

## Supplementary information

### **Design and synthesis of 6,7-methylenedioxy-4-substituted phenylquinolin-2(1H)-one derivatives as novel anticancer agents that induce apoptosis with cell cycle arrest at G2/M phase**

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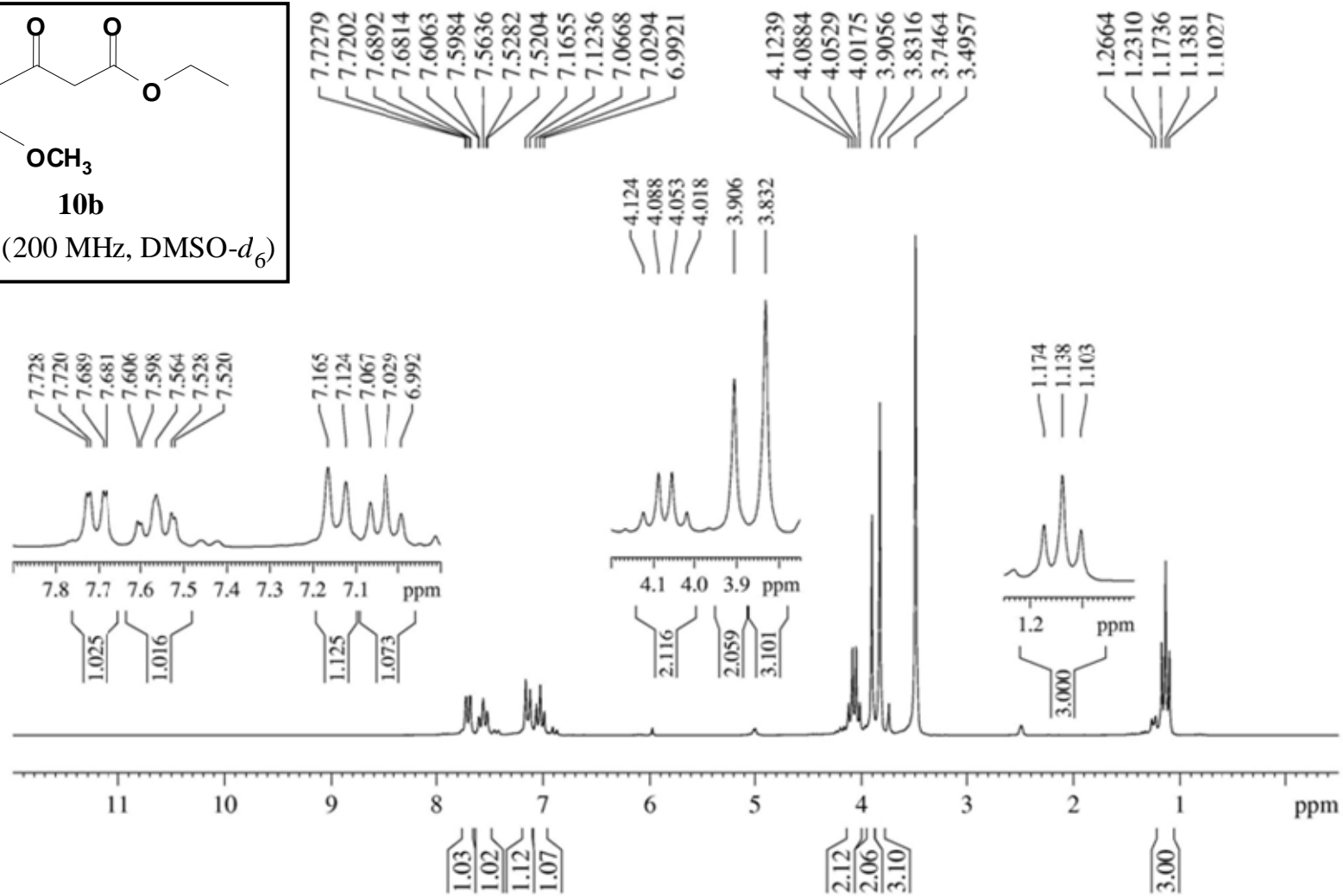
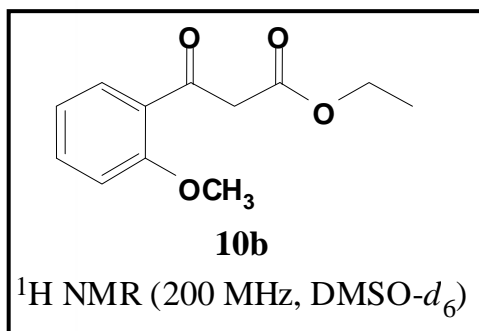
<sup>b</sup>*Graduate Institute of Pharmaceutical Chemistry, China Medical University, No.91 Hsueh-Shih Road, Taichung, Taiwan 40402, R.O.C.*

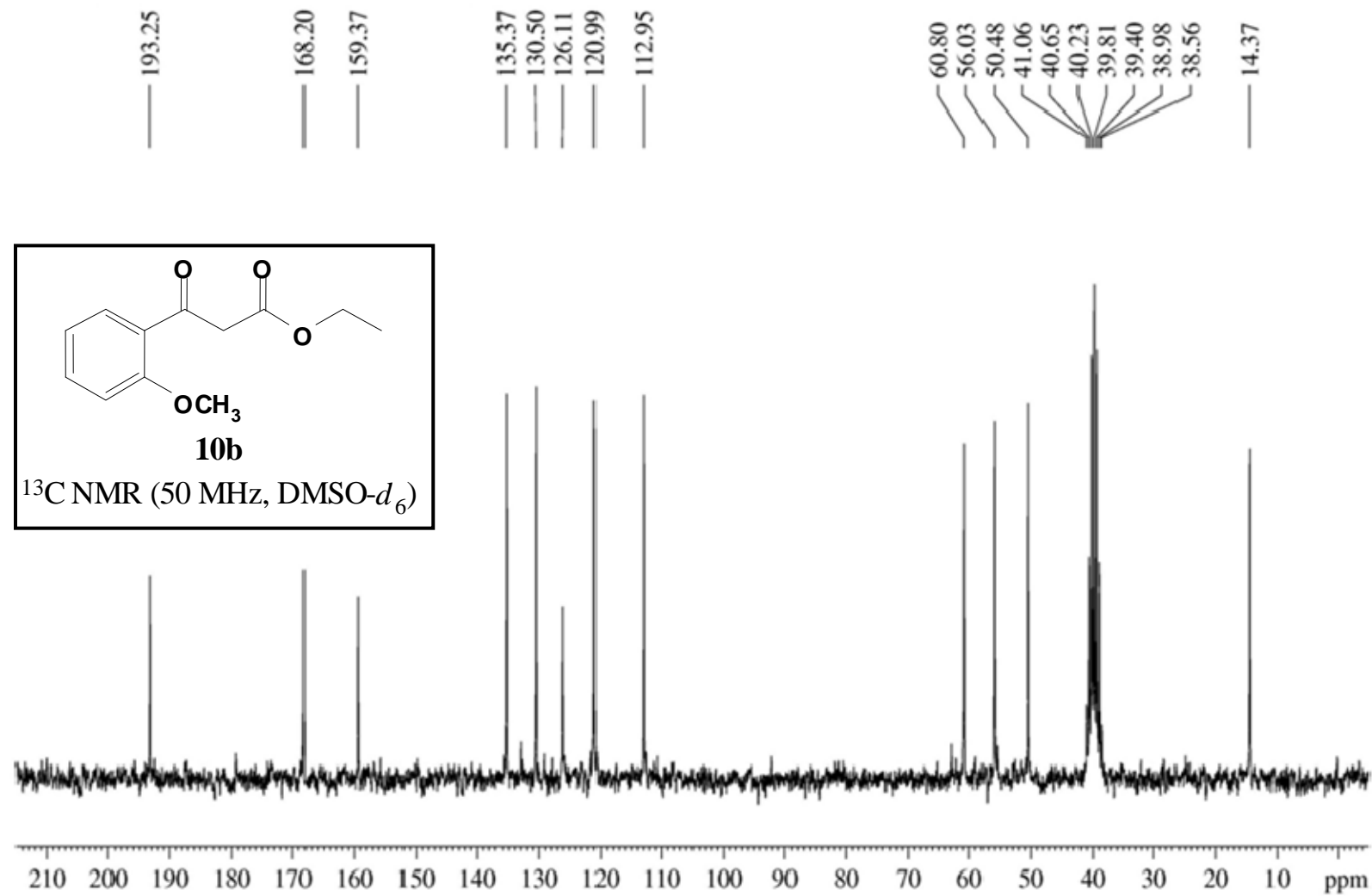
<sup>c</sup>*Department of Biochemistry, School of Medicine, China Medical University, No.91 Hsueh-Shih Road, Taichung, Taiwan 40402, R.O.C.*

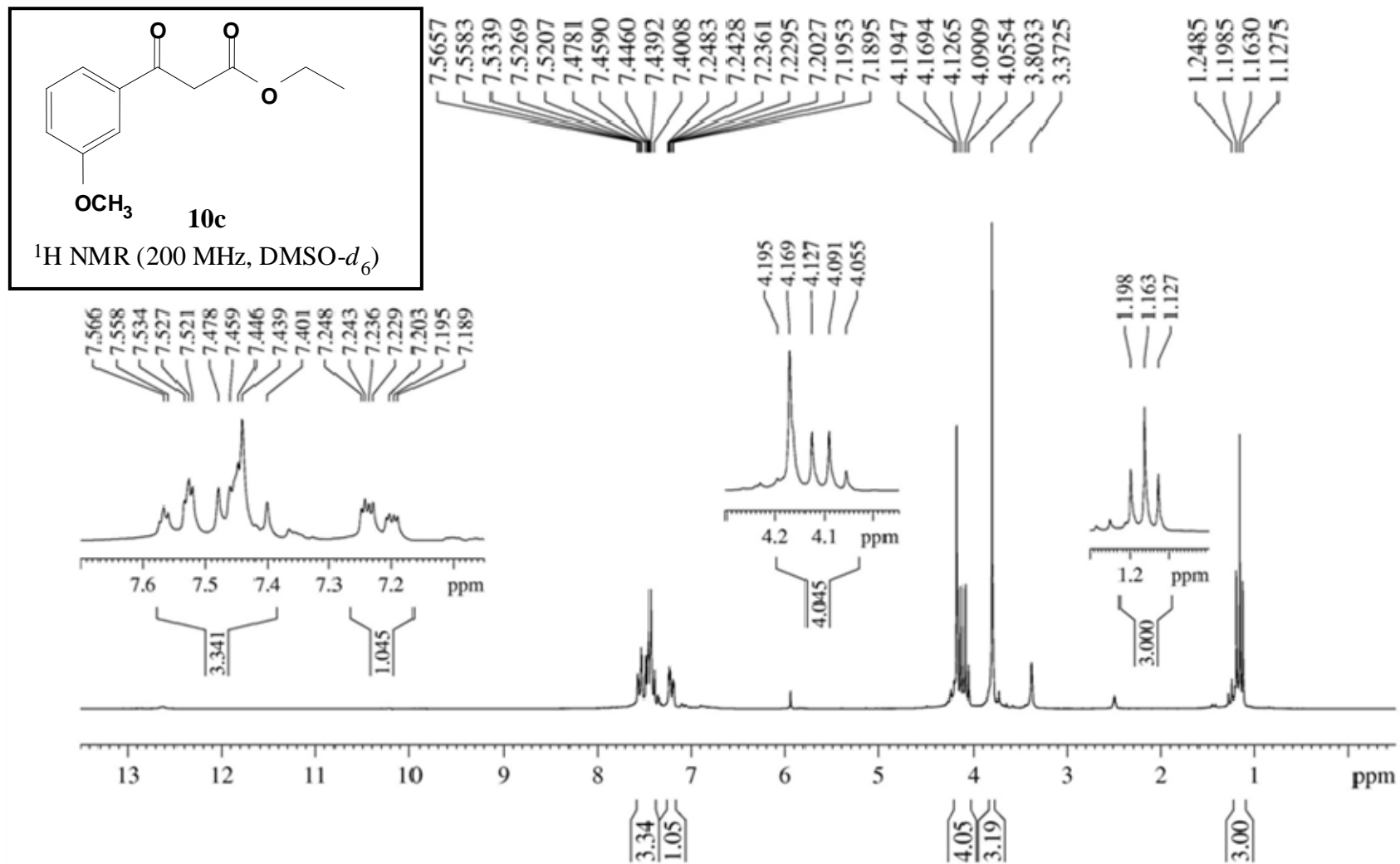
<sup>d</sup>*Natural Products Research Laboratories, Eshelman School of Pharmacy, University of North Carolina, Chapel Hill, North Carolina 27599-7568, USA*

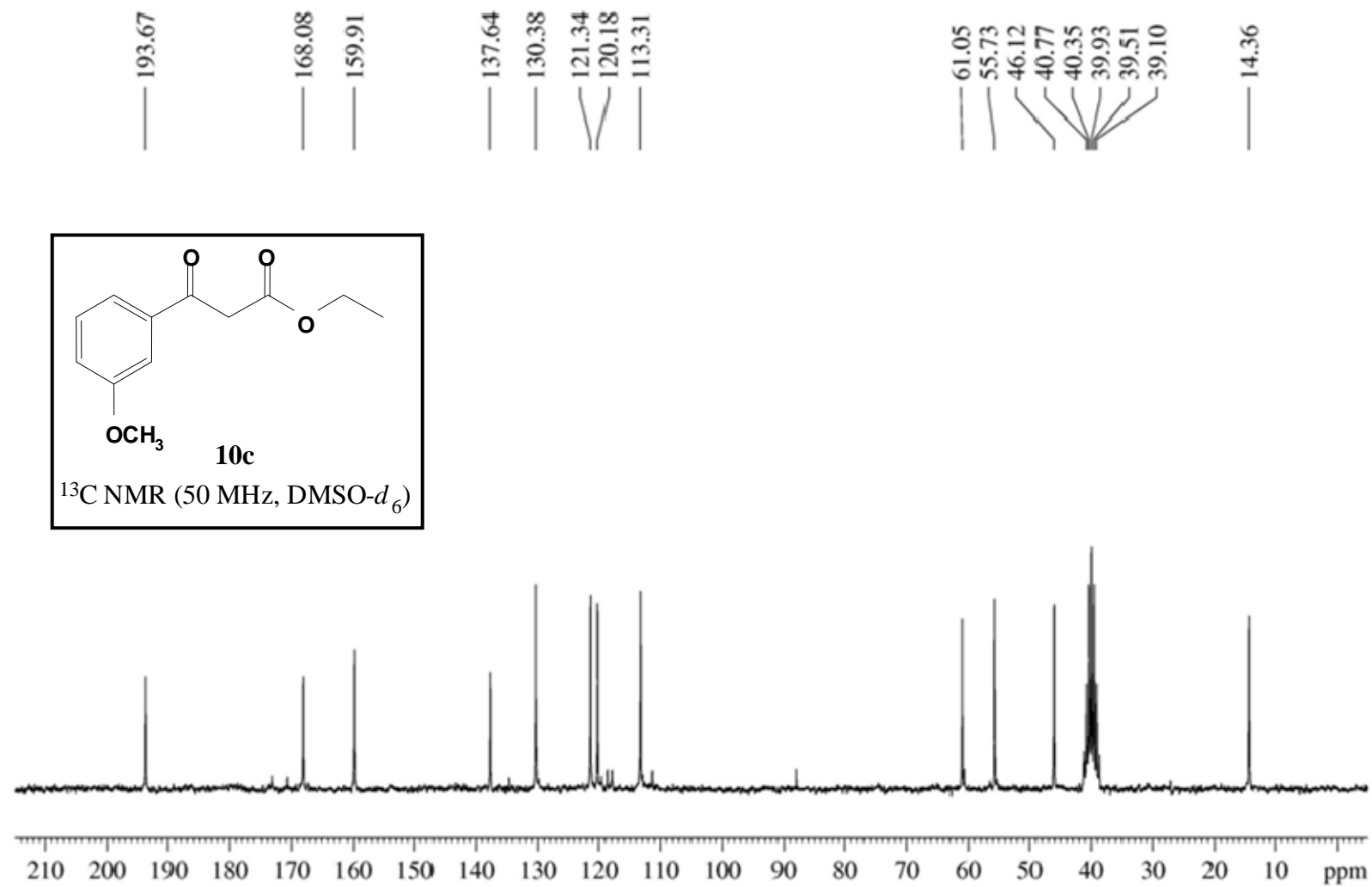
<sup>e</sup>*Chinese Medicine Research and Development Center, China Medical University Hospital, Taichung, Taiwan 40402, R.O.C.*

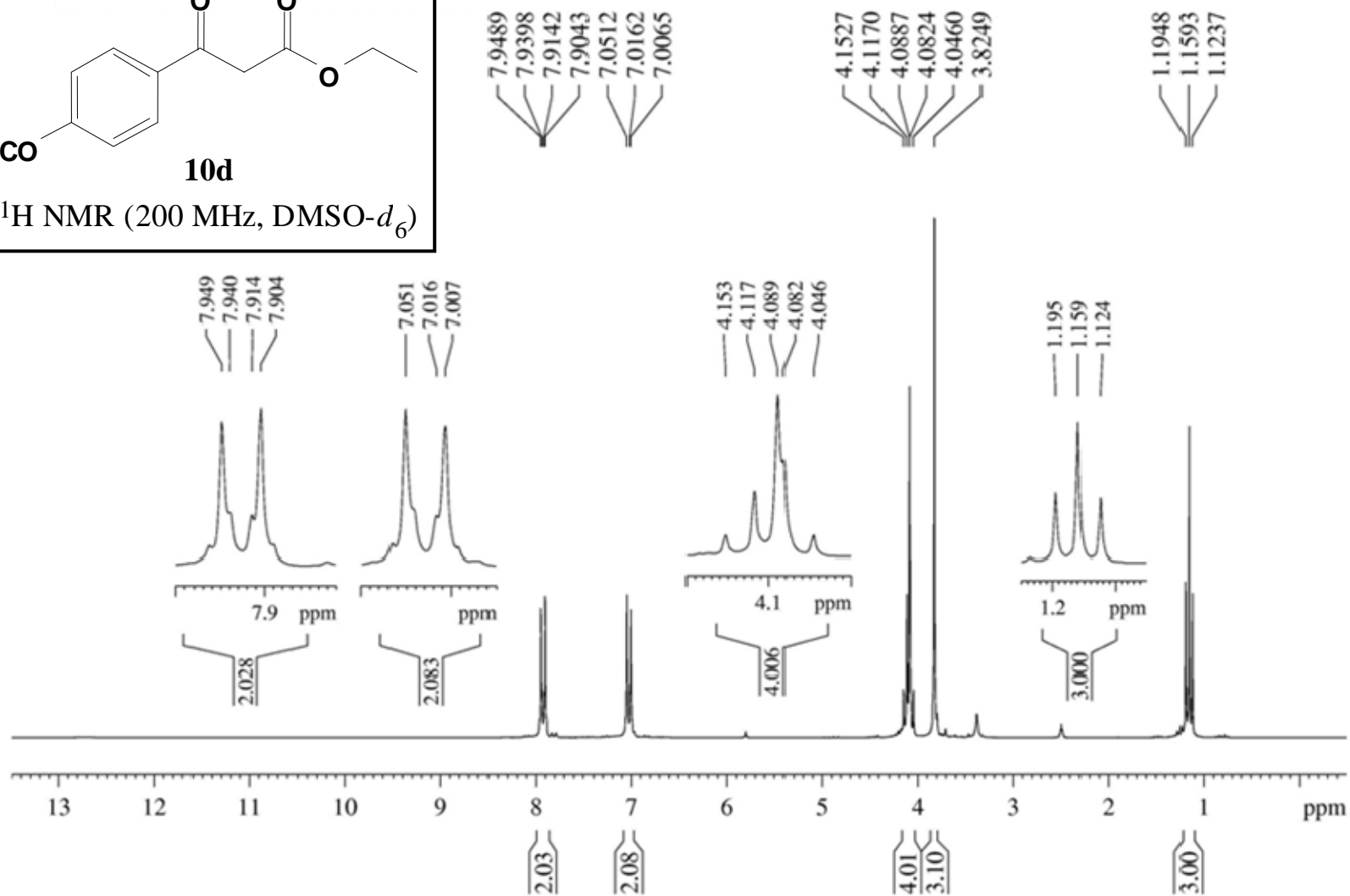
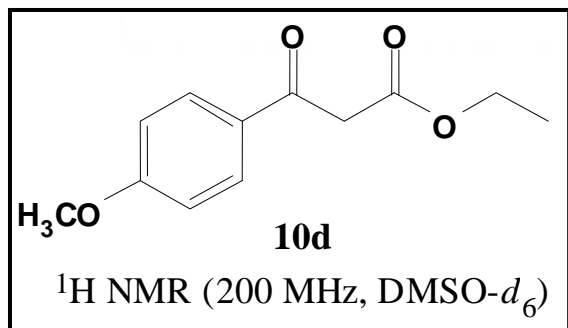
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- ◆ Spectral copies of EI-MS, HRMS of the synthetic compounds ..... S84 - S124

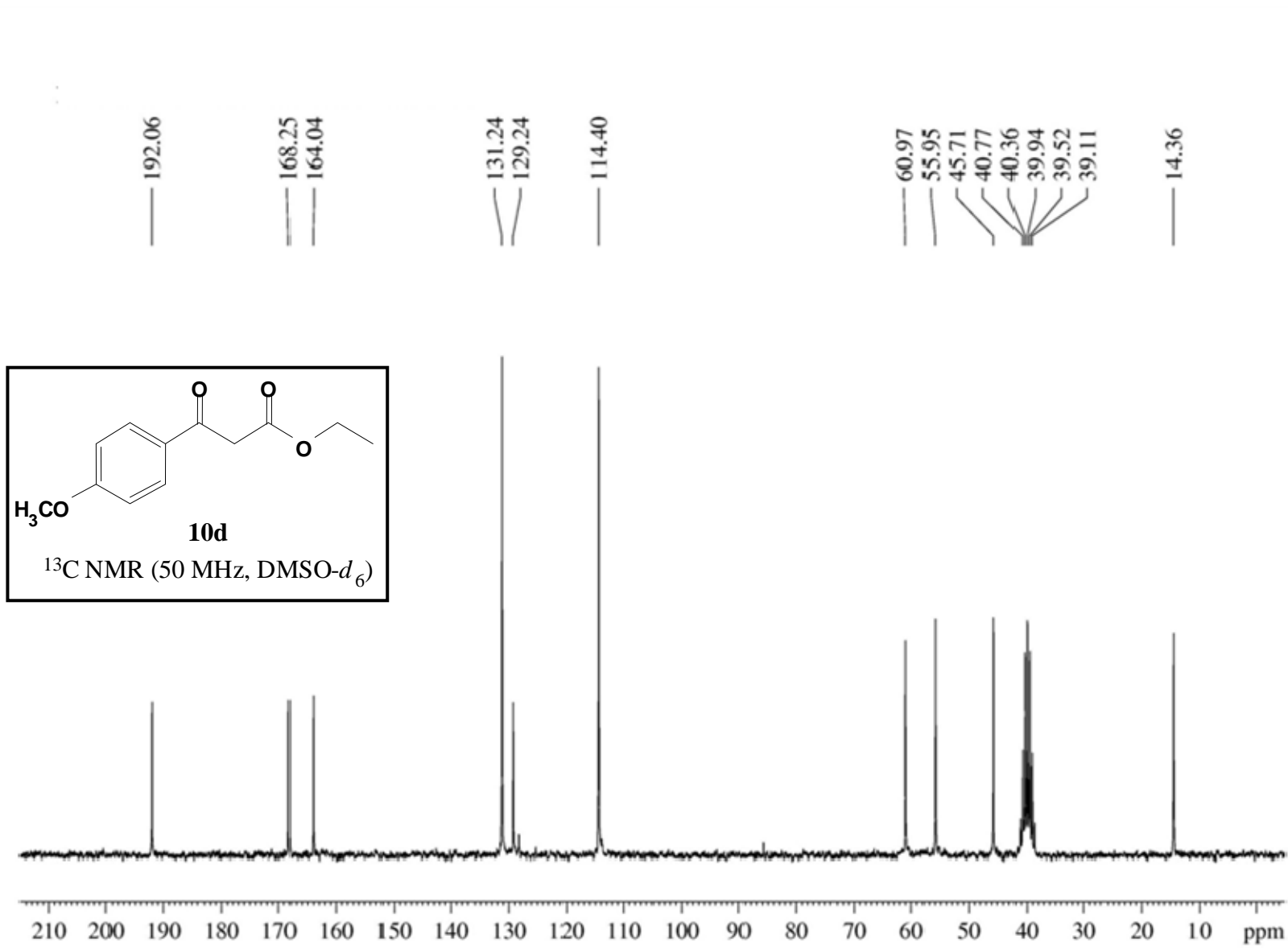


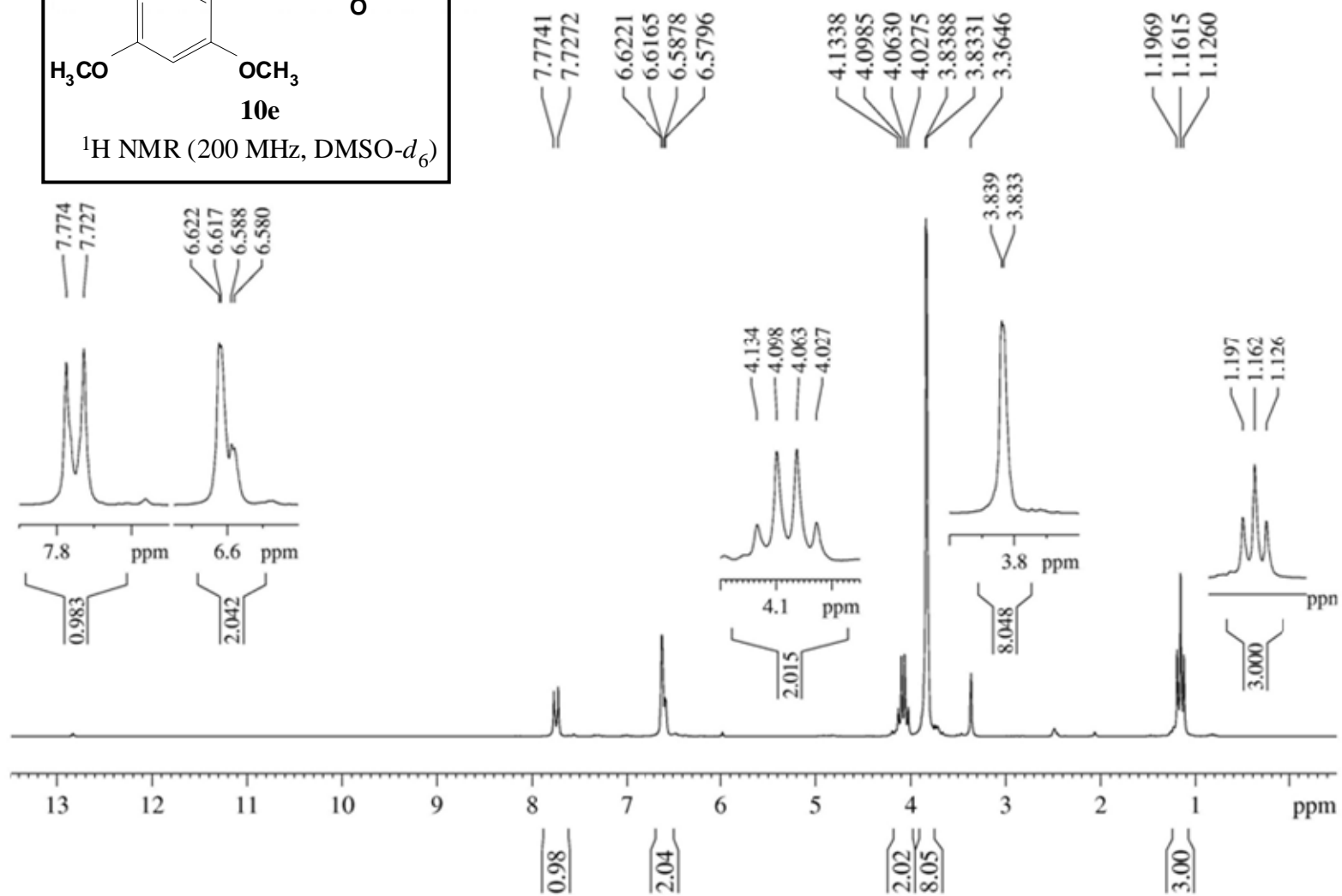
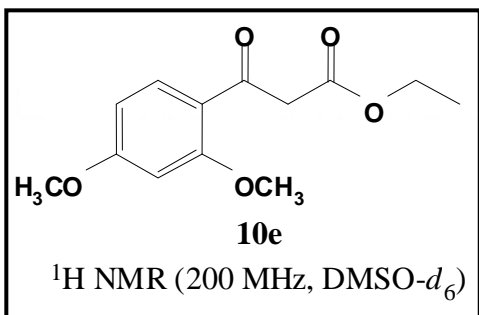




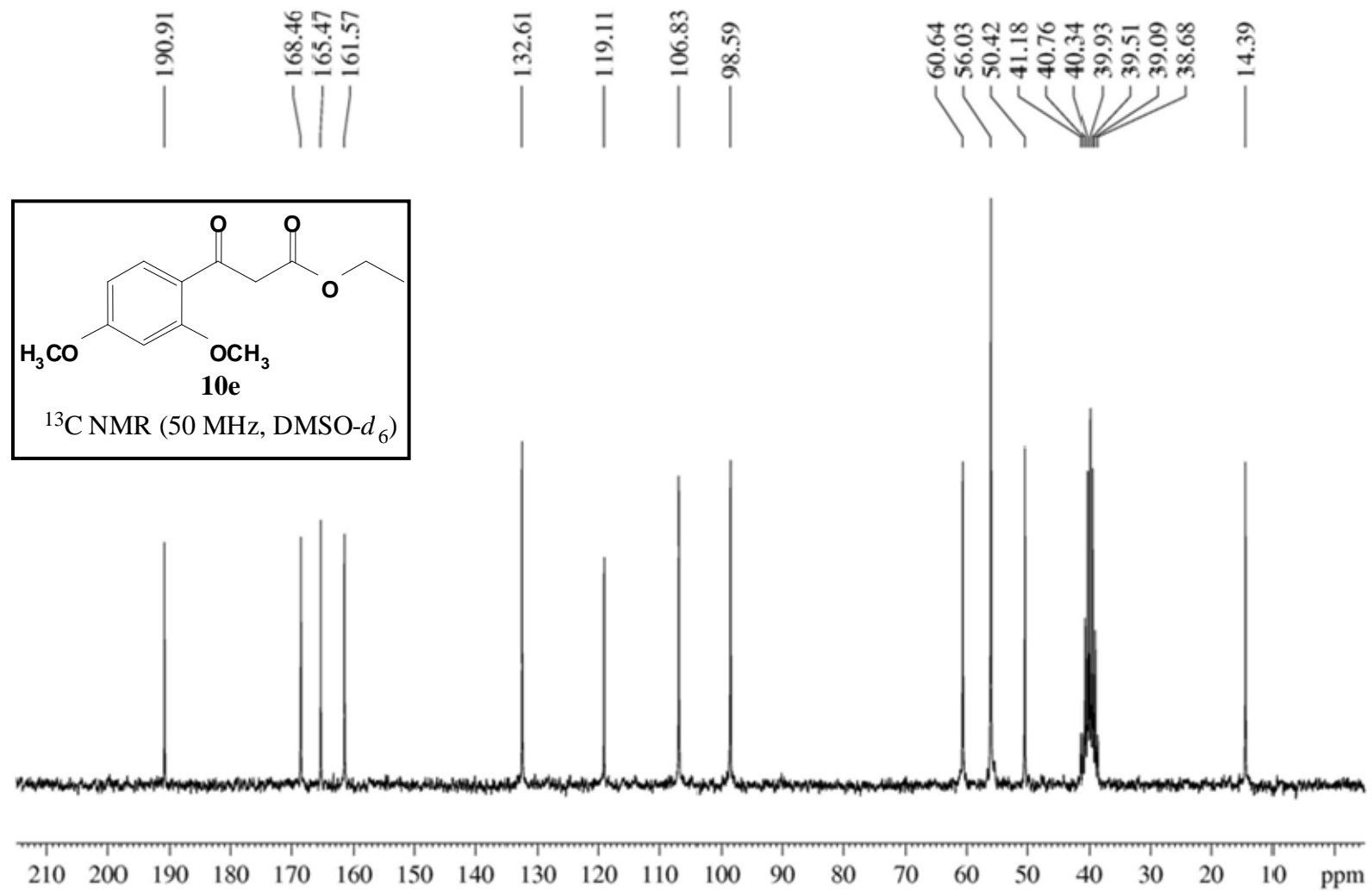


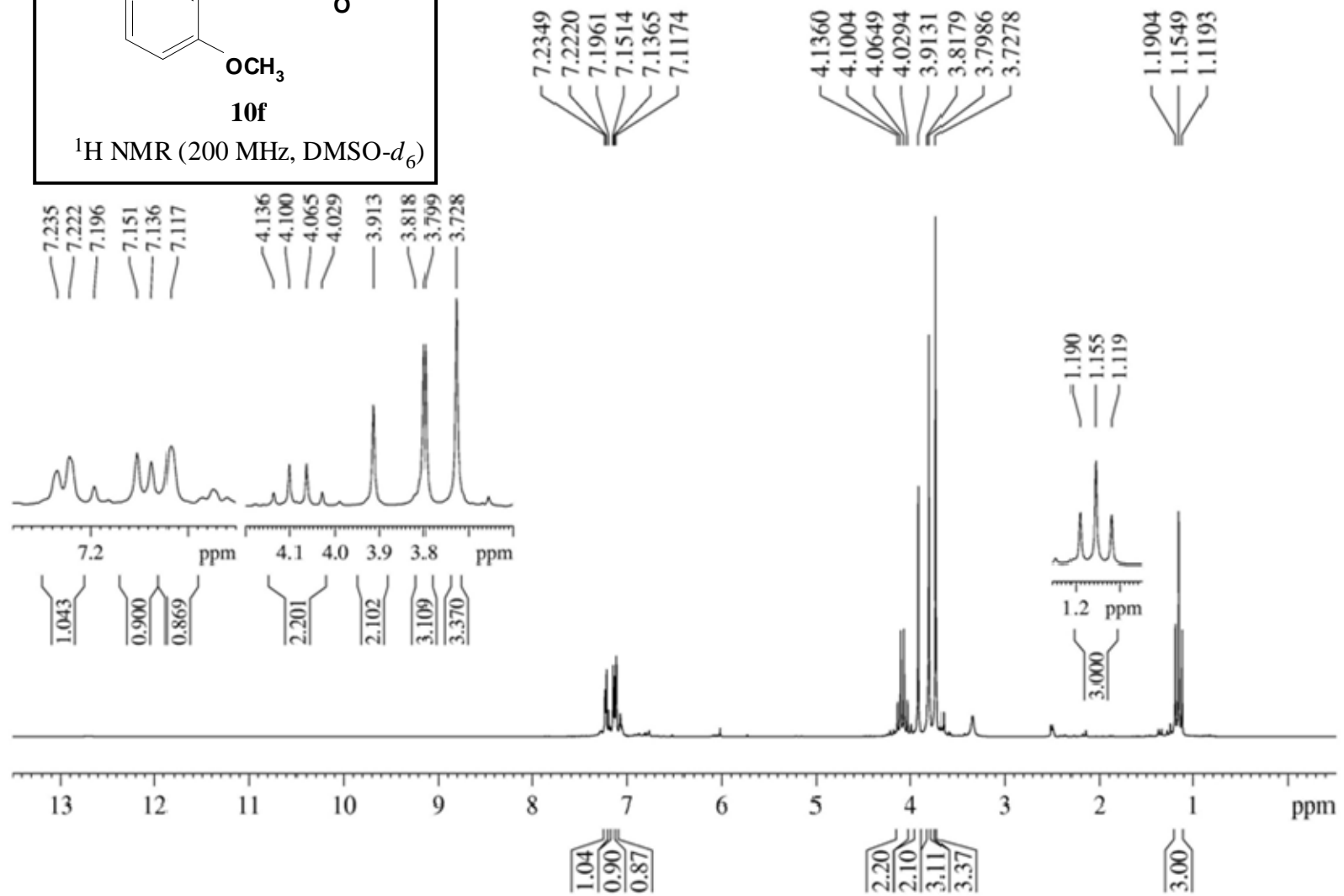
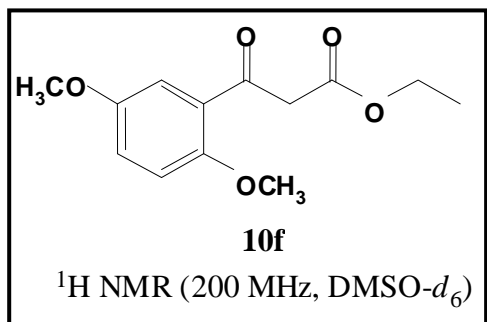


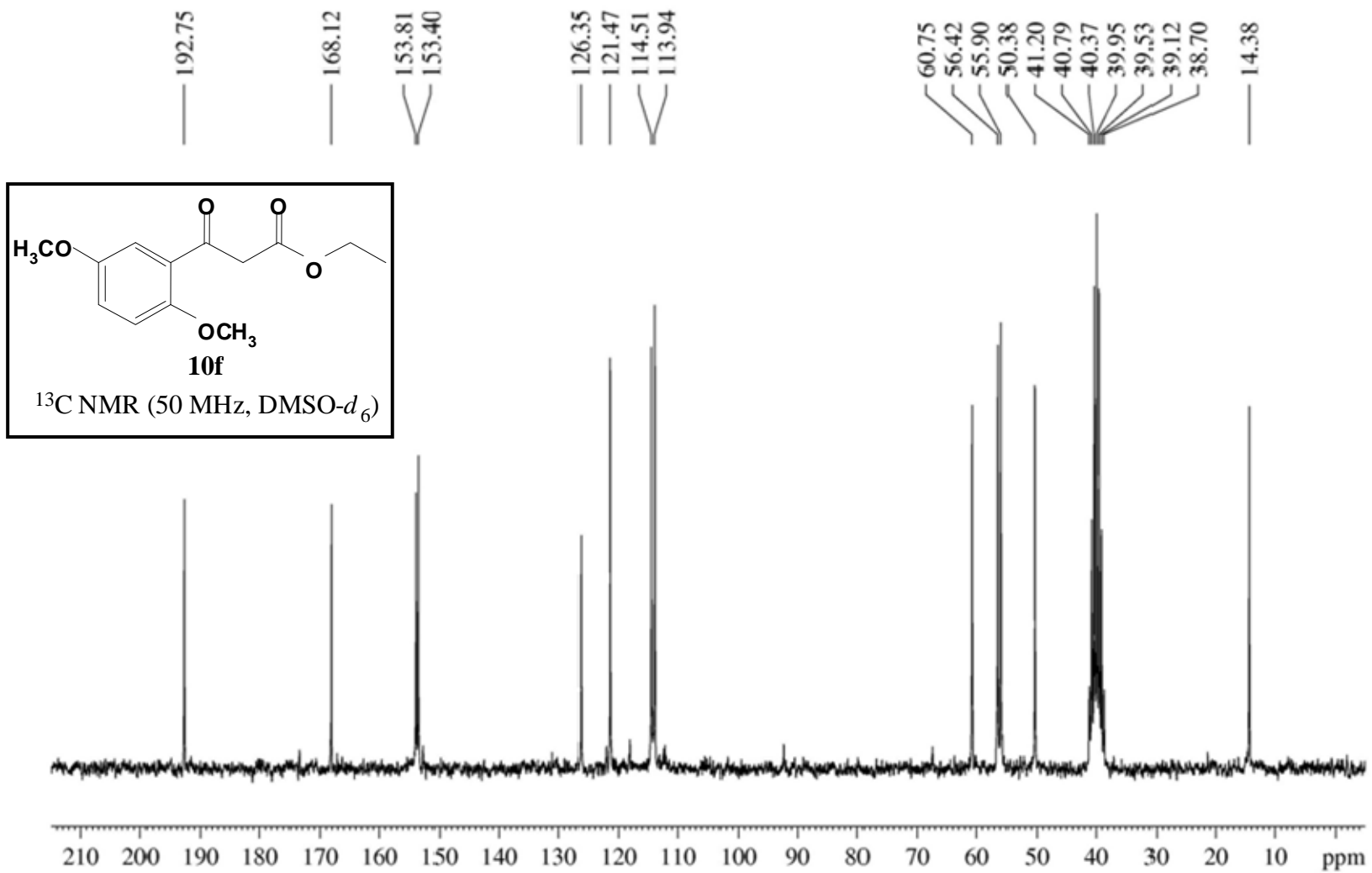


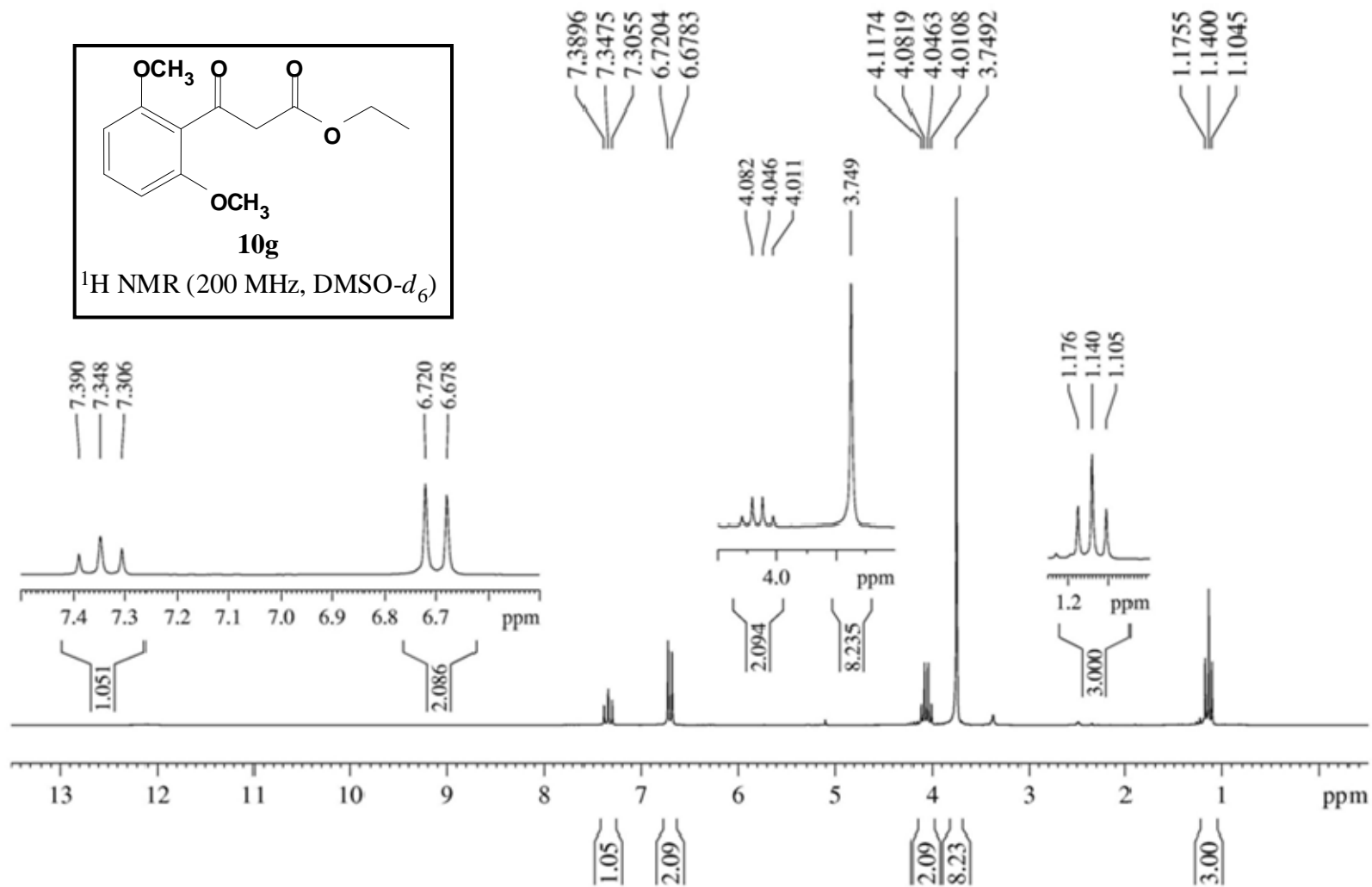
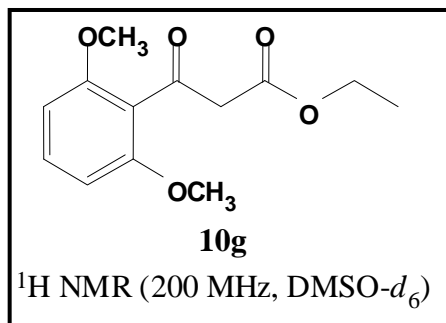


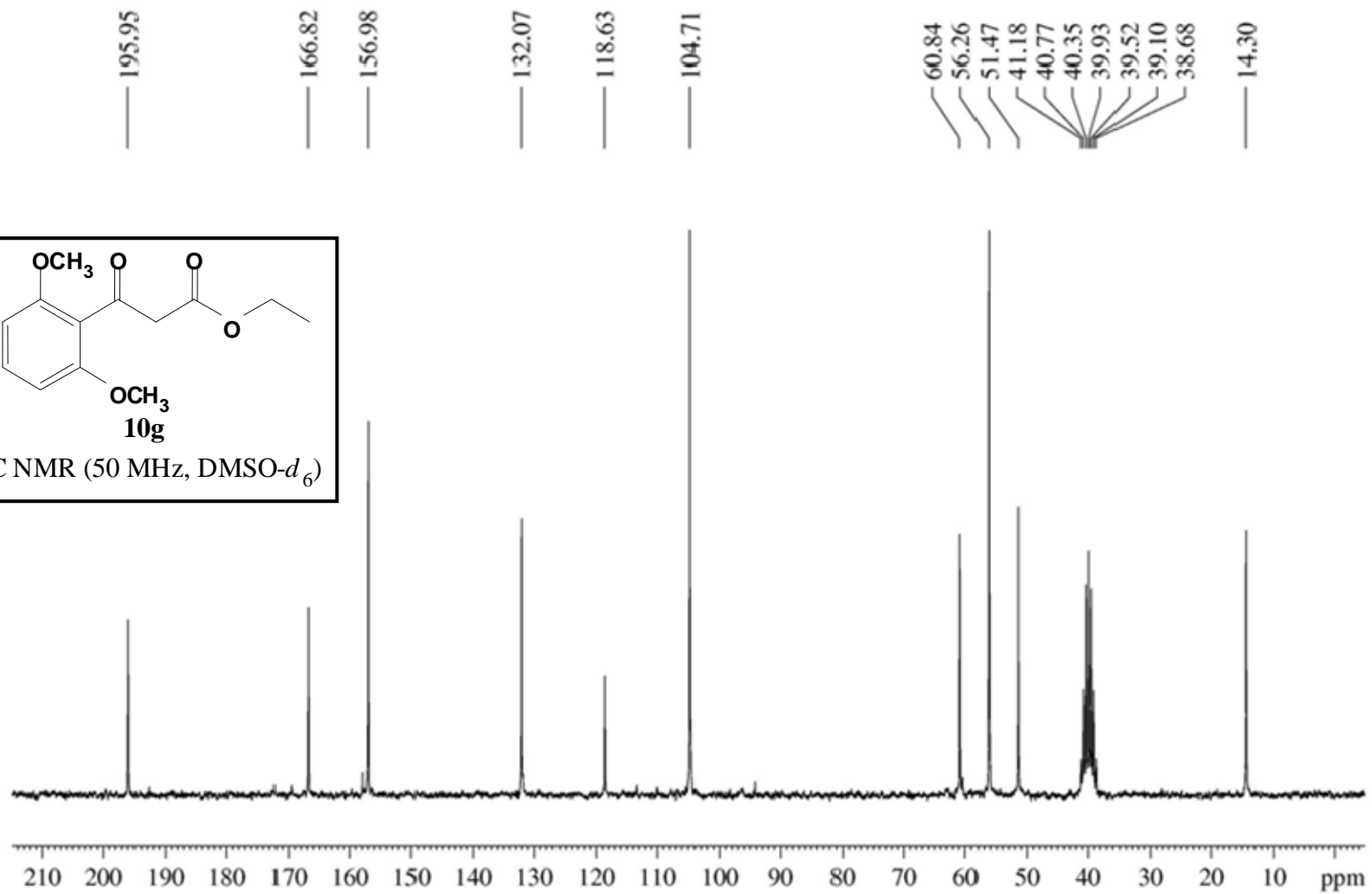
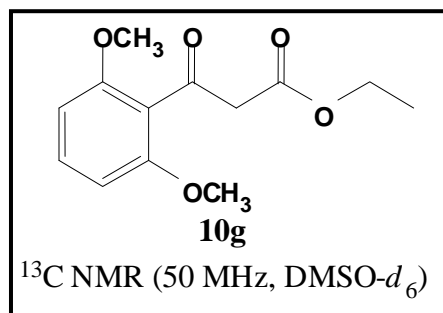


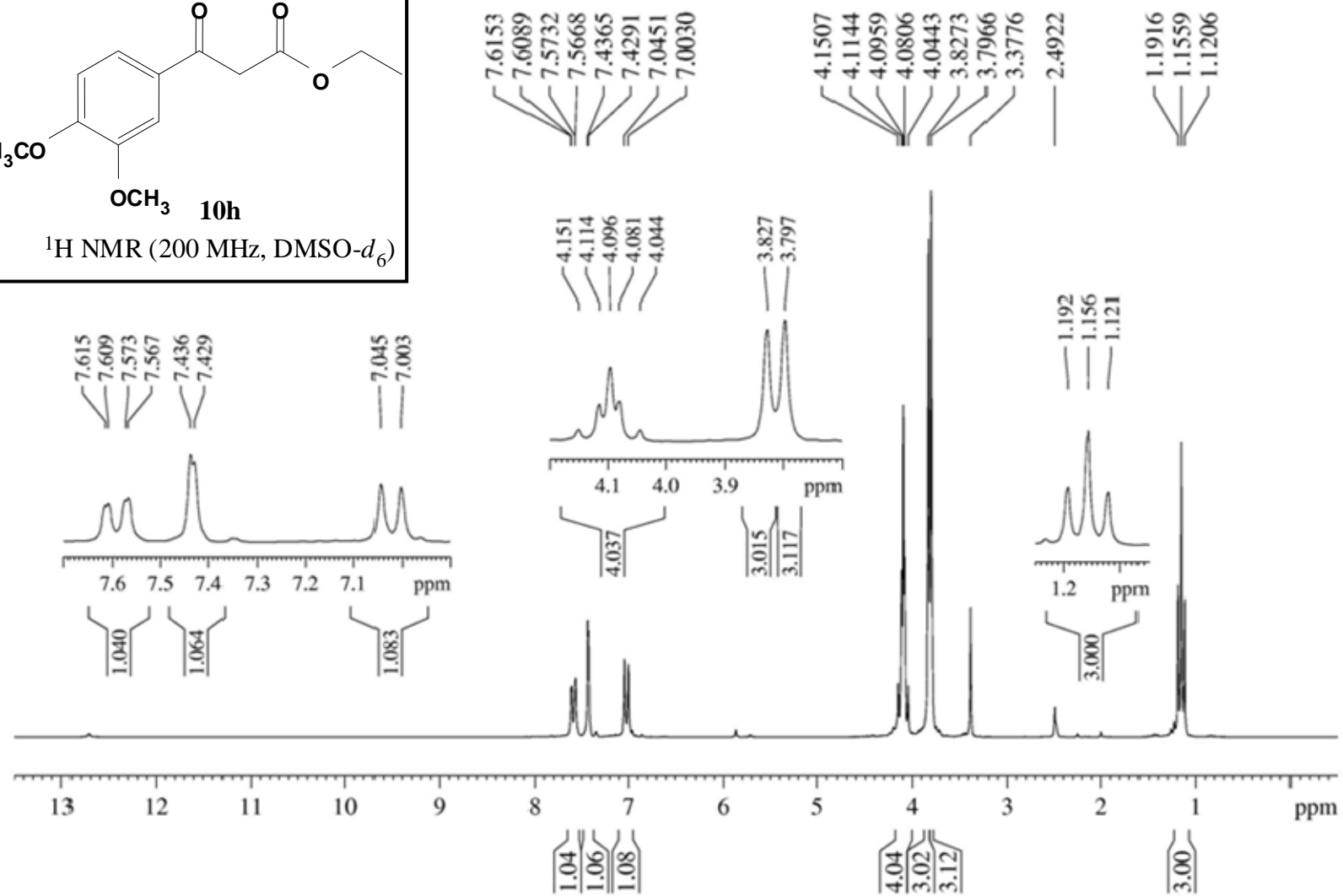
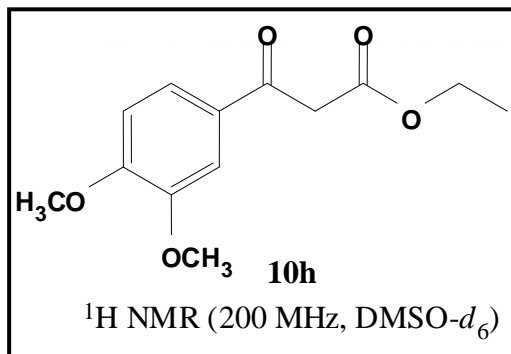


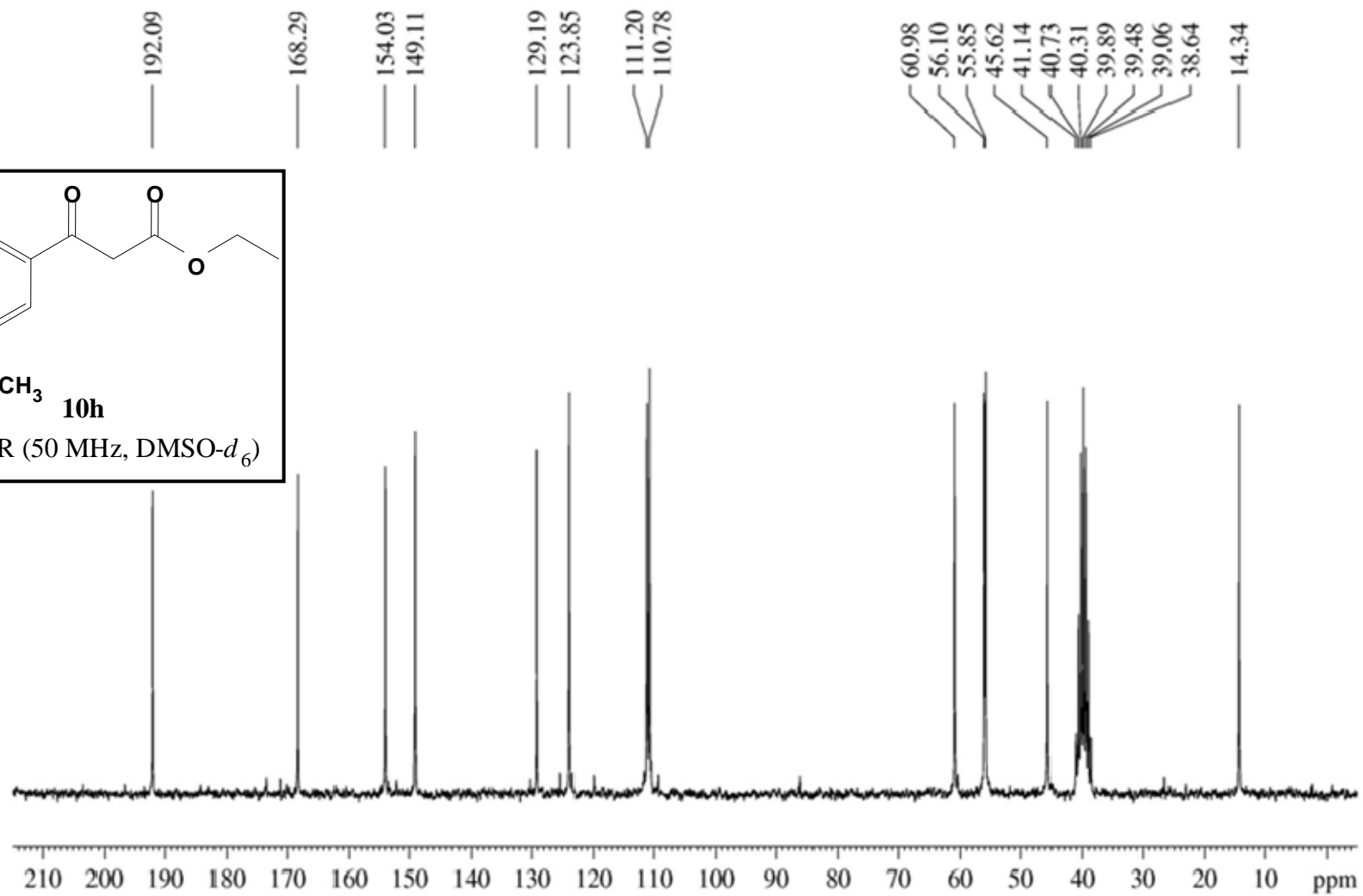
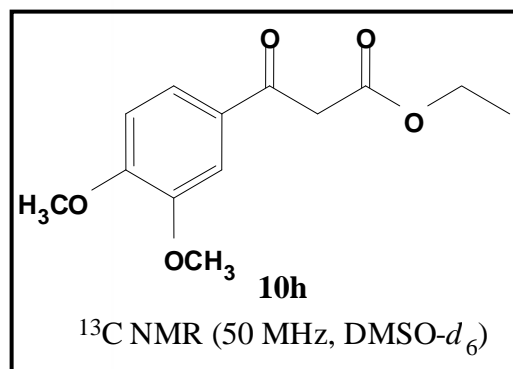


