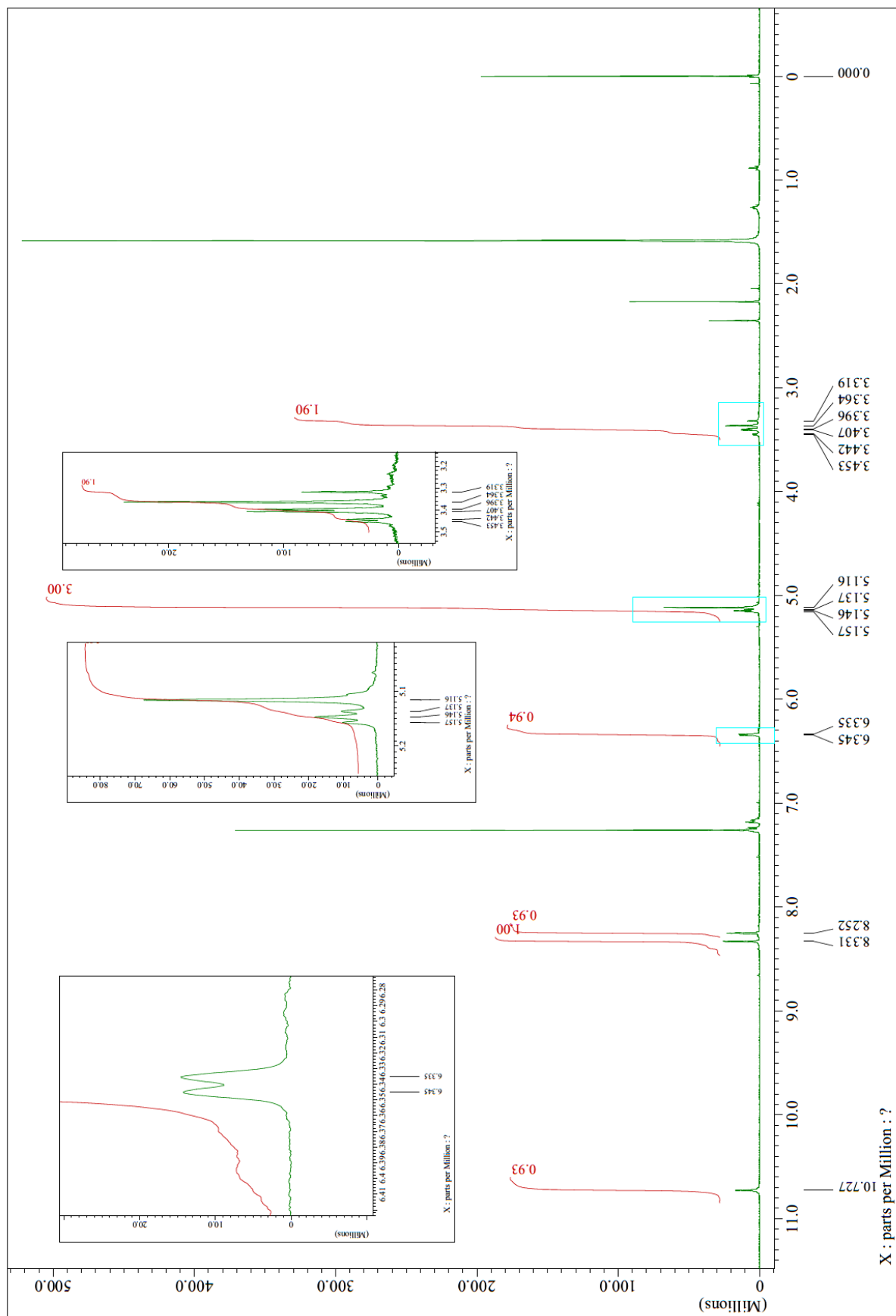
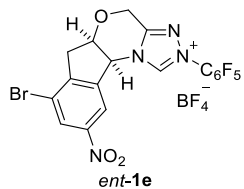
Supporting Information II

^{13}C NMR of S4



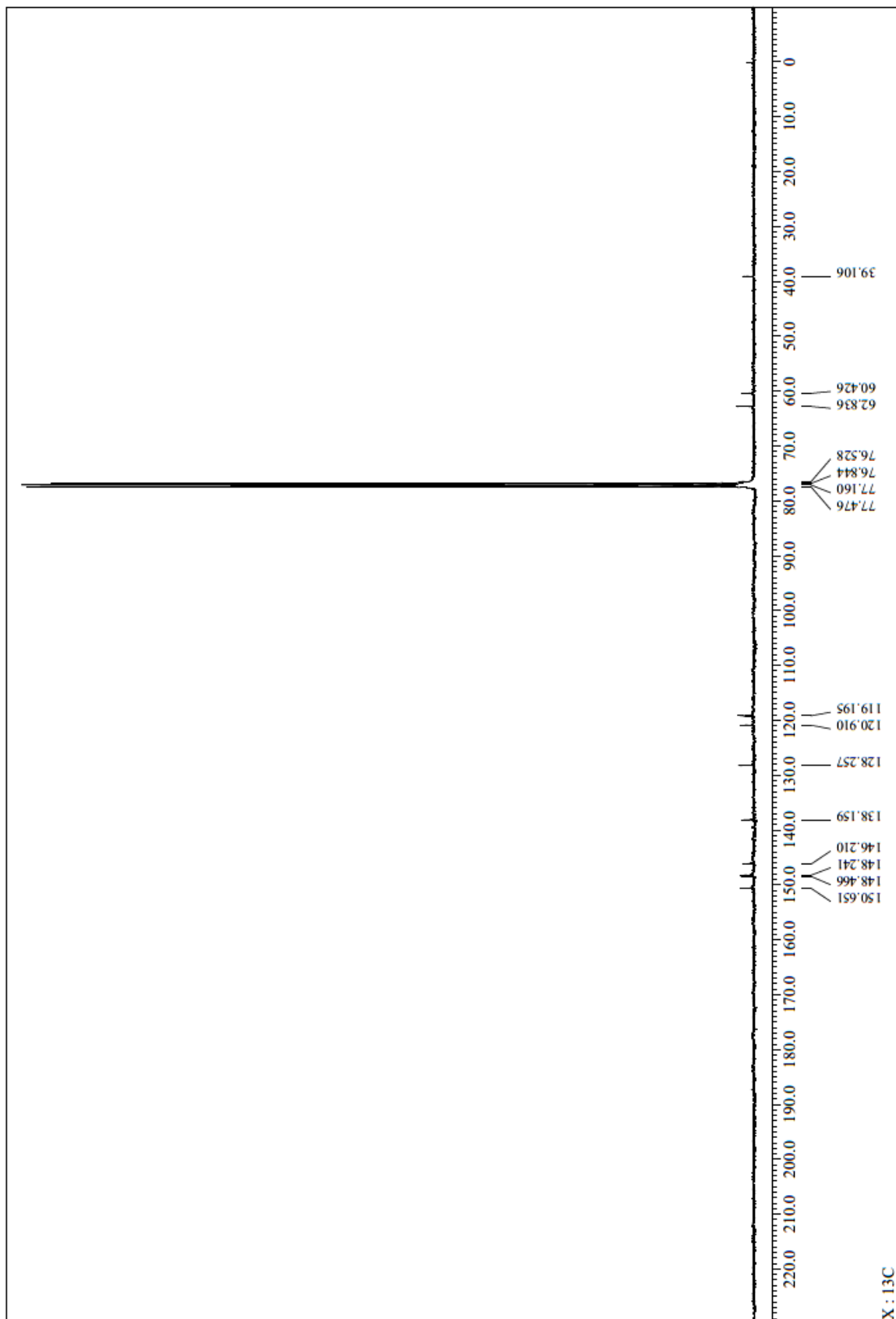
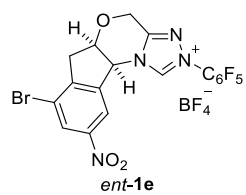
Supporting Information II

¹H NMR of *ent-1e*



Supporting Information II

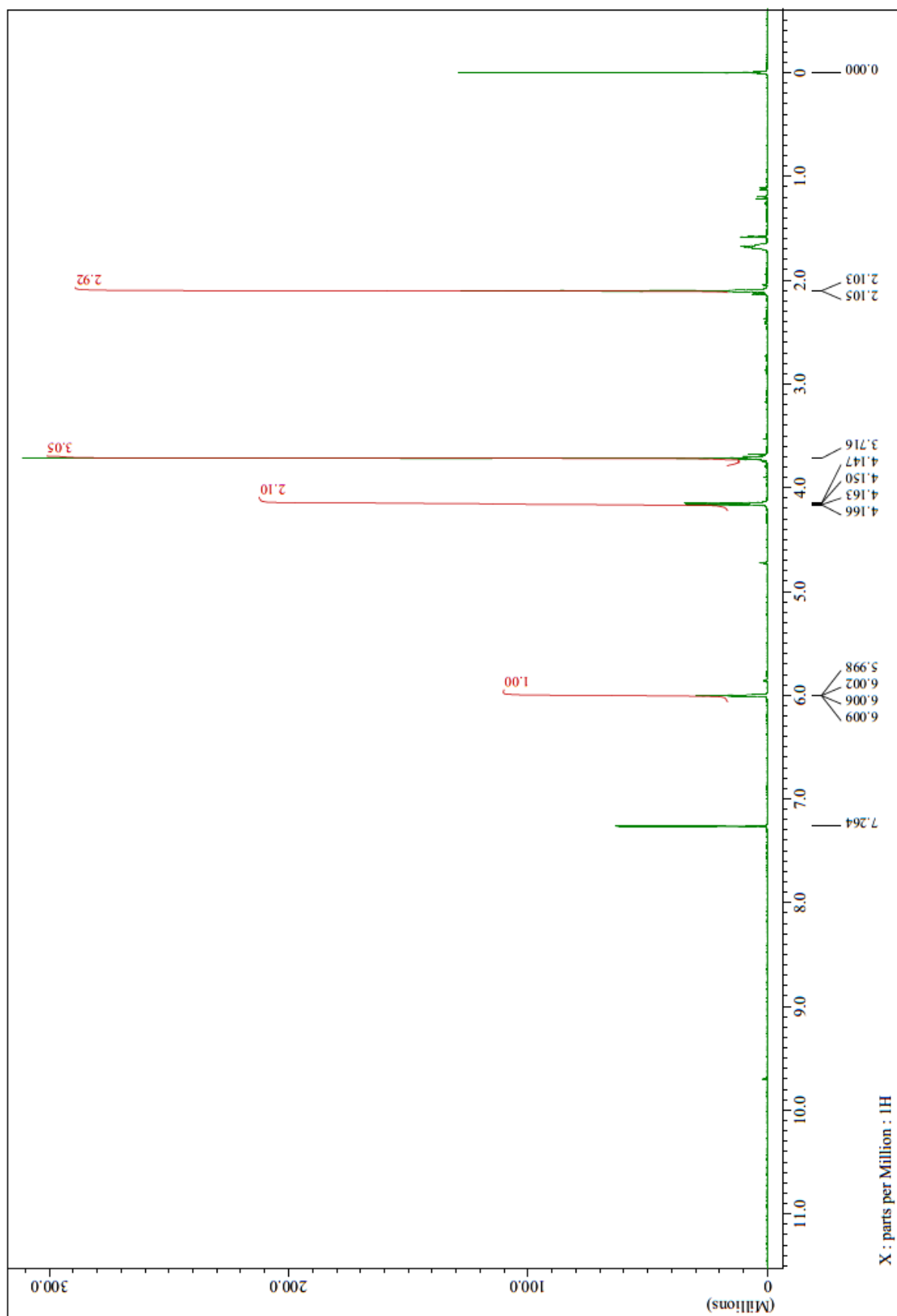
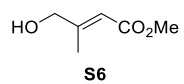
^{13}C NMR of *ent-1e*



X: 13C

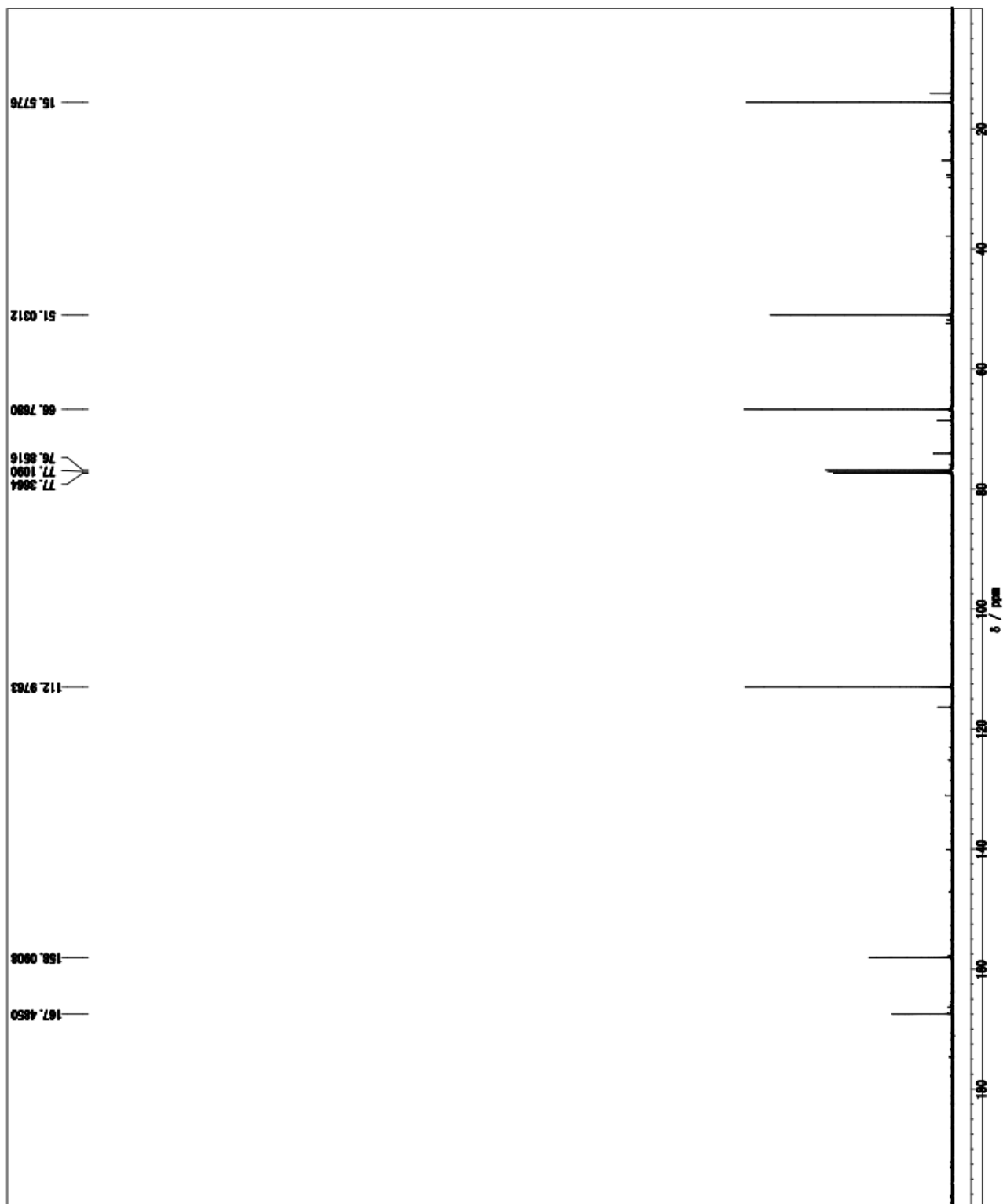
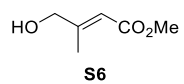
Supporting Information II

