

## Supporting Information

### 1,2,3-Benzoxathiazine-2,2-dioxides – effective inhibitors of human carbonic anhydrases

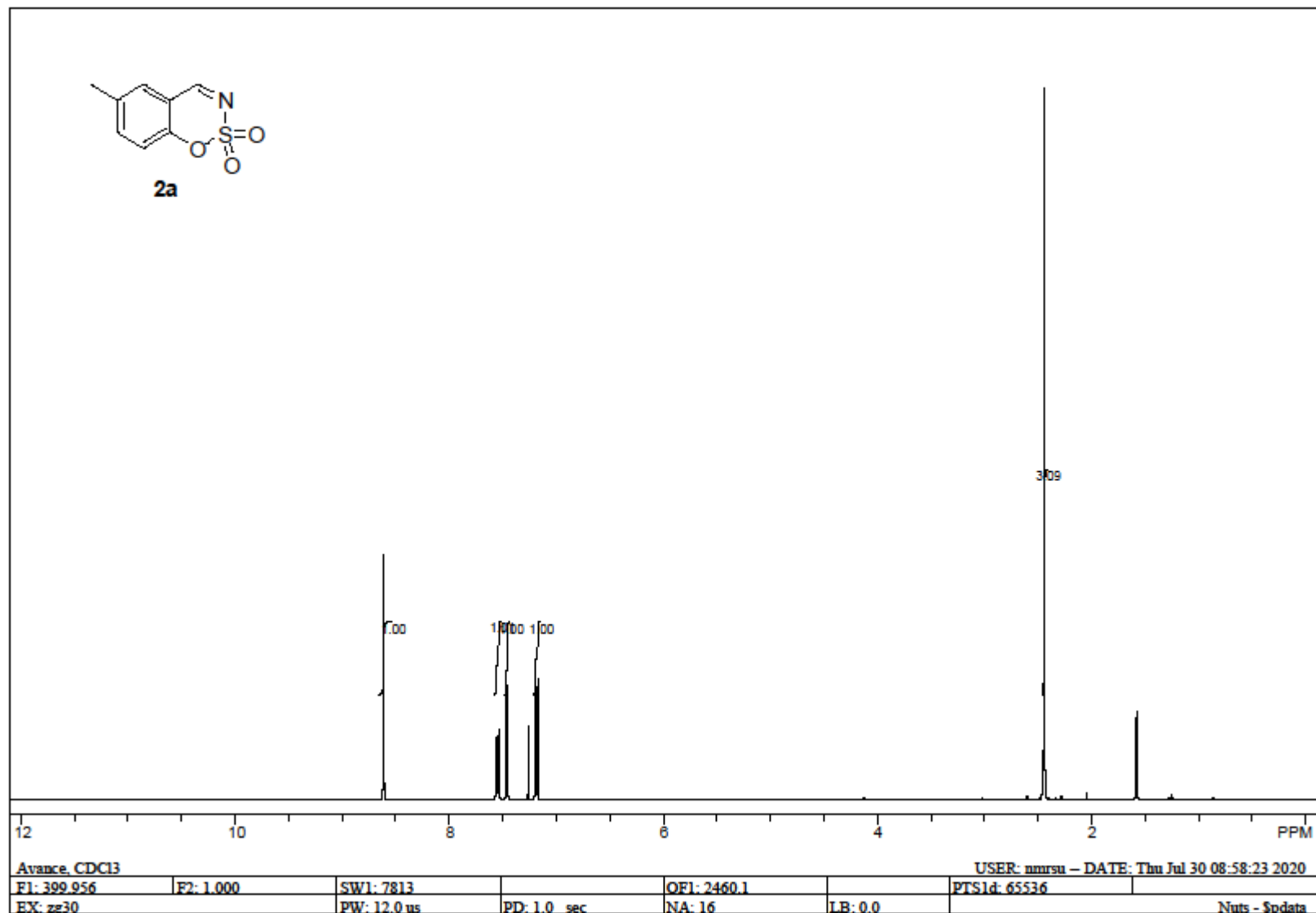
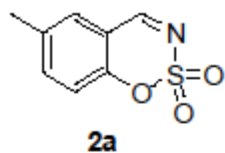
Jekaterīna Ivanova,<sup>1</sup> Morteza Abdoli,<sup>2</sup> Alessio Nocentini,<sup>3</sup> Raivis Žalubovskis, <sup>\*,1,2</sup> Claudiu T. Supuran<sup>3</sup>

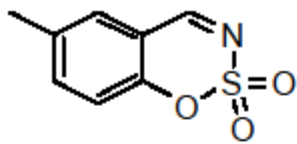
<sup>1</sup> Latvian Institute of Organic Synthesis, Riga, Latvia;

<sup>2</sup> Institute of Technology of Organic Chemistry, Faculty of Materials Science and Applied Chemistry, Riga Technical University, Riga, Latvia;

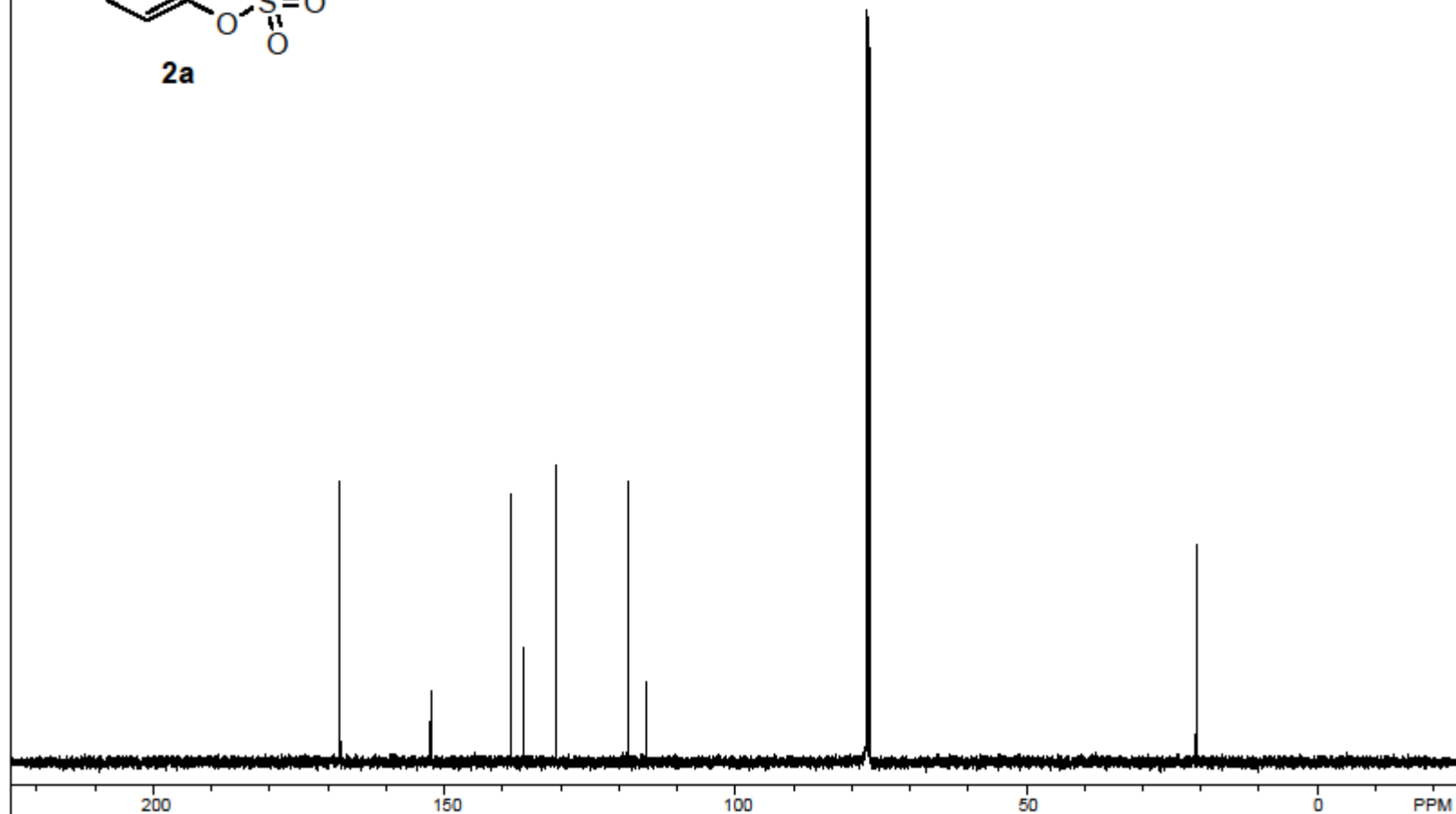
<sup>3</sup> Neurofarba Department, Università degli Studi di Firenze, Florence, Italy;

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2a



Avance, CDCl3

USER: nmrsu - DATE: Thu Jul 30 09:57:58 2020

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F2: 1.000

SW1: 25000

OF1: 10068.7

PTS1d: 32768

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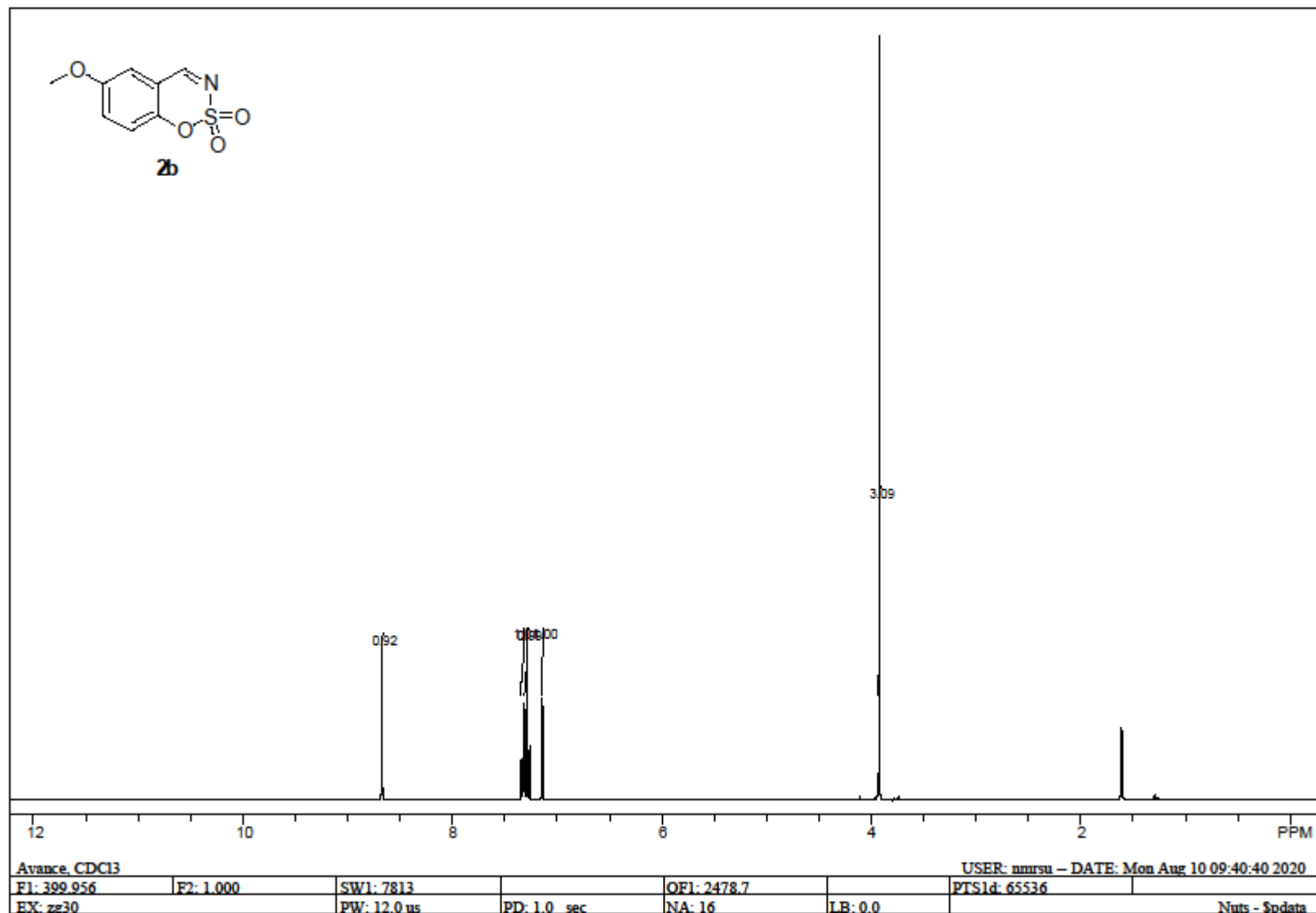
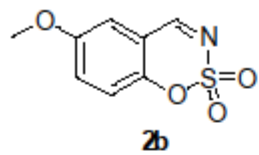
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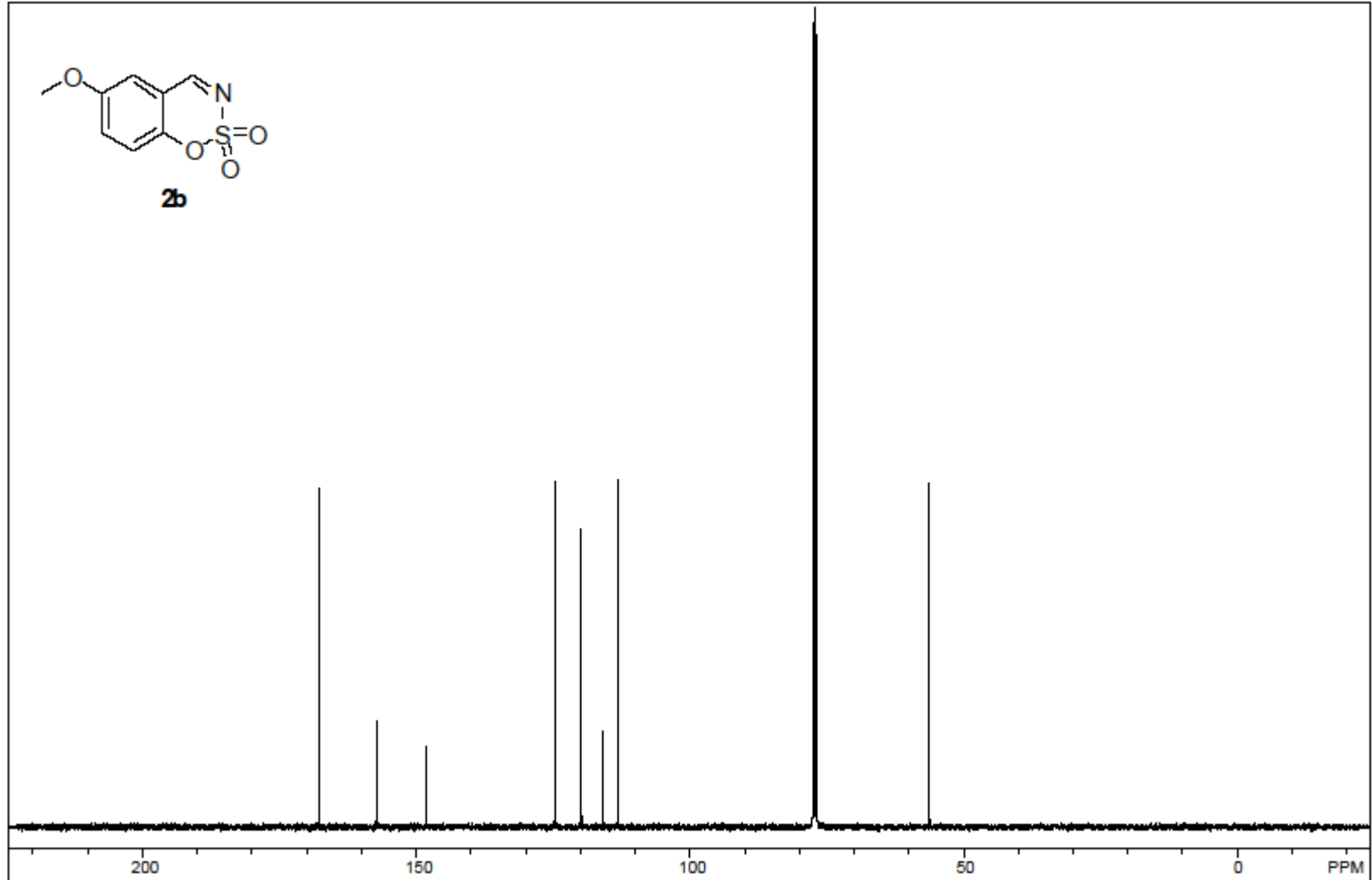
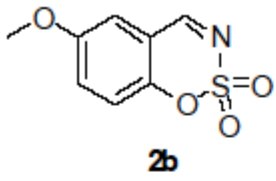
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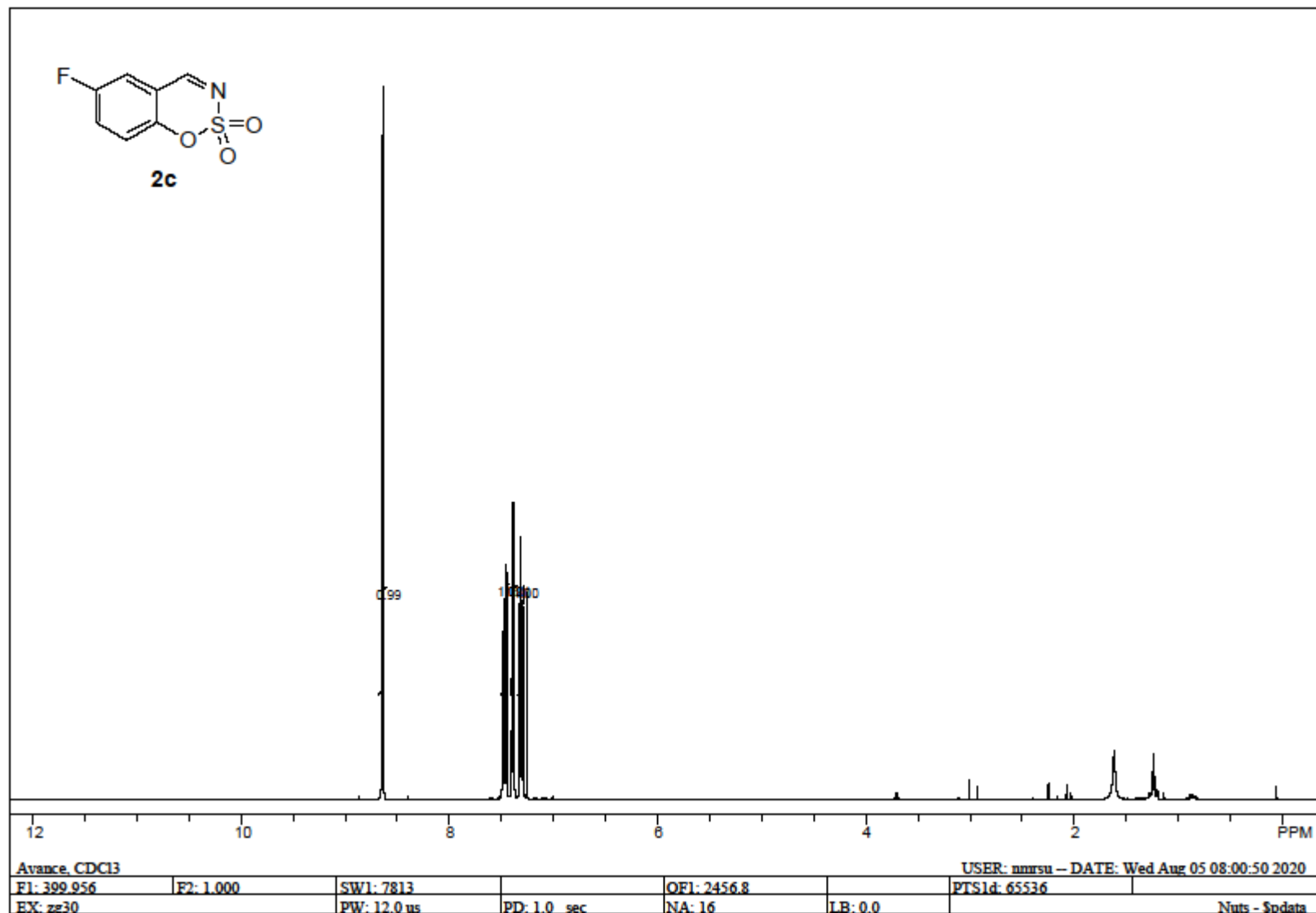
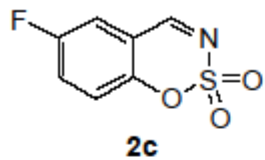
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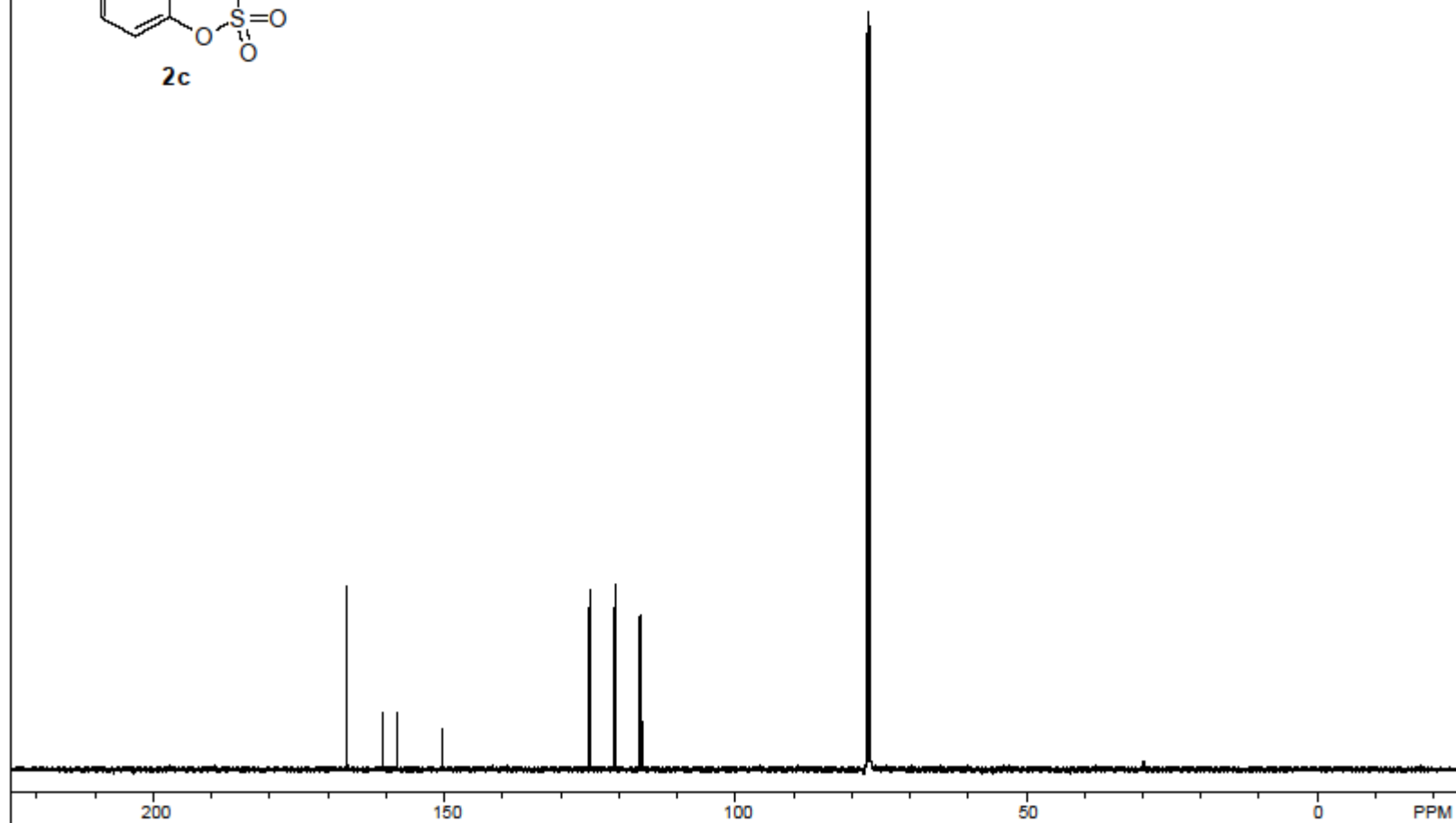
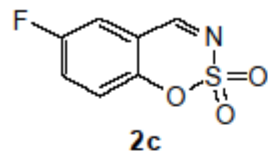
Nuts - \$pdata



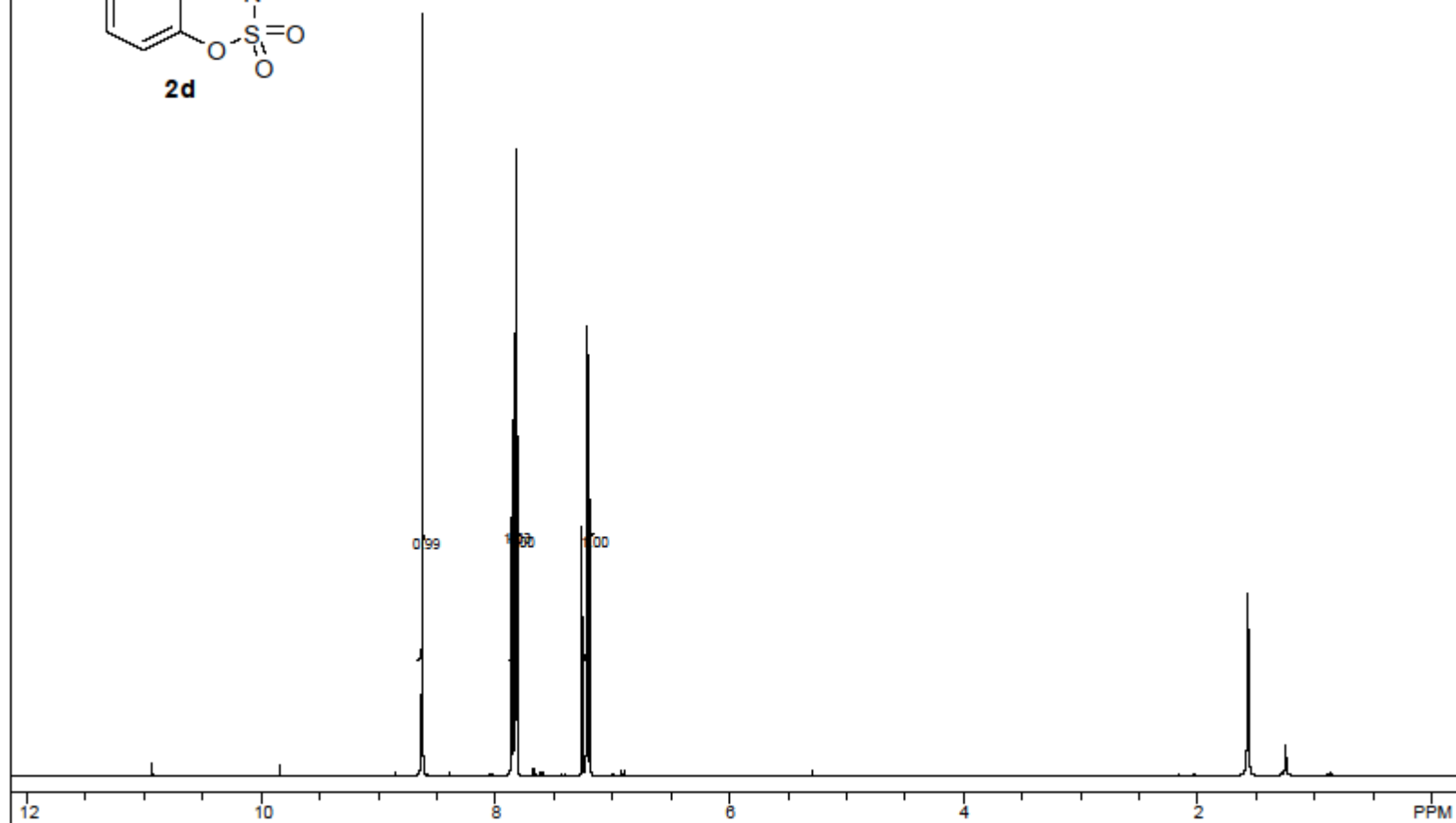
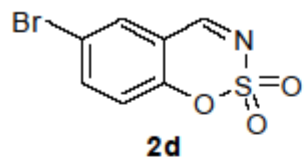


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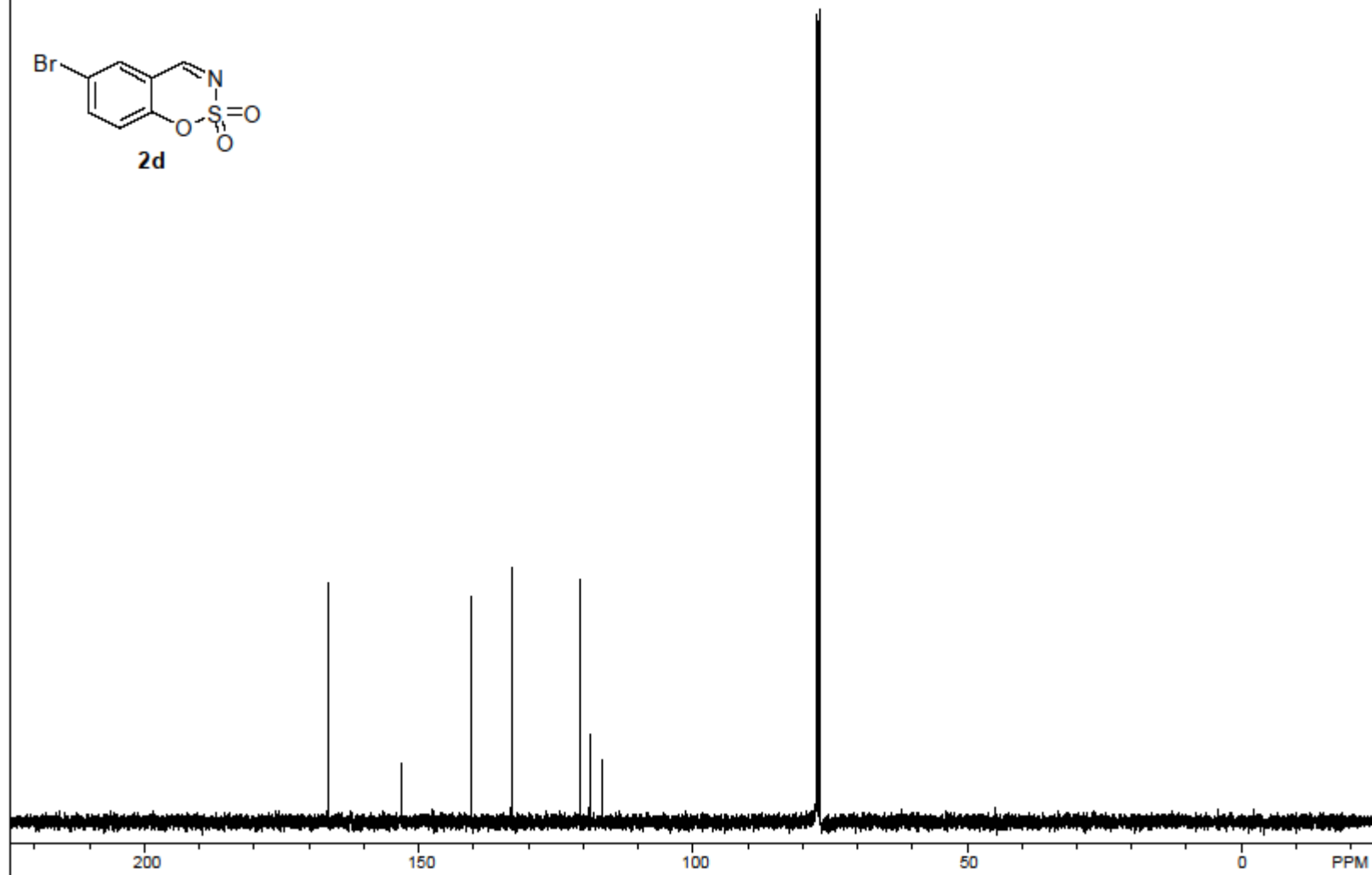
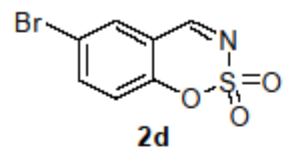




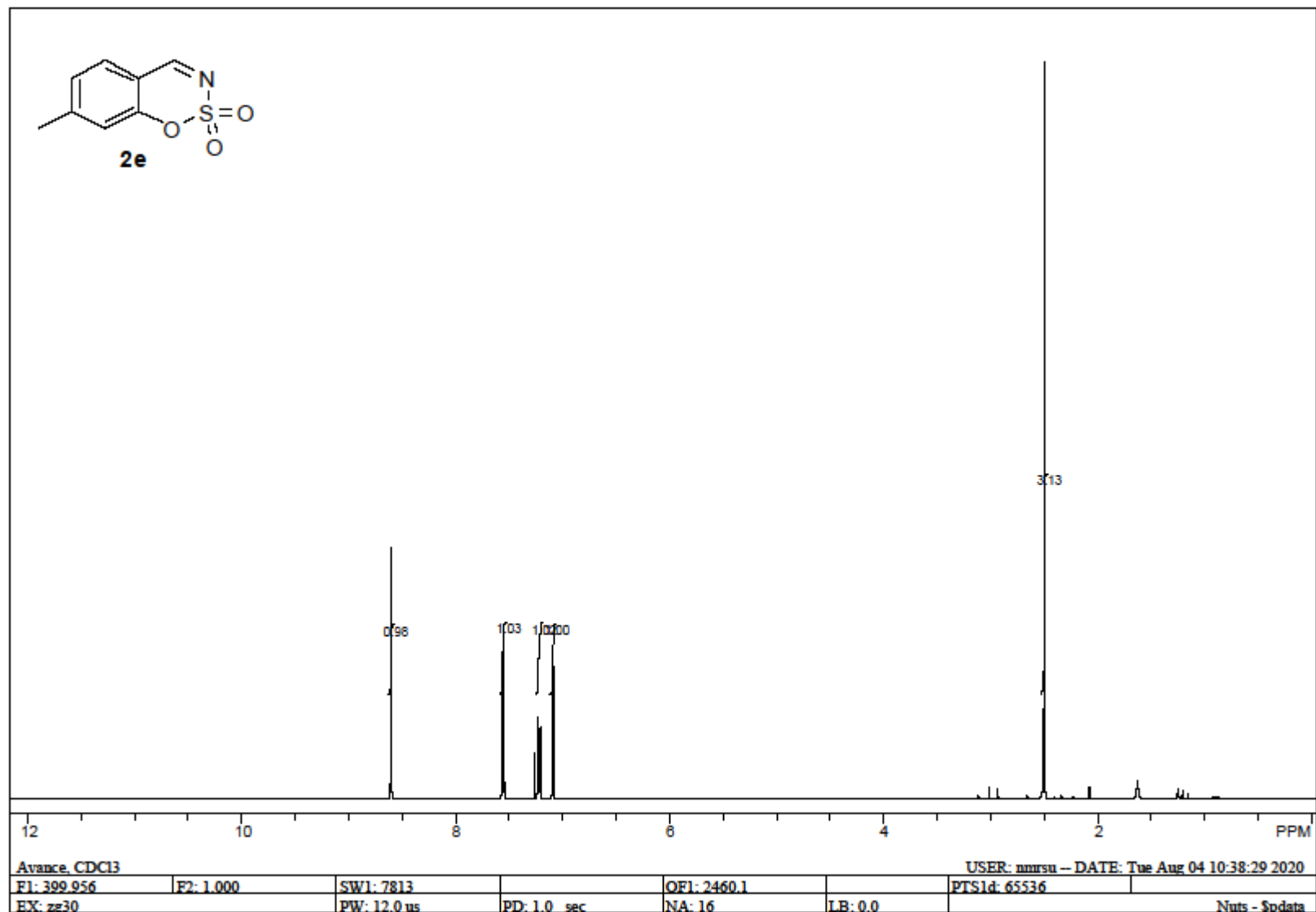
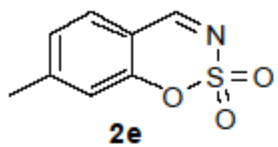
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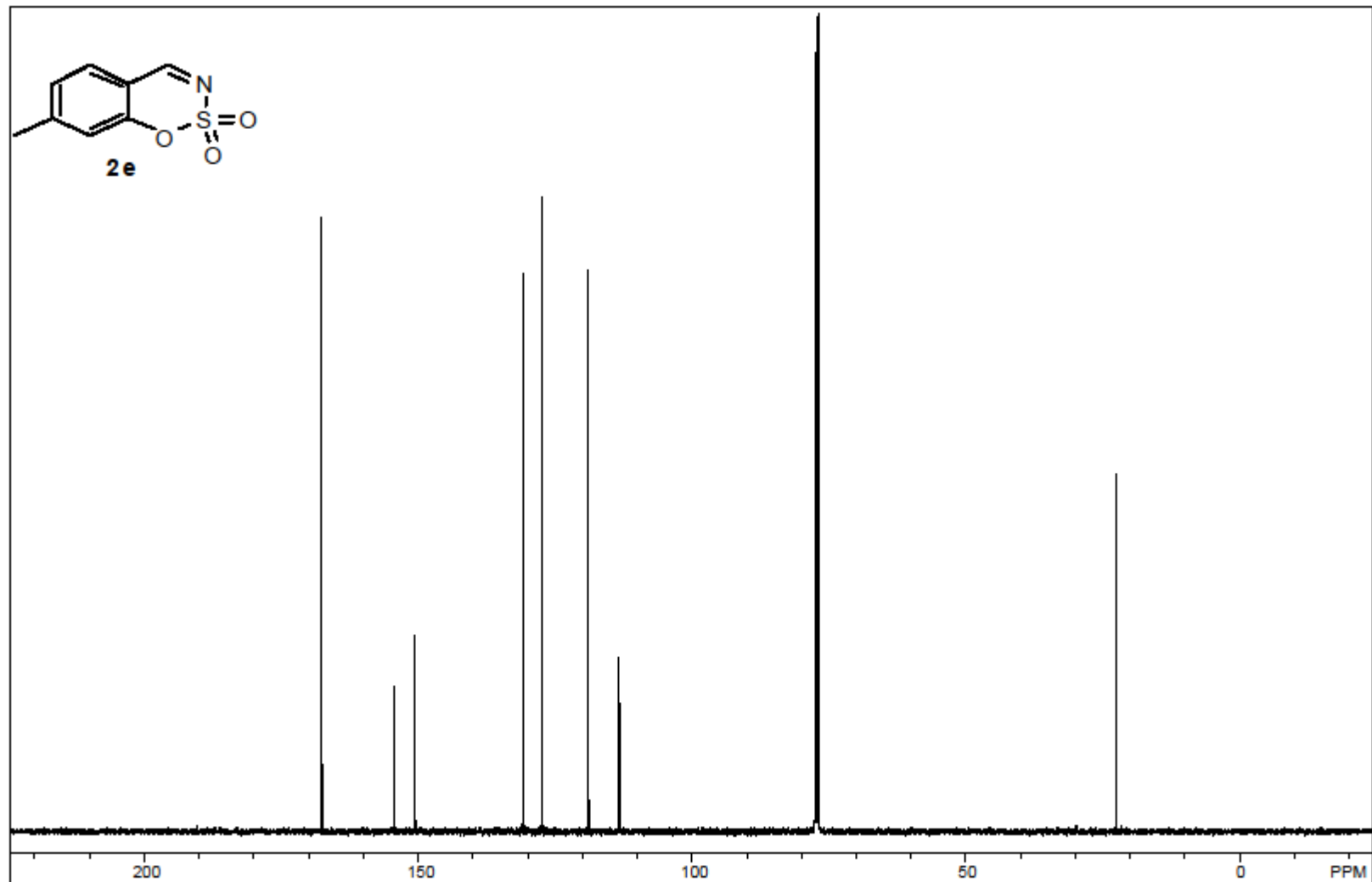
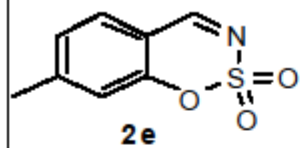