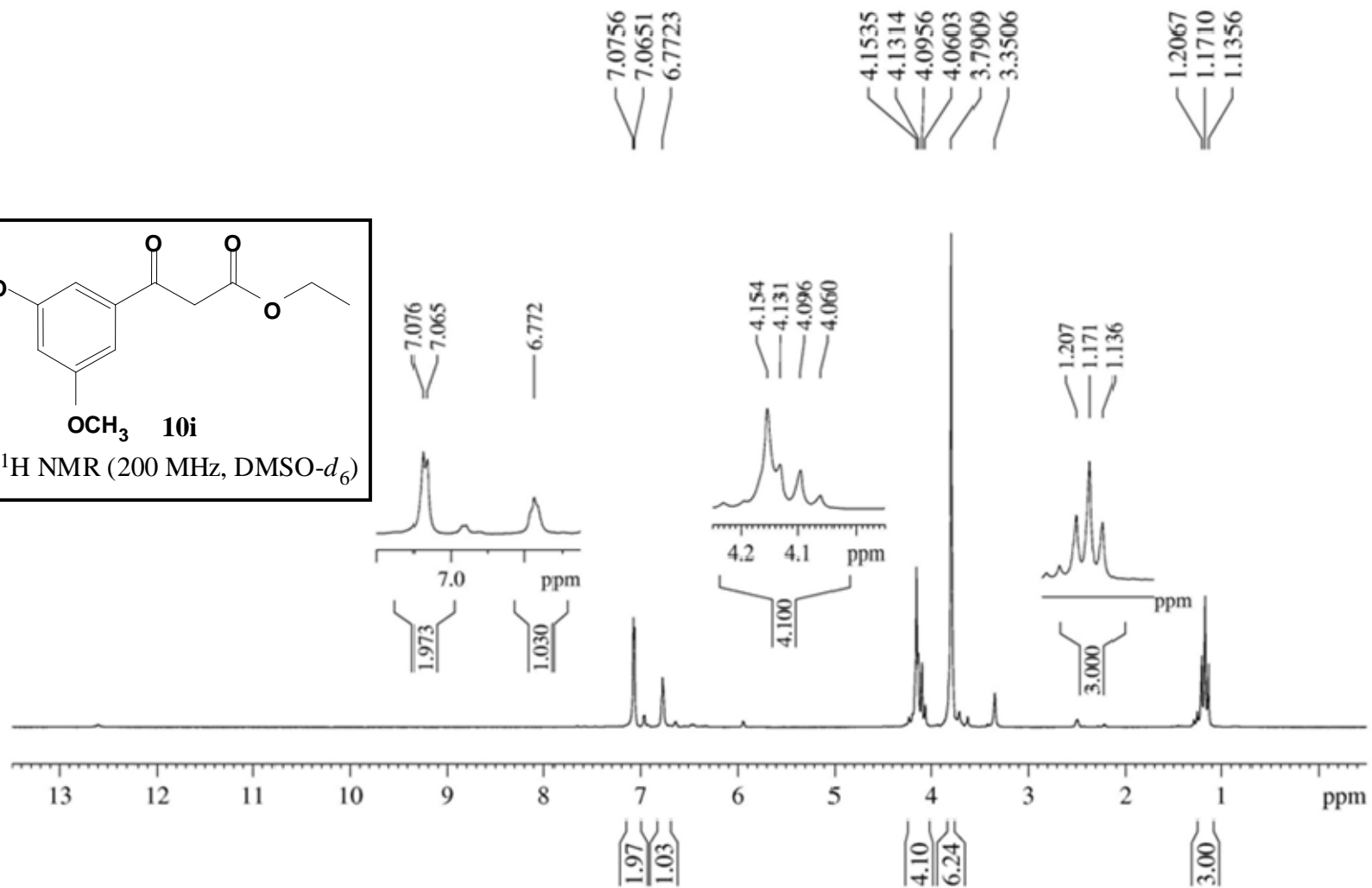
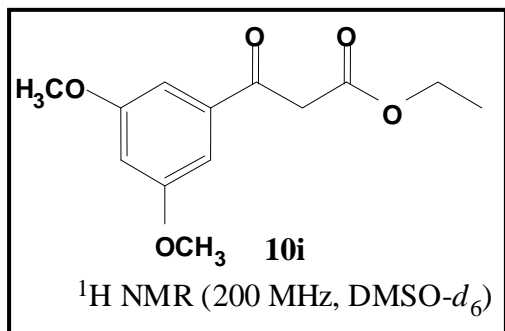




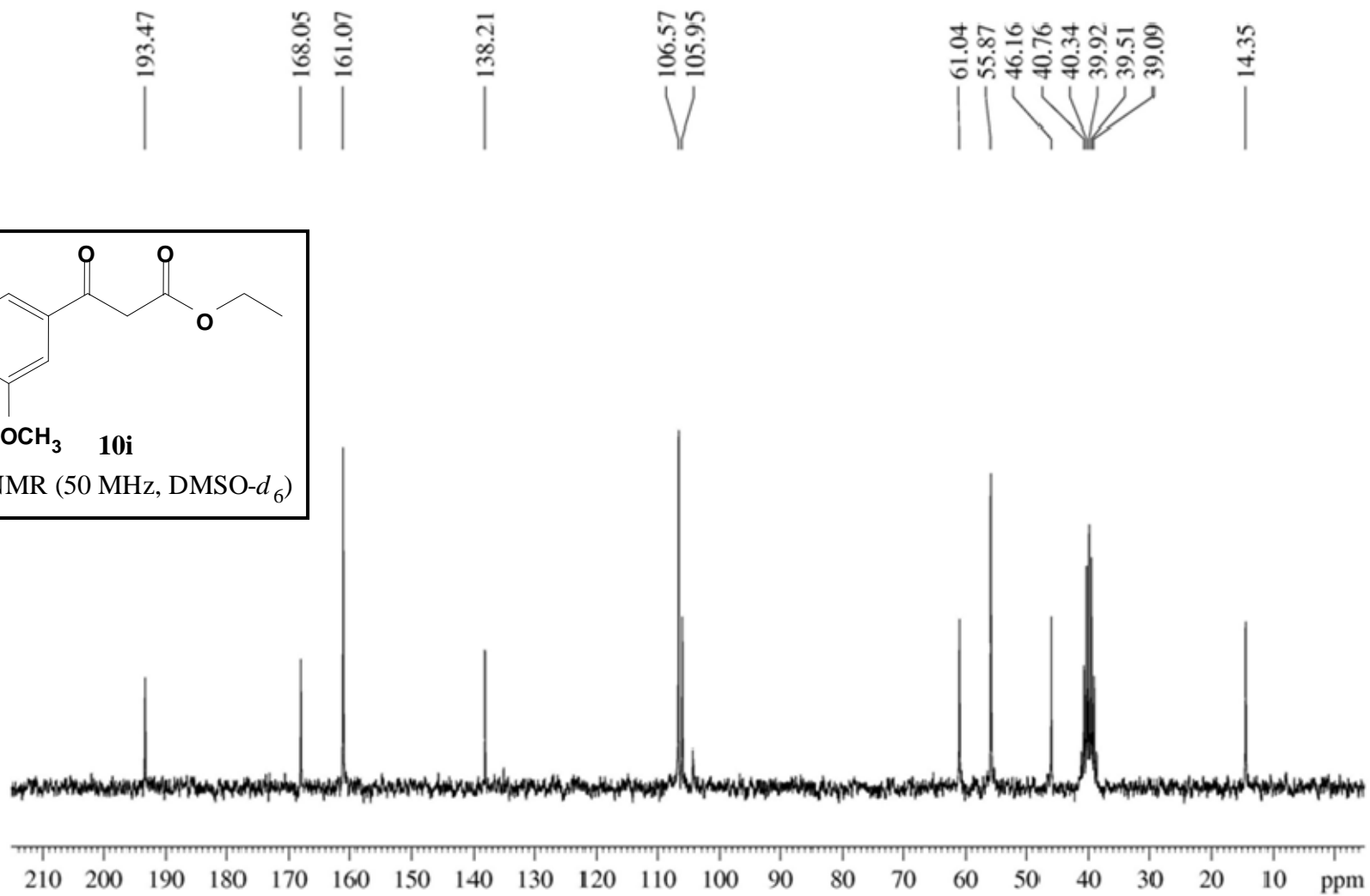
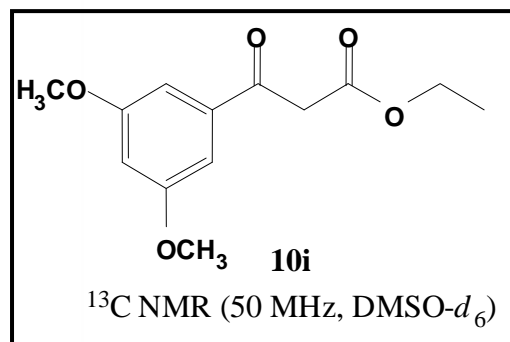


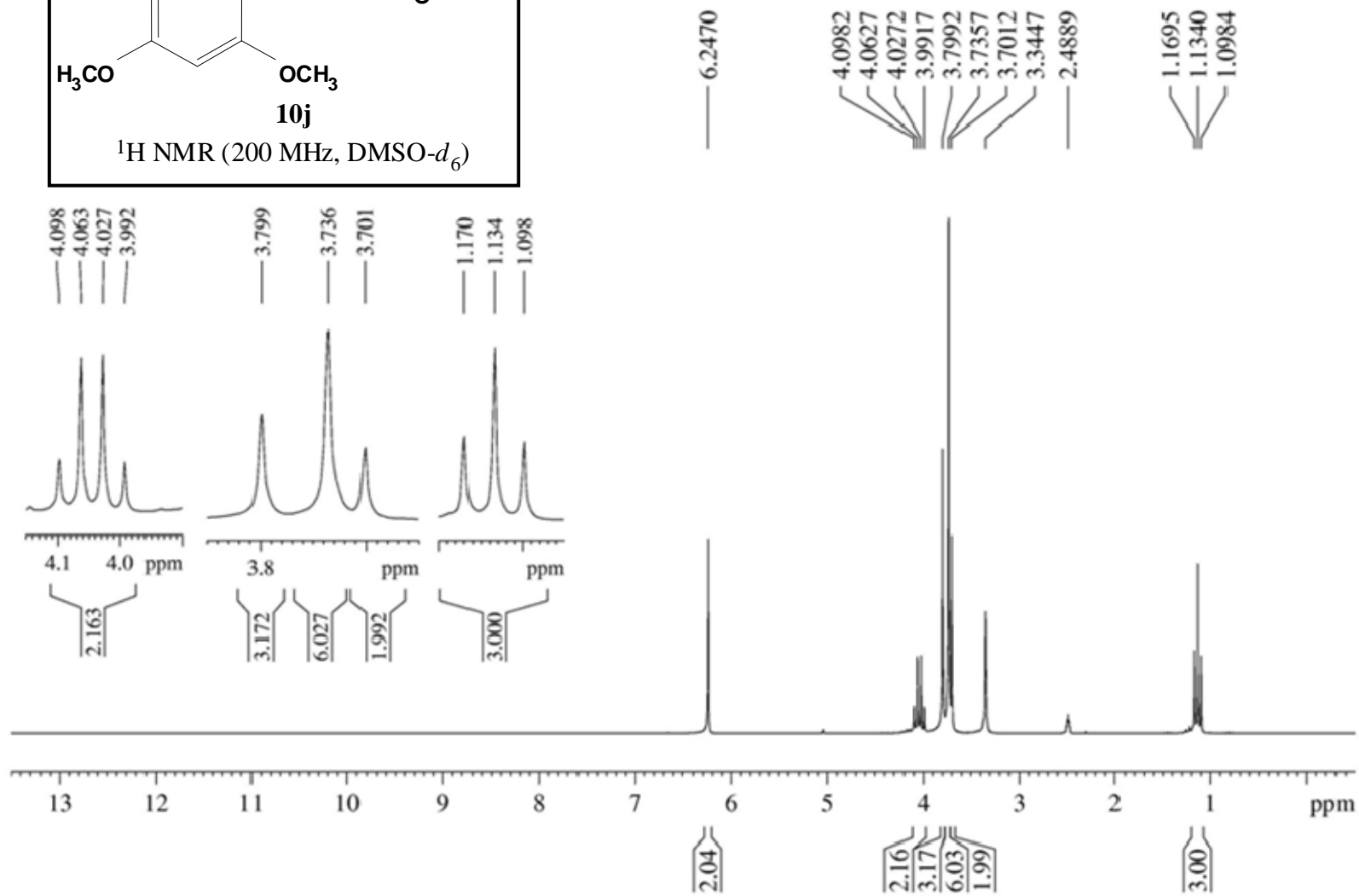
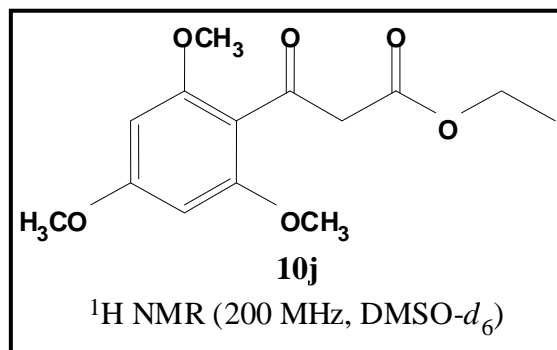


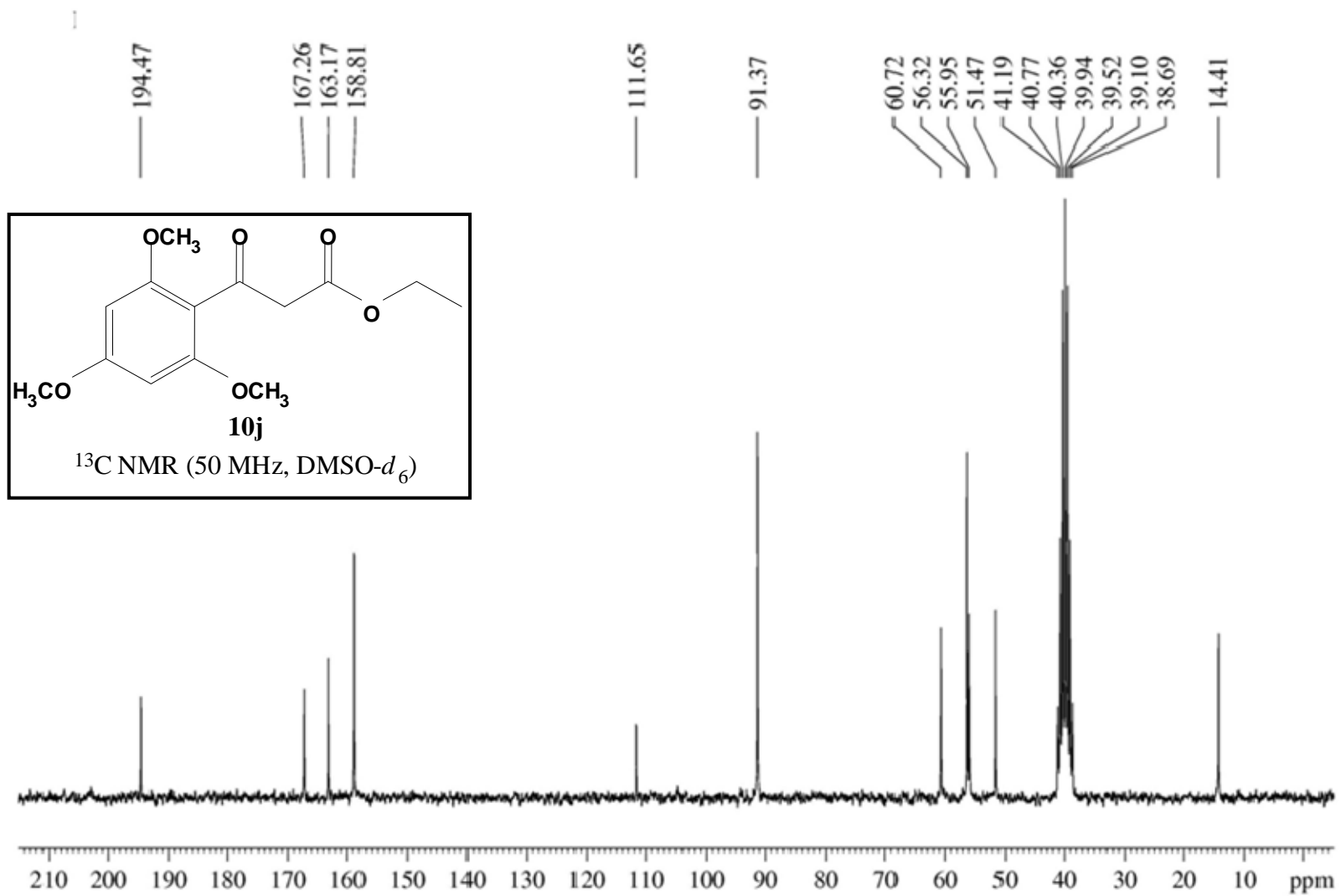


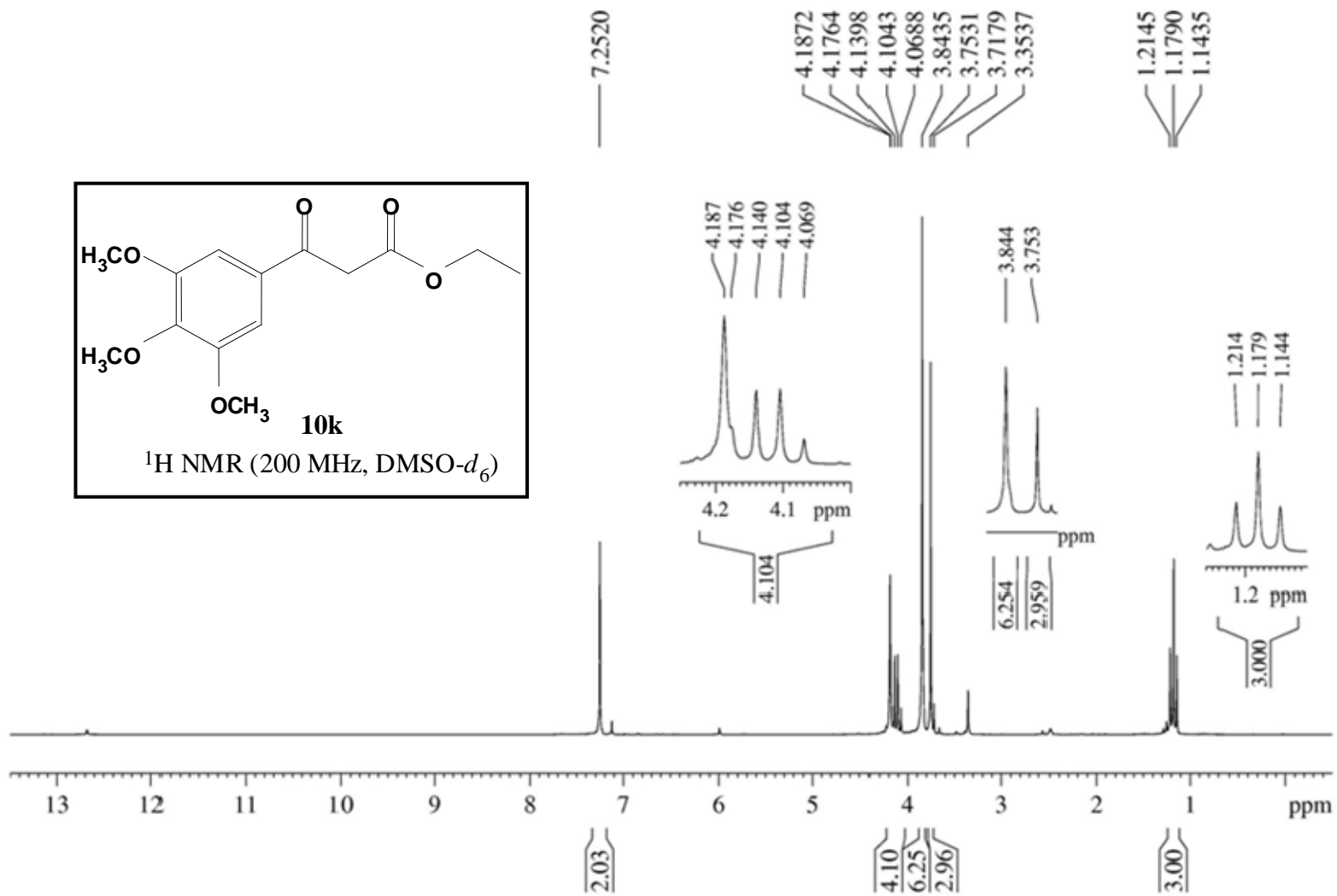


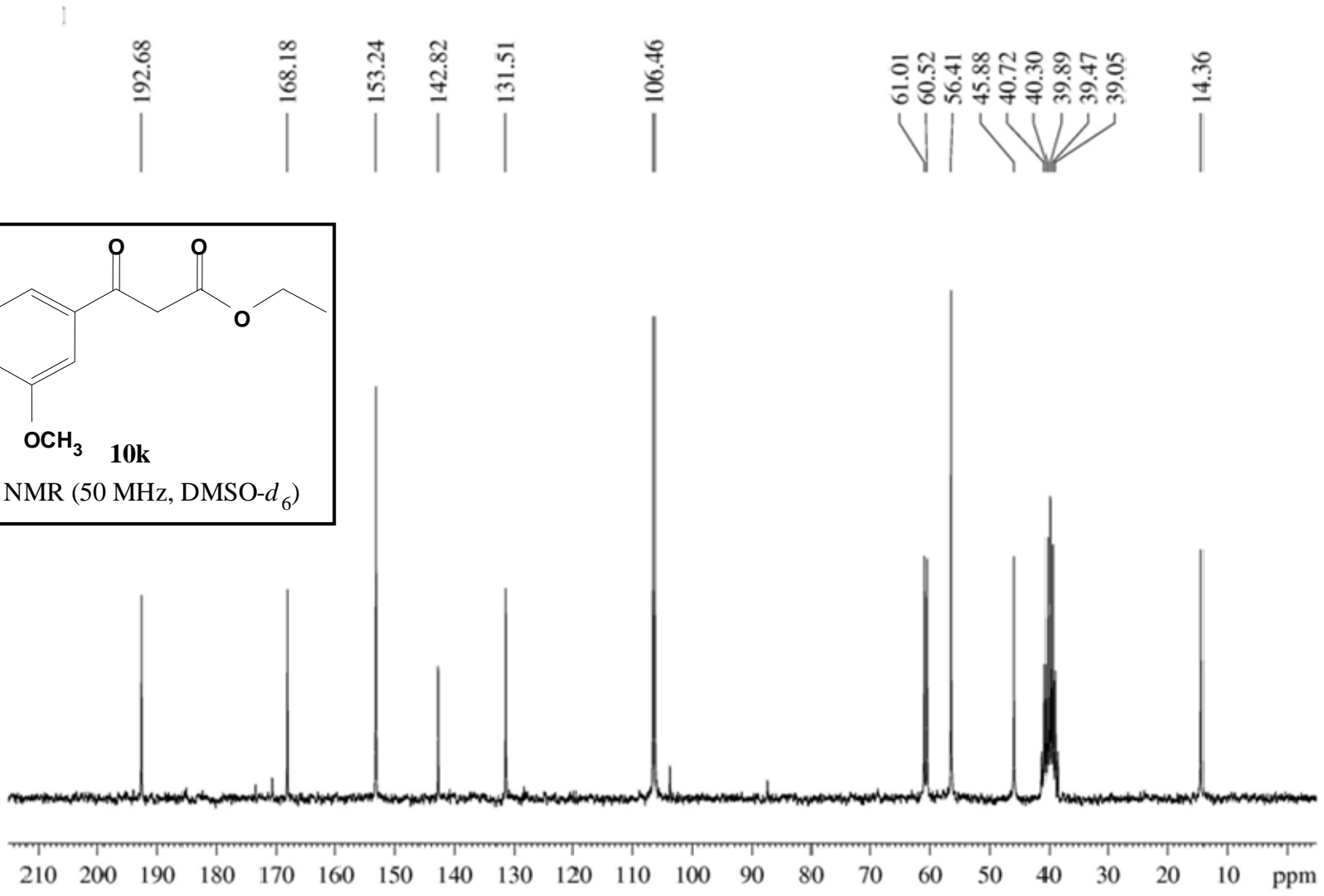
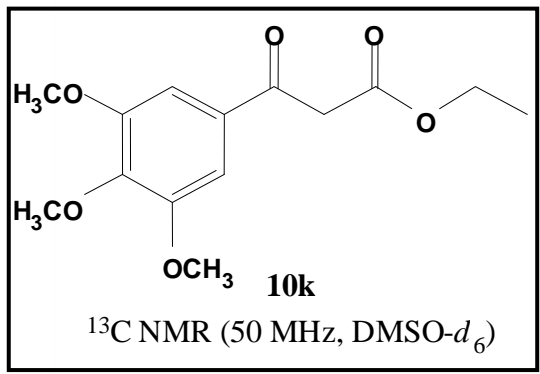


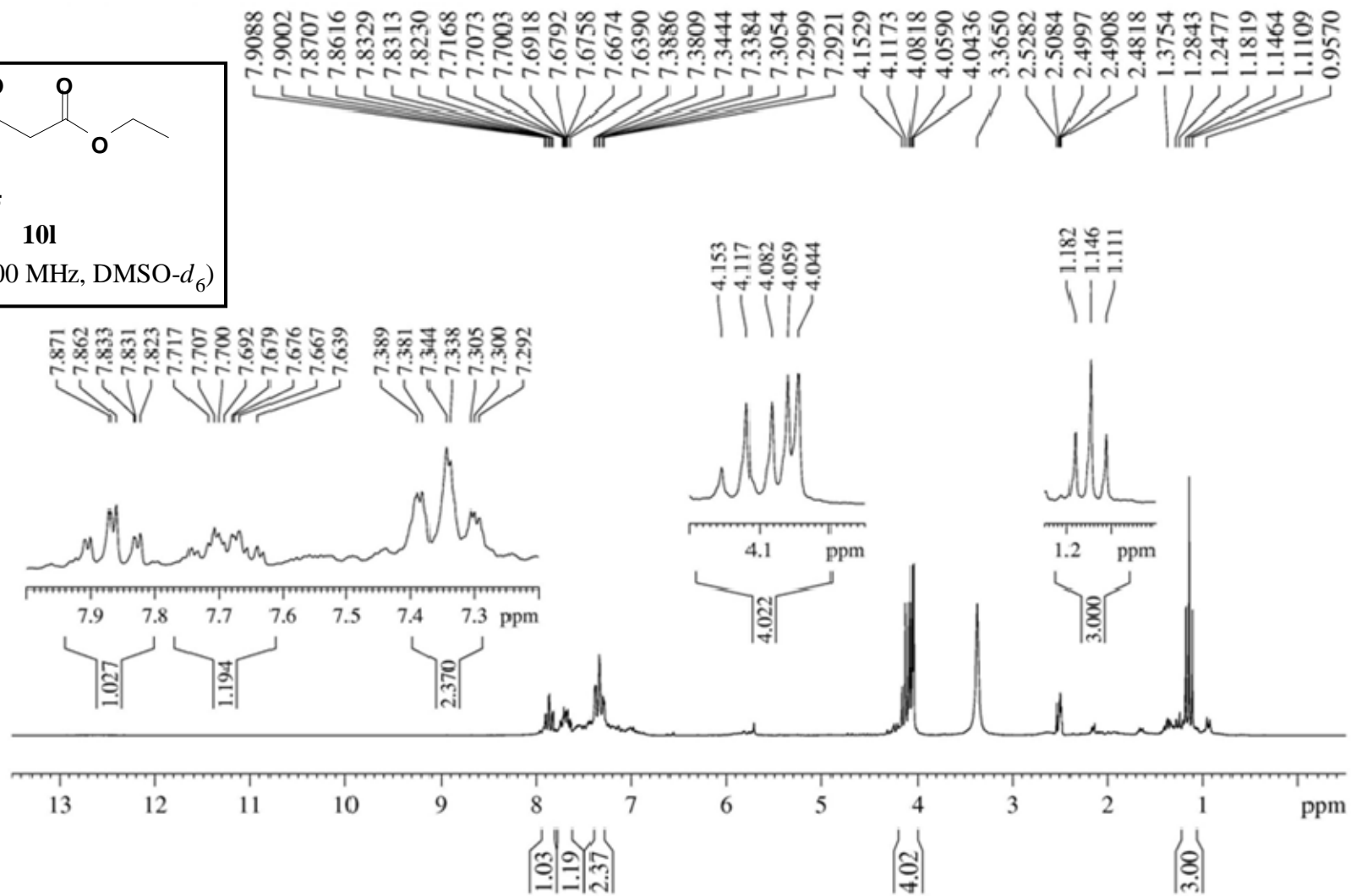
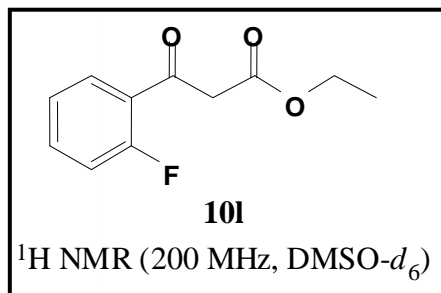


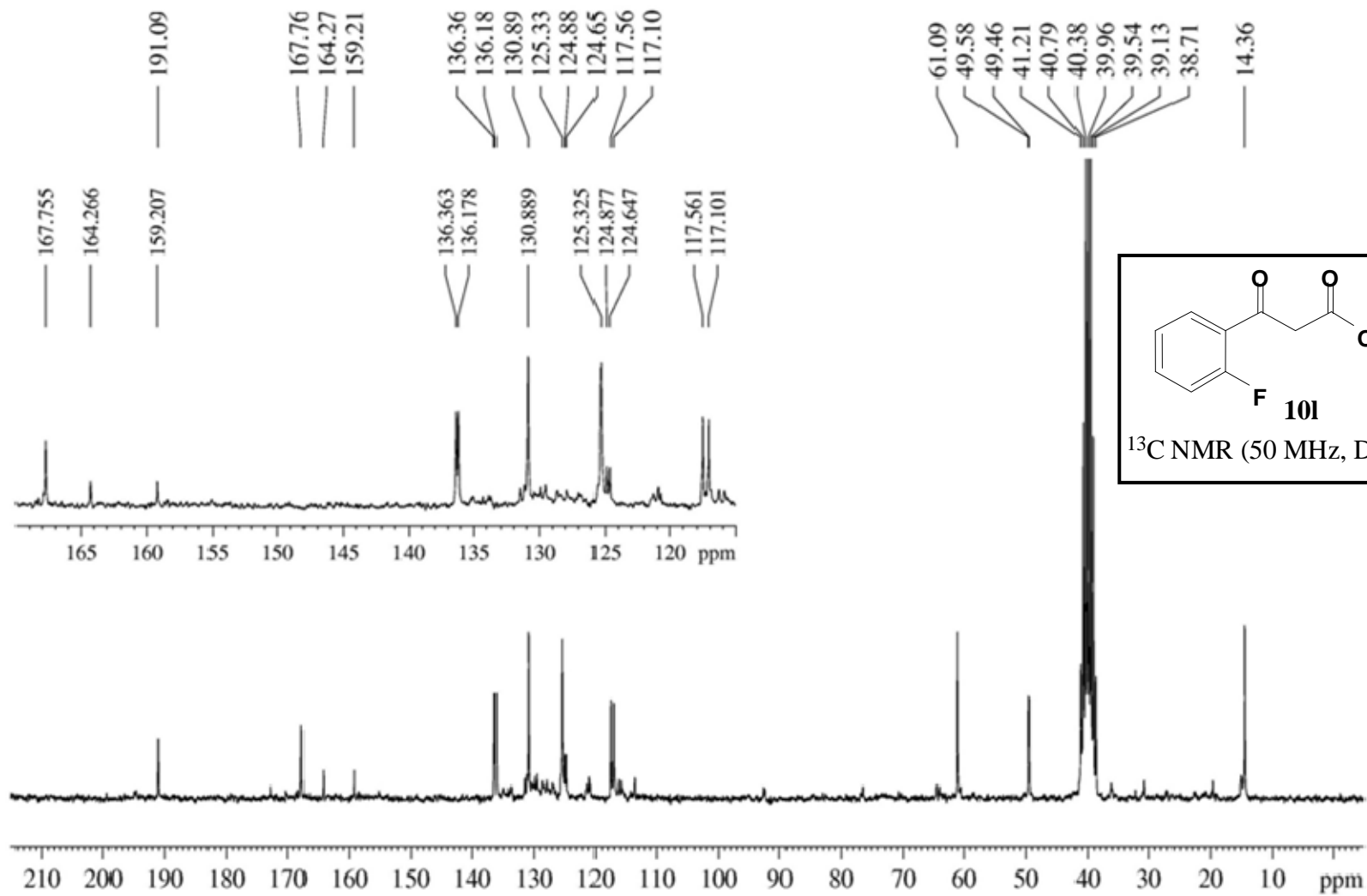


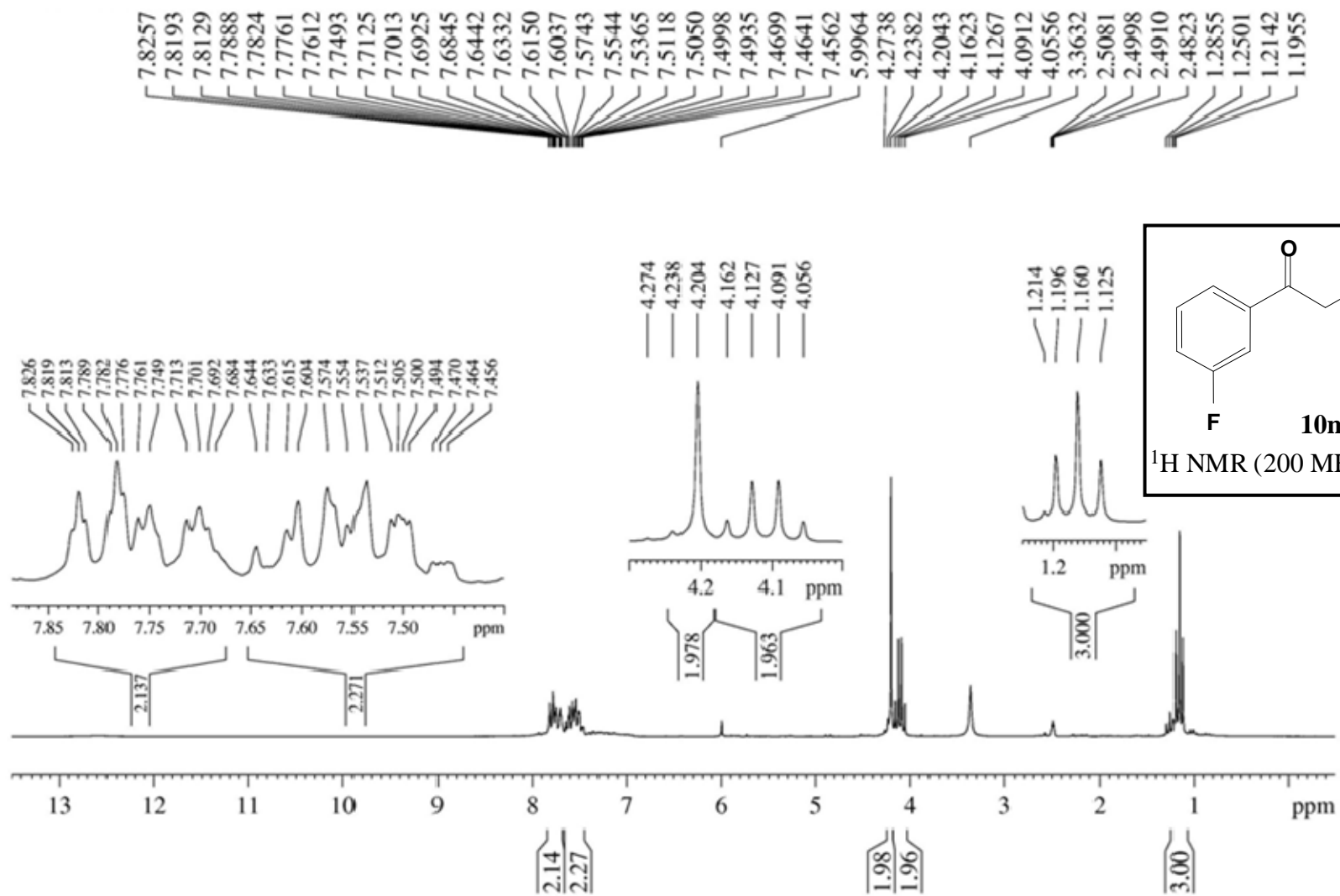




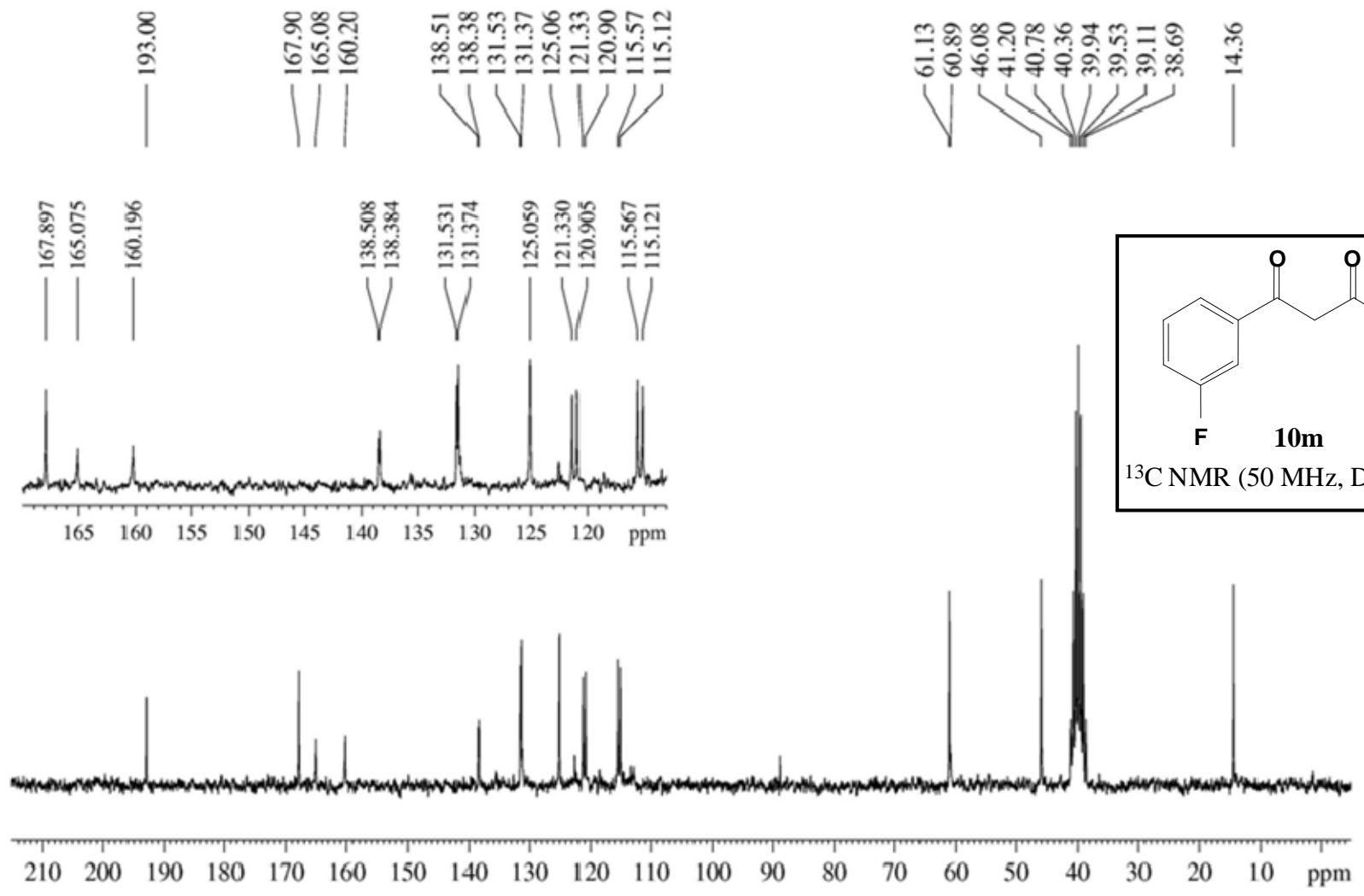


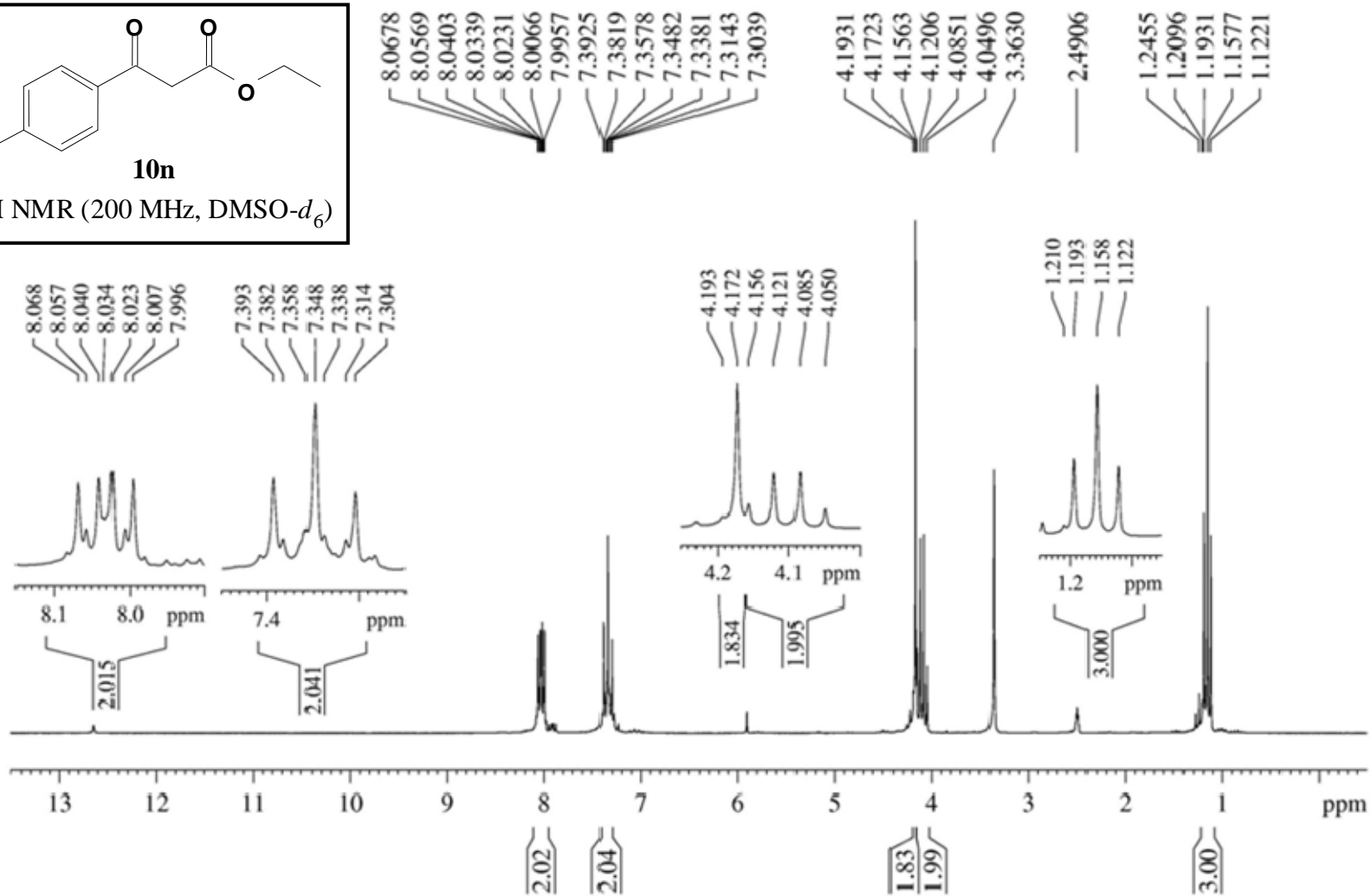
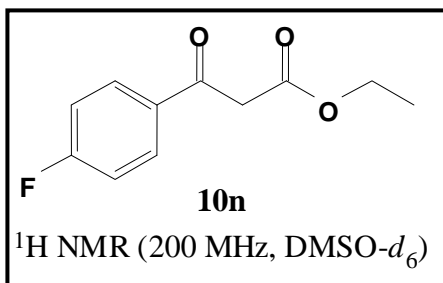


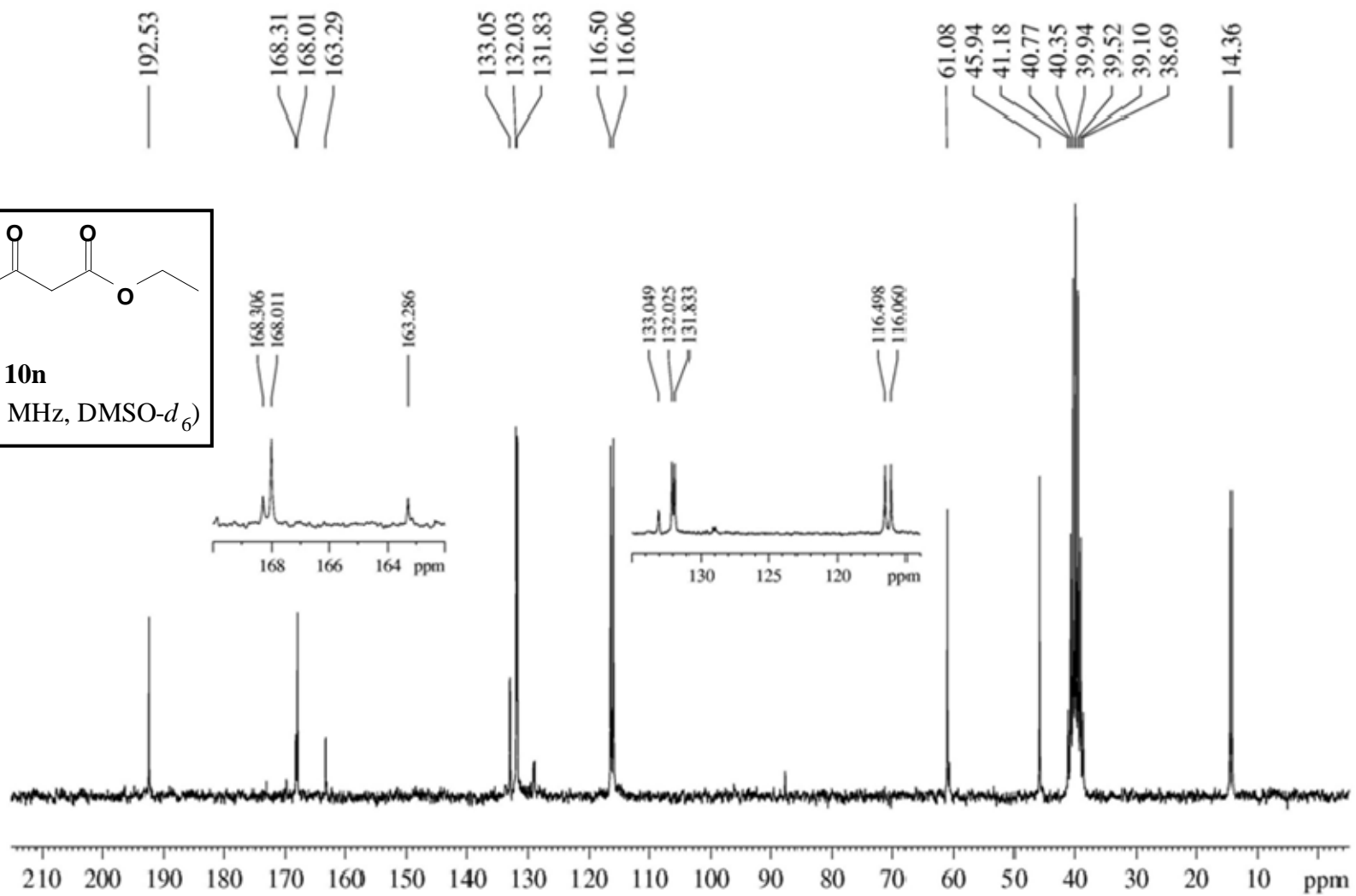
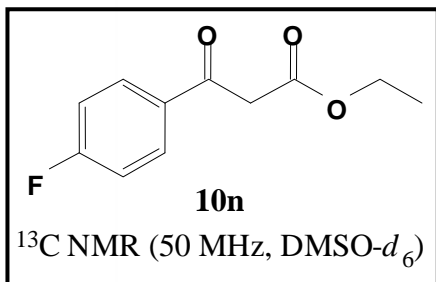