^1H NMR of S6



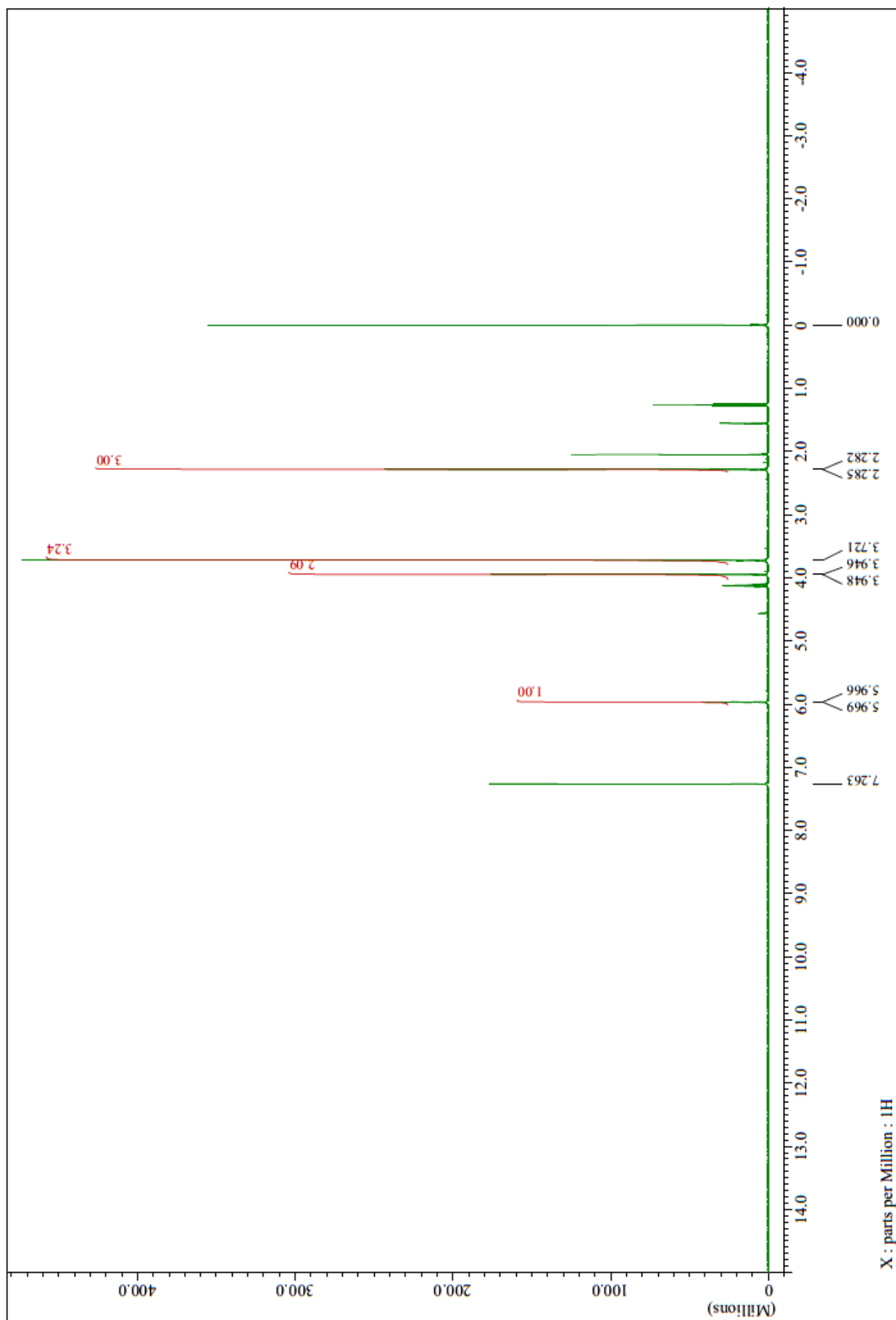
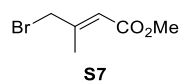
Supporting Information II

^{13}C NMR of S6



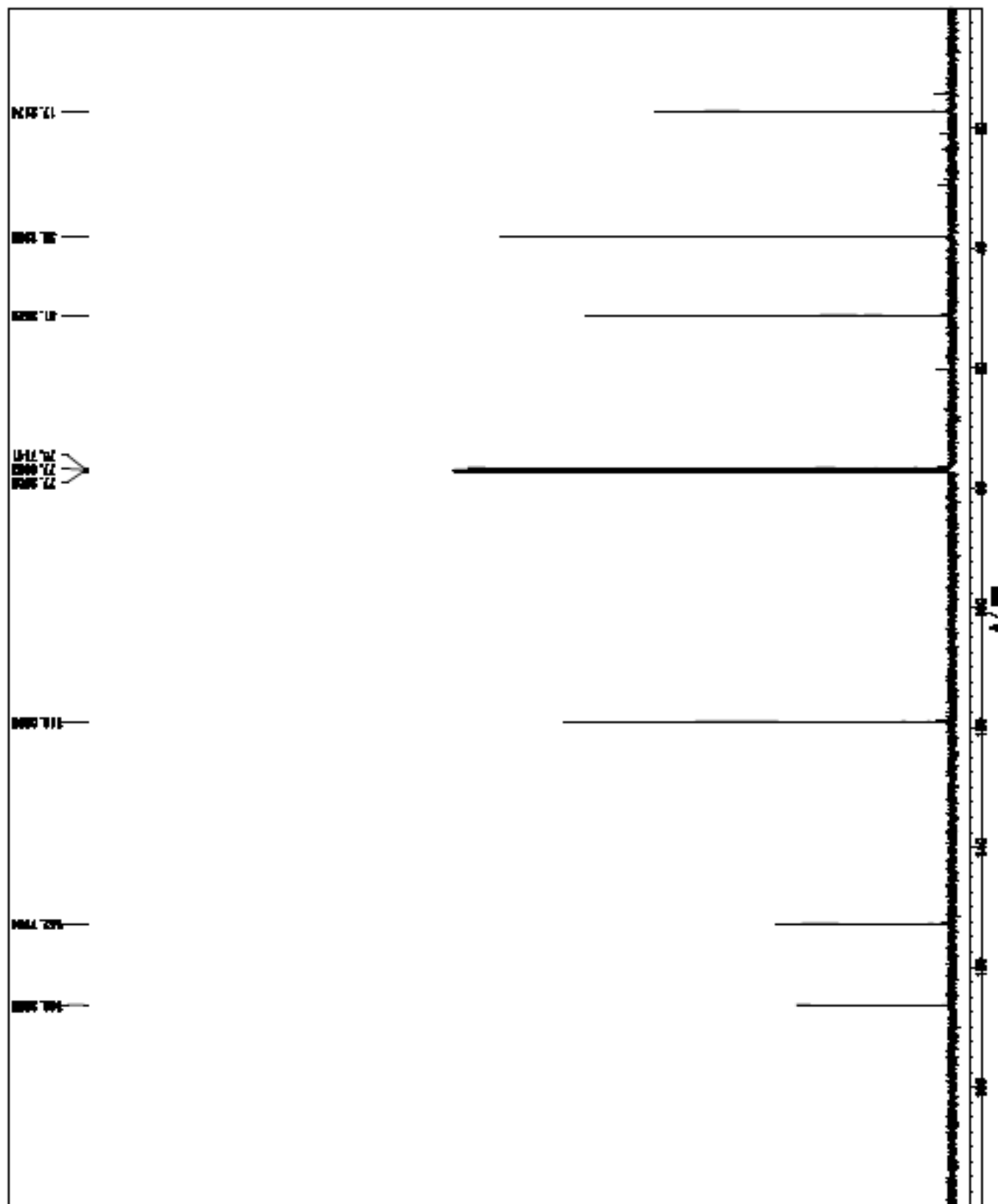
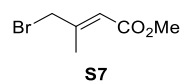
Supporting Information II

^1H NMR of S7



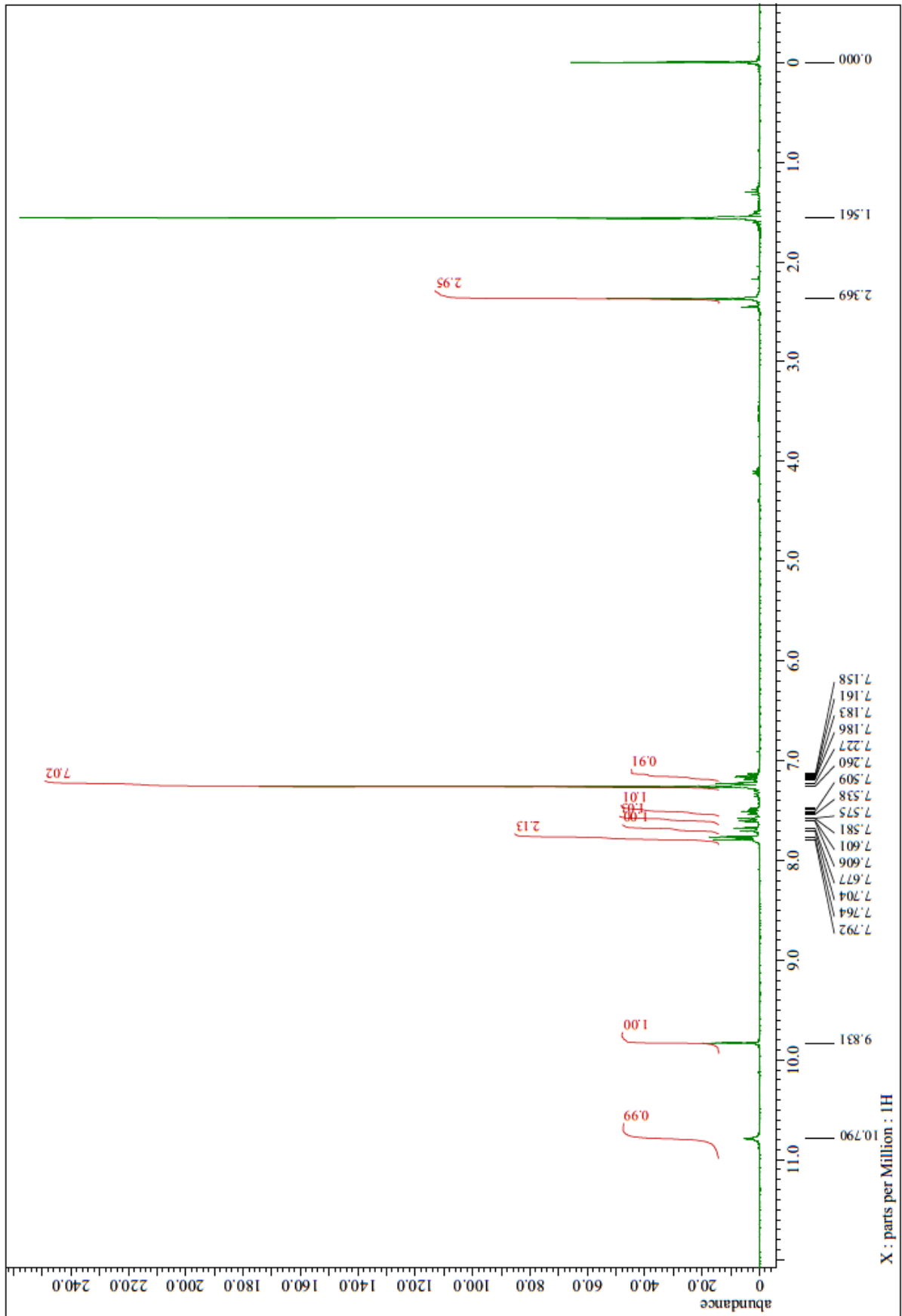
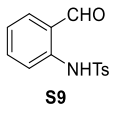
Supporting Information II