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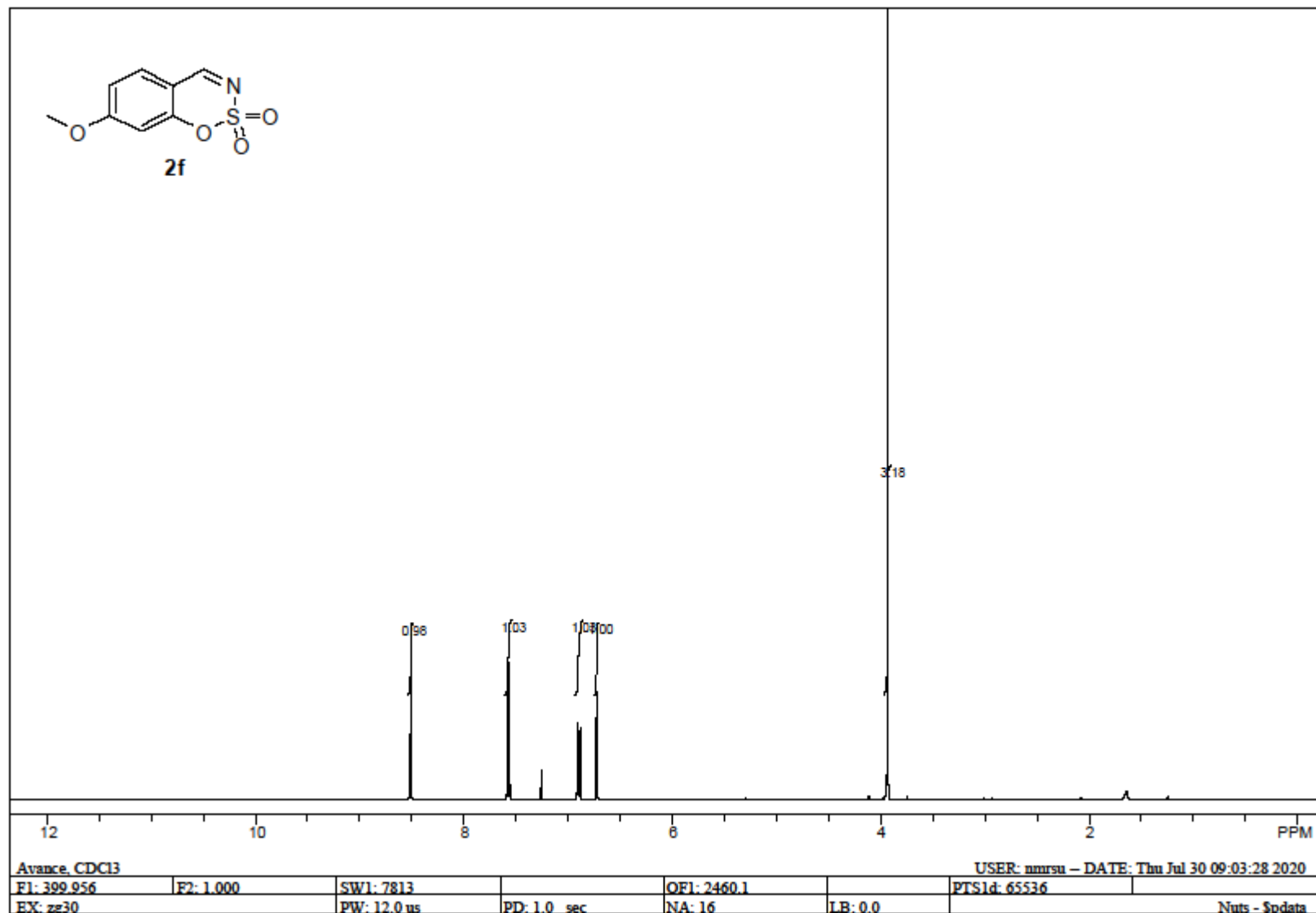
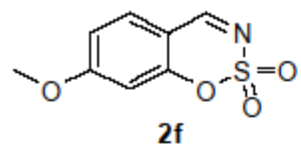


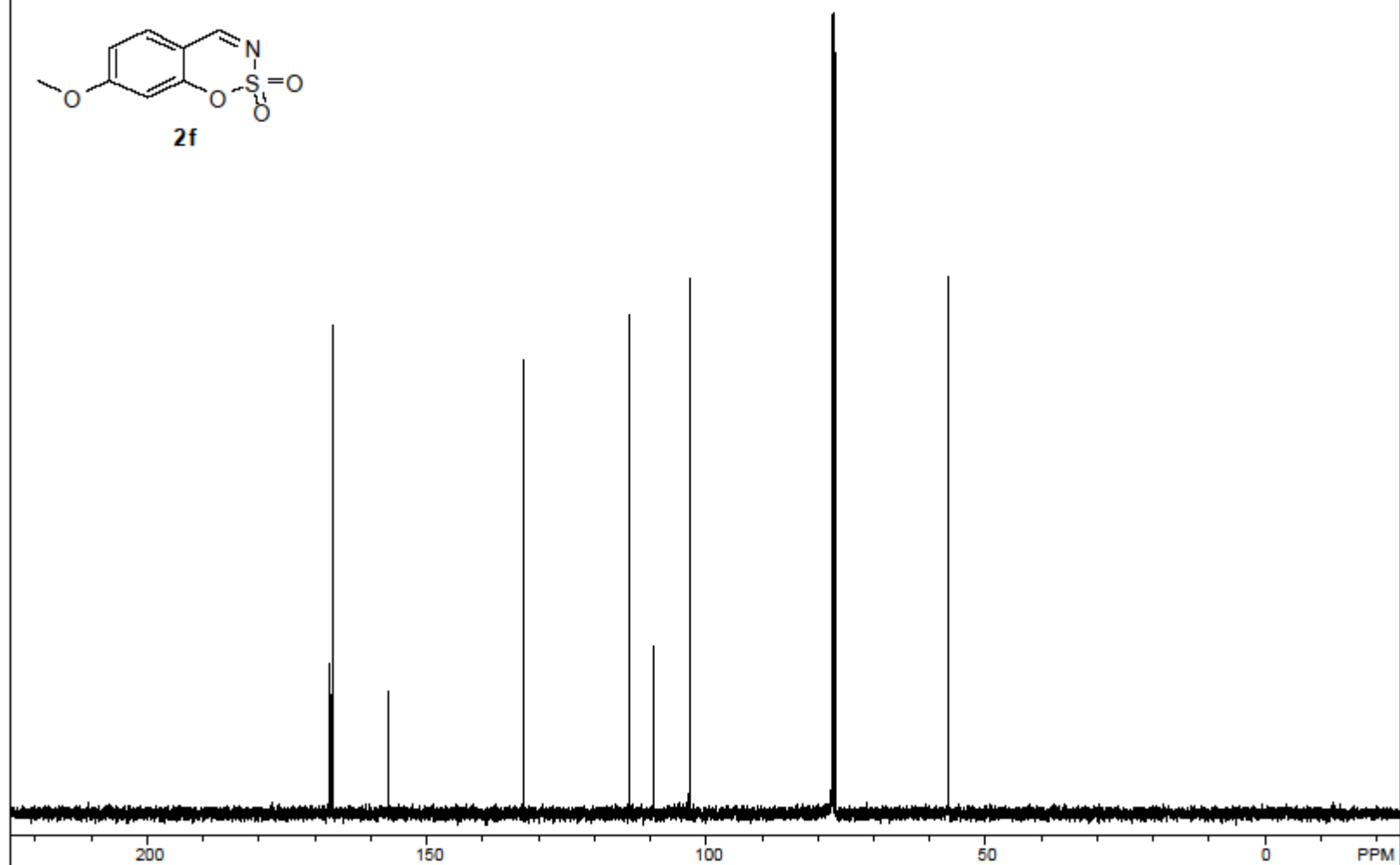
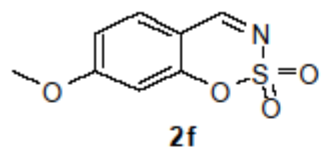
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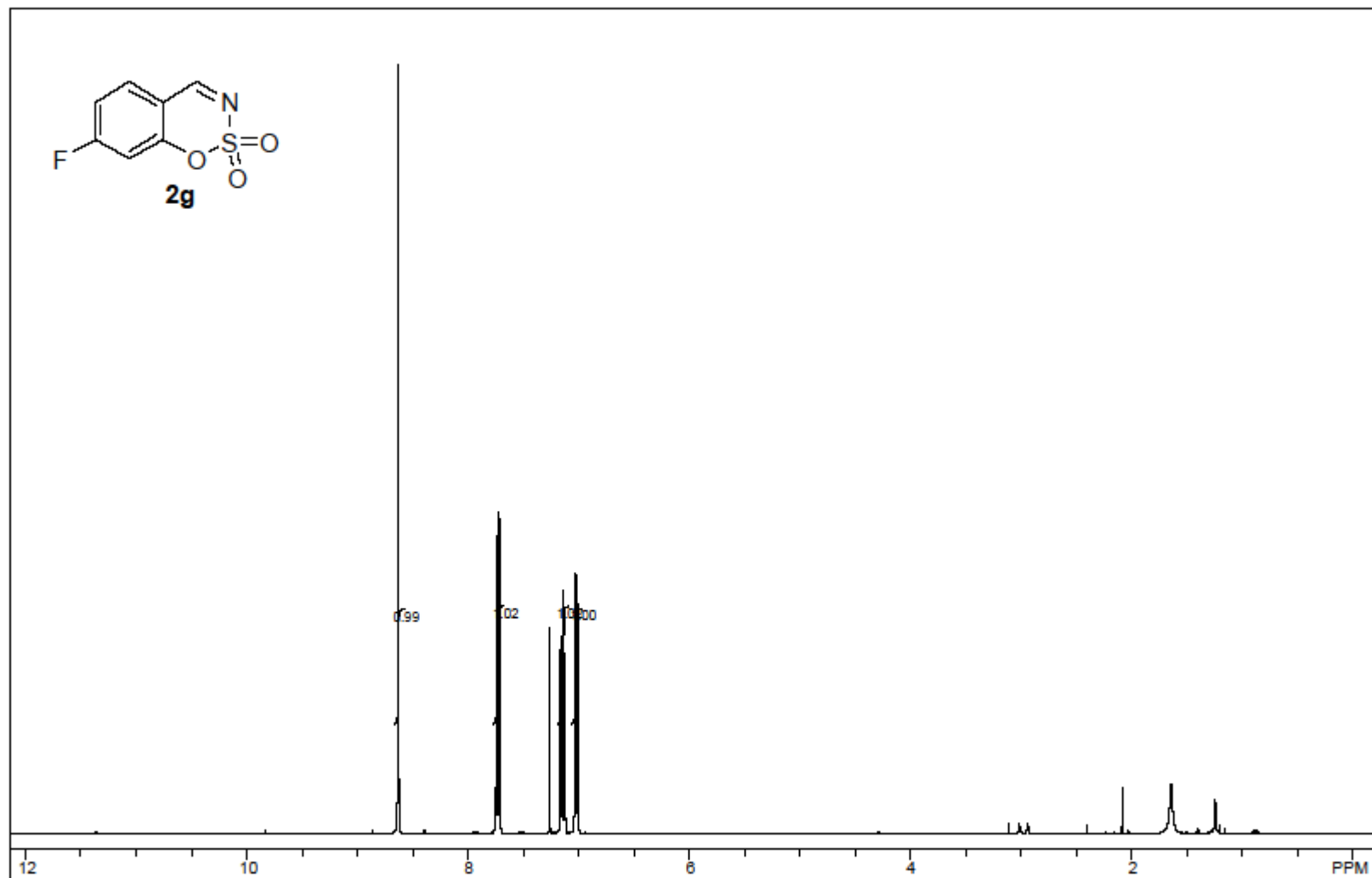
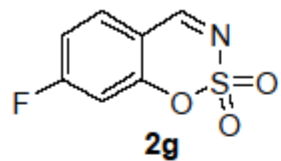


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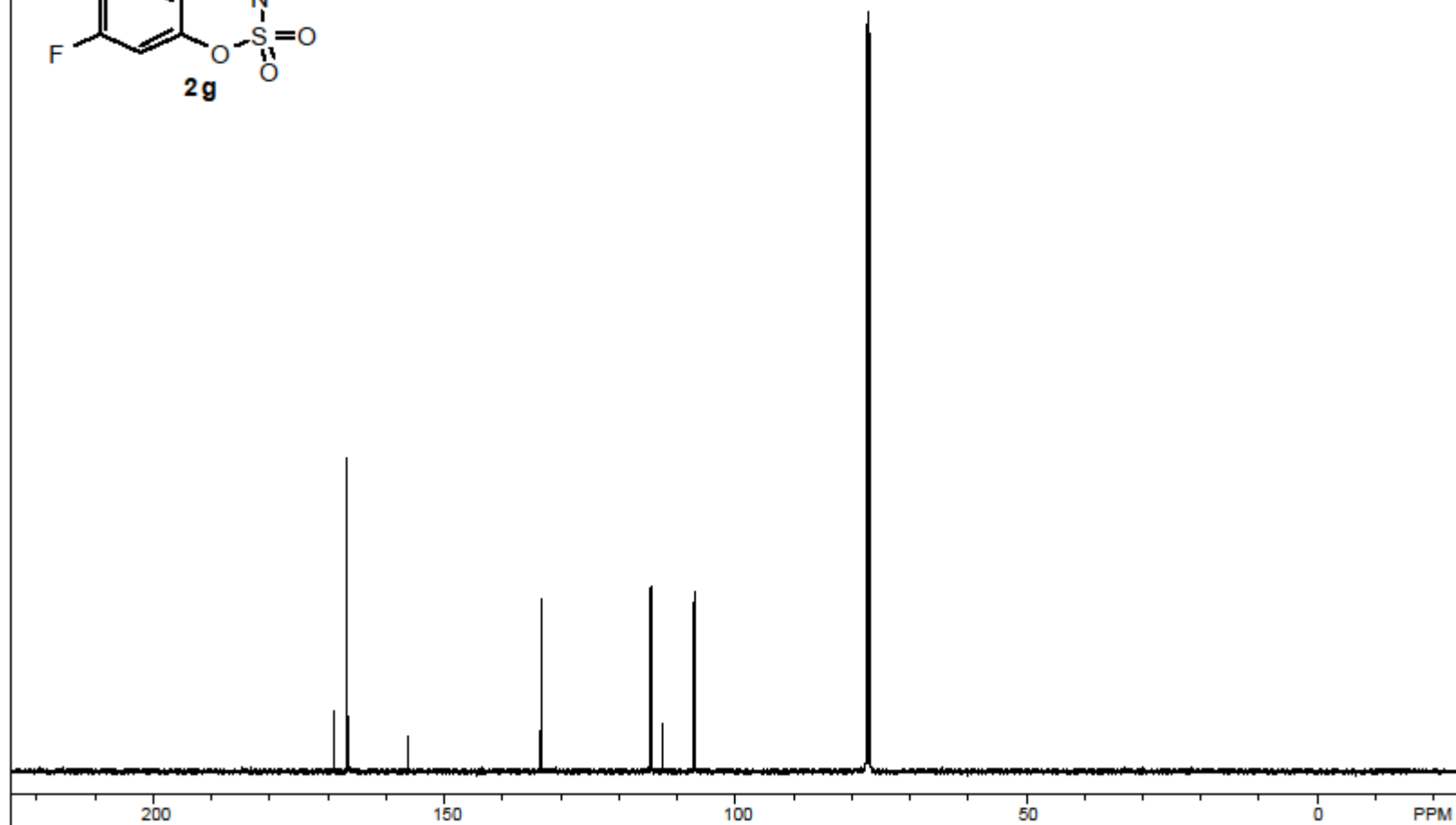
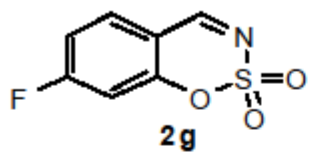




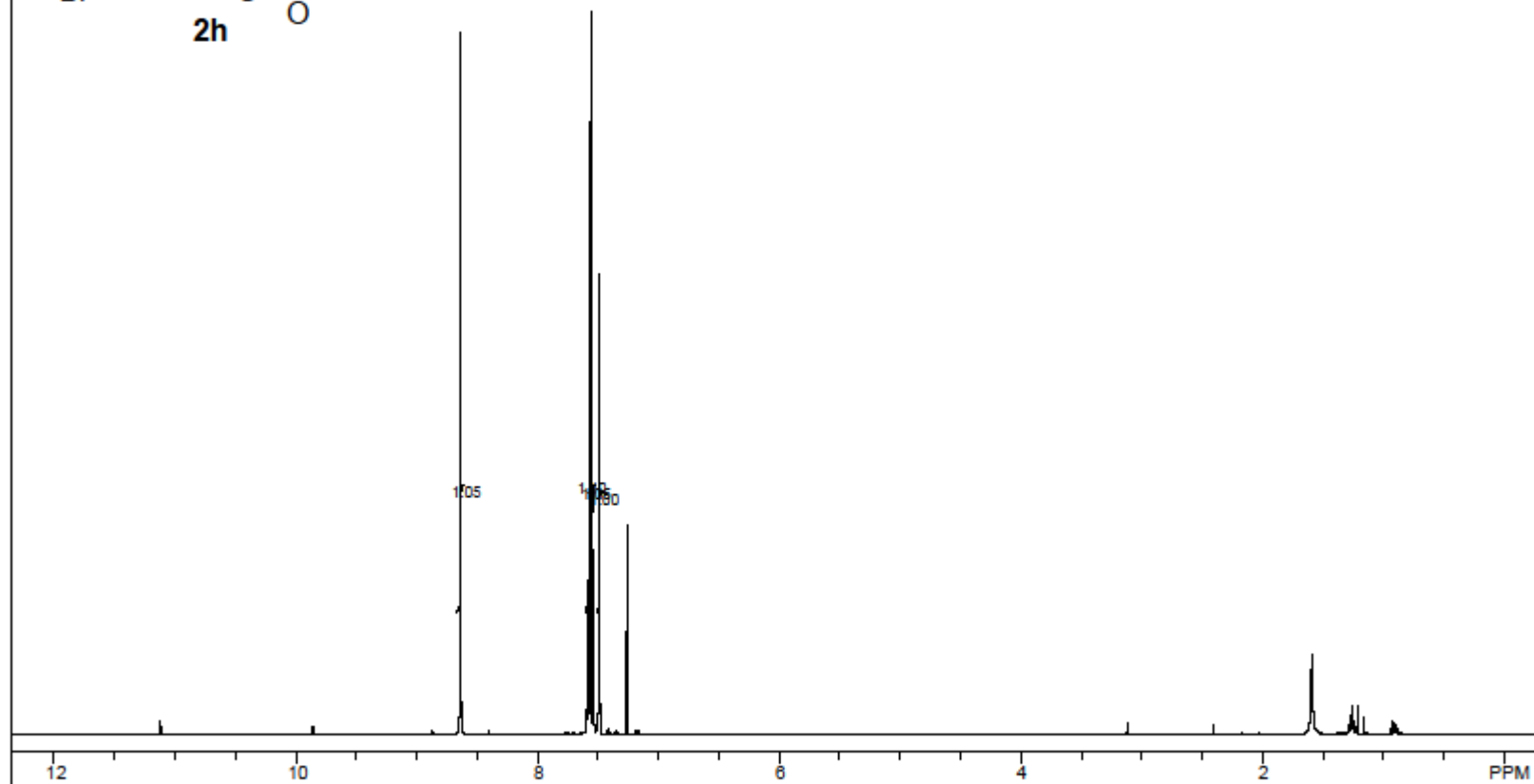
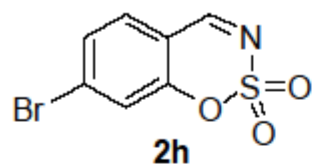
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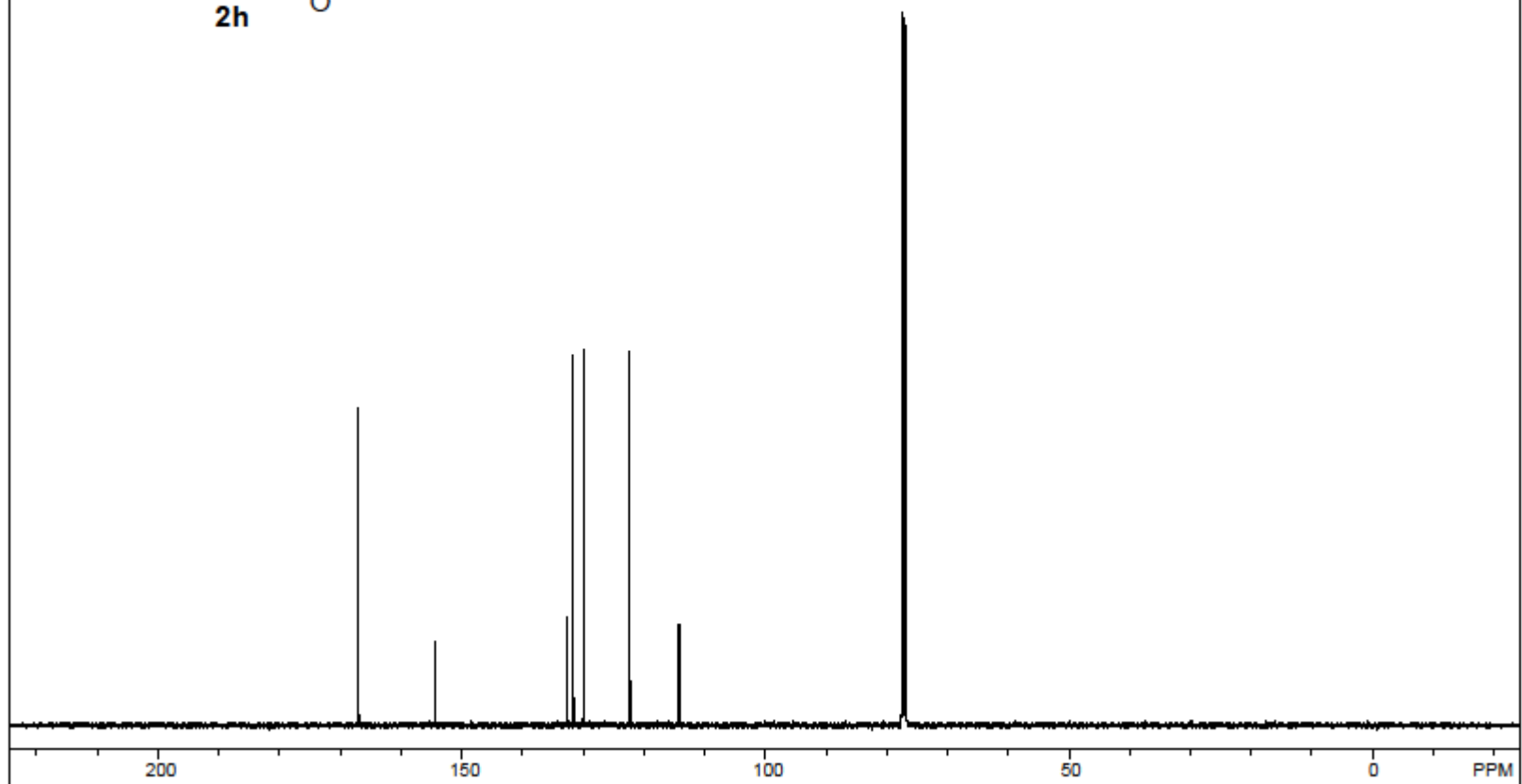
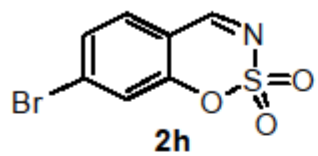
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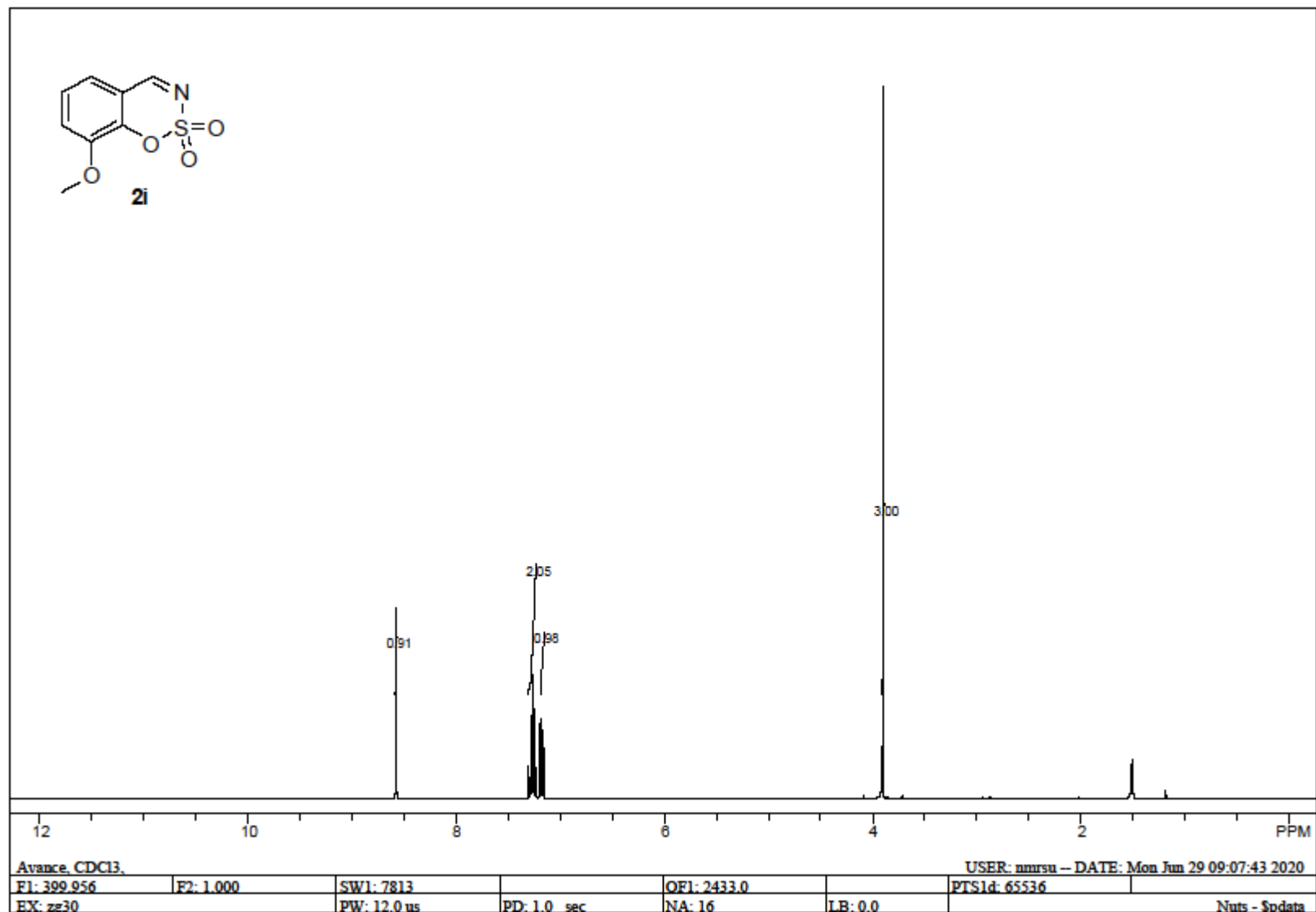
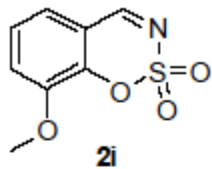
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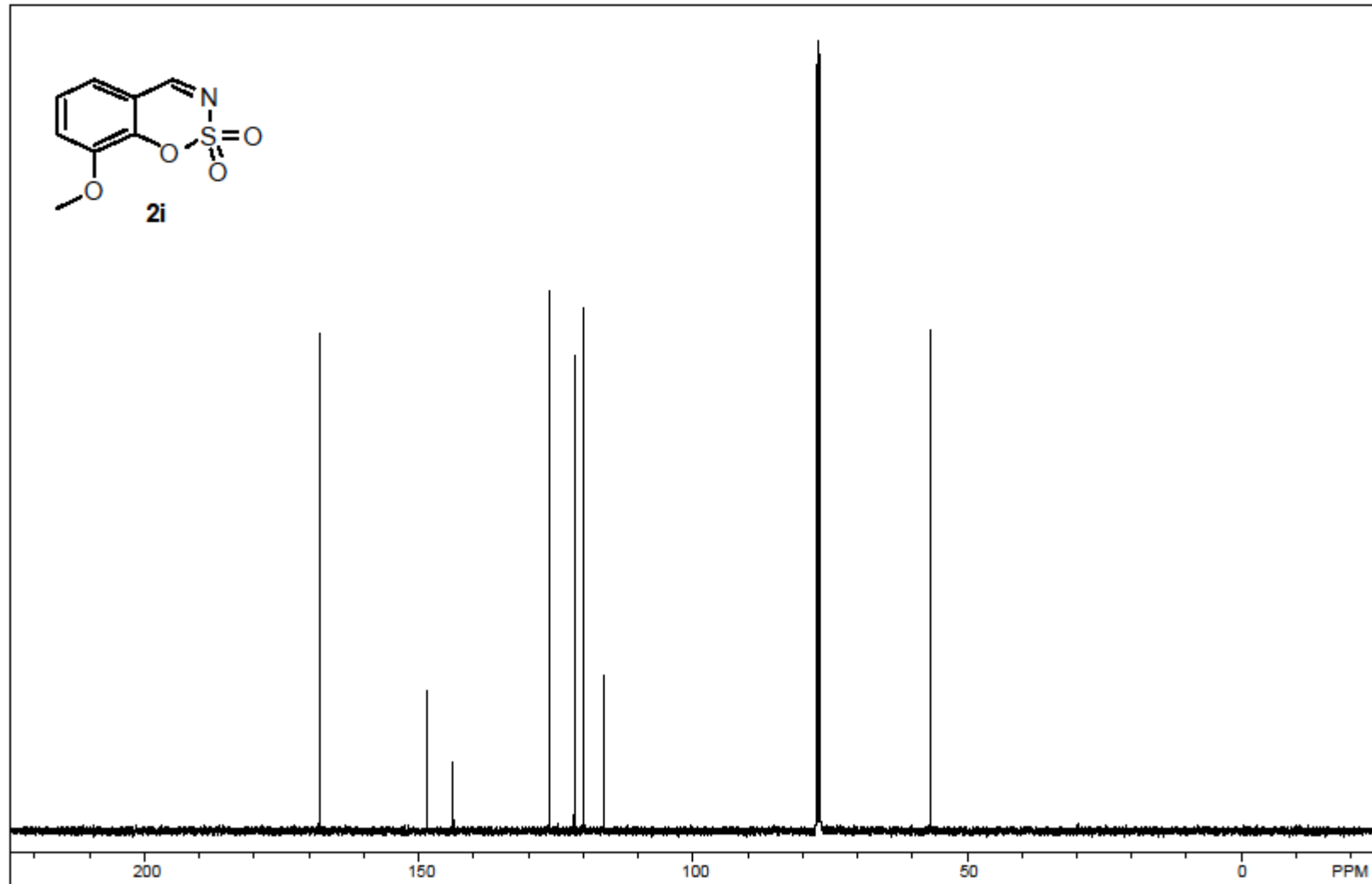
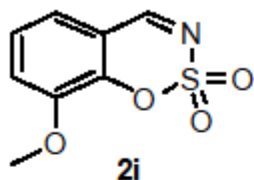


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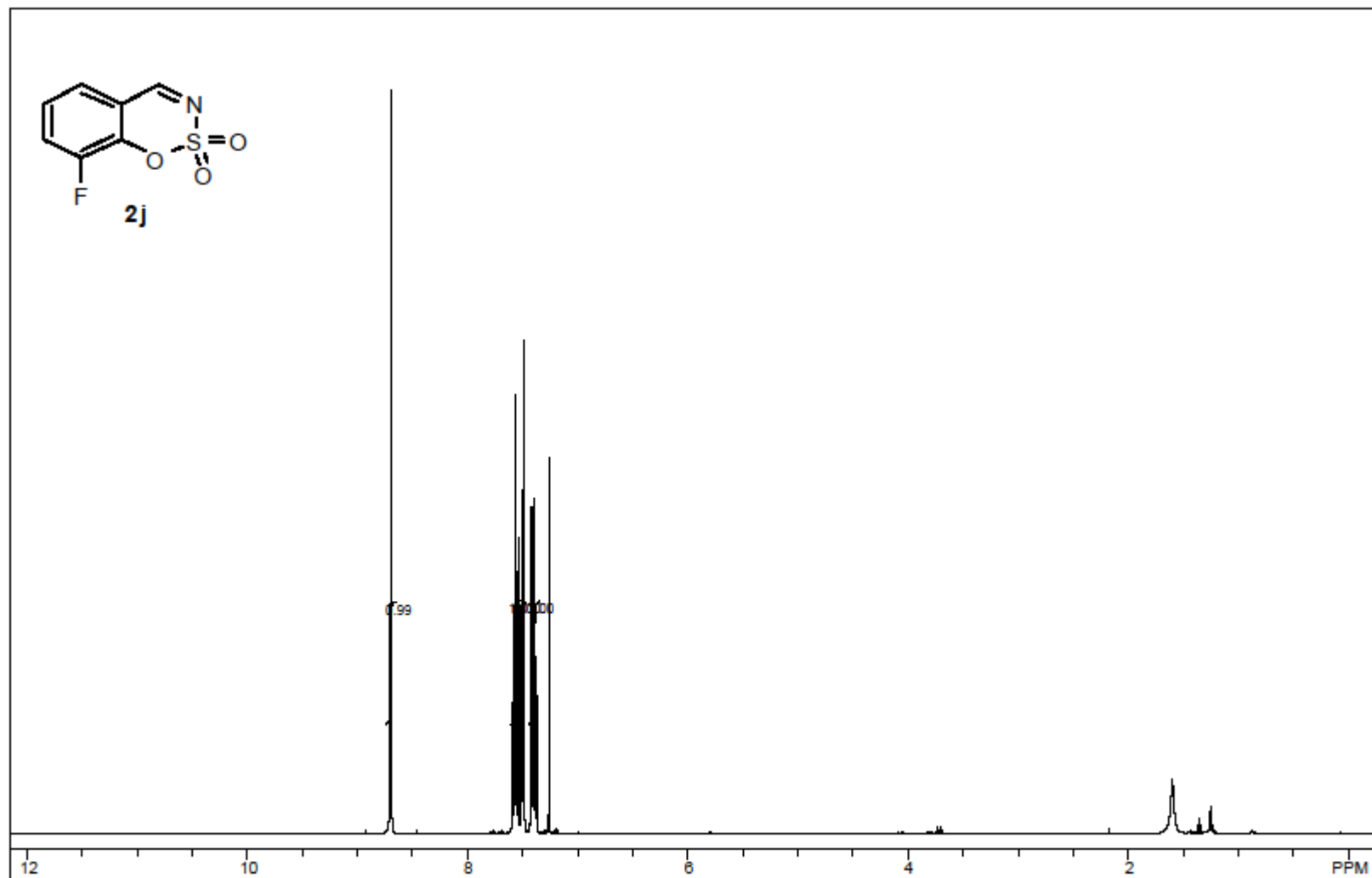
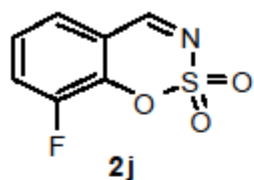