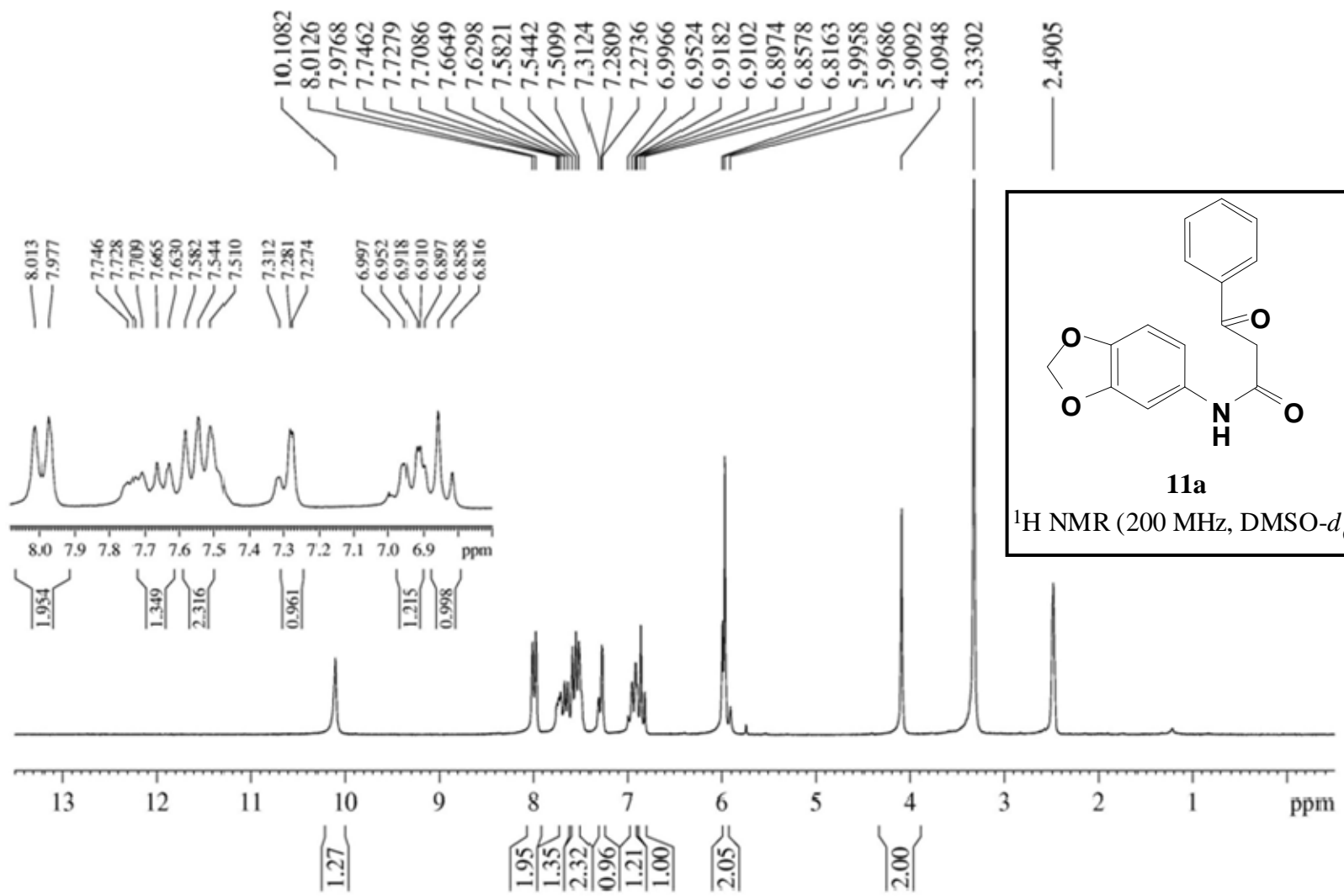


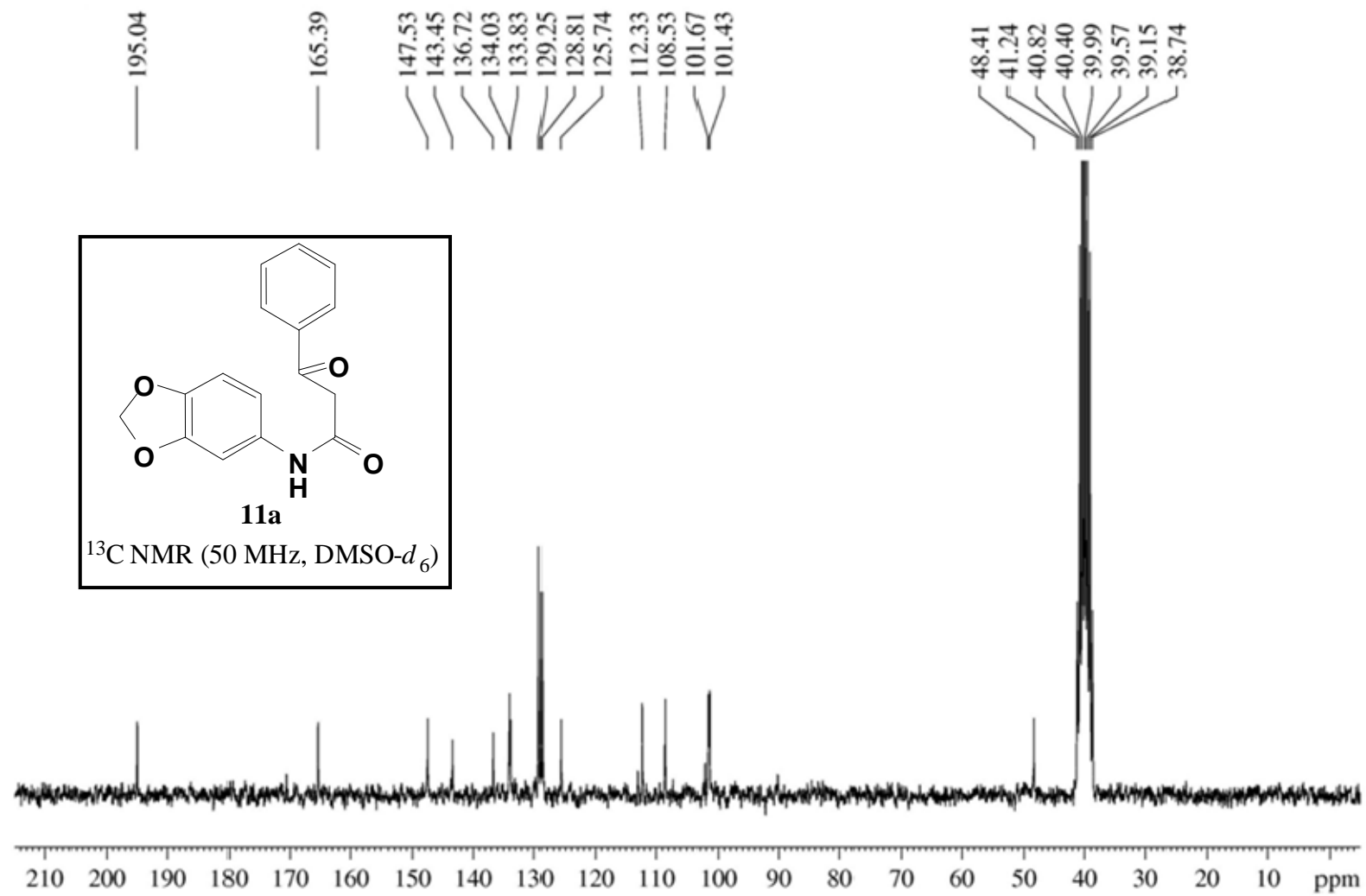


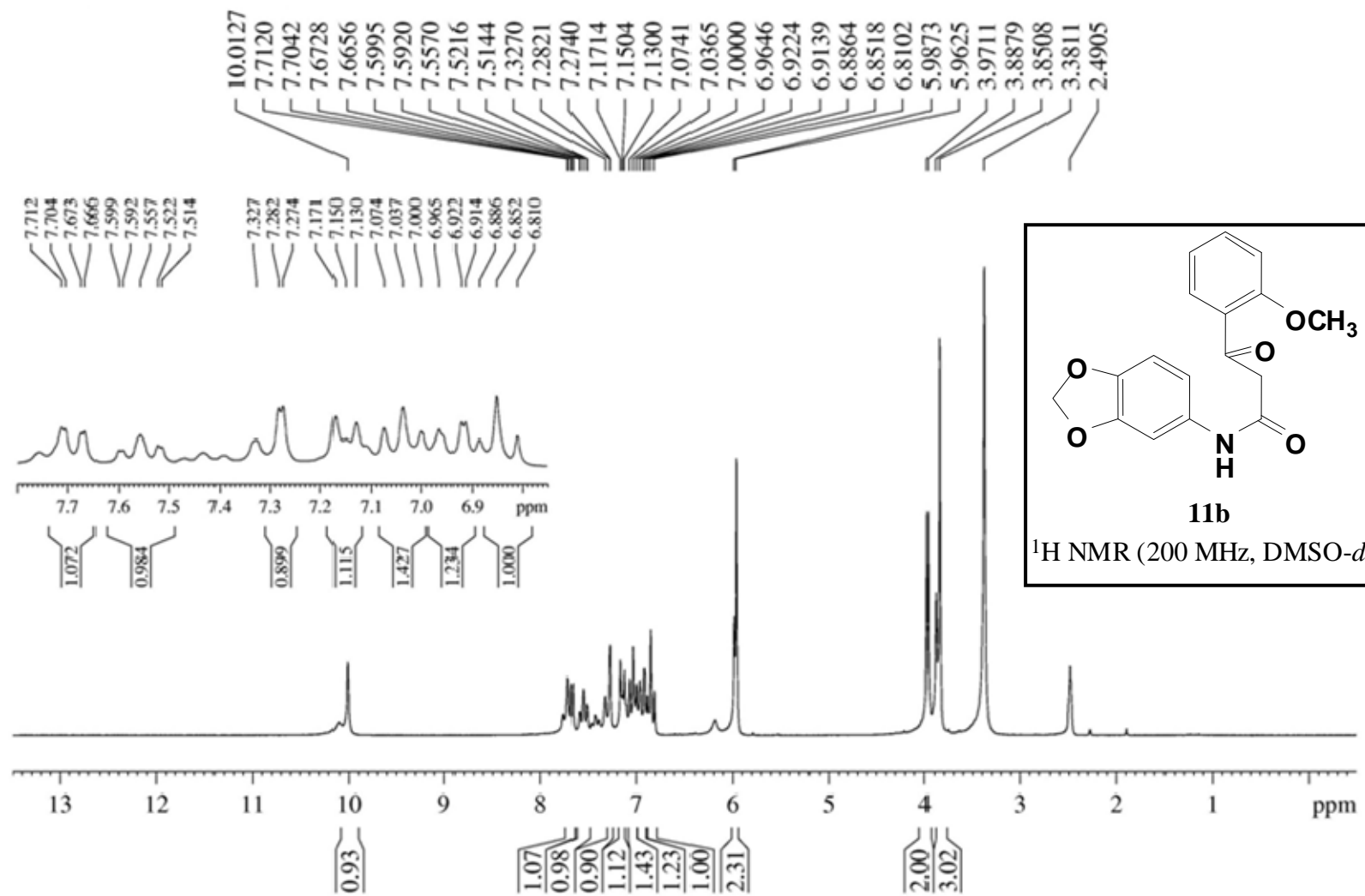


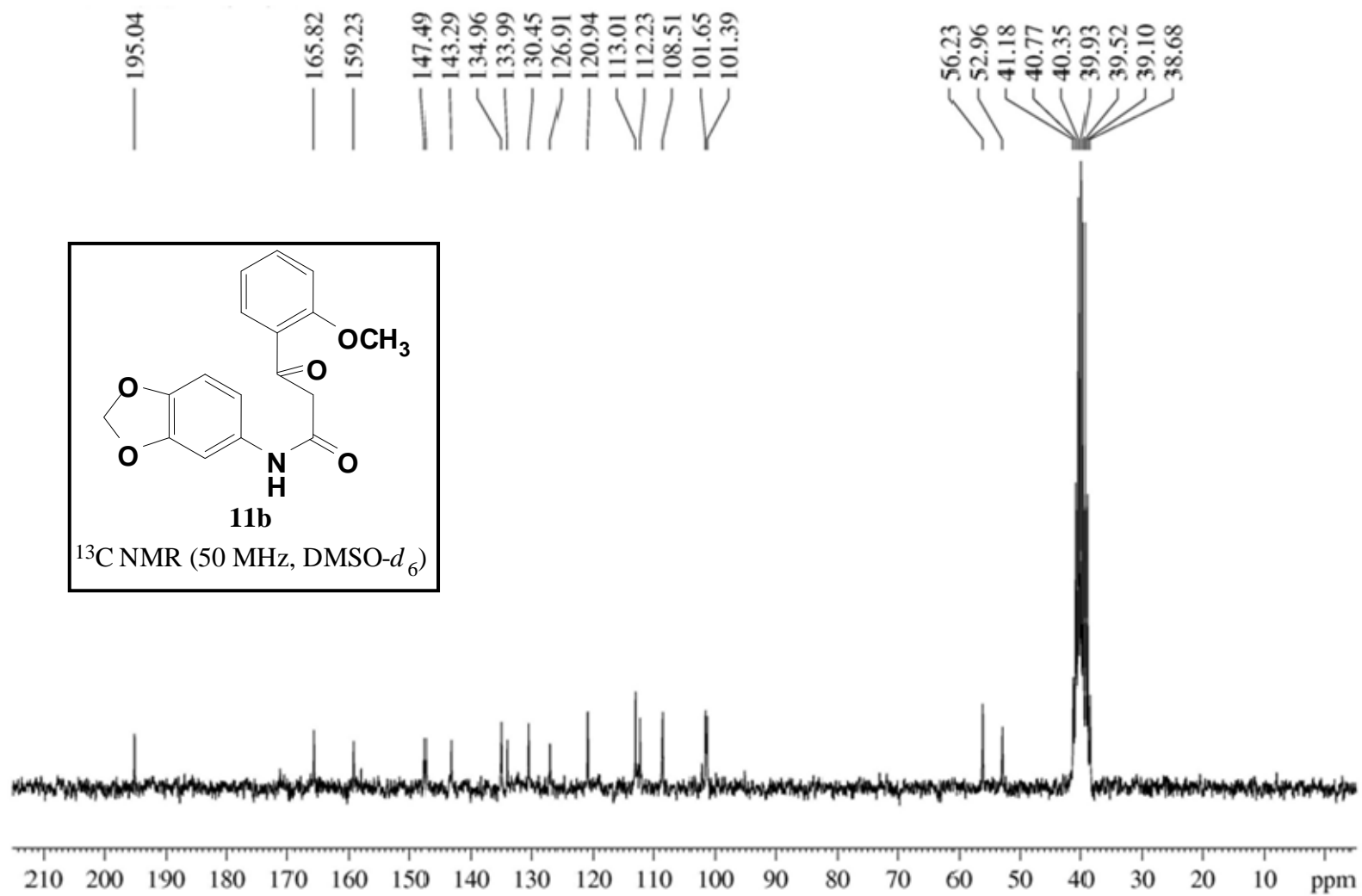


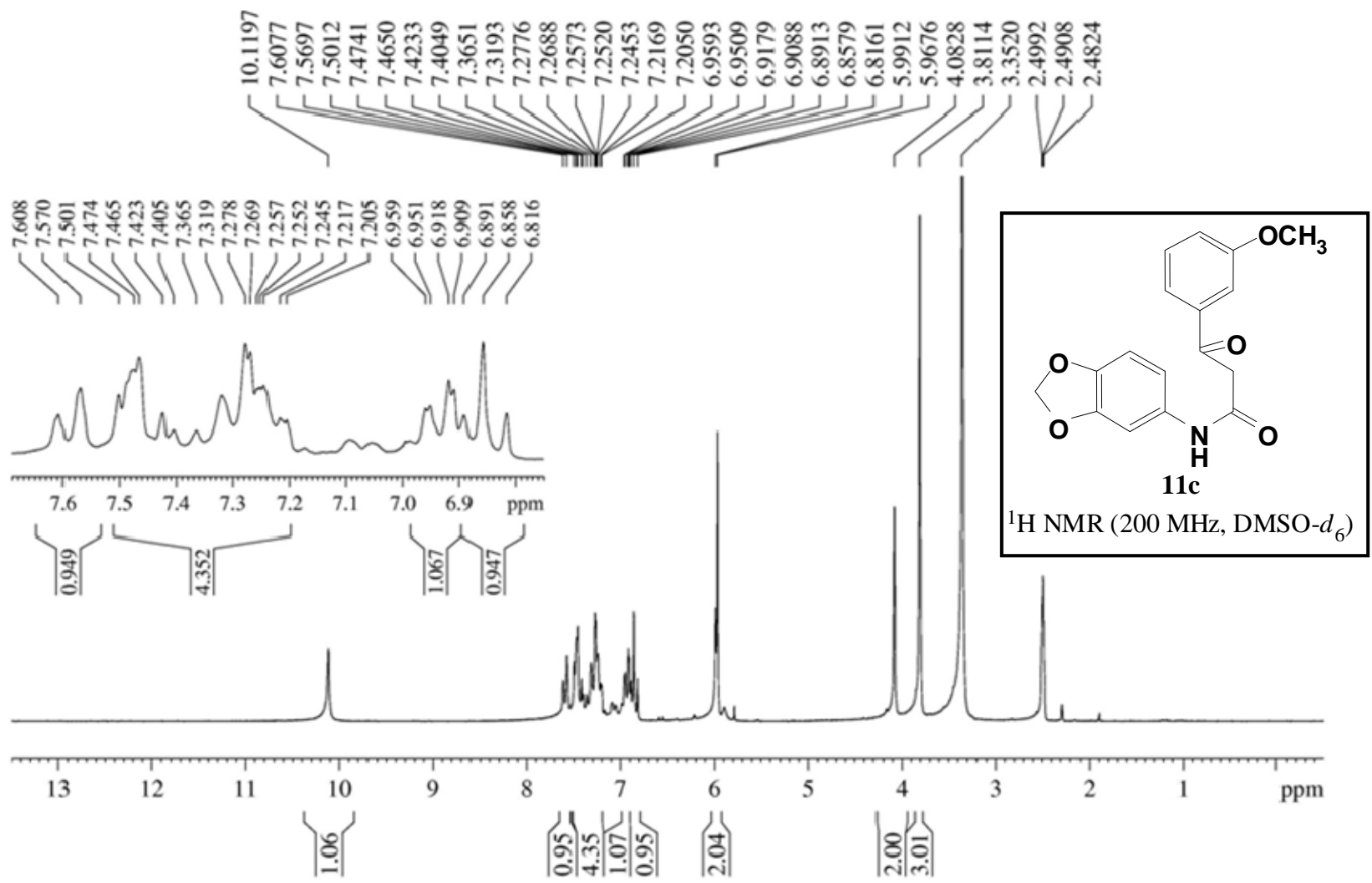




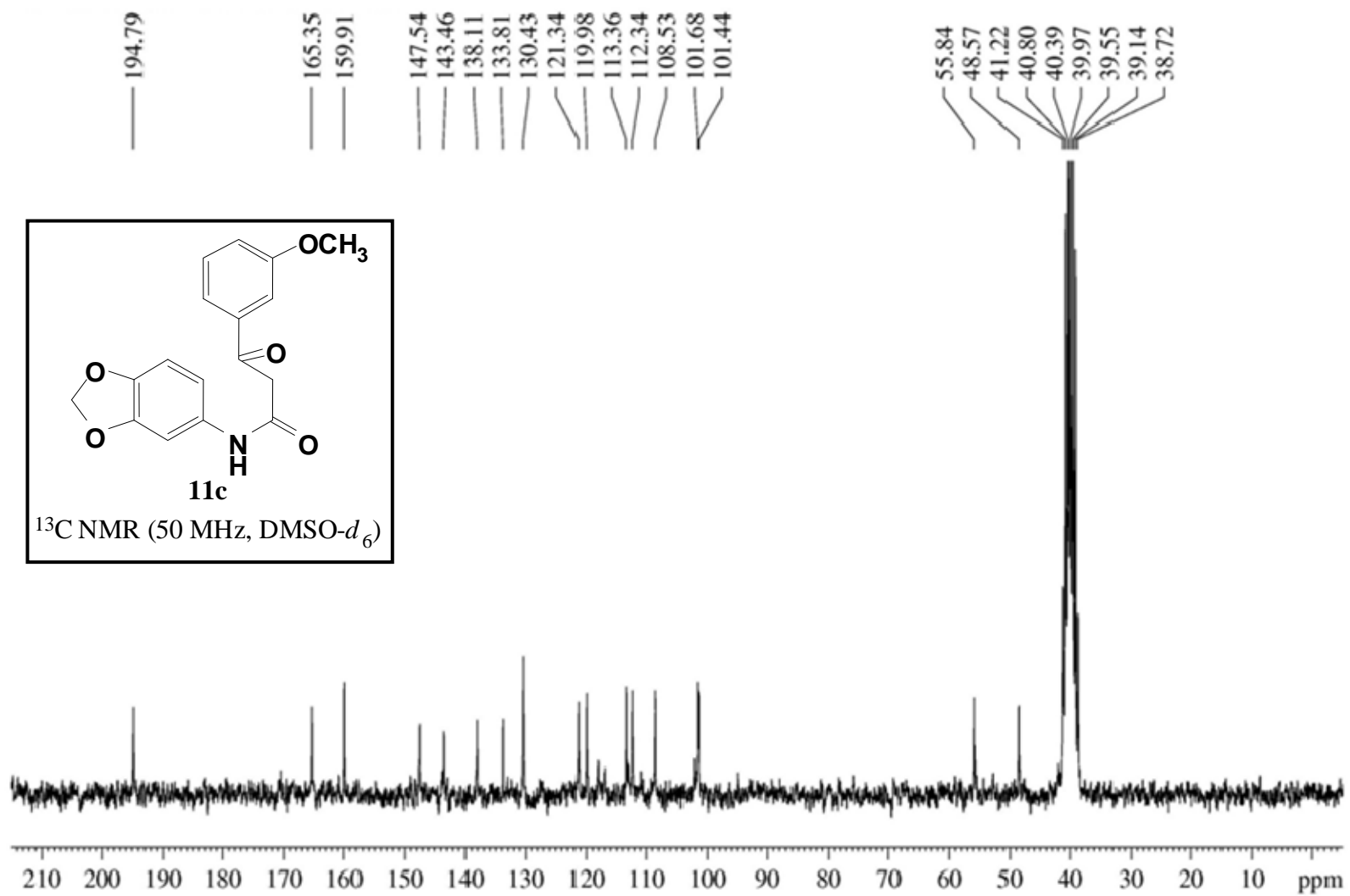


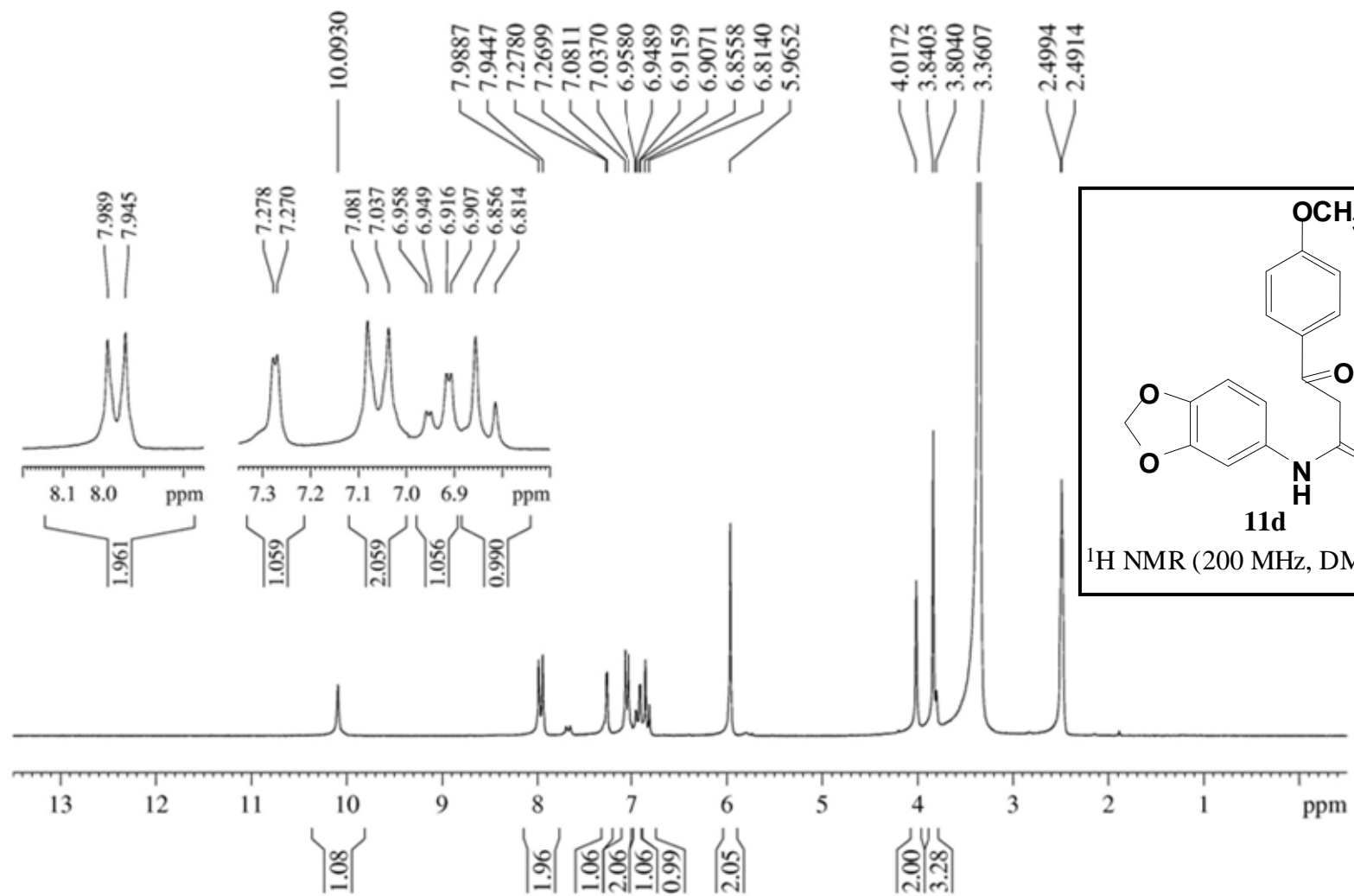


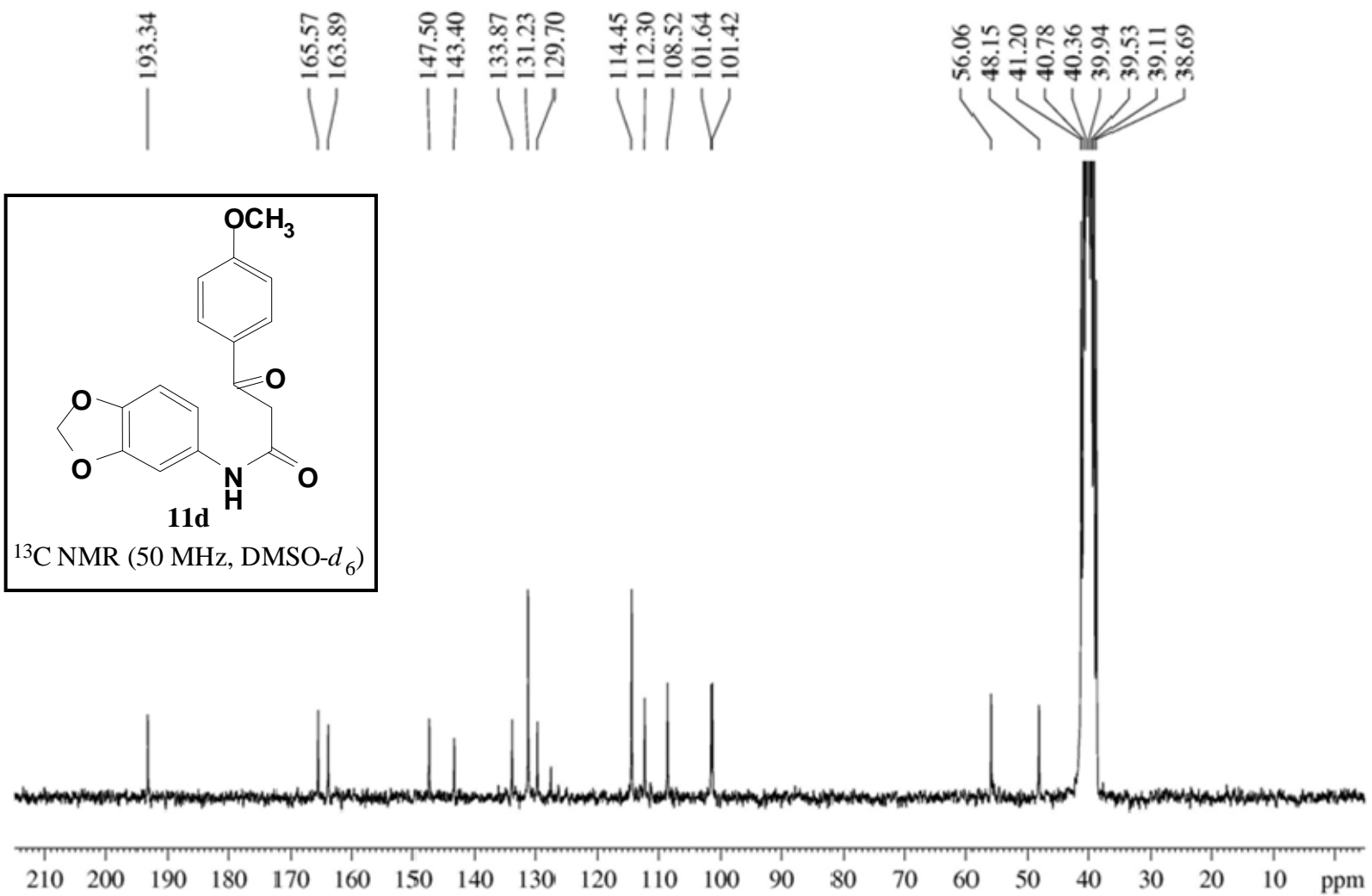


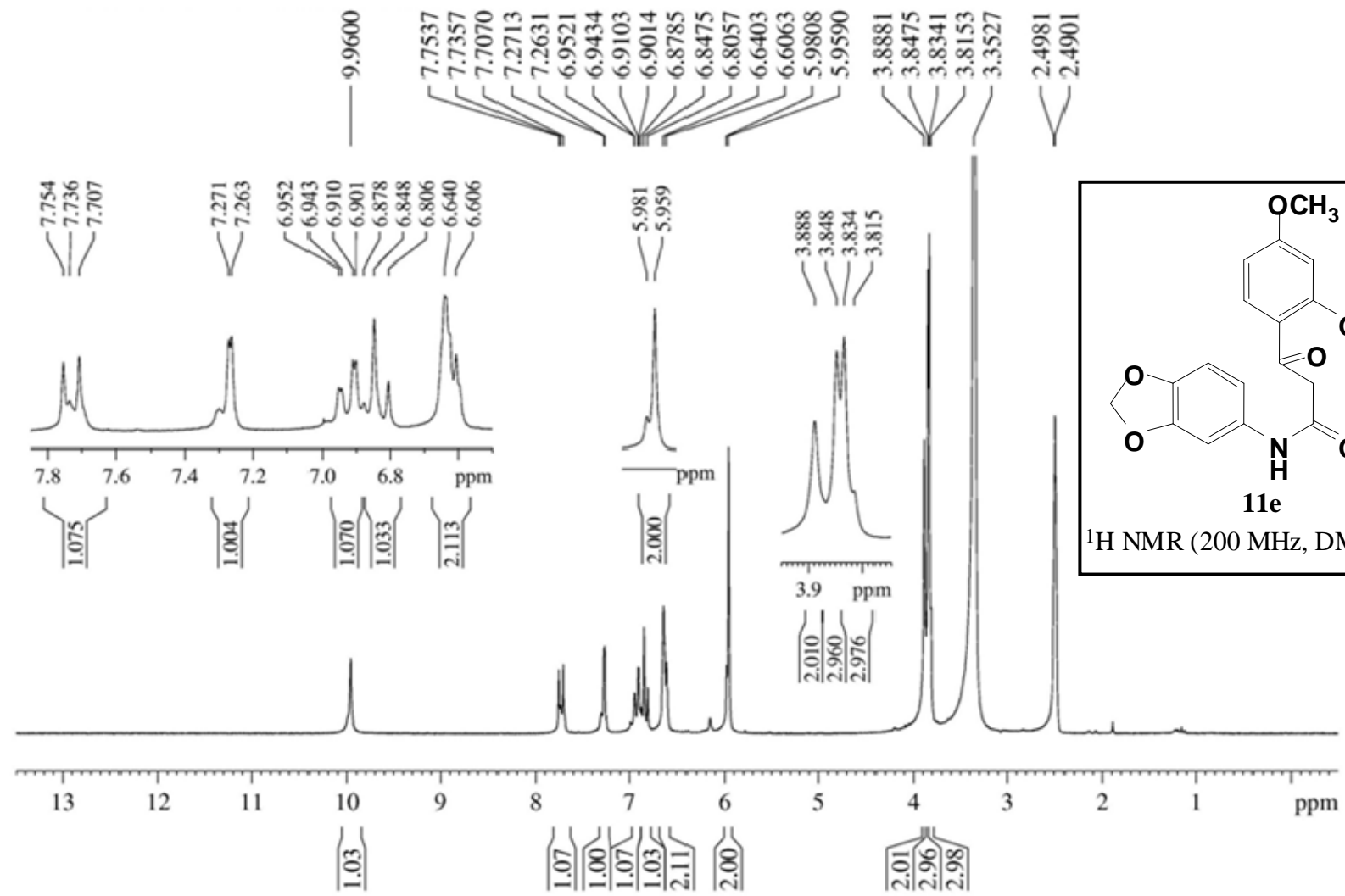


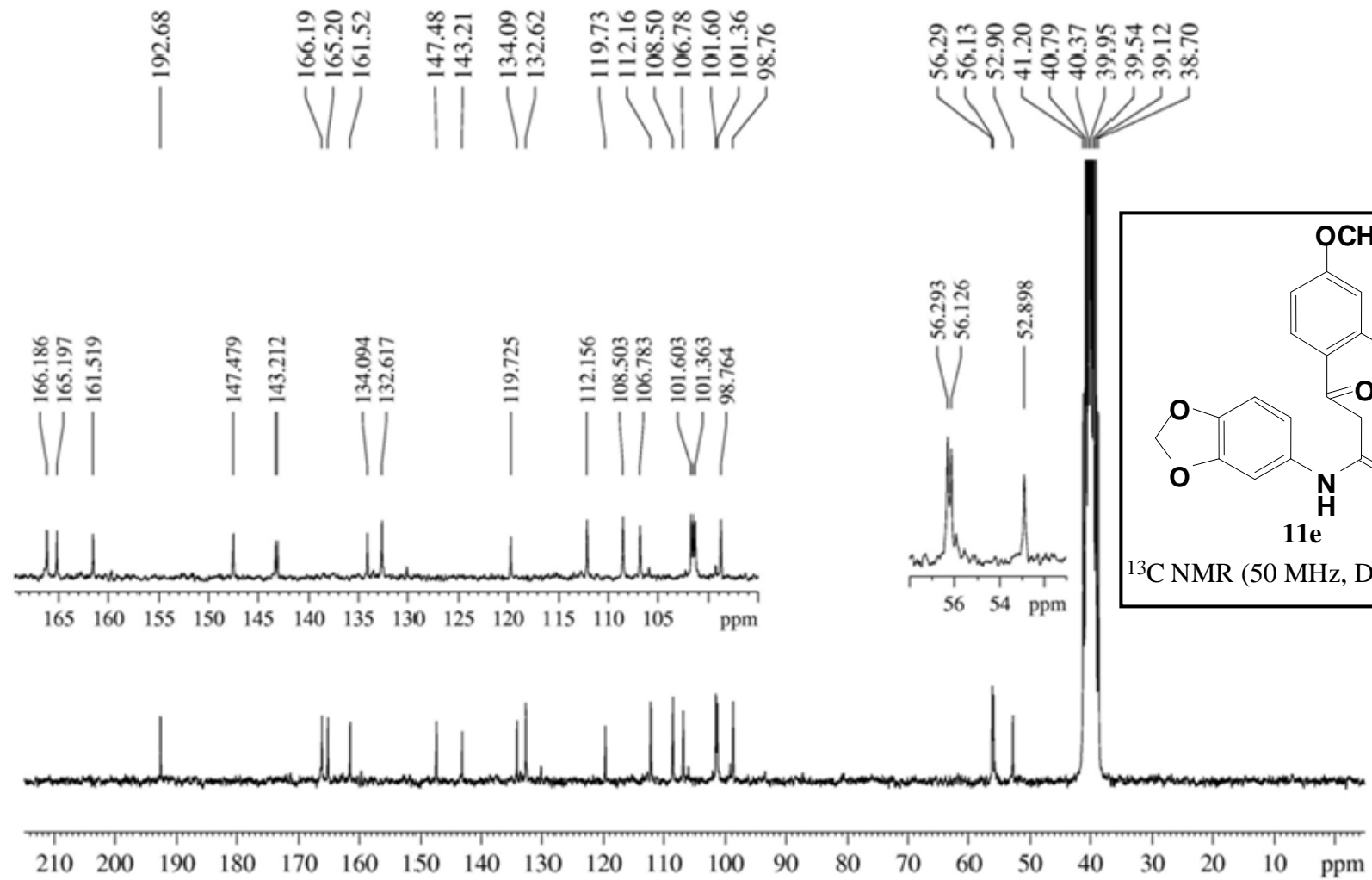


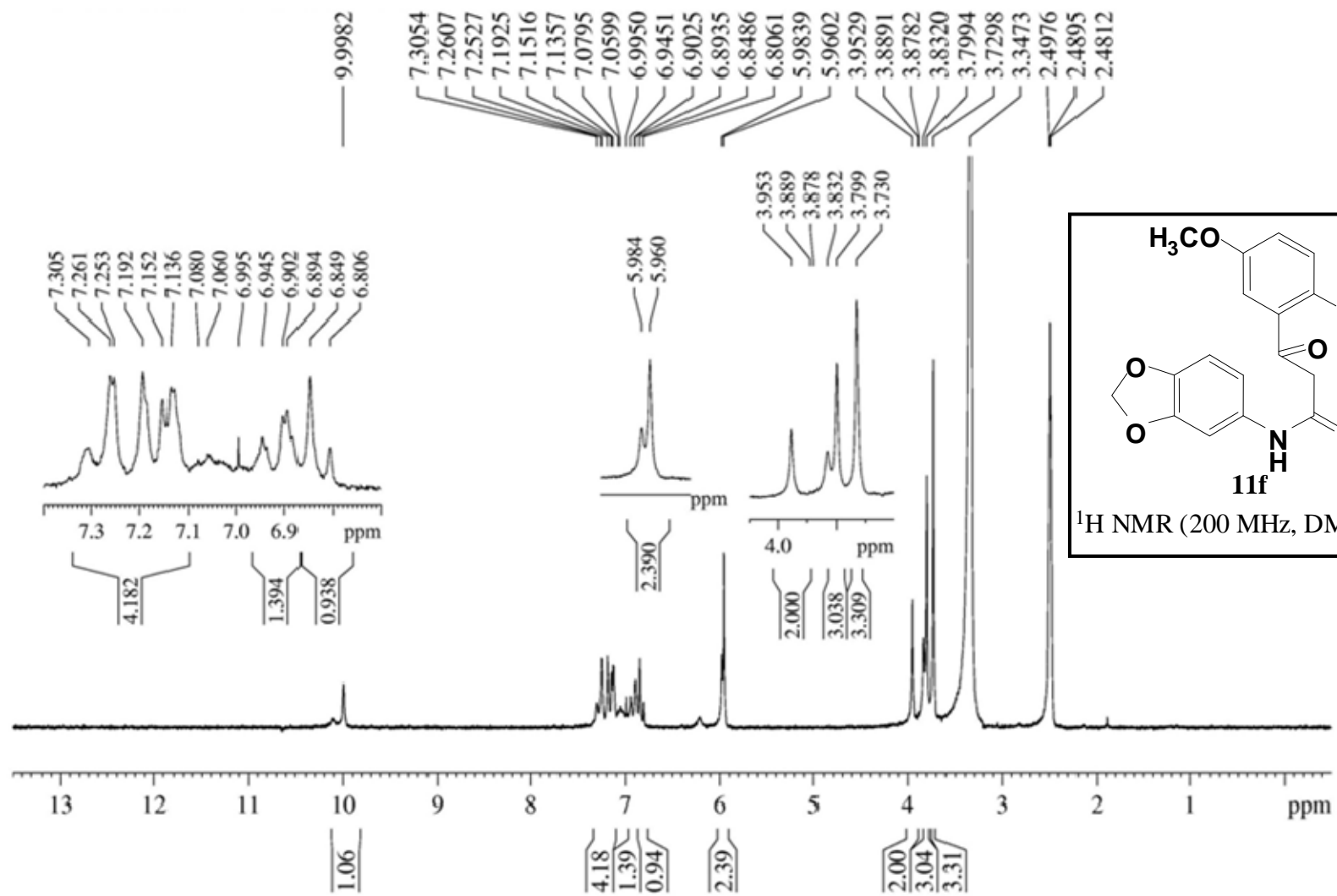


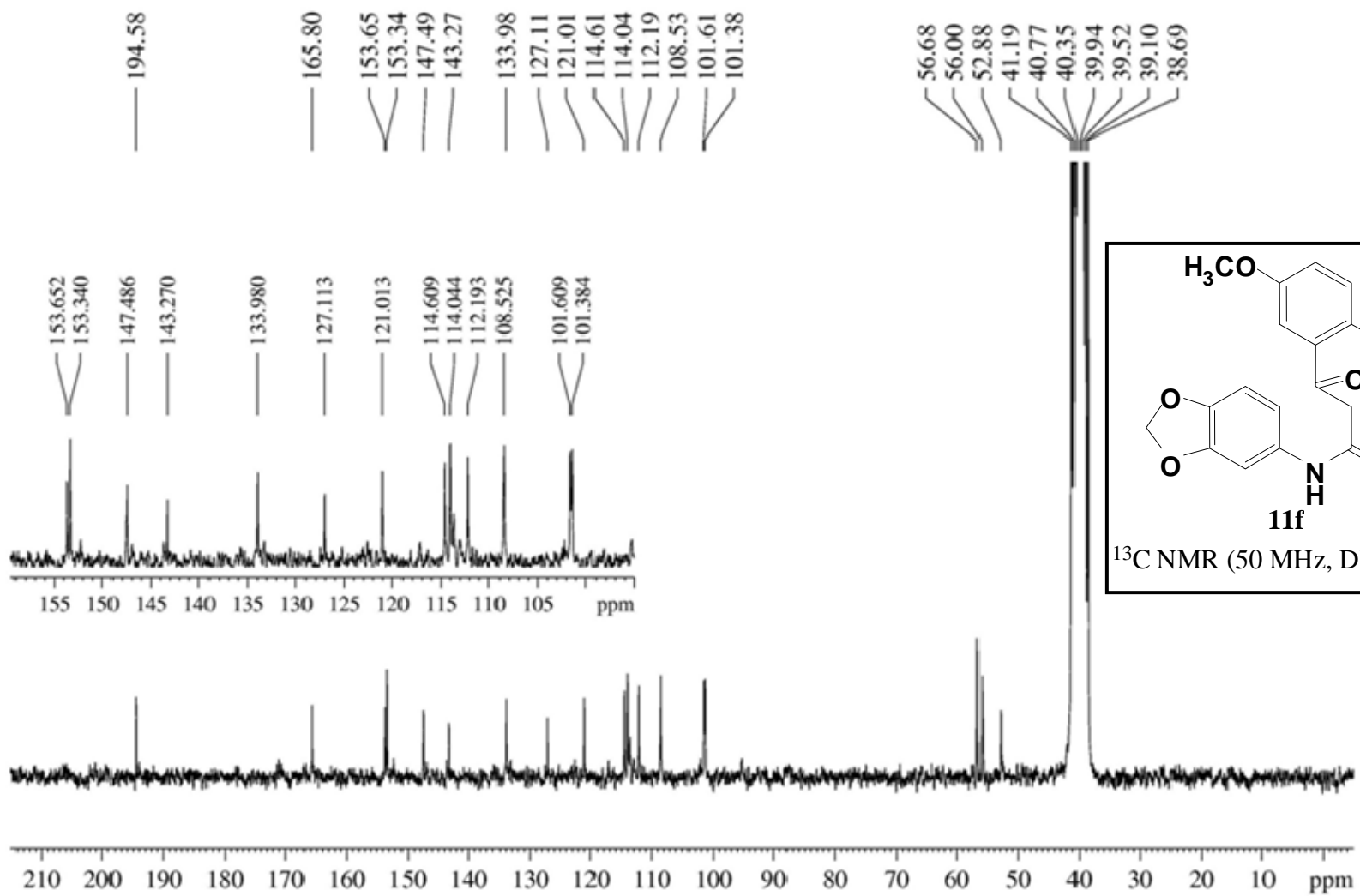


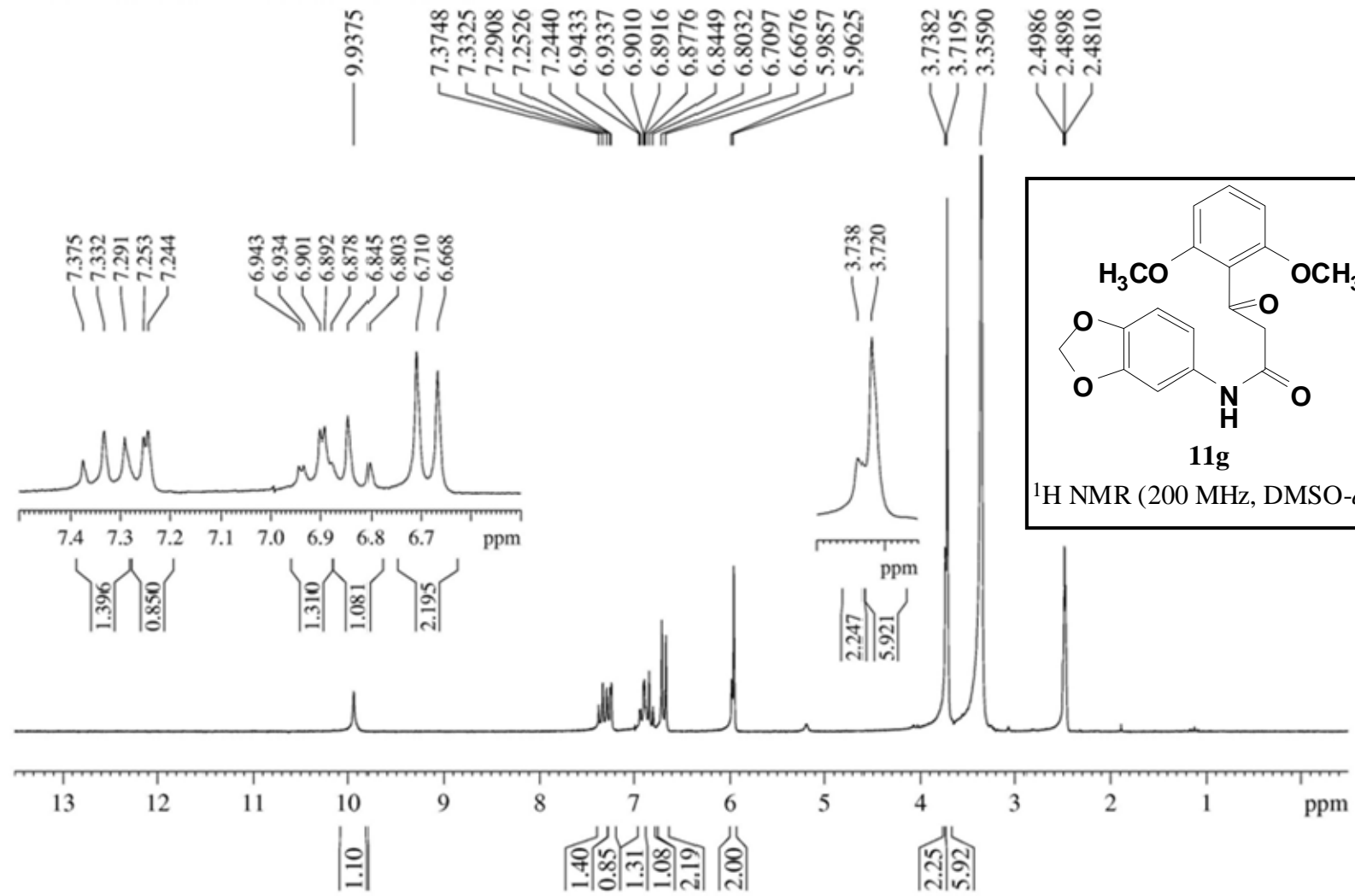




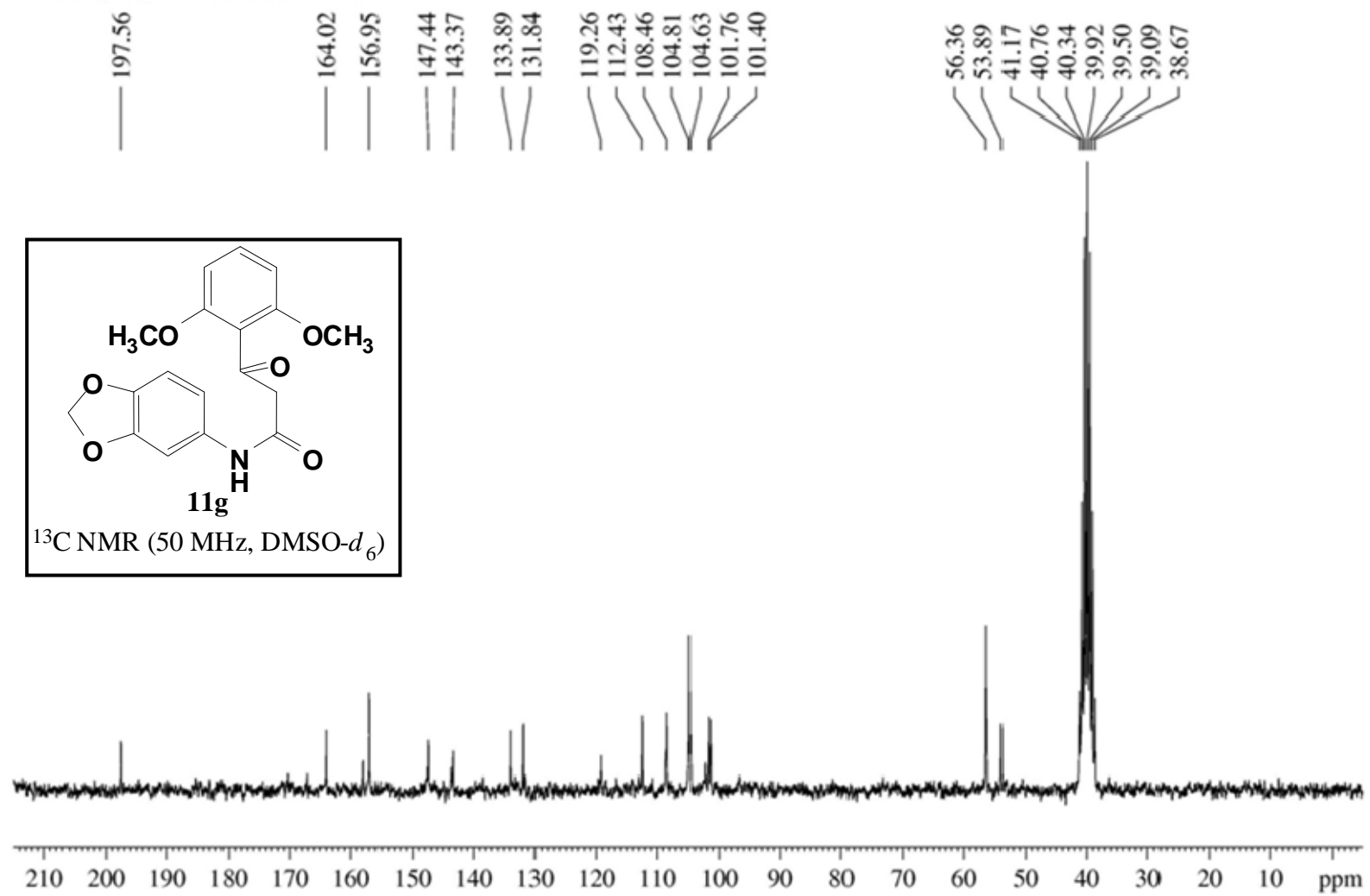


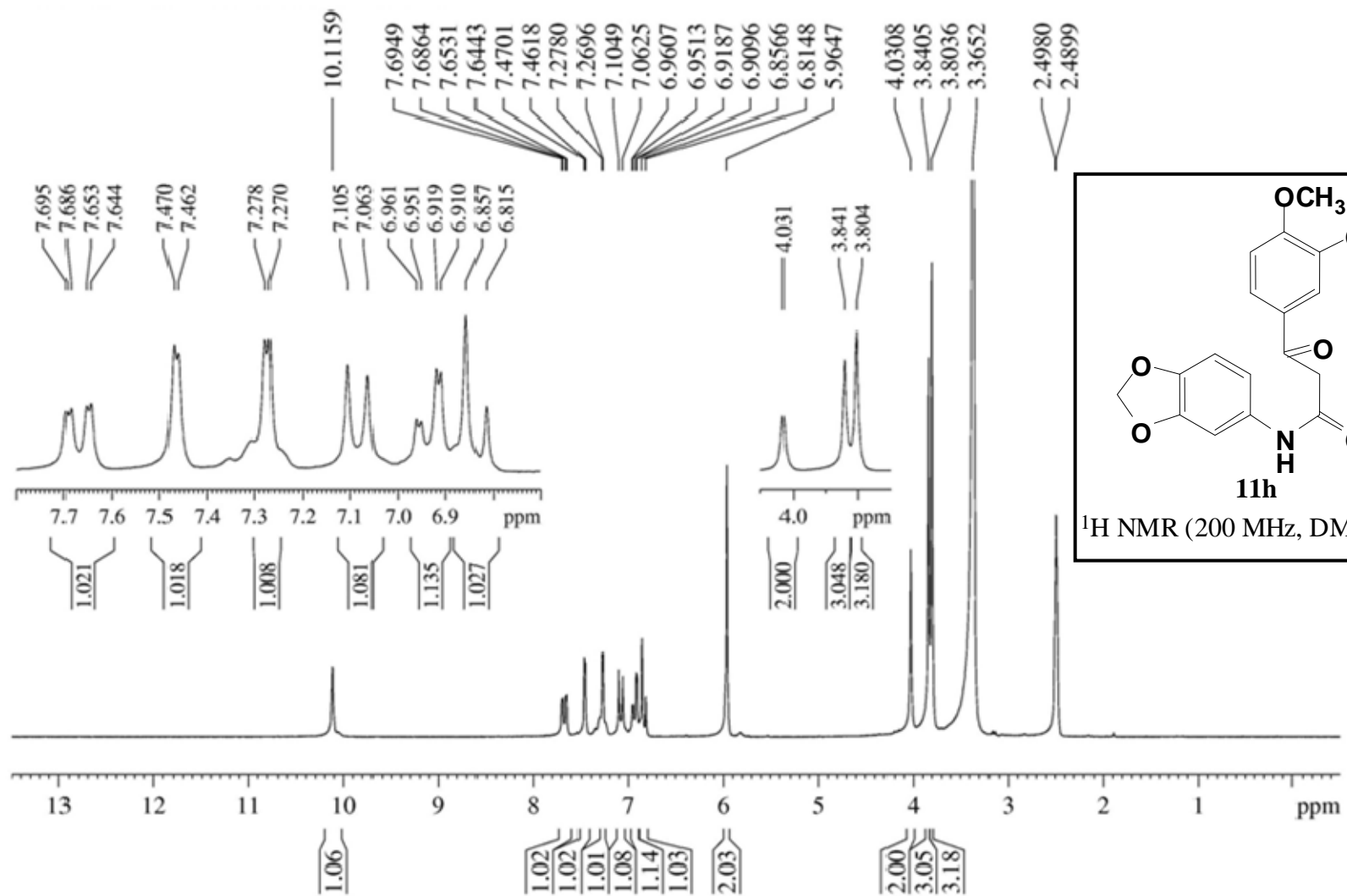


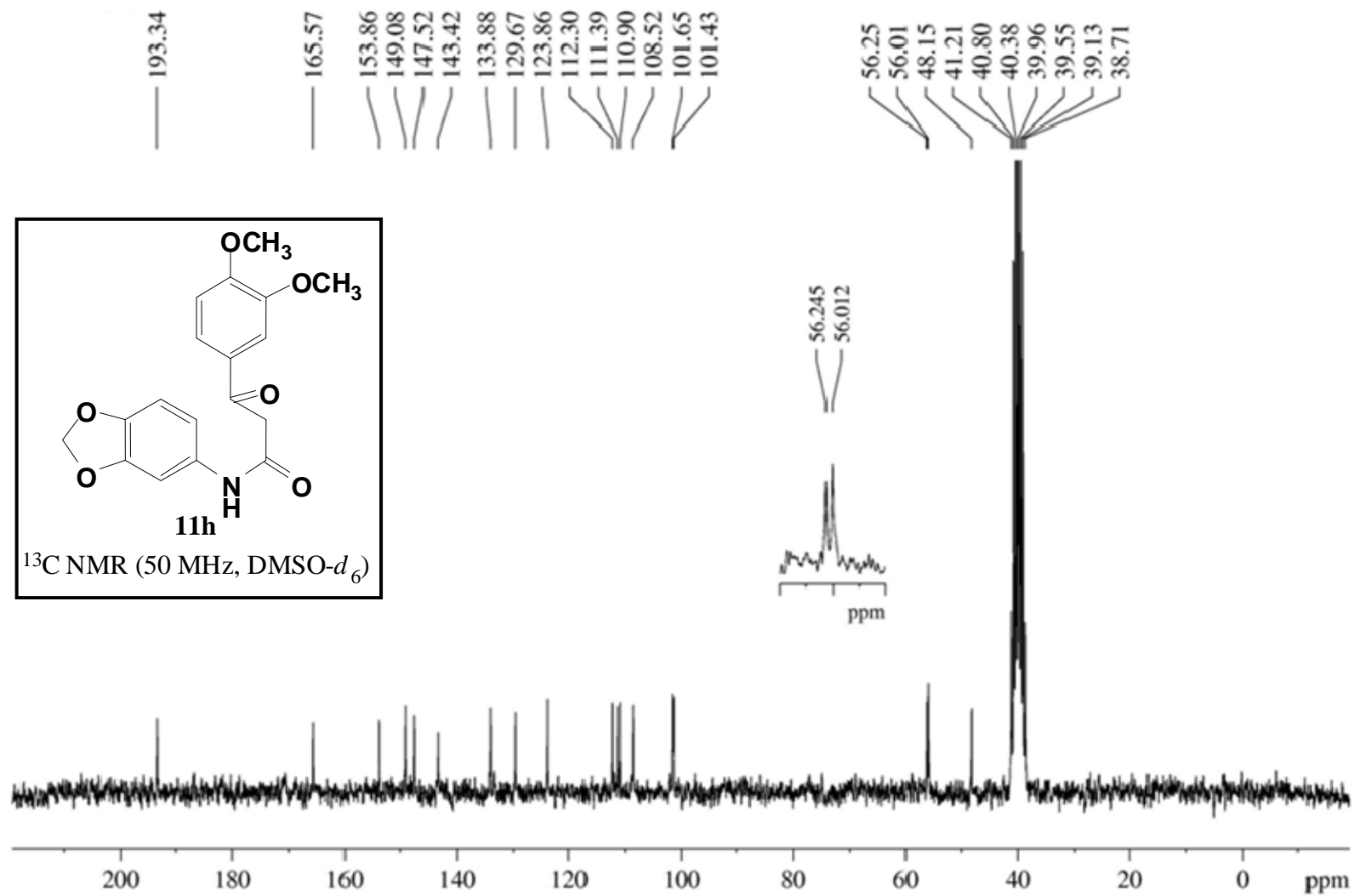


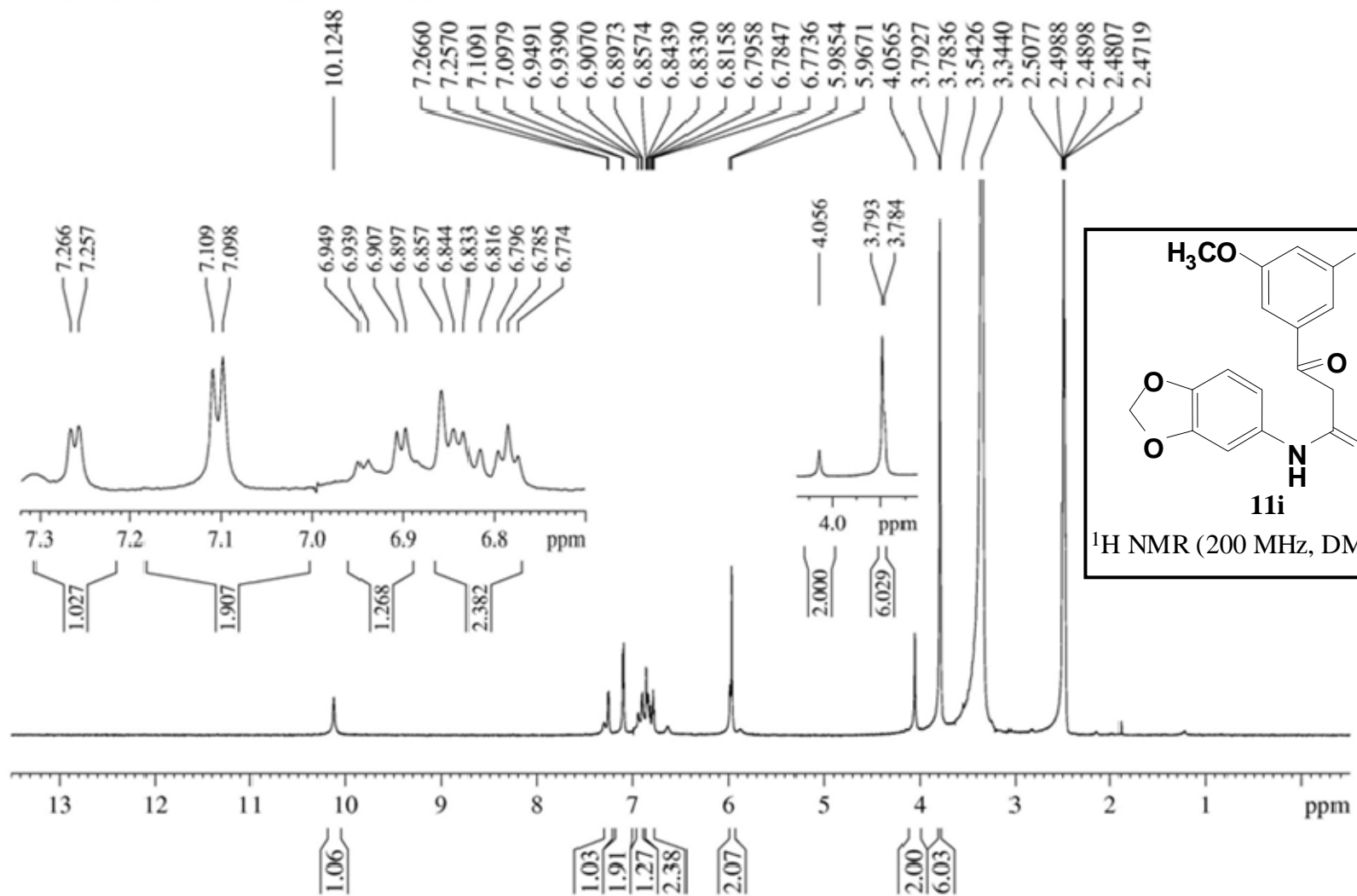


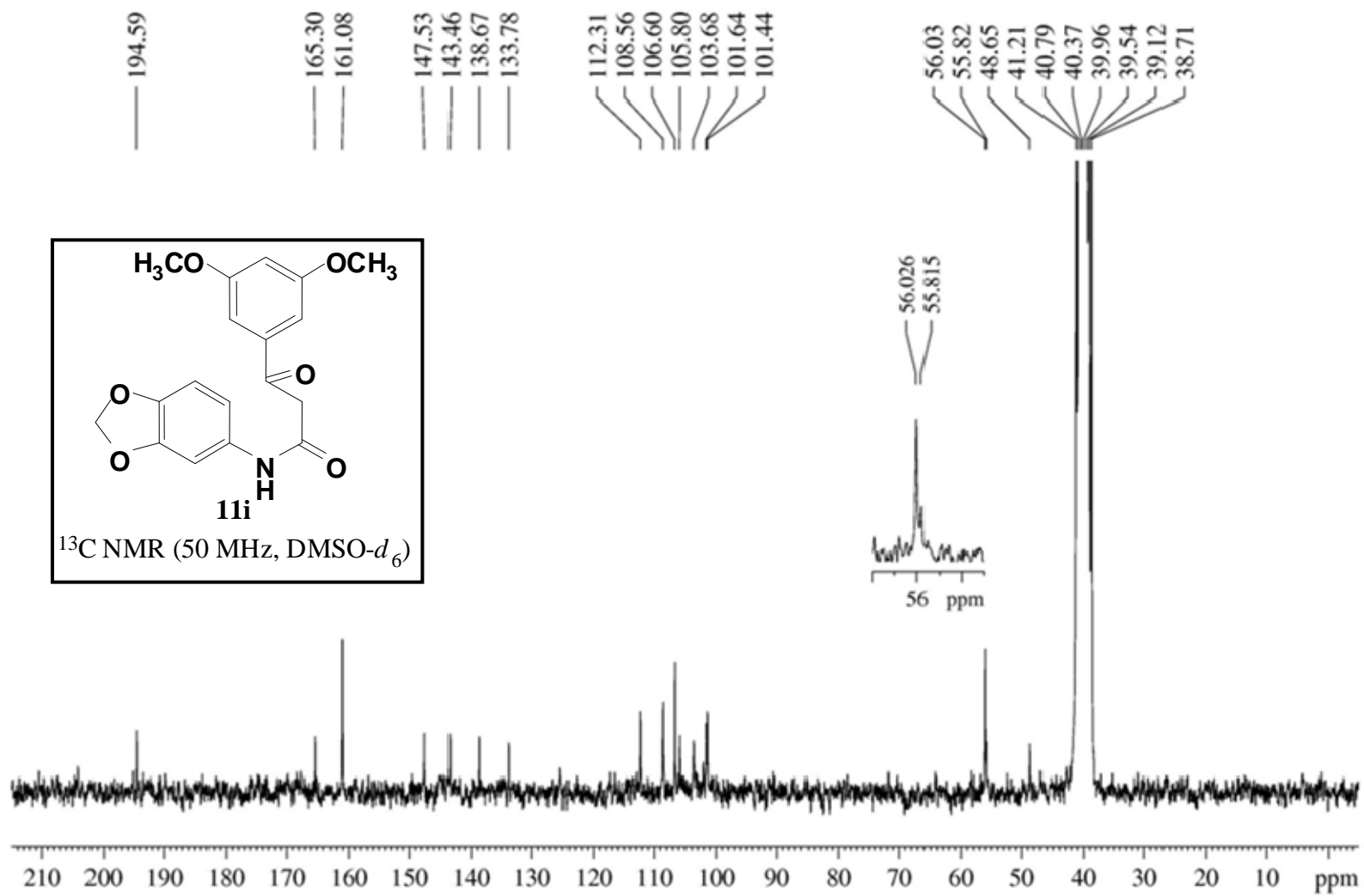


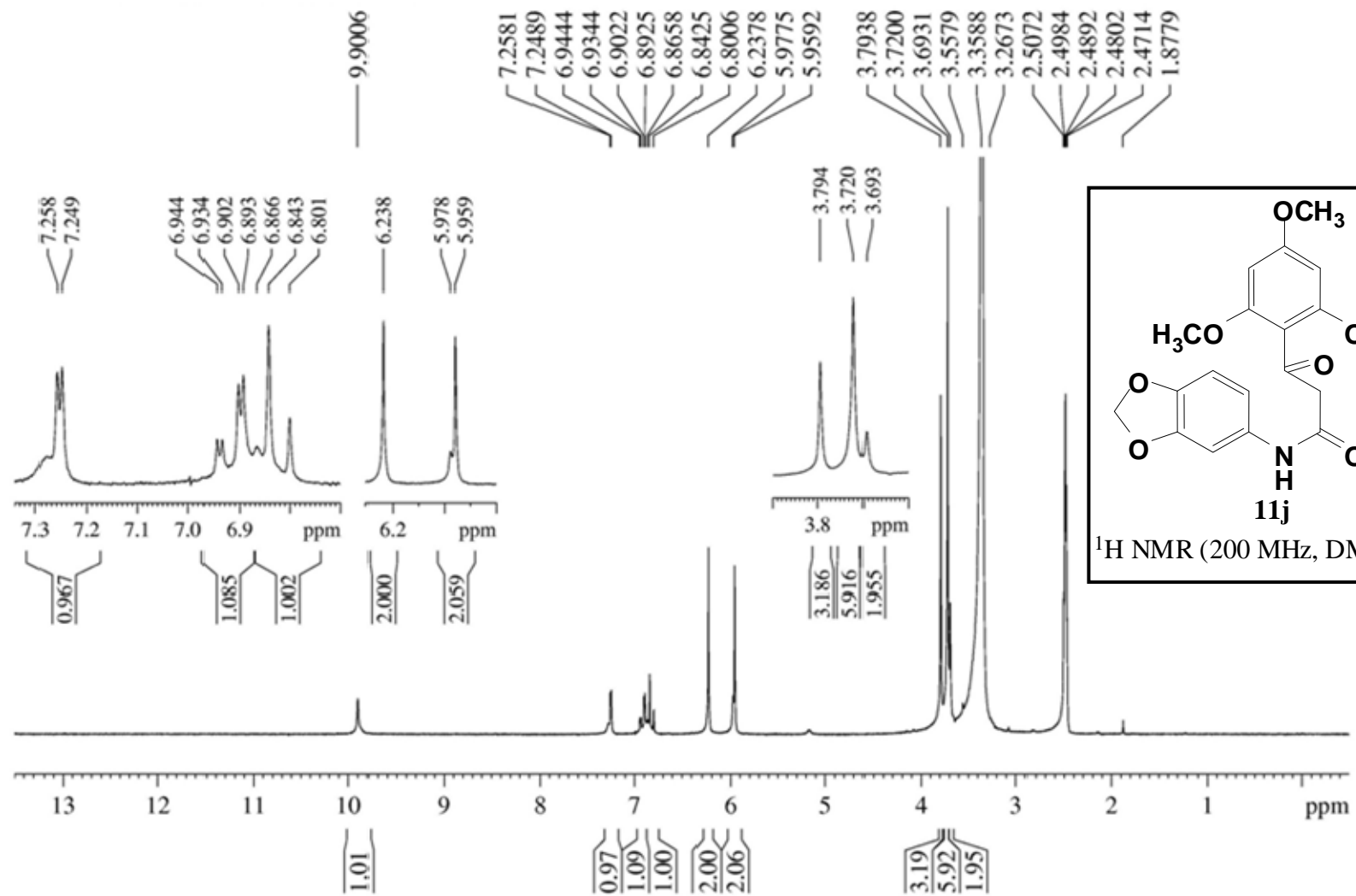


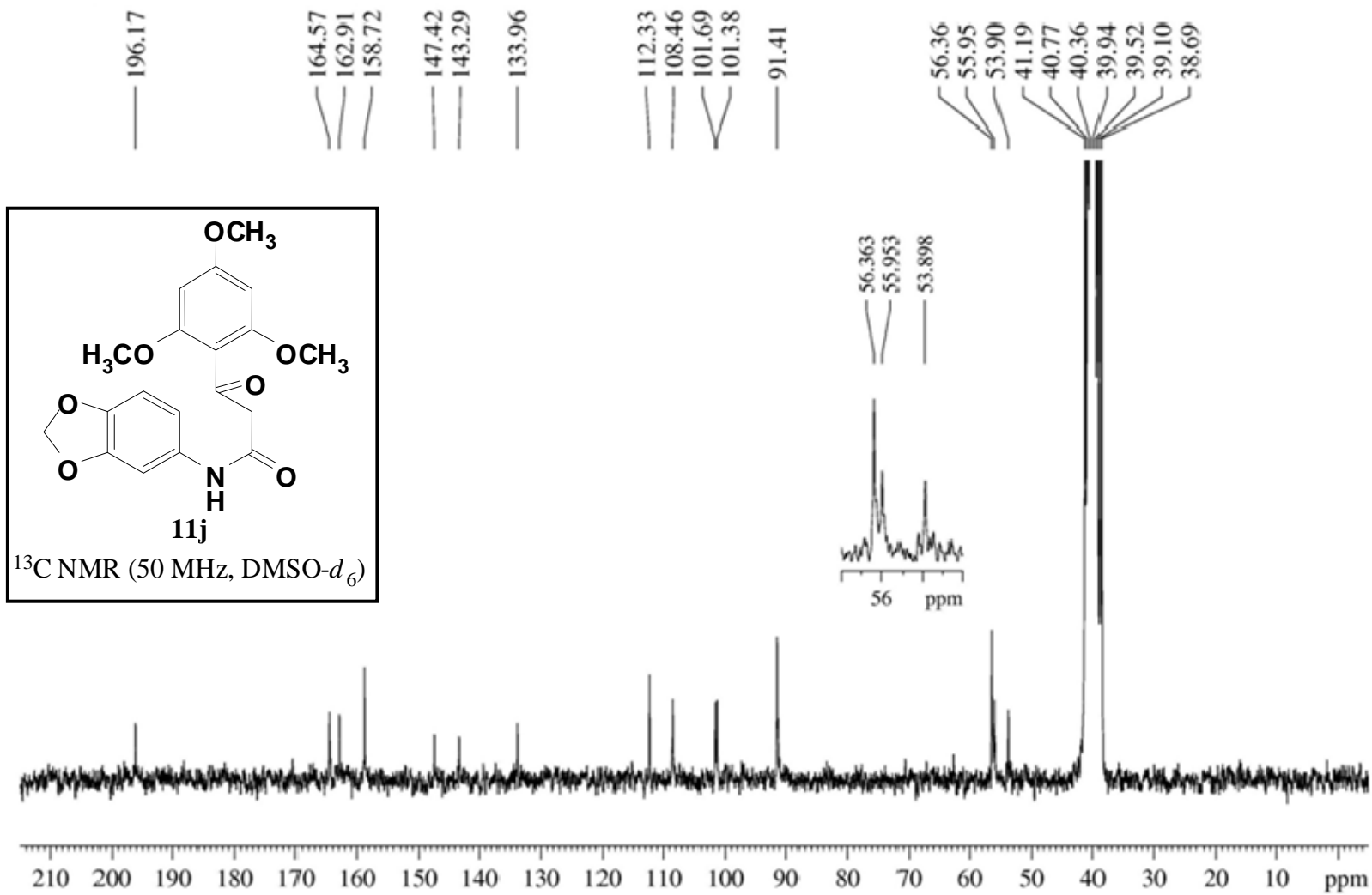


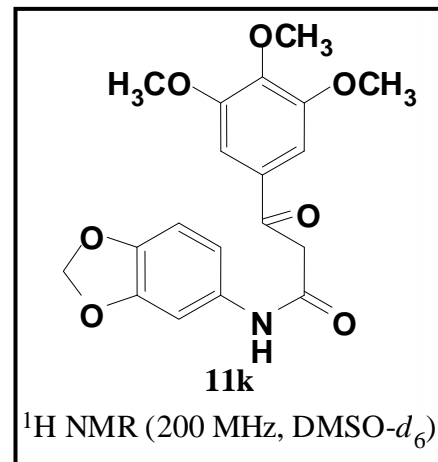
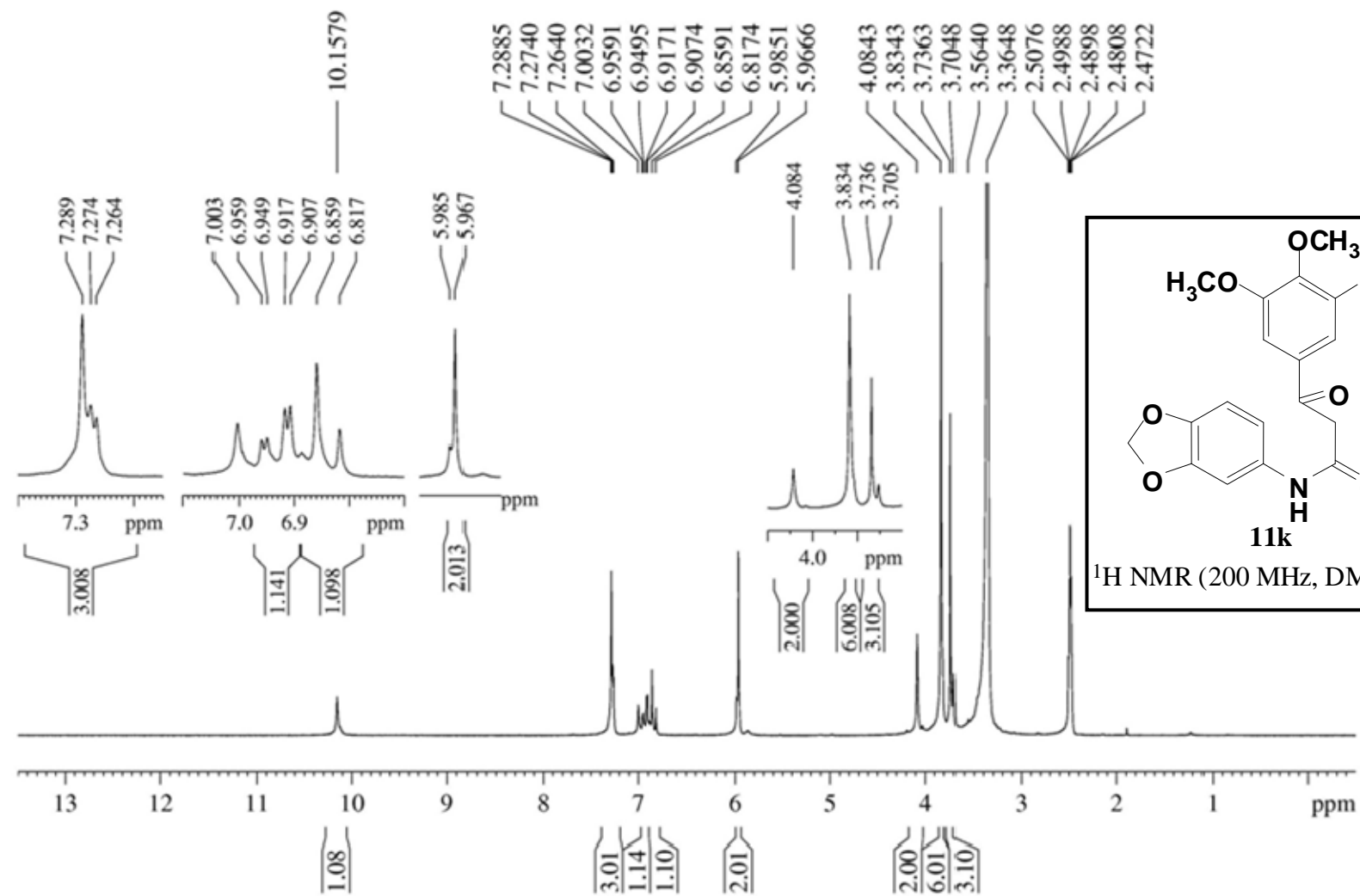