^{13}C NMR of S7



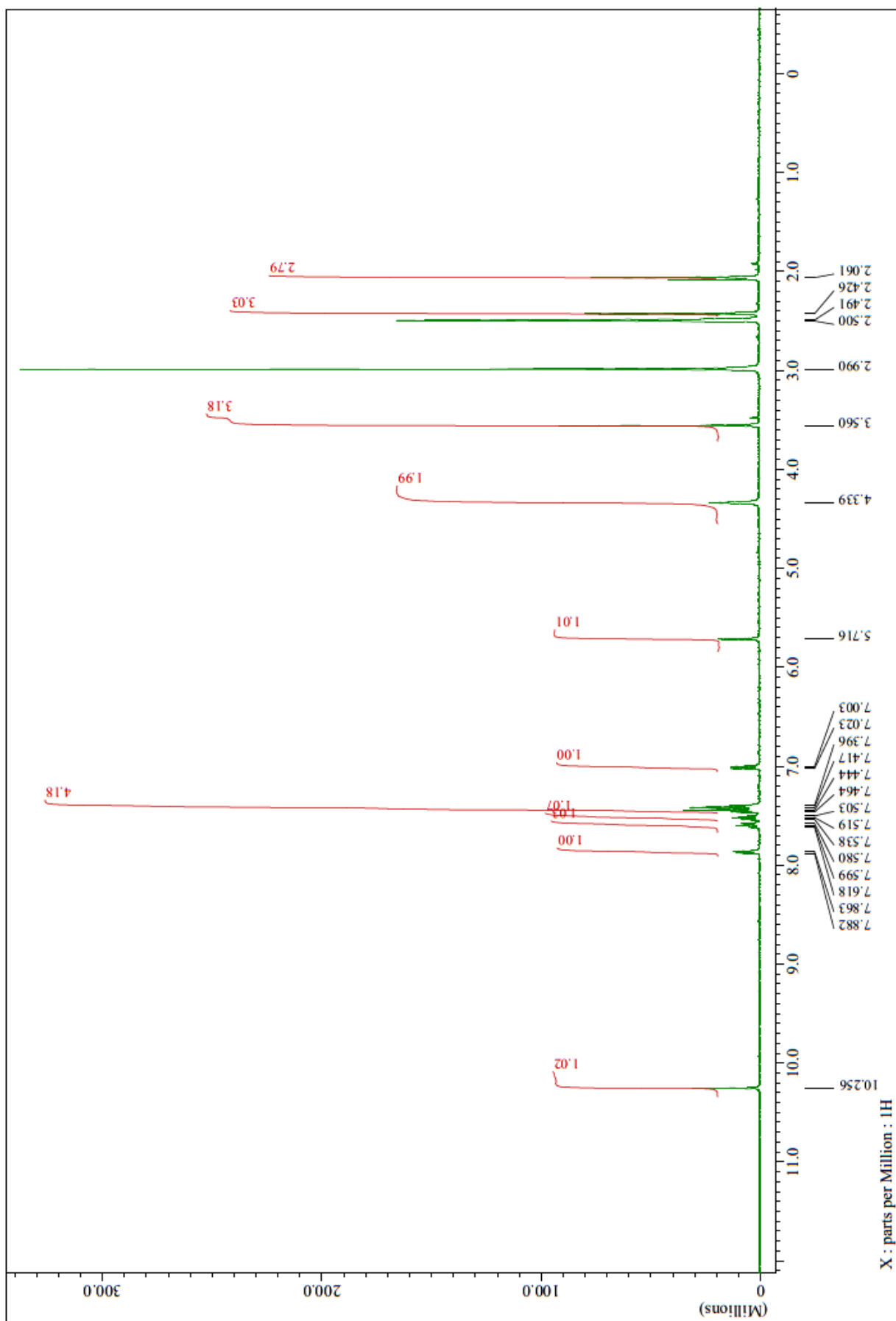
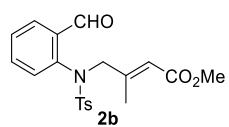
Supporting Information II

¹H NMR of S9



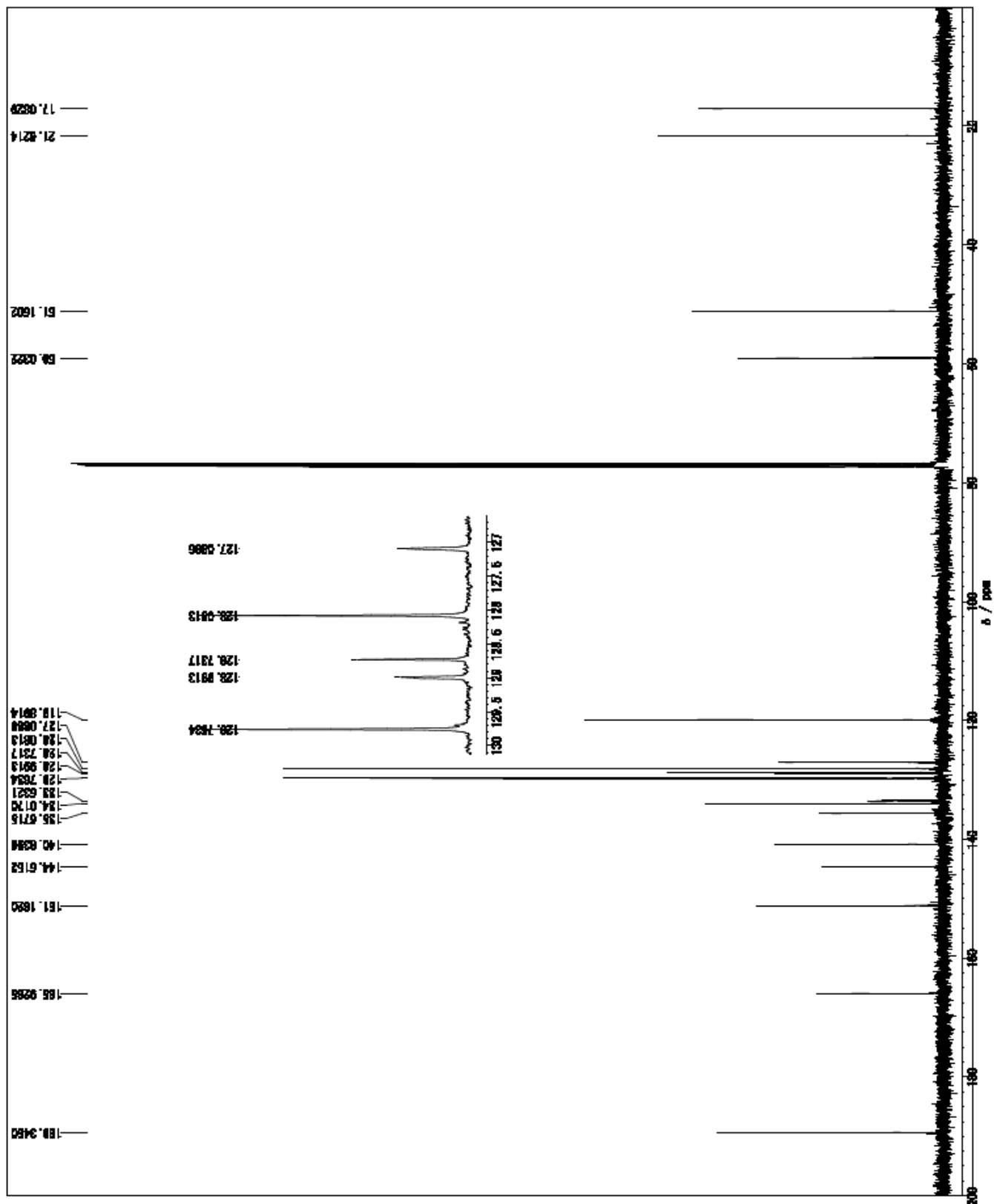
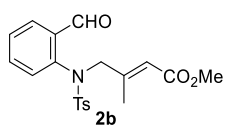
Supporting Information II

¹H NMR of 2b



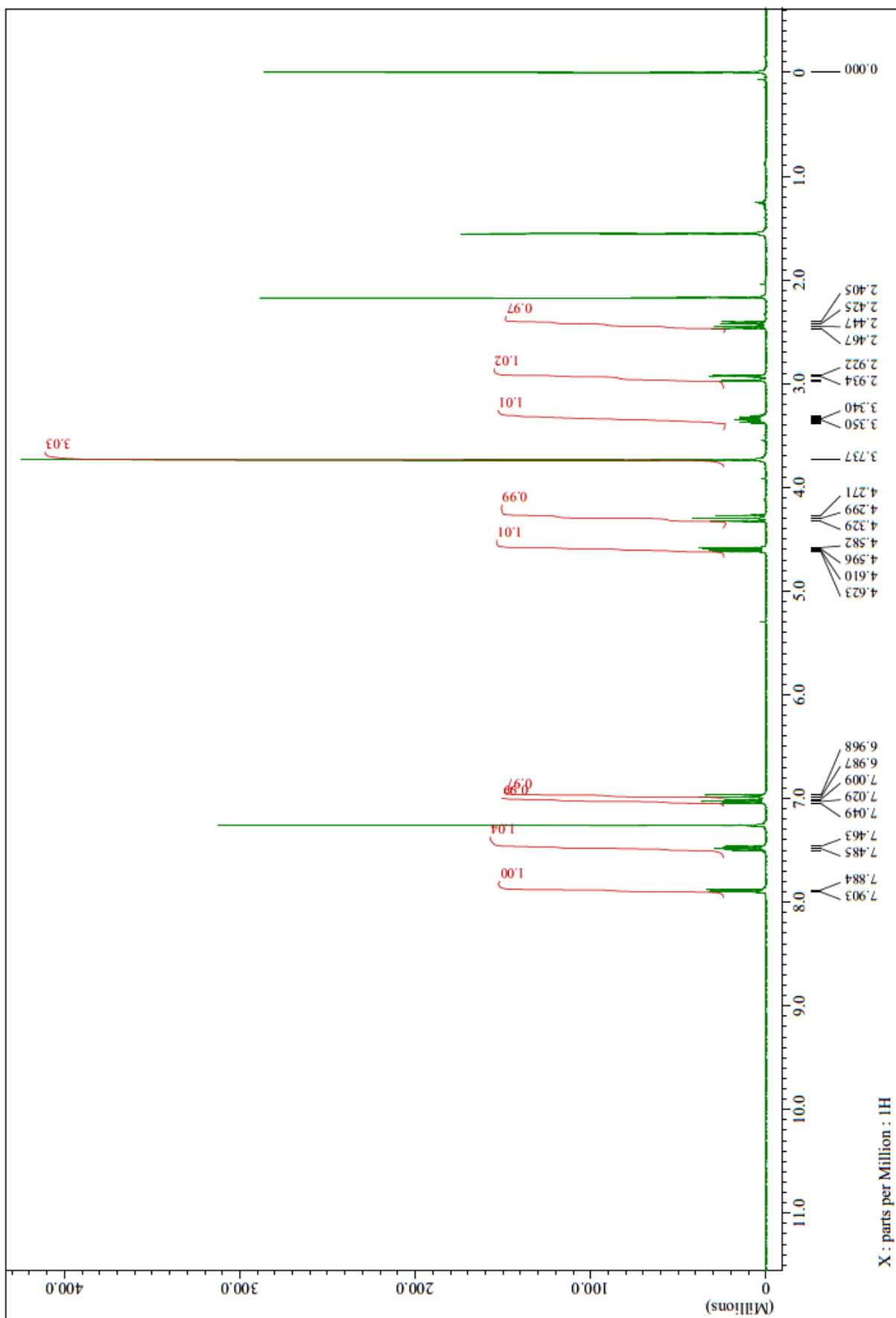
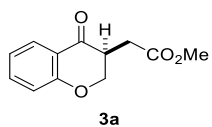
Supporting Information II

¹³C NMR of 2b



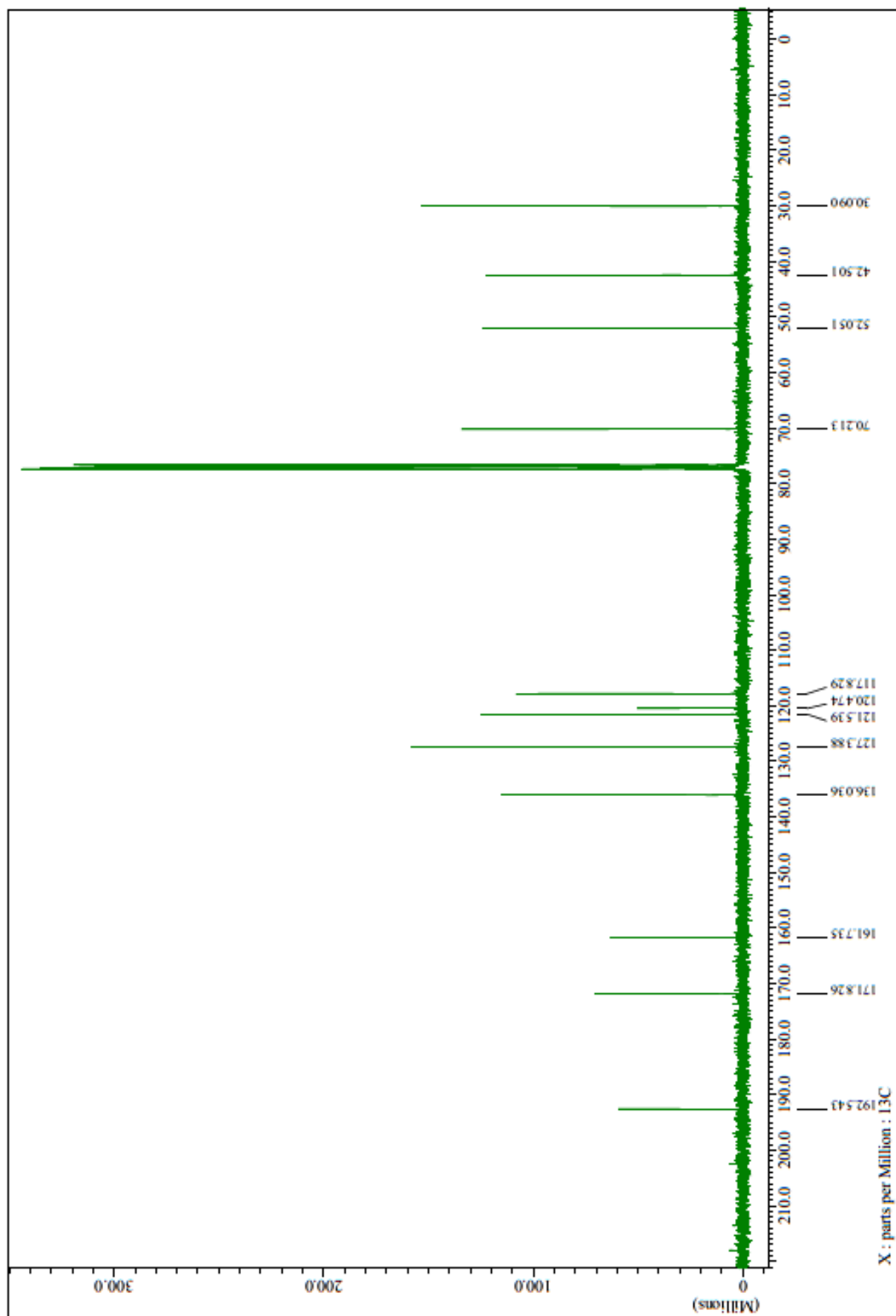
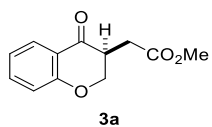
Supporting Information II