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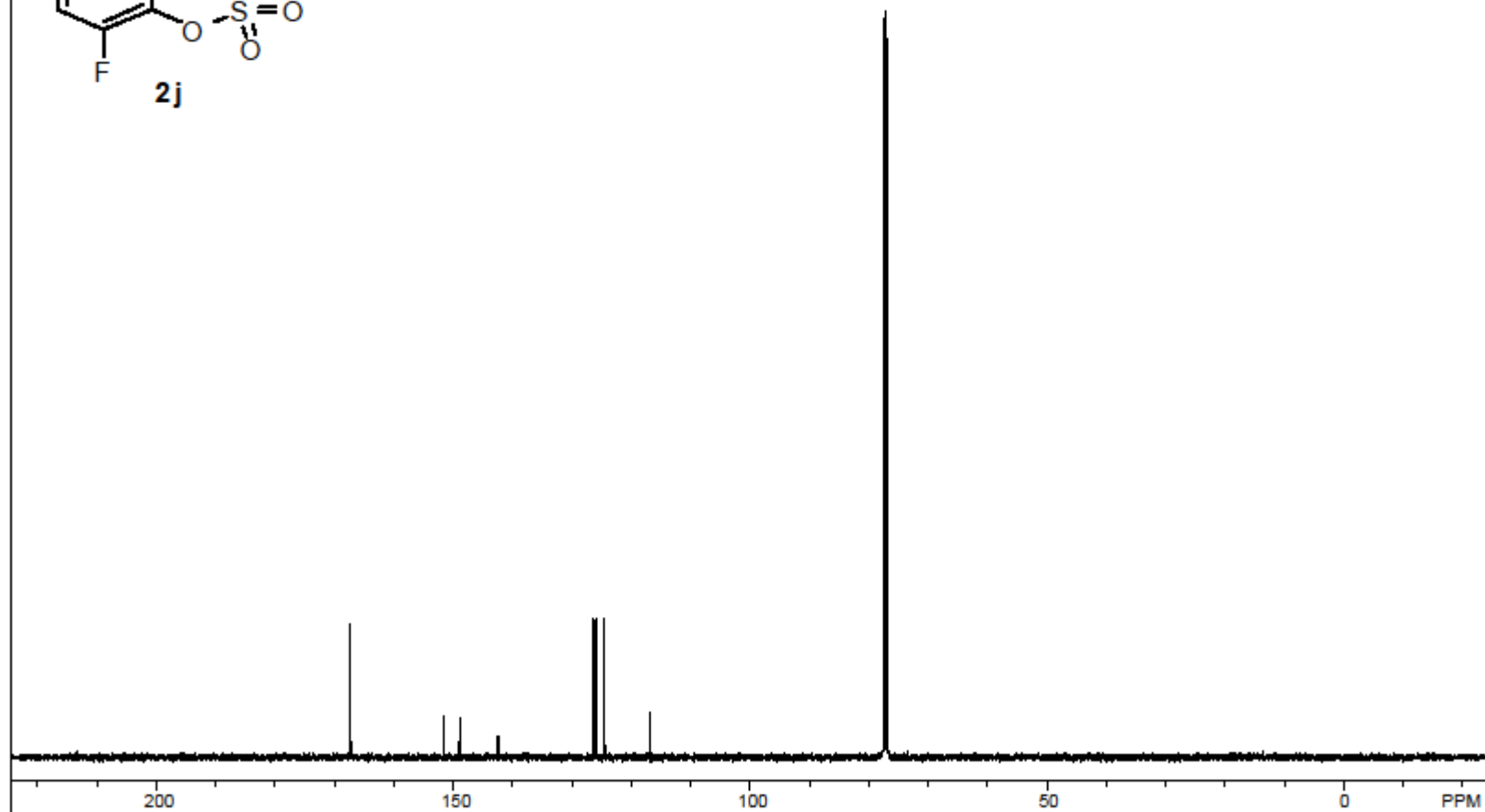
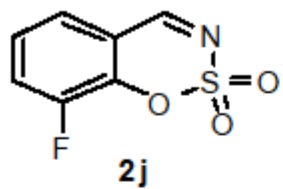




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Avance CDCl3

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SW1: 25000

OF1: 10069.4

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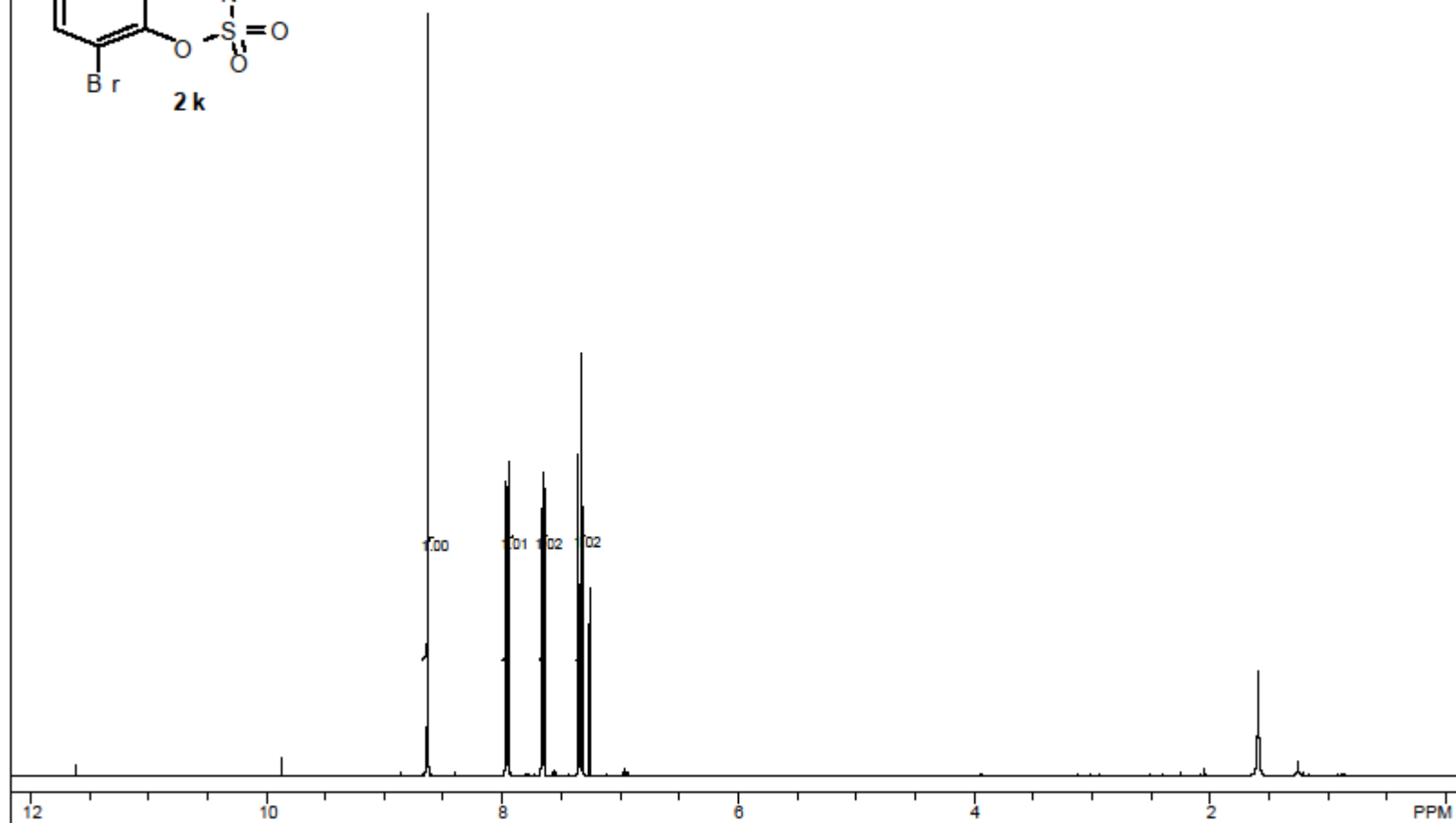
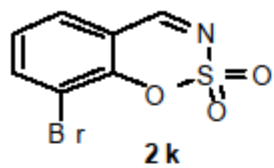
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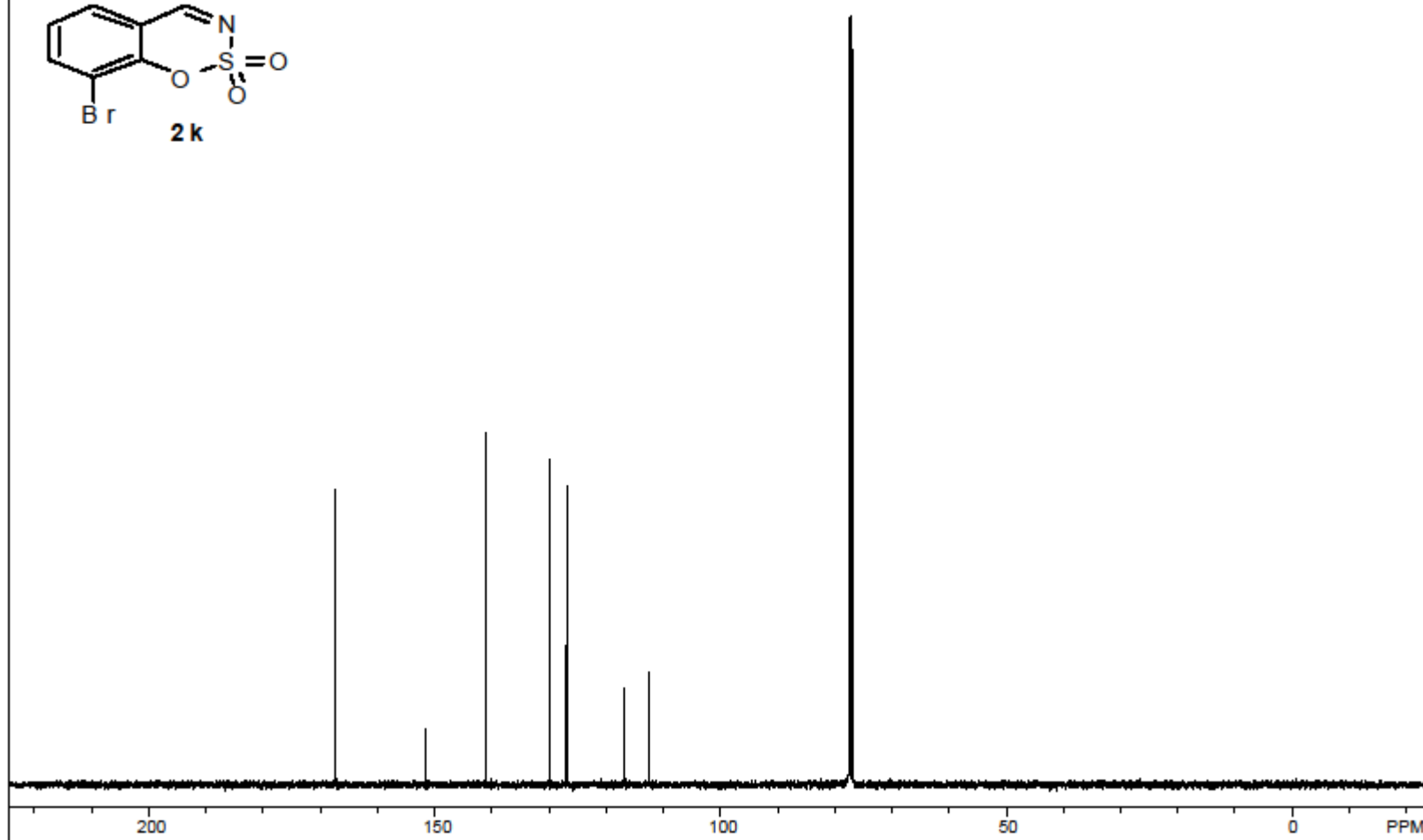
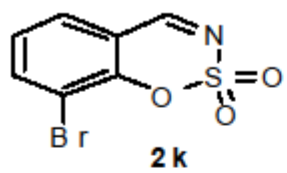
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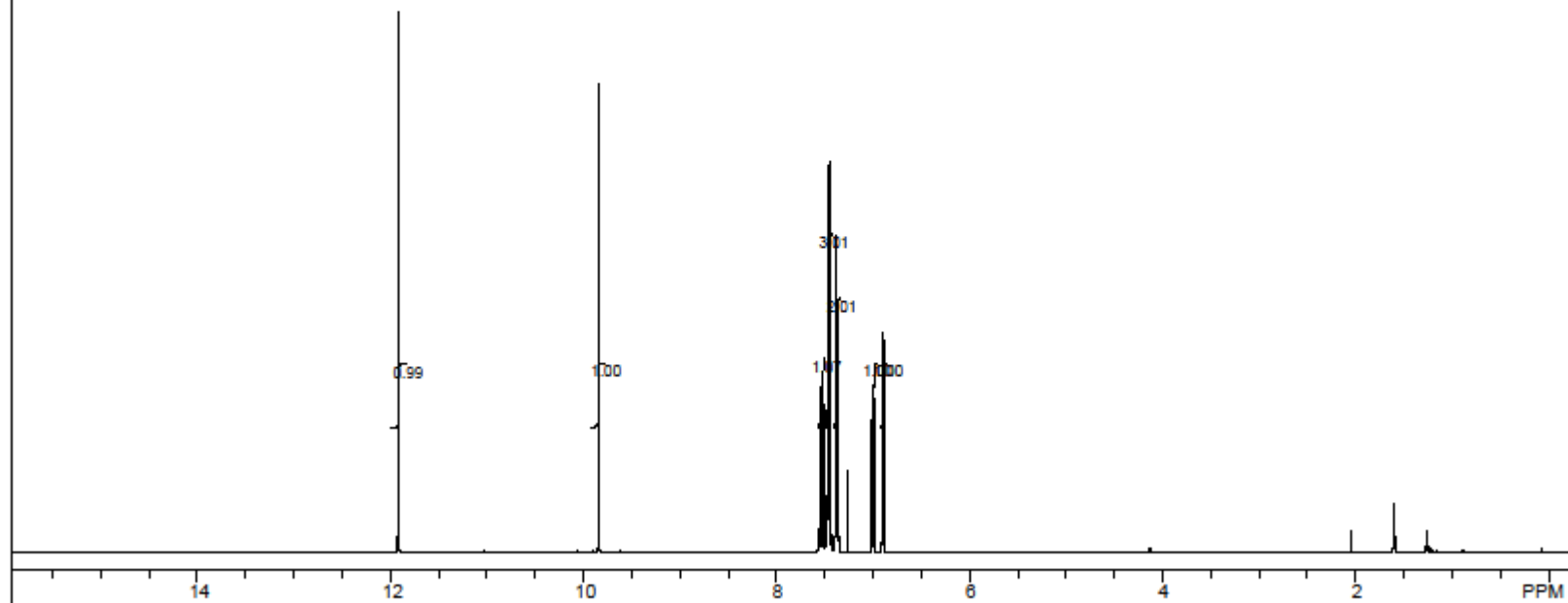
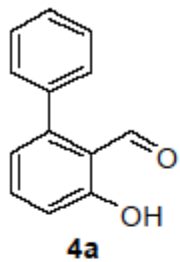
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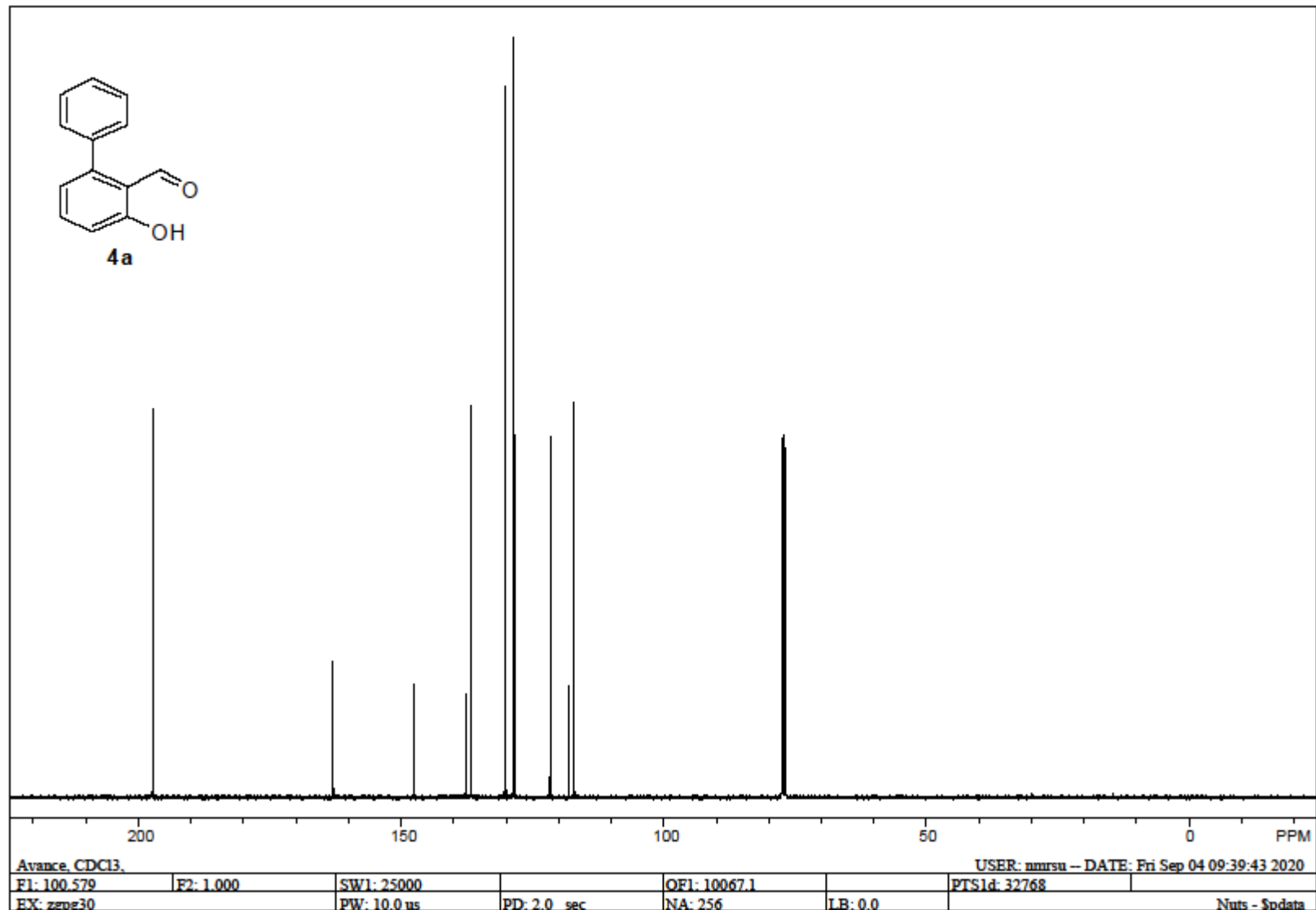
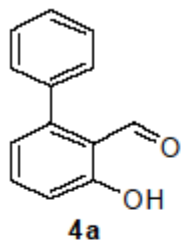
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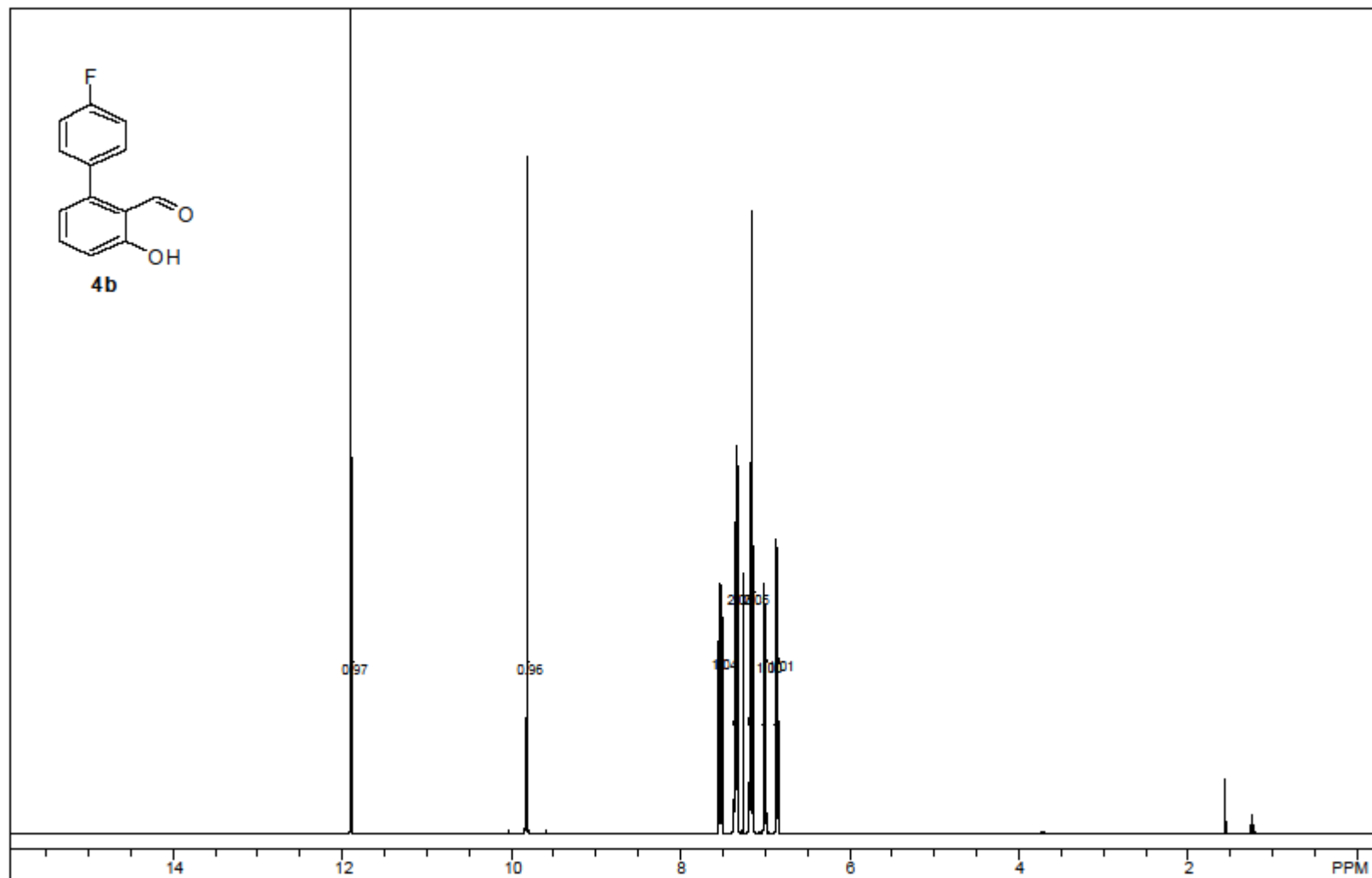
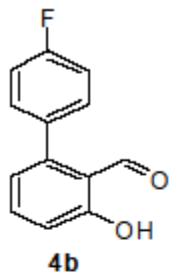


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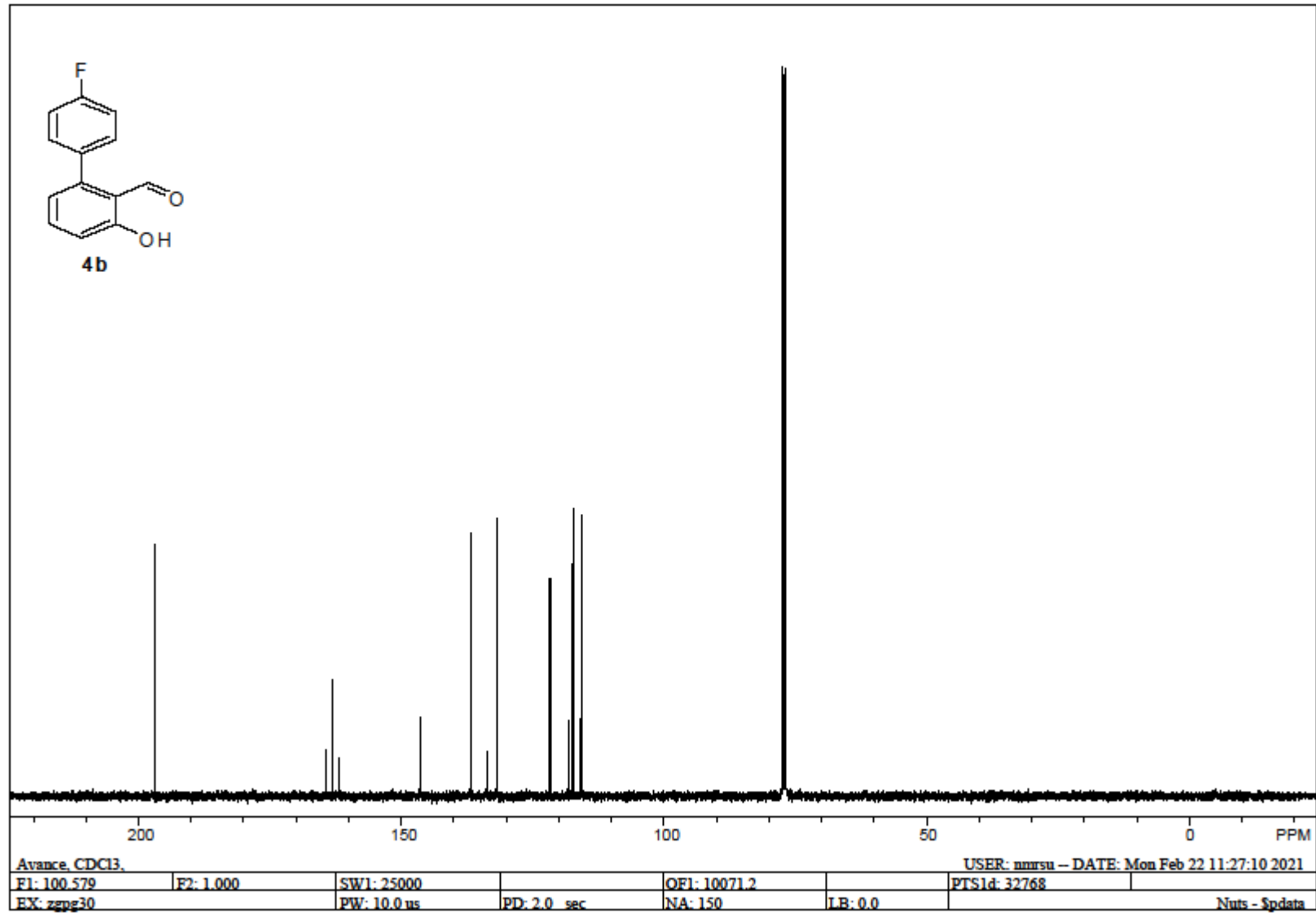
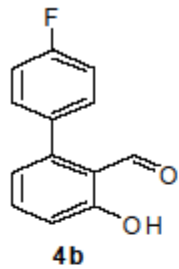


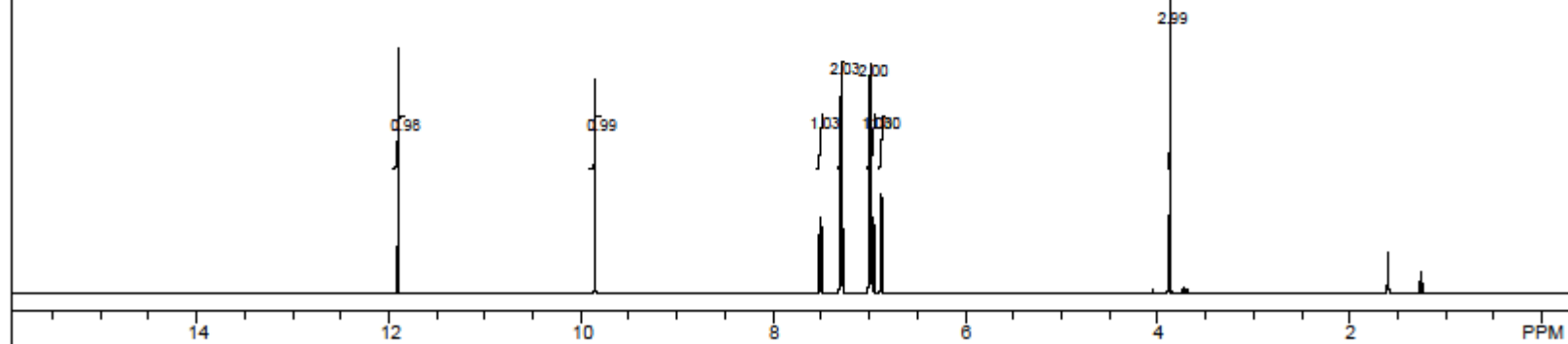
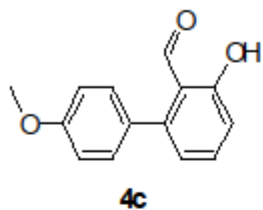
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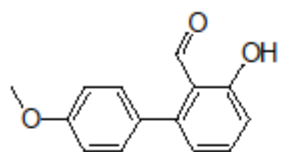


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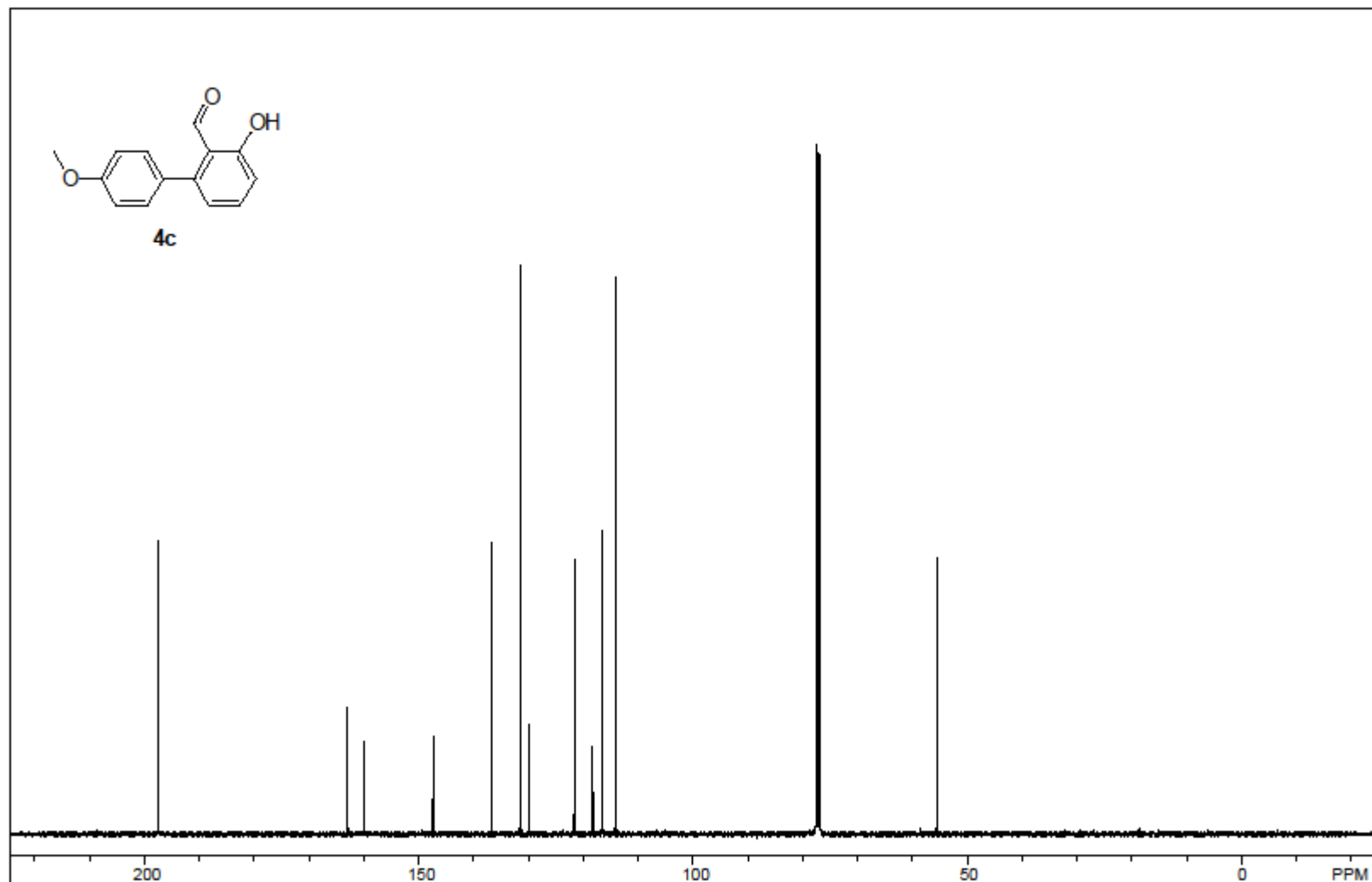