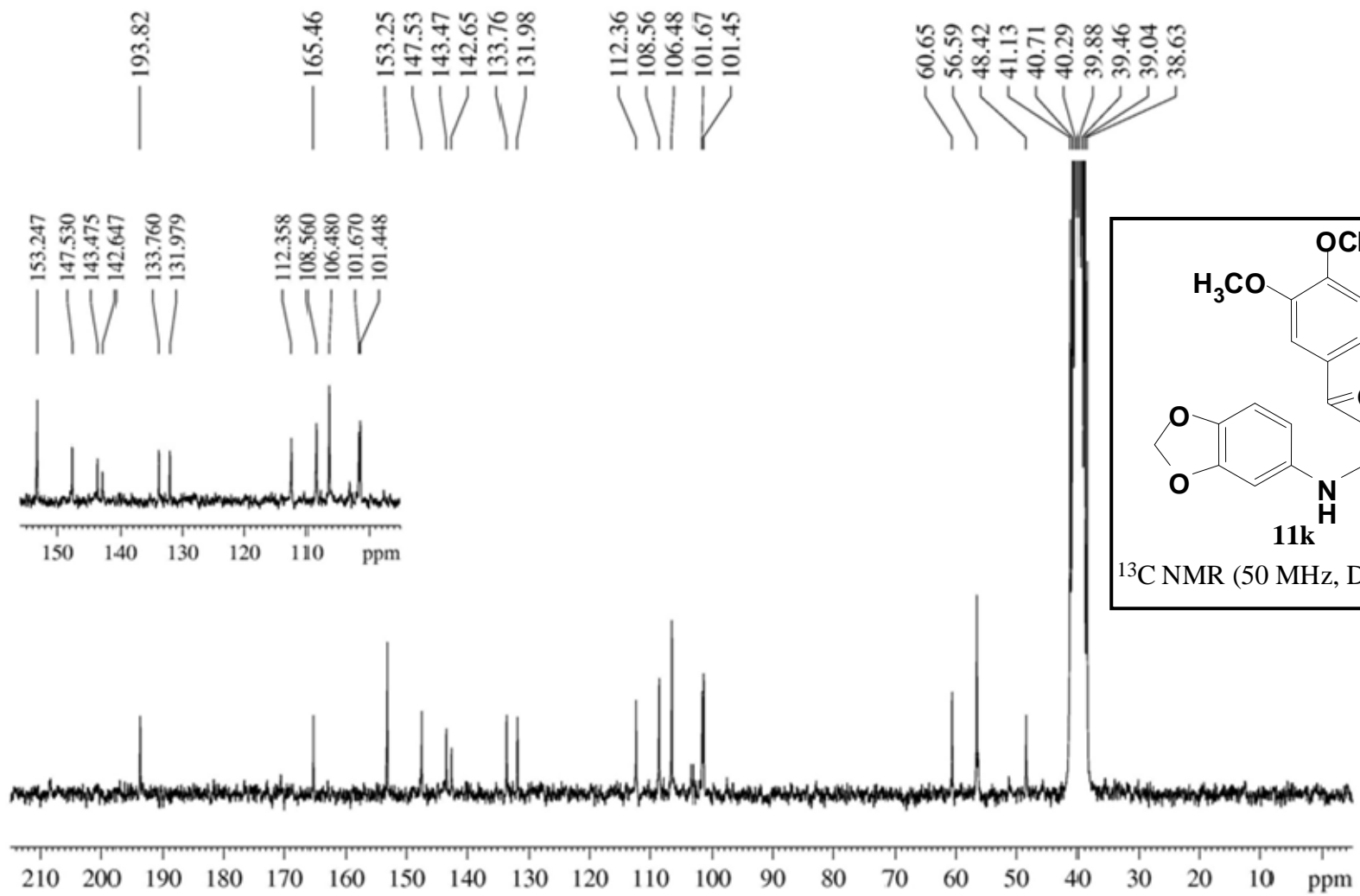


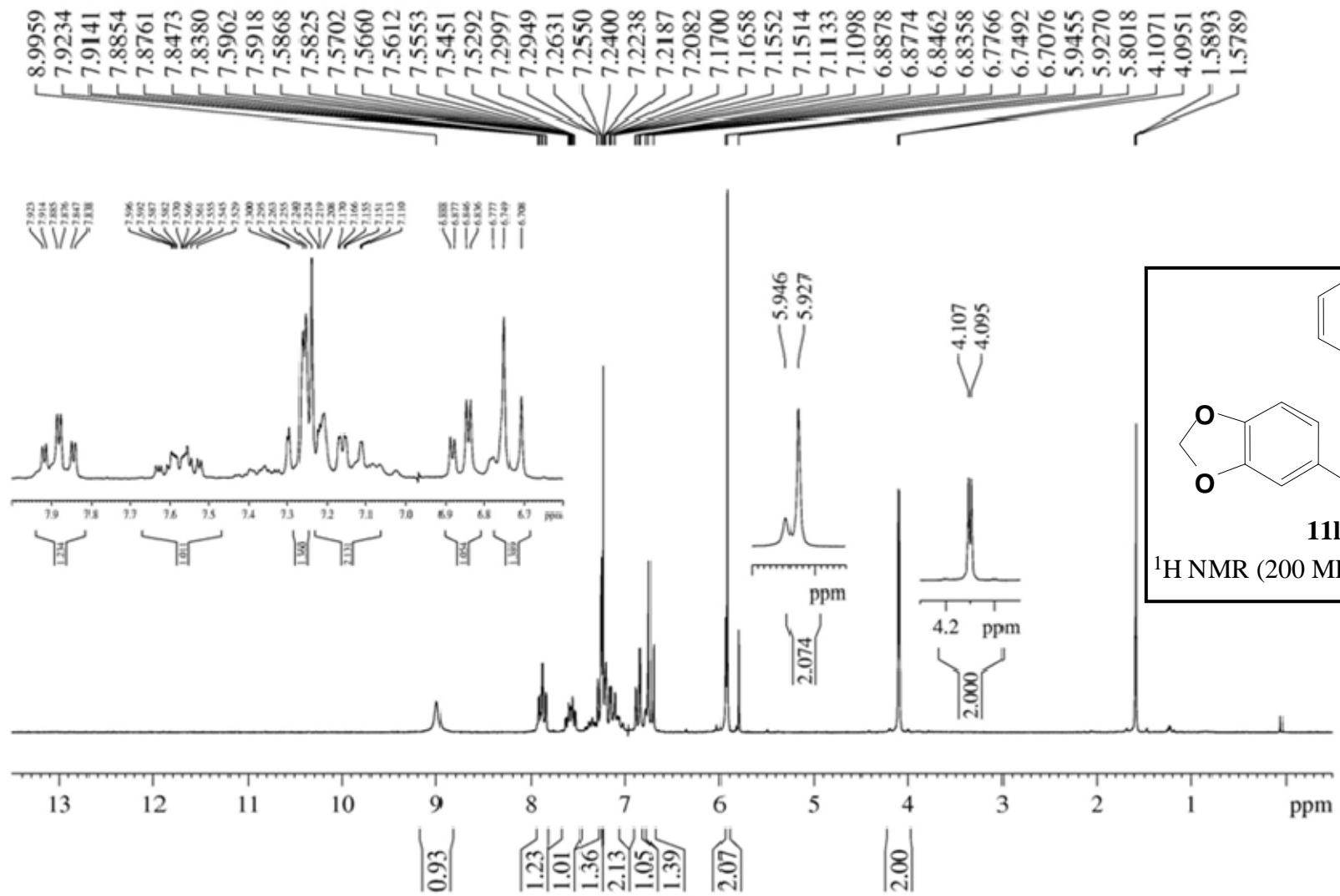


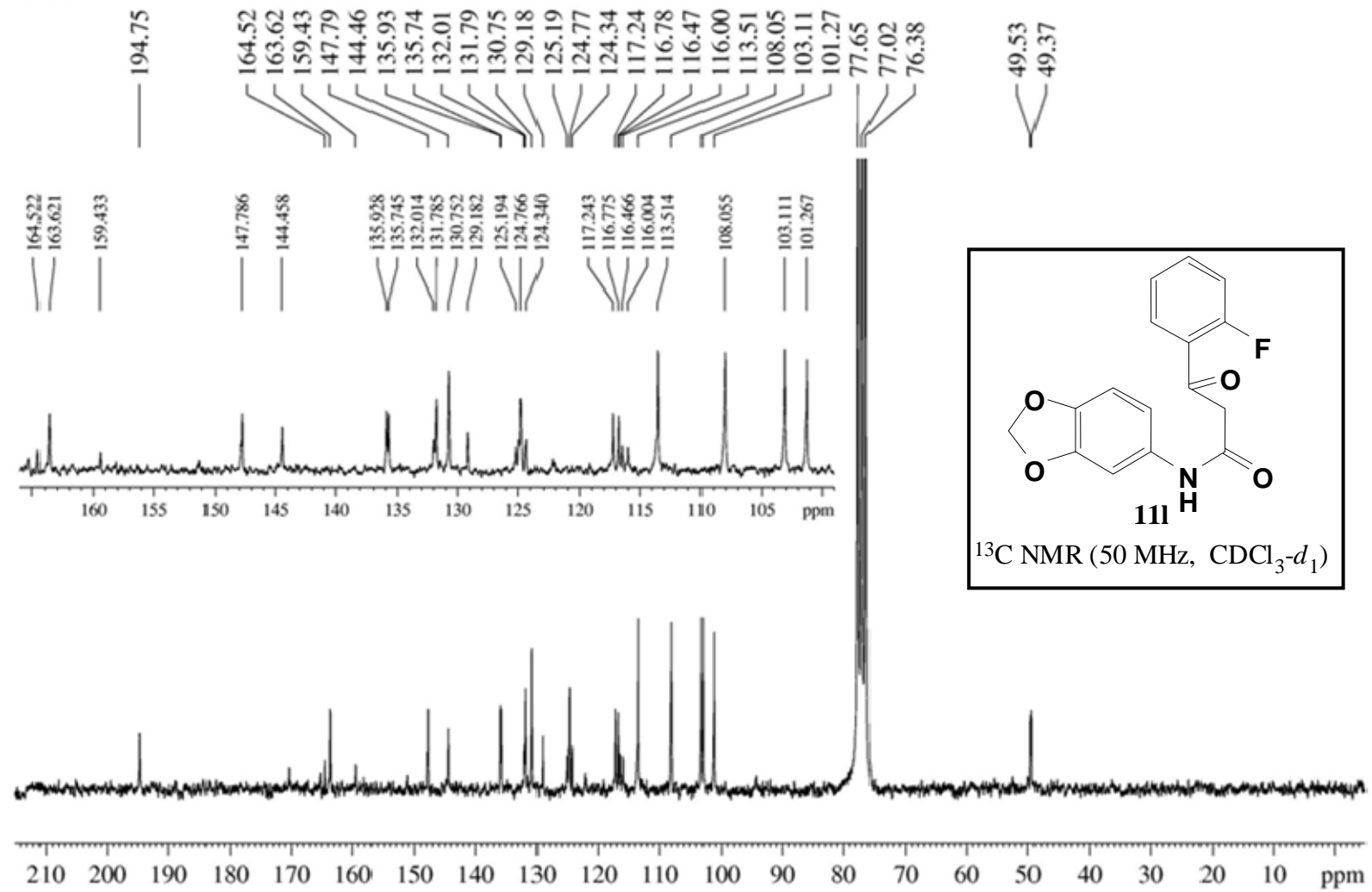


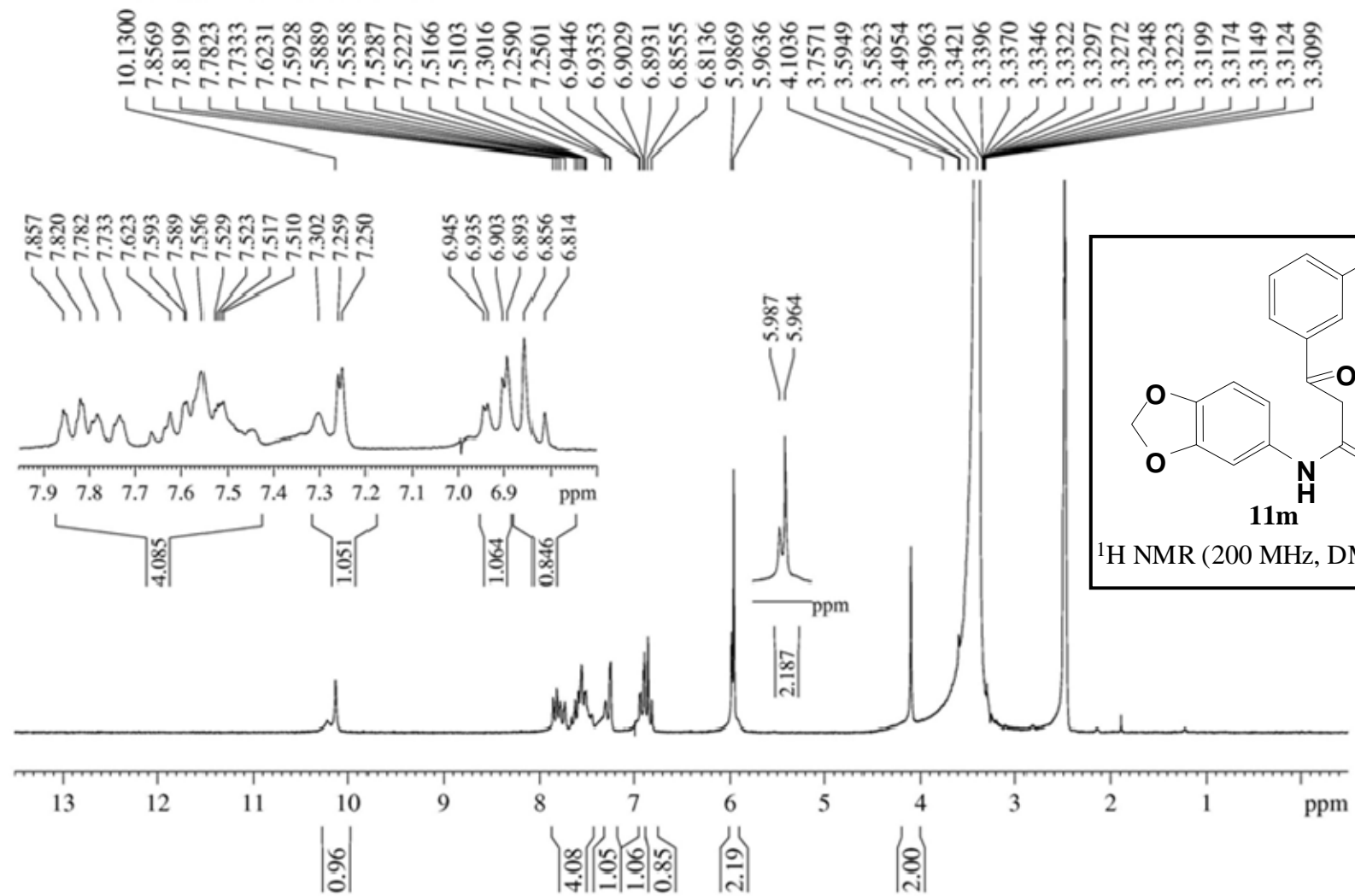


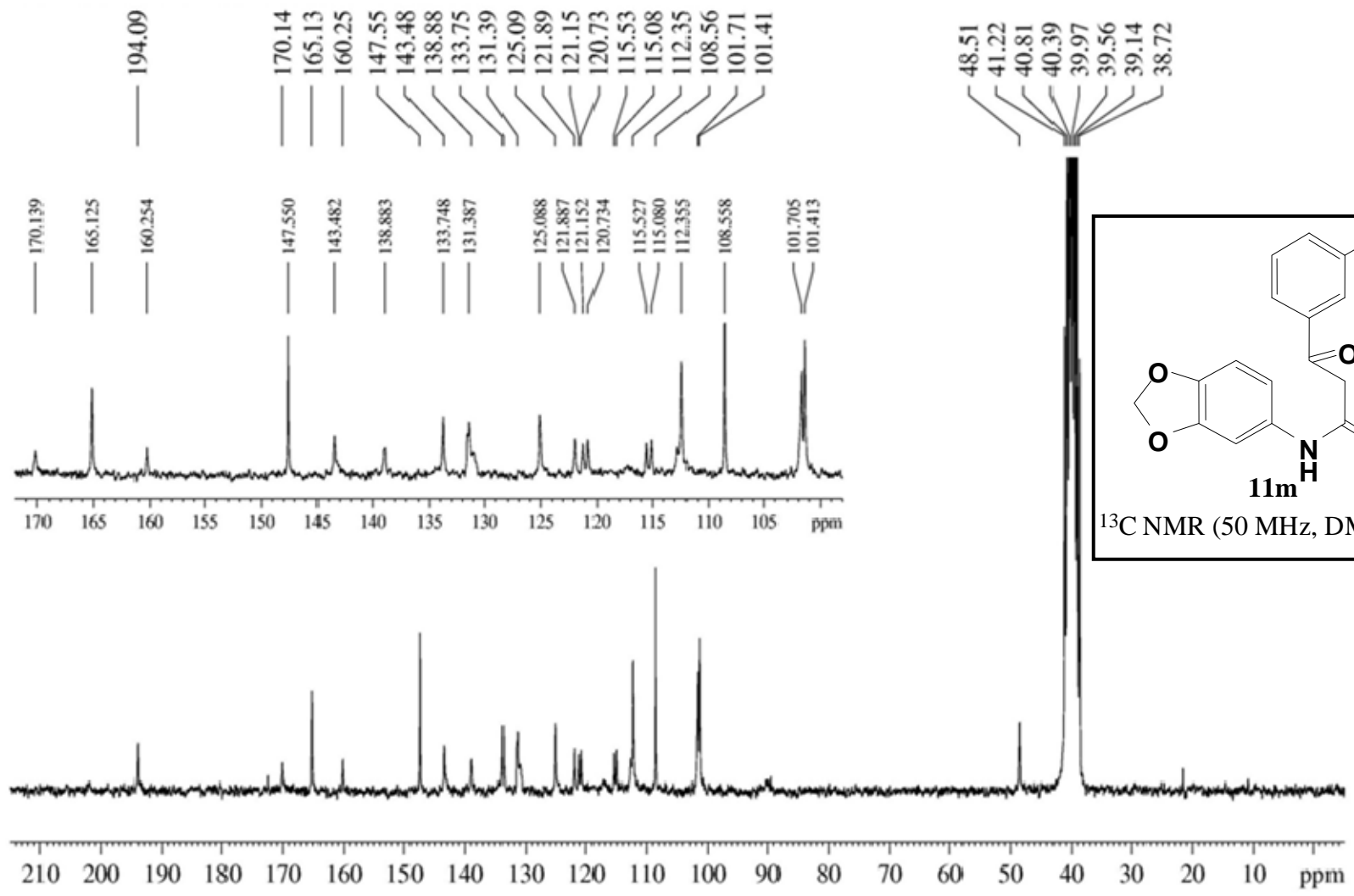


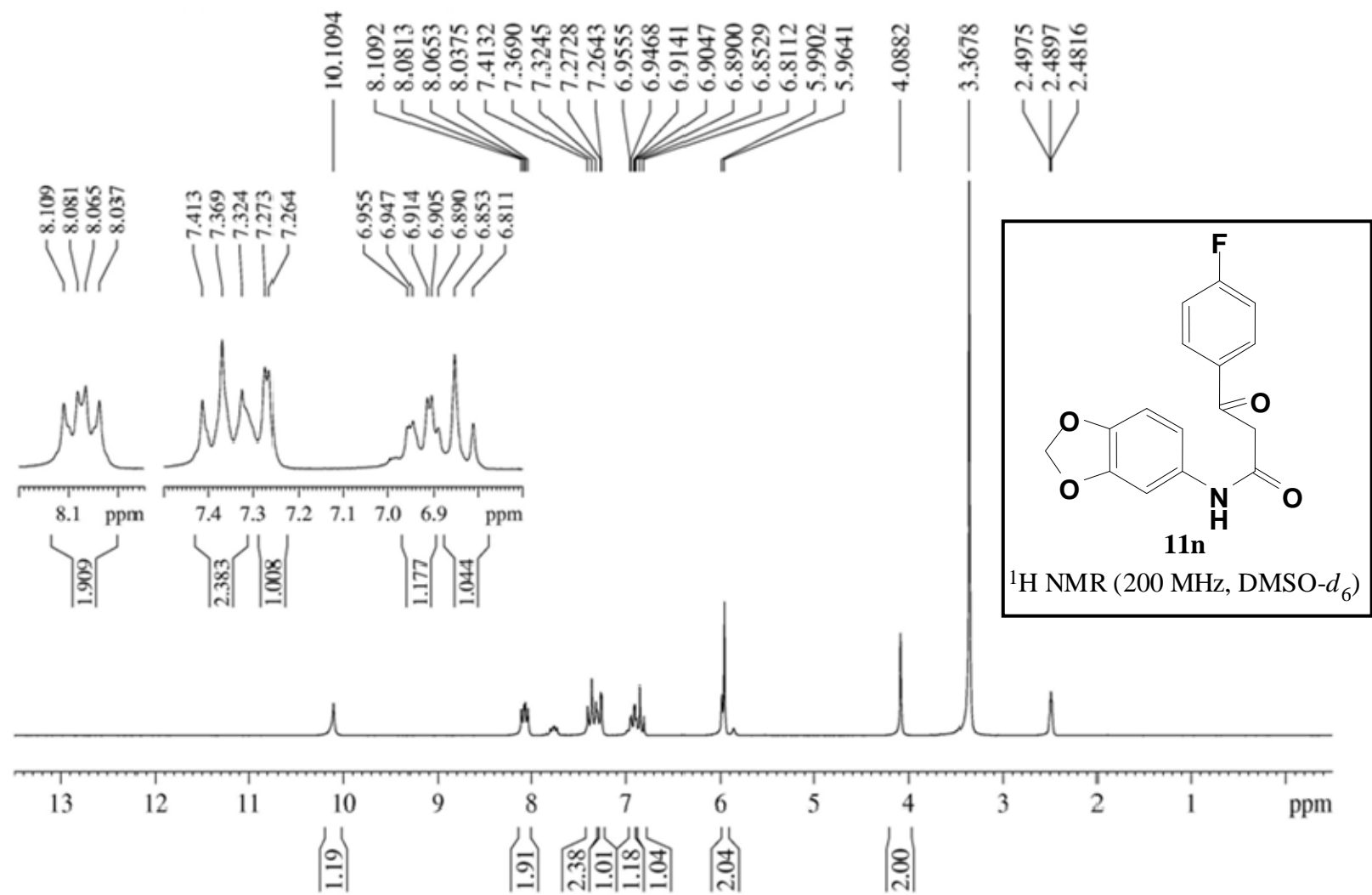


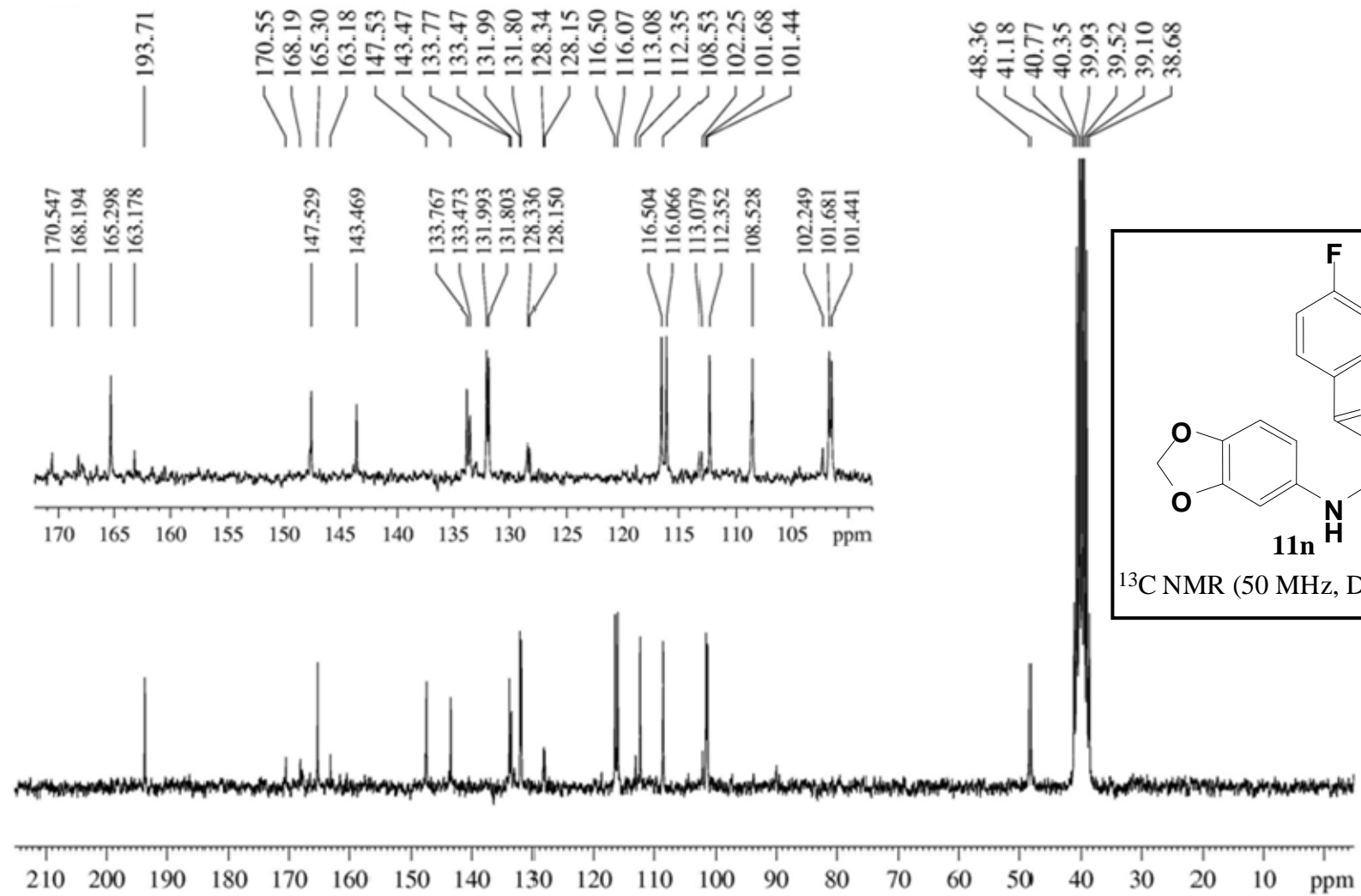


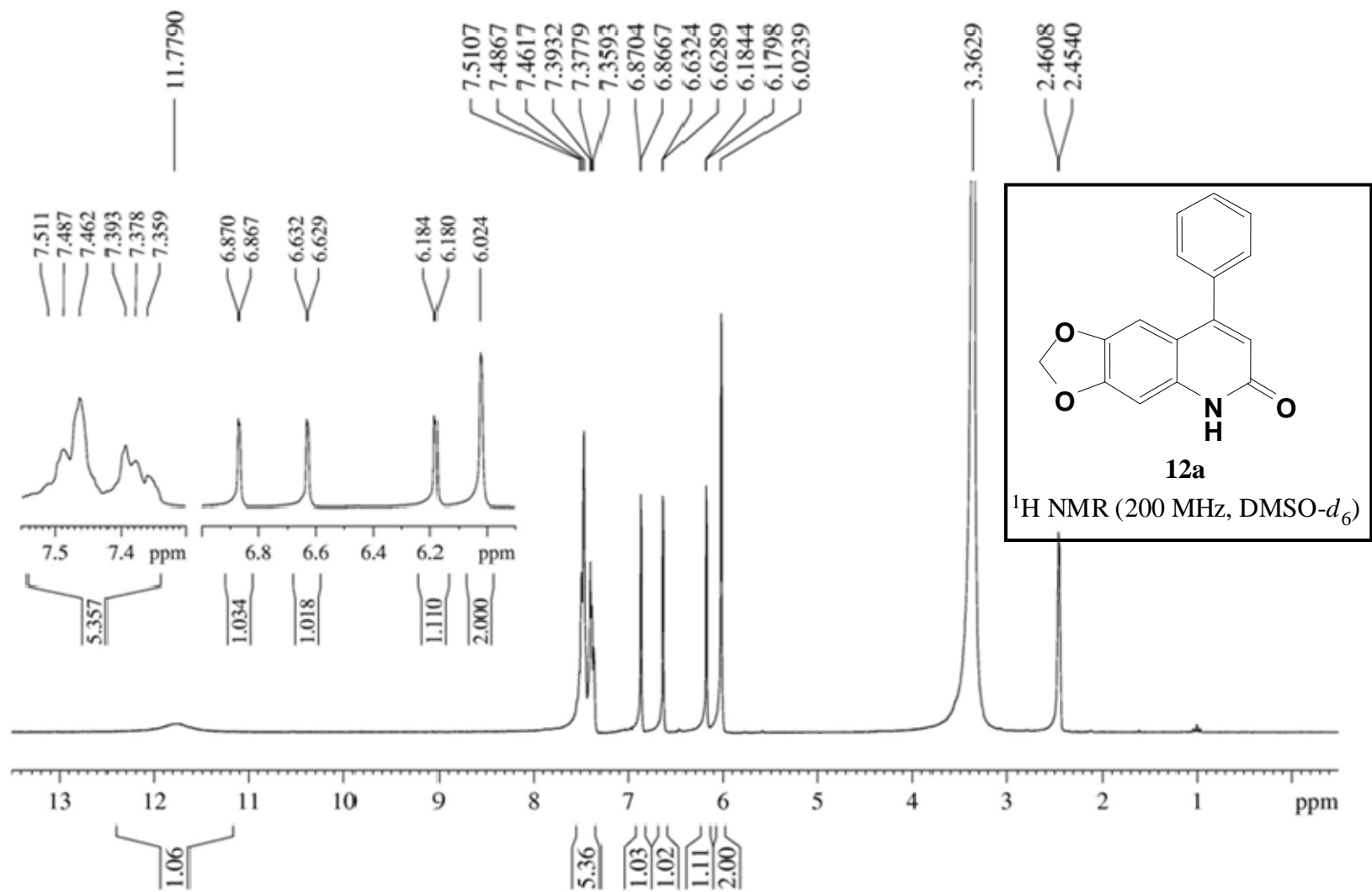




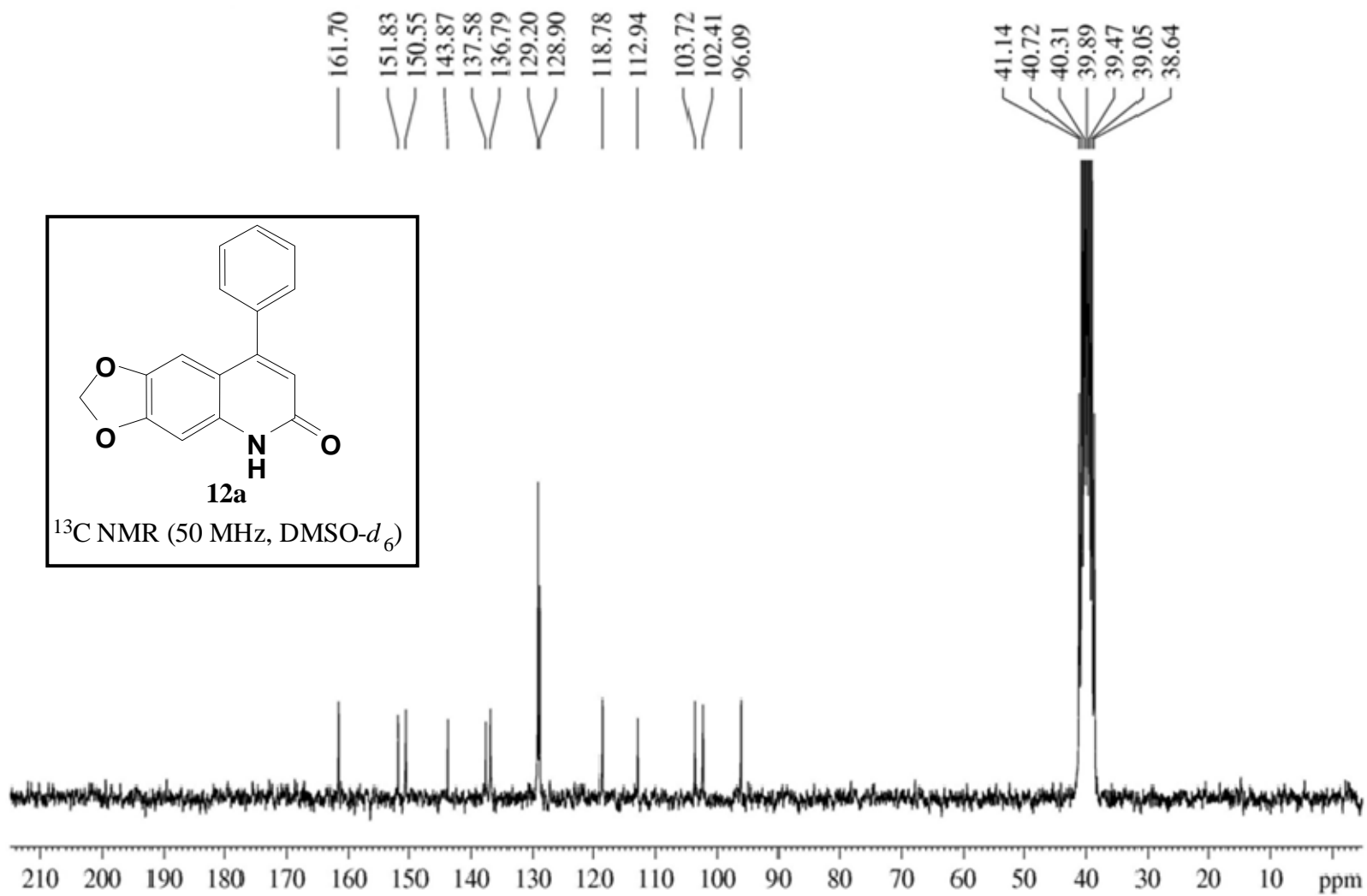


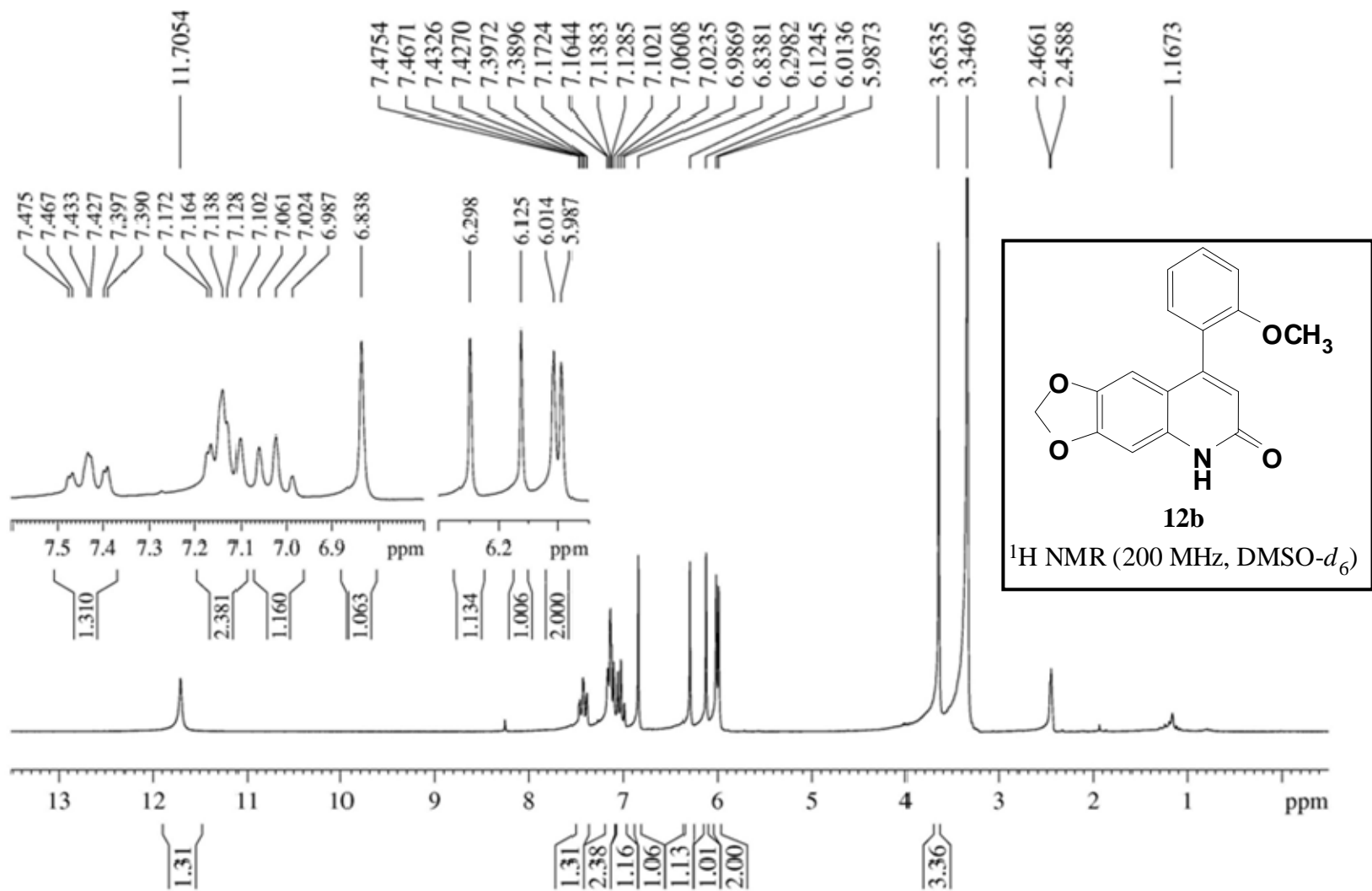


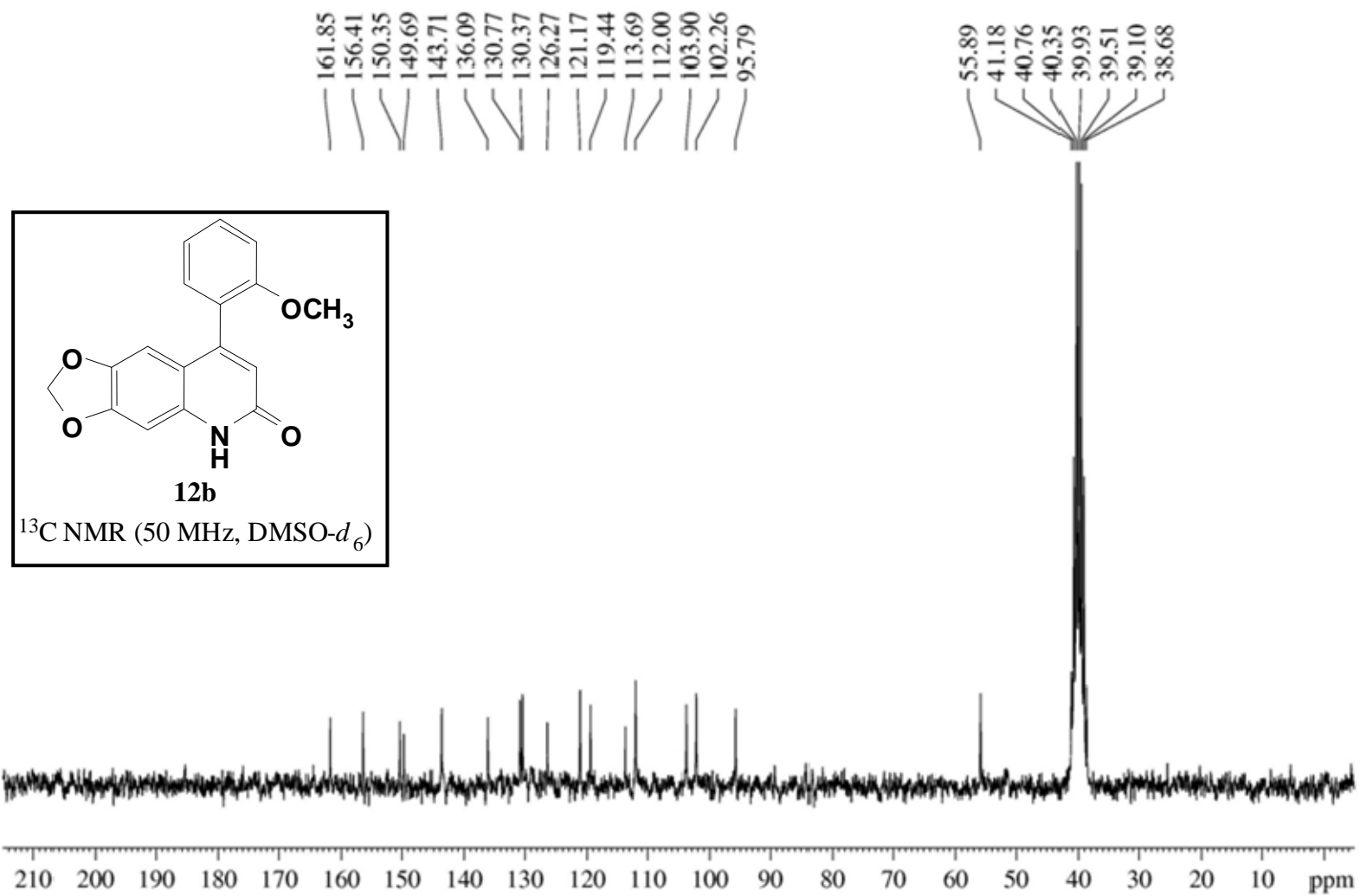


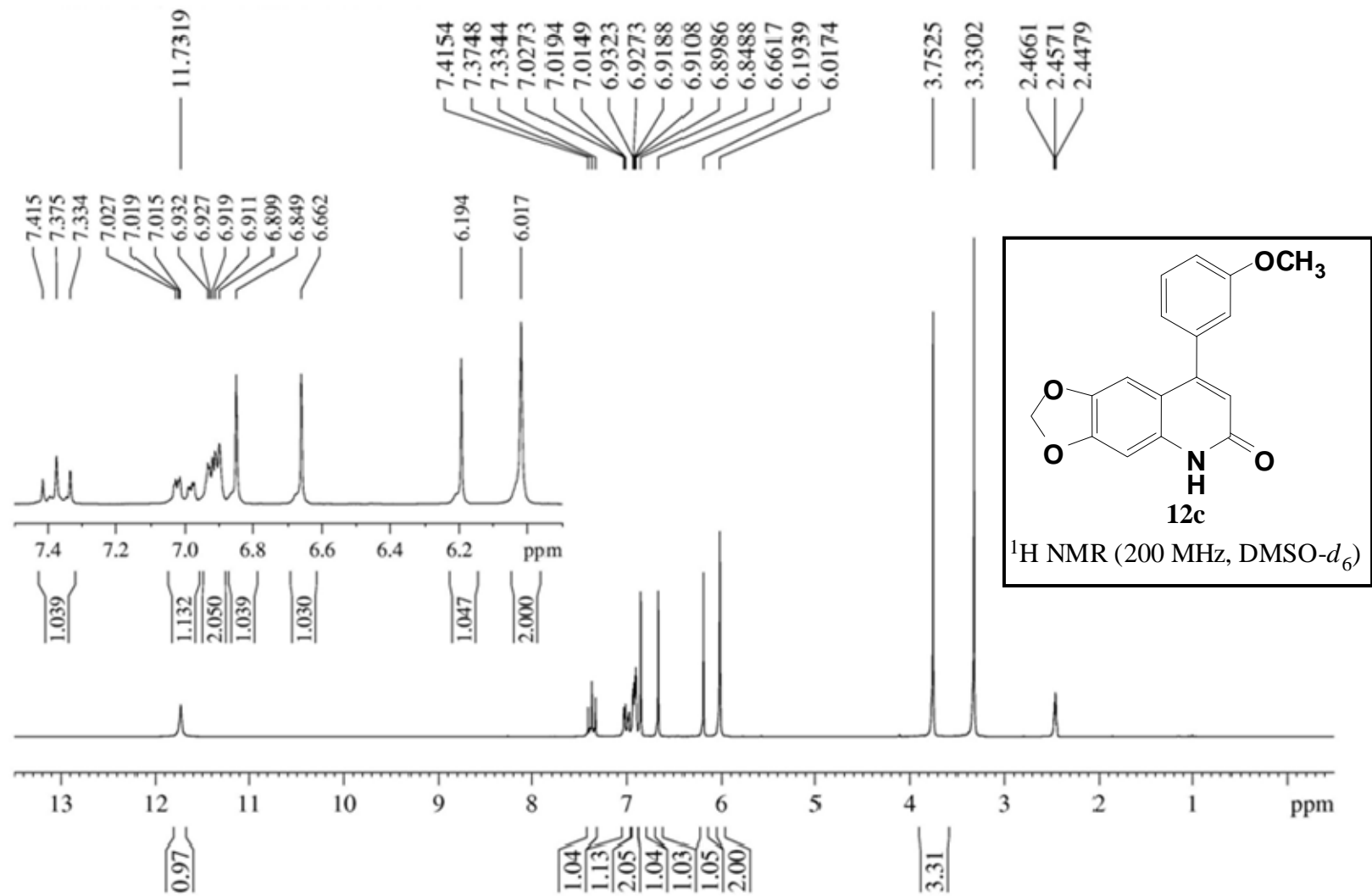


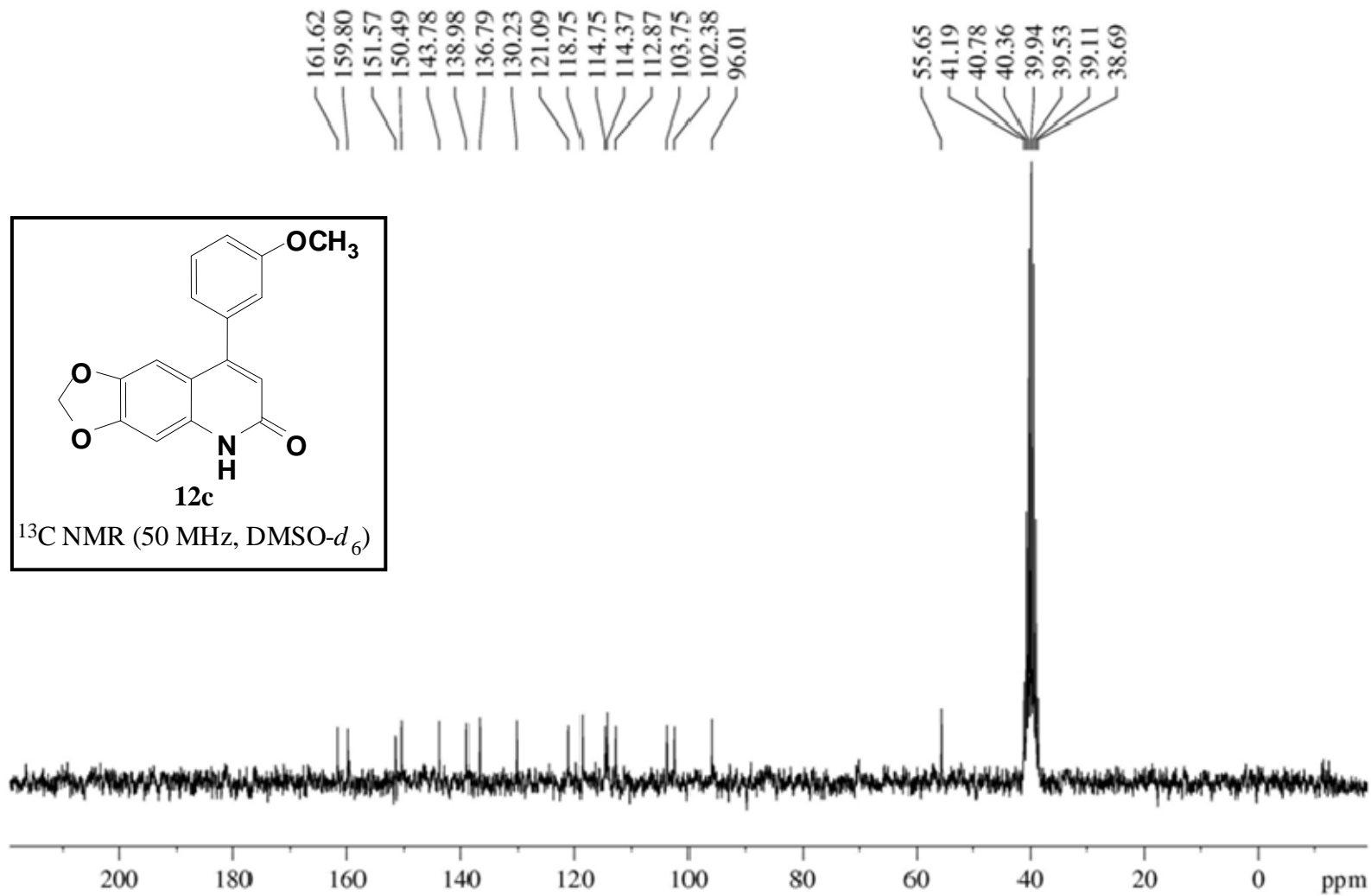