¹H NMR of 3a



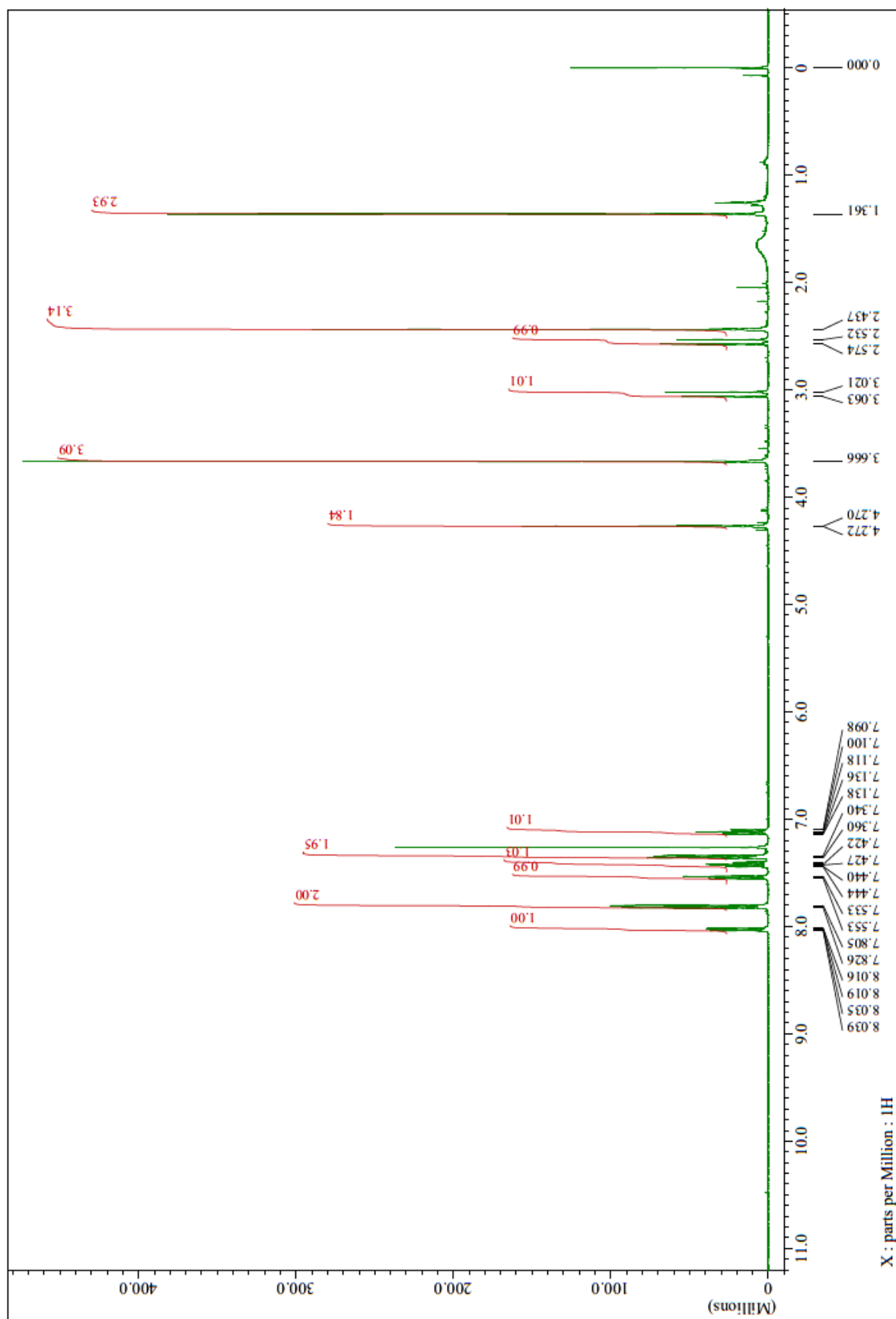
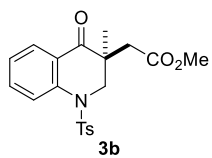
Supporting Information II

^{13}C NMR of 3a



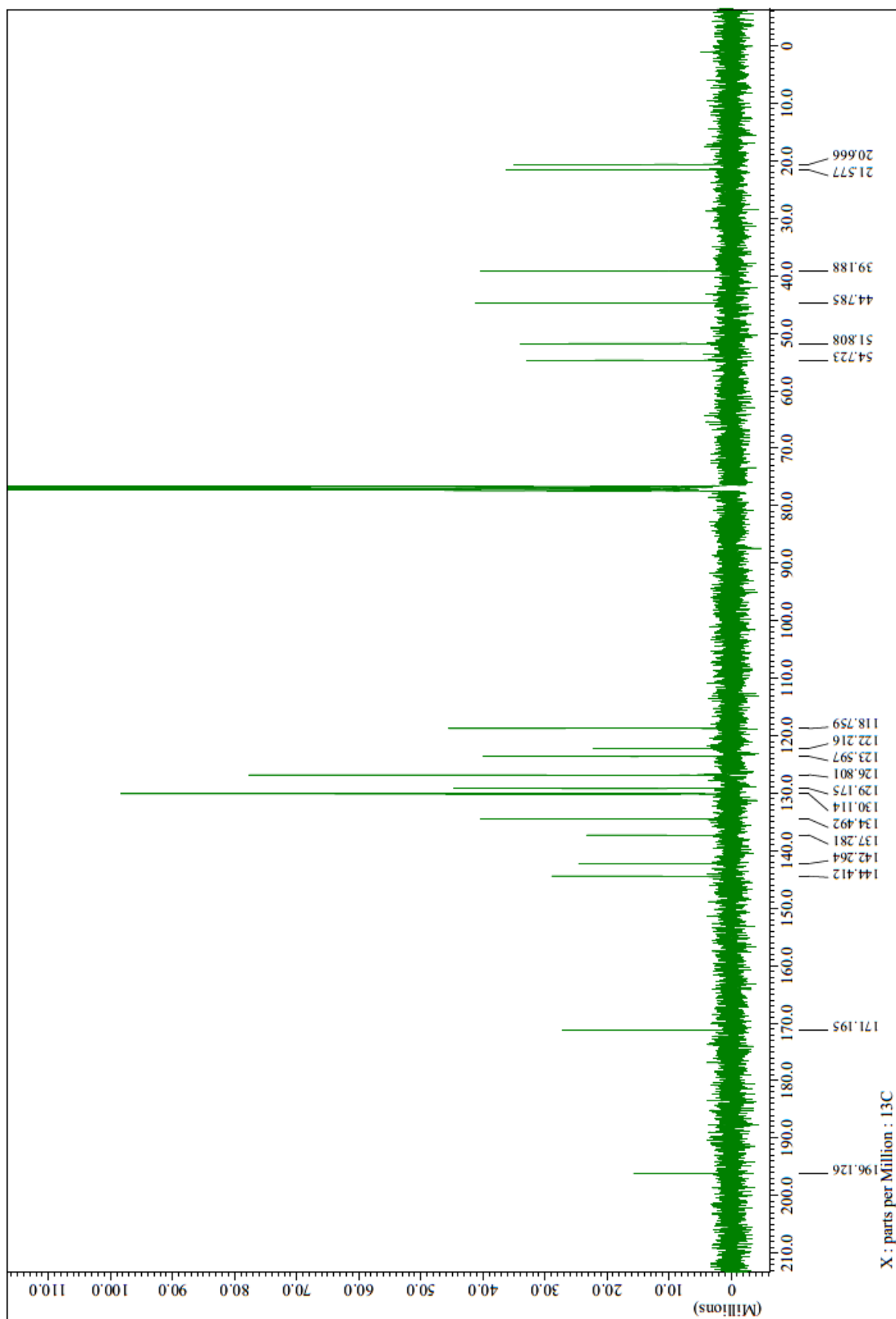
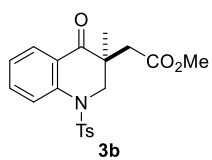
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¹H NMR of 3b



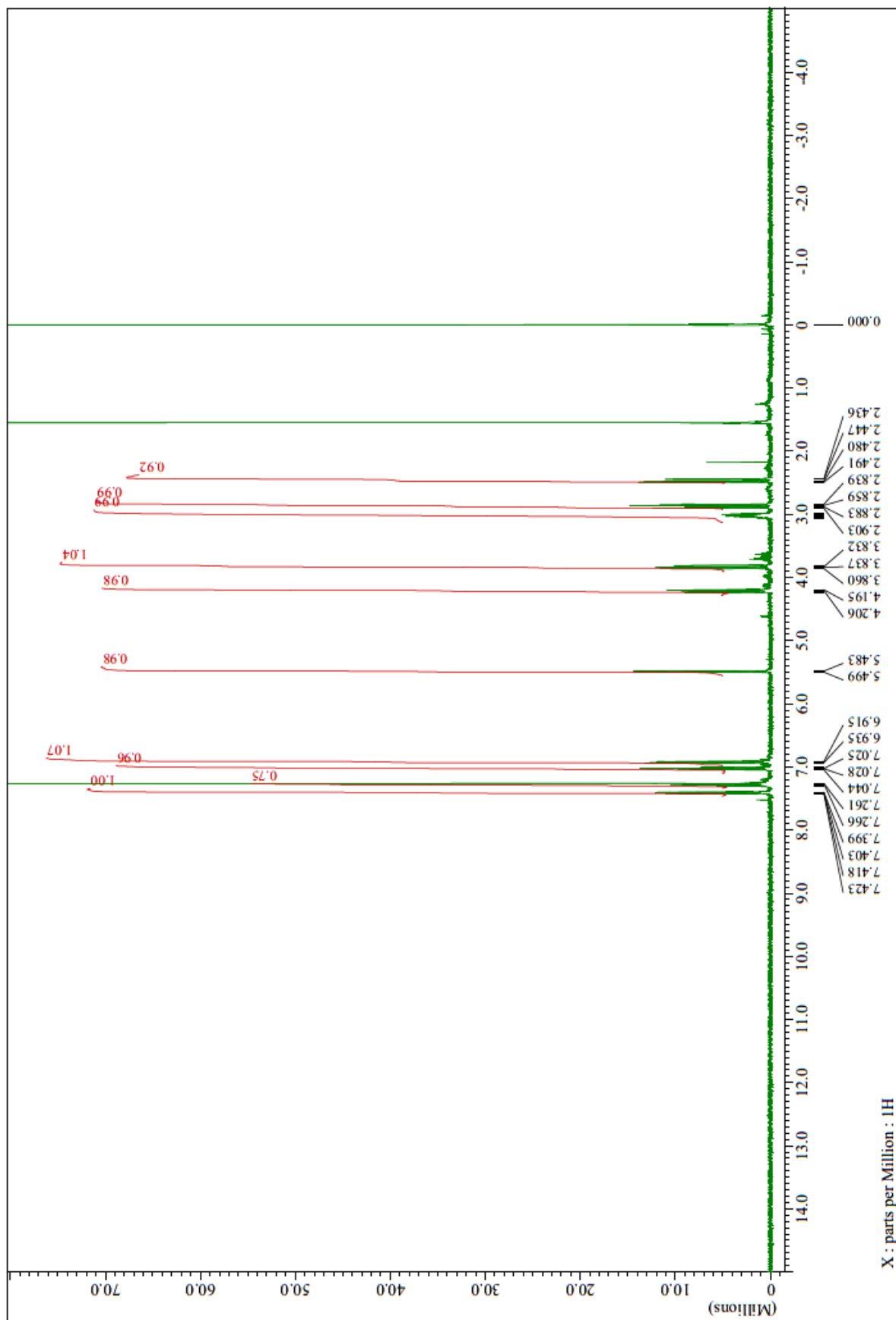
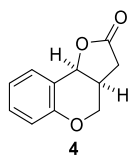
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^{13}C NMR of 3b



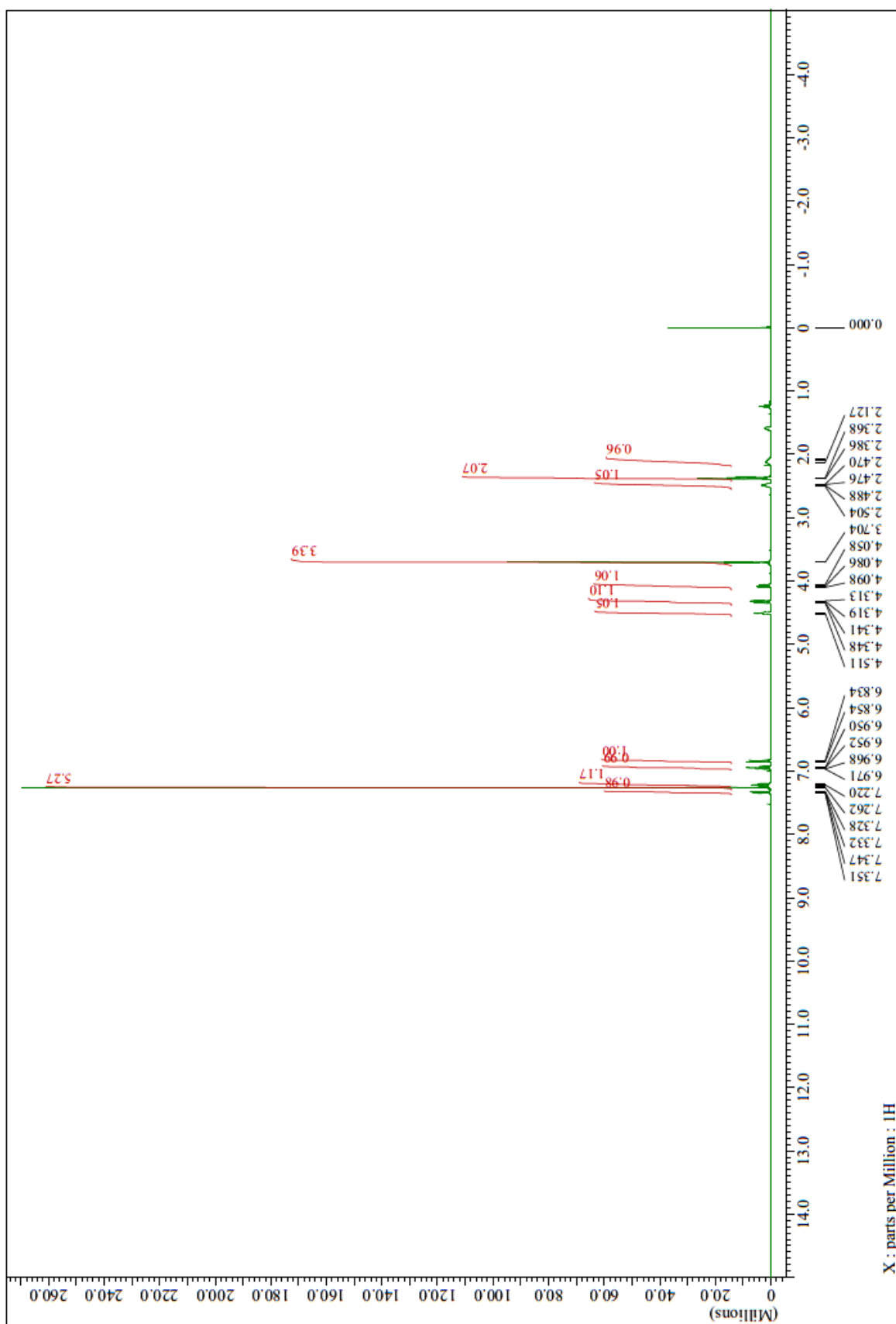
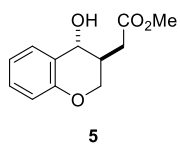
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¹H NMR of 4