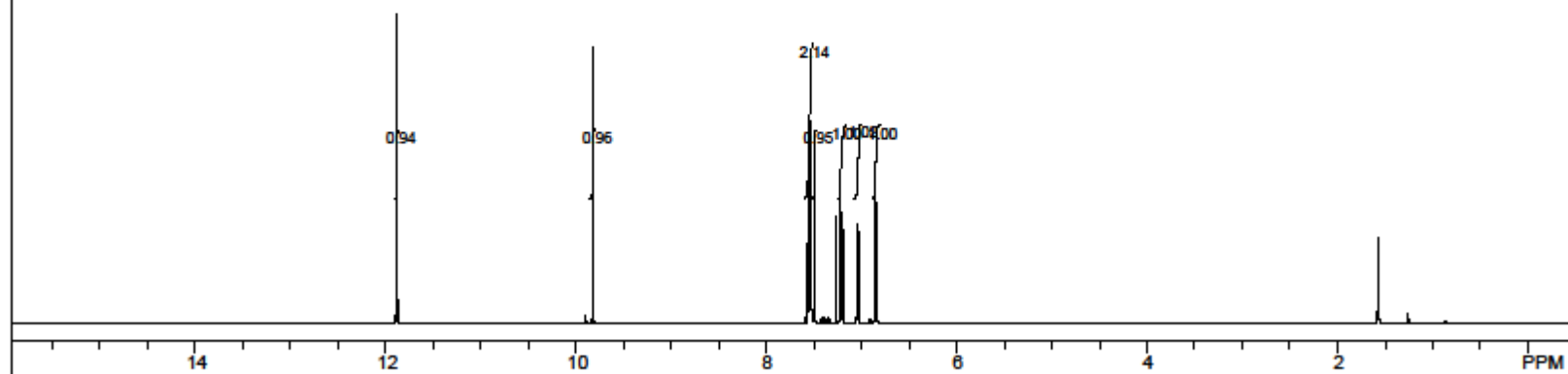
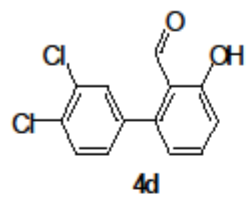
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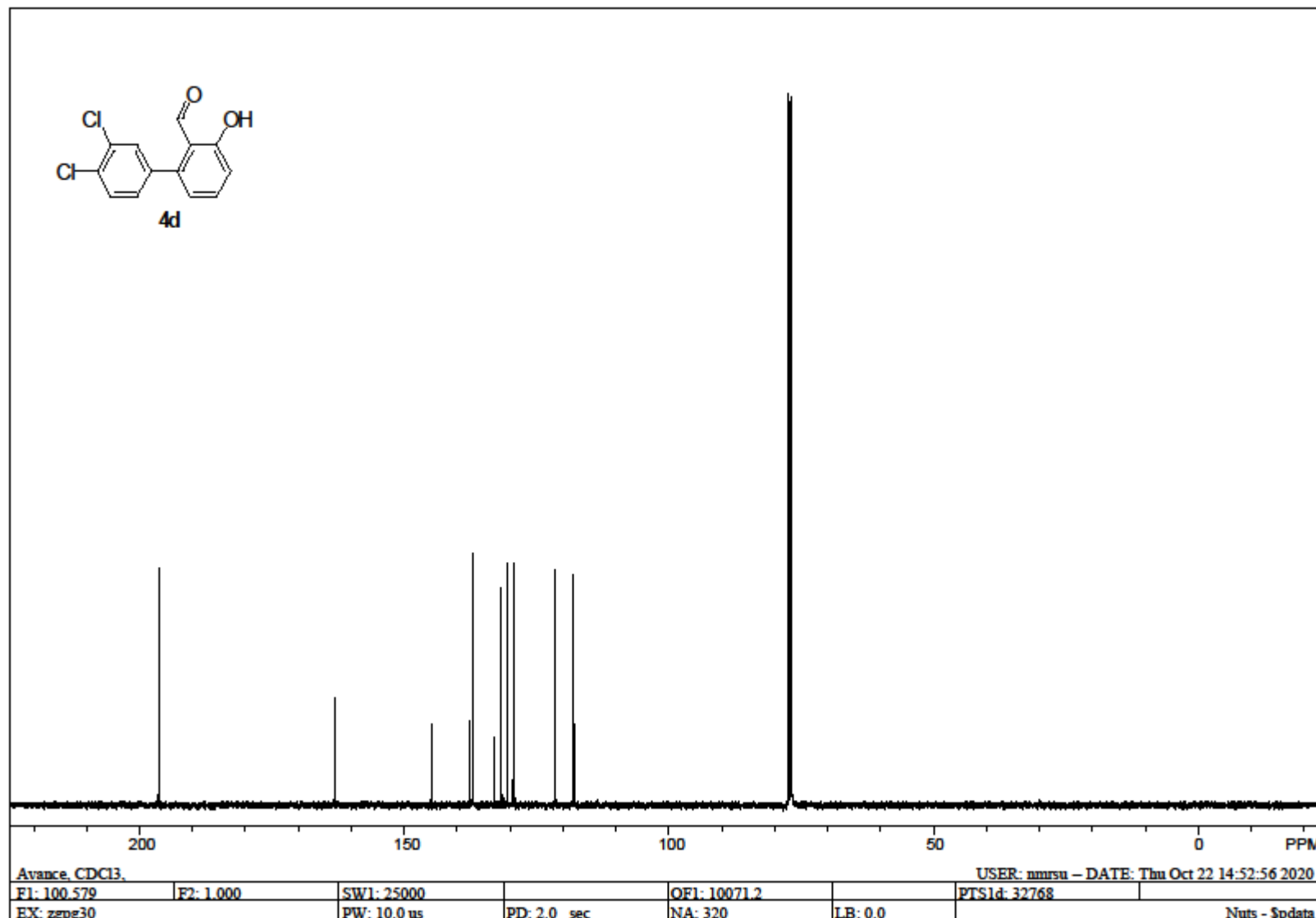
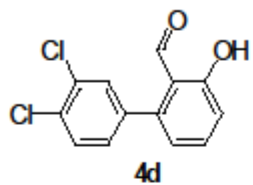
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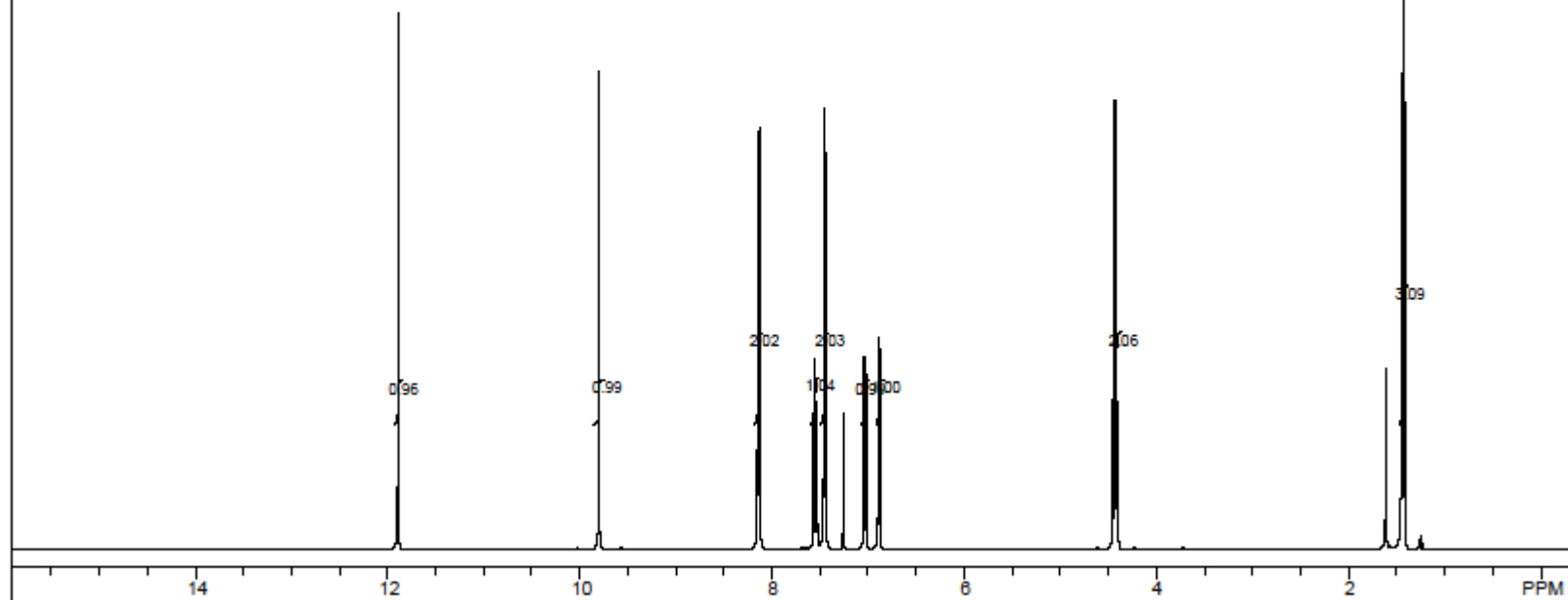
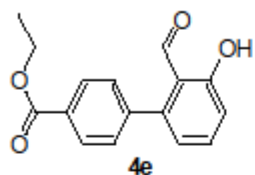


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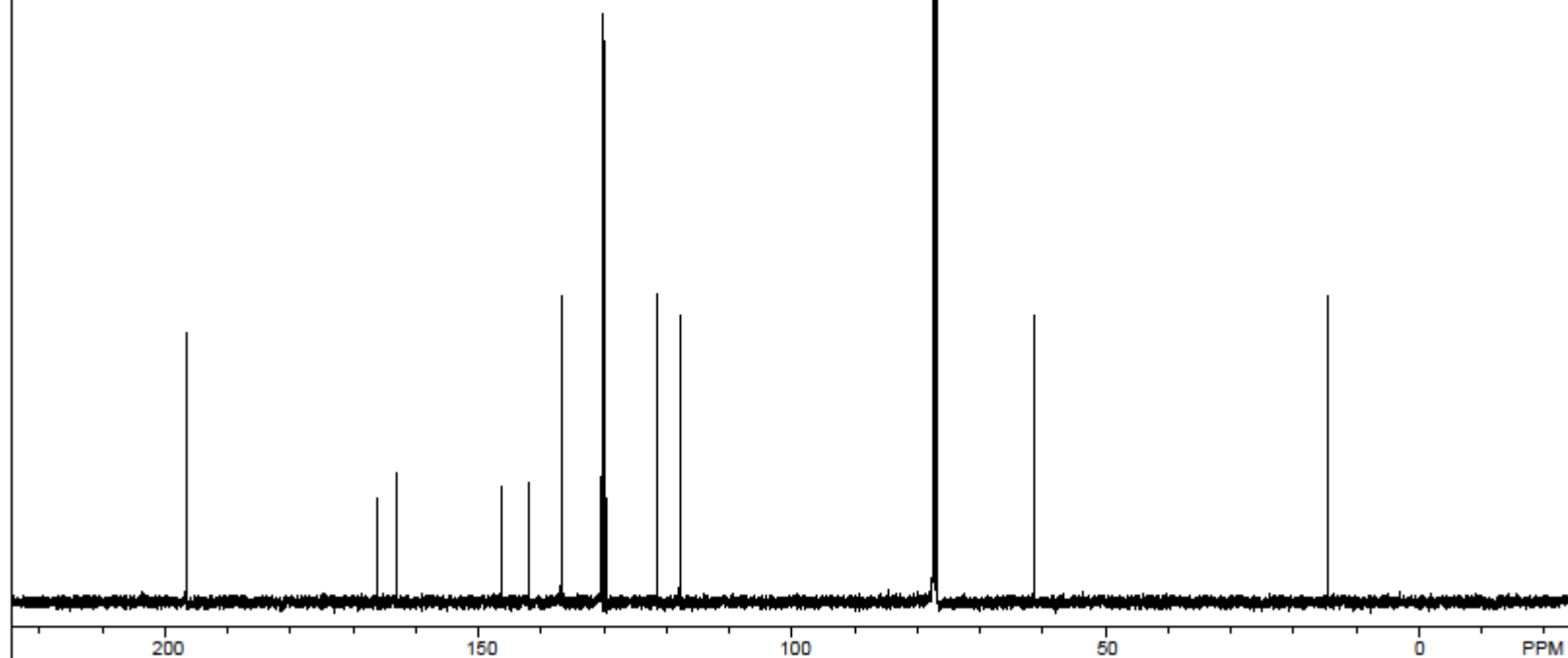
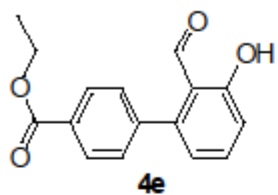


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EX: zg30		PW: 12.0 us	PD: 1.0 sec	NA: 16	LB: 0.0	Nuts - Spdata

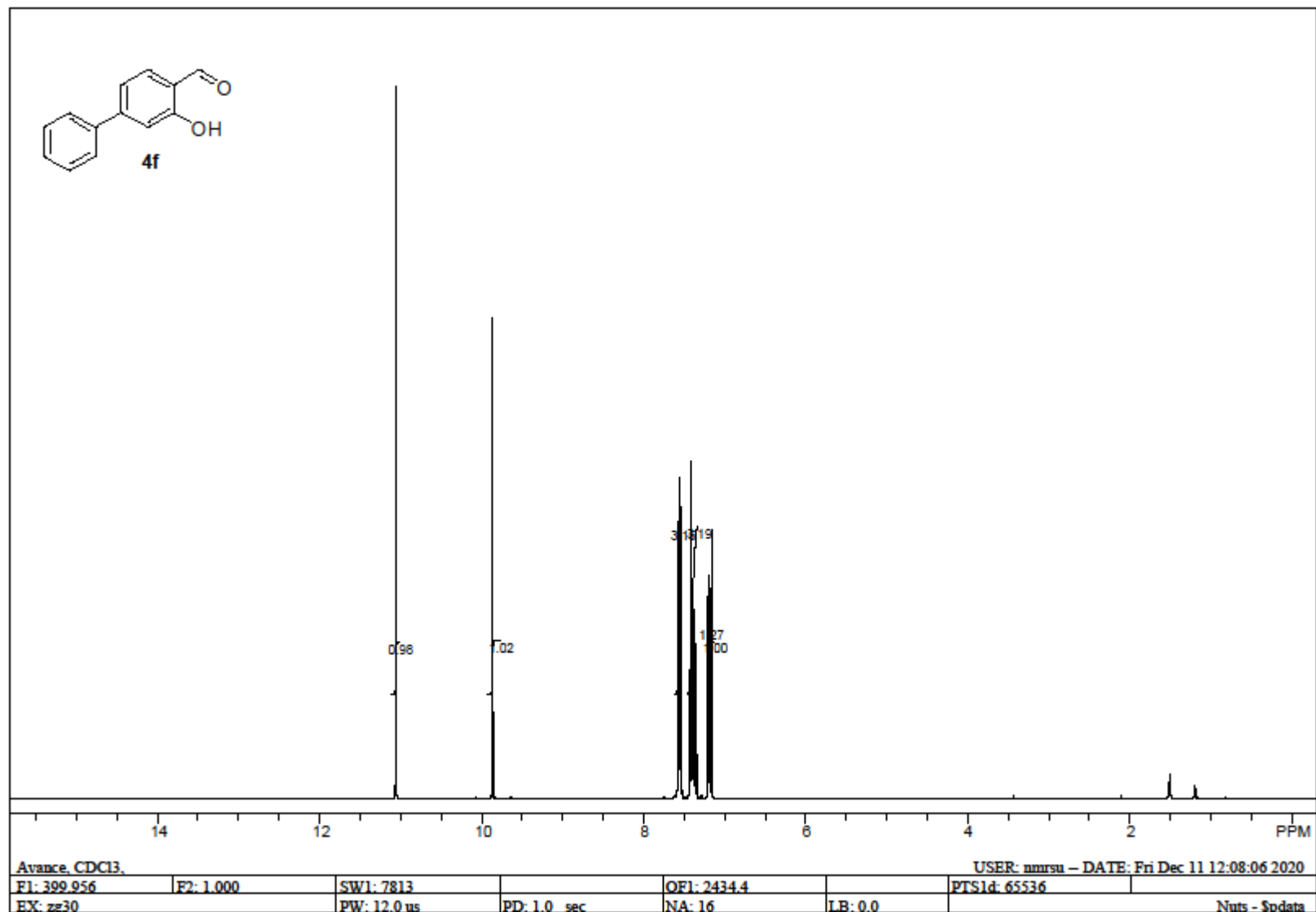
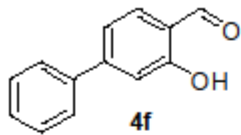


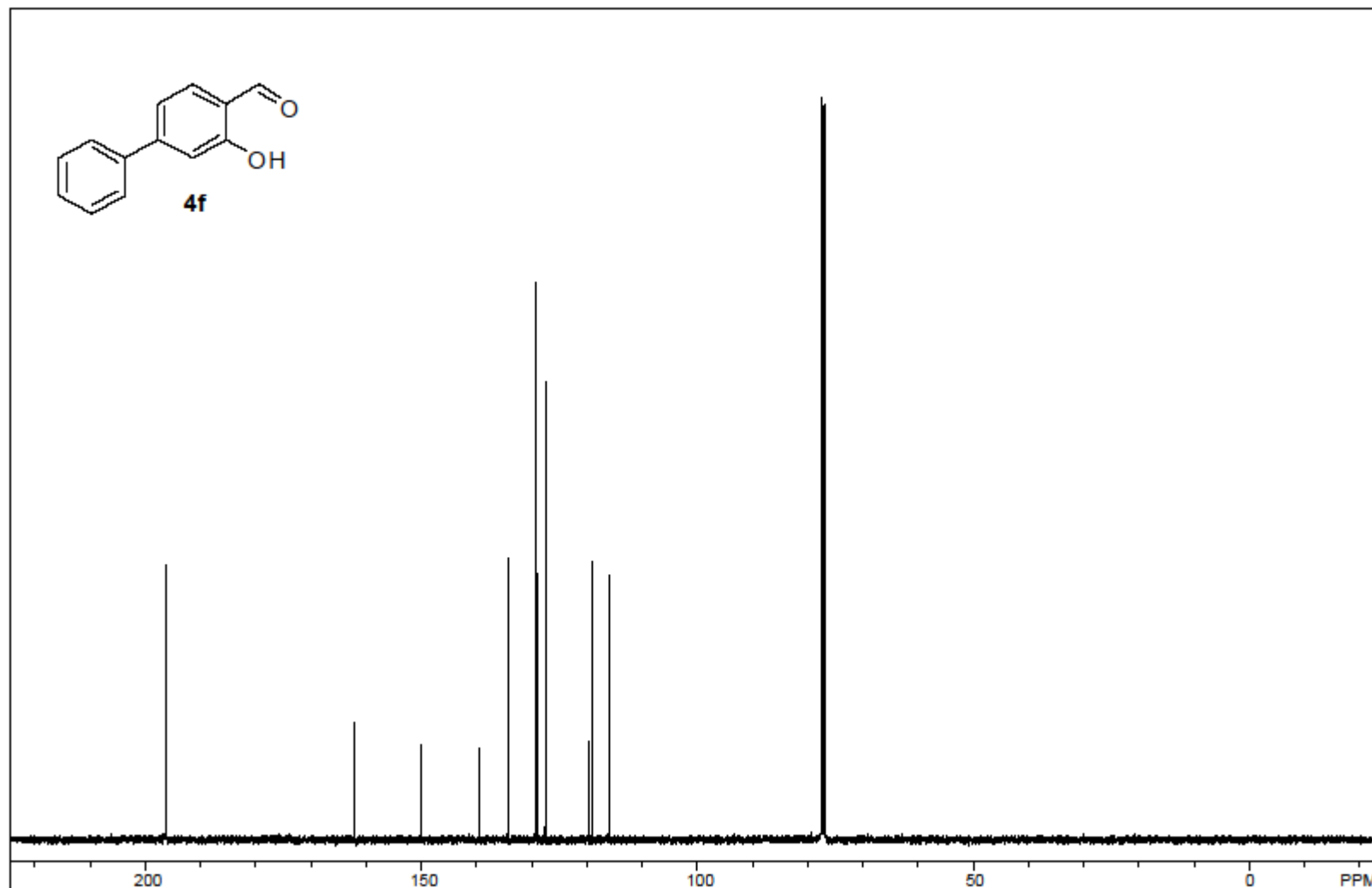
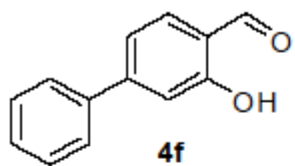


Avance CDCl3			USER: nmrsu - DATE: Thu Oct 22 17:02:19 2020			
F1: 399.956	F2: 1.000	SW1: 7813		OF1: 2460.3		PTS1d: 65536
EX: zg30		PW: 12.0 us	PD: 1.0 sec	NA: 16	LB: 0.0	Nuts - Spdata

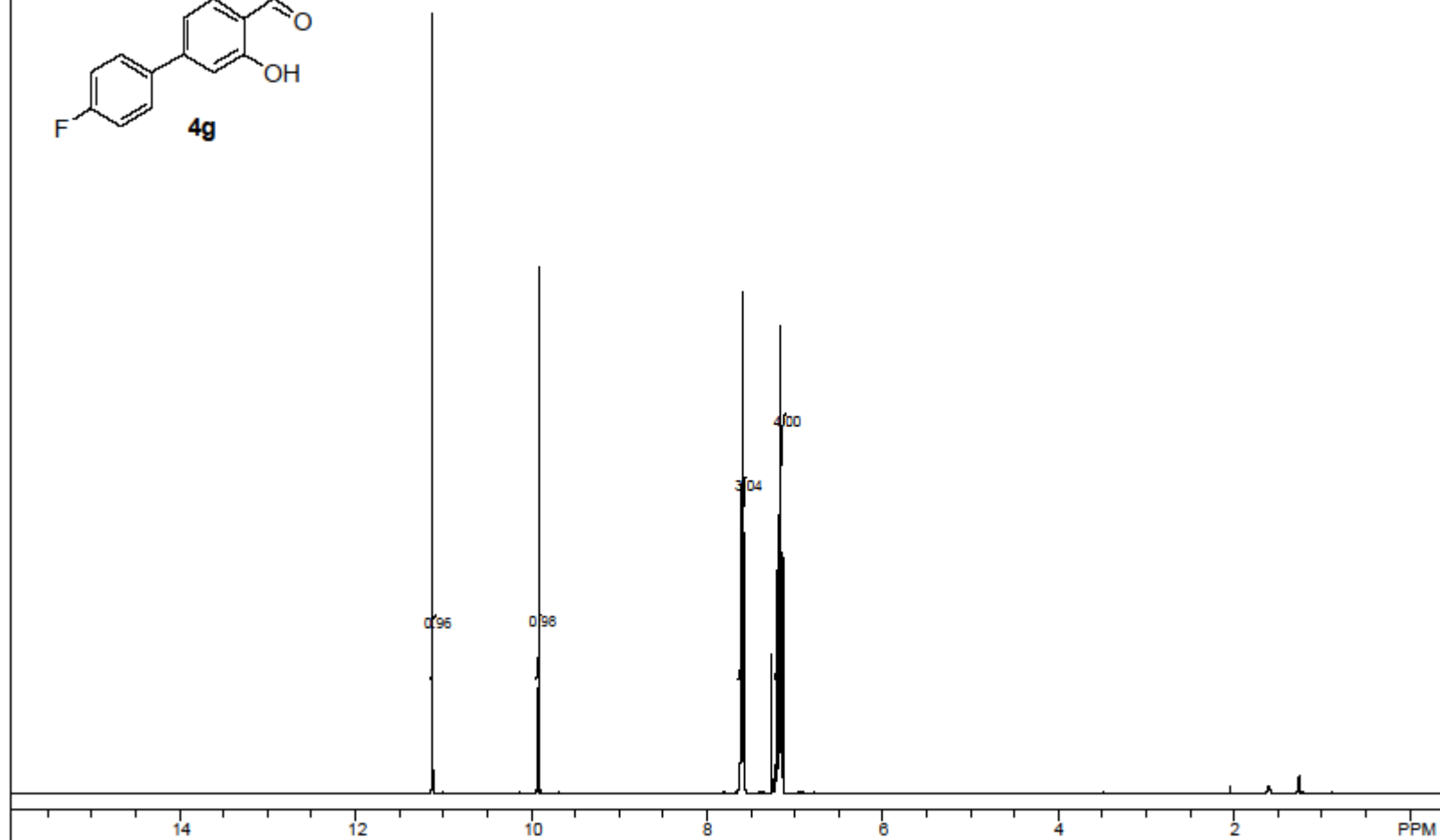
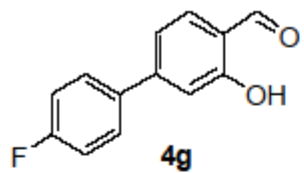


Avance CDCl <sub>3</sub>			USER: nmrsu - DATE: Thu Oct 22 17:11:48 2020			
F1: 100.579	F2: 1.000	SW1: 25000		OF1: 10070.1		PTS1d: 32768
EX: zgpg30		PW: 10.0 us	PD: 2.0 sec	NA: 160	LB: 0.0	Nuts - \$pdata

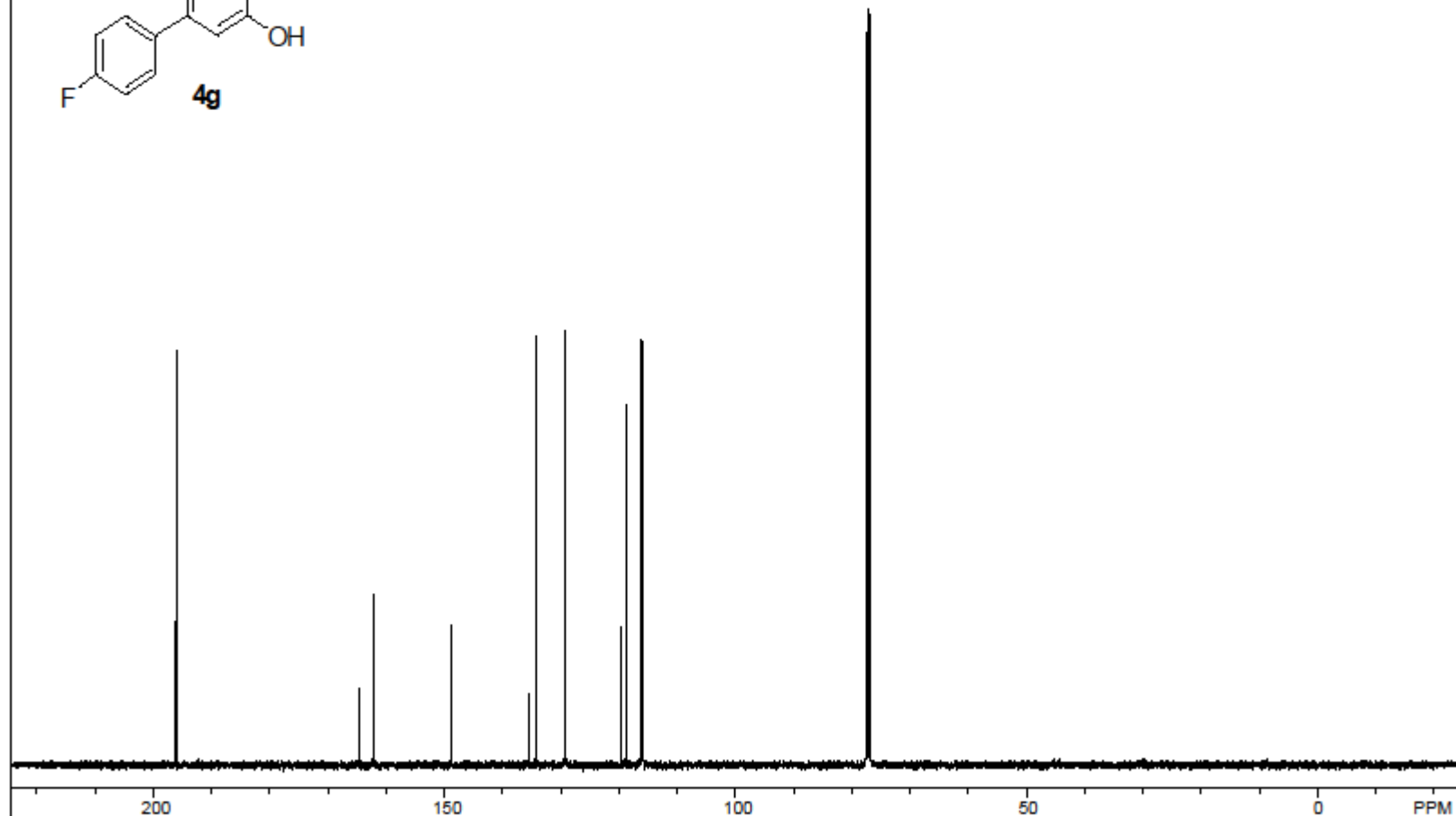
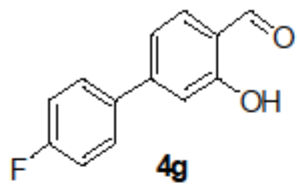




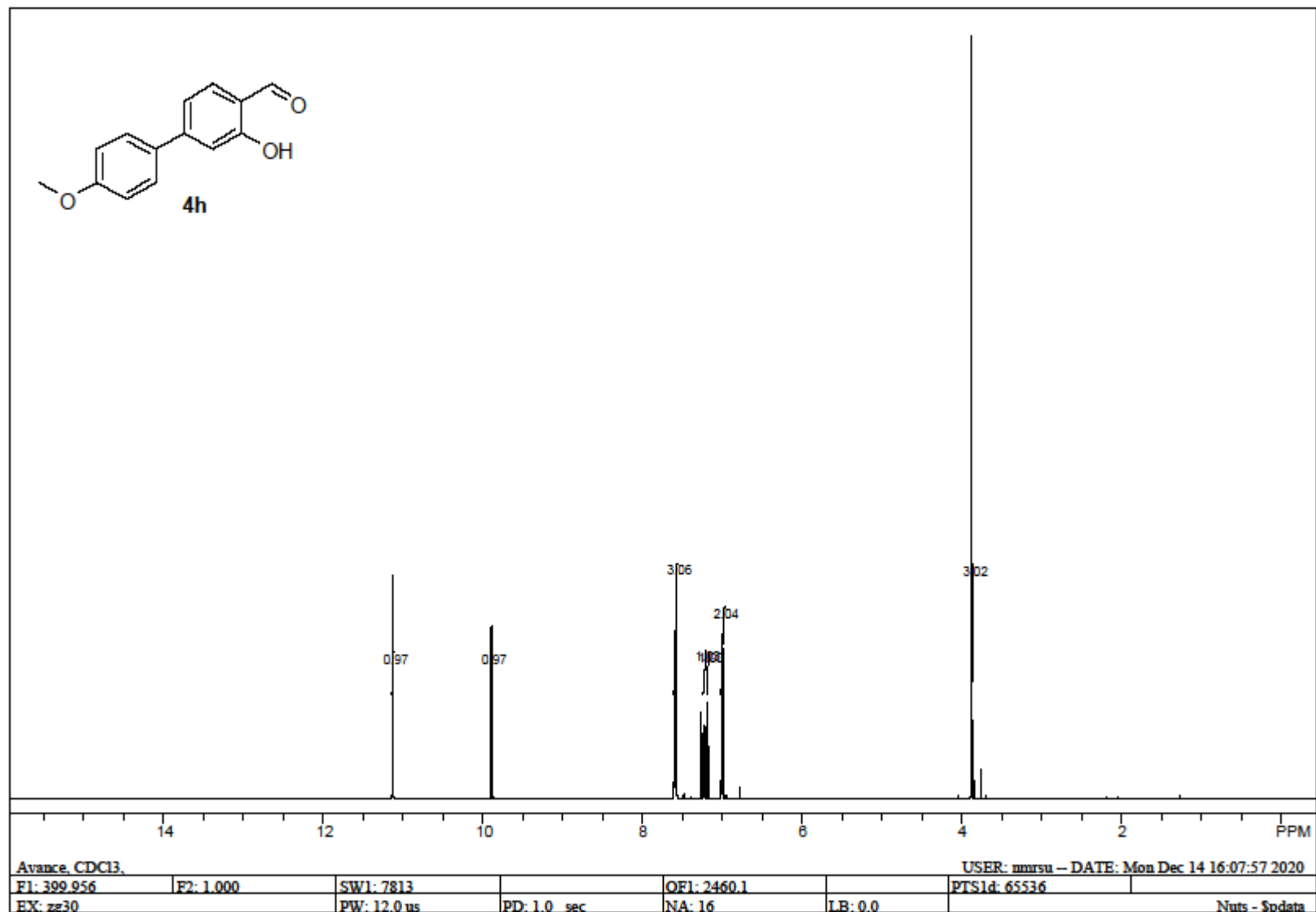
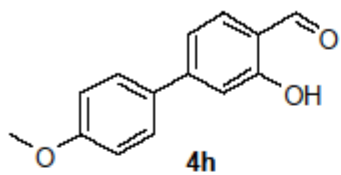
Avance, CDCl <sub>3</sub>			USER: nmrsu - DATE: Fri Dec 11 12:21:08 2020			
F1: 100.579	F2: 1.000	SW1: 25000		OF1: 10070.5		PTS1d: 32768
EX: zgpg30		PW: 10.0 us	PD: 2.0 sec	NA: 256	LB: 0.0	Nuts - Spdata

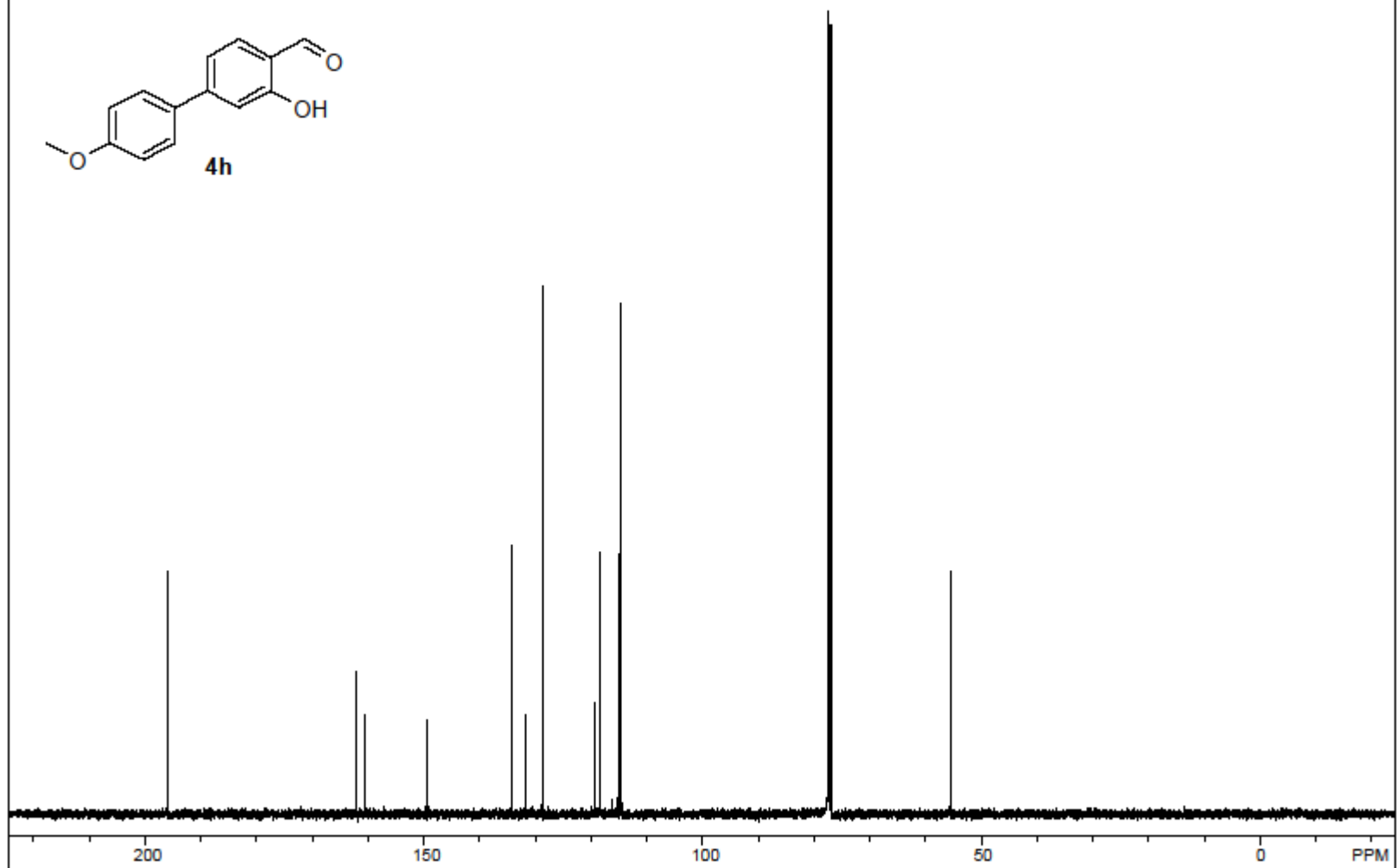
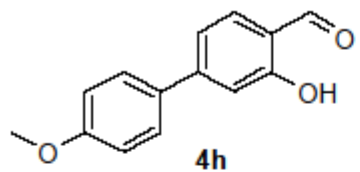


Avance CDCl3			USER: nmrsu - DATE: Fri Dec 11 11:50:19 2020			
F1: 399.956	F2: 1.000	SW1: 7813		OF1: 2460.1		PTS1d: 65536
EX: zg30		PW: 12.0 us	PD: 1.0 sec	NA: 16	LB: 0.0	Nuts - Spdata