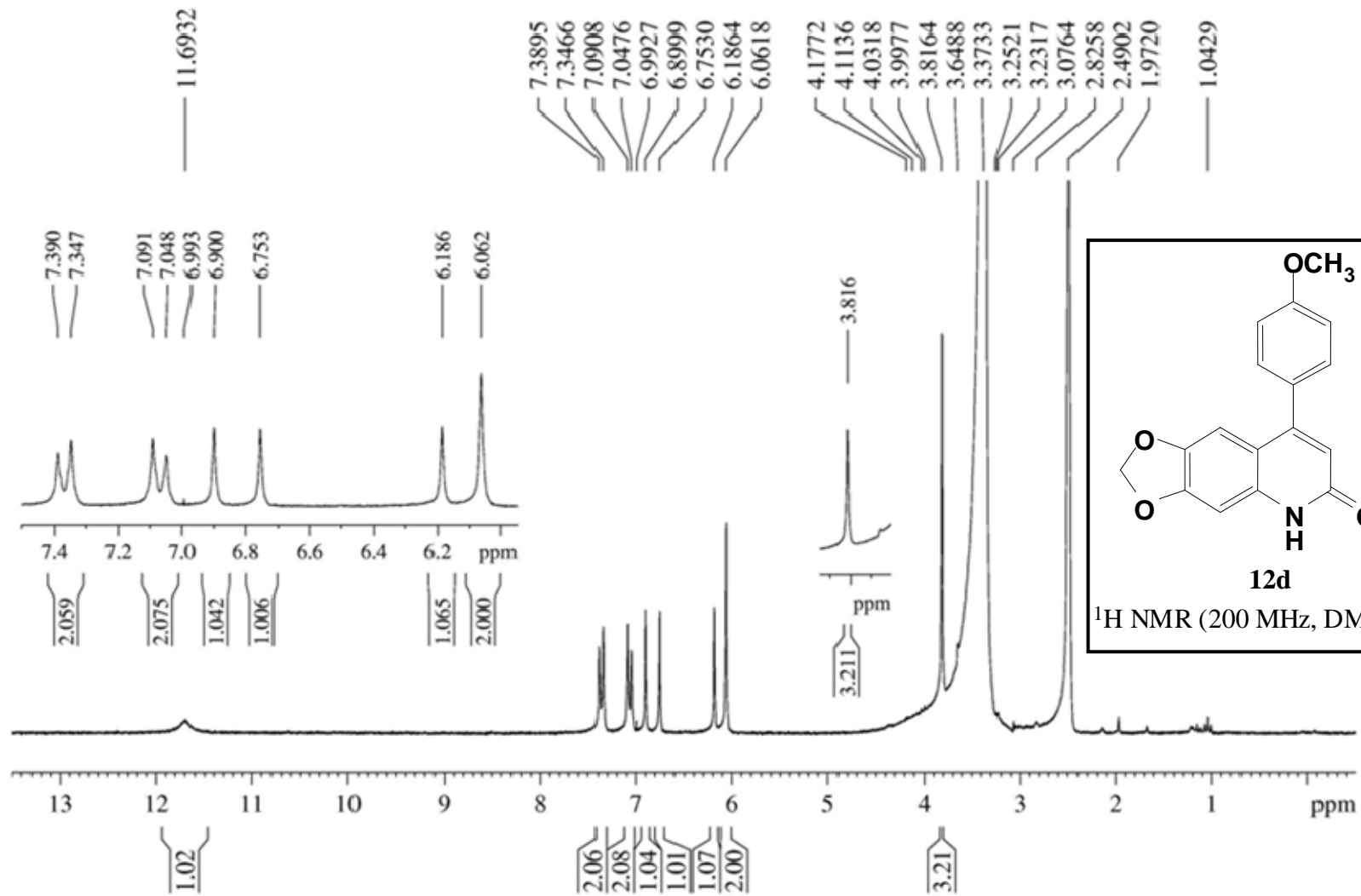


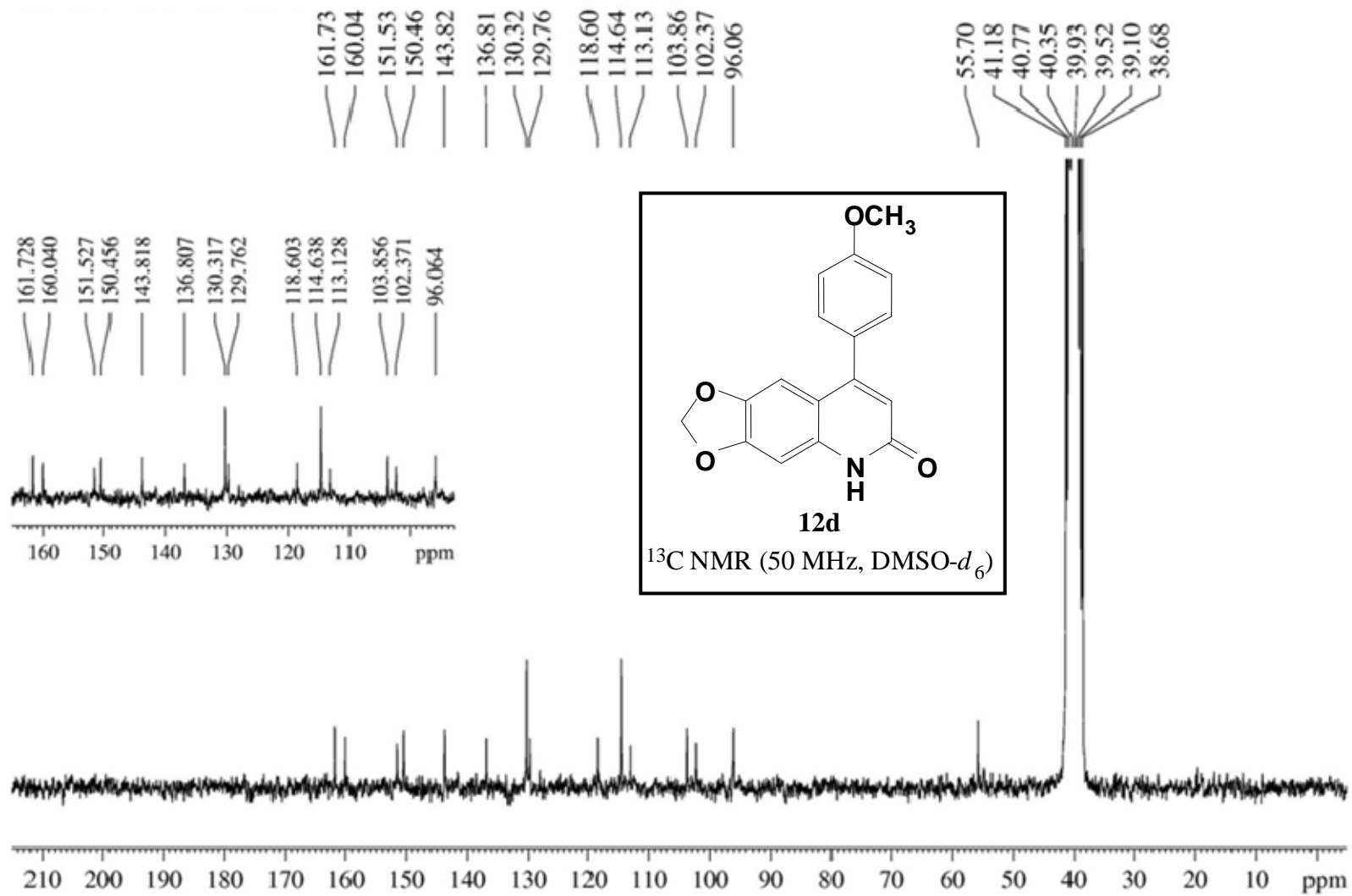


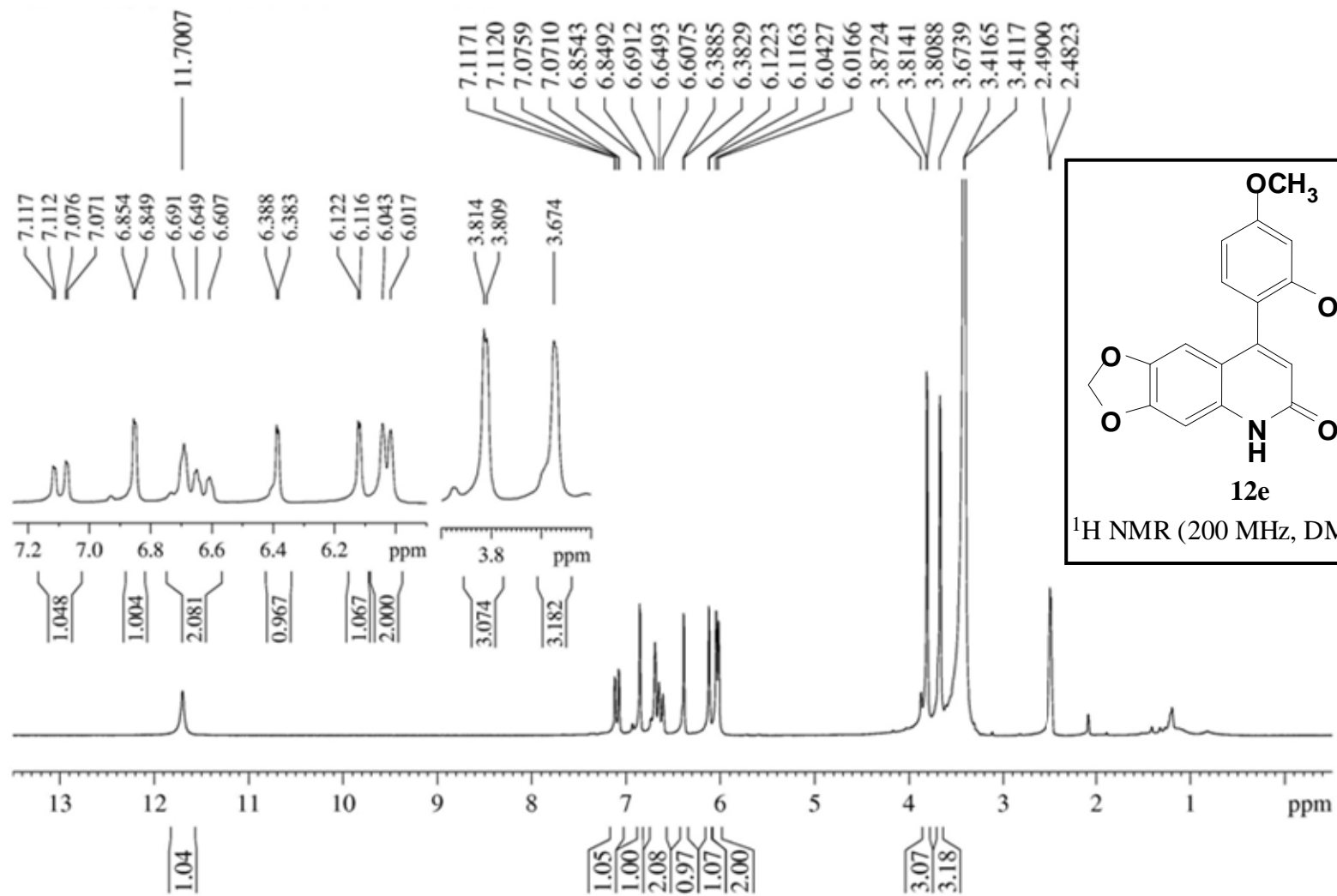




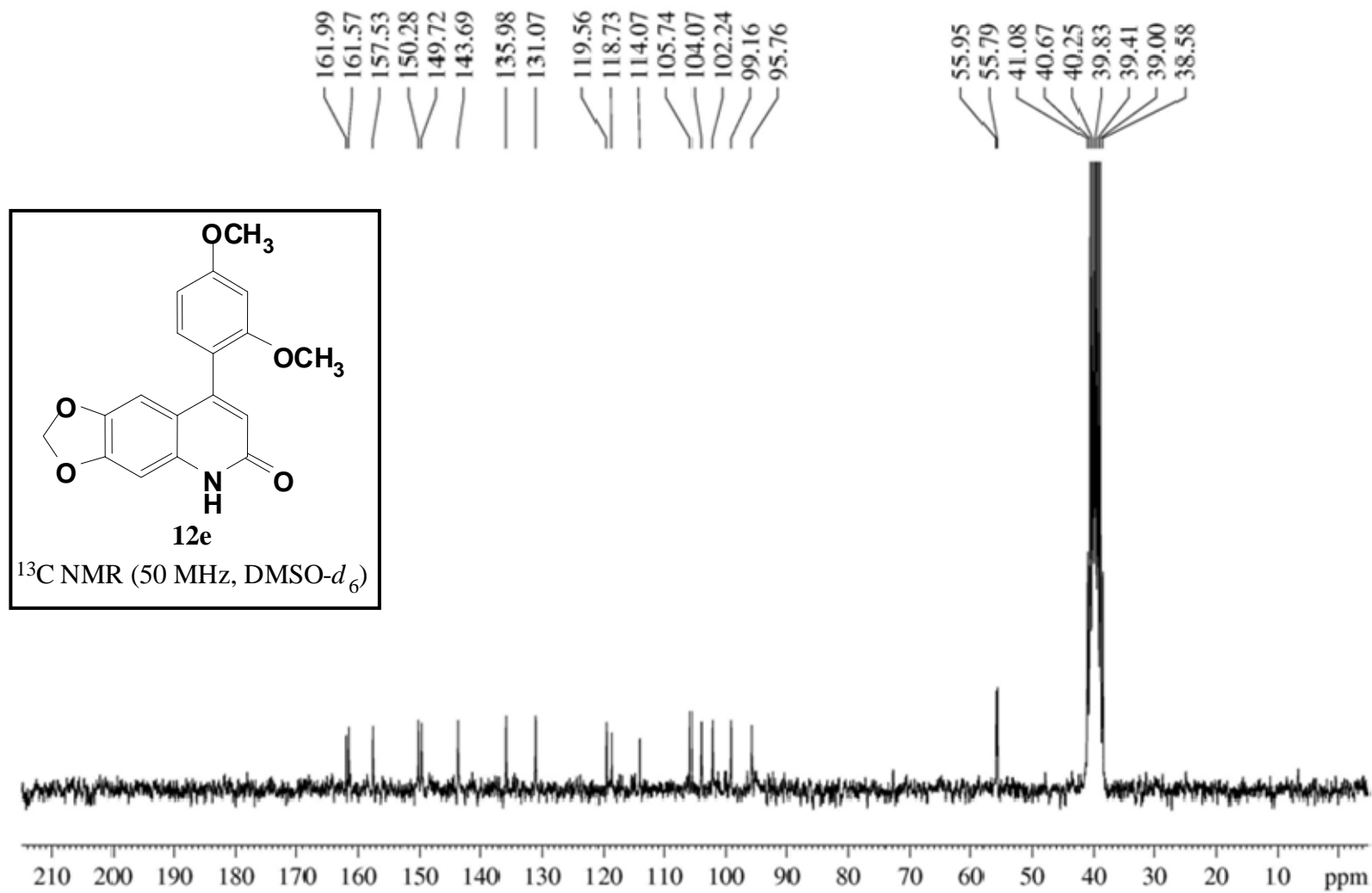


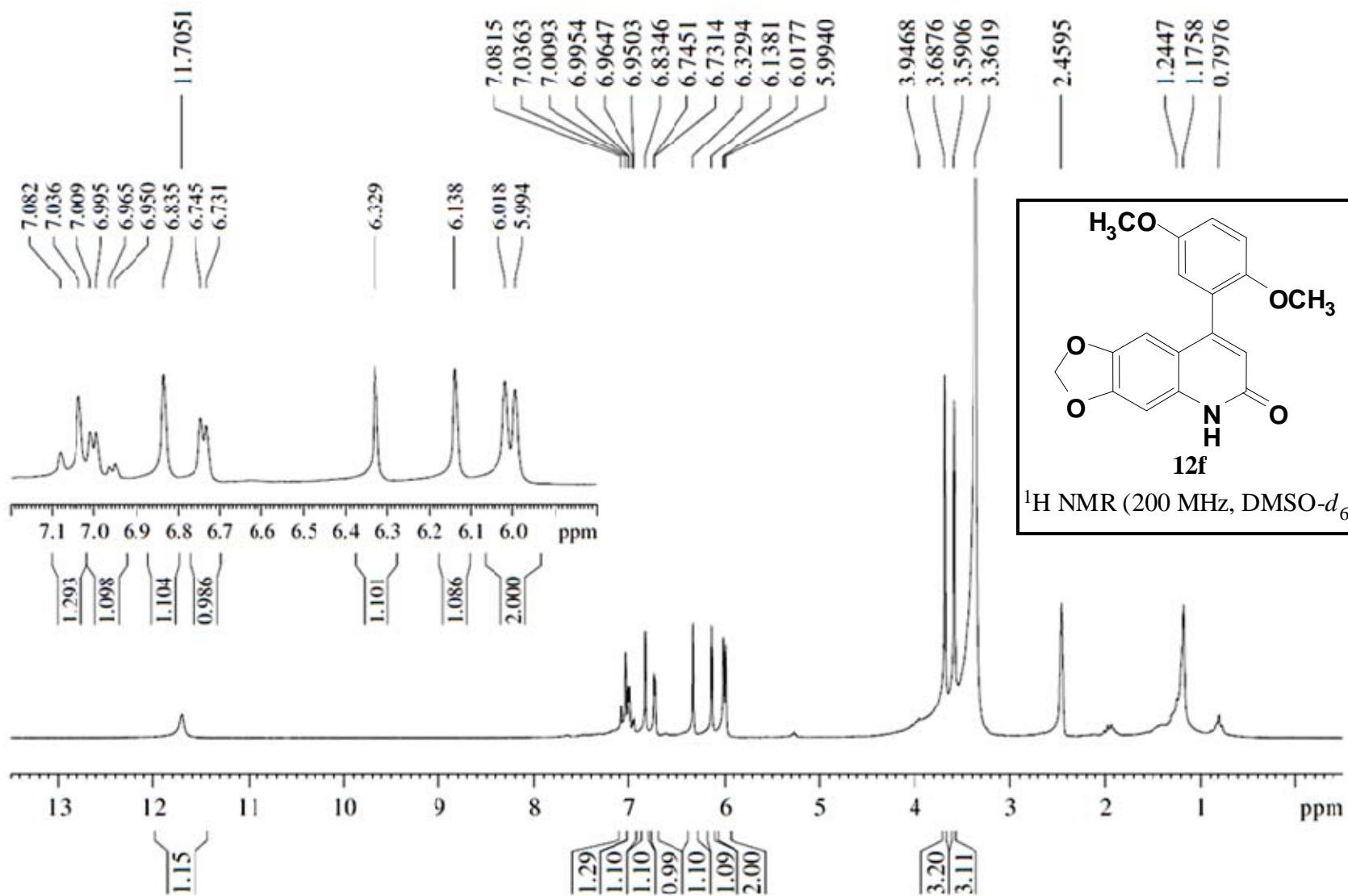


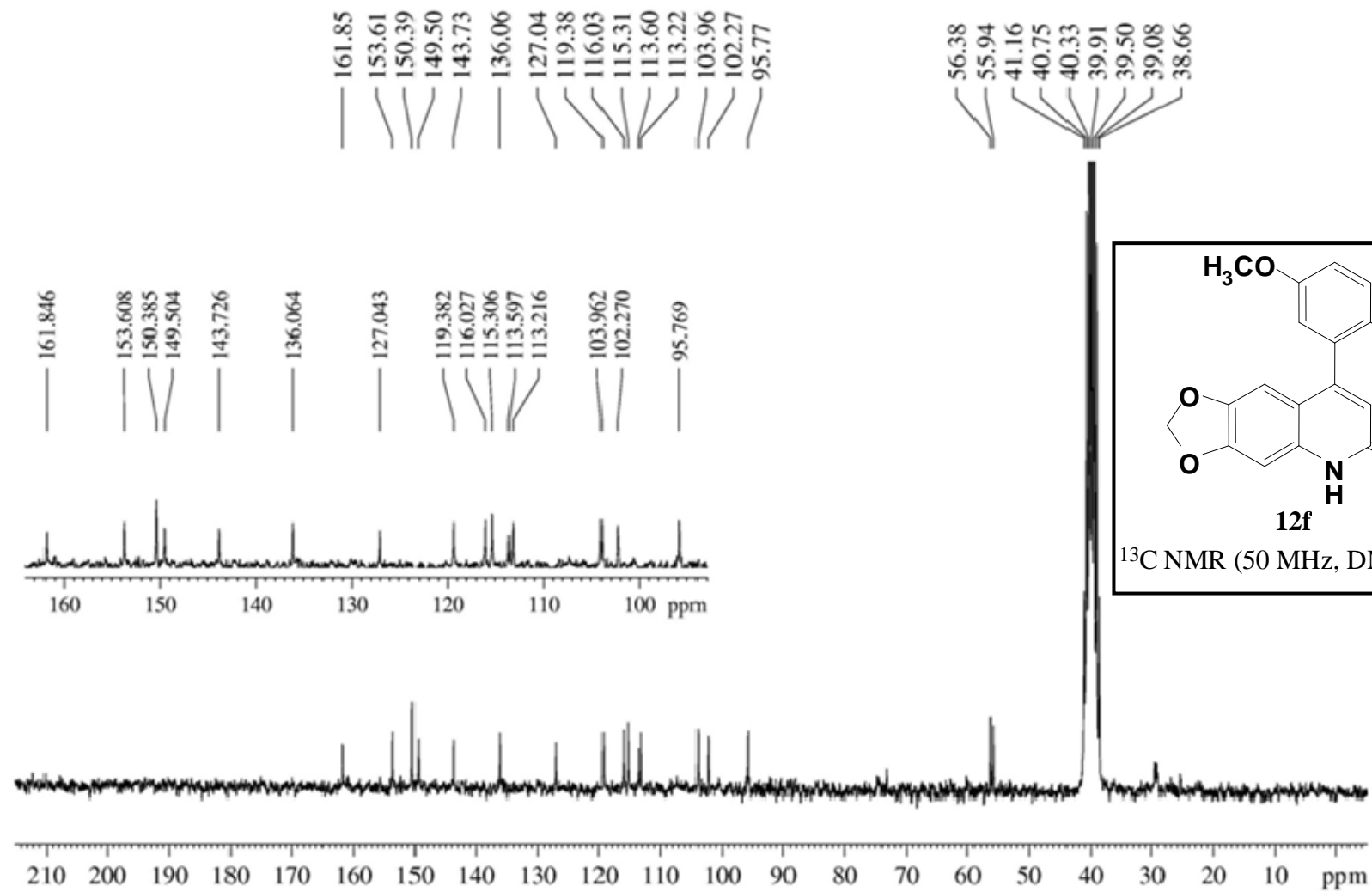


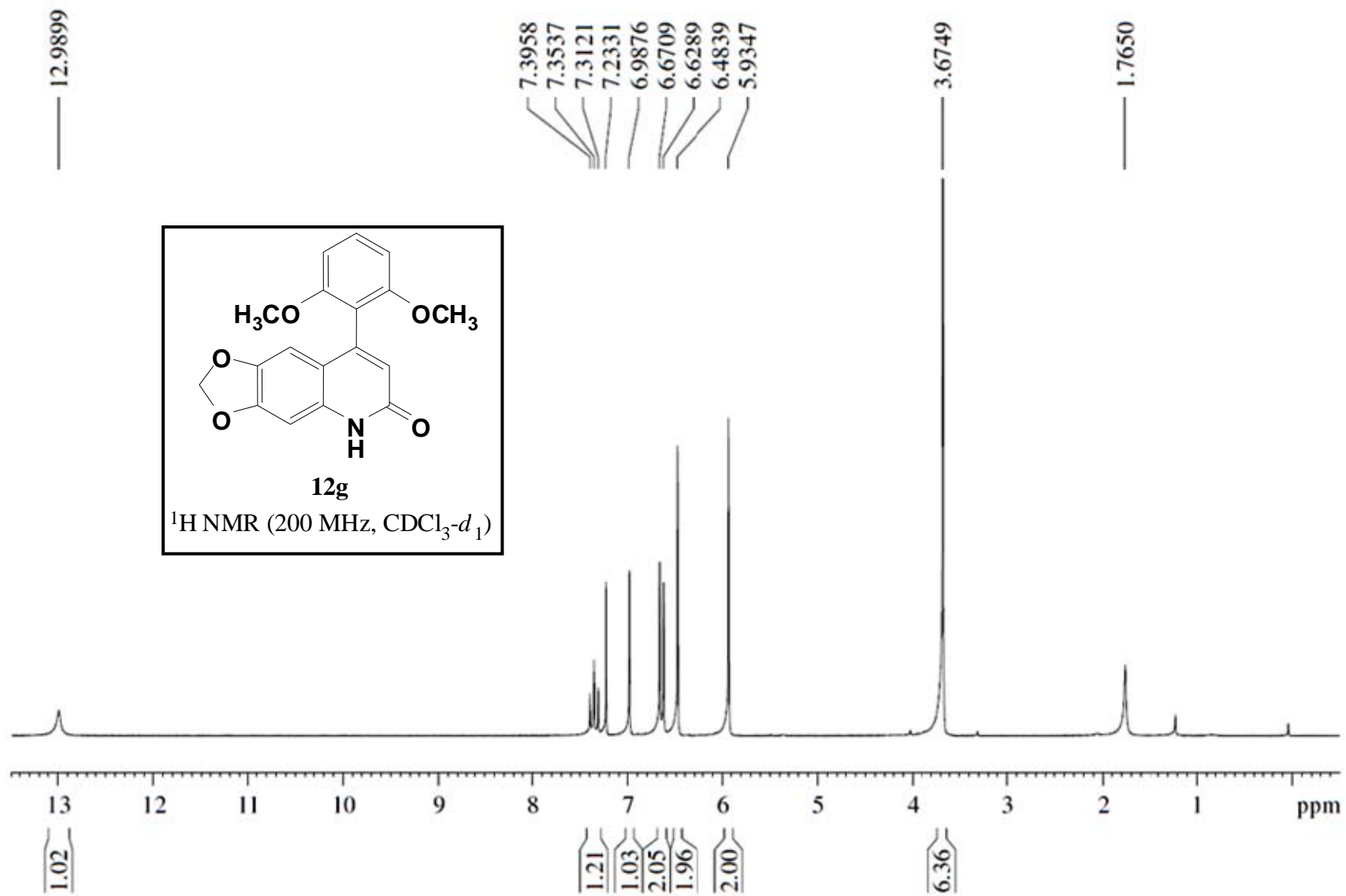


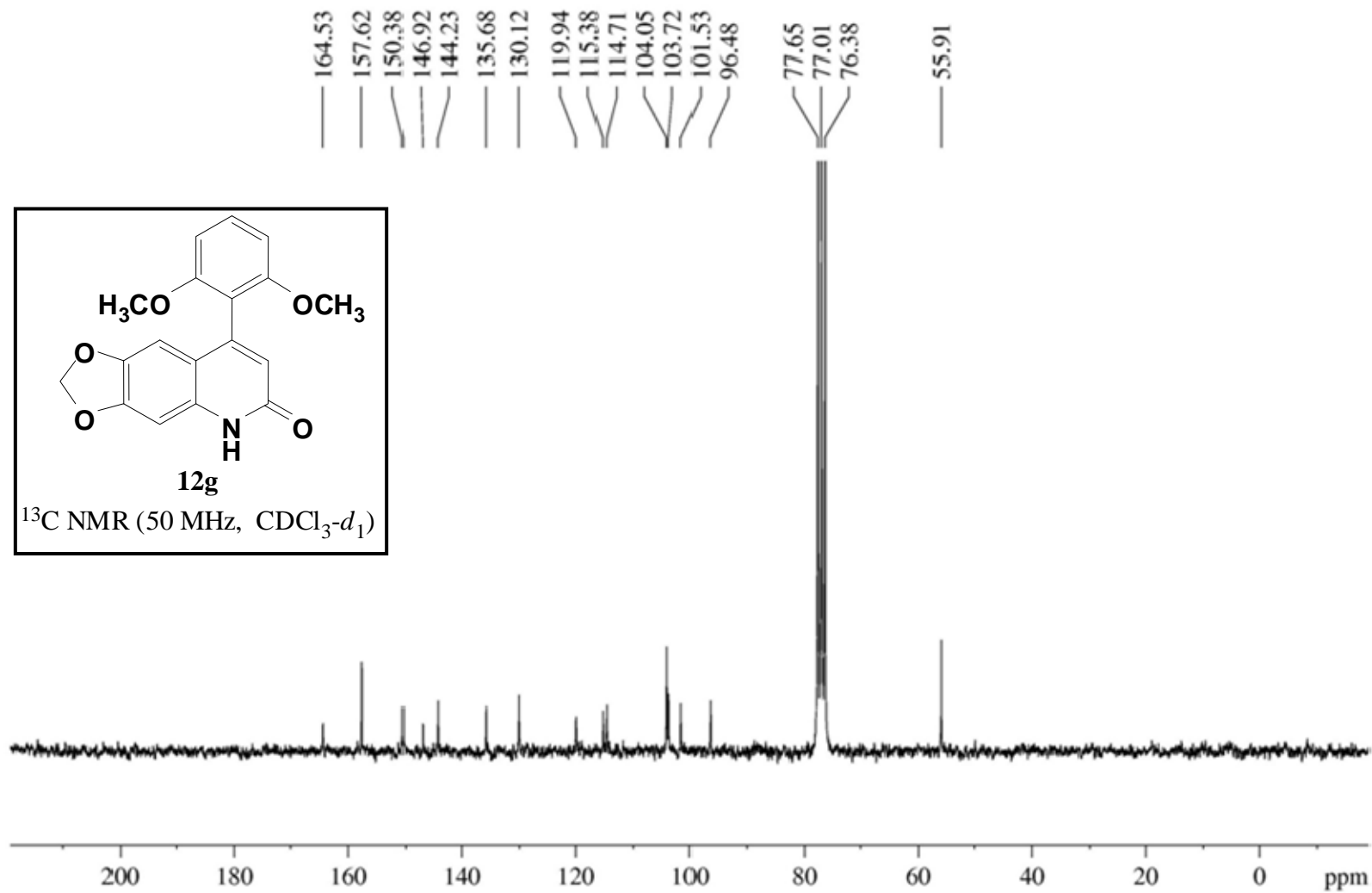


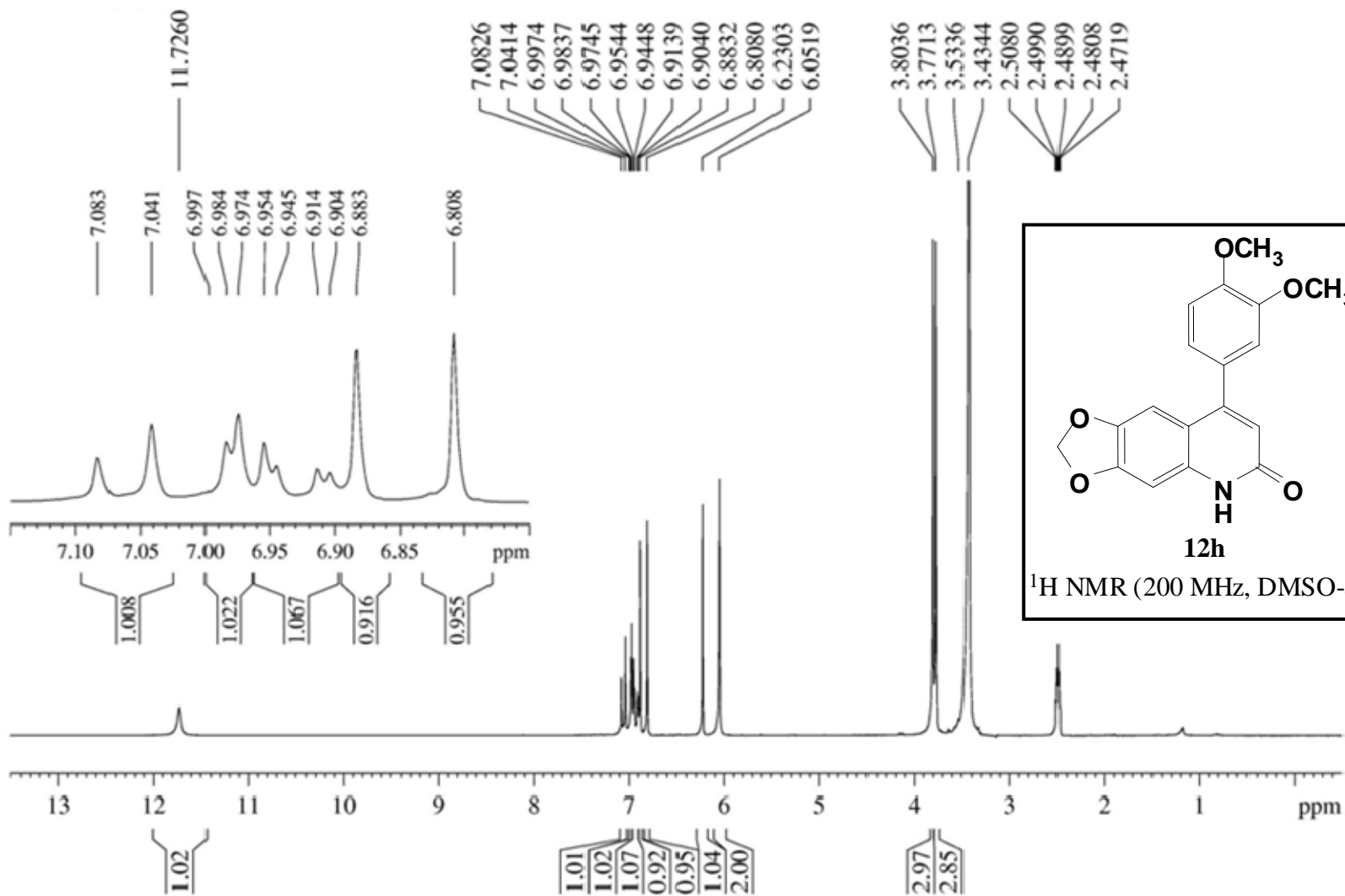


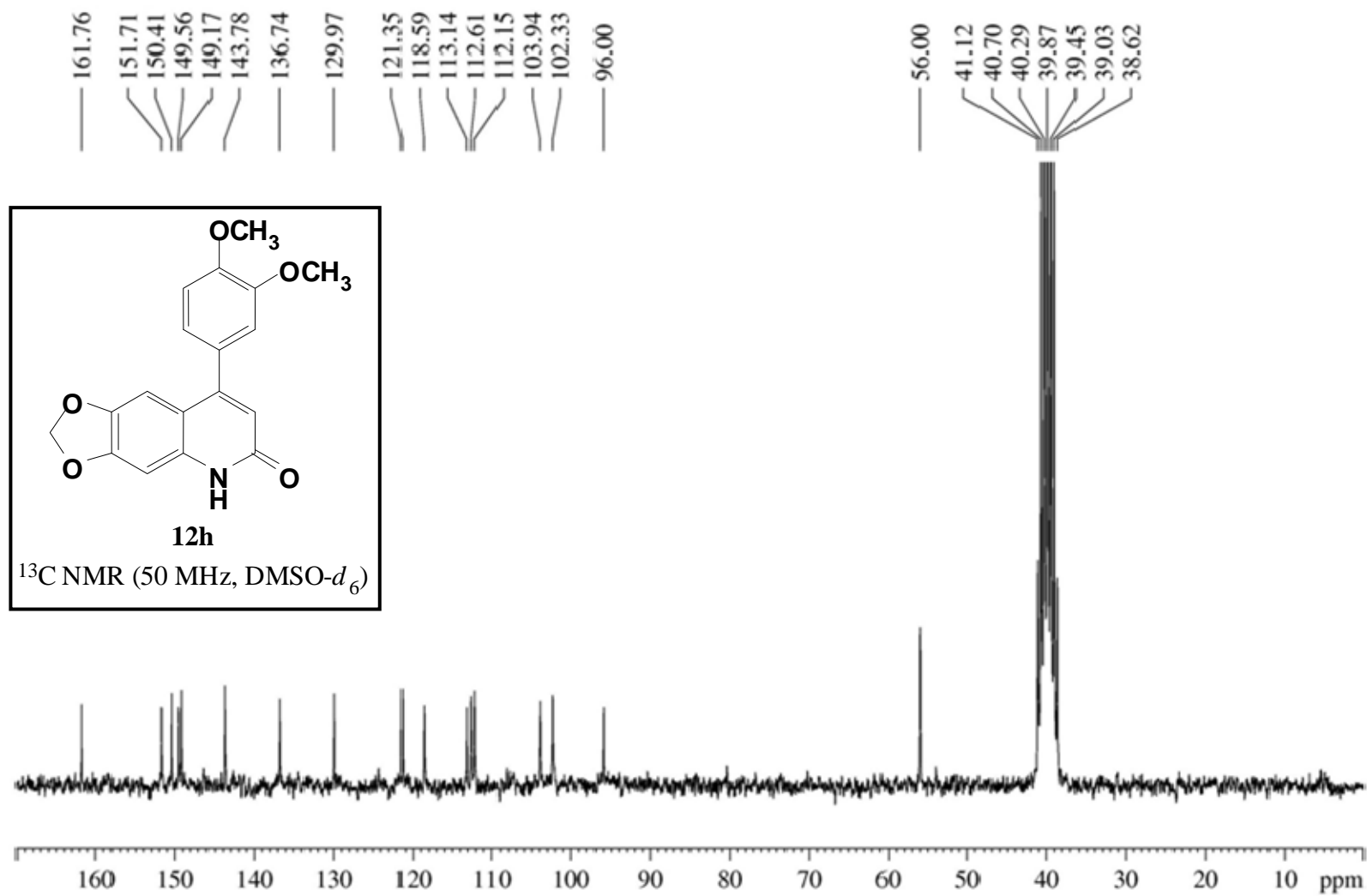


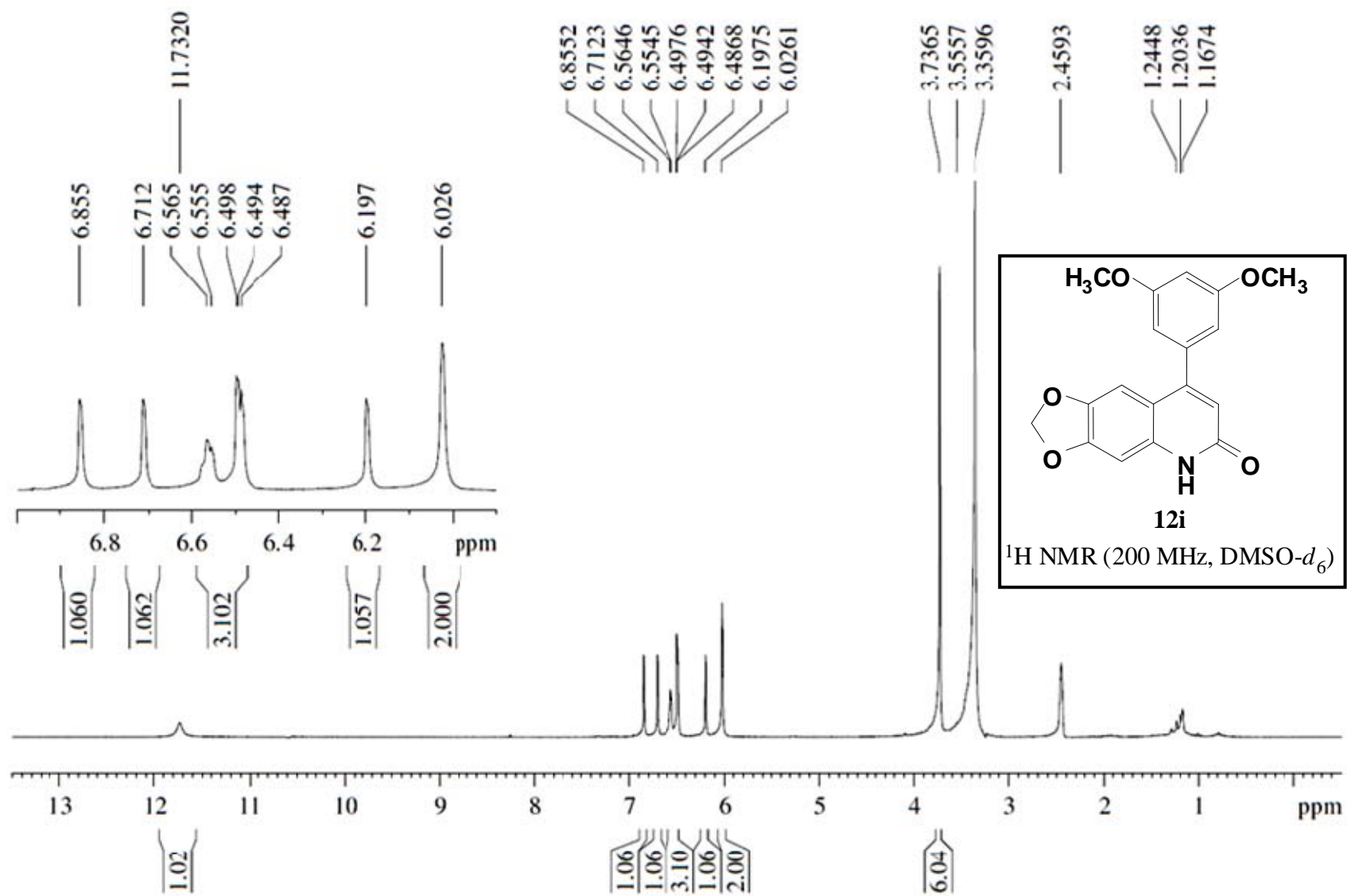




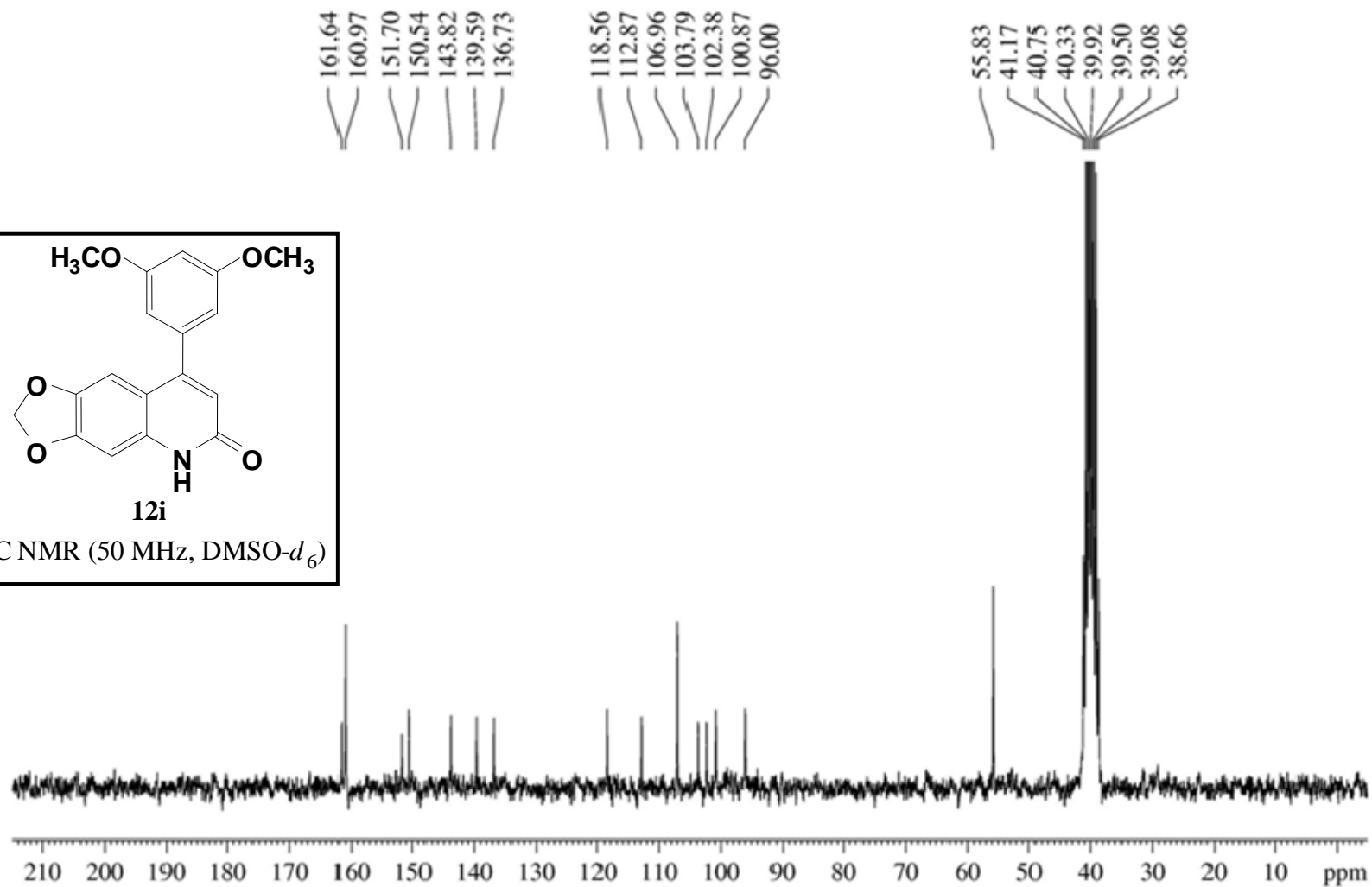
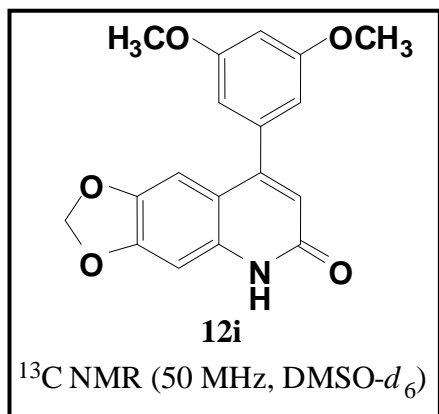