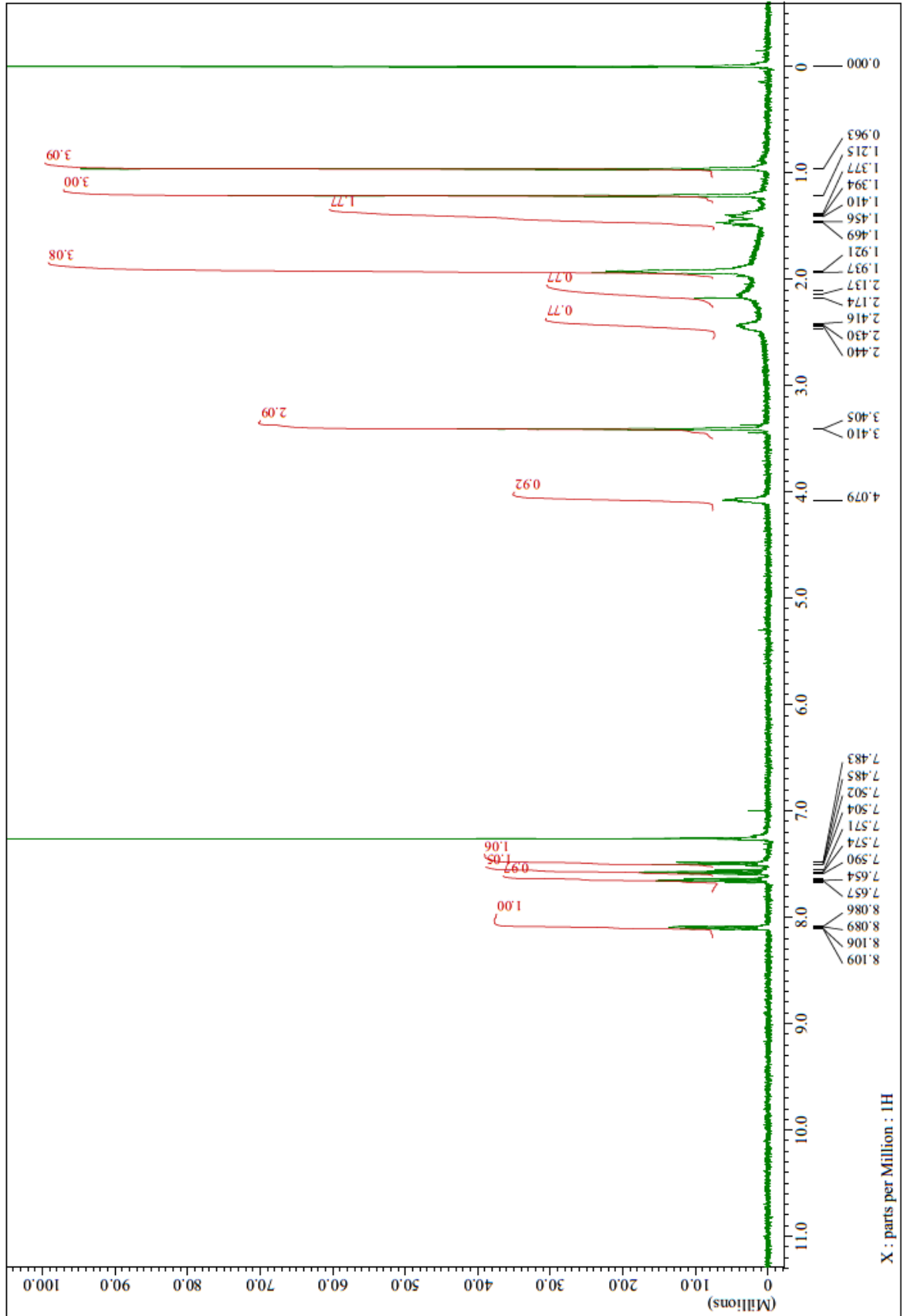
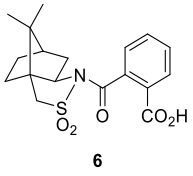
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¹H NMR of 5



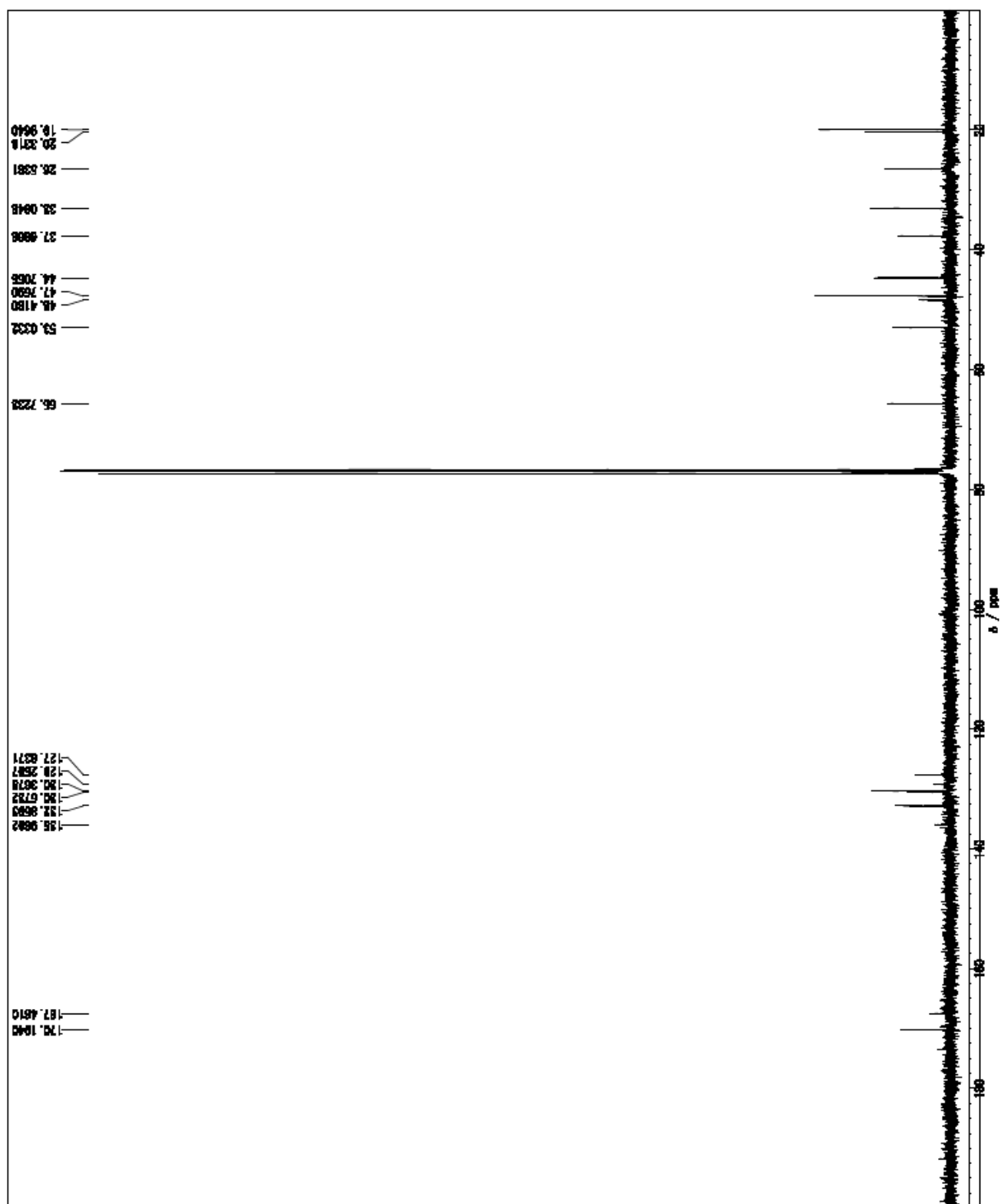
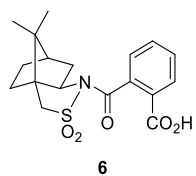
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¹H NMR of 6



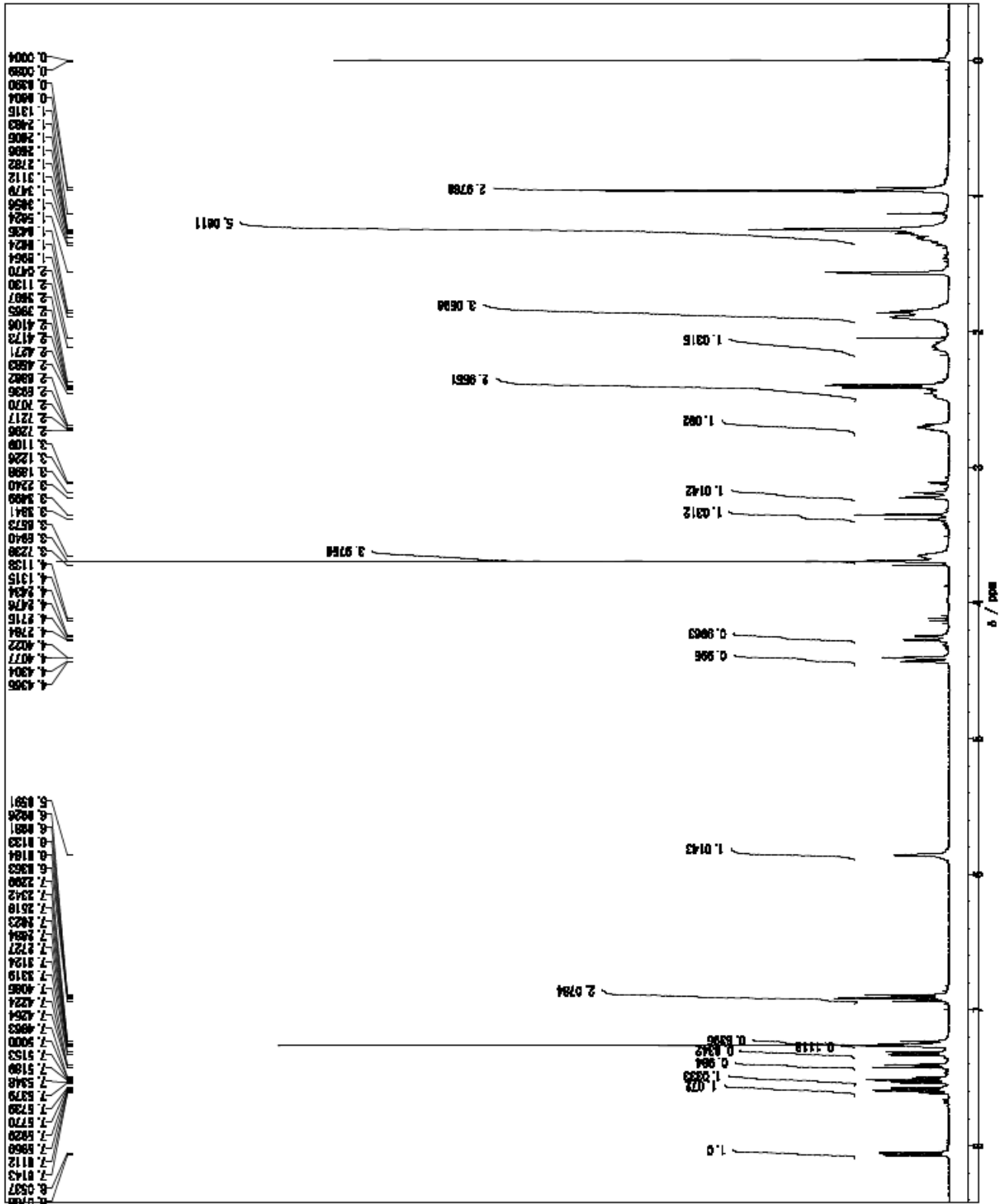
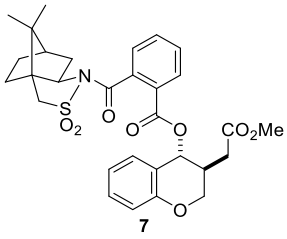
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^{13}C NMR of 6



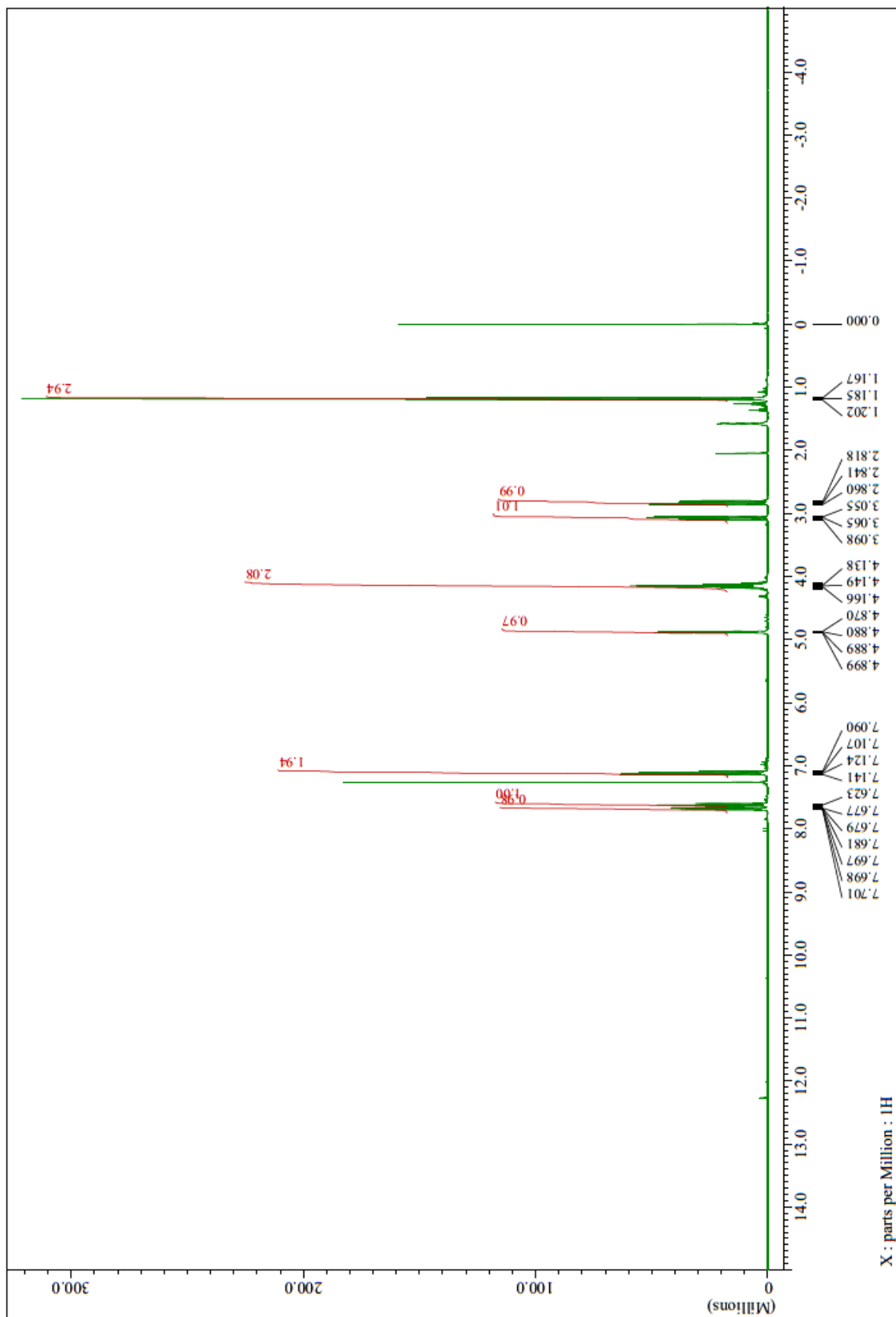
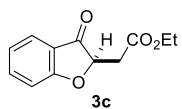
Supporting Information II