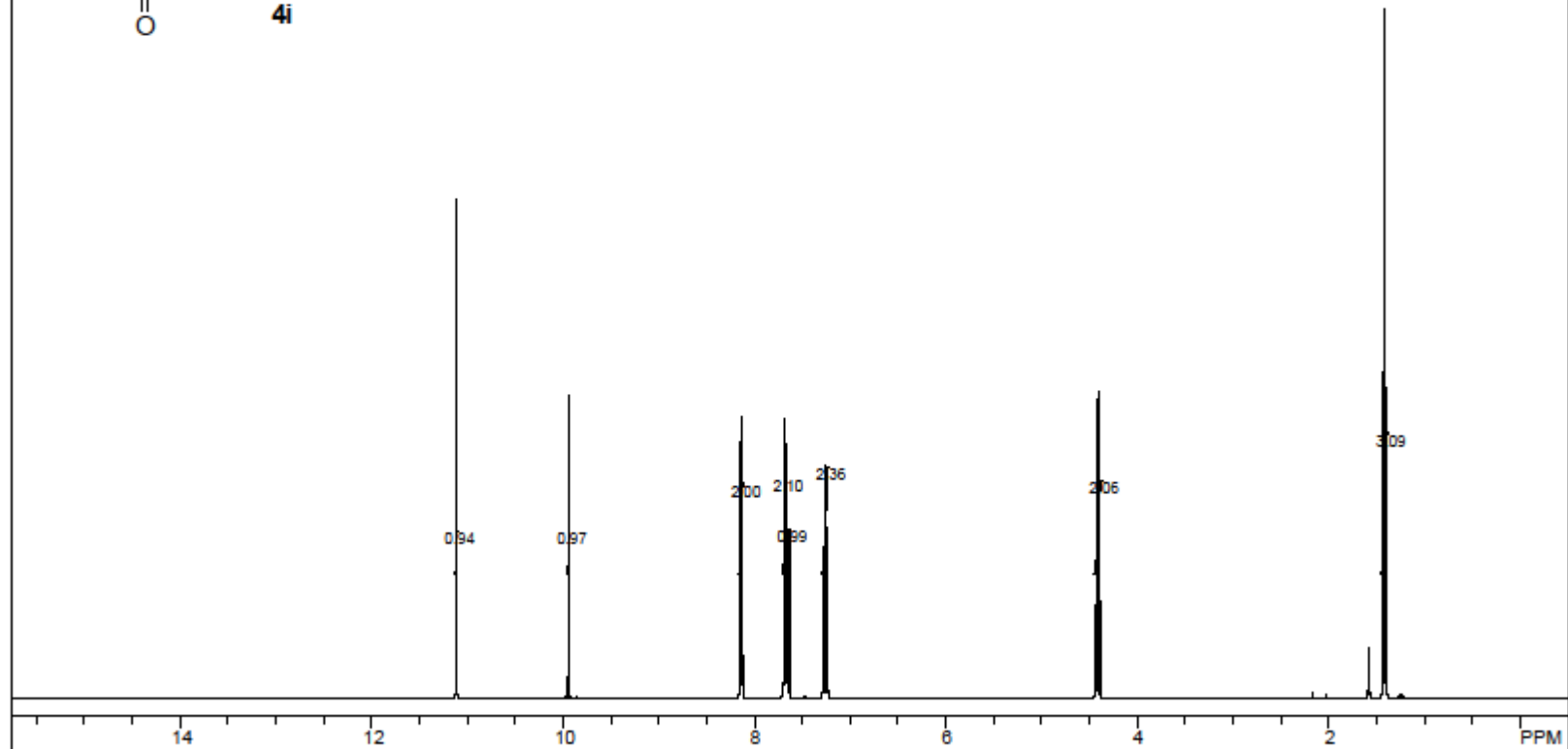
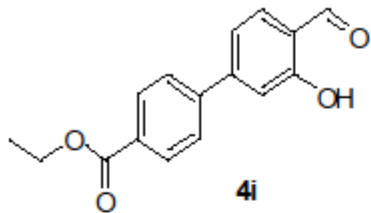


Avance CDCl <sub>3</sub>			USER: nmrsu - DATE: Fri Dec 11 12:03:38 2020			
F1: 100.579	F2: 1.000	SW1: 25000		OFl: 10069.2		PTS1d: 32768
EX: zgpg30		PW: 10.0 us	PD: 2.0 sec	NA: 256	LB: 0.0	Nuts - \$pdata

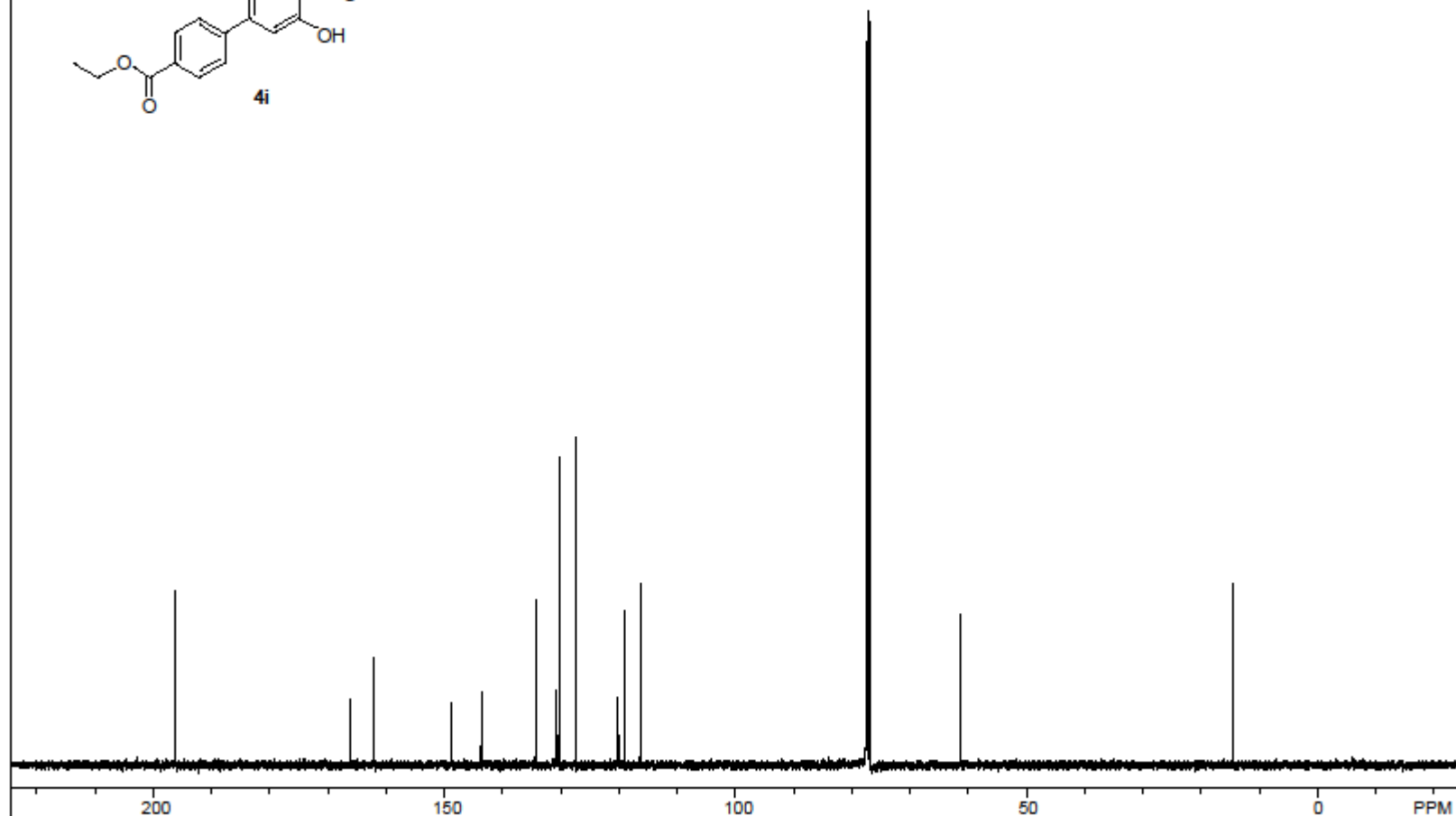
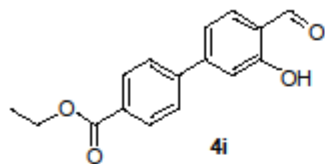




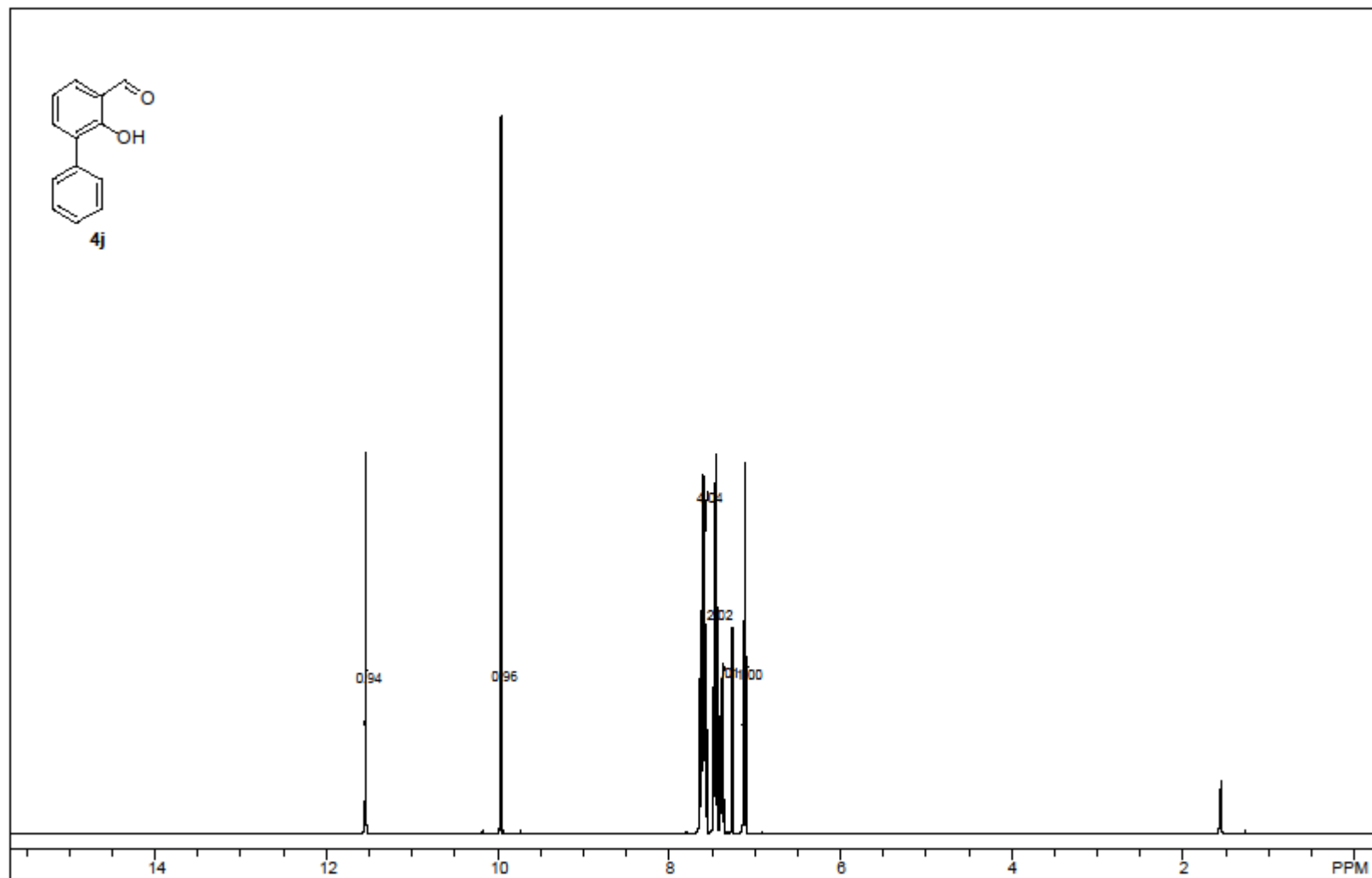
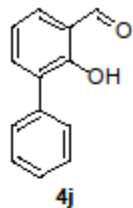
Avance CDCl3			USER: nmrsu -- DATE: Mon Dec 14 16:17:47 2020			
F1: 100.579	F2: 1.000	SW1: 25000		OF1: 10070.5		PTS1d: 32768
EX: zgpg30		PW: 10.0 us	PD: 2.0 sec	NA: 180	LB: 0.0	Nuts - \$pdata



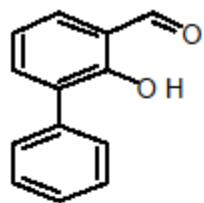
Avance CDCl <sub>3</sub>		USER: nmrsu -- DATE: Mon Dec 14 16:37:46 2020			
F1: 399.956	F2: 1.000	SW1: 7813	OF1: 2460.1	PTS1d: 65536	
EX: zg30		PW: 12.0 us	PD: 1.0 sec	NA: 16	LB: 0.0
					Nuts - Spdata



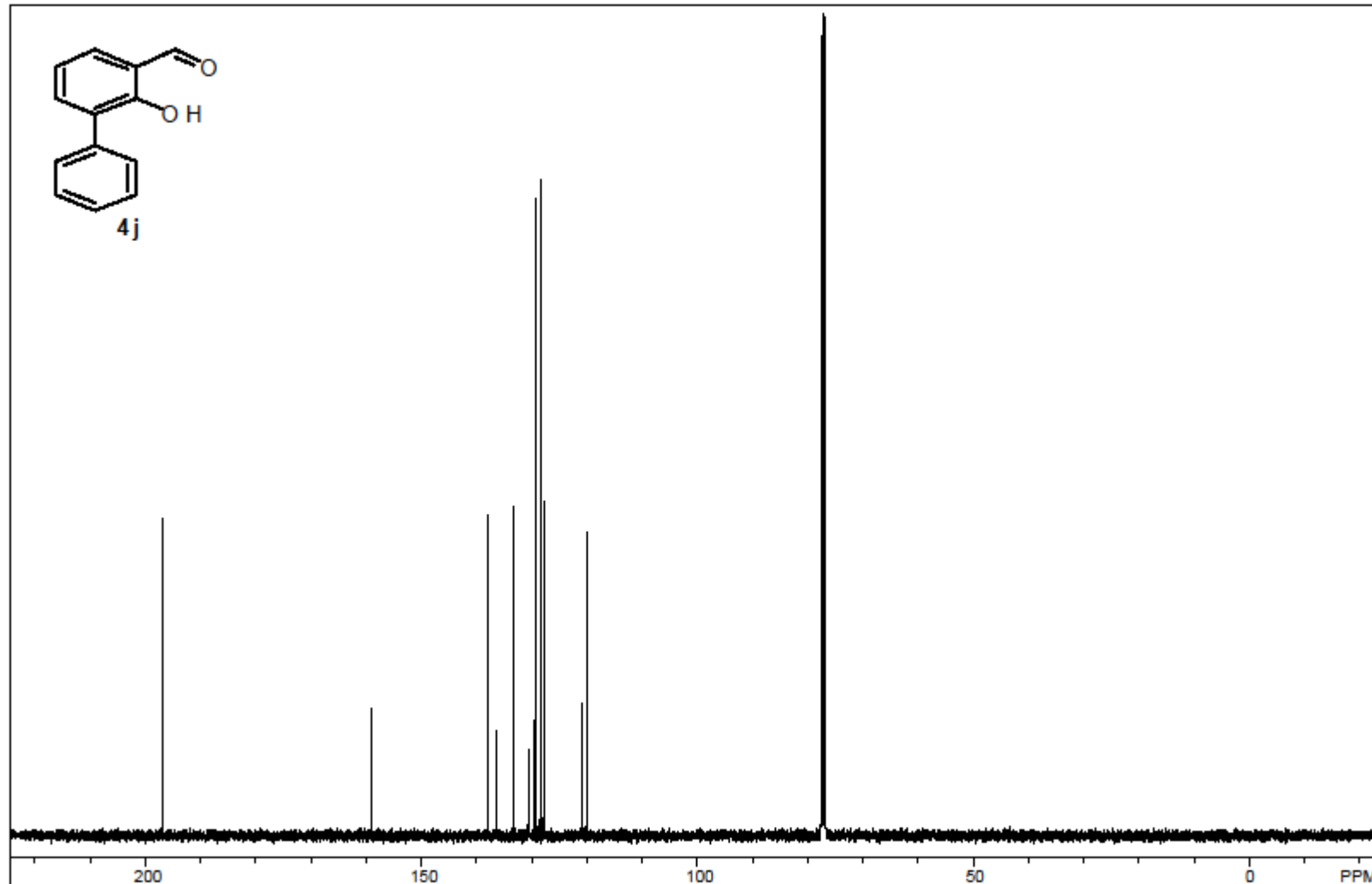
Avance, CDCl <sub>3</sub>						USER: nmrsu -- DATE: Mon Dec 14 16:47:39 2020	
F1: 100.579	F2: 1.000	SW1: 25000		OF1: 10070.2		PTS1d: 32768	
EX: zgpg30		PW: 10.0 us	PD: 2.0 sec	NA: 180	LB: 0.0		Nuts - \$pdata



Avance CDCl3			USER: nmsu -- DATE: Mon Jan 11 11:57:07 2021			
F1: 399.956	F2: 1.000	SW1: 7813		OF1: 2459.9		PTS1d: 65536
EX: zg30		PW: 12.0 us	PD: 1.0 sec	NA: 16	LB: 0.0	Nuts - Spdata



4j



Avance, CDCl3,

USER: nrsu -- DATE: Mon Jan 11 12:06:45 2021

F1: 100.579 F2: 1.000

SW1: 25000

OF1: 10069.3

PTS1d: 32768

EX: zgpg30

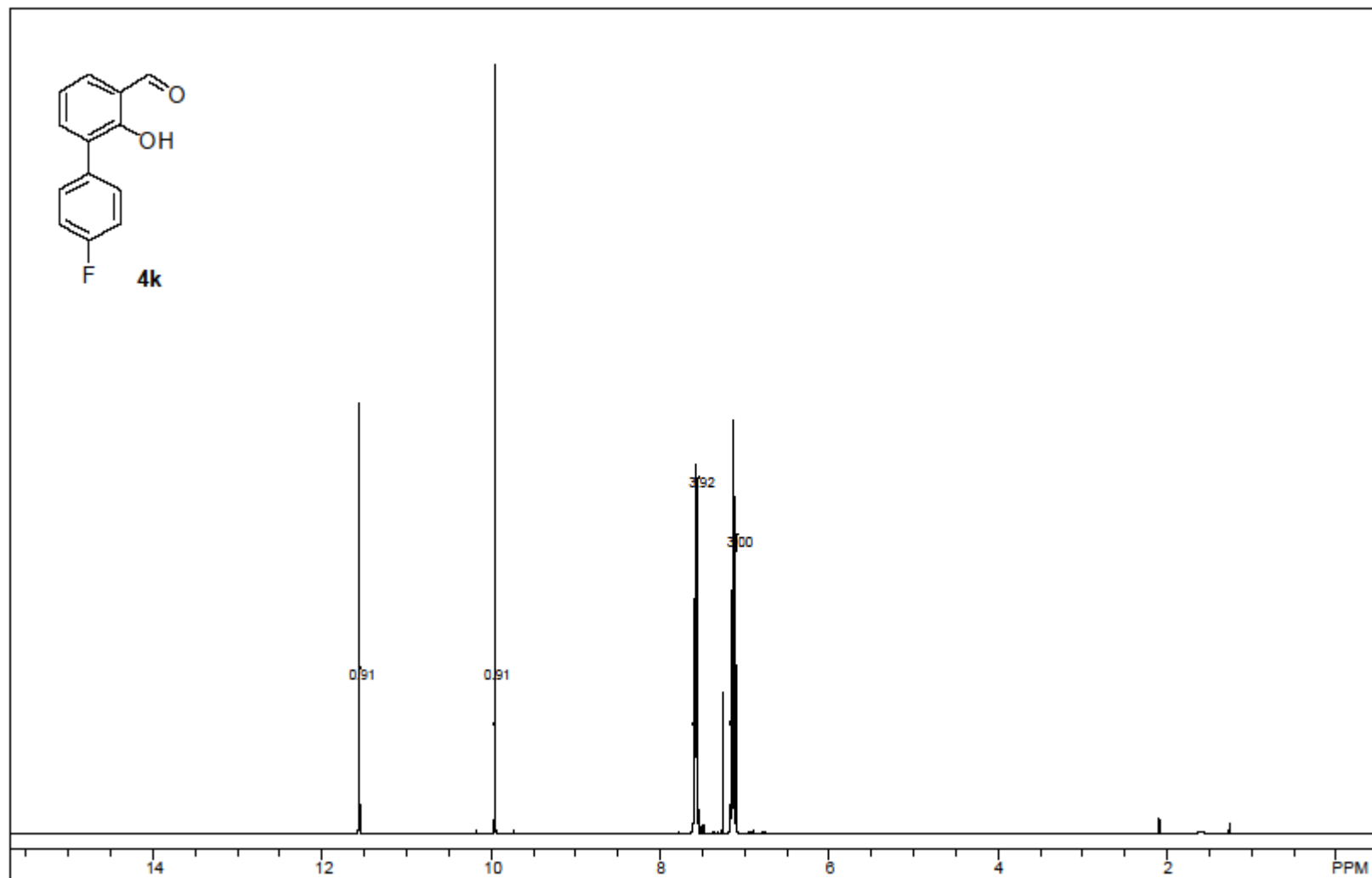
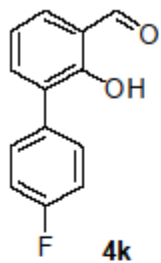
PW: 10.0 us

PD: 2.0 sec

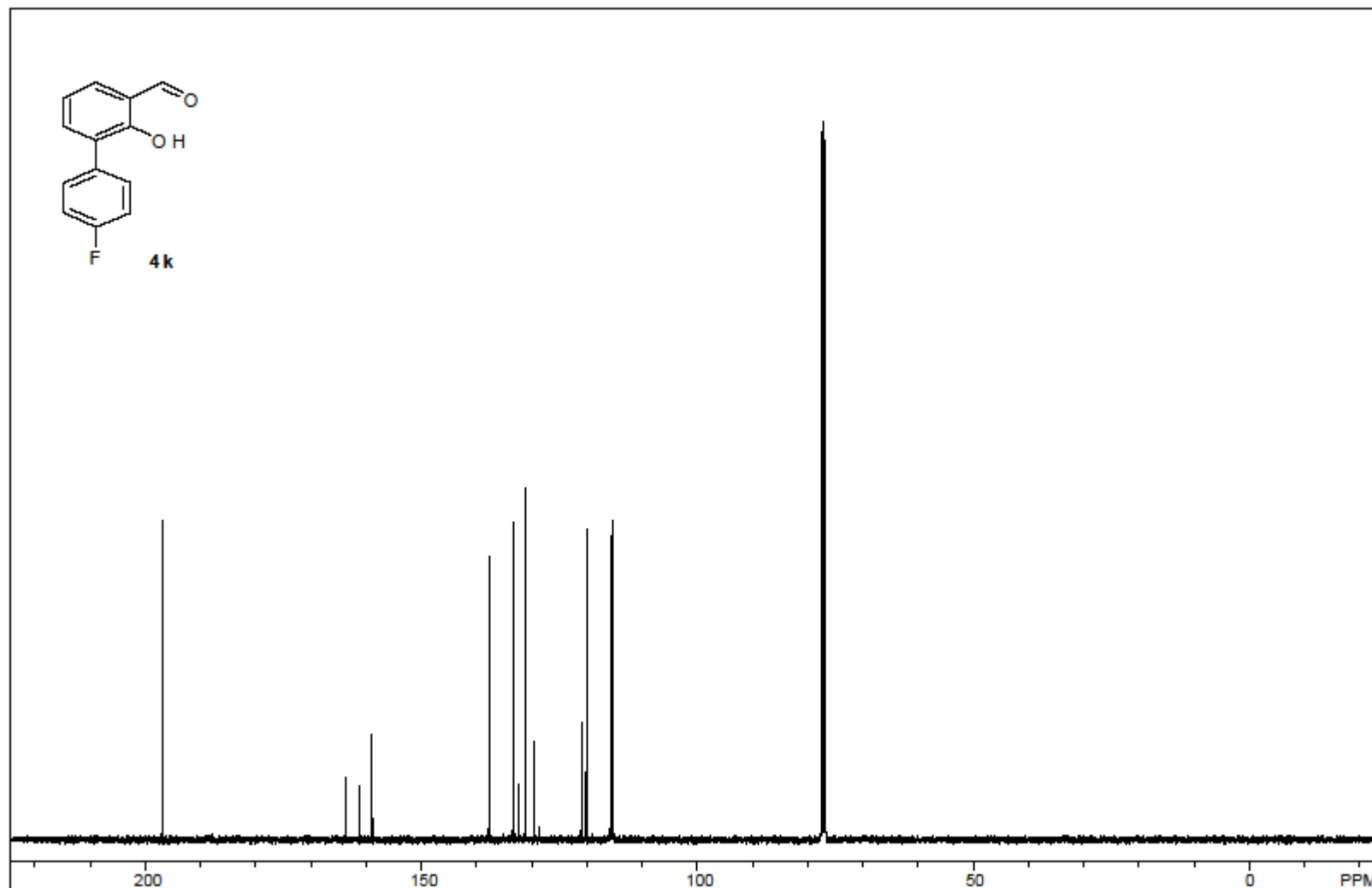
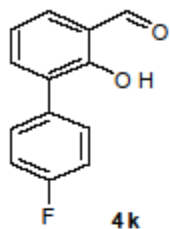
NA: 183

LB: 0.0

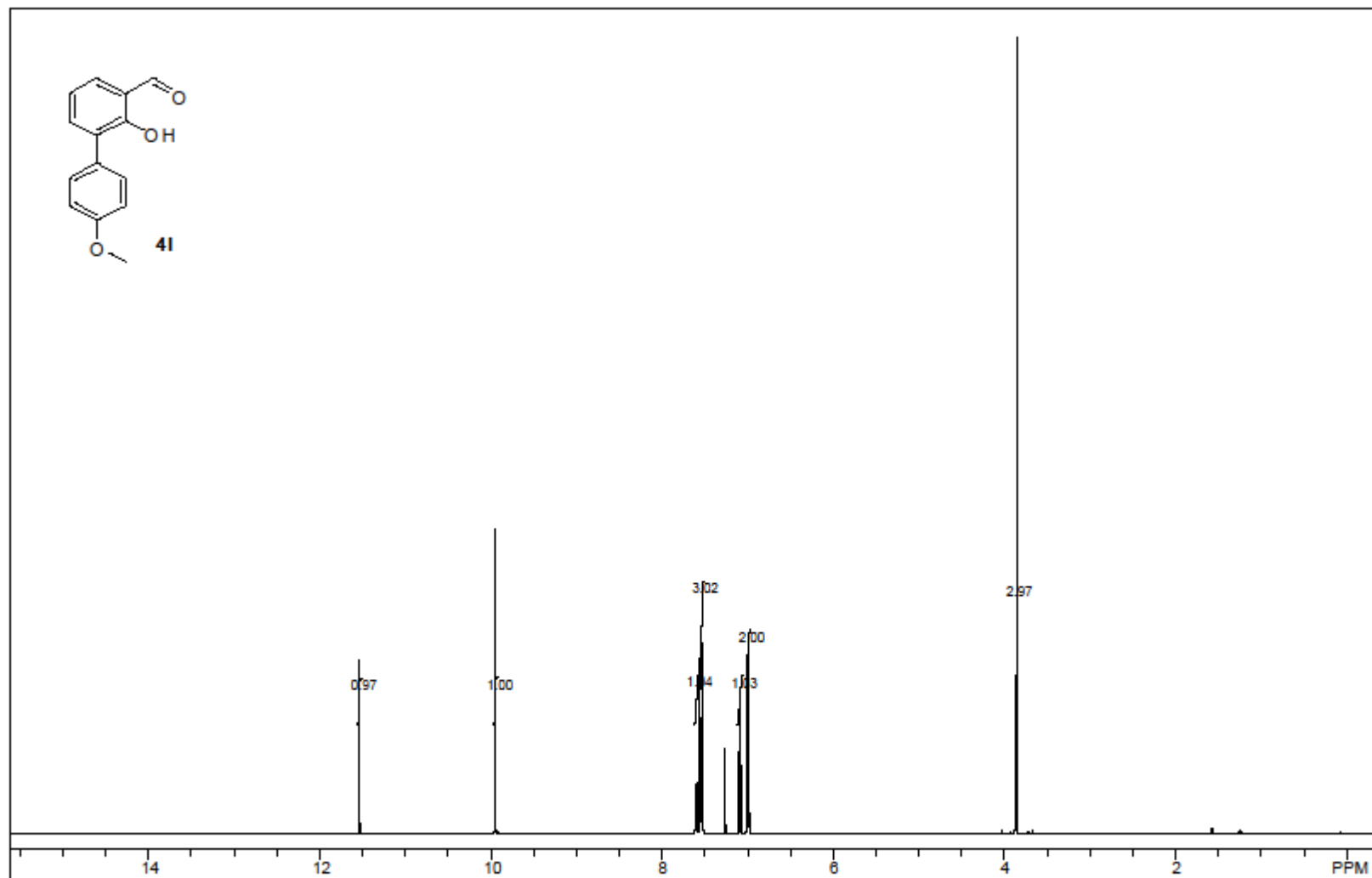
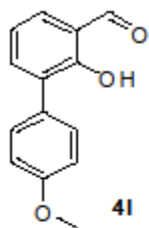
Nuts - \$pdata



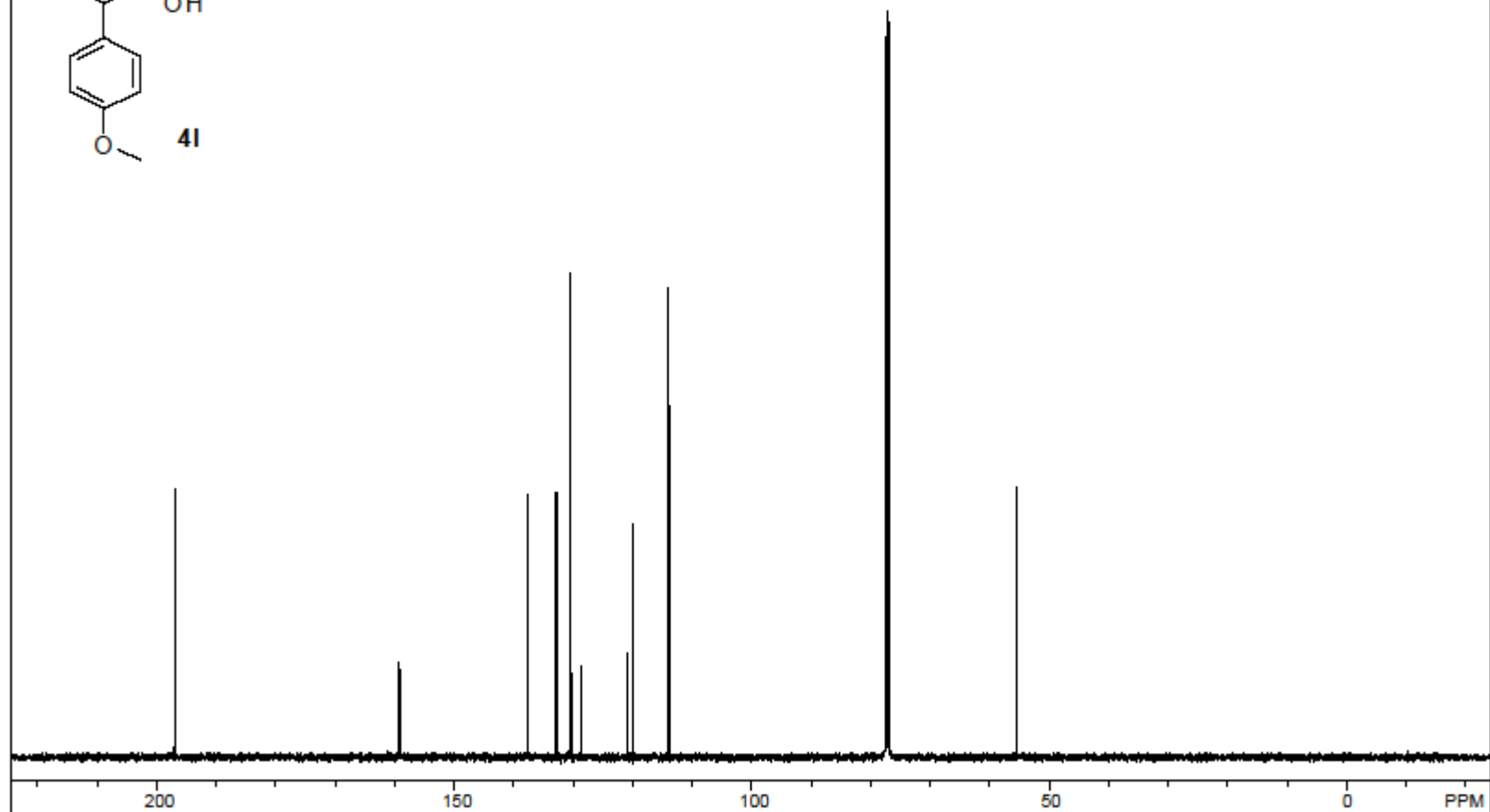
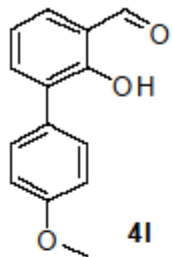
Avance CDCl3			USER: nrsu -- DATE: Mon Jan 11 11:39:12 2021			
F1: 399.956	F2: 1.000	SW1: 7813		OF1: 2460.0		PTS1d: 65536
EX: zg30		PW: 12.0 us	PD: 1.0 sec	NA: 16	LB: 0.0	Nuts - Spdata



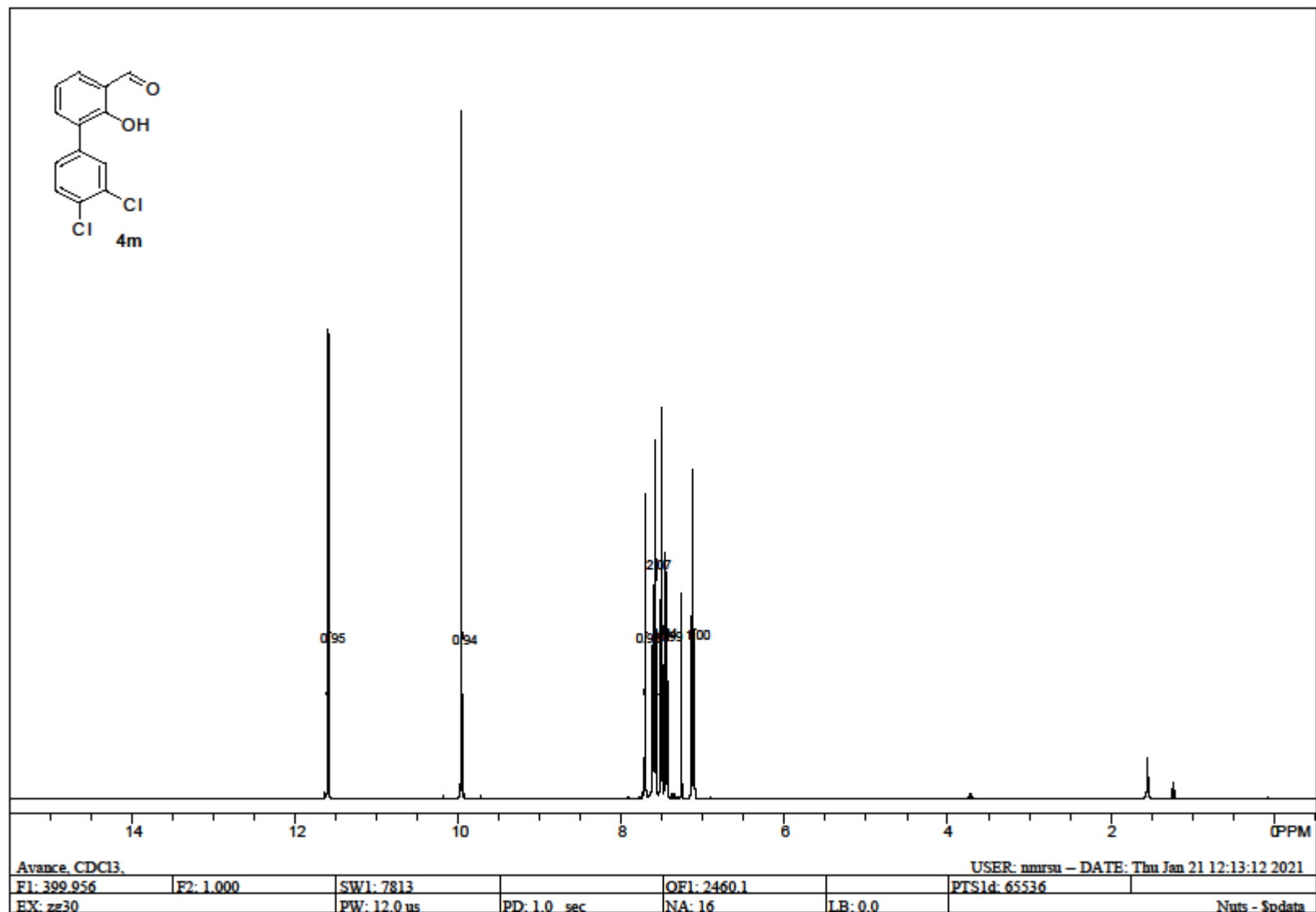
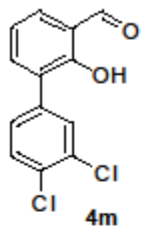
Avance CDCl <sub>3</sub>			USER: nrsu -- DATE: Mon Jan 11 11:52:40 2021			
F1: 100.579	F2: 1.000	SW1: 25000		OF1: 10069.2		PTS1d: 32768
EX: zgpg30		PW: 10.0 us	PD: 2.0 sec	NA: 256	LB: 0.0	Nuts - \$pdata