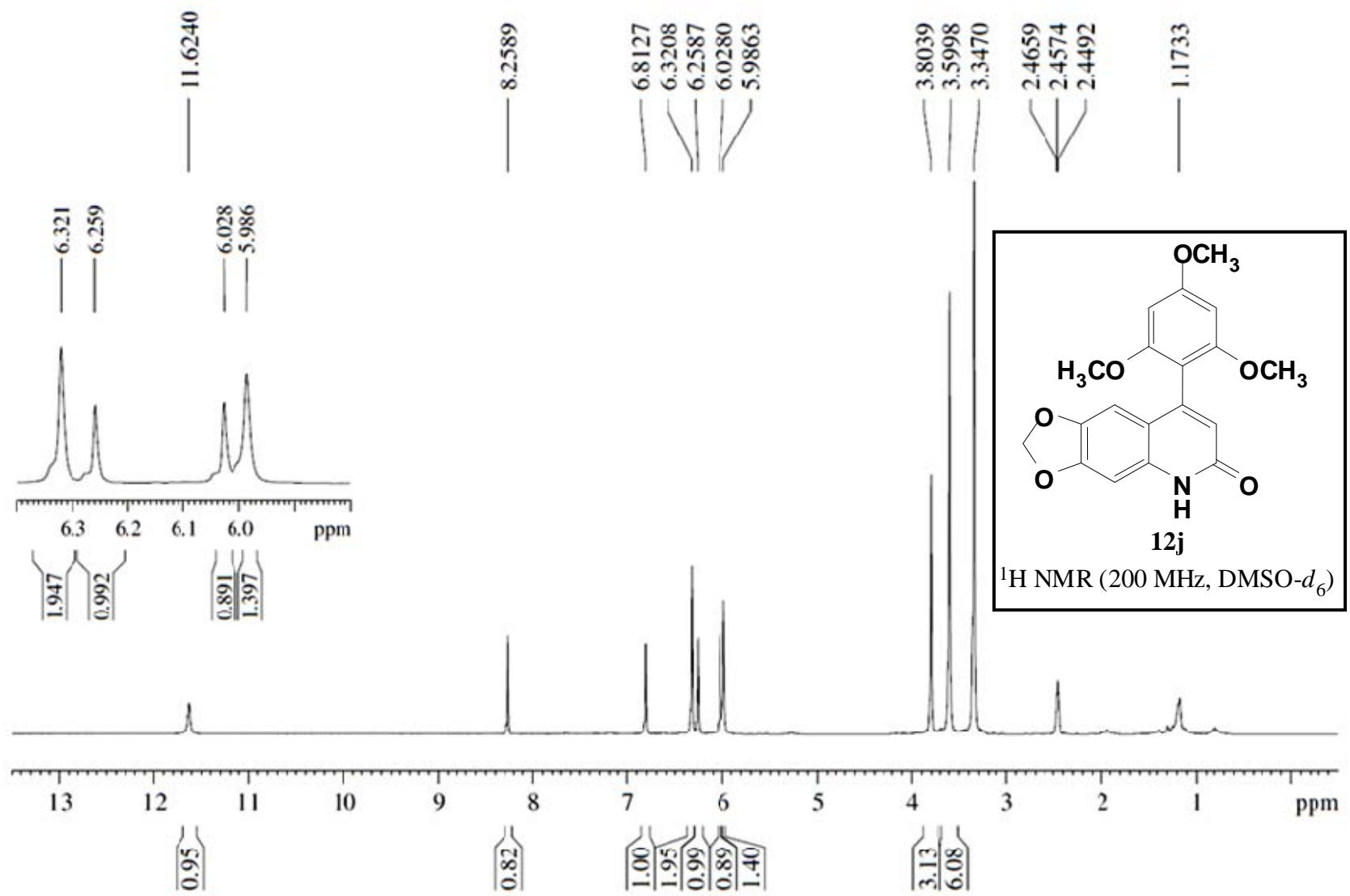


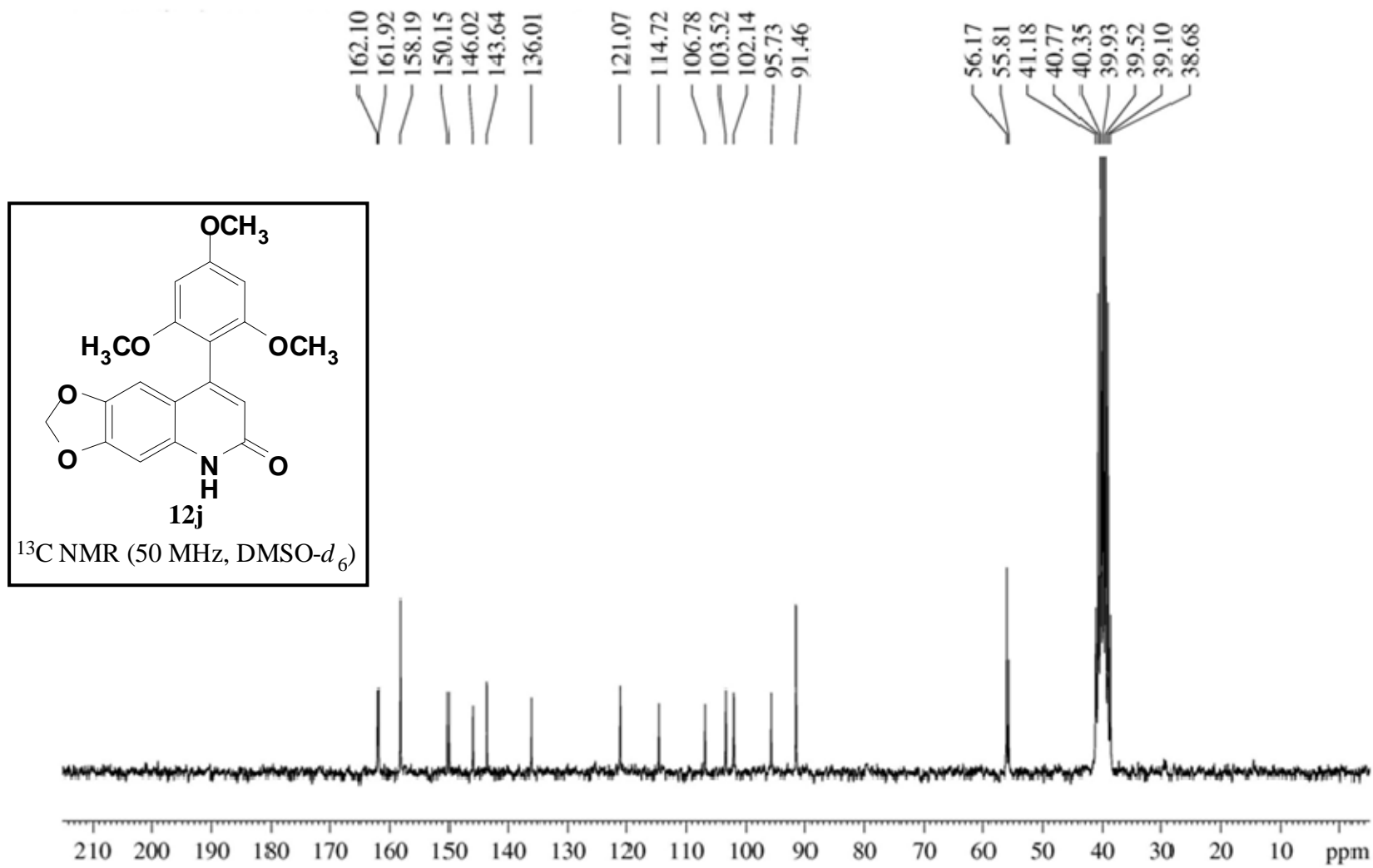


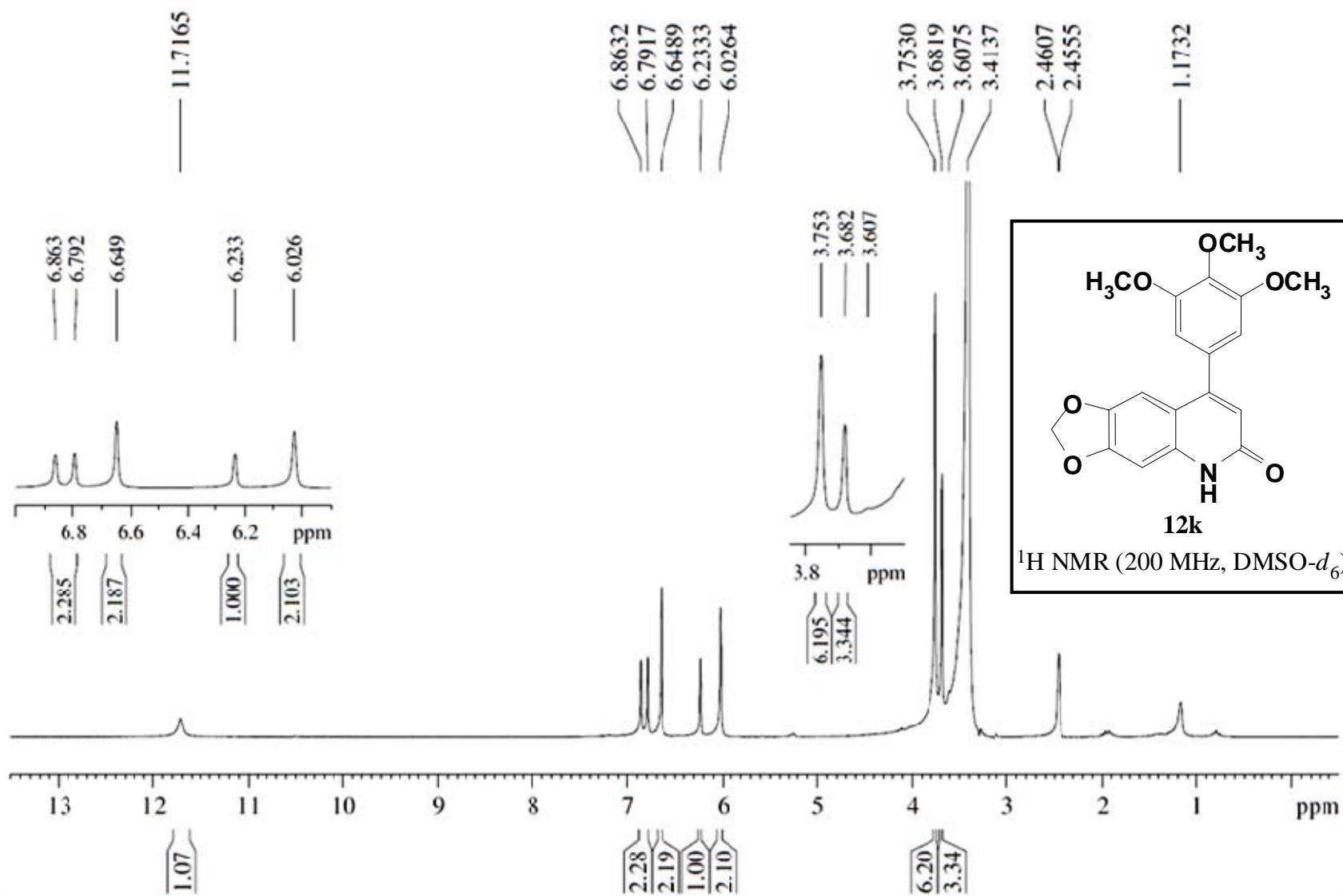


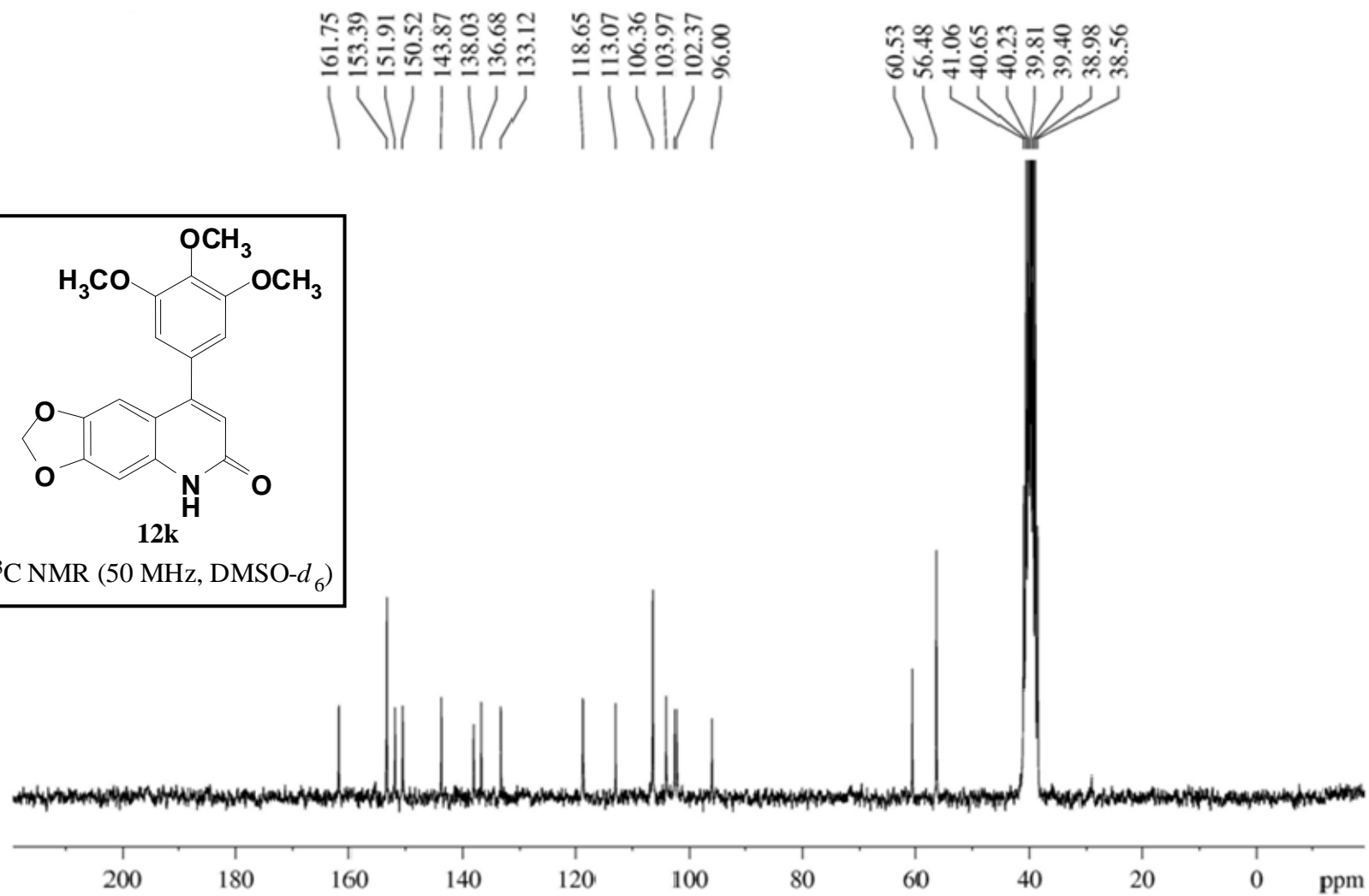
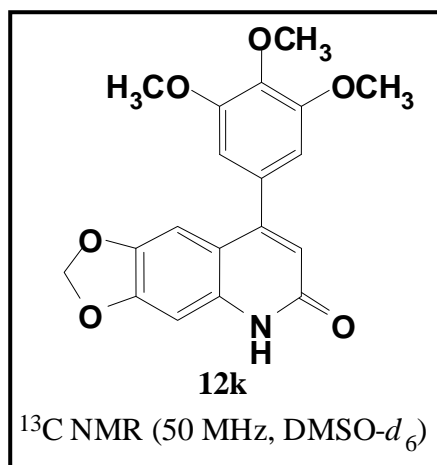


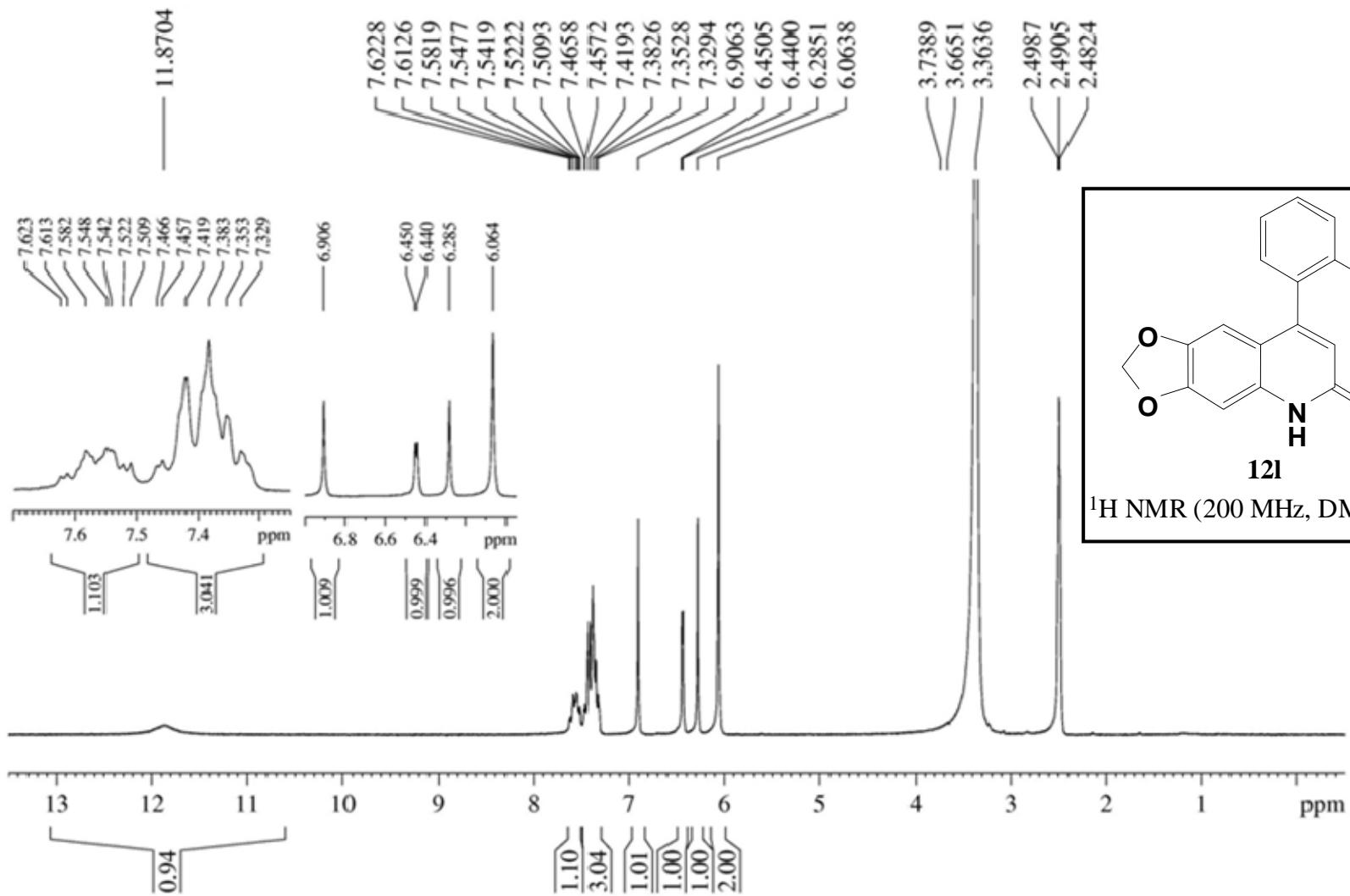


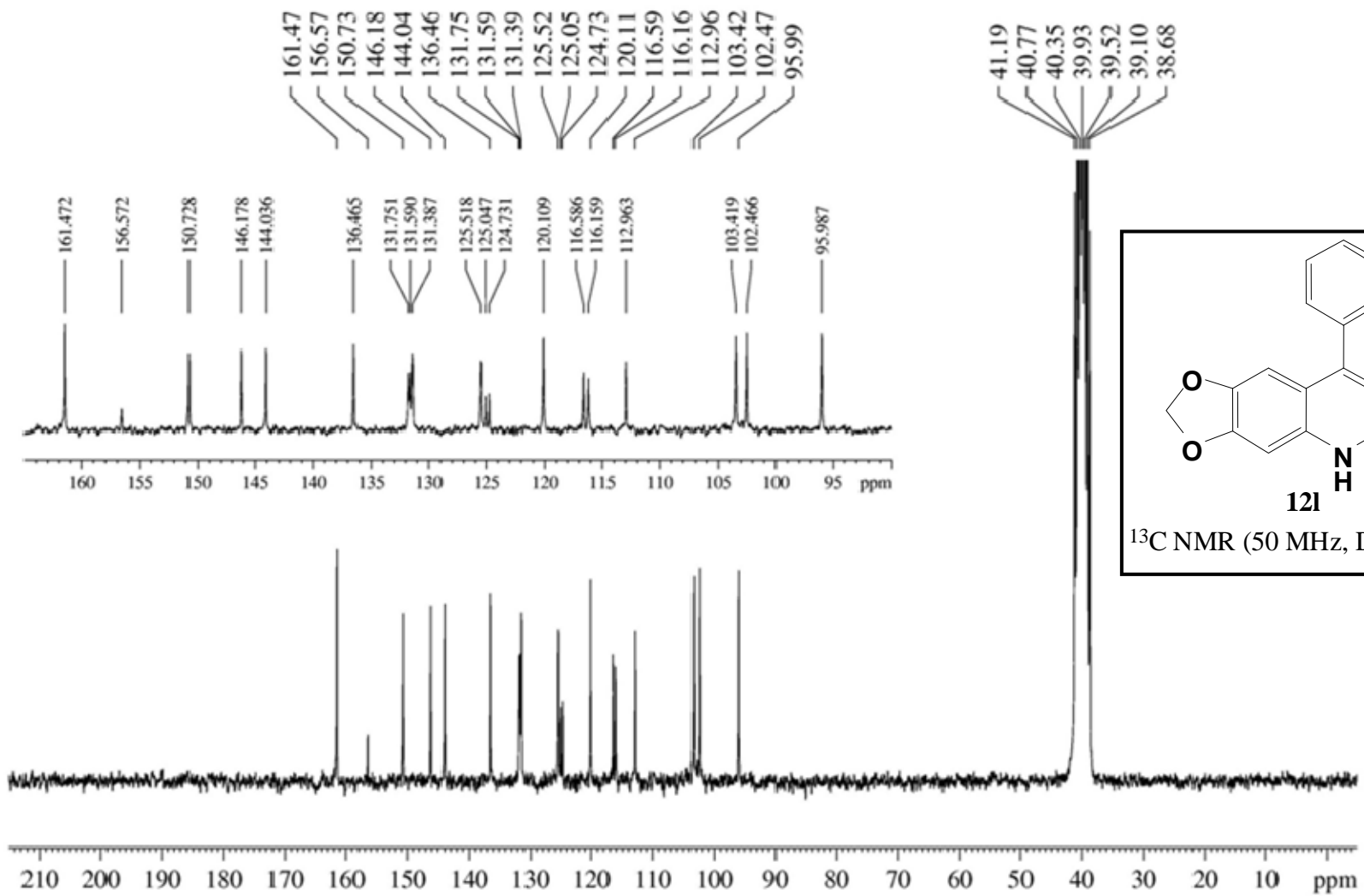


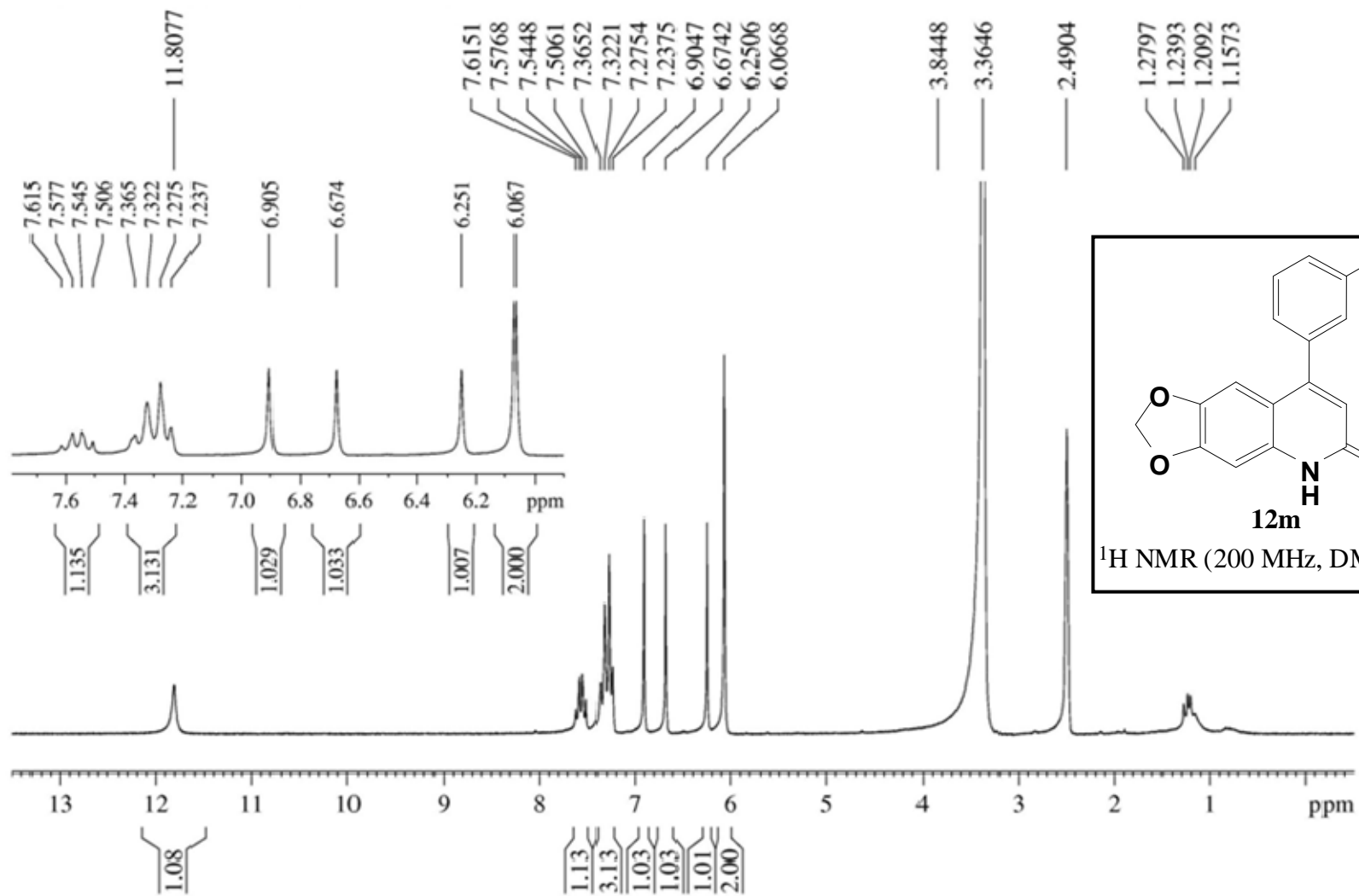




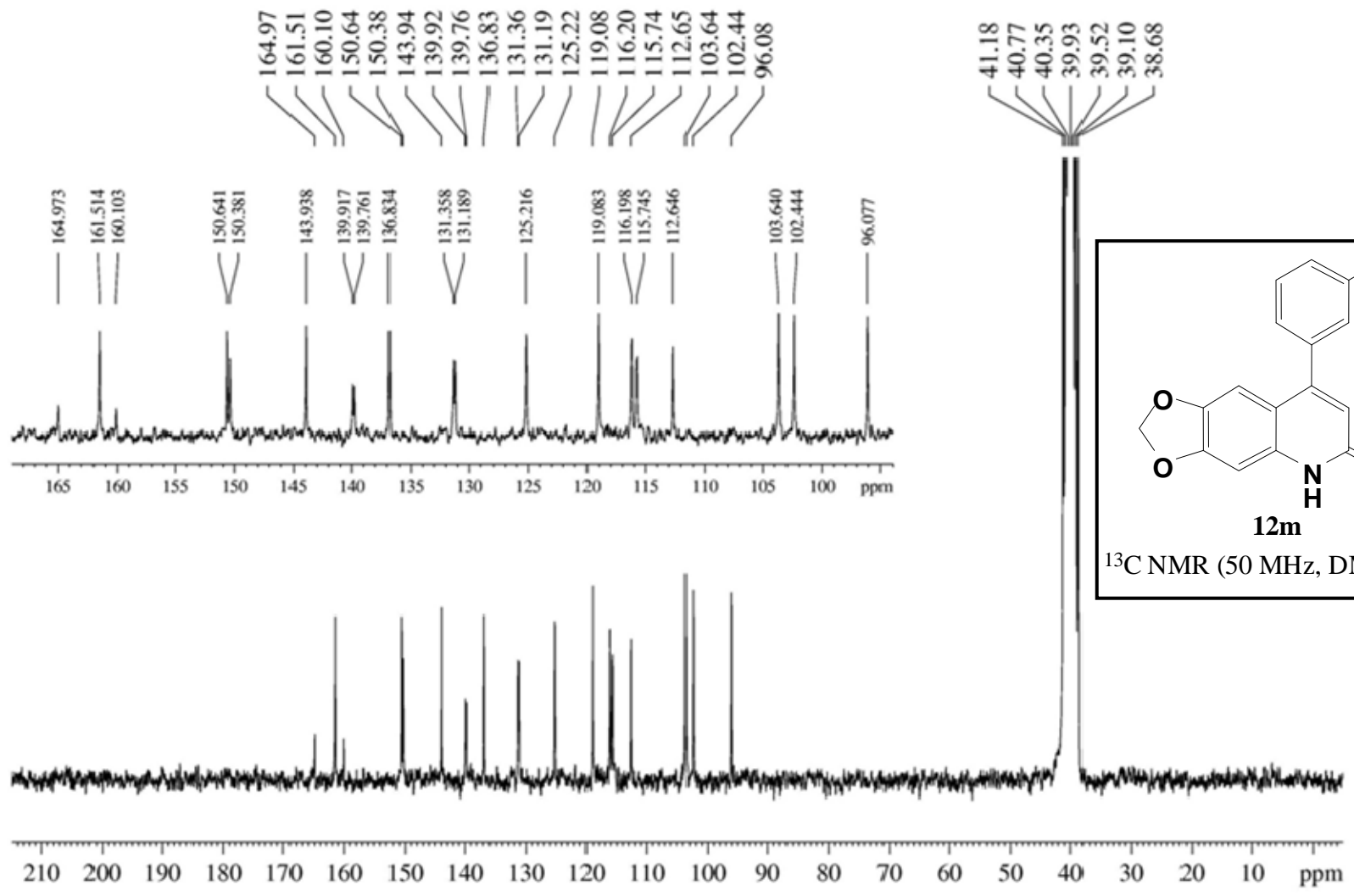


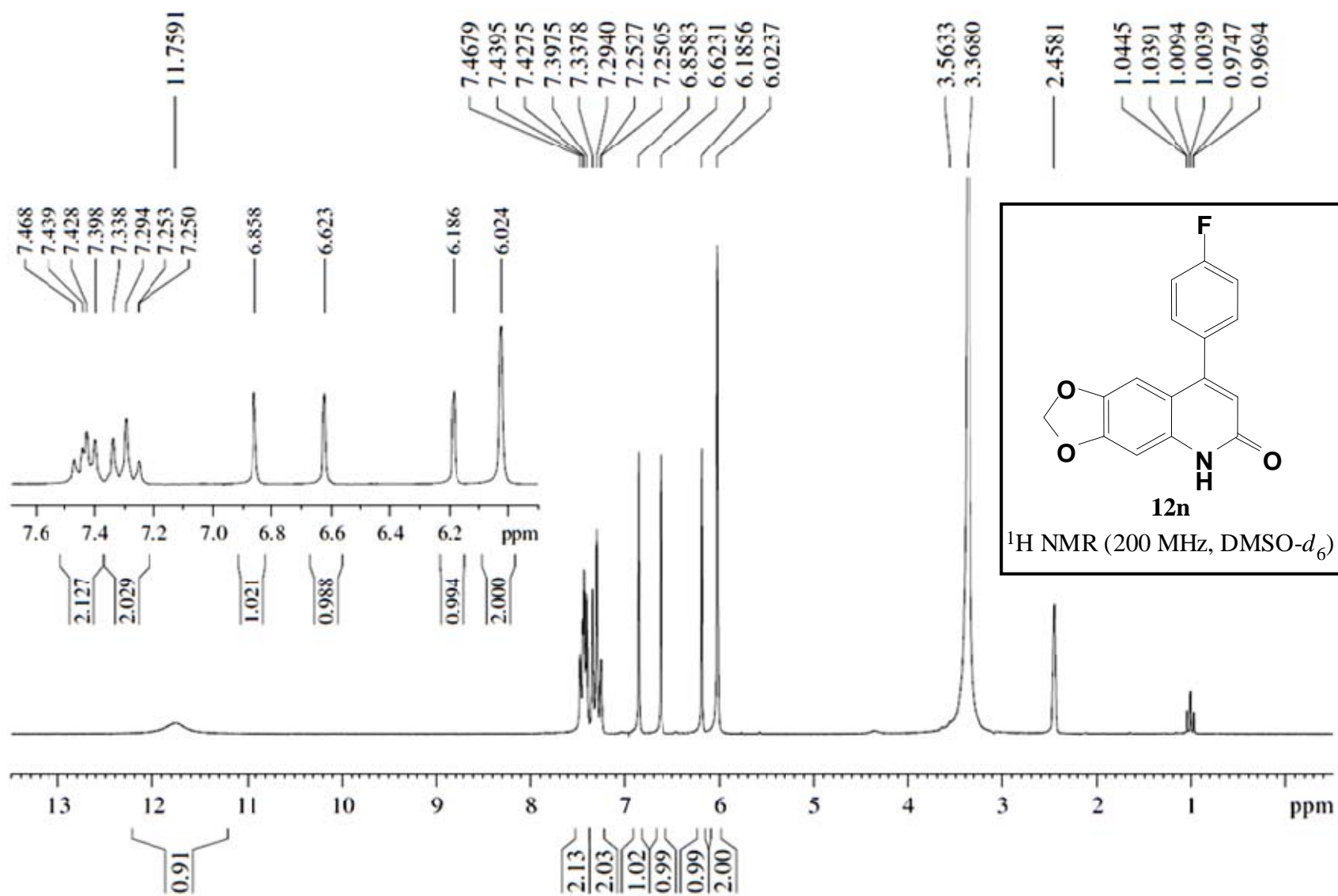


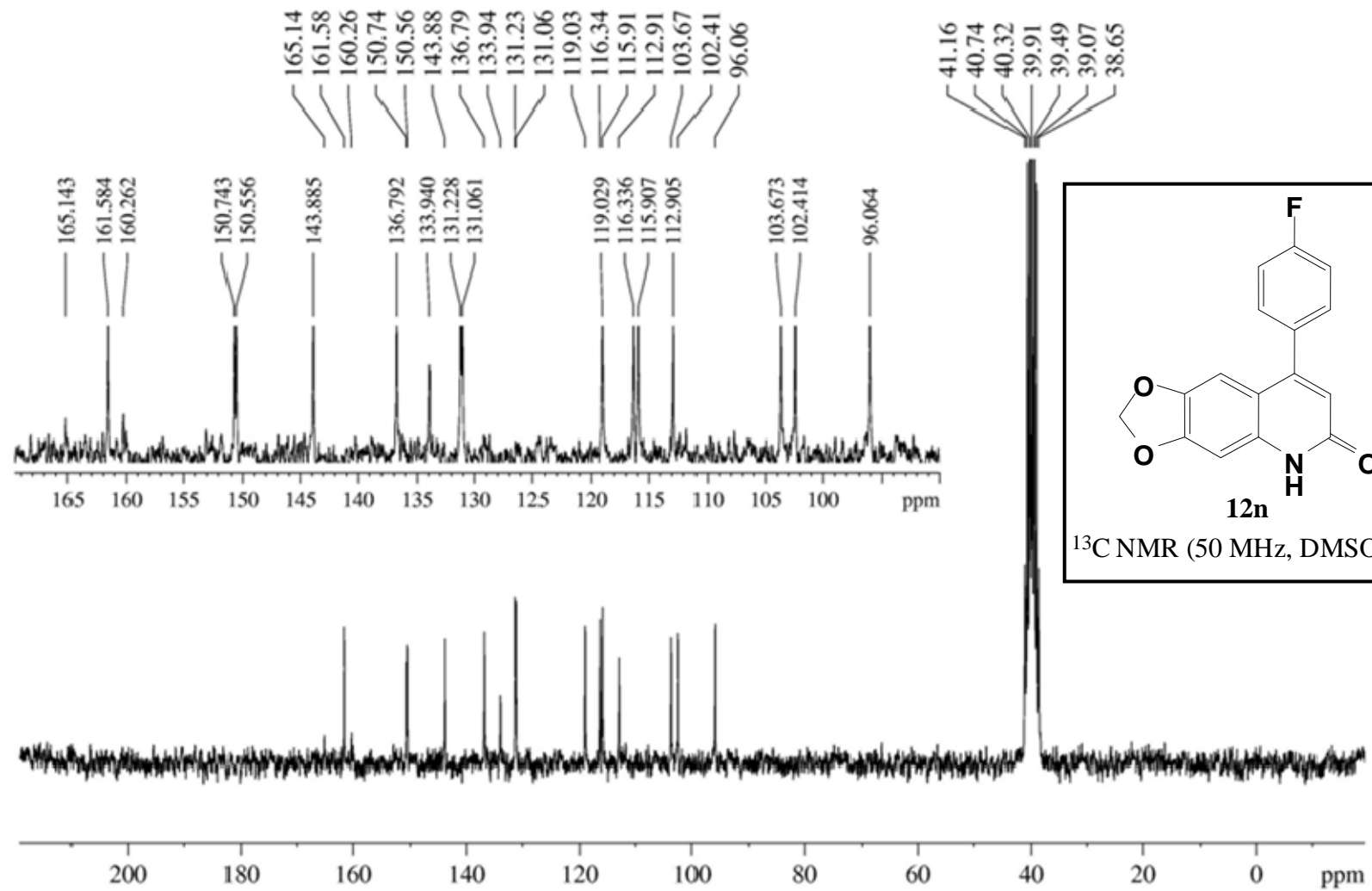






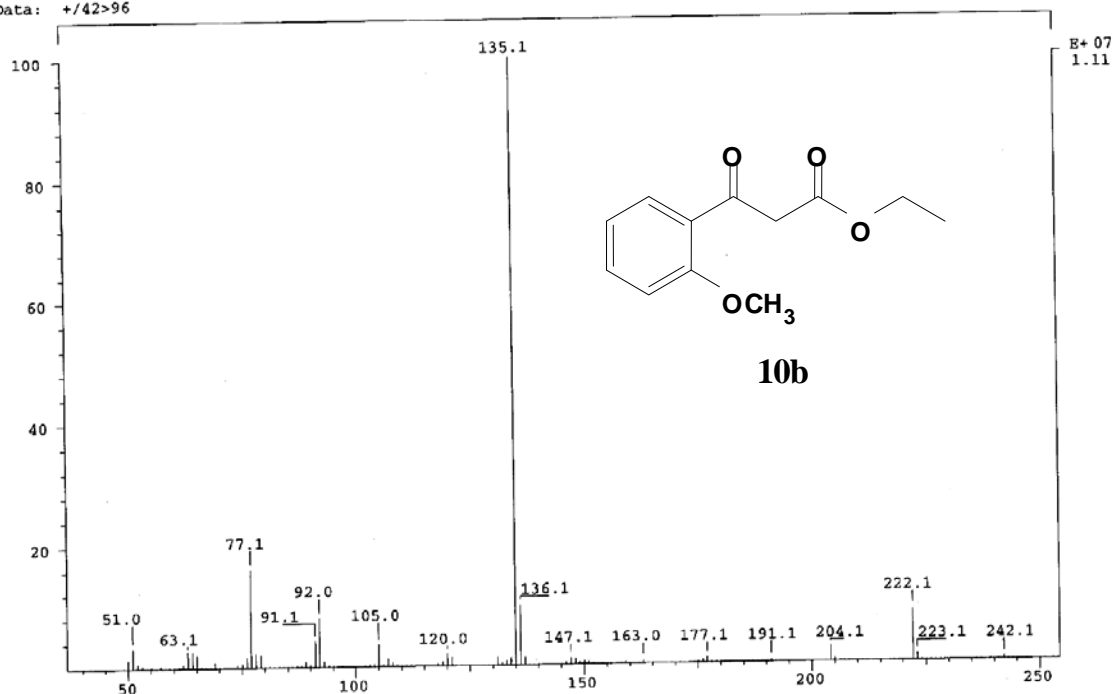






### EI-MS spectra of compound 10b.

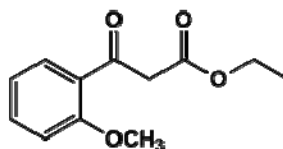
SPEC: lei7454\_hpk2c  
 REG : 01:32.2 #9  
 Samp: Start : 207  
 Mode: EI +VE +LMR BSCAN (EXP) UP LR NRM  
 Oper: Inlet :  
 Base: 135.1 Inten : 11093385 Masses: 45 > 260  
 Norm: 135.1 RIC : 23923874 #peaks: 202  
 Peak: 1000.00 mmu  
 Data: +/42>96



### HRMS spectra of compound 10b.

LIST: hei6494\_hpk2c-c1 09-Oct-12 REG : 04:14.9 #9  
 Samp: Start : 17:35:33 3918  
 Mode: EI +VE +LMR ESCAN (EXP) UP HR NRM  
 Oper: Inlet :  
 Limt: ( 0)  
 : (353) C21.H21.O5  
 Peak: 1000.00 mmu R+D: -2.0 > 60.0  
 Data: +/718>1075 (CMASS : converted |CMASS : converted |CMASS : conv

Mass	Intensity	%RA	Flags	Delta	R+D	Composition
222.0884	24320	81.18	#	0.8	6.0	C12.H14.O4



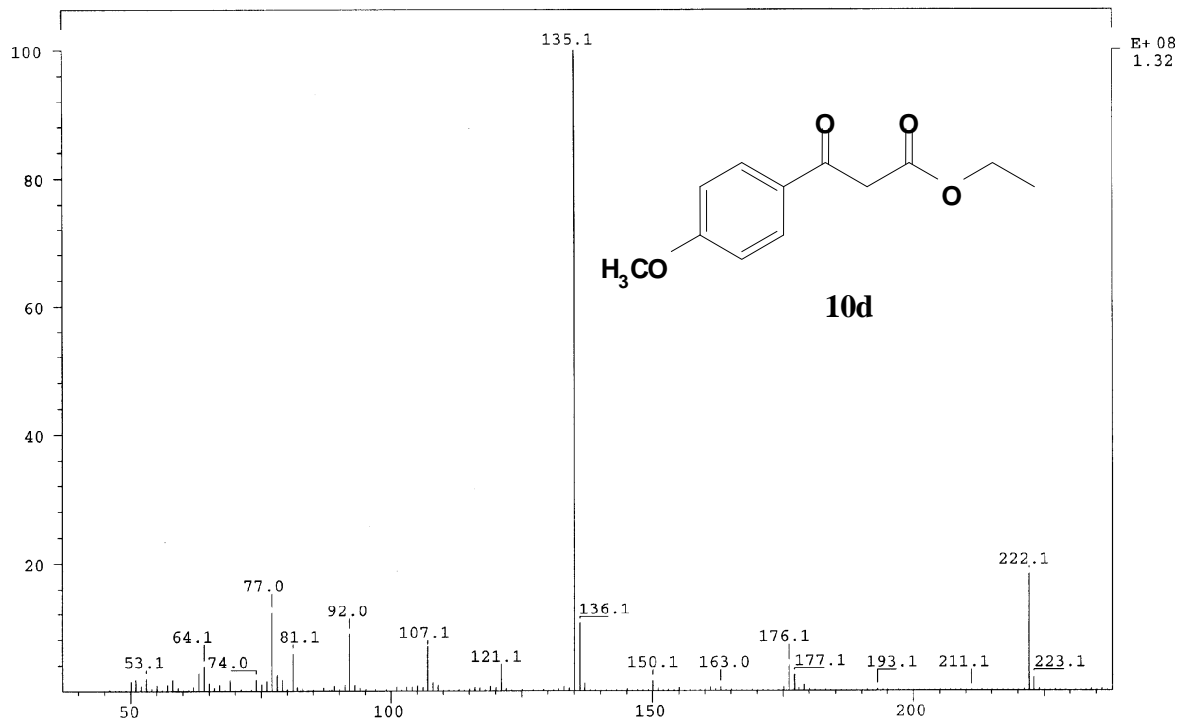
10b

calculated for C<sub>12</sub>H<sub>14</sub>O<sub>4</sub>: 222.0892;  
 found: 222.0884



### EI-MS spectra of compound 10d.

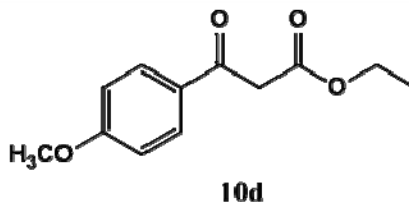
SPEC: lei7457\_hpk4c                      03-Oct-12    REG : 01:28.5    #9  
 Samp:    Start : 10:09:19    156  
 Mode: EI +VE +LMR    BSCAN (EXP) UP LR NRM  
 Oper:    Inlet :  
 Base: 135.1                                      Inten : 131912448    Masses: 45 > 260  
 Norm: 135.1                                      RIC : 316407282    #peaks: 236  
 Peak: 1000.00 mmu  
 Data: +/27>86



### HRMS spectra of compound 10d.

LIST: hei6497\_hpk4c-c2                      09-Oct-12    REG : 09:23.2    #9  
 Samp:    Start : 19:30:11    3626  
 Mode: EI +VE +LMR    ESCAN (EXP) UP HR NRM  
 Oper:    Inlet :  
 Limt: ( 0)  
       : (353) C21.H21.O5  
 Peak: 1000.00 mmu    R+D: -2.0 > 60.0  
 Data: +/1629>2320    (CMASS : converted |CMASS : converted

Mass	Intensity	%RA	Flags	Delta	R+D	Composition
222.0899	29440	100.00	#	-0.7	6.0	C12.H14.O4



calculated for C<sub>12</sub>H<sub>14</sub>O<sub>4</sub>: 222.0892:  
 found: 222.0899

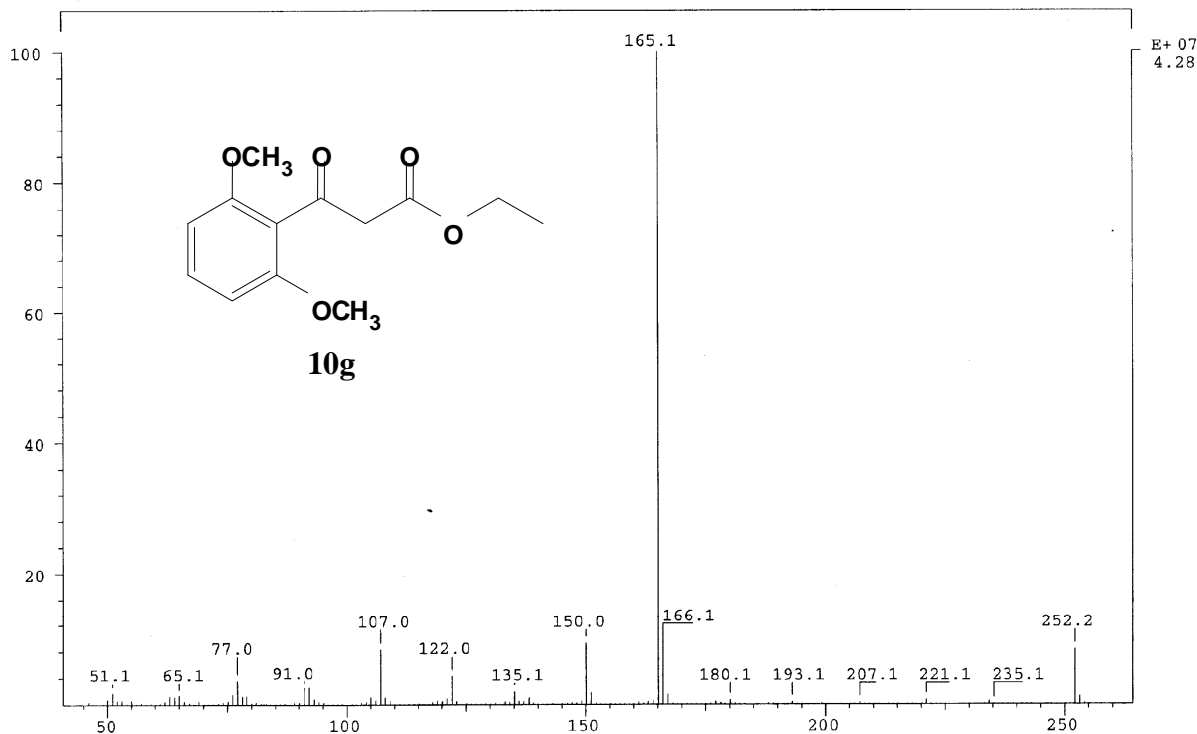






### EI-MS spectra of compound 10g.

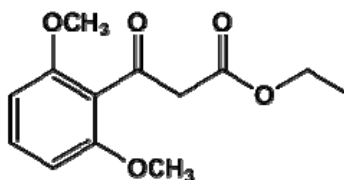
SPEC: lei7460\_hpk7c                      03-Oct-12    REG : 00:35.9    #9  
 Samp:    Start : 14:00:46    147  
 Mode: EI +VE +LMR BSCAN (EXP) UP LR NRM                      Inlet :  
 Oper:    Inten : 42829996                      Masses: 45 > 260  
 Base: 165.1                                      RIC : 84182743                      #peaks: 232  
 Norm: 165.1  
 Peak: 1000.00 mmu  
 Data: +/9>29



### HRMS spectra of compound 10g.

LIST: hei6500\_hpk7c-c4                      11-Oct-12    REG : 05:32.9    #9  
 Samp:    Start : 11:55:46    1949  
 Mode: EI +VE +LMR ESCAN (EXP) UP HR NRM                      Inlet :  
 Oper:    Inten :  
 Limt: ( 0)  
 : (353) C21.H21.O5  
 Peak: 1000.00 mmu    R+D: -2.0 > 60.0  
 Data: +/980>1309 (CMASS : converted |CMASS : converted |CMASS : conv

Mass	Intensity	%RA	Flags	Delta	R+D	Composition
252.1006	935245	100.00	#	-0.8	6.0	C13.H16.O5

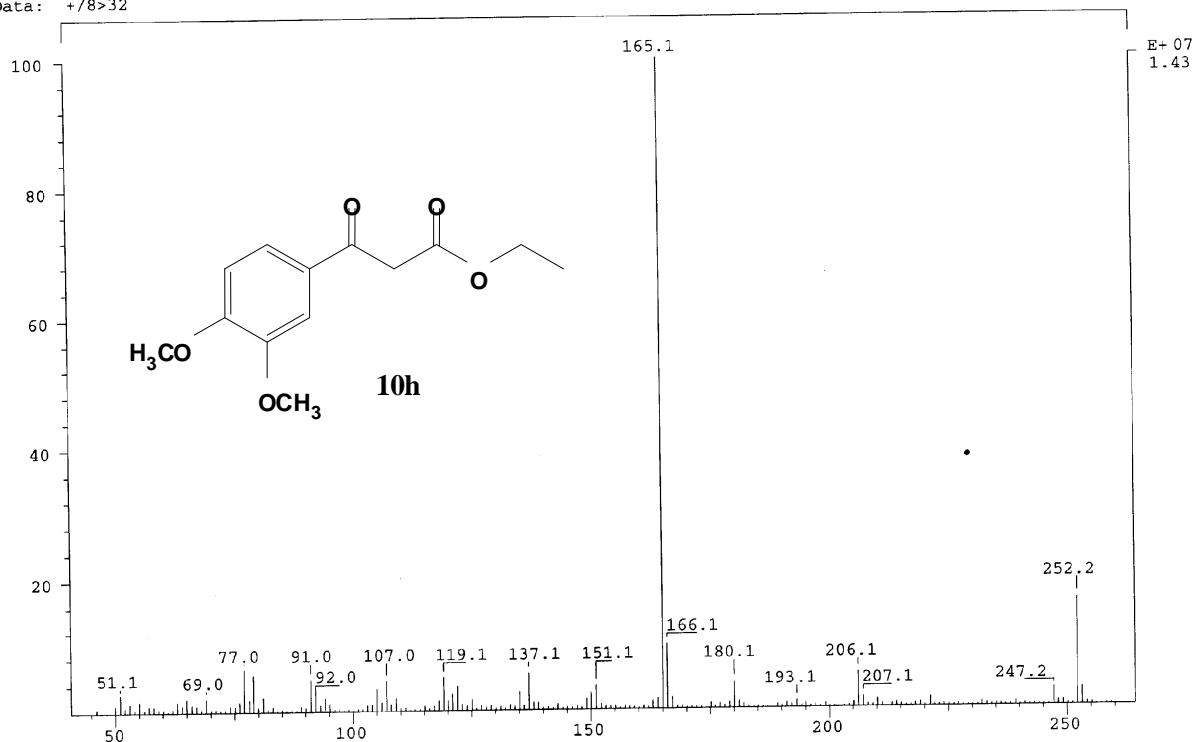


10g

calculated for C<sub>13</sub>H<sub>16</sub>O<sub>5</sub> : 252.0998;  
 found: 252.1006

### EI-MS spectra of compound 10h.

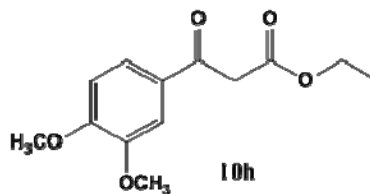
SPEC: lei7461\_hpk8c                      03-Oct-12    REG : 00:29.9       #9  
 Samp:    Start : 14:29:21    174  
 Mode: EI +VE +LMR    BSCAN (EXP) UP LR NRM  
 Oper:    Inlet :  
 Base: 165.1                                      Inten : 14331549    Masses: 45 > 260  
 Norm: 165.1                                      RIC : 43370973     #peaks: 236  
 Peak: 1000.00    mmu  
 Data: +/8>32



### HRMS spectra of compound 10h.

LIST: hei6501\_hpk8c-c3                      11-Oct-12    REG : 02:32.1       #9  
 Samp:    Start : 13:48:43    2368  
 Mode: EI +VE +LMR    ESCAN (EXP) UP HR NRM  
 Oper:    Inlet :  
 Limt: ( 0)  
       : (366) C21.H34.O5  
 Peak: 1000.00    mmu    R+D: -2.0 > 60.0  
 Data: +/448>721    (CMASS : converted |CMASS : converted |CMASS : conve

Mass	Intensity	%RA	Flags	Delta (mmu)	R+D	Composition
252.1003	3733939	100.00	#	-0.6	6.0	C13.H16.O5

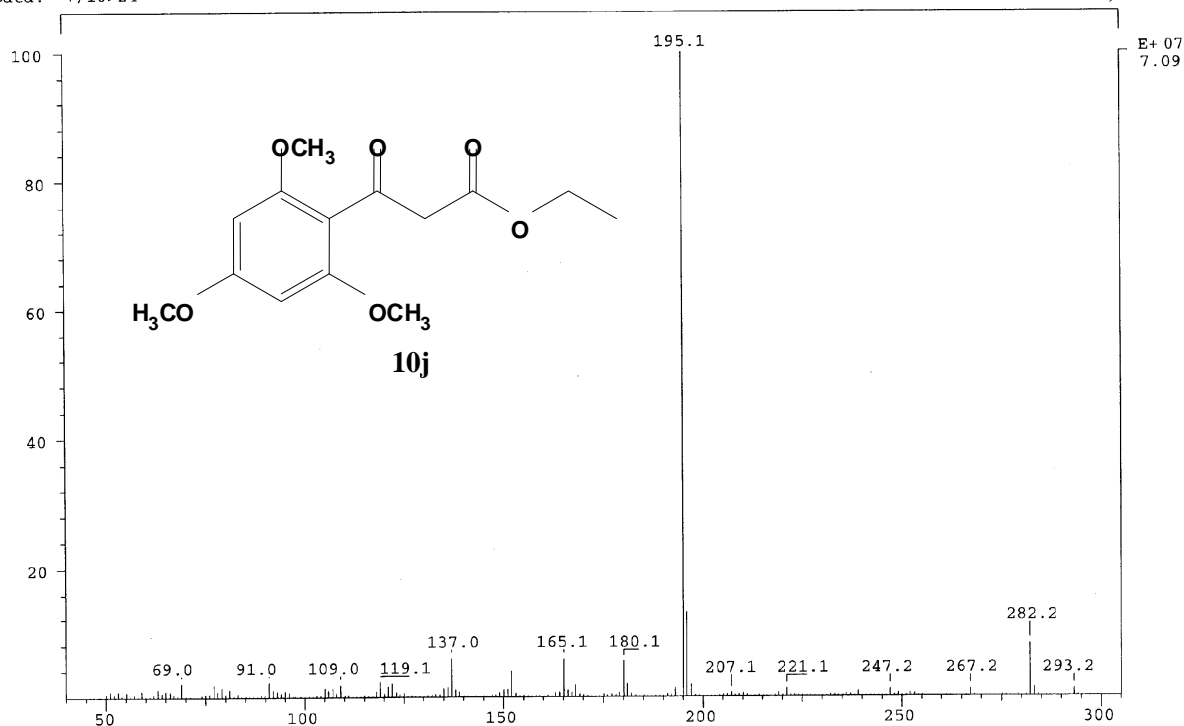


calculated for C<sub>13</sub>H<sub>16</sub>O<sub>5</sub> : 252.0998;  
 found: 252.1003



### EI-MS spectra of compound 10j.

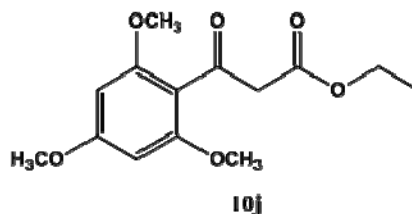
SPEC: lei7463\_hpkl0c                      03-Oct-12    REG : 00:35.8    #9  
 Samp:    Start : 15:30:53    108  
 Mode: EI +VE +LMR BSCAN (EXP) UP LR NRM  
 Oper:    Inlet :  
 Base: 195.1                                      Inten : 70878328    Masses: 45 > 300  
 Norm: 195.1                                      RIC : 164875549    #peaks: 255  
 Peak: 1000.00 mmu  
 Data: +/10>24



### HRMS spectra of compound 10j.

LIST: hei6503\_hpkl0c-c2                      11-Oct-12    REG : 04:23.6    #9  
 Samp:    Start : 14:51:03    1925  
 Mode: EI +VE +LMR ESCAN (EXP) UP HR NRM  
 Oper:    Inlet :  
 Limt: ( 0)  
       : (414) C21.H34.O8  
 Peak: 1000.00 mmu    R+D: -2.0 > 60.0  
 Data: +/820>1001 (CMASS : converted |CMASS : converted |CMASS : conv

Mass	Intensity	%RA	Flags	Delta	R+D	Composition
282.1106	26813	14.05	#	-0.3	6.0	C14.H18.O6