¹H NMR of 7



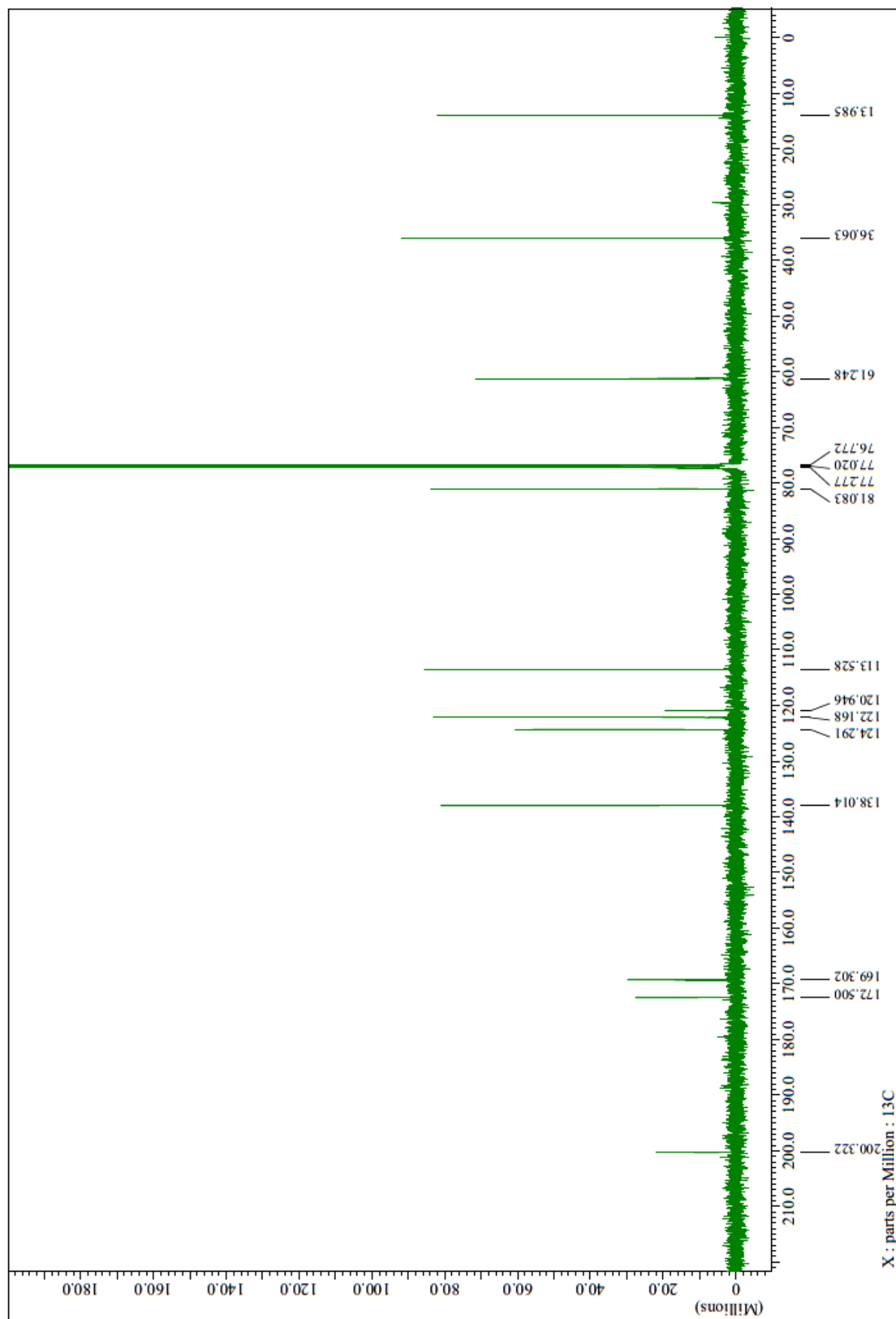
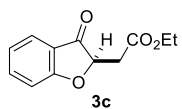
Supporting Information II

¹H NMR of 3c



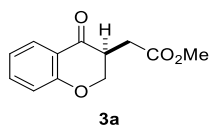
Supporting Information II

^{13}C NMR of 3c

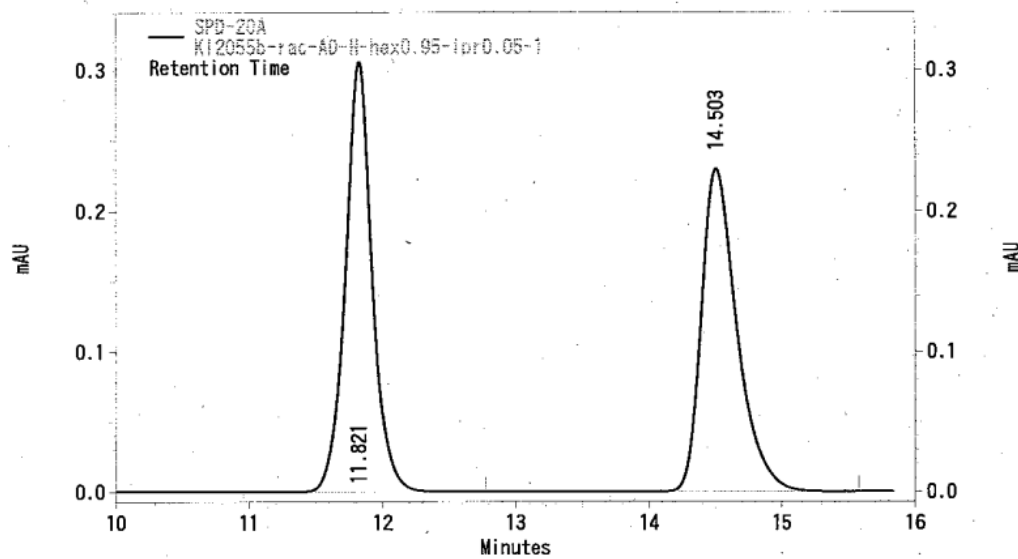


Supporting Information II

2. Copies of HPLC charts



(±)-3a

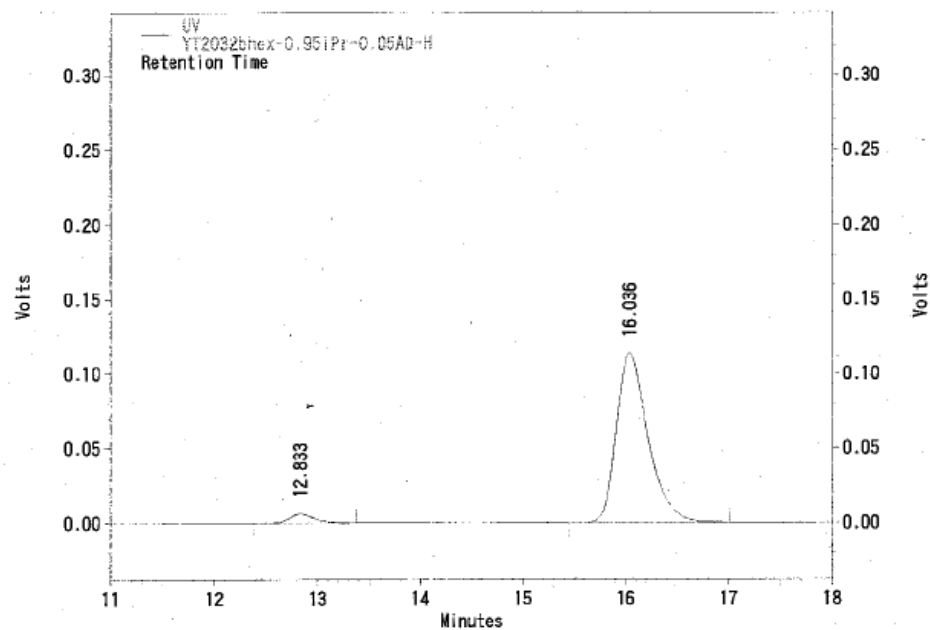


4

Name	Retention Time	Area	Area Percent	Height
1	11.821	4250382	49.843	305876
2	14.503	4277135	50.157	229890
Totals		8527517	100.000	535766

V

R-3a in Table 1, Entry 1 (92% ee, *ent*-1c was used)

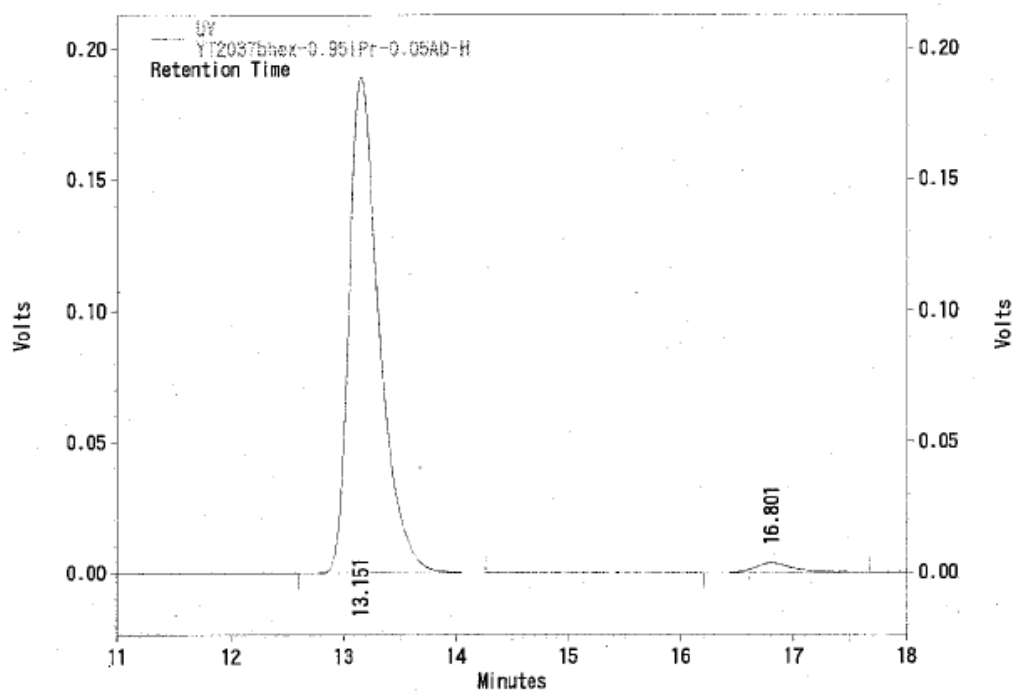


SPD-20A Results

Retention Time	Area	Area %	Height
12.833	100774	4.013	6135
16.036	2410566	95.987	113259
Totals		2511340	119394

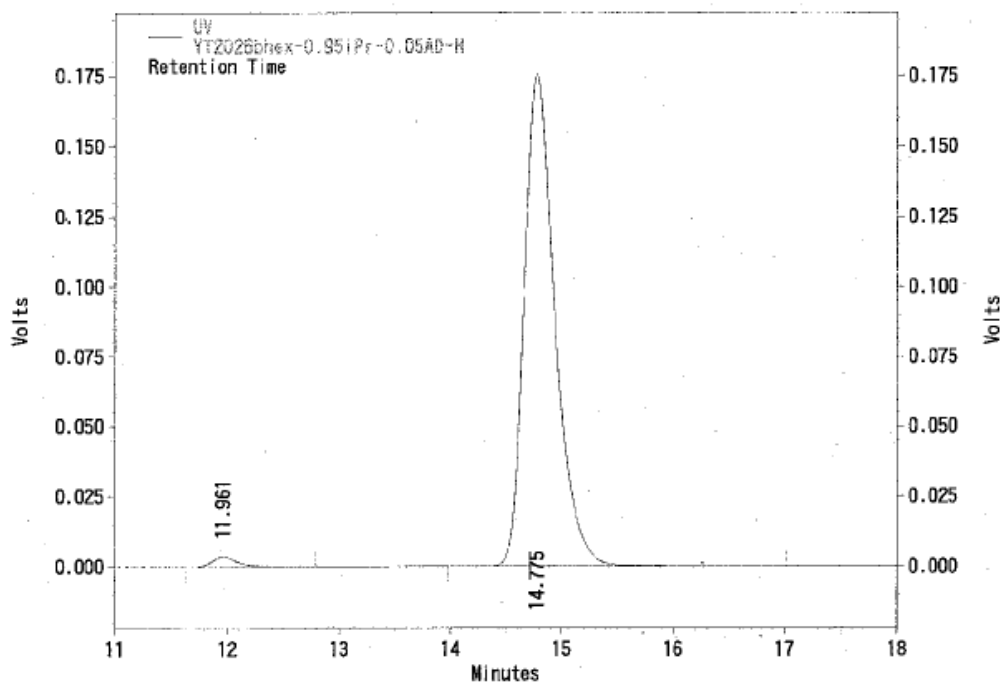
Supporting Information II

S-3a in Table 1, Entry 2 (96% ee)



SPD-20A Results			
Retention Time	Area	Area %	Height
13.151	3487547	97.750	189153
16.801	80273	2.250	3508
Totals	3567820	100.000	192661