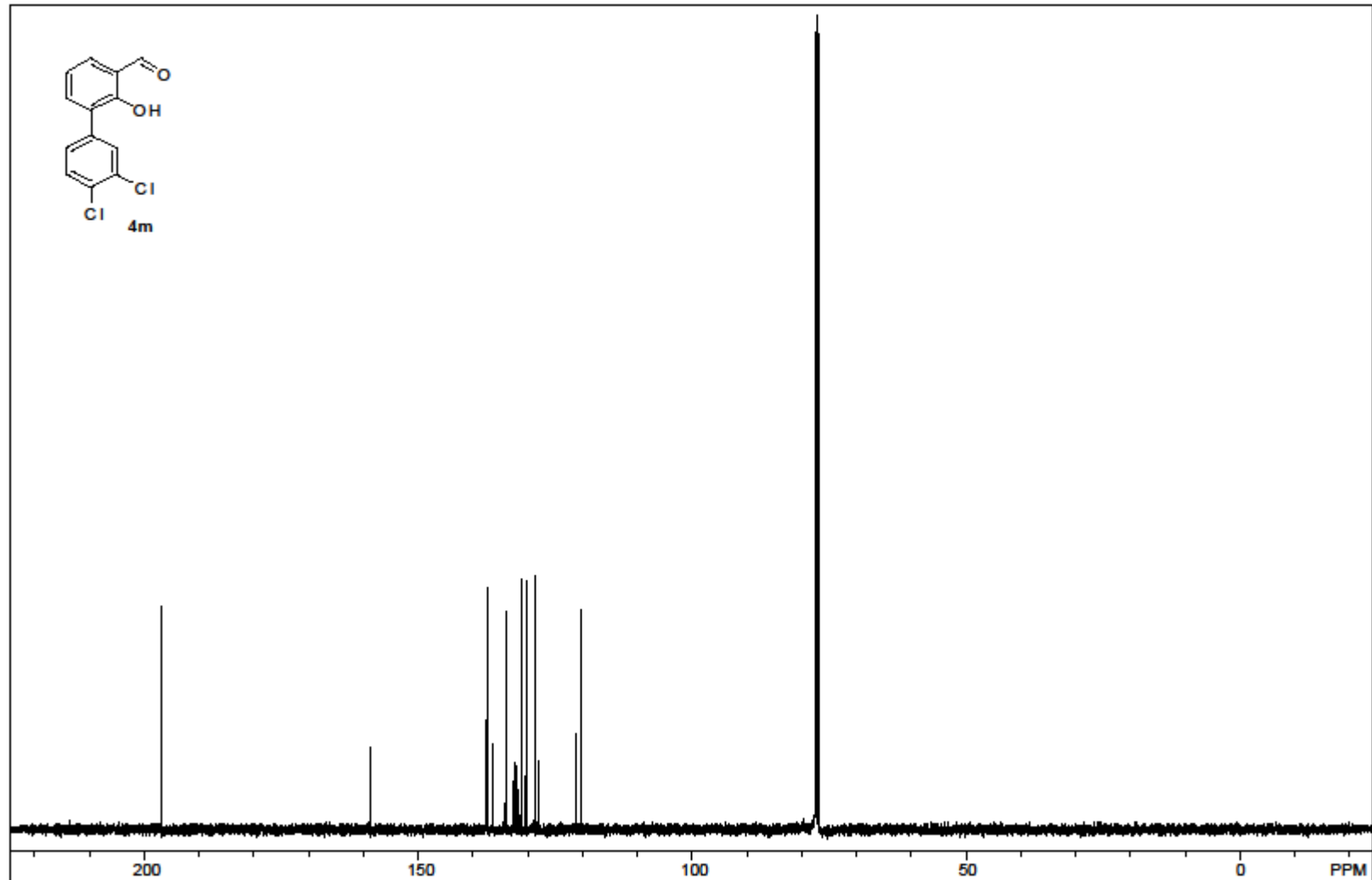
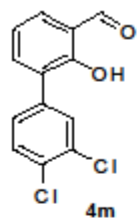


Avance, CDCl <sub>3</sub>			USER: nmrsv -- DATE: Wed Jan 20 15:05:51 2021			
F1: 399.956	F2: 1.000	SW1: 7813		OF1: 2460.1		PTS1d: 65536
EX: zg30		PW: 12.0 us	PD: 1.0 sec	NA: 16	LB: 0.0	Nuts - Spdata

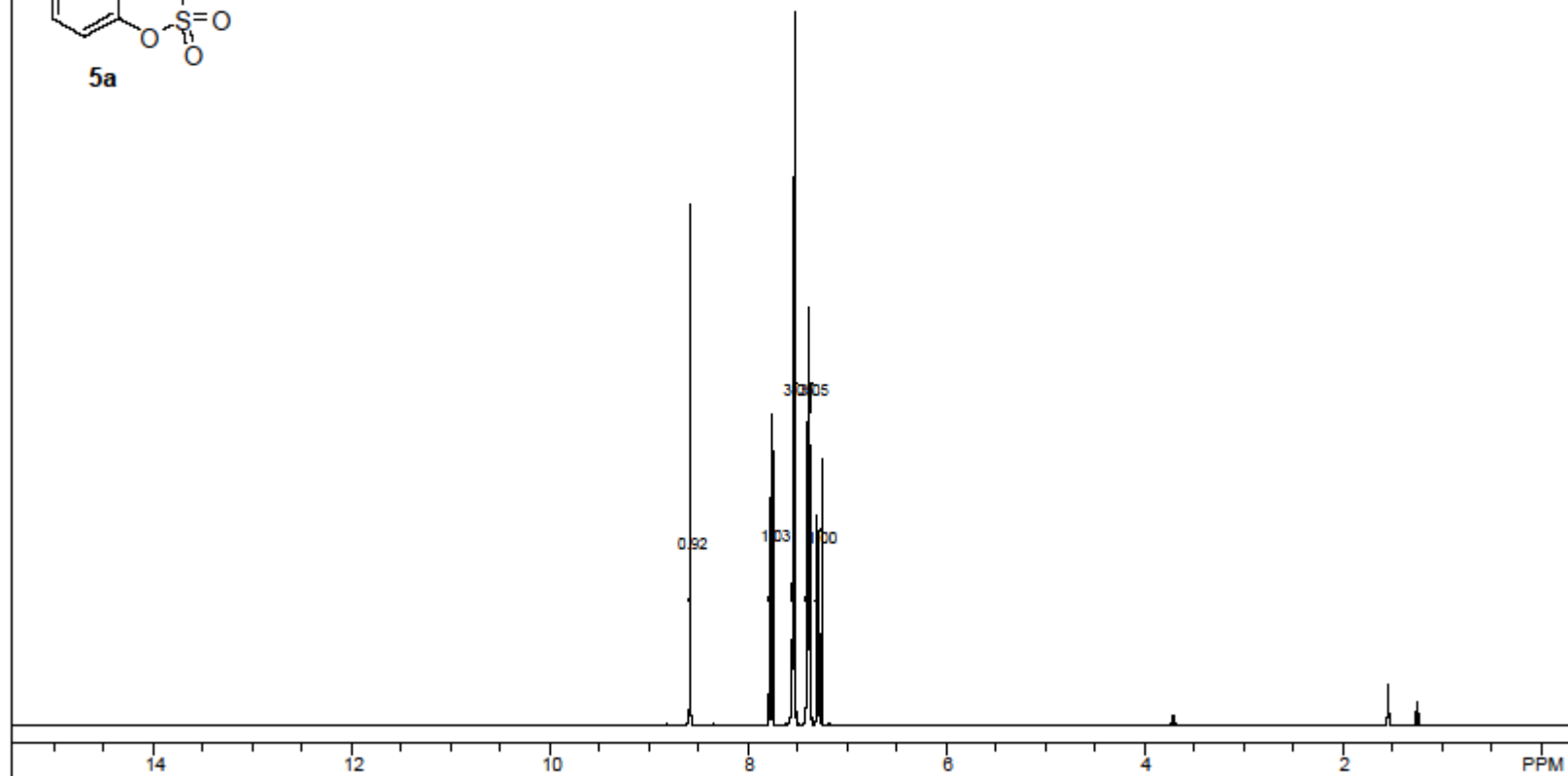
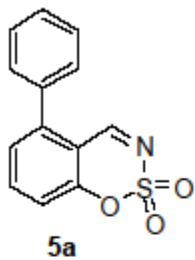


Avance, CDCl <sub>3</sub>			USER: nrsu -- DATE: Wed Jan 20 15:18:24 2021			
F1: 100.579	F2: 1.000	SW1: 25000		OF1: 10069.2		PTS1d: 32768
EX: zgpg30		PW: 10.0 us	PD: 2.0 sec	NA: 256	LB: 0.0	Nuts - \$pdata





Avance, CDCl <sub>3</sub>			USER: nmrsu - DATE: Thu Jan 21 12:20:50 2021			
F1: 100.579	F2: 1.000	SW1: 25000		OF1: 10069.7		PTS1d: 32768
EX: zgpg30		PW: 10.0 us	PD: 2.0 sec	NA: 135	LB: 0.0	Nuts - \$pdata



Avance, CDCl<sub>3</sub>

USER: nmrsu - DATE: Fri Oct 23 15:41:02 2020

F1: 399.956 F2: 1.000

SW1: 7813

OF1: 2460.1

PTS1d: 65536

EX: zg30

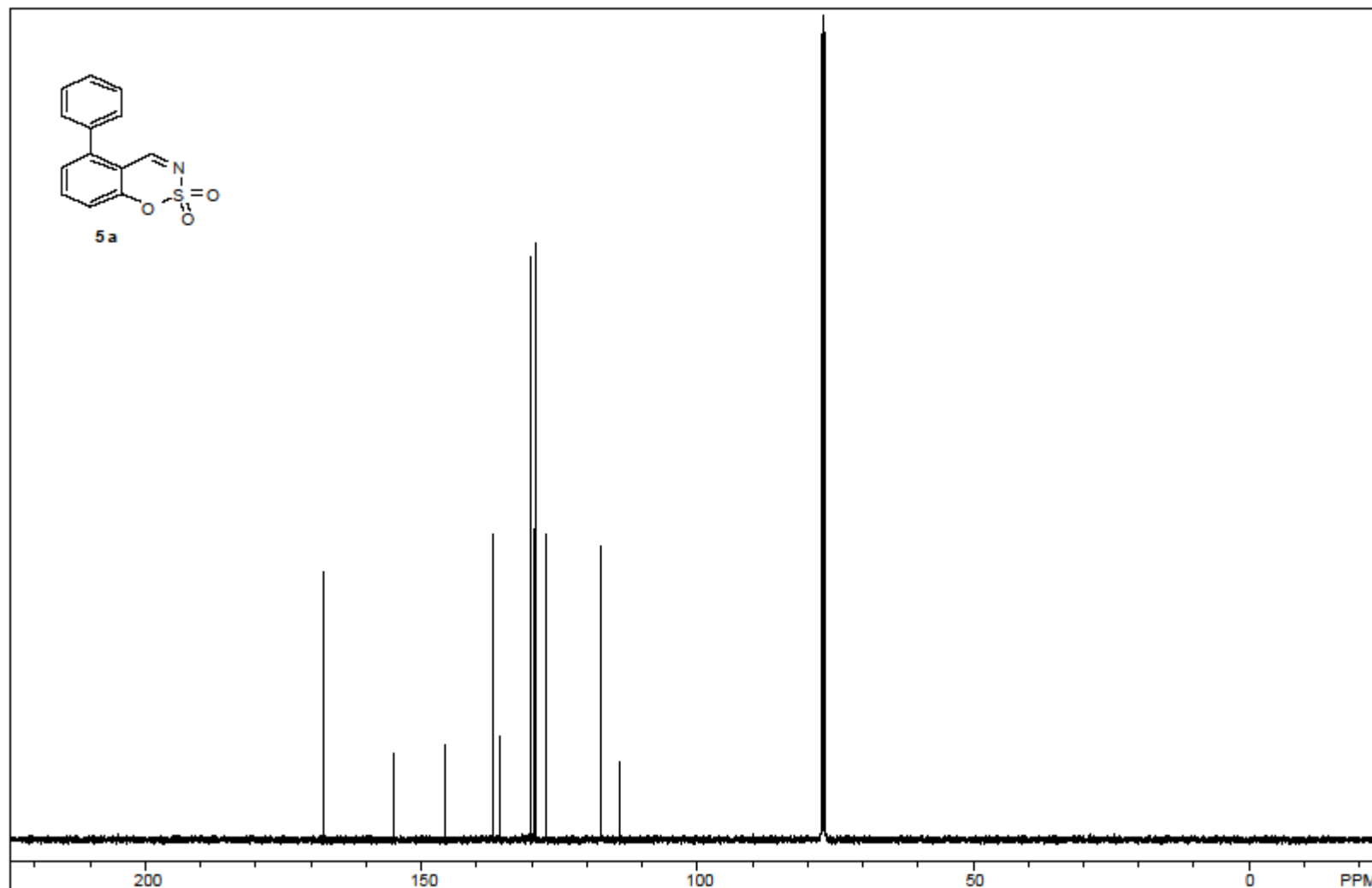
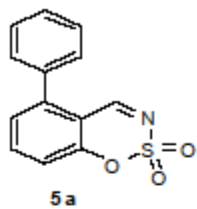
PW: 12.0 us

PD: 1.0 sec

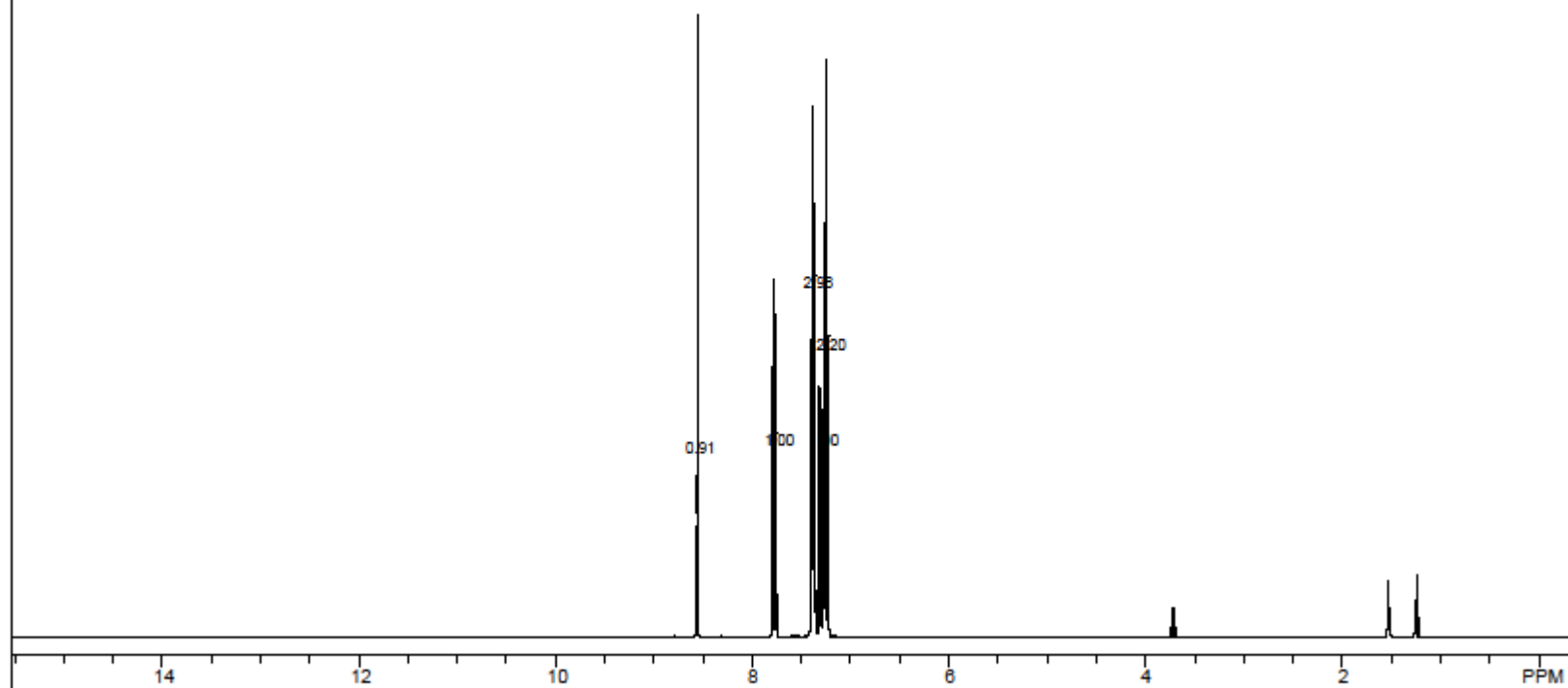
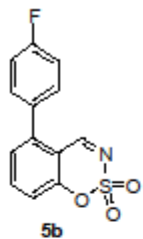
NA: 16

LB: 0.0

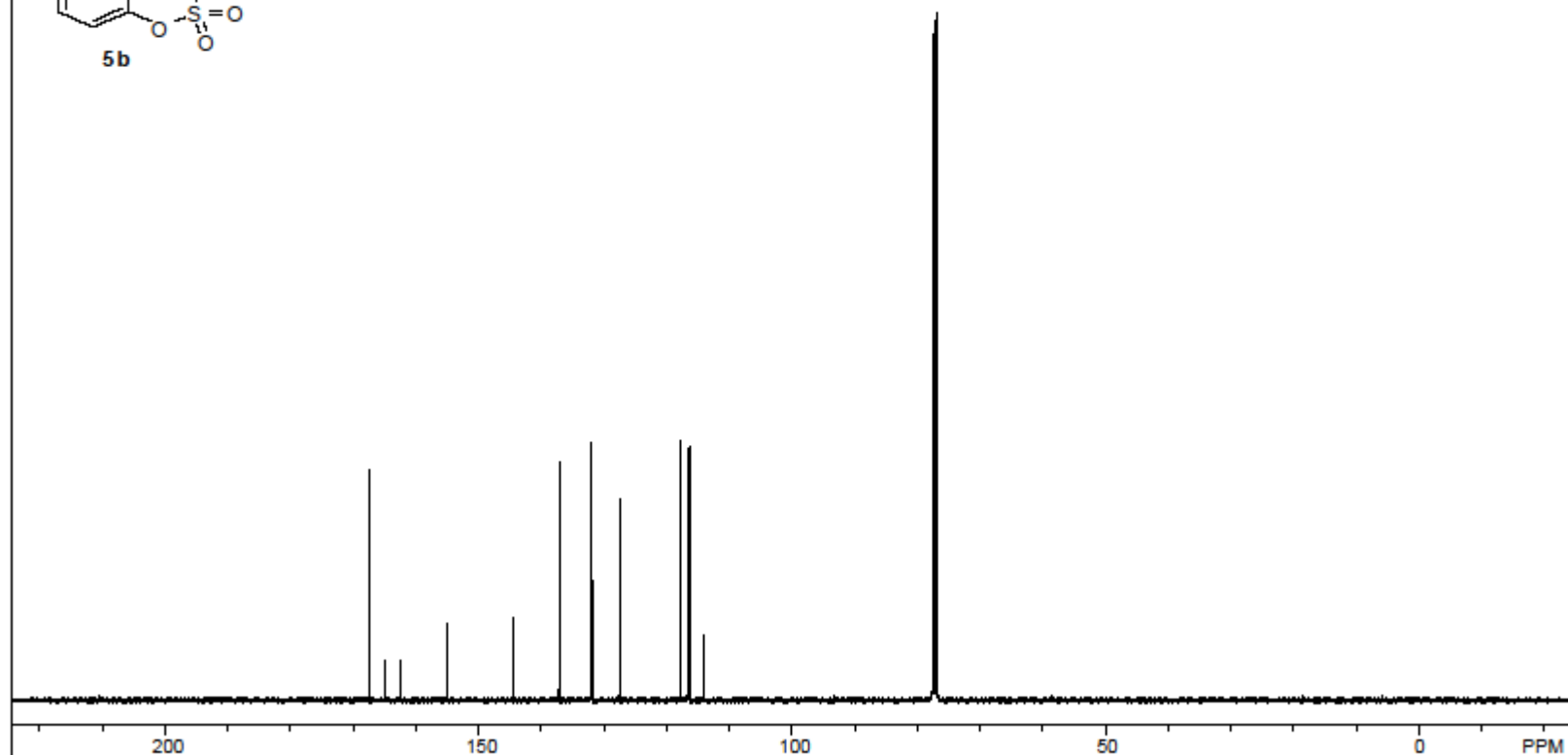
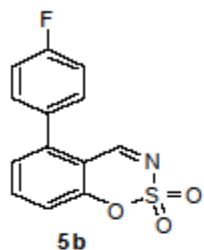
Nuts - Spdata



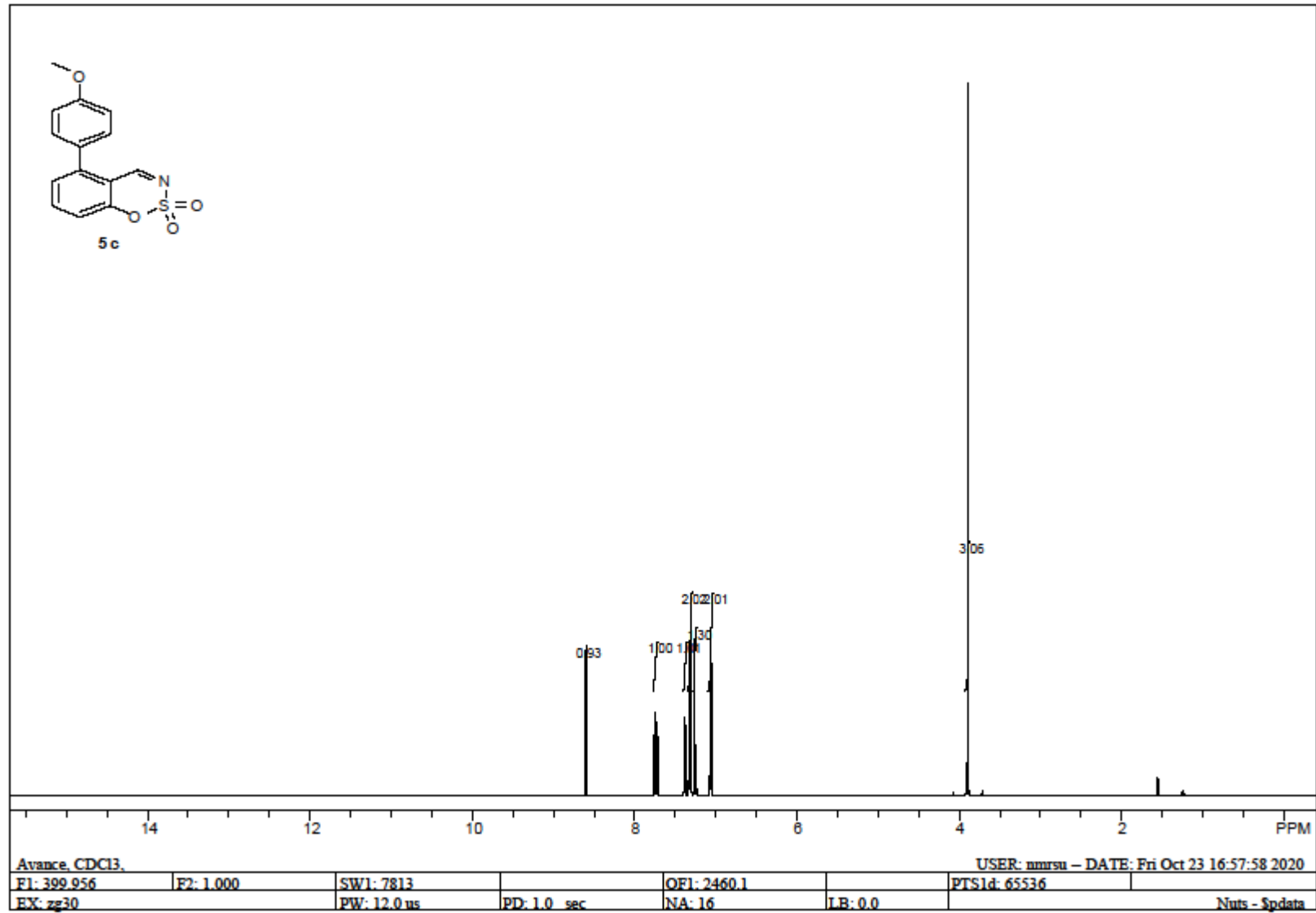
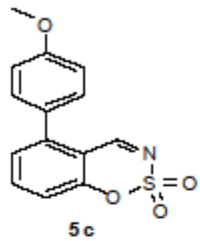
Avance, CDCl <sub>3</sub>			USER: nmrsu - DATE: Fri Oct 23 15:59:24 2020			
F1: 100.579	F2: 1.000	SW1: 25000		OFl: 10069.0		PTS1d: 32768
EX: zgpg30		PW: 10.0 us	PD: 2.0 sec	NA: 350	LB: 0.0	Nuts - Spdata

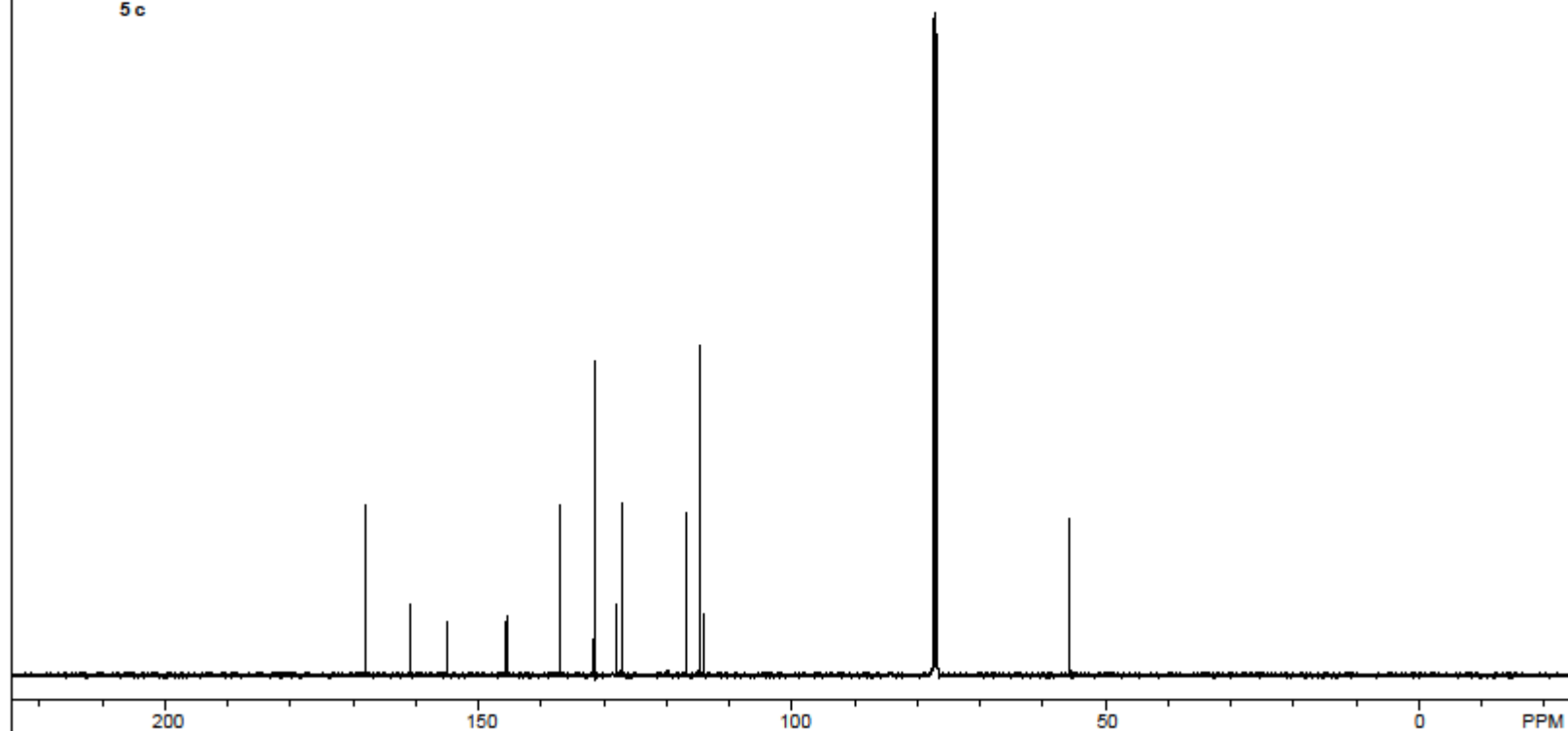
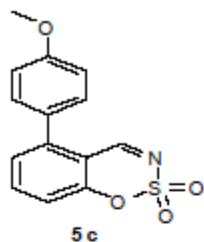


Avance, CDCl <sub>3</sub>			USER: nmrsu - DATE: Fri Oct 23 17:27:42 2020			
F1: 399.956	F2: 1.000	SW1: 7813		OF1: 2460.5		PTS1d: 65536
EX: zg30		PW: 12.0 us	PD: 1.0 sec	NA: 16	LB: 0.0	Nuts - Spdata

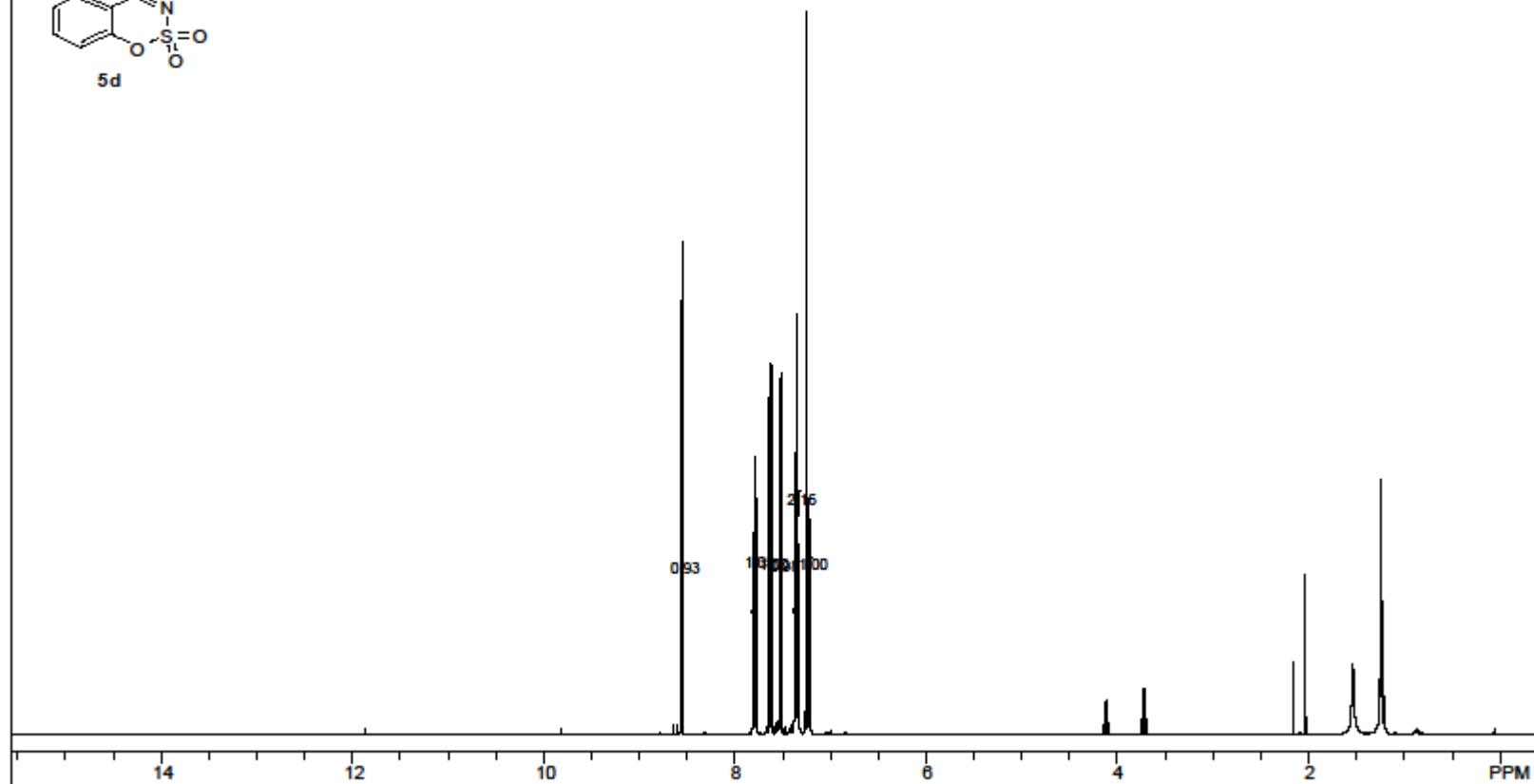
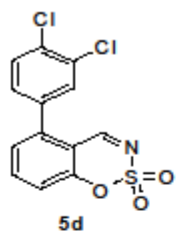


Avance CDCl3			USER: nmrsu - DATE: Fri Oct 23 17:52:03 2020			
F1: 100.579	F2: 1.000	SW1: 25000		OF1: 10069.7		PTS1d: 32768
EX: zgpg30		PW: 10.0 us	PD: 2.0 sec	NA: 512	LB: 0.0	Nuts - Spdata

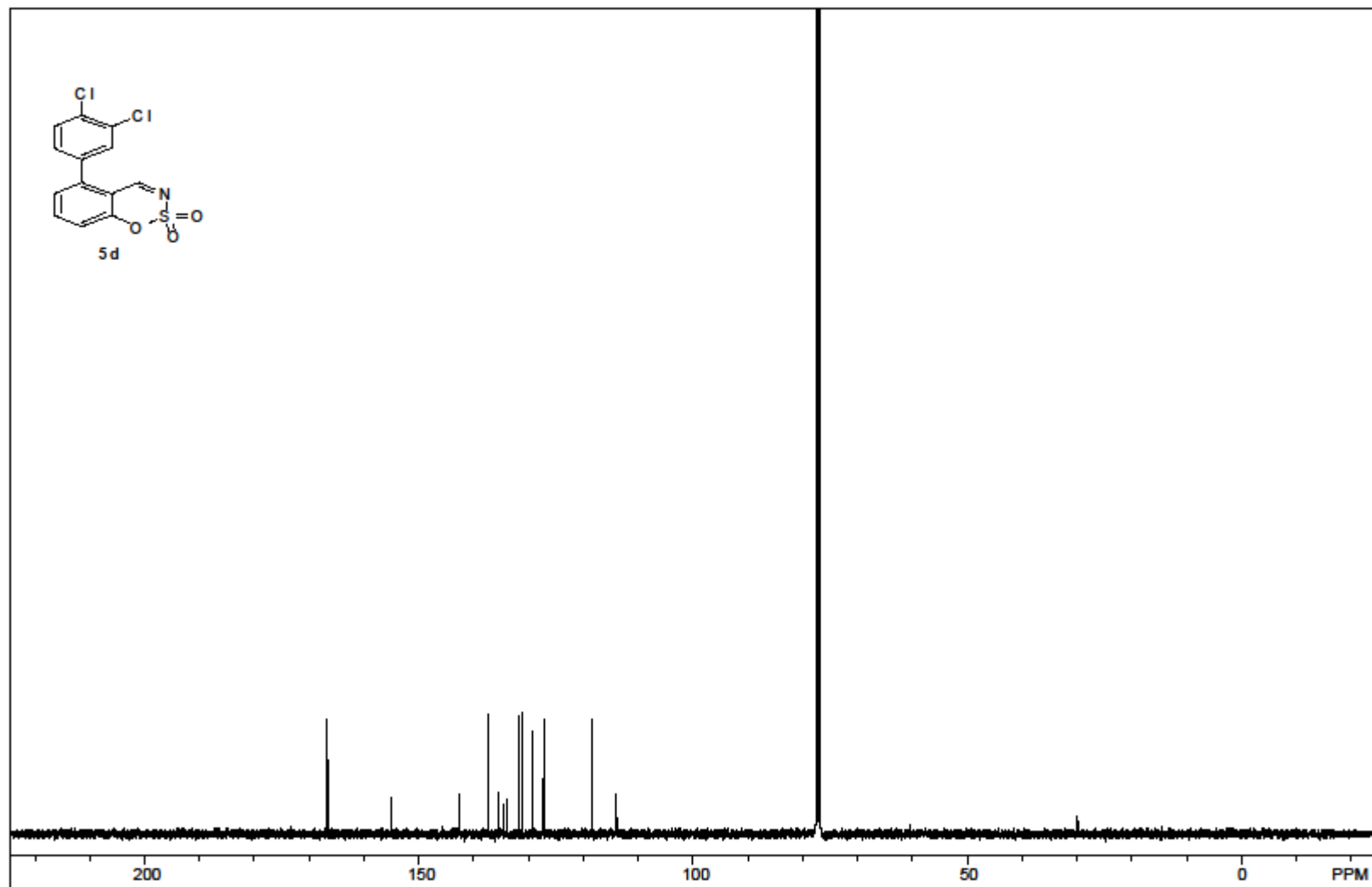
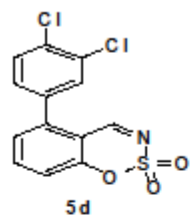