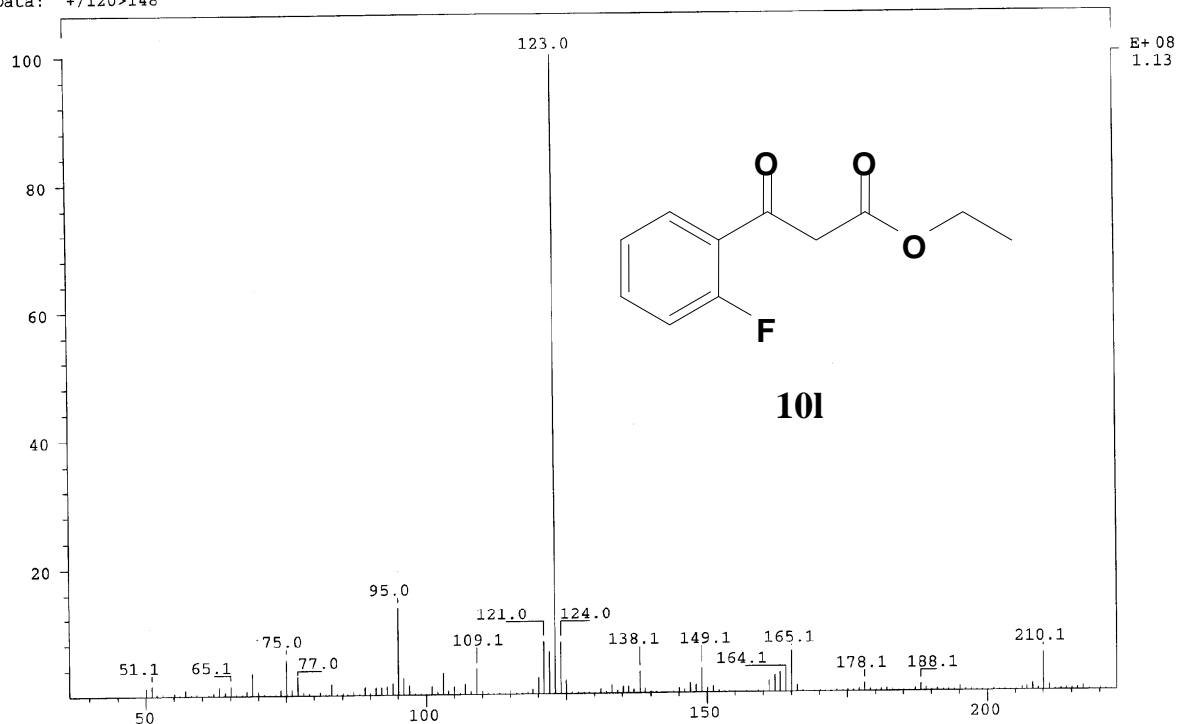


calculated for C<sub>14</sub>H<sub>18</sub>O<sub>6</sub>: 282.1103;  
 found: 282.1106



### EI-MS spectra of compound 101.

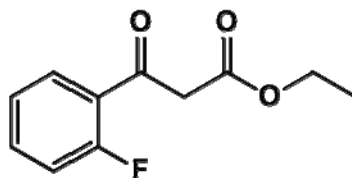
SPEC: lei7465\_hpk12c  
 03-Oct-12 REG : 07:04.7 #9  
 Samp: Start : 16:13:26 183  
 Mode: EI +VE +LMR BSCAN (EXP) UP LR NRM  
 Oper: Inlet :  
 Base: 123.0 Inten : 112560760 Masses: 45 > 300  
 Norm: 123.0 RIC : 300463964 #peaks: 322  
 Peak: 1000.00 mmu  
 Data: +/120>148



### HRMS spectra of compound 101.

LIST: hei6505\_hpk12c-c3 11-Oct-12 REG : 02:05.6 #9  
 Samp: Start : 16:10:51 1099  
 Mode: EI +VE +LMR ESCAN (EXP) UP HR NRM  
 Oper: Inlet :  
 Limt: ( 0)  
 : (248) C12.H21.F.O4  
 Peak: 1000.00 mmu R+D: -2.0 > 60.0  
 Data: +/309>438 (CMASS : converted; CMASS : converted; CMASS : conve

Mass	Intensity	%RA	Flags	Delta	R+D	Composition
210.0700	46234	100.00	#	-0.8	6.0	C11.H11.F.O3

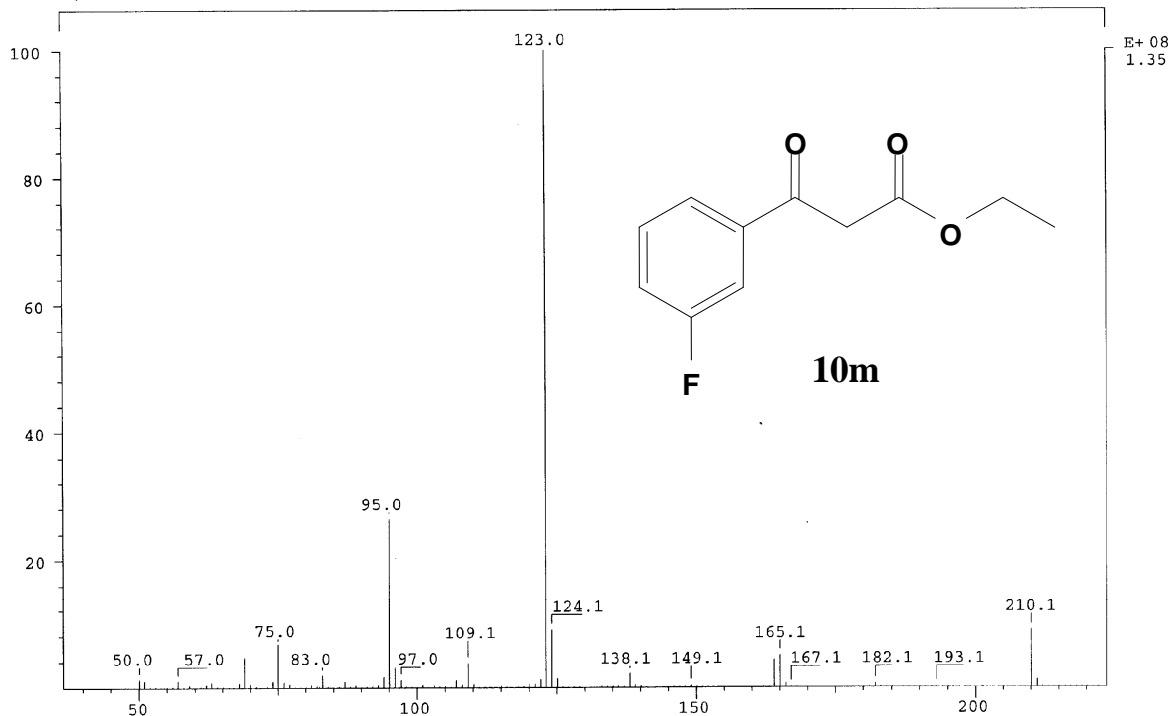


**101**

calculated for  $C_{11}H_{11}FO_3$  : 210.0692:  
 found: 210.0700

### EI-MS spectra of compound 10m.

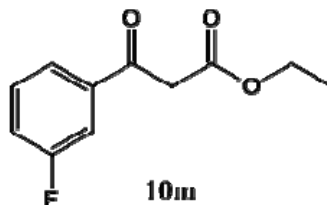
SPEC: lei7466\_hp13c                      03-Oct-12    REG : 00:25.4    #9  
 Samp:    Start : 16:30:55    49  
 Mode: EI +VE +LMR BSCAN (EXP) UP LR NRM  
 Oper:    Inlet :  
 Base: 123.0                                      Inten : 135011312    Masses: 45 > 300  
 Norm: 123.0                                      RIC : 280353385    #peaks: 276  
 Peak: 1000.00 mmu  
 Data: +/6>11



### HRMS spectra of compound 10m.

LIST: hei6506\_hp13c-c3                      11-Oct-12    REG : 09:38.4    #9  
 Samp:    Start : 16:40:57    1579  
 Mode: EI +VE +LMR ESCAN (EXP) UP HR NRM  
 Oper:    Inlet :  
 Limt: ( 19)                                      .F.  
       : (372) C21.H21.F.O5  
 Peak: 1000.00 mmu                              R+D: -2.0 > 60.0  
 Data: +/1433>1537 (CMASS : converted |CMASS : converted |CMASS : con

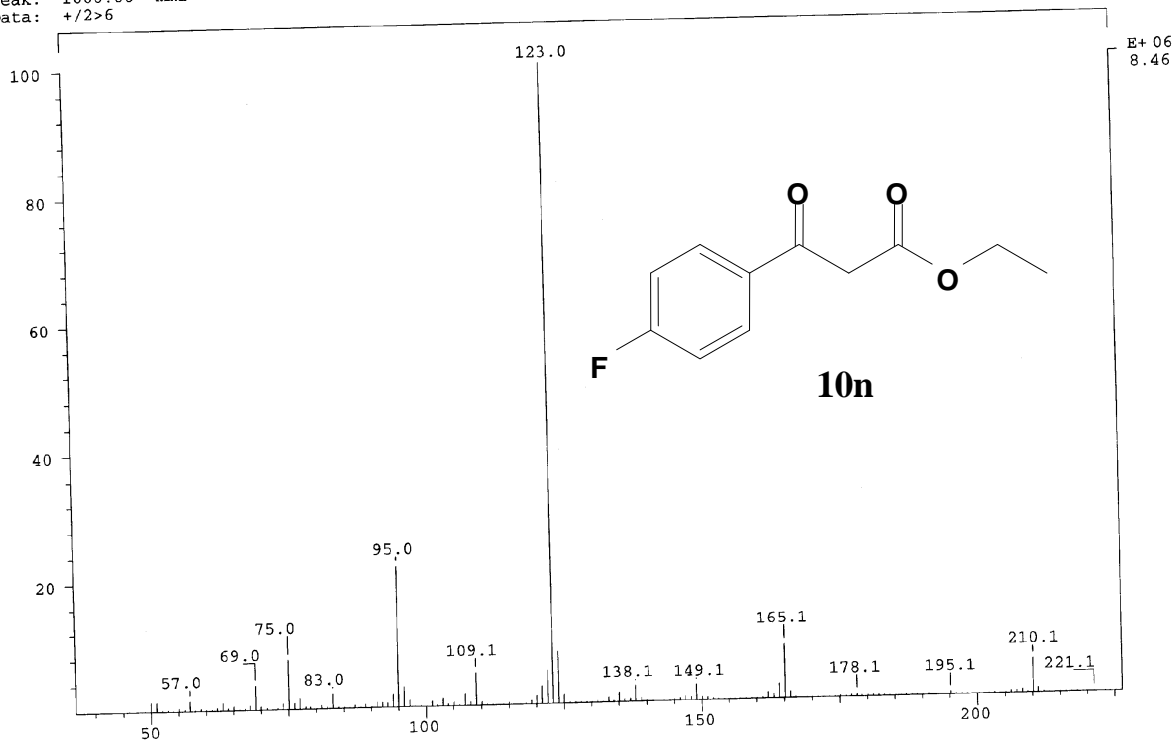
Mass	Intensity	%RA	Flags	Delta	R+D	Composition
210.0695	9211	62.88	#	-0.3	6.0	C11.H11.F.O3



calculated for C<sub>11</sub>H<sub>11</sub>FO<sub>3</sub> : 210.0692:  
 found: 210.0695

### EI-MS spectra of compound 10n.

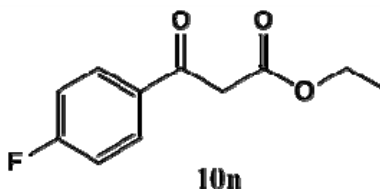
SPEC: lei7467\_hpkl4c  
 03-Oct-12 REG : 00:11.5 #9  
 Start : 17:03:15 30  
 Samp: Mode: EI +VE +LMR BSCAN (EXP) UP LR NRM  
 Oper: Inlet :  
 Base: 123.0 Inten : 8461338 Masses: 45 > 300  
 Norm: 123.0 RIC : 19788048 #peaks: 262  
 Peak: 1000.00 mmu  
 Data: +/2>6



### HRMS spectra of compound 10n.

LIST: hei6507\_hpkl4c-cl 11-Oct-12 REG : 07:21.5 #9  
 Start : 19:48:24 2498  
 Samp: Mode: EI +VE +LMR ESCAN (EXP) UP HR NRM  
 Oper: Inlet :  
 Limit: ( 19) .F.  
 : (372) C21.H21.F.O5  
 Peak: 1000.00 mmu R+D: -2.0 > 60.0  
 Data: +/1093>1187 (CMASS : converted |CMASS : converted |CMASS : con

Mass	Intensity	%RA	Flags	Delta (mmu)	R+D	Composition
210.0701	21808	100.00	#	-0.9	6.0	C11.H11.F.O3

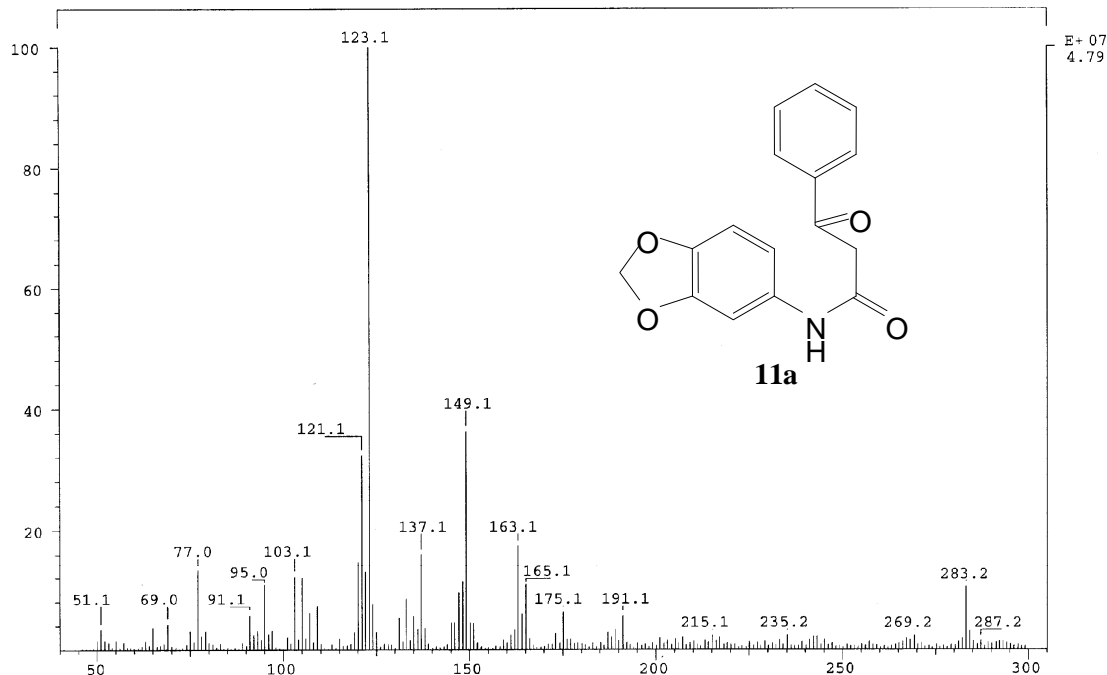


calculated for C<sub>11</sub>H<sub>11</sub>FO<sub>3</sub> : 210.0692;  
 found: 210.0701



### EI-MS spectra of compound 11a.

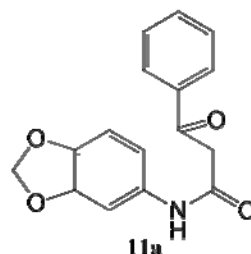
SPEC: lei7468\_hpk2e 04-Oct-12 REG : 04:36.9 #9  
 Samp: Start : 09:00:49 216  
 Mode: EI +VE +LMR BSCAN (EXP) UP LR NRM  
 Oper: Inlet :  
 Base: 123.1 Inten : 47884352 Masses: 45 > 300  
 Norm: 123.1 RTC : 310804439 #peaks: 458  
 Peak: 1000.00 mmu  
 Data: +/79>127



### HRMS spectra of compound 11a.

LIST: hei6489\_hpk2e-c2 09-Oct-12 REG : 03:59.9 #9  
 Samp: Start : 14:40:45 5998  
 Mode: EI +VE +LMR ESCAN (EXP) UP HR NRM  
 Oper: Inlet :  
 Limit: ( 0)  
 : (322) C17.H21.N.F.O4  
 Peak: 1000.00 mmu R+D: -2.0 > 60.0  
 Data: +/745>848 (CMASS : converted |CMASS : converted |CMASS : conve

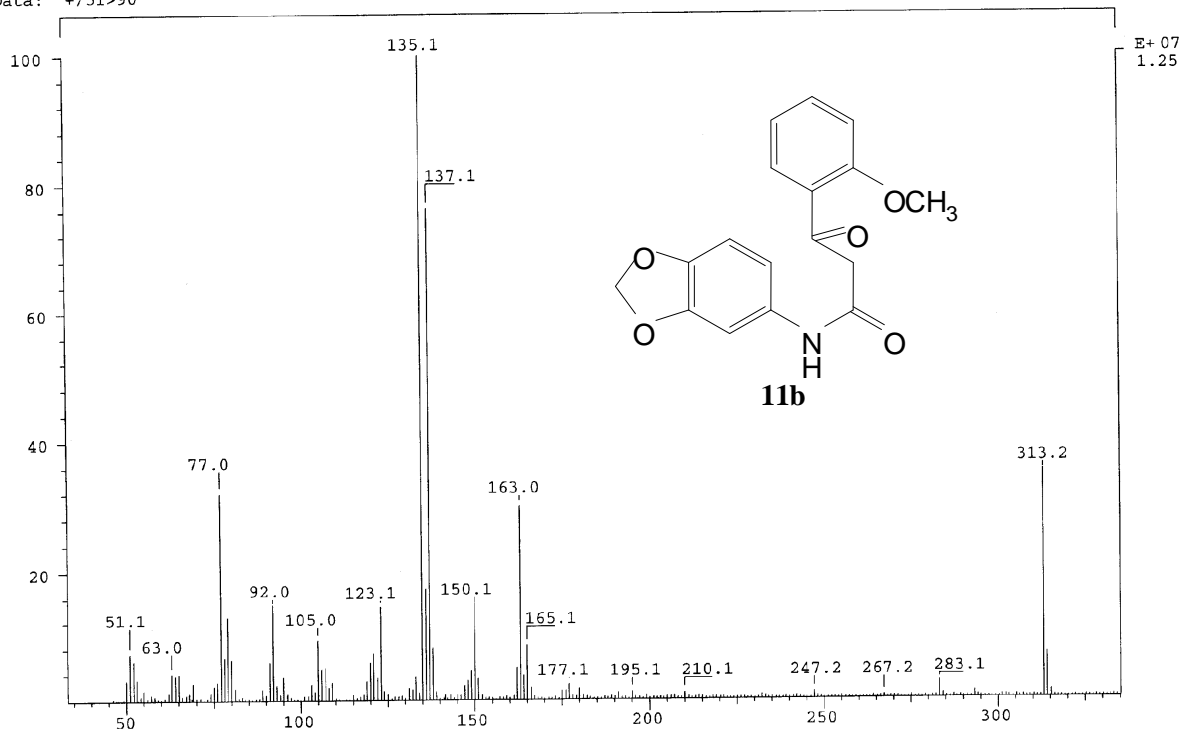
Mass	Intensity	%RA	Flags	Delta	R+D	Composition
283.0836	9348	45.00	#	0.8	11.0	C16.H13.N.O4



calculated for C<sub>16</sub>H<sub>13</sub>NO<sub>4</sub>: 283.0845;  
 found: 283.0836

### EI-MS spectra of compound **11b**.

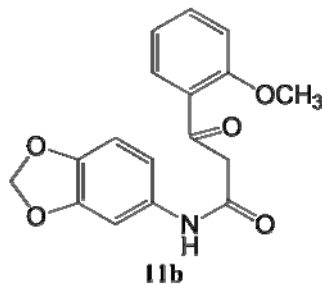
SPEC: lei7469\_hpk3e                      04-Oct-12    REG : 03:12.7    #9  
 Samp:    Start : 09:42:46    177  
 Mode: EI +VE +LMR BSCAN (EXP) UP LR NRM                      Inlet :  
 Oper:    Masses: 45 > 350  
 Base: 135.1                                      Inten : 12457353                      #peaks: 403  
 Norm: 135.1                                      RIC : 77023609  
 Peak: 1000.00 mmu  
 Data: +/51>90



### HRMS spectra of compound **11b**.

LIST: hei6467\_hpk3e-c6                      08-Oct-12    REG : 15:00.7    #9  
 Samp:    Start : 10:10:56    3460  
 Mode: EI +VE +LMR ESCAN (EXP) UP HR NRM                      Inlet :  
 Oper:      
 Limt: ( 0)  
 : (411) C22.H21.N.O7  
 Peak: 1000.00 mmu                      R+D: -2.0 > 60.0  
 Data: +/2845>3148                      (CMASS : converted; CMASS : con

Mass	Intensity	%RA	Flags	Delta	R+D	Composition
313.0959	1294	17.80	#	-0.8	11.0	C17.H15.N.O5

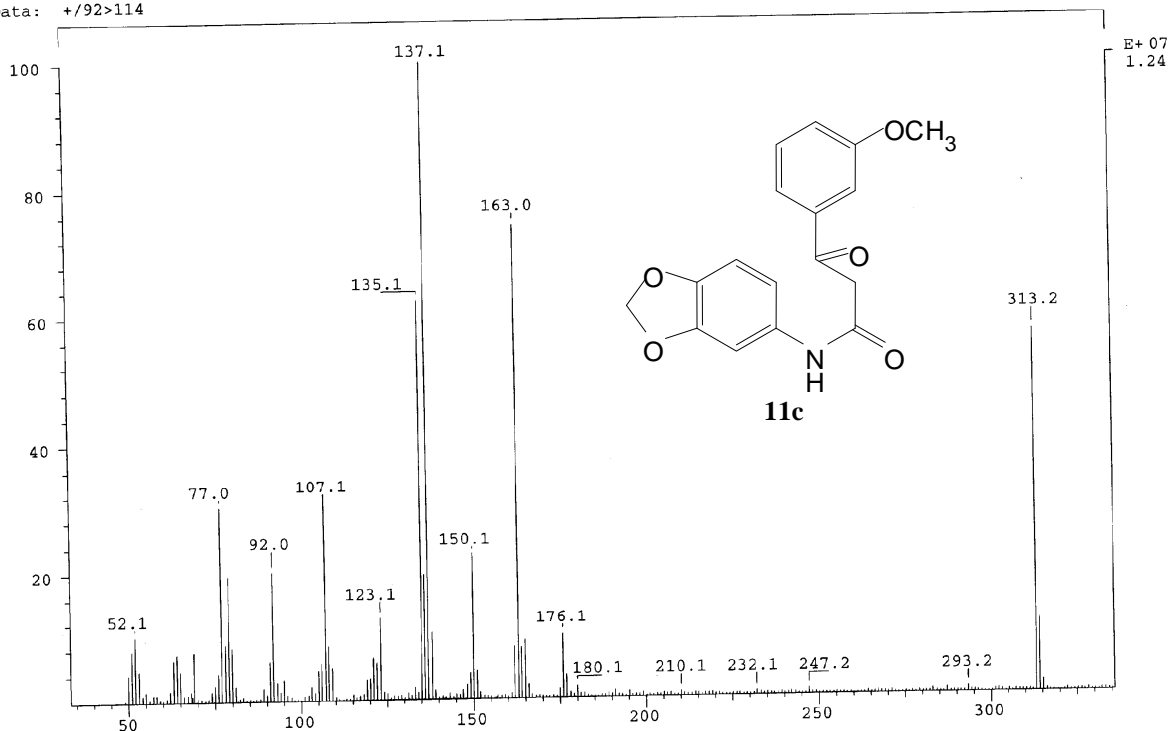


calculated for C<sub>17</sub>H<sub>15</sub>NO<sub>5</sub>: 313.0950;  
 found: 313.0959

### EI-MS spectra of compound 11c.

SPEC: lei7470\_hpk4e  
 Mode: EI +VE +LMR BSCAN (EXP) UP LR NRM  
 Oper: Base: 137.1 Inten: 12442348  
 Norm: 137.1 RIC: 97126495  
 Peak: 1000.00 mmu  
 Data: +/92>114

04-Oct-12 REG: 05:50.7 #9  
 Start: 09:55:45 160  
 Inlet:  
 Masses: 45 > 350  
 #peaks: 397

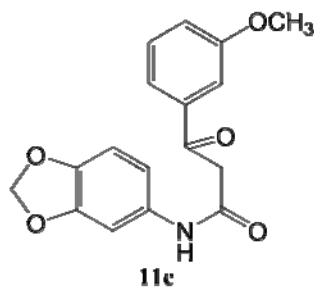


### HRMS spectra of compound 11c.

LIST: hei6469\_hpk4e-c8  
 Mode: EI +VE +LMR ESCAN (EXP) UP HR NRM  
 Oper: Limt: ( 0)  
 : (411) C22.H21.N.O7  
 Peak: 1000.00 mmu R+D: -2.0 > 60.0  
 Data: +/665>834 (CMASS : converted; CMASS : conve

08-Oct-12 REG: 03:27.9 #9  
 Start: 10:53:01 2241  
 Inlet:

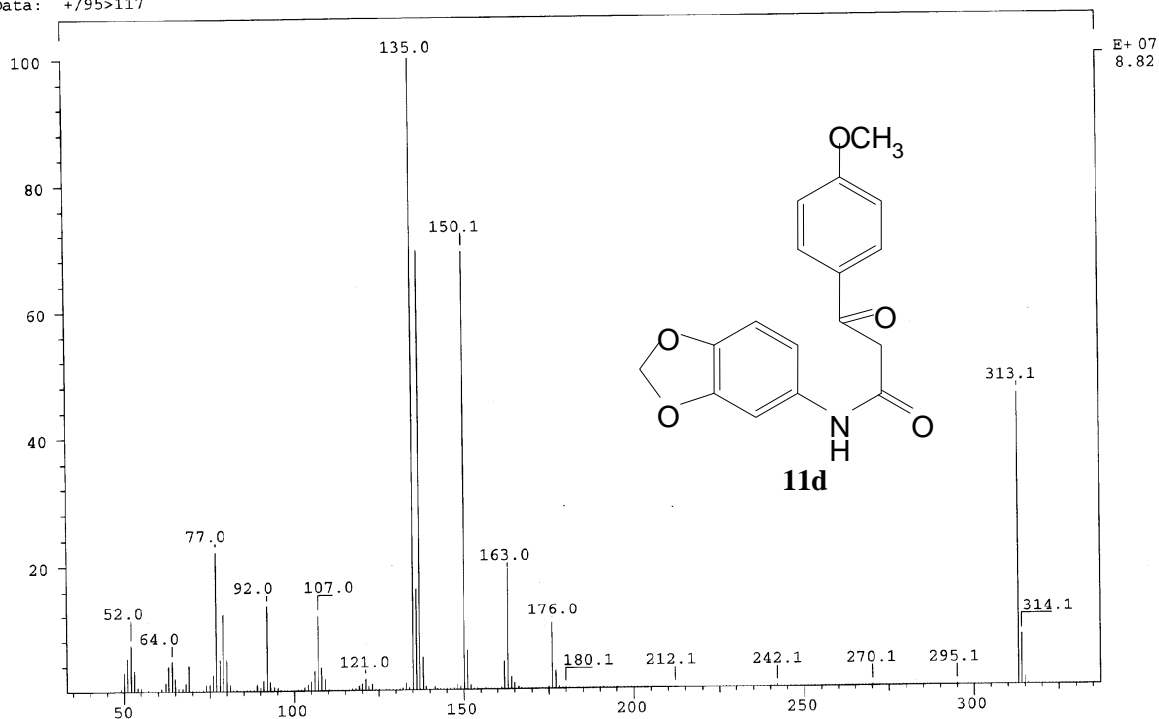
Mass	Intensity	%RA	Flags	Delta	R+D	Composition
313.0958	299518	20.54	#	-0.8	11.0	C17.H15.N.O5



calculated for C<sub>17</sub>H<sub>15</sub>NO<sub>5</sub>: 313.0950;  
 found: 313.0958

### EI-MS spectra of compound 11d.

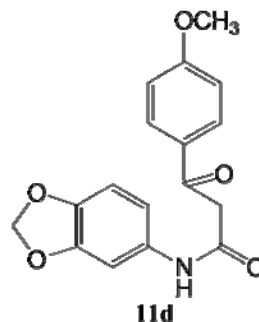
SPEC: lei7471\_hpk5e                      04-Oct-12    REG : 06:03.9    #9  
 Samp:    Start : 10:20:16    187  
 Mode: EI +VE +LMR    BSCAN (EXP) UP LR NRM                      Inlet :  
 Oper:    Masses: 45 > 350  
 Base: 135.0                      Inten : 88158928                      #peaks: 428  
 Norm: 135.0                      RIC : 457082367  
 Peak: 1000.00 mmu  
 Data: +/95>117



### HRMS spectra of compound 11d.

LIST: hei6469\_hpk5e-c5                      08-Oct-12    REG : 08:52.8    #9  
 Samp:    Start : 11:40:57    2758  
 Mode: EI +VE +LMR    ESCAN (EXP) UP HR NRM                      Inlet :  
 Oper:      
 Limt: ( 0)  
       : (411) C22.H21.N.O7  
 Peak: 1000.00 mmu    R+D: -2.0 > 60.0  
 Data: +/1710>2016    (CMASS : converted; CMASS : converted; CMASS : con

Mass	Intensity	%RA	Flags	Delta	R+D	Composition
313.0944	5617	96.93	#	0.6	11.0	C17.H15.N.O5

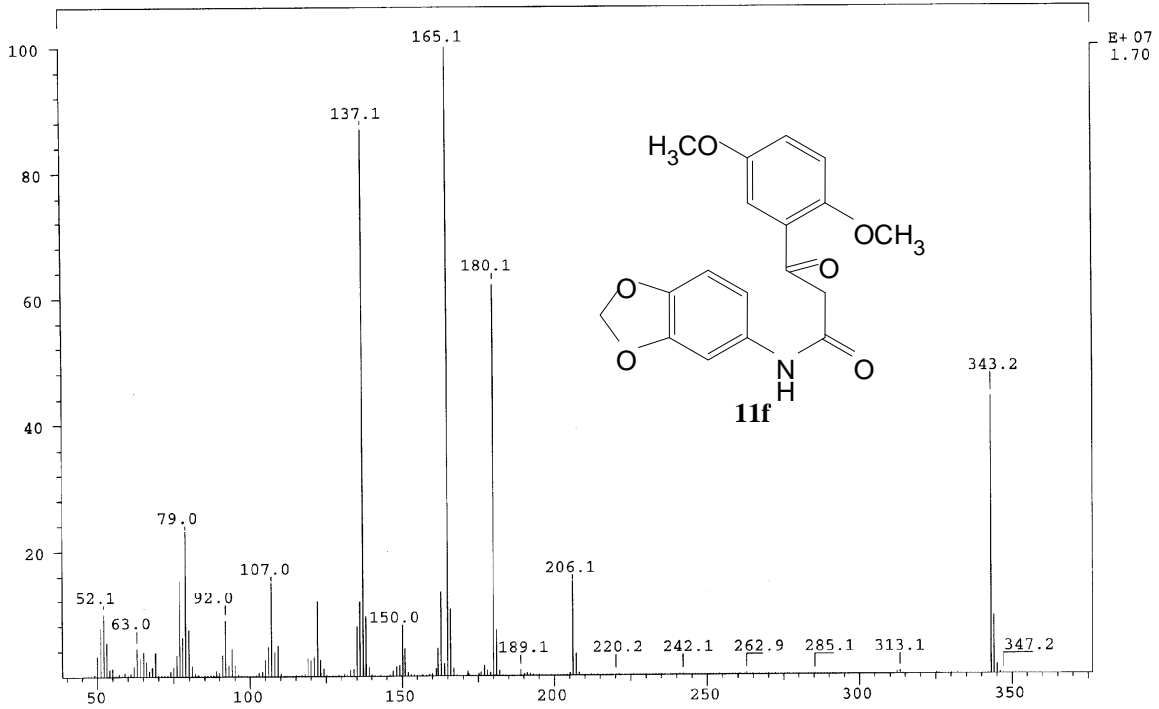


calculated for C<sub>17</sub>H<sub>15</sub>NO<sub>5</sub>: 313.0950;  
 found: 313.0944



### EI-MS spectra of compound **11f**.

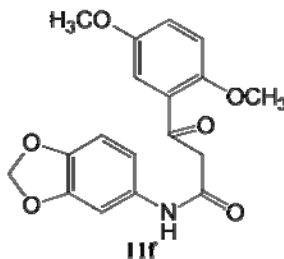
SPEC: lei7474\_hpk9e                      04-Oct-12    REG : 04:20.8    #9  
 Samp:    Start : 13:45:53    159  
 Mode: EI +VE +LMR BSCAN (EXP) UP LR NRM                      Inlet :  
 Oper:    Masses: 45 > 370  
 Base: 165.1                                      Inten : 17013894                      #peaks: 380  
 Norm: 165.1                                      RIC : 107803540  
 Peak: 1000.00 mmu  
 Data: +/66>95



### HRMS spectra of compound **11f**.

LIST: hei6473\_hpk9e-c2                      08-Oct-12    REG : 07:00.5    #9  
 Samp:    Start : 14:39:39    3643  
 Mode: EI +VE +LMR ESCAN (EXP) UP HR NRM                      Inlet :  
 Oper:      
 Limt: ( 0)  
       : (399) C21.H21.N.O7  
 Peak: 1000.00 mmu                      R+D: -2.0 > 60.0  
 Data: +/1405>1774                      (CMASS : converted; CMASS : converted | CMASS : con

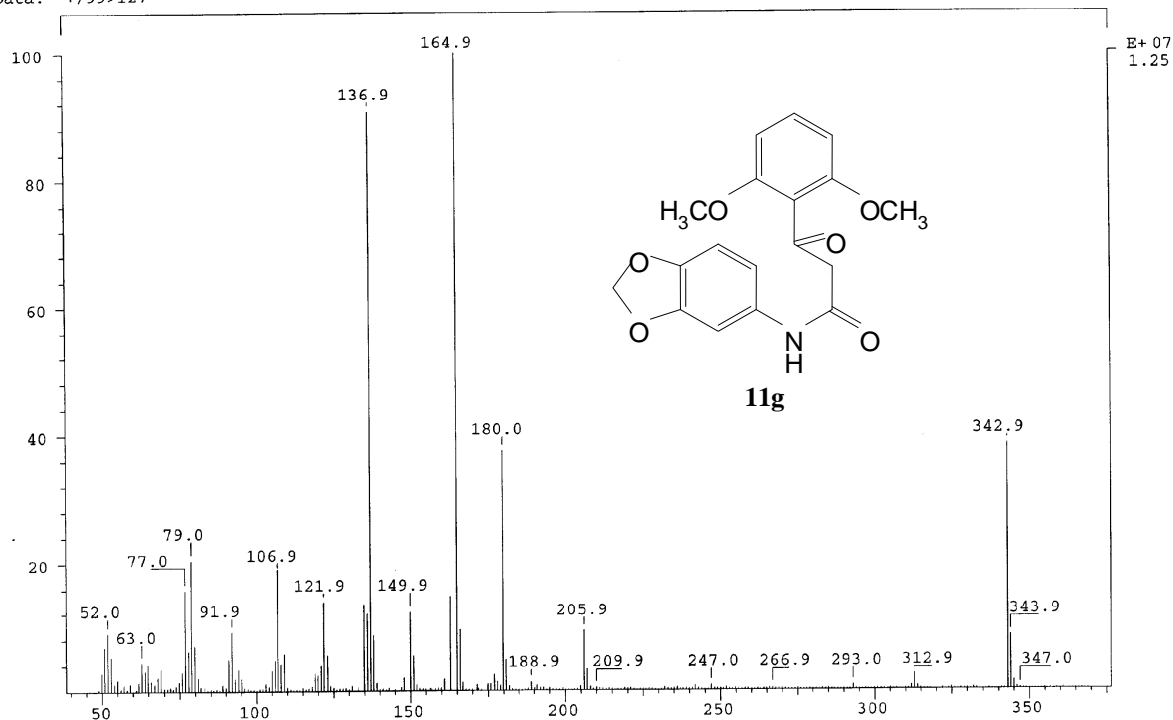
Mass	Intensity	%RA	Flags	Delta	R+D	Composition
343.1051	266341	20.08	#	0.5	11.0	C18.H17.N.O6



calculated for C<sub>18</sub>H<sub>17</sub>NO<sub>6</sub>: 343.1056;  
 found: 343.1051

### EI-MS spectra of compound **11g**.

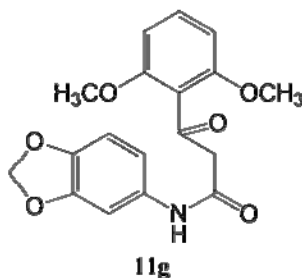
SPEC: lei7475\_hpk10e                      04-Oct-12    REG : 06:26.9    #9  
 Samp:    Start : 14:21:49    181  
 Mode: EI +VE +LMR BSCAN (EXP) UP LR NRM                      Inlet :  
 Oper:    Masses: 45 > 370  
 Base: 164.9                                      Inten : 12528154                      #peaks: 325  
 Norm: 164.9                                      RIC : 82983014  
 Peak: 1000.00 mmu  
 Data: +/-99>127



### HRMS spectra of compound **11g**.

LIST: hei6474\_hpk10e-c4                      08-Oct-12    REG : 09:18.9    #9  
 Samp:    Start : 15:20:26    2509  
 Mode: EI +VE +LMR ESCAN (EXP) UP HR NRM                      Inlet :  
 Oper:     
 Limt: ( 0)  
 : (399) C21.H21.N.O7  
 Peak: 1000.00 mmu    R+D: -2.0 > 60.0  
 Data: +/-1869>2292 (CMASS : converted |CMASS : converted |CMASS : con

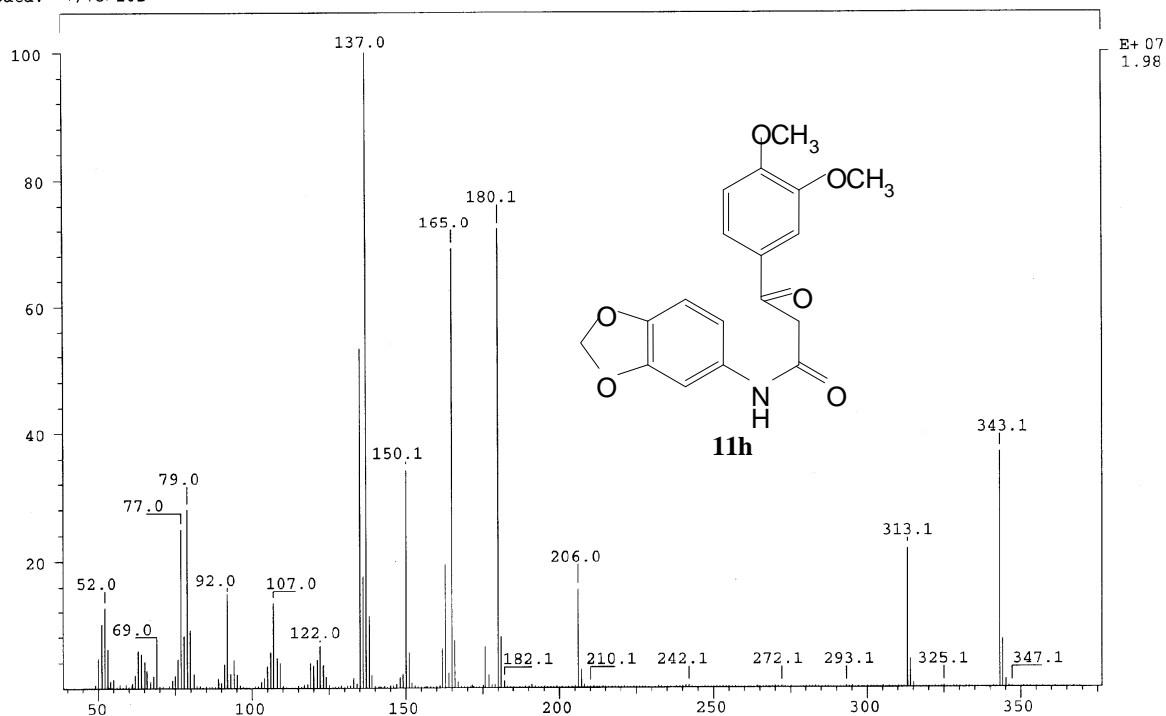
Mass	Intensity	%RA	Flags	(mmu)	Delta	R+D	Composition
343.1062	38655	100.00	#	-0.6	11.0		C18.H17.N.O6



calculated for C<sub>18</sub>H<sub>17</sub>N<sub>2</sub>O<sub>6</sub>: 343.1056;  
 found: 343.1062

### EI-MS spectra of compound **11h**.

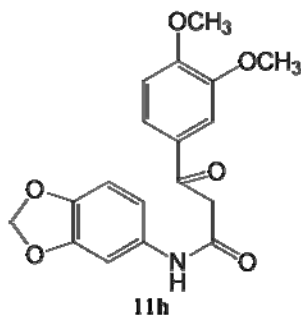
SPEC: lei7472\_hpk7e                      04-Oct-12    REG : 05:14.6    #9  
 Samp:    Start : 11:01:44    205  
 Mode: EI +VE +LMR BSCAN (EXP) UP LR NRM  
 Oper:    Inlet :  
 Base: 137.0                                      Inten : 19758102    Masses: 45 > 370  
 Norm: 137.0                                      RIC : 155505600    #peaks: 398  
 Peak: 1000.00 mmu  
 Data: +/75>101



### HRMS spectra of compound **11h**.

LIST: hei6471\_hpk7e-c3                      08-Oct-12    REG : 11:26.9    #9  
 Samp:    Start : 13:14:29    3387  
 Mode: EI +VE +LMR ESCAN (EXP) UP HR NRM  
 Oper:    Inlet :  
 Limt: ( 0)  
 : (399) C21.H21.N.O7  
 Peak: 1000.00 mmu    R+D: -2.0 > 60.0  
 Data: +/2295>2826    (CMASS : converted |CMASS : converted |CMASS : con

Mass	Intensity	%RA	Flags	Delta	R+D	Composition
343.1050	22858	100.00	#	0.6	11.0	C18.H17.N.O6

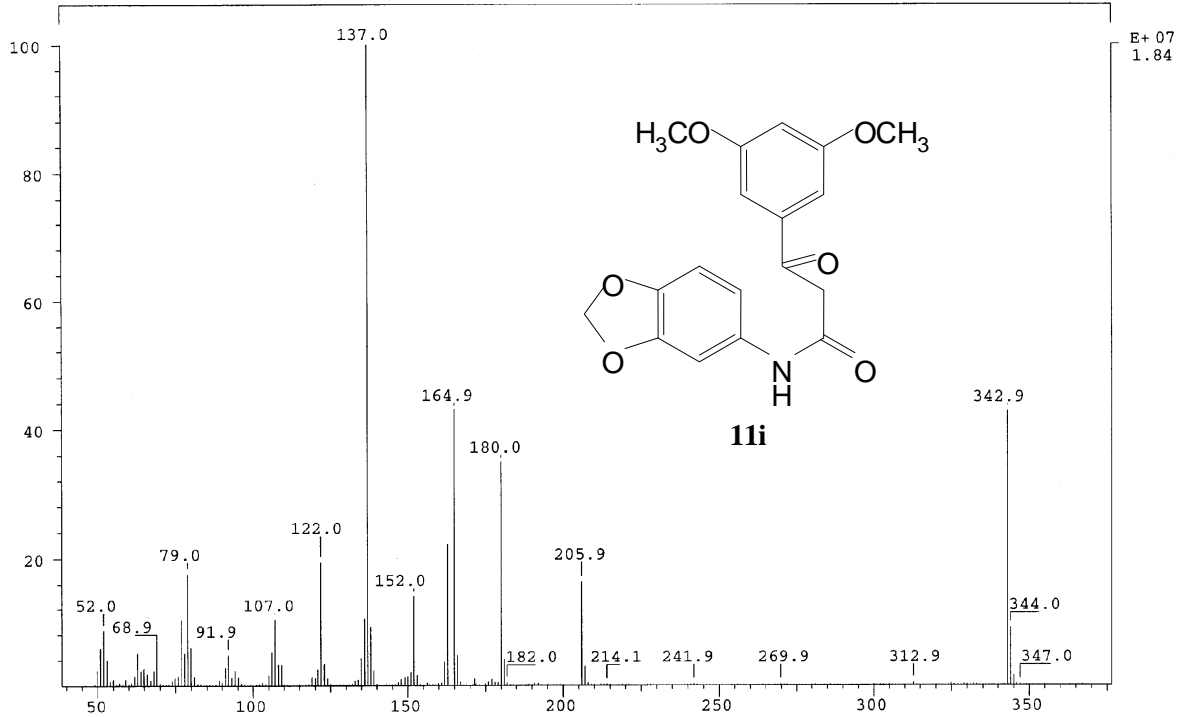


calculated for C<sub>18</sub>H<sub>17</sub>NO<sub>6</sub>: 343.1056;  
 found: 343.1050



### EI-MS spectra of compound **11i**.

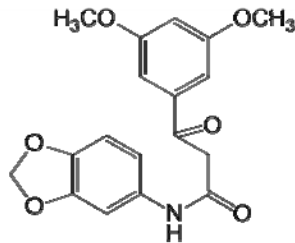
SPEC: lei7476\_hpk11e                      04-Oct-12    REG : 04:30.2    #9  
 Samp:    Start : 15:01:02    158  
 Mode: EI +VE +LMR BSCAN (EXP) UP LR NRM                      Inlet :  
 Oper:    Masses: 45 > 370  
 Base: 137.0                                      Inten : 18415296                      #peaks: 325  
 Norm: 137.0                                      RIC : 97209887  
 Peak: 1000.00 mmu  
 Data: +/69>94



### HRMS spectra of compound **11i**.

LIST: hei6475\_hpk11e-c4                      08-Oct-12    REG : 09:28.7    #9  
 Samp:    Start : 16:00:33    2307  
 Mode: EI +VE +LMR ESCAN (EXP) UP HR NRM                      Inlet :  
 Oper:      
 Limit: ( 0 )  
 : (399) C21.H21.N.07  
 Peak: 1000.00 mmu                      R+D: -2.0 > 60.0  
 Data: +/1902>2154                      (CMASS : converted; CMASS : converted |CMASS : con

Mass	Intensity	%RA	Flags	Delta (mmu)	R+D	Composition
343.1059	8935	23.59	#	-0.3	11.0	C18.H17.N.O6

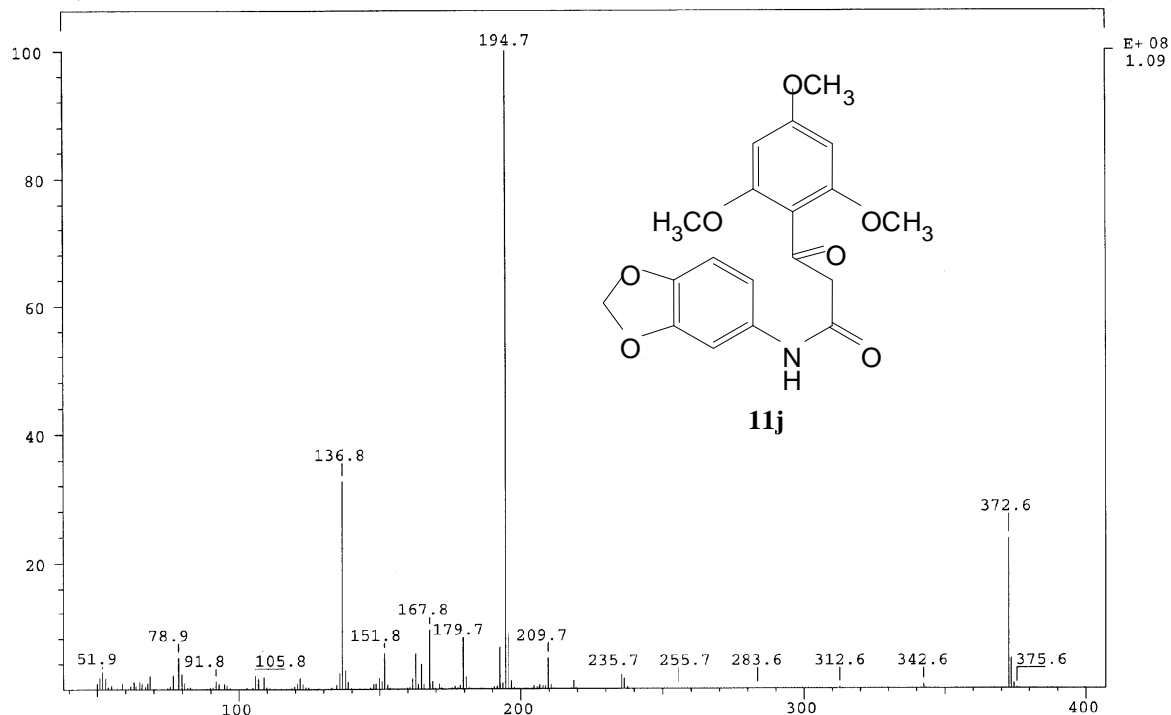


**11i**

calculated for C<sub>18</sub>H<sub>17</sub>NO<sub>6</sub>: 343.1056  
 found: 343.1059

### EI-MS spectra of compound **11j**.

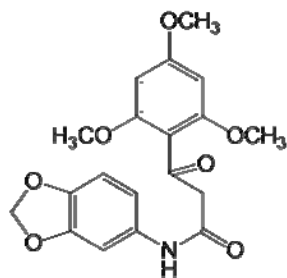
SPEC: lei7478\_hpkl3e                      04-Oct-12    REG : 04:18.9    #9  
 Samp:    Start : 16:21:01    138  
 Mode: EI +VE +LMR BSCAN (EXP) UP LR NRM                      Inlet :  
 Oper:    Masses: 45 > 400  
 Base: 194.7                                      Inten : 108730264                      #peaks: 371  
 Norm: 194.7                                      RIC : 358191561  
 Peak: 1000.00 mmu  
 Data: +/63>85



### HRMS spectra of compound **11j**.

LIST: hei6480\_hpkl3e-c2                      08-Oct-12    REG : 04:07.9    #9  
 Samp:    Start : 17:24:54    911  
 Mode: EI +VE +LMR ESCAN (EXP) UP HR NRM                      Inlet :  
 Oper:     
 Limt: ( 0)  
       : (399) C21.H21.N.07  
 Peak: 1000.00 mmu                      R+D: -2.0 > 60.0  
 Data: +/782>870 (CMASS : converted; CMASS : converted)

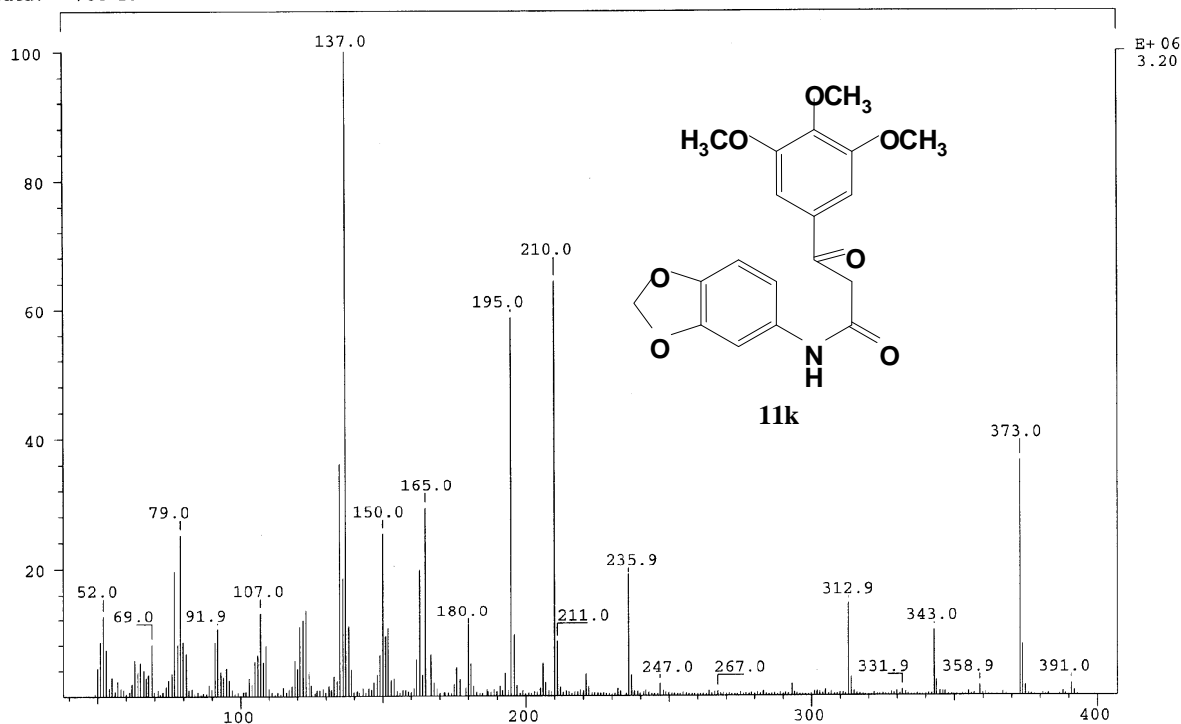
Mass	Intensity	%RA	Flags	Delta	R+D	Composition
373.1166	61787	43.86	#	-0.5	11.0	C19.H19.N.07



calculated for C<sub>19</sub>H<sub>19</sub>NO<sub>7</sub>: 373.1162;  
 found: 373.1166

### EI-MS spectra of compound 11k.

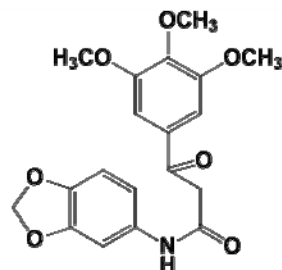
SPEC: lei7477\_hp12e                      04-Oct-12    REG : 03:43.1    #9  
 Samp:    Start : 15:41:58    170  
 Mode: EI +VE +LMR BSCAN (EXP) UP LR NRM                      Inlet :  
 Oper:    Masses: 45 > 400  
 Base: 137.0                                      Inten : 3197062                      #peaks: 354  
 Norm: 137.0                                      RIC : 32098551  
 Peak: 1000.00 mmu  
 Data: +/54>102



### HRMS spectra of compound 11k.

LIST: hei6477\_hp12e-c2                      08-Oct-12    REG : 02:07.9    #9  
 Samp:    Start : 16:34:48    1641  
 Mode: EI +VE +LMR ESCAN (EXP) UP HR NRM                      Inlet :  
 Oper:      
 Limt: ( 0)  
       : (399) C21.H21.N.07  
 Peak: 1000.00 mmu                      R+D: -2.0 > 60.0  
 Data: +/402>676 (CMASS : not converted; CMASS : not converted |CMASS

Mass	Intensity	%RA	Flags	Delta	R+D	Composition
373.1170	590	91.76	#?	-0.9	11.0	C19.H19.N.07



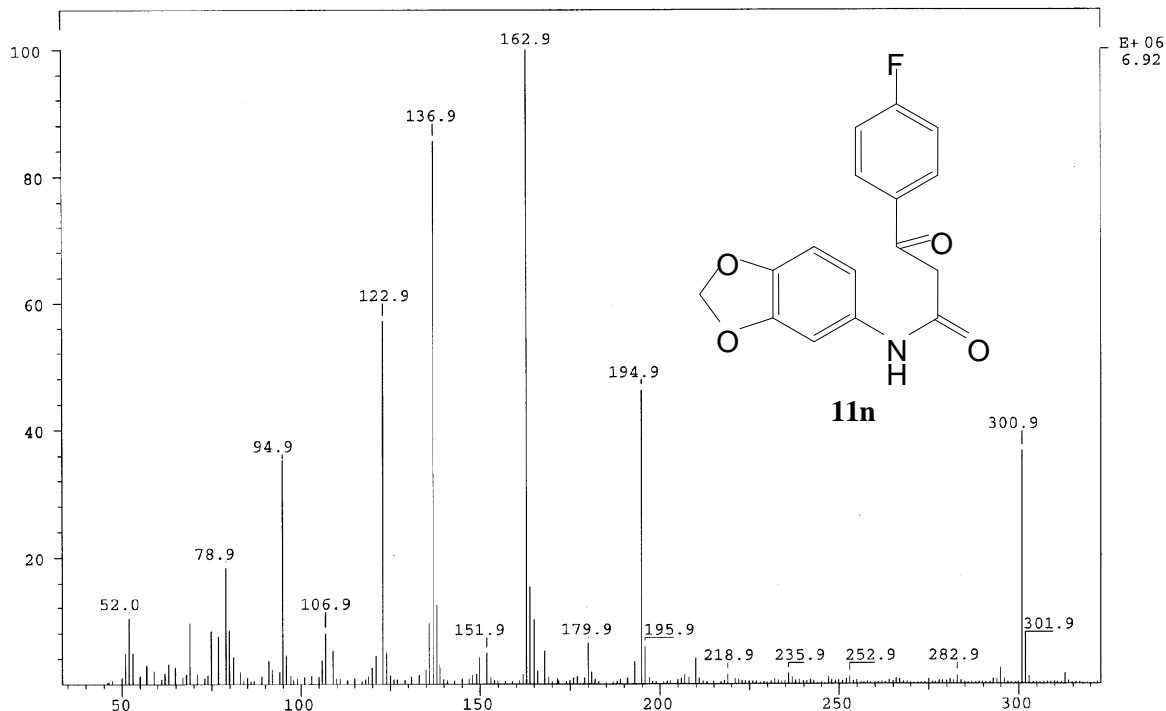
11k  
 calculated for C<sub>19</sub>H<sub>19</sub>NO<sub>7</sub>: 373.1162;  
 found: 373.1170