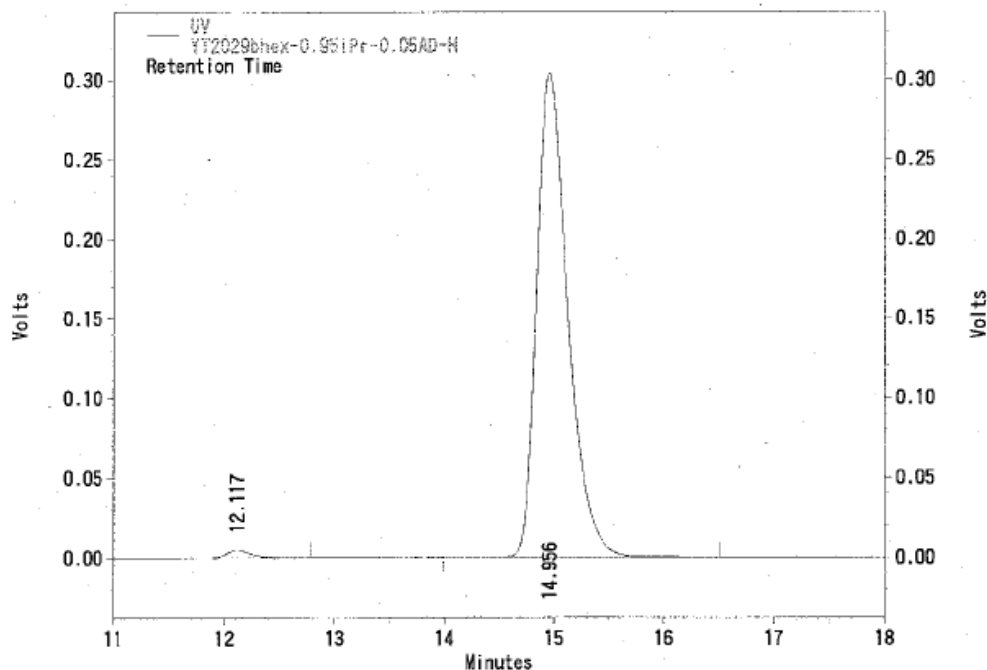
R-3a in Table 1, Entry 3 (97% ee, *ent-1a* was used)



SPD-20A Results			
Retention Time	Area	Area %	Height
11.961	52326	1.527	3632
14.775	3373897	98.473	175492
Totals	3426223	100.000	179124

Supporting Information II

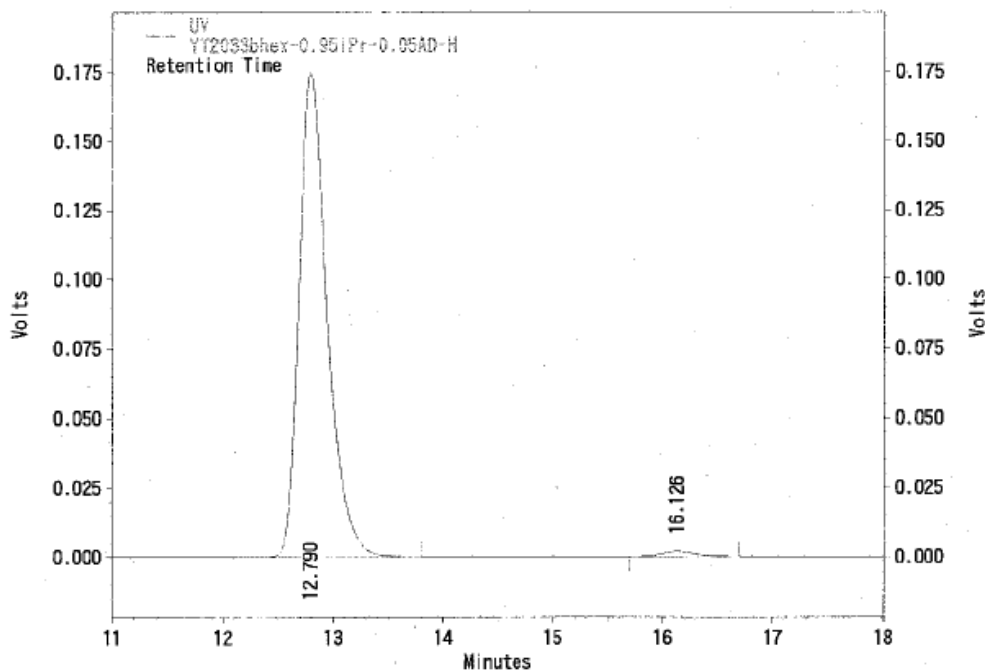
R-3a in Table 1, Entry 4 (98% ee, *ent*-1d was used)



SPD-20A Results			
Retention Time	Area	Area %	Height
12.117	71864	1.189	5027
14.956	5969976	98.811	303800

Totals	Area	Area %	Height
	6041840	100.000	308827

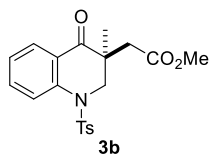
S-3a in Table 1, Entry 5 (98% ee)



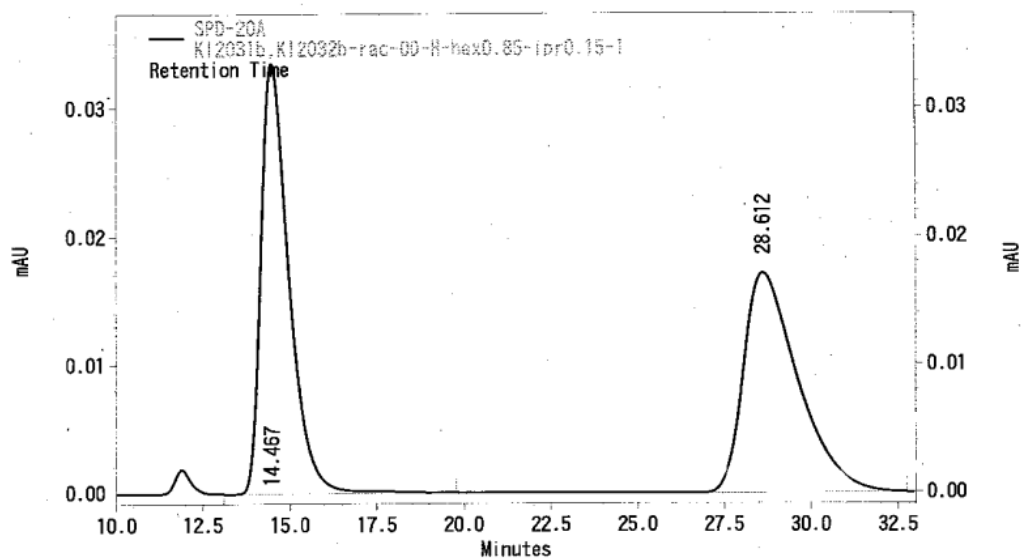
SPD-20A Results			
Retention Time	Area	Area %	Height
12.790	3078441	98.761	174645
16.126	38625	1.239	1872

Totals	Area	Area %	Height
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Supporting Information II



(±)-**3b**

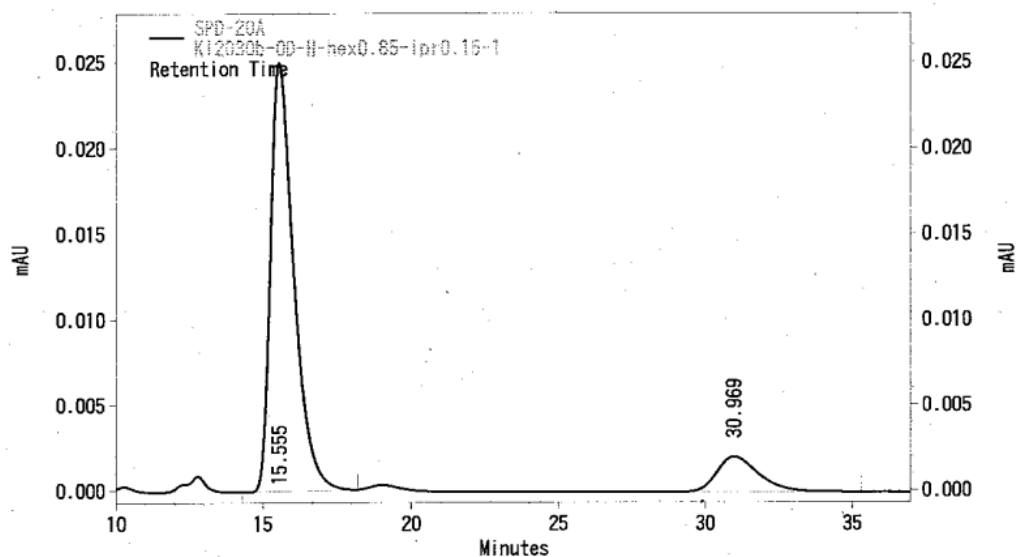


4

Name	Retention Time	Area	Area Percent	Height
1	14.467	1884952	50.265	33548
2	28.612	1865113	49.735	17150
Totals		3750065	100.000	50698

v

R-**3b** in Table 1, Entry 6 (74% ee, *ent*-**1c** was used)



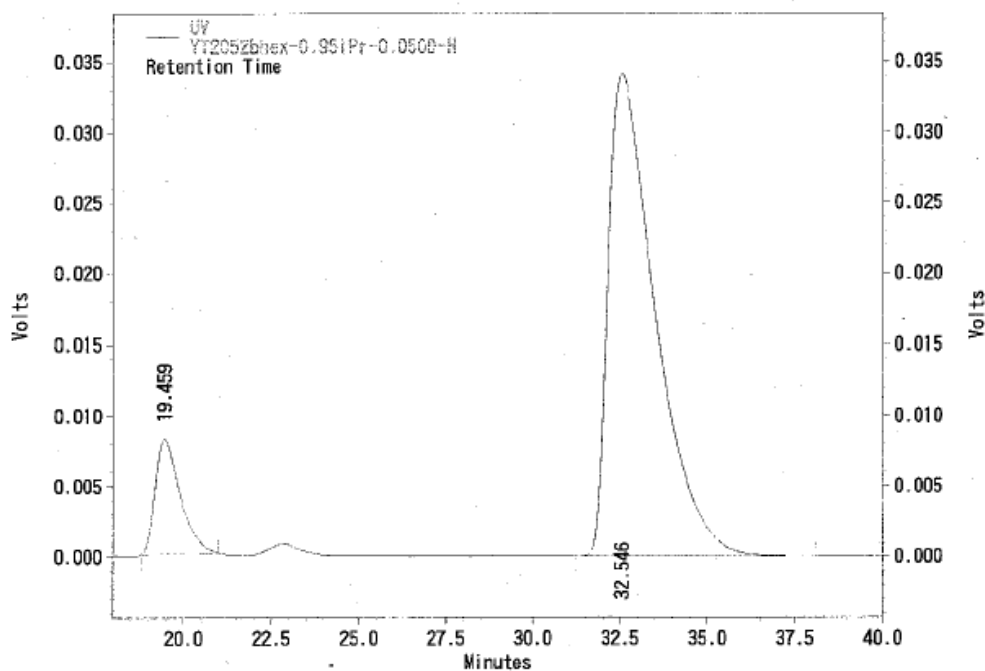
4

Name	Retention Time	Area	Area Percent	Height
1	15.555	1377977	86.969	24996
2	30.969	206465	13.031	2076
Totals		1584442	100.000	27072

v

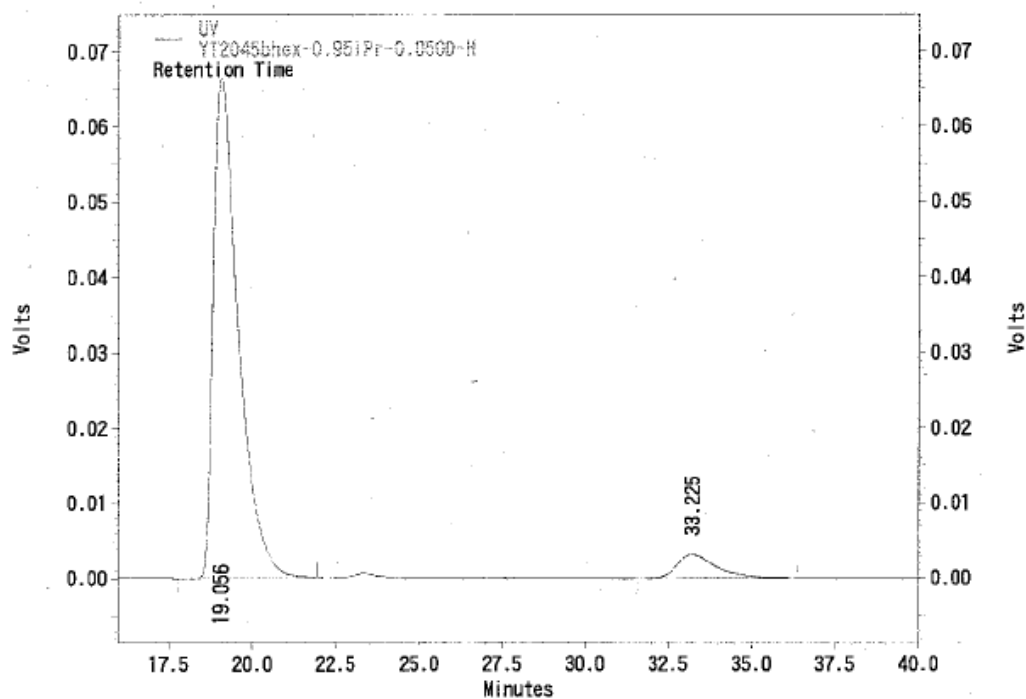
Supporting Information II

S-3b in Table 1, Entry 7 (78% ee)



SPD-20A Results			
Retention Time	Area	Area %	Height
19.459	405852	11.239	8181
32.546	3205194	88.761	34104
Totals	3611046	100.000	42285