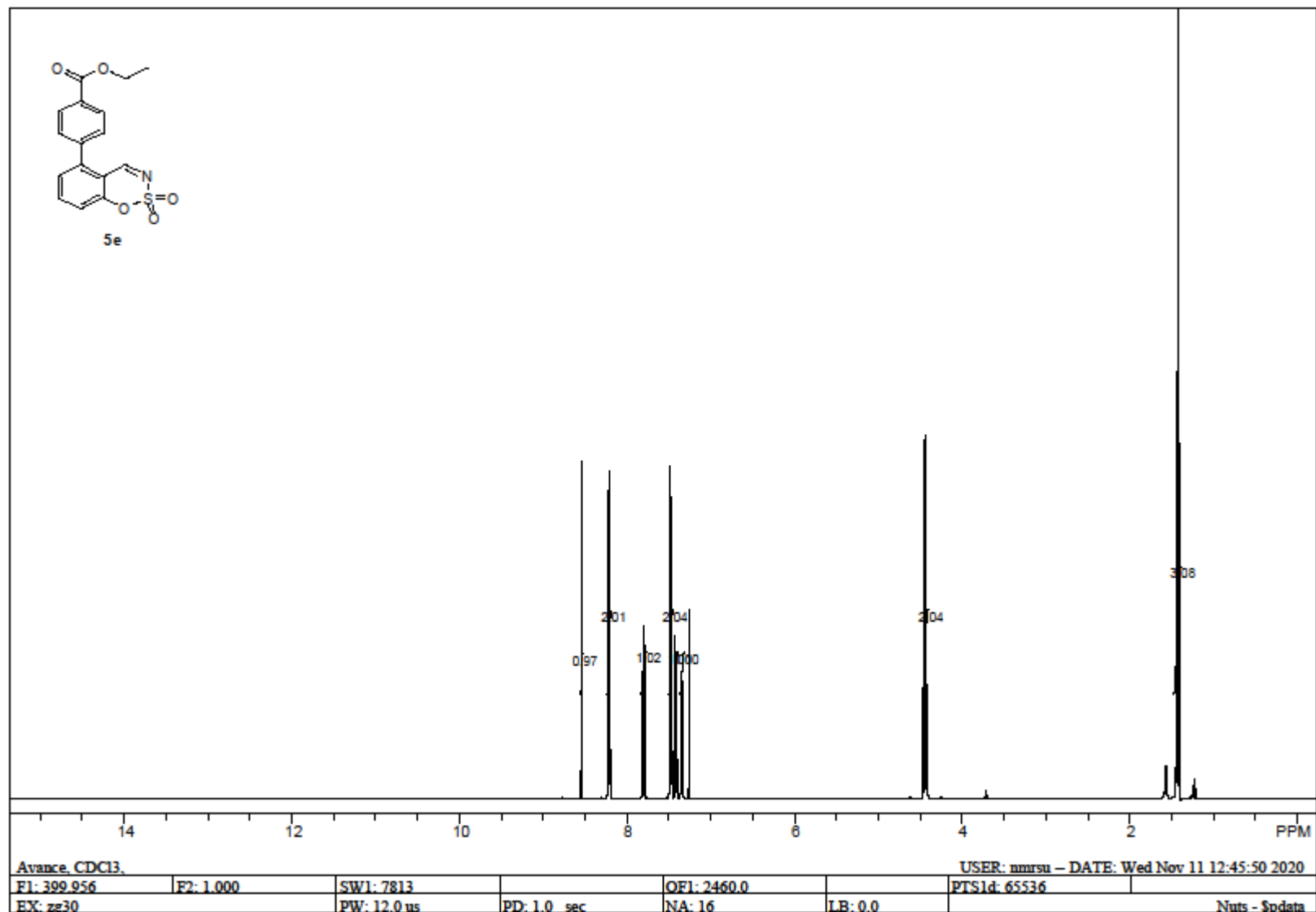
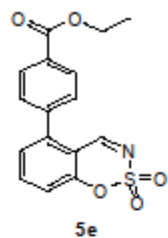
Avance CDCl <sub>3</sub>			USER: nmrsu - DATE: Fri Oct 23 17:22:52 2020			
F1: 100.579	F2: 1.000	SW1: 25000		OF1: 10070.1		PTS1d: 32768
EX: zgpg30		PW: 10.0 us	PD: 2.0 sec	NA: 512	LB: 0.0	Nuts - Spdata

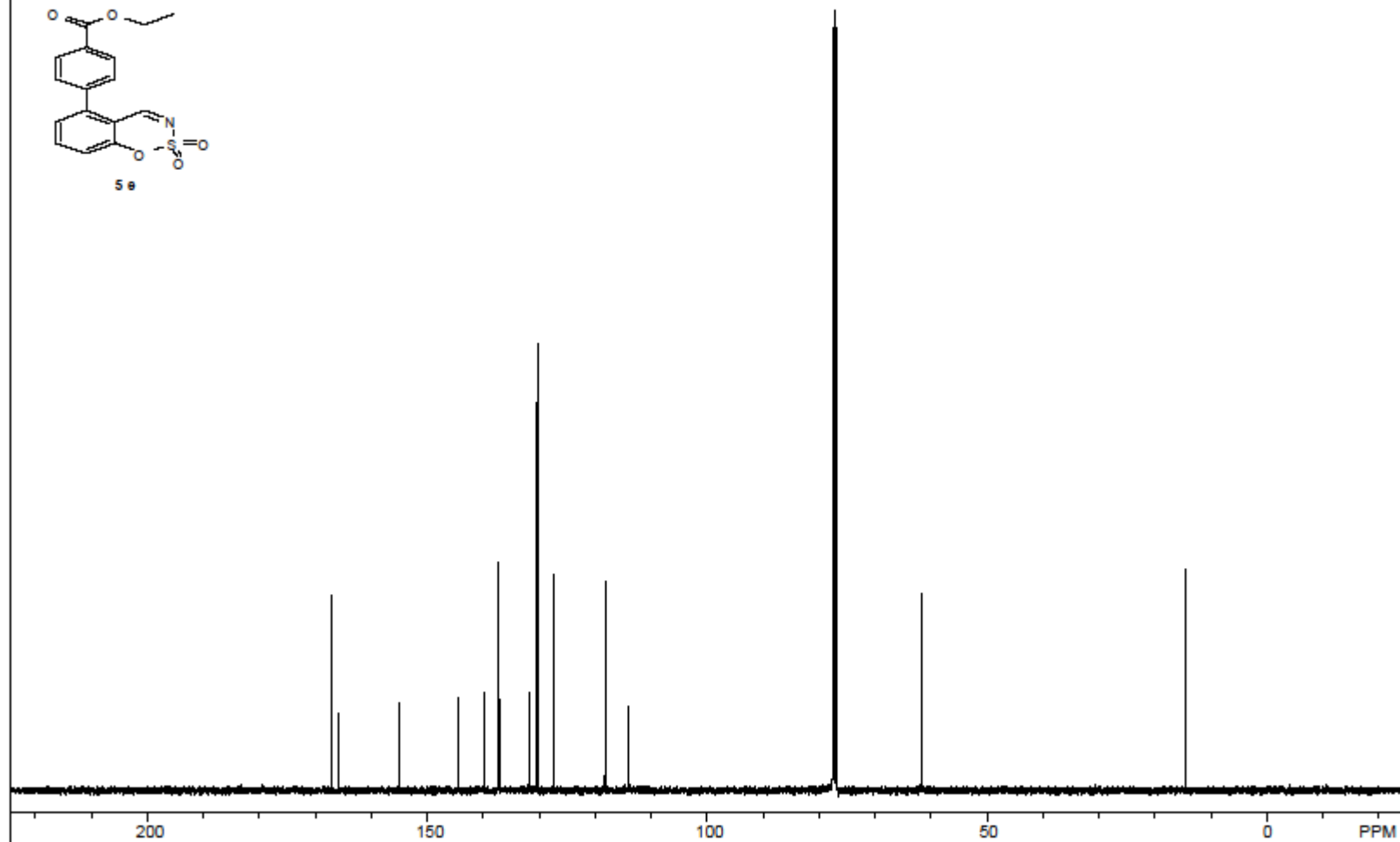
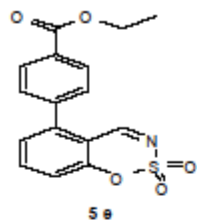


Avance CDCl <sub>3</sub>			USER: nmrsu - DATE: Wed Nov 11 12:22:23 2020			
F1: 399.956	F2: 1.000	SW1: 7813		OF1: 2460.0		PTS1d: 65536
EX: zg30		PW: 12.0 us	PD: 1.0 sec	NA: 16	LB: 0.0	Nuts - Spdata

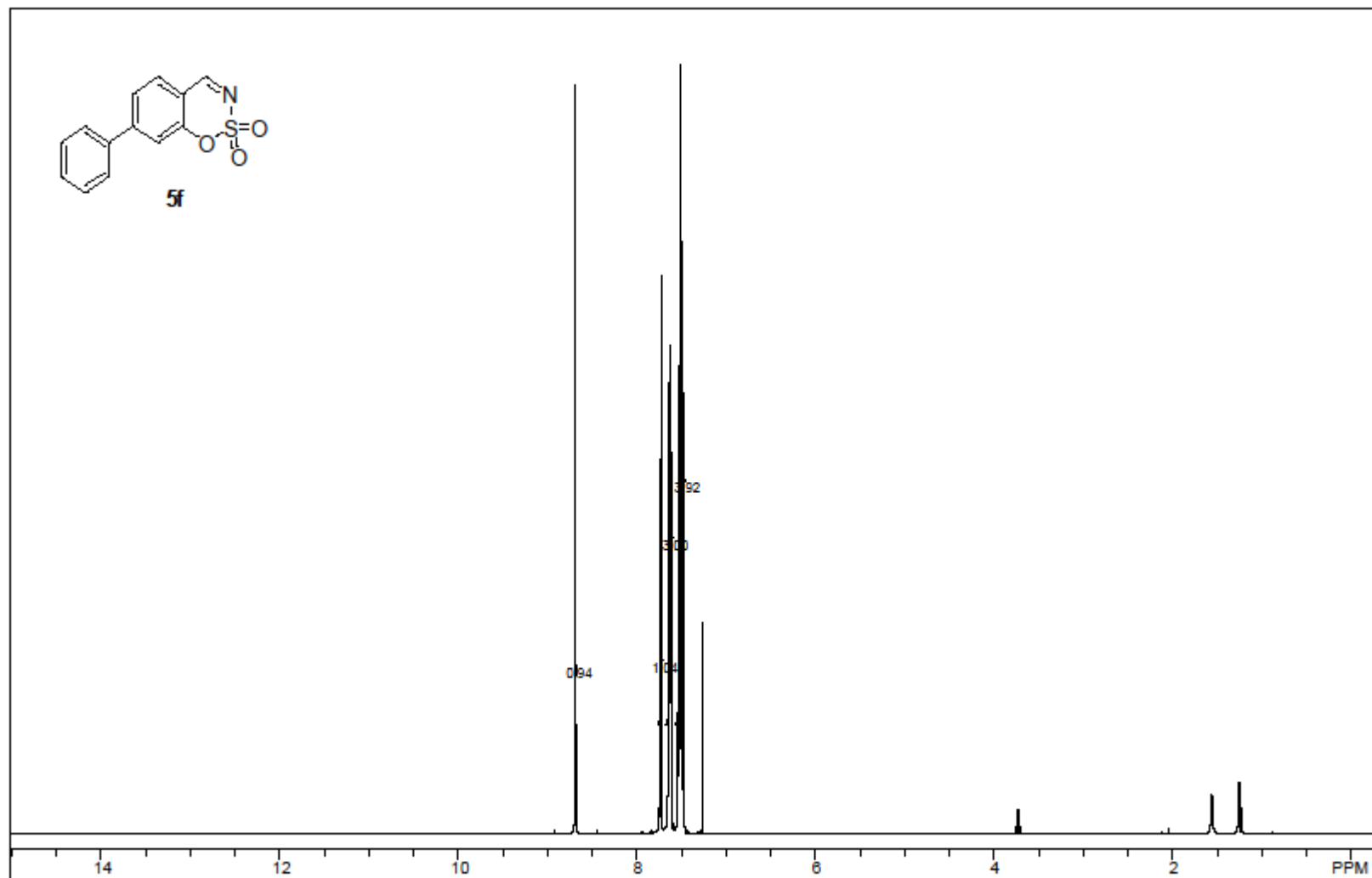


Avance, CDCl <sub>3</sub>						USER: nmsu - DATE: Wed Nov 11 12:35:31 2020	
F1: 100.579	F2: 1.000	SW1: 25000		OF1: 10070.6		PTS1d: 32768	
EX: zgpg30		PW: 10.0 us	PD: 2.0 sec	NA: 256	LB: 0.0		Nuts - \$pdata

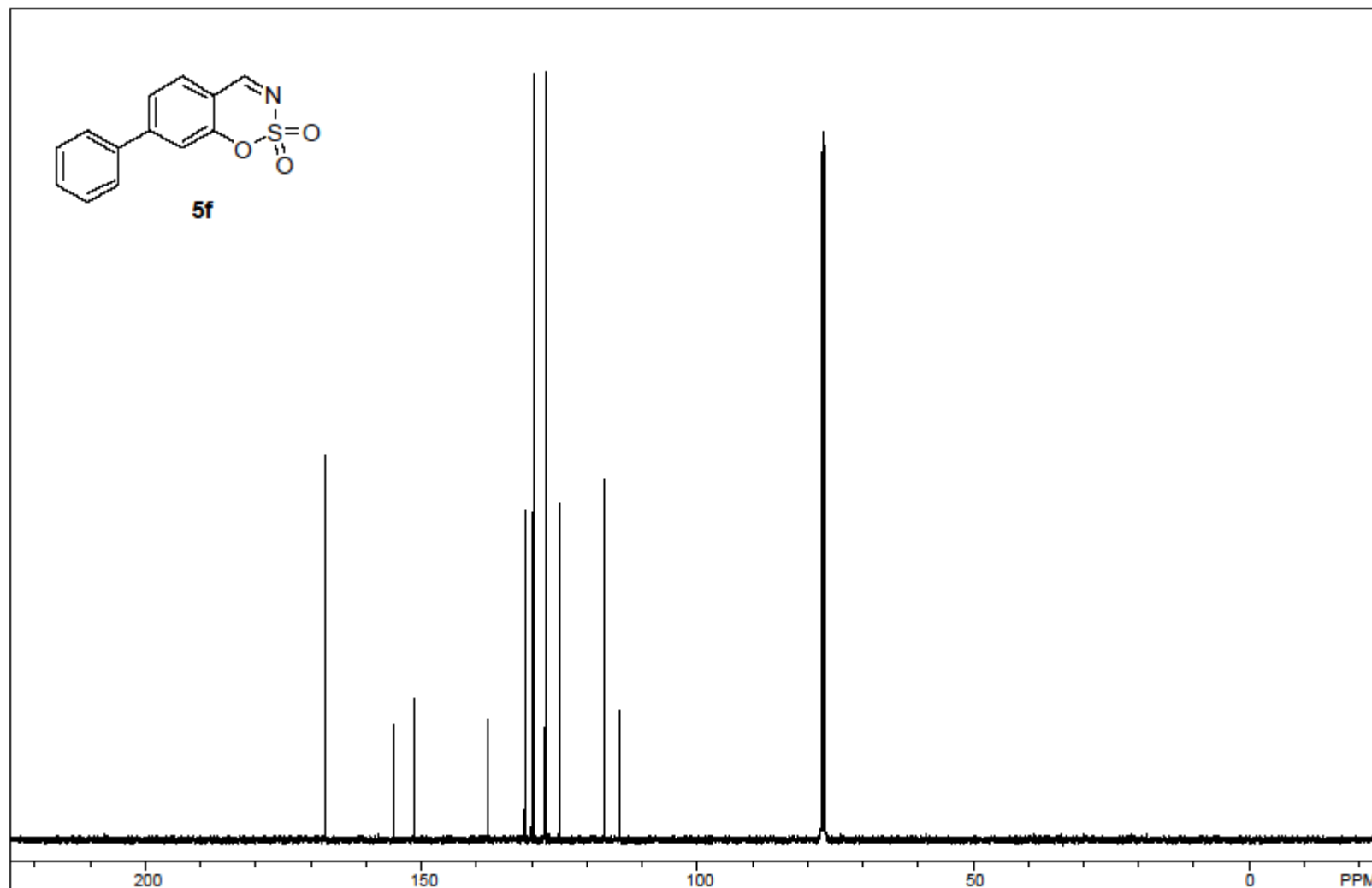
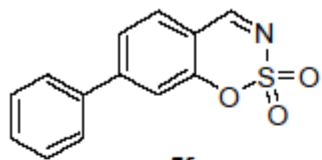




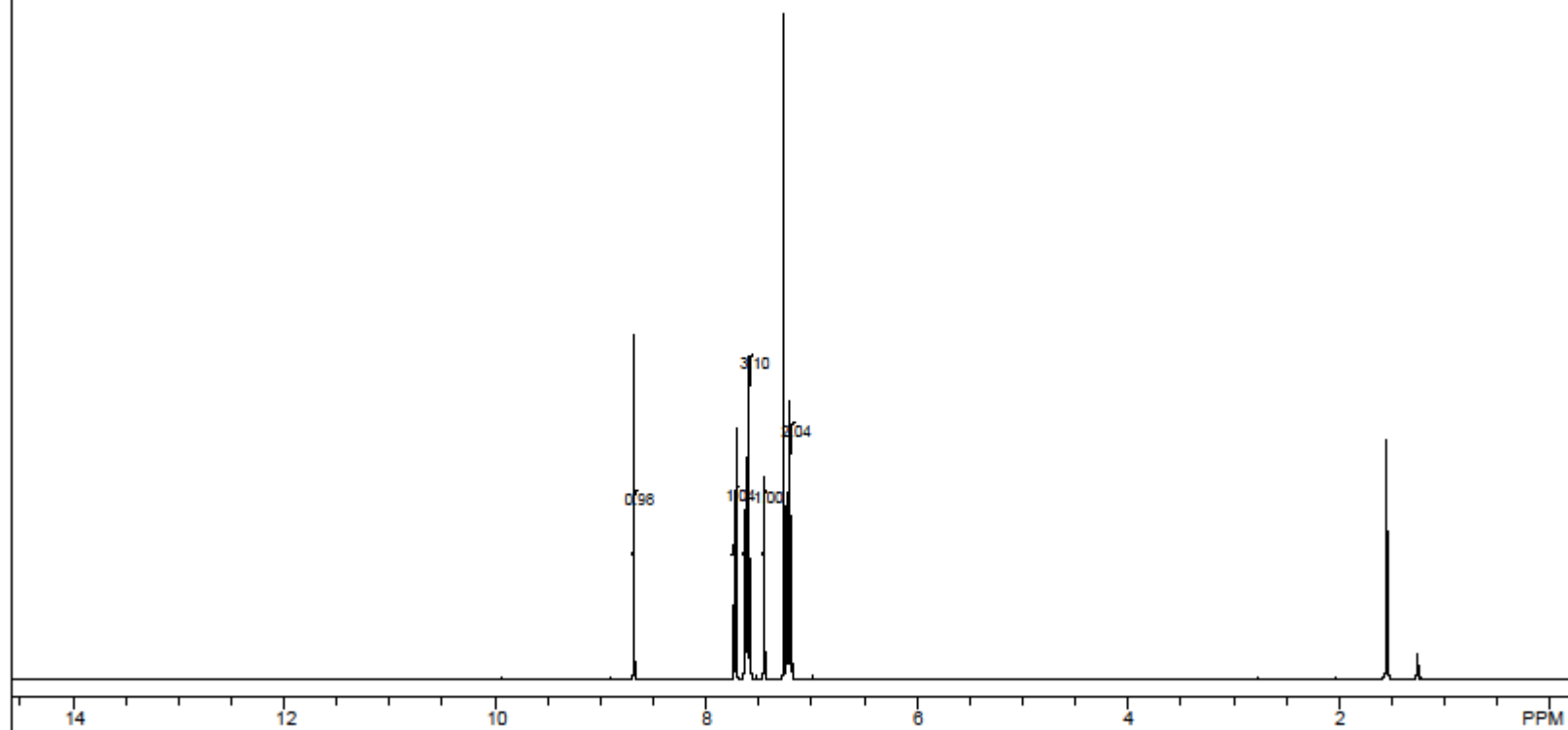
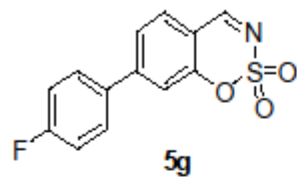
Avance CDCl <sub>3</sub>		USER: nmrsu - DATE: Wed Nov 11 12:58:24 2020			
F1: 100.579	F2: 1.000	SW1: 25000	OF1: 10069.0	PTS1d: 32768	
EX: zgpg30	PW: 10.0 us	PD: 2.0 sec	NA: 256	LB: 0.0	Nuts - \$pdata



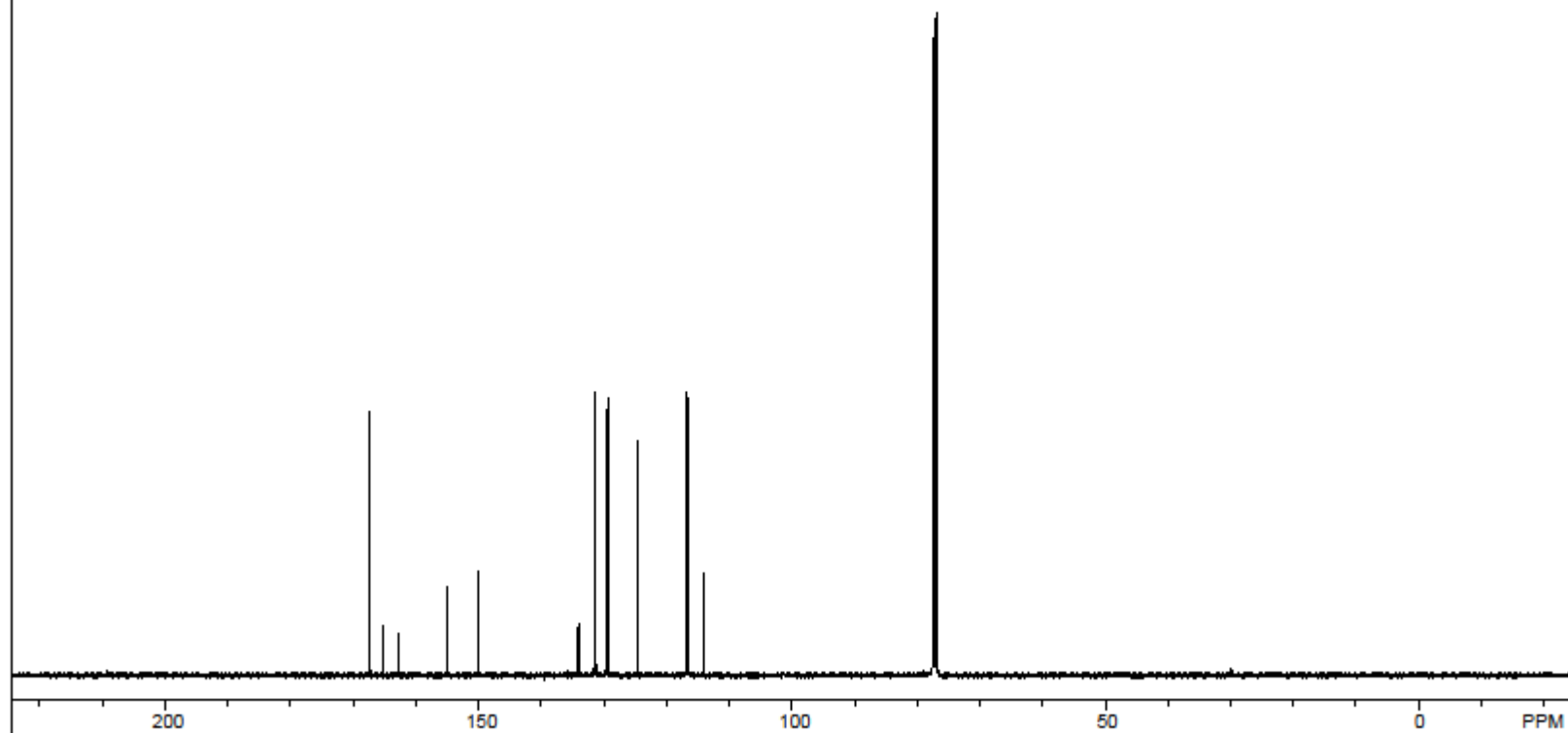
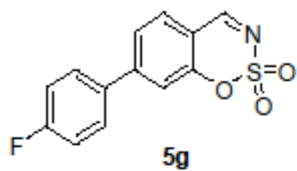
Avance, CDCl <sub>3</sub>			USER: nmrsu -- DATE: Thu Nov 26 19:47:56 2020			
F1: 399.956	F2: 1.000	SW1: 7813		OF1: 2459.8		PTS1d: 65536
EX: zg30		PW: 12.0 us	PD: 1.0 sec	NA: 16	LB: 0.0	Nuts - Spdata



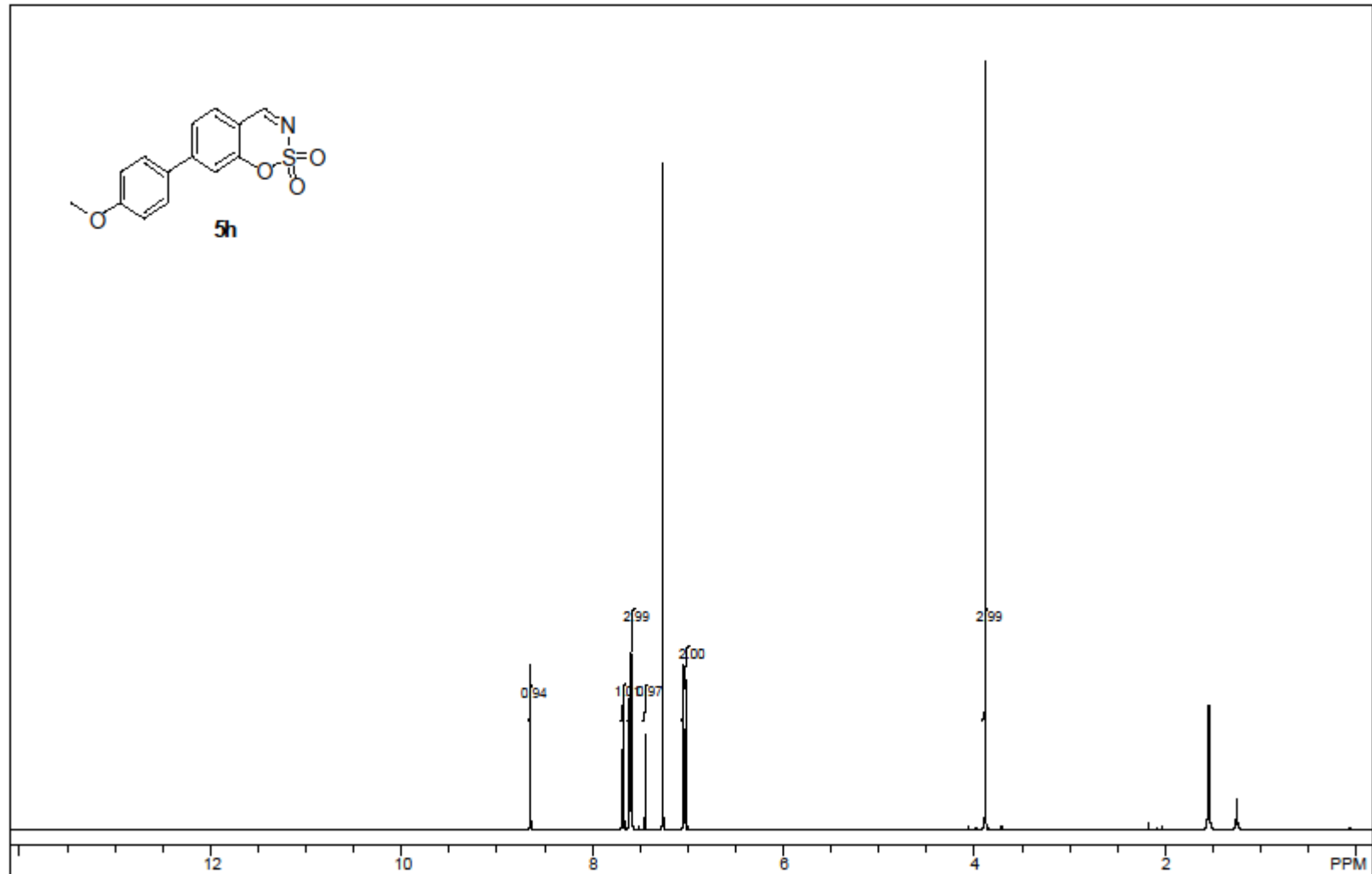
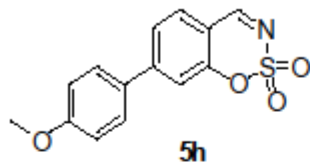
Avance CDCl3			USER: mmrsu -- DATE: Thu Nov 26 20:00:54 2020			
F1: 100.579	F2: 1.000	SW1: 25000		OF1: 10067.5		PTS1d: 32768
EX: zgpg30		PW: 10.0 us	PD: 2.0 sec	NA: 256	LB: 0.0	Nuts - \$pdata



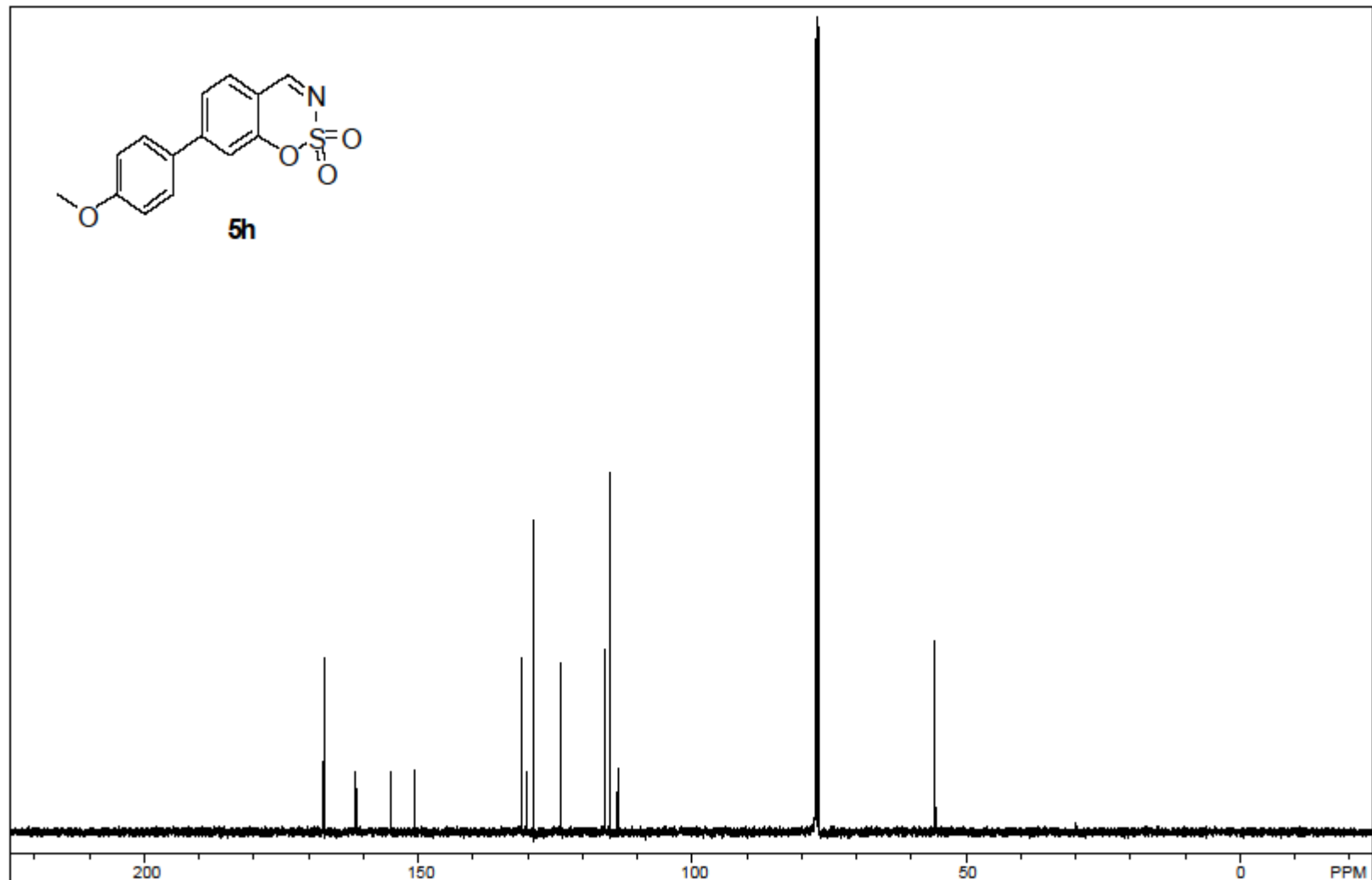
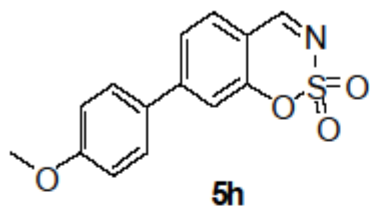
Avance, CDCl <sub>3</sub>			USER: nmrsl - DATE: Wed Dec 16 10:37:00 2020			
F1: 399.956	F2: 1.000	SW1: 7813		OF1: 2459.1		PTS1d: 65536
EX: zg30		PW: 12.0 us	PD: 1.0 sec	NA: 16	LB: 0.0	Nuts - Spdata



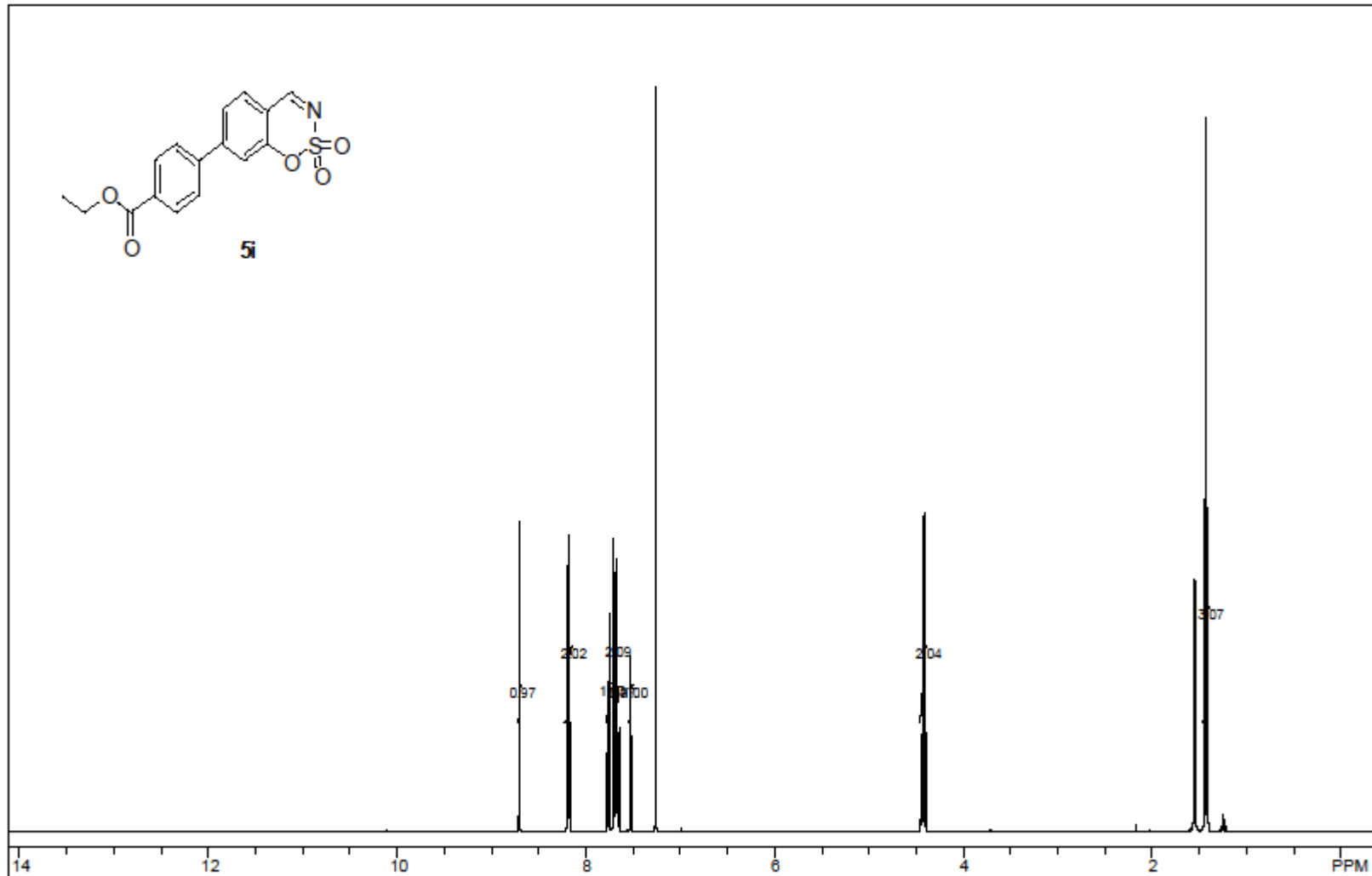
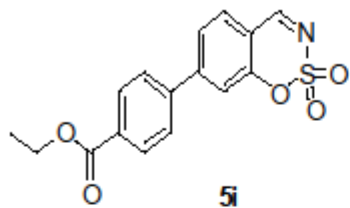
Avance, CDCl3,			USER: nrsu -- DATE: Thu Dec 17 15:33:24 2020			
F1: 100.579	F2: 1.000	SW1: 25000		OF1: 10068.9		PTS1d: 32768
EX: zgpg30		PW: 10.0 us	PD: 2.0 sec	NA: 512	LB: 0.0	Nuts - \$pdata