### EI-MS spectra of compound **11n**.

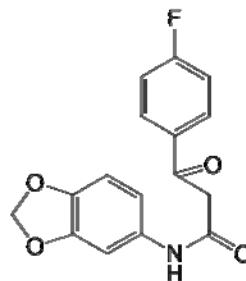
SPEC: lei7481\_hpkl6e                      04-Oct-12    REG : 04:54.5    #9  
 Samp:    Start : 18:50:28    119  
 Mode: EI +VE +LMR    BSCAN (EXP) UP LR NRM  
 Oper:    Inlet :  
 Base: 162.9                                      Inten : 6923549    Masses: 45 > 350  
 Norm: 162.9                                      RIC : 59958946    #peaks: 306  
 Peak: 1000.00    mmu  
 Data: +/52>77



### HRMS spectra of compound **11n**.

LIST: hei6485\_hpkl6e-c3                      09-Oct-12    REG : 32:37.9    #9  
 Samp:    Start : 11:24:34    8511  
 Mode: EI +VE +LMR    ESCAN (EXP) UP HR NRM                      Inlet :  
 Oper:    :  
 Limt: ( 0)  
 : (338) C17.H21.N.F.O5  
 Peak: 1000.00    mmu    R+D: -2.0 > 60.0  
 Data: +/6221>6991    (CMASS : converted; CMASS : converted |CMASS : con

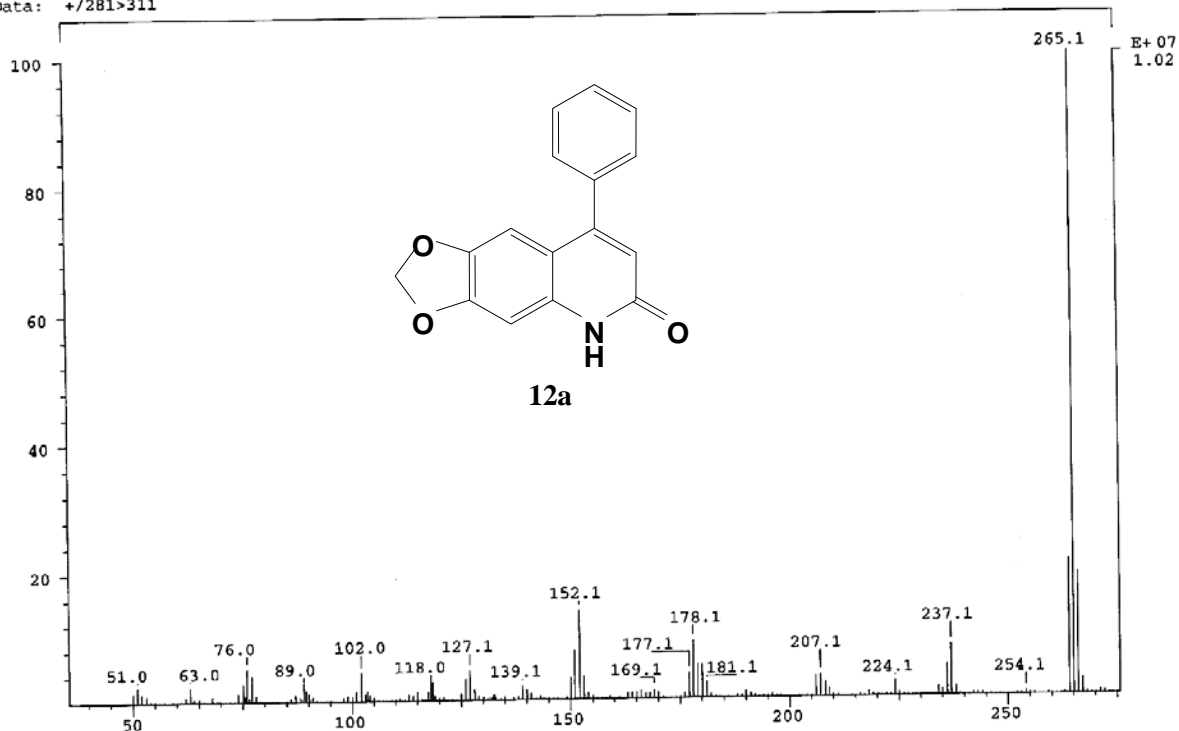
Mass	Intensity	%RA	Flags	Delta	R+D	Composition
301.0755	2354	66.74	#	-0.5	11.0	C16.H12.N.F.O4



**11n**  
 calculated for C<sub>16</sub>H<sub>12</sub>FNO<sub>4</sub>: 301.0750;  
 found: 301.0755

### EI-MS spectra of compound 12a.

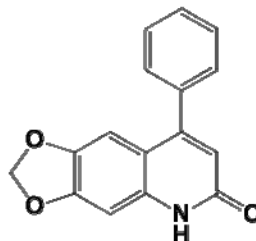
SPC: lei7368\_hpk2f                      25-Sep-12    REG : 16:22.9    #9  
 Samp:                                      Start : 09:35:55    439  
 Mode: EI +VE +LMR BSCAN (EXP) UP LR NRM                      Inlet :  
 Oper:                                      Masses: 45 > 300  
 Base: 265.1                      Inten : 10228337                      #peaks: 325  
 Norm: 265.1                      RIC : 37030683  
 Peak: 1000.00 mmu  
 Data: +/281>311



### HRMS spectra of compound 12a.

LIST: hei6451\_hpk2f-c2                      27-Sep-12    REG : 07:44.8    #9  
 Samp:                                      Start : 17:35:08    5234  
 Mode: EI +VE +LMR ESCAN (EXP) UP HR NRM                      Inlet :  
 Oper:                                        
 Limt: ( 0)  
       : (335) C21.H21.N.O3  
 Peak: 1000.00 mmu    R+D: -2.0 > 60.0  
 Data: +/1394>1717    (CMASS : converted |CMASS : converted |CMASS : con

Mass	Intensity	%RA	Flags	Delta	R+D	Composition
265.0733	50040	100.00	#	0.6	12.0	C16.H11.N.O3



**12a**

calculated for C<sub>16</sub>H<sub>11</sub>NO<sub>3</sub>: 265.0739;  
 found: 265.0733

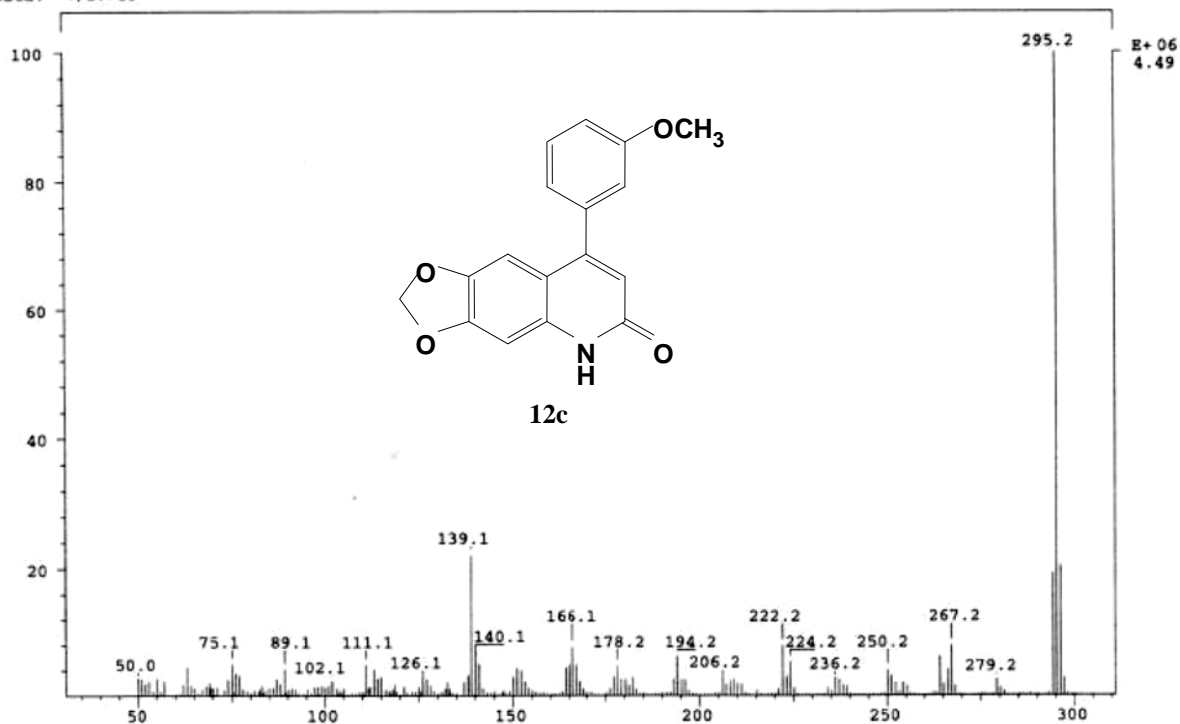




EI-MS spectra of compound 12c.

SPEC: lei0777  
 Samp: 14.HPK-057  
 Mode: EI +VE +LMR BSCAN (EXP) UP LR NRM  
 Oper:  
 Base: 295.2 Inten: 4487057  
 Norm: 295.2 RIC: 23379615  
 Peak: 1000.00 mmu  
 Data: +/57>89

21-Jun-10 REG: 05:18.3 #9  
 Start: 09:22:42 133  
 Inlet:  
 Masses: 45 > 500  
 #peaks: 517

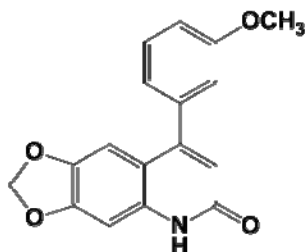


HRMS spectra of compound 12c.

LIST: hei6453\_hpk4f-c4  
 Samp:  
 Mode: EI +VE +LMR ESCAN (EXP) UP HR NRM  
 Oper:  
 Limit: ( 0)  
 : (400) C22.H26.N.O6  
 Peak: 1000.00 mmu R+D: -2.0 > 60.0  
 Data: +/2177>3108 (CMASS : converted |CMASS : converted |CMASS : con

27-Sep-12 REG: 11:25.4 #9  
 Start: 18:47:15 5451  
 Inlet:

Mass	Intensity	%RA	Flags	Delta	R+D	Composition
295.0851	20768	23.16	#	-0.7	12.0	C17.H13.N.O4

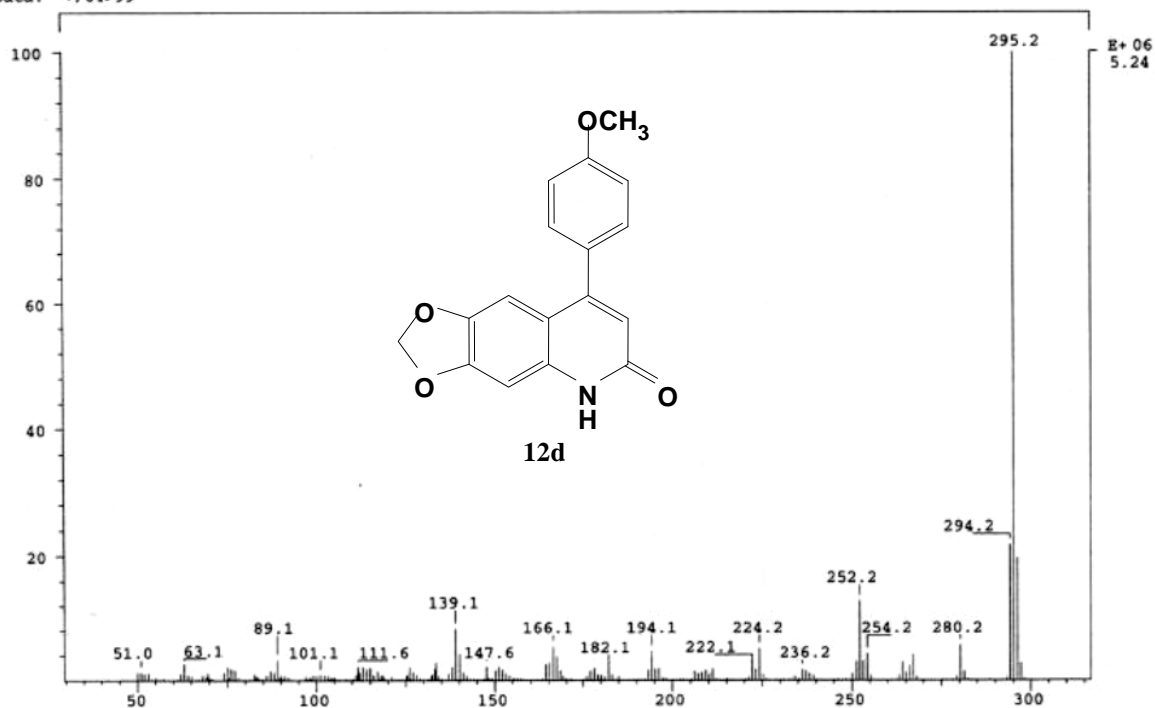


12c

calculated for C<sub>17</sub>H<sub>13</sub>NO<sub>4</sub>: 295.0845;  
 found: 295.0851

### EI-MS spectra of compound 12d.

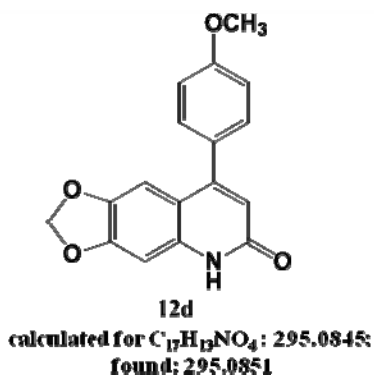
SPBC: lei0784 21-Jun-10 REG : 06:07.3 #9  
 Samp: 17HPK034 Start : 13:00:15 218  
 Mode: EI +VE +LMR BSCAN (EXP) UP LR NRM  
 Oper: Inlet :  
 Base: 295.2 Inten : 5241995 Masses : 45 > 550  
 Norm: 295.2 RIC : 20056797 #peaks: 508  
 Peak: 1000.00 mmu  
 Data: +/64>99



### HRMS spectra of compound 12d.

LIST: hei6455\_hp5f-c2 27-Sep-12 REG : 01:10.3 #9  
 Samp: Start : 20:32:48 2749  
 Mode: EI +VE +LMR ESCAN (EXP) UP HR NRM  
 Oper: Inlet :  
 Limt: ( 0)  
 : (367) C21.H21.N.O5  
 Peak: 1000.00 mmu R+D: -2.0 > 60.0  
 Data: +/221>376 (CMASS : converted |CMASS : converted |CMASS : conve

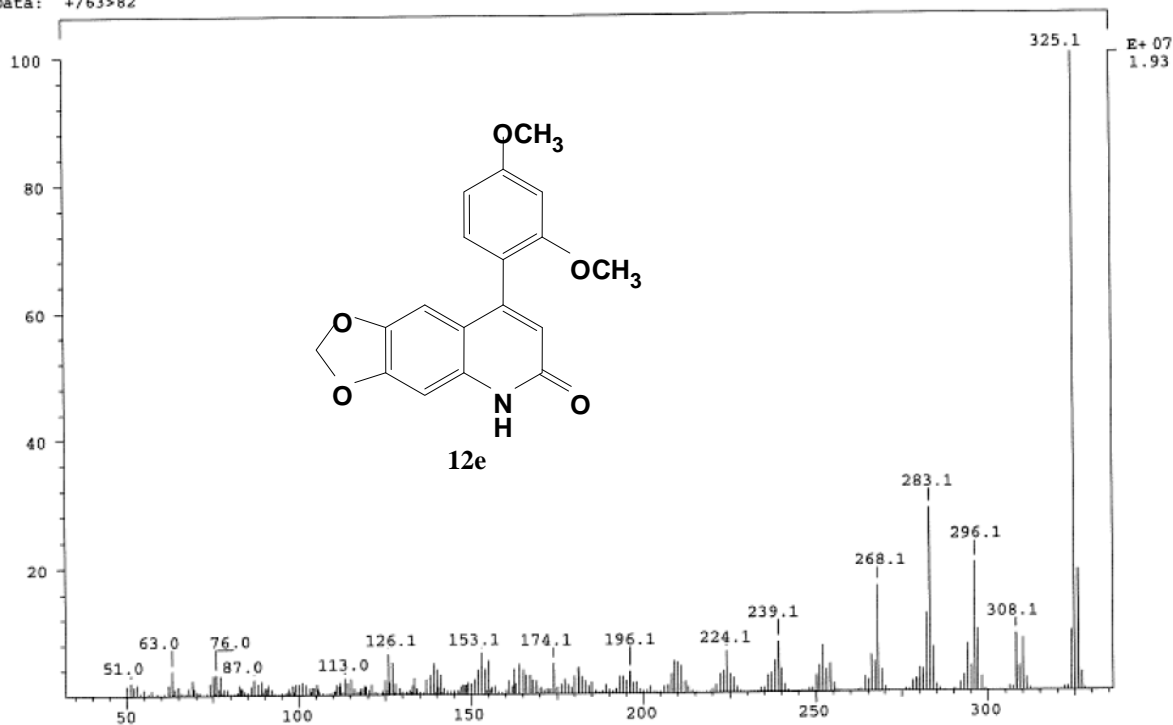
Mass	Intensity	%RA	Flags	Delta (mmu)	R+D	Composition
295.0851	1040	71.38	#	-0.7	12.0	C17.H13.N.O4



### EI-MS spectra of compound 12e.

SPEC: lei0381  
 Samp: HPK048  
 Mode: EI +VE +LMR BSCAN (EXP) UP LR NRM  
 Oper:  
 Base: 325.1 Inten: 19306180  
 Norm: 325.1 RIC: 131768682  
 Peak: 1000.00 mmu  
 Data: +/63>82

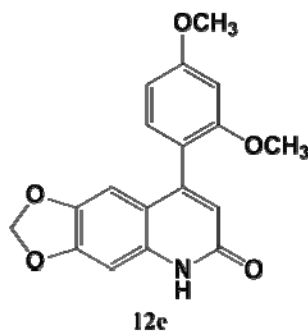
17-May-10 REG: 06:18.7 #9  
 Start: 16:47:33 168  
 Inlet:  
 Masses: 45 > 400  
 #peaks: 478



### HRMS spectra of compound 12e.

LIST: hei6460\_hpk8f-c2  
 Samp: 28-Sep-12 REG: 04:39.7 #9  
 Mode: EI +VE +LMR ESCAN (EXP) UP HR NRM  
 Oper: Start: 10:38:40 1266  
 Inlet:  
 Limt: ( 0)  
 : (331) C18.H21.N.O5  
 Peak: 1000.00 mmu R+D: -2.0 > 60.0  
 Data: +/914>1104 (CMASS: converted; CMASS: conv

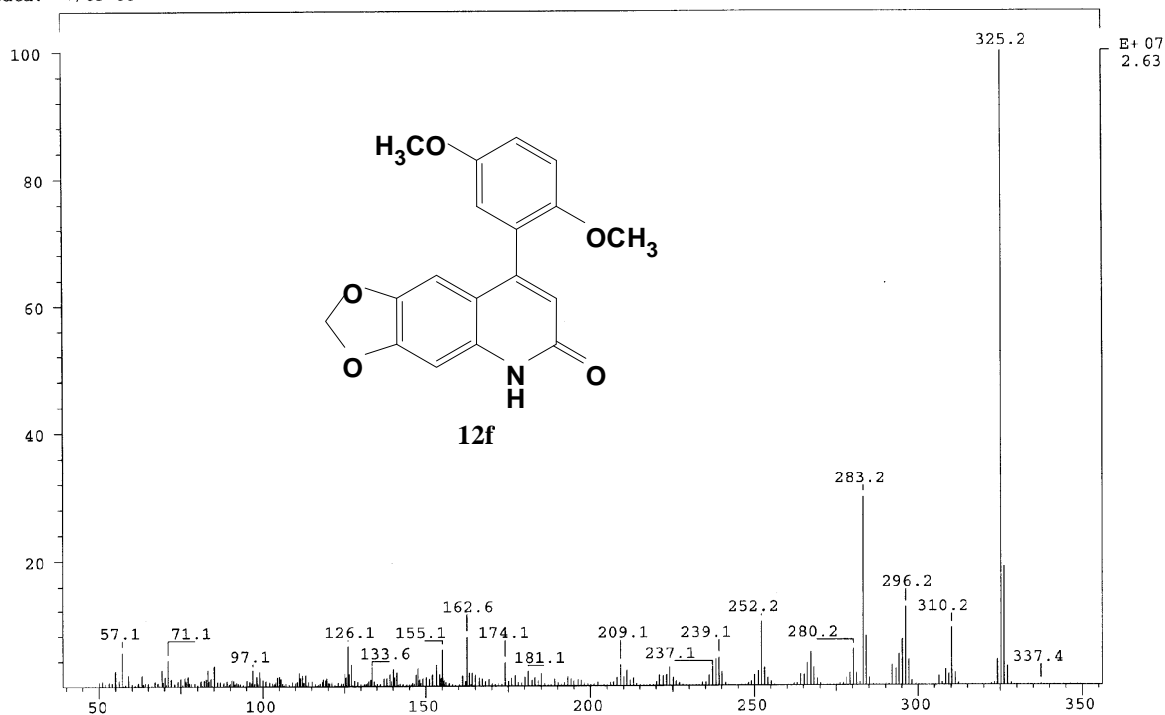
Mass	Intensity	%RA	Flags	Delta	R+D	Composition
325.0954	2483	100.00	#?	-0.3	12.0	C18.H15.N.O5



calculated for C<sub>18</sub>H<sub>15</sub>NO<sub>5</sub>: 325.0950  
 found: 325.0954

### EI-MS spectra of compound 12f.

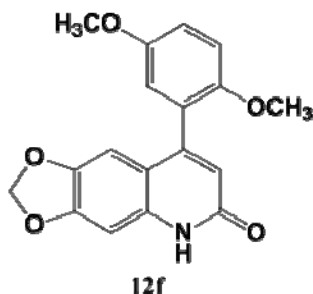
SPEC: lei7483\_hp9f                      04-Oct-12    REG : 05:49.7    #9  
 Samp:                                      Start : 19:34:15    109  
 Mode: EI +VE +LMR BSCAN (EXP) UP LR NRM  
 Oper:                                      Inlet :  
 Base: 325.2                                Inten : 26255760                      Masses: 45 > 350  
 Norm: 325.2                                RIC : 139765211                      #peaks: 440  
 Peak: 1000.00 mmu  
 Data: +/63>80



### HRMS spectra of compound 12f.

LIST: hei6491\_hp9f-c2                      09-Oct-12    REG : 02:24.7    #9  
 Samp:                                      Start : 15:41:39    3807  
 Mode: EI +VE +LMR ESCAN (EXP) UP HR NRM                      Inlet :  
 Oper:                                      Inlet :  
 Limt: ( 0)  
 : (383) C21.H21.N.06  
 Peak: 1000.00 mmu    R+D: -2.0 > 60.0  
 Data: +/471>771 (CMASS : converted |CMASS : converted |CMASS : conve

Mass	Intensity	%RA	Flags	Delta (mmu)	R+D	Composition
325.0959	8317	84.79	#	-0.8	12.0	C18.H15.N.O5

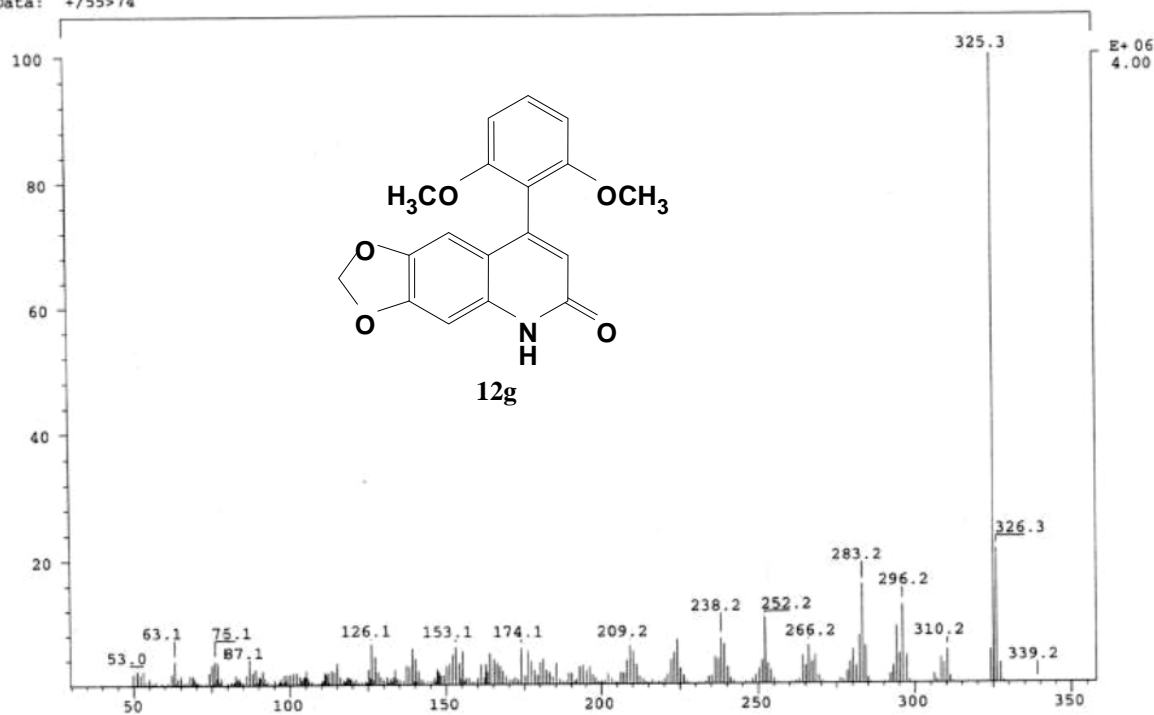


calculated for C<sub>18</sub>H<sub>15</sub>NO<sub>5</sub>: 325.0950;  
 found: 325.0959

### EI-MS spectra of compound 12g.

SPEC: lei0780  
 Samp: 15.HPK052  
 Mode: EI +VE +LMR BSCAN (EXP) UP LR NRM  
 Oper:  
 Base: 325.3 Inten: 4004443  
 Norm: 325.3 RIC: 26551980  
 Peak: 1000.00 mmu  
 Data: +/55>74

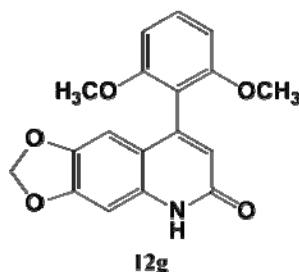
21-Jun-10 REG: 05:05.7 #9  
 Start: 10:29:45 116  
 Inlet:  
 Masses: 45 > 500  
 #peaks: 482



### HRMS spectra of compound 12g.

LIST: hei6459\_hpk10f-c1  
 Samp: 28-Sep-12 REG: 02:34.8 #9  
 Start: 10:00:28 1321  
 Mode: EI +VE +LMR ESCAN (EXP) UP HR NRM  
 Oper:  
 Inlet:  
 Limit: ( 0)  
 : (363) C18.H21.N.O7  
 Peak: 1000.00 mmu R+D: -2.0 > 60.0  
 Data: +/505>791 (CMASS : converted |CMASS : converted |CMASS : conve

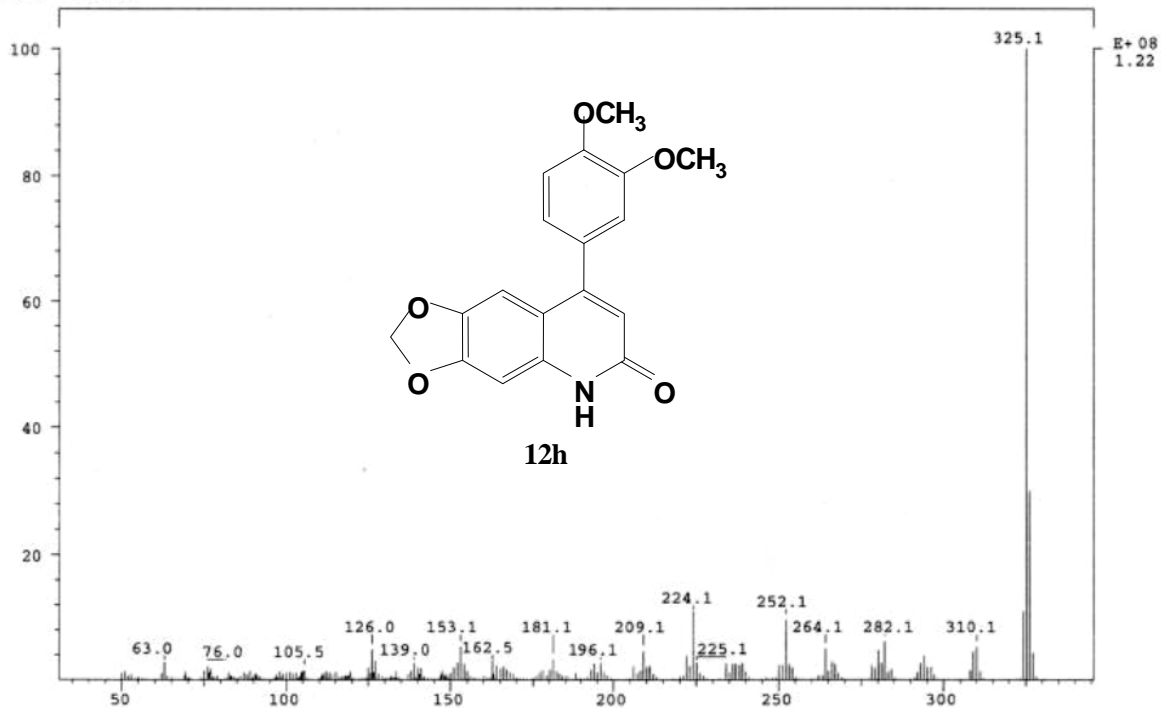
Mass	Intensity	%RA	Flags	Delta (mmu)	R+D	Composition
325.0954	58896	100.00	#	-0.3	12.0	C18.H15.N.O5



calculated for C<sub>18</sub>H<sub>15</sub>NO<sub>5</sub>: 325.0950;  
 found: 325.0954

EI-MS spectra of compound 12h.

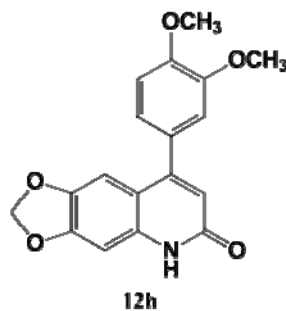
SPEC: lei9643 04-Jan-10 REG : 05:15.1 #9  
 Samp: HPK031 Start : 22:38:12 243  
 Mode: EI +VE +LMR BSCAN (EXP) UP LR NRM  
 Oper: Inlet :  
 Base: 325.1 Inten : 121888792 Masses : 45 > 450  
 Norm: 325.1 RIC : 533939880 #peaks: 532  
 Peak: 1000.00 mmu  
 Data: +/59>82



HRMS spectra of compound 12h.

LIST: hei6459\_hp7f-c2 27-Sep-12 REG : 01:42.9 #9  
 Samp: Start : 22:28:39 872  
 Mode: EI +VE +LMR ESCAN (EXP) UP HR NRM  
 Oper: Inlet :  
 Limit: ( 0)  
 : (331) C18.H21.N.O5  
 Peak: 1000.00 mmu R+D: -2.0 > 60.0  
 Data: +/334>571 (CMASS : converted; CMASS : converted | CMASS : conve

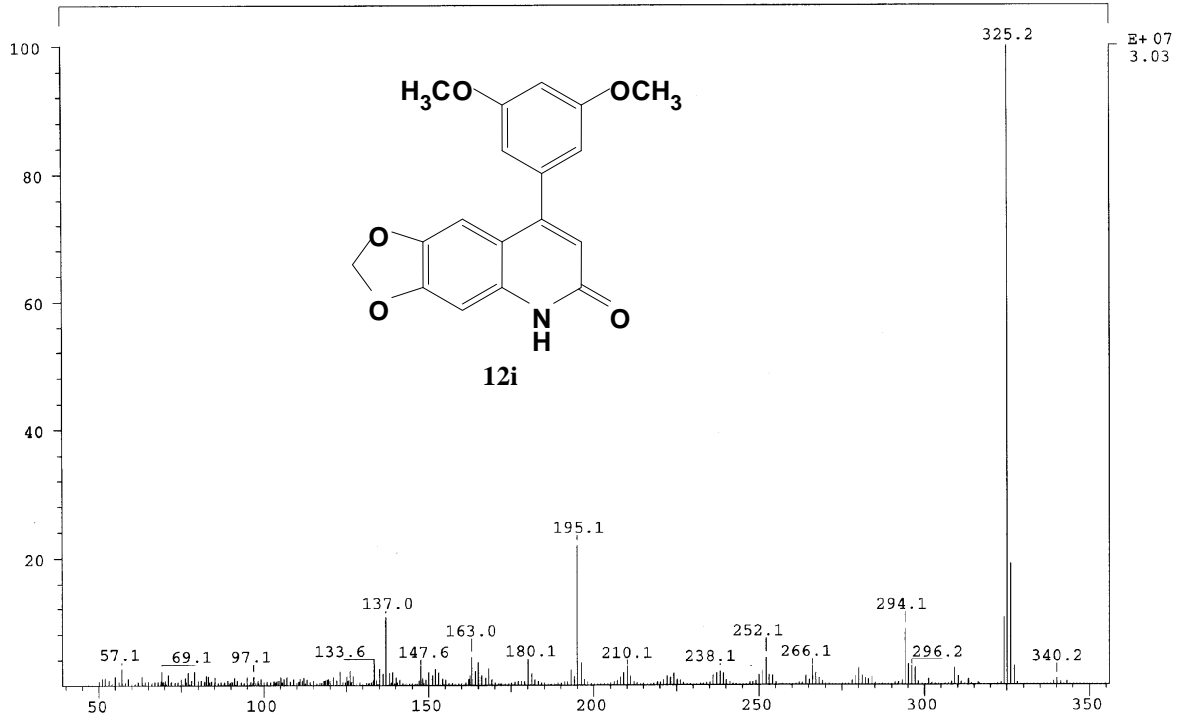
Mass	Intensity	%RA	Flags	(mmu)	Delta	R+D	Composition
325.0954	27450	100.00	#	-0.4	12.0		C18.H15.N.O5



calculated for C<sub>18</sub>H<sub>15</sub>NO<sub>5</sub>: 325.0950:  
 found: 325.0954

### EI-MS spectra of compound 12i.

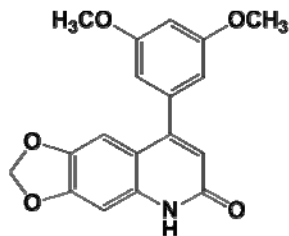
SPEC: lei7484\_hpkl1f                      04-Oct-12    REG : 06:55.1    #9  
 Samp:    Start : 20:10:53    173  
 Mode: EI +VE +LMR BSCAN (EXP) UP LR NRM                      Inlet :  
 Oper:    Masses: 45 > 350  
 Base: 325.2                      Inten : 30282032                      #peaks: 512  
 Norm: 325.2                      RIC : 126375269  
 Peak: 1000.00 mmu  
 Data: +/73>96



### HRMS spectra of compound 12i.

LIST: hei6492\_hpkl1f-c2                      09-Oct-12    REG : 00:08.8    #9  
 Samp:    Start : 16:40:47    5632  
 Mode: EI +VE +LMR ESCAN (EXP) UP HR NRM                      Inlet :  
 Oper:      
 Limt: ( 0)  
 : (383) C21.H21.N.06  
 Peak: 1000.00 mmu    R+D: -2.0 > 60.0  
 Data: +/27>141 (CMASS : converted |CMASS : converted |CMASS : conver

Mass	Intensity	%RA	Flags	Delta (mmu)	R+D	Composition
325.0954	6556	76.82	#	-0.4	12.0	C18.H15.N.05

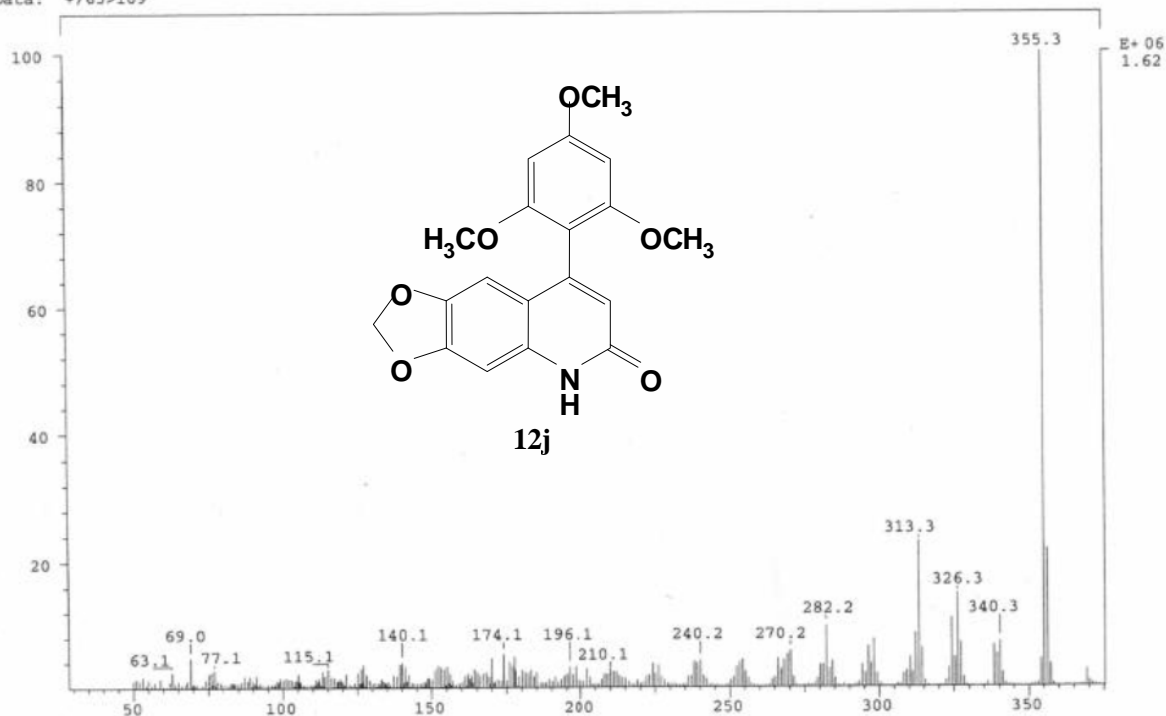


calculated for  $C_{18}H_{15}NO_5$ : 325.0950:  
 found: 325.0954

### EI-MS spectra of compound 12j.

SPEC: lei0783  
 Samp: 16HPK049  
 Mode: EI +VE +LMR BSCAN (EXP) UP LR NRM  
 Oper:  
 Base: 355.3 Inten: 1622770  
 Norm: 355.3 RIC: 11614454  
 Peak: 1000.00 mmu  
 Data: +/65>109

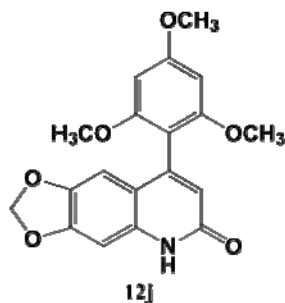
21-Jun-10 REG: 06:07.1 #9  
 Start: 12:20:20 396  
 Inlet:  
 Masses: 45 > 550  
 #peaks: 522



### HRMS spectra of compound 12j.

LIST: hei6462\_hpk13f-c1  
 Samp: 28-Sep-12 REG: 05:19.9 #9  
 Mode: EI +VE +LMR ESCAN (EXP) UP HR NRM  
 Oper: Start: 12:01:39 4962  
 Inlet:  
 Limit: ( 0)  
 : (411) C22.H21.N.O7  
 Peak: 1000.00 mmu R+D: -2.0 > 60.0  
 Data: +/1076>1923 (CMASS: converted |CMASS: converted |CMASS: con

Mass	Intensity	%RA	Flags	Delta	R+D	Composition
355.1048	128473	100.00	#	0.8	12.0	C19.H17.N.O6



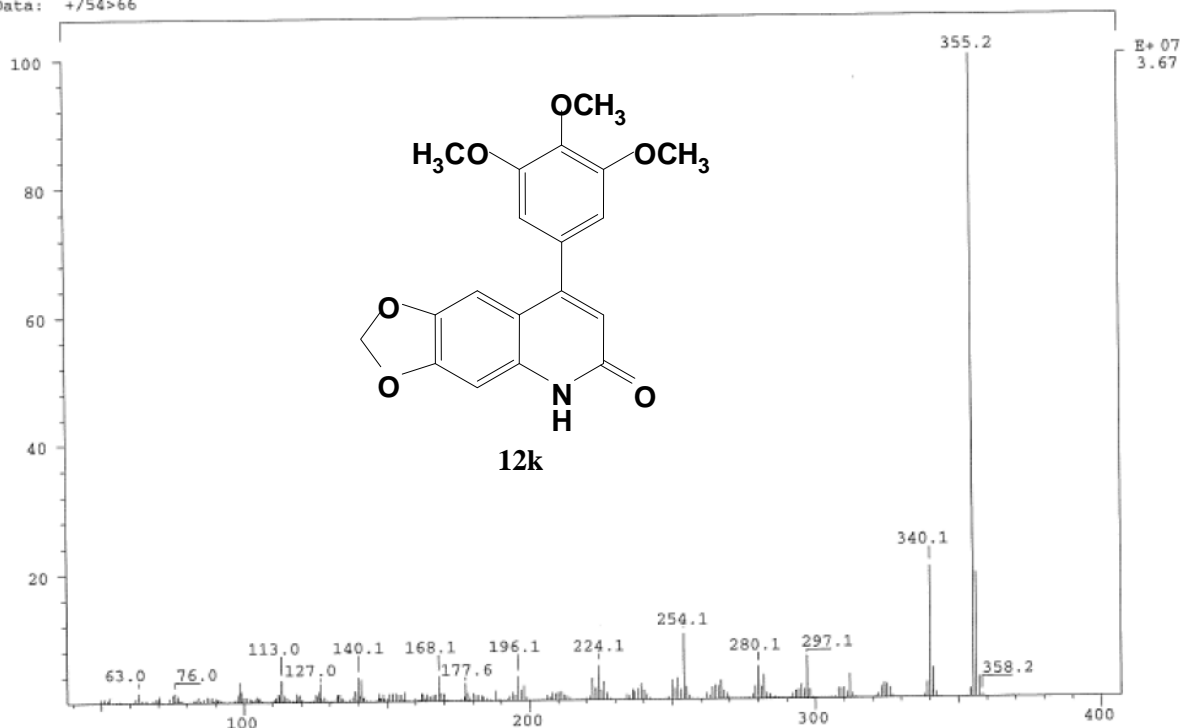
12j  
 calculated for C<sub>19</sub>H<sub>17</sub>NO<sub>6</sub>: 355.1056;  
 found: 355.1048



### EI-MS spectra of compound 12k.

SPEC: 1e10380  
 Samp: HPK042  
 Mode: EI +VE +LMR BSCAN (EXP) UP LR NRM  
 Oper:  
 Base: 355.2 Inten: 36692048  
 Norm: 355.2 RIC: 151121470  
 Peak: 1000.00 mmu  
 Data: +/54>66

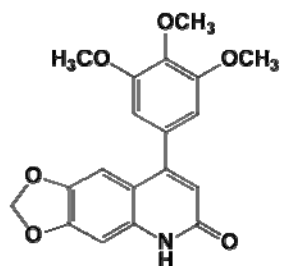
17-May-10 REG: 05:24.6 #9  
 Start: 16:32:27 133  
 Inlet:  
 Masses: 45 > 400  
 #peaks: 475



### HRMS spectra of compound 12k.

LIST: hei6461\_hpk12f-c2  
 Samp: 28-Sep-12 REG: 06:58.6 #9  
 Mode: EI +VE +LMR ESCAN (EXP) UP HR NRM  
 Oper: Inlet:  
 Limit: ( 0)  
 : (411) C22.H21.N.O7  
 Peak: 1000.00 mmu R+D: -2.0 > 60.0  
 Data: +/1411>2070 (CMASS : converted |CMASS : converted |CMASS : con

Mass	Intensity	%RA	Flags	Delta	R+D	Composition
355.1050	463773	100.00	#	0.6	12.0	C19.H17.N.O6

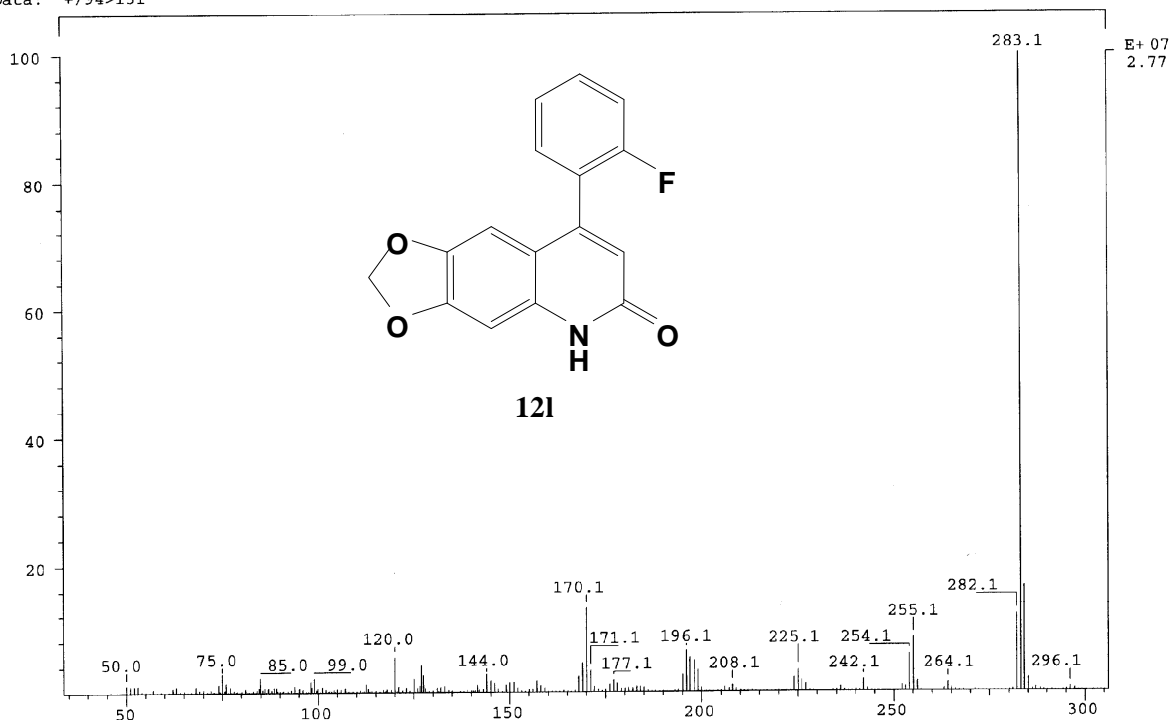


12k

calculated for C<sub>19</sub>H<sub>17</sub>N<sub>1</sub>O<sub>6</sub>: 355.1056  
 found: 355.1050

### EI-MS spectra of compound 121.

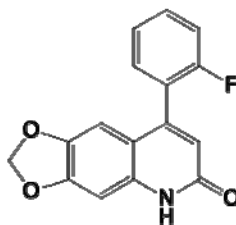
SPEC: lei7365\_hpkl4f                      24-Sep-12    REG : 06:05.8    #9  
 Samp:    Start : 16:20:34    232  
 Mode: EI +VE +LMR BSCAN (EXP) UP LR NRM                      Inlet :  
 Oper:    Masses: 45 > 360  
 Base: 283.1                      Inten : 27734898                      #peaks: 426  
 Norm: 283.1                      RIC : 90801246  
 Peak: 1000.00 mmu  
 Data: +/94>131



### HRMS spectra of compound 121.

LIST: hei6457\_hpkl4f-c2                      27-Sep-12    REG : 10:09.7    #9  
 Samp:    Start : 21:03:02    4871  
 Mode: EI +VE +LMR ESCAN (EXP) UP HR NRM                      Inlet :  
 Oper:     
 Limt: ( 0)  
 : (322) C17.H37.N.F.O3  
 Peak: 1000.00 mmu    R+D: -2.0 > 60.0  
 Data: +/1897>2661 (CMASS : converted |CMASS : converted |CMASS : con

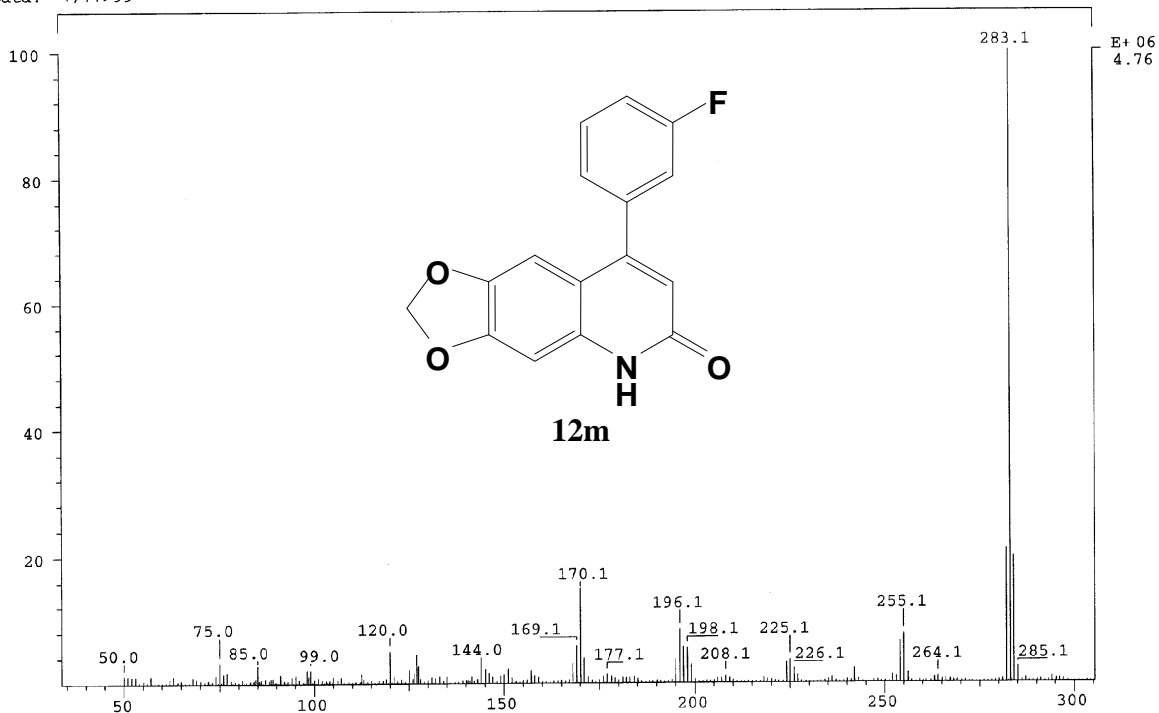
Mass	Intensity	%RA	Flags	Delta	R+D	Composition
283.0641	3674	57.91	#?	0.3	12.0	C16.H10.N.F.O3



**121**  
 calculated for C<sub>16</sub>H<sub>10</sub>FNO<sub>3</sub>: 283.0645;  
 found: 283.0641

### EI-MS spectra of compound 12m.

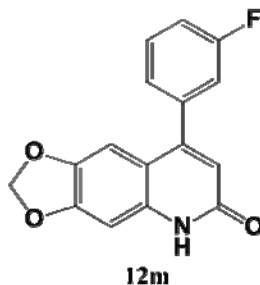
SPEC: lei7367\_hpkl5f                      25-Sep-12    REG : 05:00.9    #9  
 Samp:    Start : 09:18:04    255  
 Mode: EI +VE +LMR    BSCAN (EXP) UP LR NRM  
 Oper:    Inlet :  
 Base: 283.1                                      Inten : 4760491                      Masses: 45 > 360  
 Norm: 283.1                                      RIC : 18889528                      #peaks: 405  
 Peak: 1000.00    mmu  
 Data: +/77>99



### HRMS spectra of compound 12m.

LIST: hei6458\_hpkl5f-c4                      27-Sep-12    REG : 07:30.7    #9  
 Samp:    Start : 21:29:26    5012  
 Mode: EI +VE +LMR    ESCAN (EXP) UP HR NRM  
 Oper:    Inlet :  
 Limt: ( 0)  
       : (322) C17.H37.N.F.O3  
 Peak: 1000.00    mmu    R+D: -2.0 > 60.0  
 Data: +/1405>2082    (CMASS : converted |CMASS : converted |CMASS : con

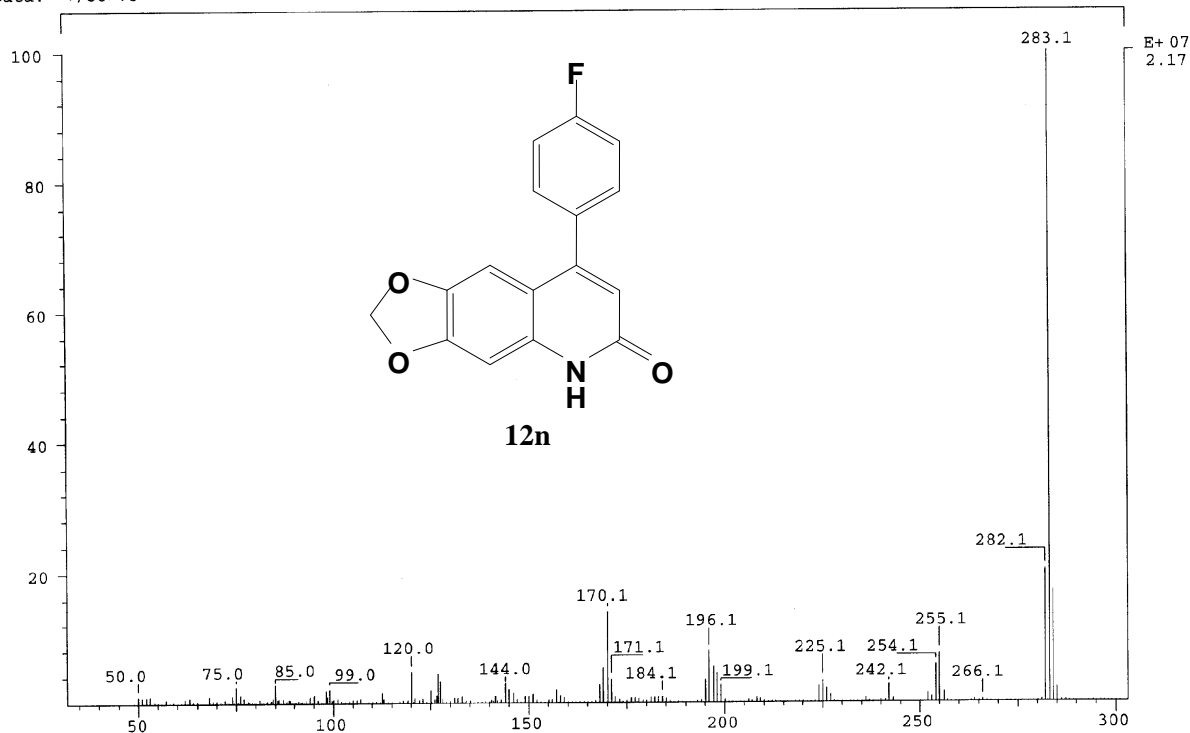
Mass	Intensity	%RA	Flags	Delta	R+D	Composition
283.0648	64505	17.01	#	-0.3	12.0	C16.H10.N.F.O3



calculated for C<sub>16</sub>H<sub>10</sub>FNO<sub>3</sub>: 283.0645:  
 found: 283.0648

### EI-MS spectra of compound 12n.

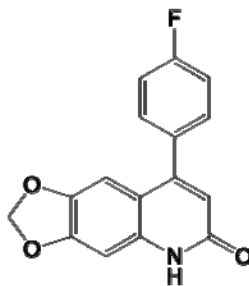
SPEC: lei7363\_hpk16f                      24-Sep-12 REG : 04:10.7    #9  
 Samp:    Start : 15:11:50    754  
 Mode: EI +VE +LMR BSCAN (EXP) UP LR NRM                      Inlet :  
 Oper:    Masses: 45 > 450  
 Base: 283.1                                      Inten : 21724394    #peaks: 463  
 Norm: 283.1                                      RIC : 71177110  
 Peak: 1000.00 mmu  
 Data: +/58>75



### HRMS spectra of compound 12n.

LIST: hei6459\_hpk16f-c3                      27-Sep-12 REG : 18:37.1    #9  
 Samp:    Start : 21:56:29    3792  
 Mode: EI +VE +LMR ESCAN (EXP) UP HR NRM                      Inlet :  
 Oper:     
 Limt: ( 0)  
       : (322) C17.H37.N.F.O3  
 Peak: 1000.00 mmu    R+D: -2.0 > 60.0  
 Data: +/3485>3537 (CMASS : converted |CMASS : converted |CMASS : con

Mass	Intensity	%RA	Flags	Delta	R+D	Composition
283.0636	28738	100.00	#	0.9	12.0	C16.H10.N.F.O3



calculated for C<sub>16</sub>H<sub>10</sub>FNO<sub>3</sub>: 283.0645;  
 found: 283.0636