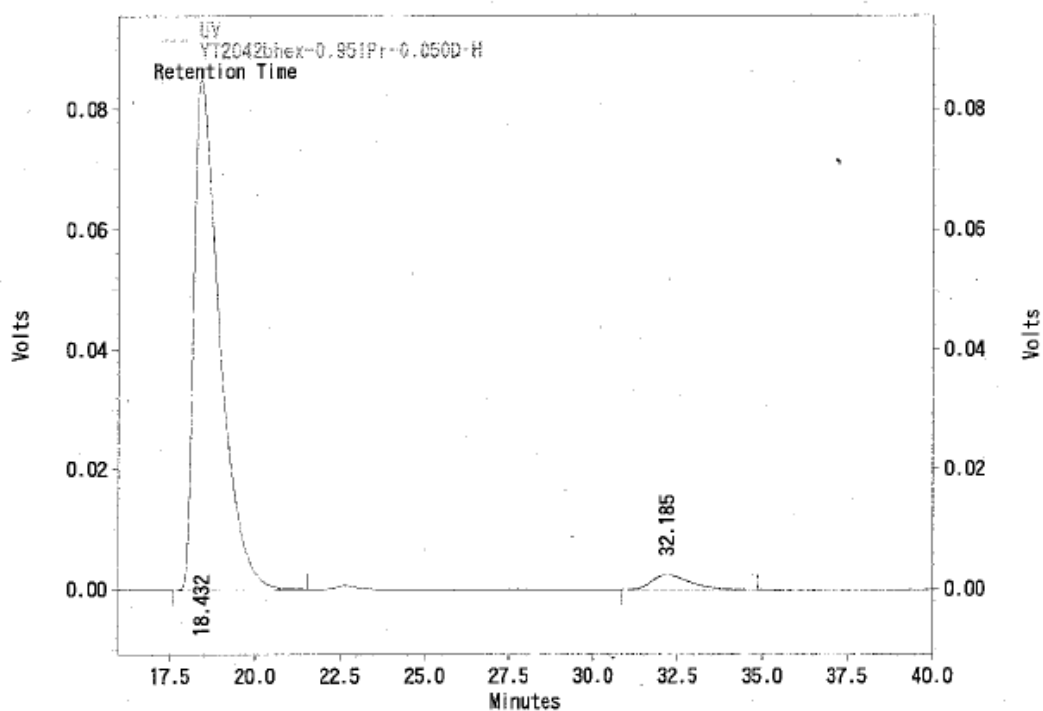
R-3b in Table 1, Entry 8 (86% ee, *ent-1a* was used)



SPD-20A Results			
Retention Time	Area	Area %	Height
19.056	3443457	93.091	66503
33.225	255565	6.909	3210
Totals	3699022	100.000	69713

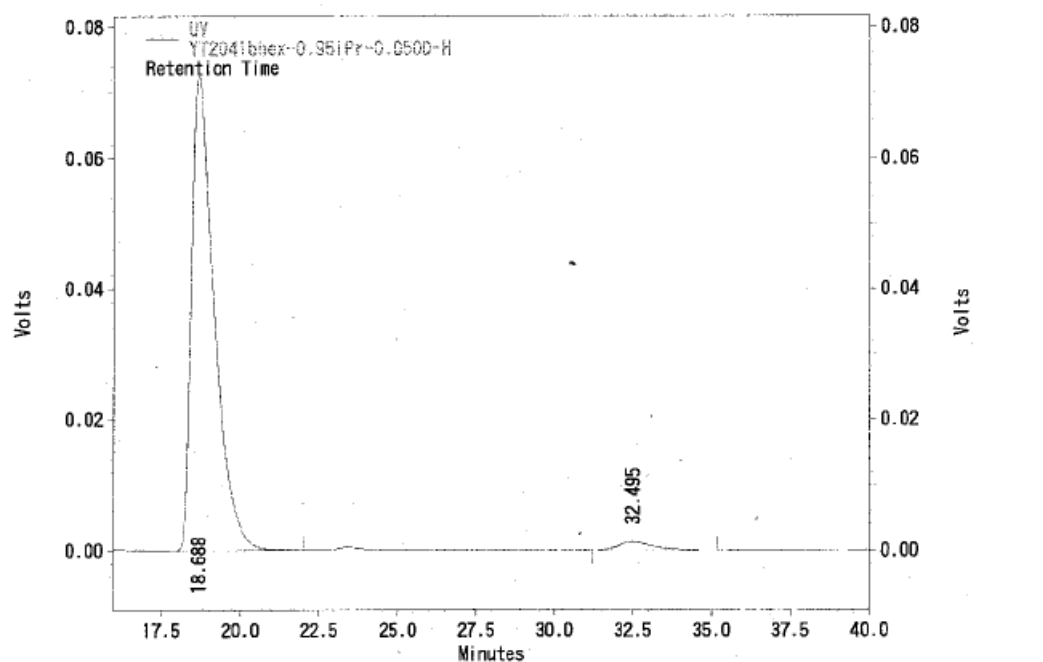
Supporting Information II

R-3b in Table 1, Entry 9 (92% ee, *ent*-1d was used)



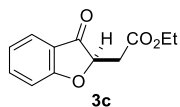
SPD-20A Results			
Retention Time	Area	Area %	Height
18.432	4499703	95.876	84988
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Totals	4693254	100.000	87442

R-3b in Table 1, Entry 10 (95% ee, *ent*-1e was used)

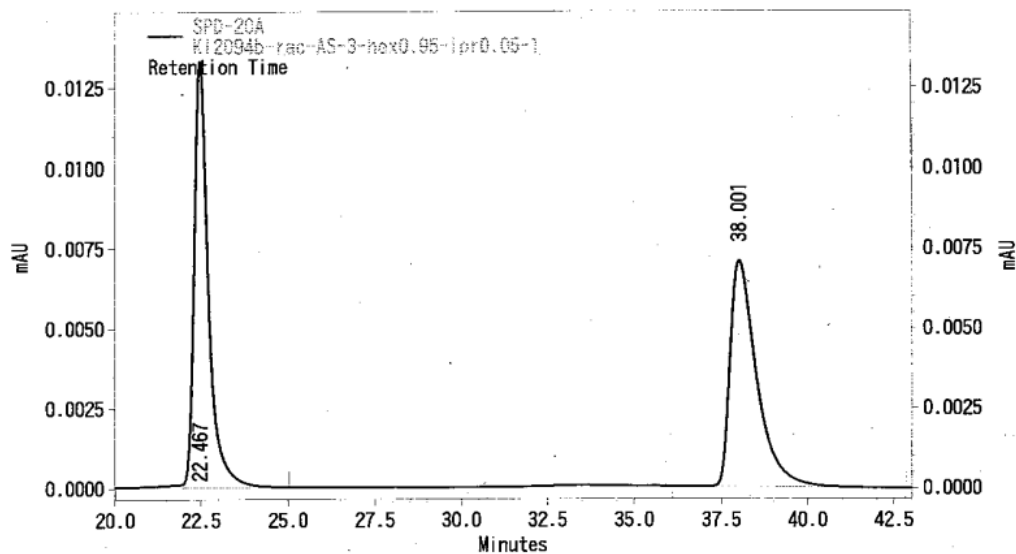


SPD-20A Results			
Retention Time	Area	Area %	Height
18.688	3606491	97.333	72515
32.495	98805	2.667	1286
Totals	3705296	100.000	73801

Supporting Information II



(±)-**3c**

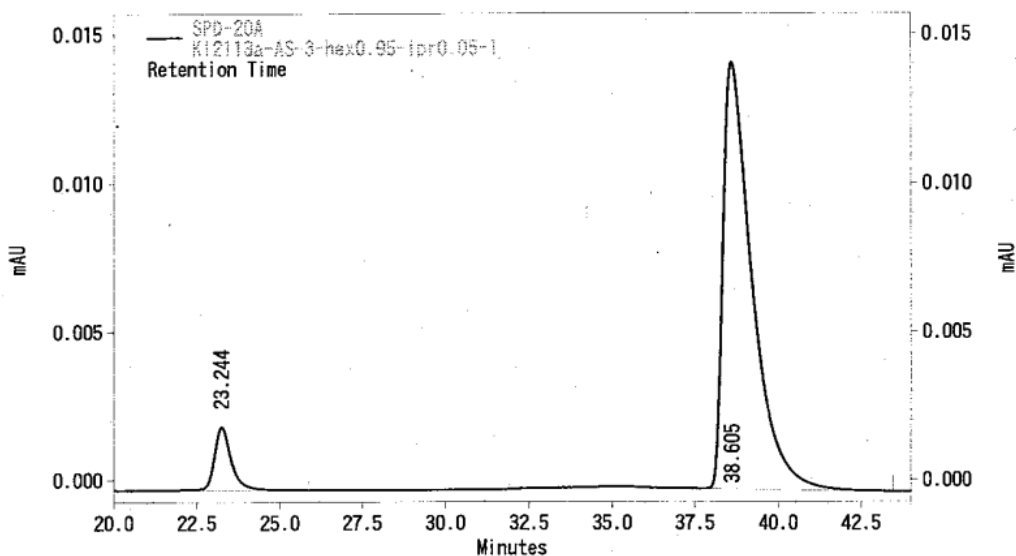


4

Name	Retention Time	Area	Area Percent	Height
1	22.467	383638	50.447	13299
2	38.001	376832	49.553	7065
Totals		760470	100.000	20364

v

S-**3c** synthesized in the presence of **1a** for 2 h (84% ee)



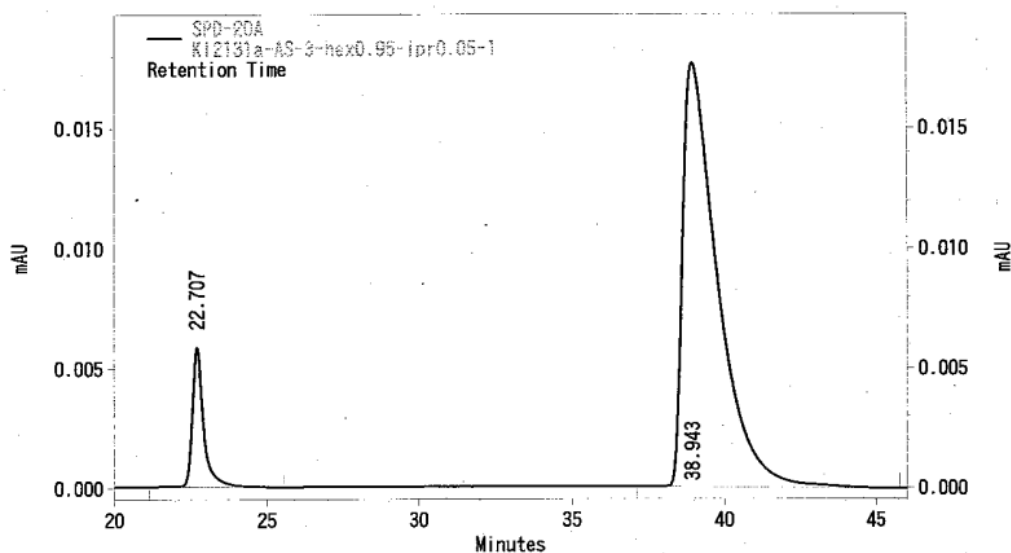
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Name	Retention Time	Area	Area Percent	Height
1	23.244	76815	8.157	2134
2	38.605	864849	91.843	14361
Totals		941664	100.000	16495

v

Supporting Information II

S-**3c** synthesized in the presence of **1a** for 4 h (81% ee)

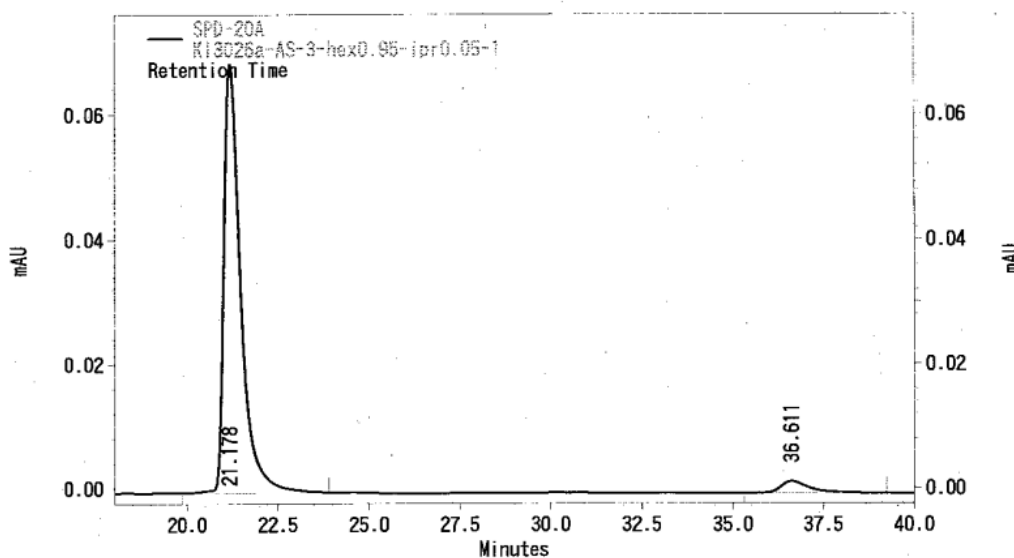


4

Name	Retention Time	Area	Area Percent	Height
1	22.707	151430	9.701	5827
2	38.943	1409565	90.299	17648
Totals		1560995	100.000	23475

v

R-**3c** synthesized in the presence of *ent*-**1e** for 2 h (91% ee)



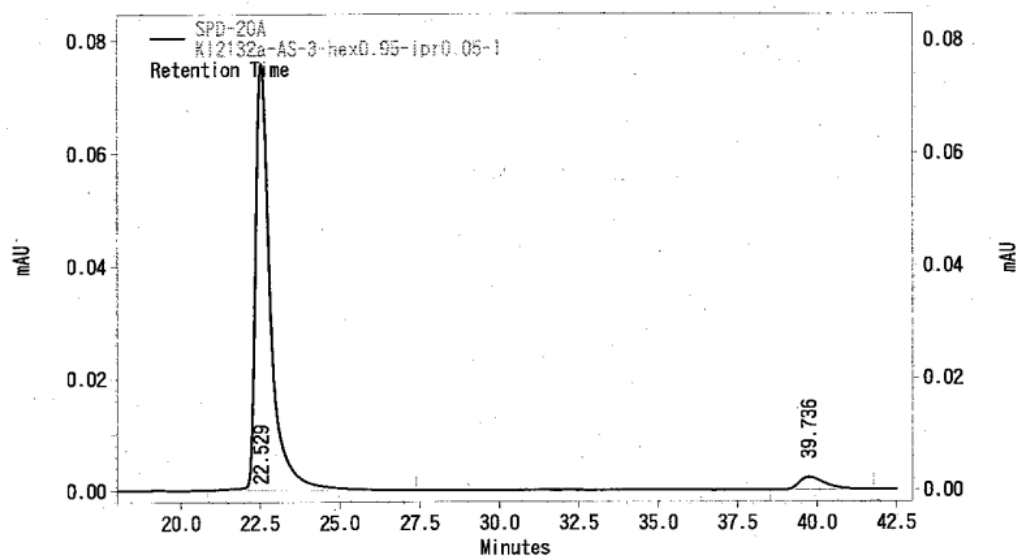
4

Name	Retention Time	Area	Area Percent	Height
1	21.178	2218229	95.521	68789
2	36.611	104016	4.479	1891
Totals		2322245	100.000	70680

v

Supporting Information II

R-3c synthesized in the presence of *ent*-1e for 4 h (90% ee)



4

Name	Retention Time	Area	Area Percent	Height
1	22.529	2479672	95.003	75808
2	39.736	130438	4.997	2261
Totals		2610110	100.000	78069

v