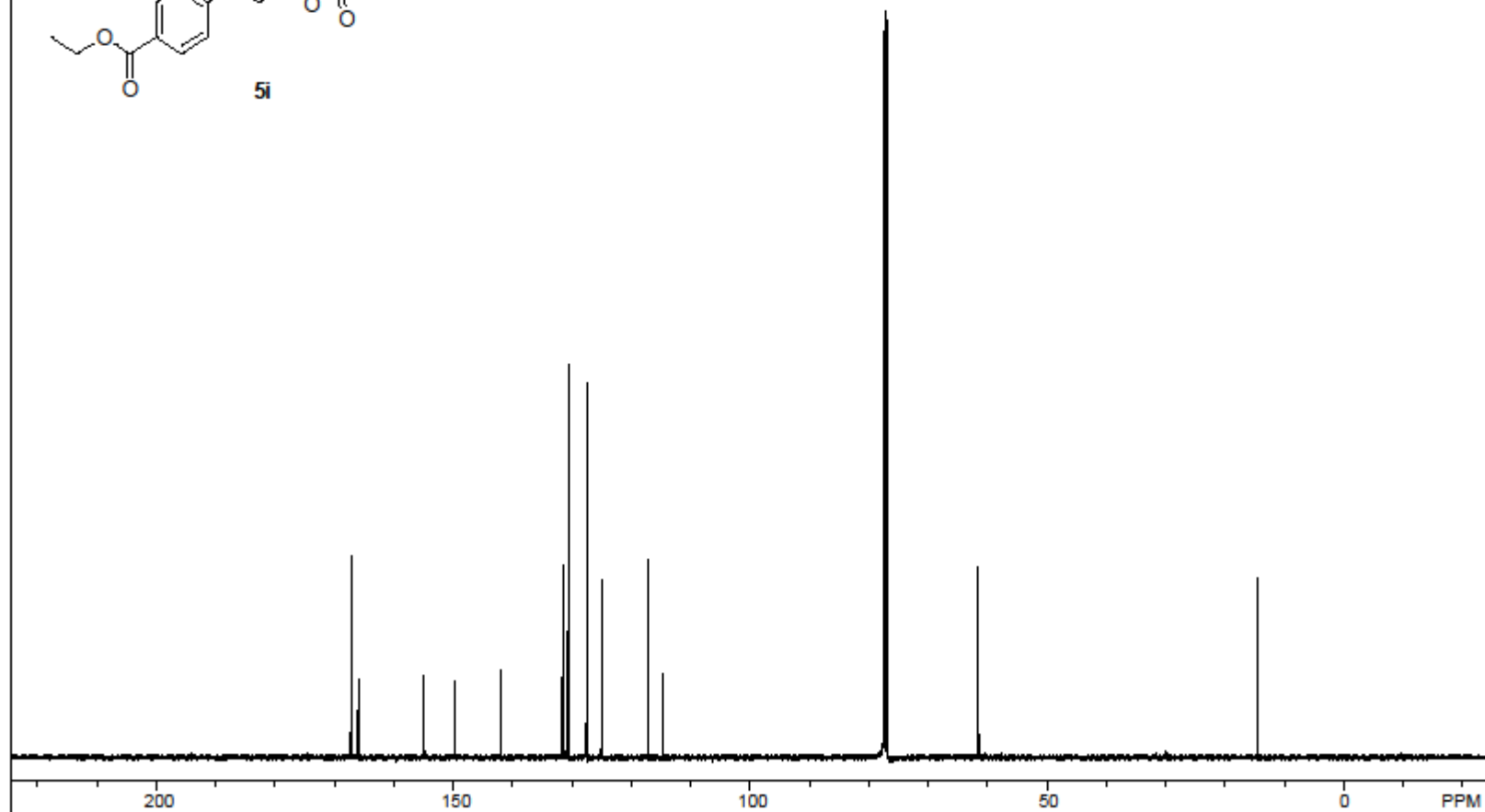
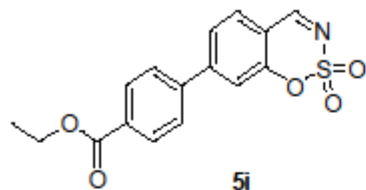
Avance CDCl3			USER: nmrsu - DATE: Wed Dec 16 08:59:27 2020			
F1: 399.956	F2: 1.000	SW1: 7813		OF1: 2460.1		PTS1d: 65536
EX: zg30		PW: 12.0 us	PD: 1.0 sec	NA: 16	LB: 0.0	Nuts - Spdata



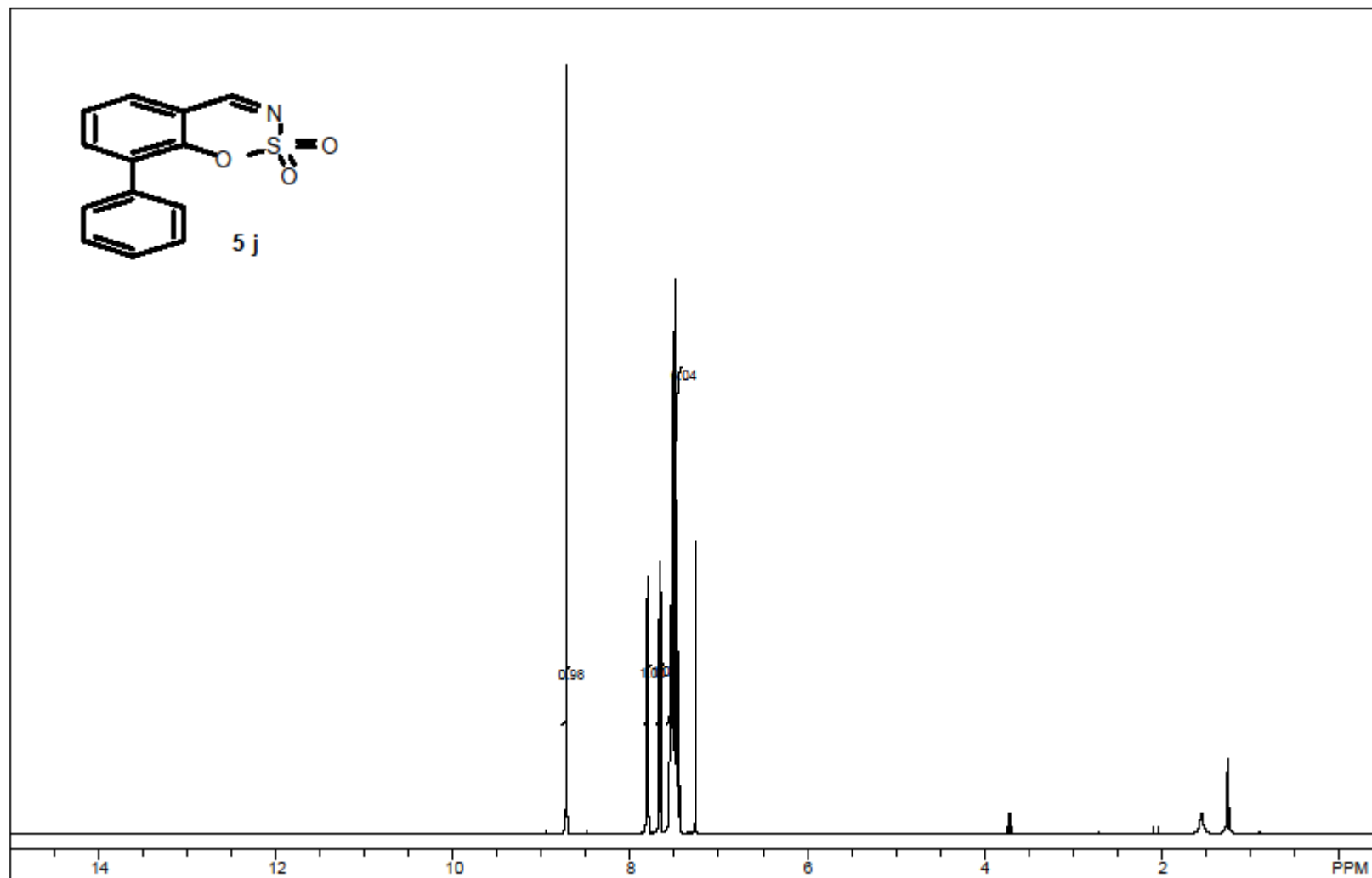
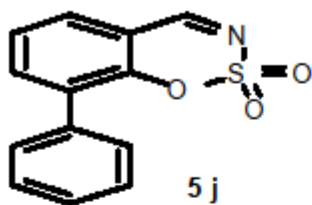
Avance CDCl3			USER: nrsu -- DATE: Thu Dec 17 14:44:52 2020			
F1: 100.579	F2: 1.000	SW1: 25000		OF1: 10069.9		PTS1d: 32768
EX: zgpg30		PW: 10.0 us	PD: 2.0 sec	NA: 240	LB: 0.0	Nuts - \$pdata



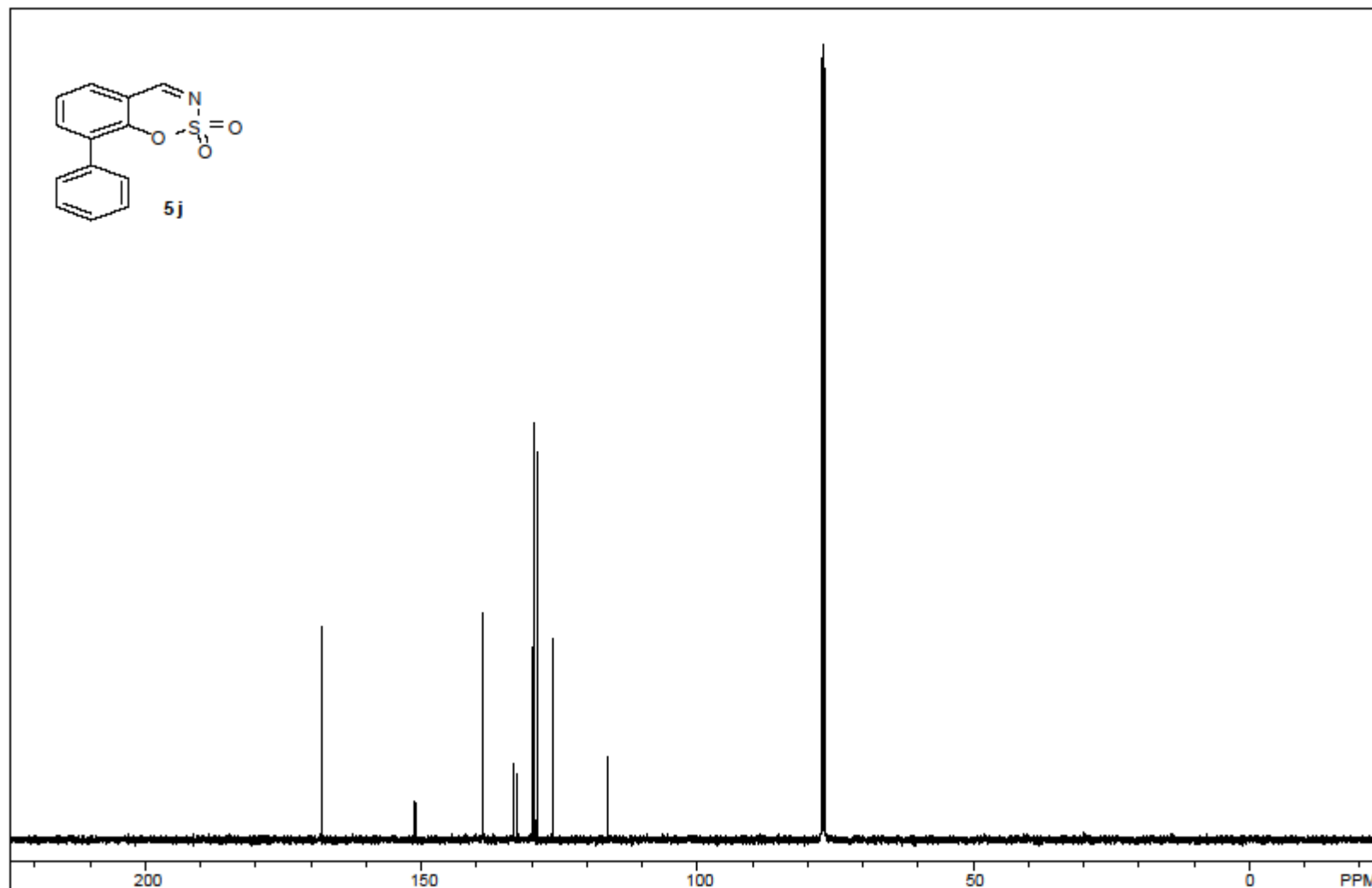
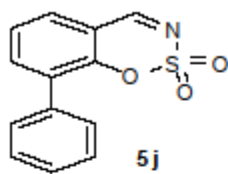
Avance CDCl <sub>3</sub>			USER: nmrsu - DATE: Wed Dec 16 09:14:07 2020			
F1: 399.956	F2: 1.000	SW1: 7813		OF1: 2460.1		PTS1d: 65536
EX: zg30		PW: 12.0 us	PD: 1.0 sec	NA: 16	LB: 0.0	Nuts - Spdata



Avance, CDCl <sub>3</sub>			USER: nrsu -- DATE: Thu Dec 17 16:38:37 2020			
F1: 100.579	F2: 1.000	SW1: 25000		OF1: 10069.2		PTS1d: 32768
EX: zgpg30		PW: 10.0 us	PD: 2.0 sec	NA: 512	LB: 0.0	Nuts - \$pdata

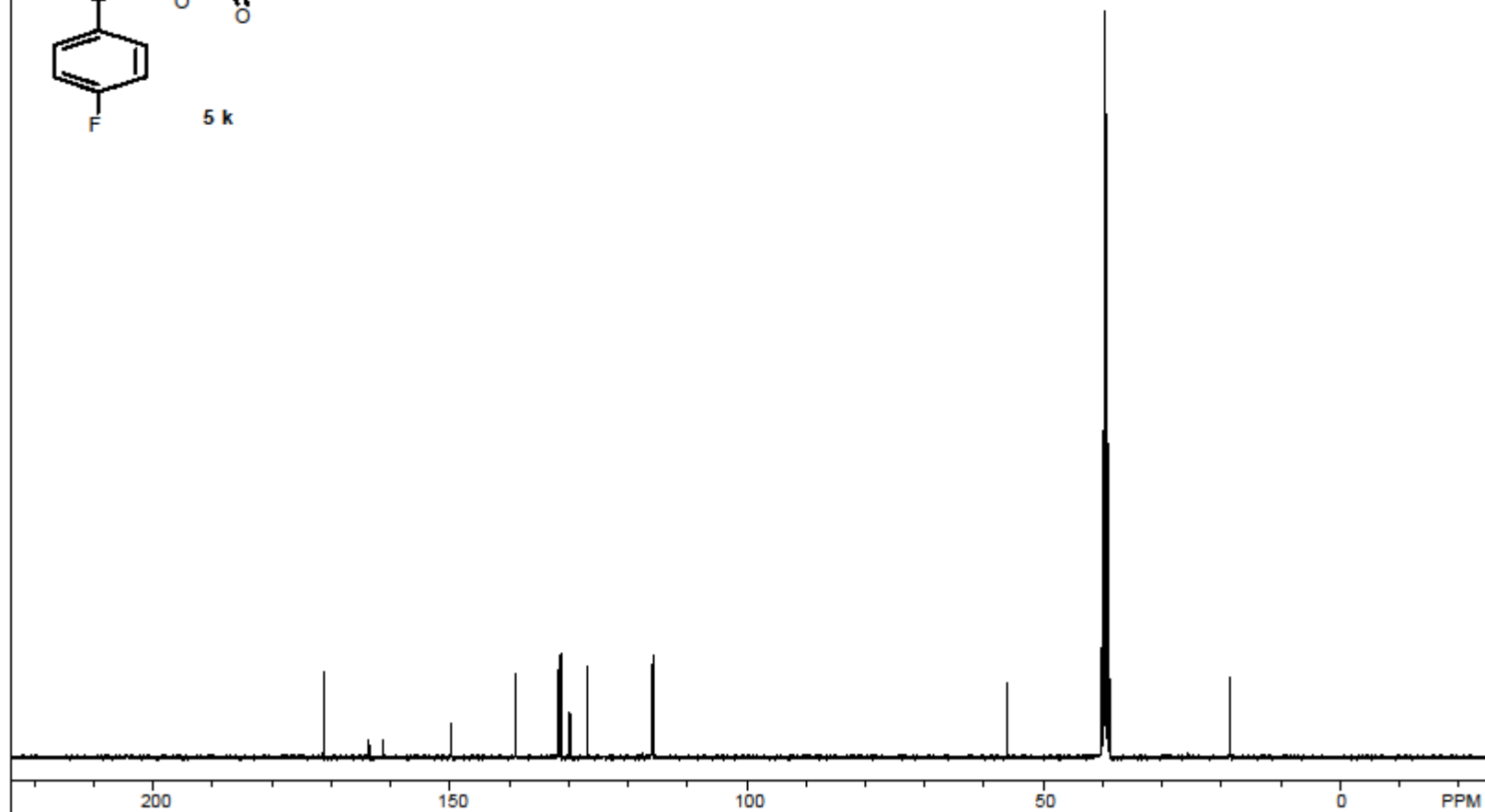
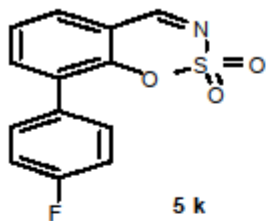


Avance CDCl3			USER: nrsu -- DATE: Mon Jan 11 11:21:31 2021			
F1: 399.956	F2: 1.000	SW1: 7813		OF1: 2460.1		PTS1d: 65536
EX: zg30		PW: 12.0 us	PD: 1.0 sec	NA: 16	LB: 0.0	Nuts - Spdata

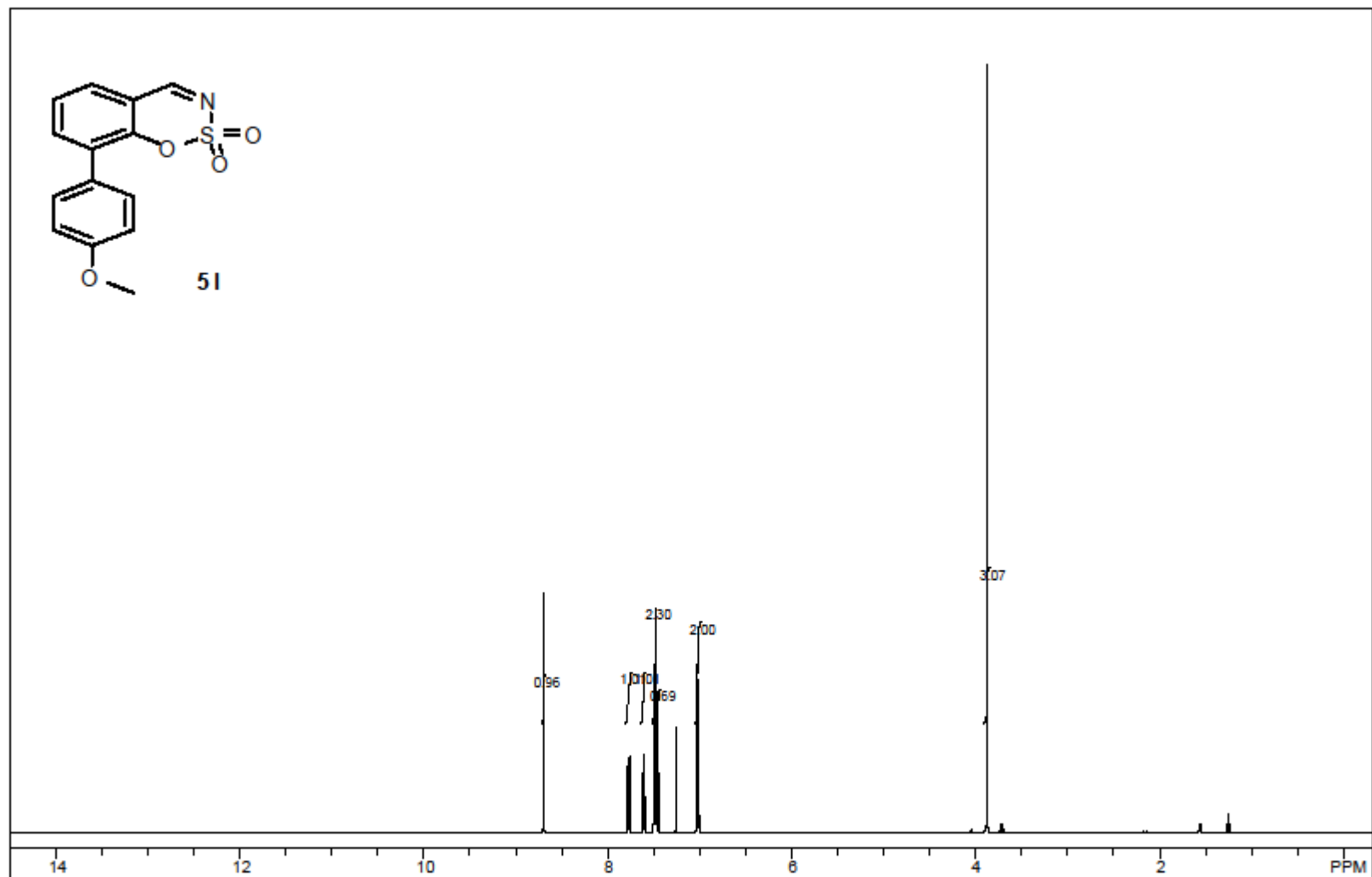
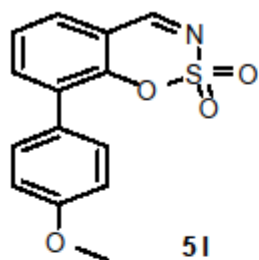


Avance CDCl3			USER: nrsu -- DATE: Mon Jan 11 11:34:17 2021			
F1: 100.579	F2: 1.000	SW1: 25000		OF1: 10069.3		PTS1d: 32768
EX: zgpg30		PW: 10.0 us	PD: 2.0 sec	NA: 256	LB: 0.0	Nuts - \$pdata

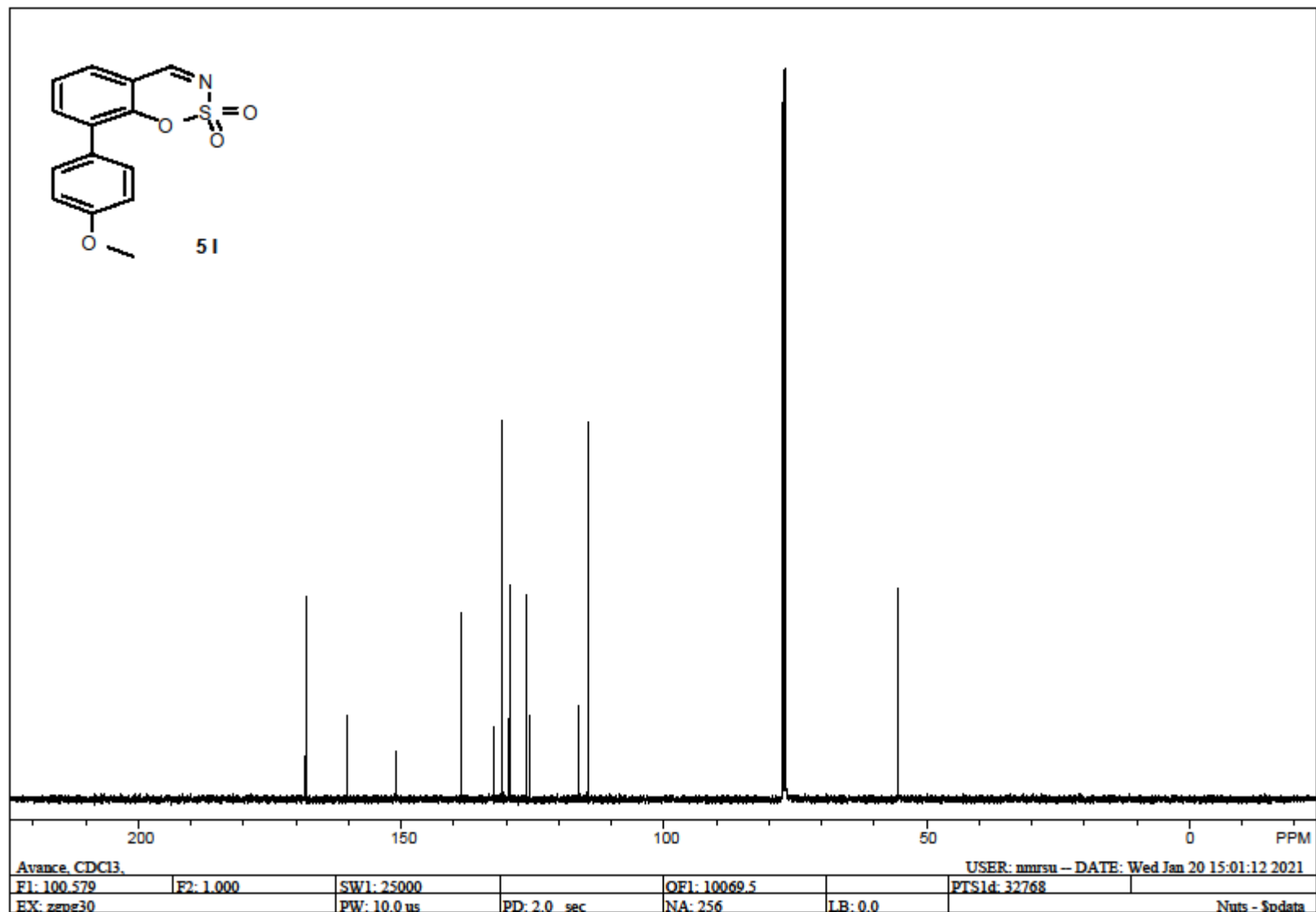
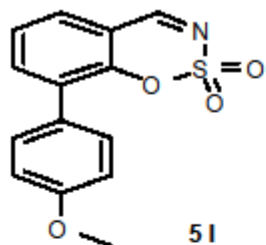


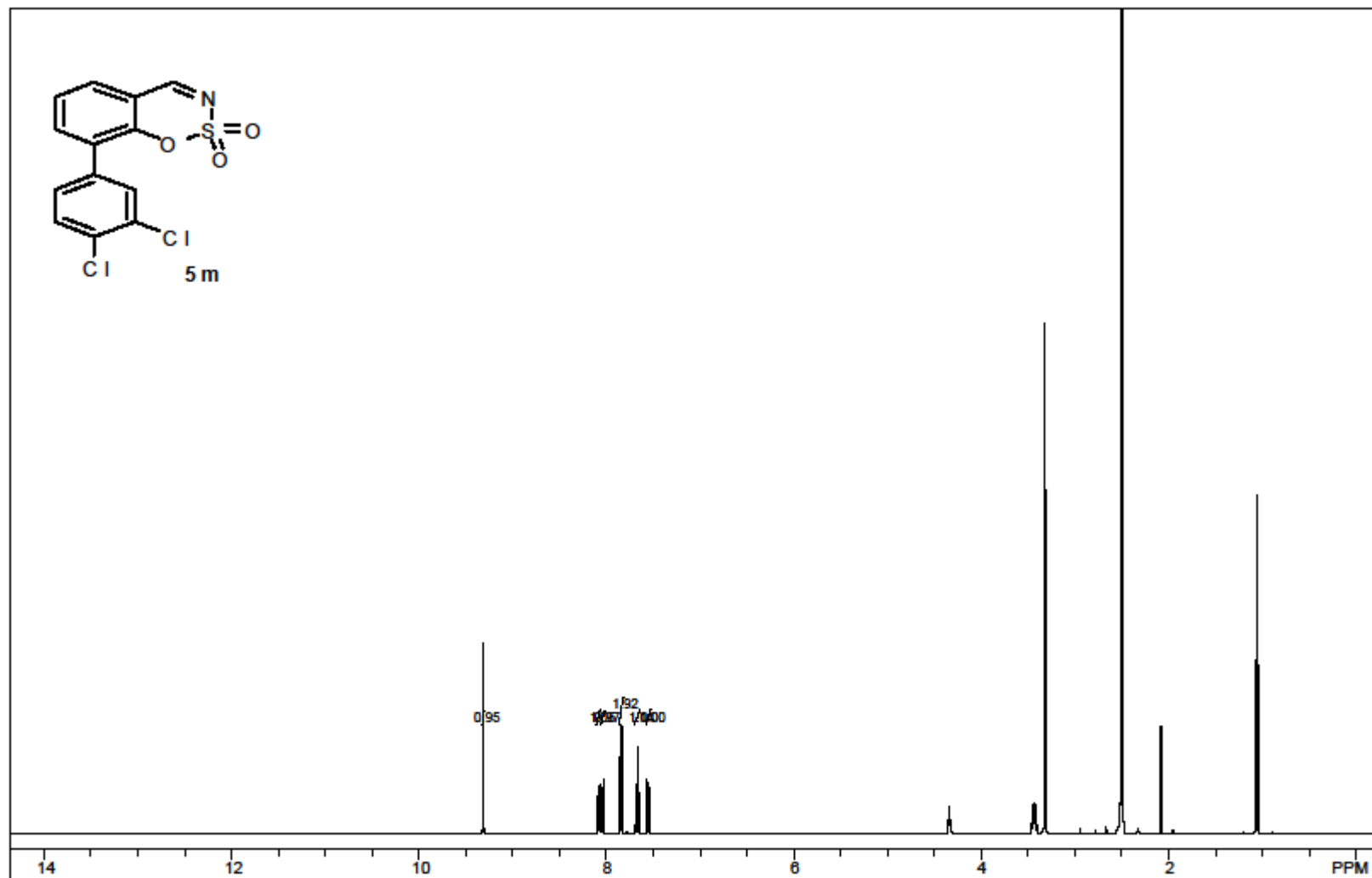
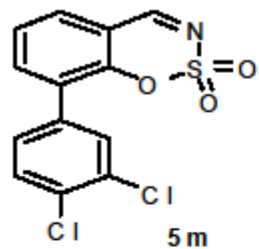


Avance DMSO			USER: nmrsu -- DATE: Tue Feb 23 12:53:26 2021			
F1: 100.579	F2: 1.000	SW1: 25000		OE1: 10012.8		PTS1d: 32768
EX: zgpg30		PW: 10.0 us	PD: 2.0 sec	NA: 256	LB: 0.0	Nuts - Spdata

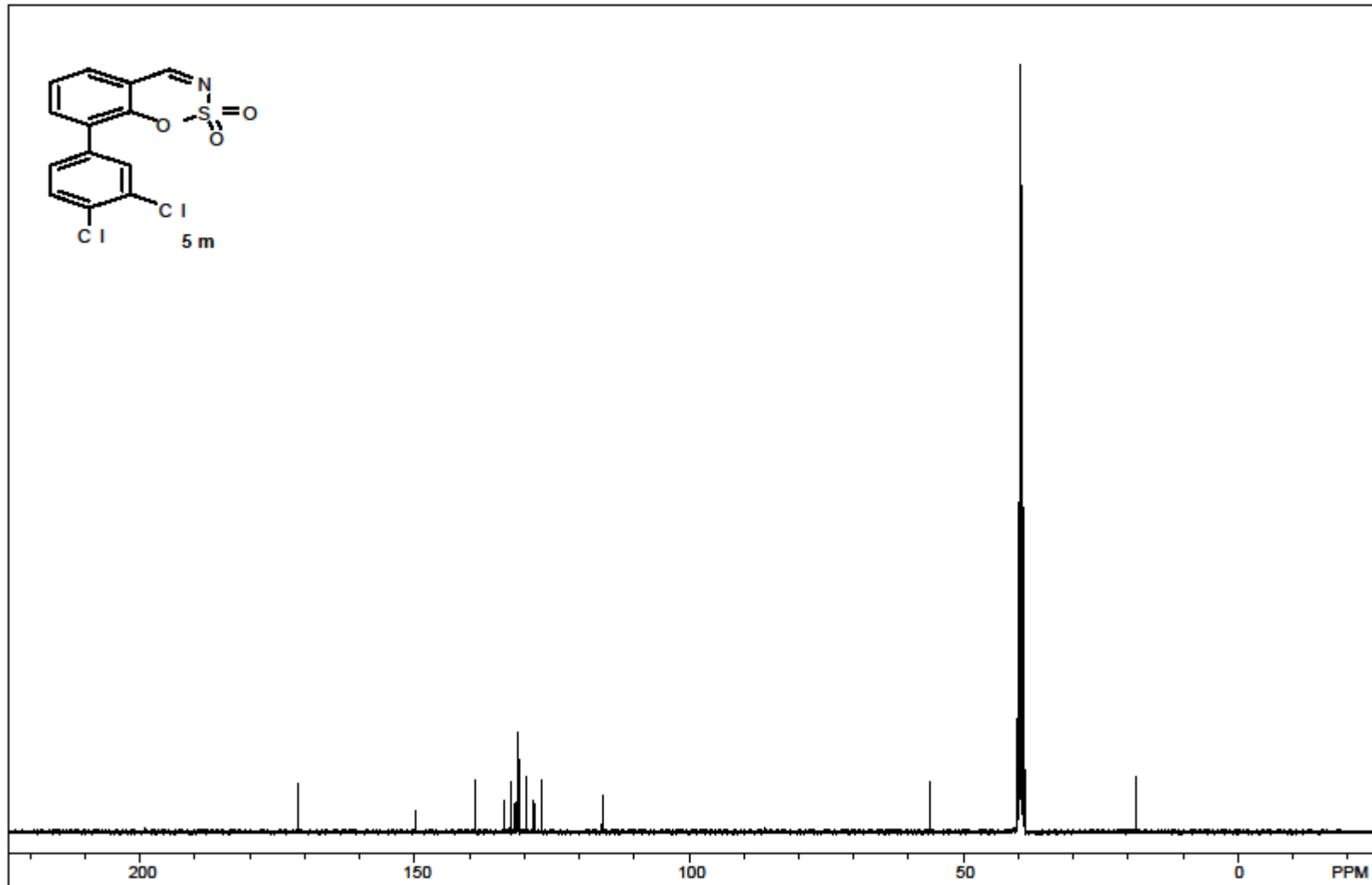
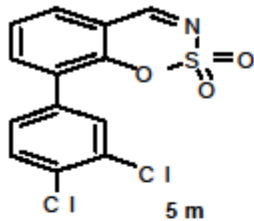


Avance, CDCl <sub>3</sub>			USER: nmrsu -- DATE: Wed Jan 20 14:30:44 2021			
F1: 399.956	F2: 1.000	SW1: 7813		OF1: 2460.1		PTS1d: 65536
EX: zg30		PW: 12.0 us	PD: 1.0 sec	NA: 16	LB: 0.0	Nuts - Spdata





Avance DMSO			USER: nmrstu -- DATE: Mon Jan 25 08:51:52 2021			
F1: 399.956	F2: 1.000	SW1: 7813		OF1: 2466.5		PTS1d: 65536
EX: zg30		PW: 12.0 us	PD: 1.0 sec	NA: 16	LB: 0.0	Nuts - Spdata



Avance DMSO			USER: nmrsu -- DATE: Tue Feb 23 12:36:17 2021			
F1: 100.579	F2: 1.000	SW1: 25000		QF1: 10012.7		PTS1d: 32768
EX: zgpg30		PW: 10.0 us	PD: 2.0 sec	NA: 256	LB: 0.0	Nuts - Spdata