Supporting Information

The diversity of alkylation/acylation products of uracil and its derivatives: synthesis and structural study

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Table S1 Input data for the regression lines using *N*MR signals of the Table 2 and the corresponding DFT calculations.

Code of the molecule	*N*ucleus	Location in the molecule	*N*MR signal	DFT predicted signal
1	*N*	*N*1	–243.5	–261.1
1	H	H1	10.48	6.60
1	C	C2	151.6	155.5
1	*N*	*N*3	–225.0	–243.1
1	H	H3	9.58	6.52

1	C	C4	164.3	167.9
1	C	C5	99.1	103.7
1	H	H5	5.21	5.20
1	C	C6	152.4	163.4
1	H	H6	.	.
1	C	CH_3atC5	.	.
1	C	CH_3atC6	18.4	21.76
1	H	HMeatC6	1.94	2.14
1	C	COOCMe_3at*N*1	.	.
1	C	COOCMe_3at*N*3	.	.
1	C	CMe_3COOat *N*1	.	.
1	C	CMe_3COOat *N*3	.	.
1	H	HMe_3at*N*1	.	.
1	H	HMe_3at*N*1	.	.
2	*N*	*N*1	–252.2	–269.7
2	H	H1	10.16	6.58
2	C	C2	151.4	155.3
2	*N*	*N*3	–223.5	–241.3
2	H	H3	9.74	6.70
2	C	C4	164.9	169.5
2	C	C5	111.7	116.4
2	H	H5	.	.
2	C	C6	136.5	145.2
2	H	H6	6.74	7.22
2	C	CH_3atC5	11.6	15.9
2	H	HmeatC5	1.61	1.81
2	C	CH_3atC6	.	.
2	H	HmeatC6	.	.
2	C	COOCMe_3at*N*1	.	.
2	C	COOCMe_3at*N*3	.	.
2	C	CMe_3COOat *N*1	.	.
2	C	CMe_3COOat *N*3	.	.
2	H	HMe_3at*N*1	.	.
2	H	HMe_3at*N*1	.	.
3	*N*	*N*1	–249.7	–266.6
3	H	H1	10.40	6.74
3	C	C2	151.3	155.5
3	*N*	*N*3	–221.3	–239.5
3	H	H3	10.16	6.65
3	C	C4	164.3	168.2
3	C	C5	100.4	104.9
3	H	H5	5.28	5.36
3	C	C6	140.6	149.7
3	H	H6	6.87	7.39
3	C	CH_3atC5	.	.
3	H	HMeatC5	.	.

3	C	CH_3atC6	.	.
3	H	HMeatC6	.	.
3	C	COOCMe_3at*N*1	.	.
3	C	COOCMe_3at*N*3	.	.
3	C	CMe_3COOat*N*1	.	.
3	C	CMe_3COOat*N*3	.	.
3	H	HMe_3at*N*1	.	.
3	H	HMe_3at*N*1	.	.
1a	*N*	*N*1	–215.4	–221.5
1a	H	H1	.	.
1a	C	C2	148.9	157.2
1a	*N*	*N*3	–227.3	–241.6
1a	H	H3	8.73	6.87
1a	C	C4	162.2	166.4
1a	C	C5	101.6	107.2
1a	H	H5	5.55	5.45
1a	C	C6	149.7	163.5
1a	H	H6	.	.
1a	C	CH_3atC5	.	.
1a	H	HMeatC5	.	.
1a	C	CH_3atC6	18.6	22.4
1a	H	HMeatC6	2.21	2.15
1a	C	COOCMe_3at*N*1	148.2	155.7
1a	C	COOCMe_3at*N*3	.	.
1a	C	CMe_3COOat*N*1	87.7	104.1
1a	C	CMe_3COOat*N*3	.	.
1a	C	CH_3CCOOat*N*1	27.4	30.5
1a	C	CH_3CCOOat*N*3	.	.
1a	H	HMe_3at*N*1	1.60	1.53
1a	H	HMe_3at*N*3	.	.
2a	*N*	*N*1	–225.6	–228.9
2a	H	H1	.	.
2a	C	C2	148.5	153.7
2a	*N*	*N*3	–225.1	–240.7
2a	H	H3	8.67	6.75
2a	C	C4	163.3	168.6
2a	C	C5	112.0	119.4
2a	H	H5	.	.
2a	C	C6	135.3	144.6
2a	H	H6	7.71	7.62
2a	C	CH_3atC5	12.4	16.2
2a	H	HMeatC5	1.96	1.87
2a	C	CH_3atC6	.	.
2a	H	HMeatC6	.	.
2a	C	COOCMe_3at*N*1	147.3	159.4
2a	C	COOCMe_3at*N*3	.	.

2a	C	CMe_3COOat*N*1	86.9	97.5
2a	C	CMe_3COOat*N*3	.	.
2a	C	$CH_3CCOOat$*N*1	27.8	28.7
2a	C	$CH_3CCOOat$*N*3	.	.
2a	H	HMe_3at*N*1	1.61	1.63
2a	H	HMe_3at*N*3	.	.
3a	*N*	*N*1	–223.9	–226.9
3a	H	H1	.	.
3a	C	C2	147.1	153.6
3a	*N*	*N*3	–223.6	–239.2
3a	H	H3	8.76	6.72
3a	C	C4	162.5	167.2
3a	C	C5	103.7	107.9
3a	H	H5	5.80	5.57
3a	C	C6	139.7	149.3
3a	H	H6	7.88	7.80
3a	C	CH_3atC5	.	.
3a	H	HMeatC5	.	.
3a	C	CH_3atC6	.	.
3a	H	HMeatC6	.	.
3a	C	$COOCMe_3at$*N*1	148.1	159.1
3a	C	$COOCMe_3at$*N*3	.	.
3a	C	CMe_3COOat*N*1	87.4	98.0
3a	C	CMe_3COOat*N*3	.	.
3a	C	$CH_3CCOOat$*N*1	27.8	28.7
3a	C	$CH_3CCOOat$*N*3	.	.
3a	H	HMe_3at*N*1	1.61	1.65
3a	H	HMe_3at*N*3	.	.
1b	*N*	*N*1	–246.8	–261.0
1b	H	H1	9.82	6.80
1b	C	C2	150.5	155.7
1b	*N*	*N*3	–193.1	–202.1
1b	H	H3	.	.
1b	C	C4	160.8	168.4
1b	C	C5	100.3	103.9
1b	H	H5	5.56	5.37
1b	C	C6	151.3	164.0
1b	H	H6	.	.
1b	C	CH_3atC5	.	.
1b	H	HMeatC5	.	.
1b	C	CH_3atC6	18.9	21.9
1b	H	HMeatC6	2.14	2.17
1b	C	$COOCMe_3at$*N*1	.	.
1b	C	$COOCMe_3at$*N*3	147.6	159.8
1b	C	CMe_3COOat*N*1	.	.
1b	C	CMe_3COOat*N*3	86.7	97.2

1b	C	$CH_3CCOOatN1$	.	.
1b	C	$CH_3CCOOatN3$	27.4	28.3
1b	H	HMe_3atN1	.	.
1b	H	HMe_3atN3	1.60	1.59
2b	*N*	*N*1	–255.6	–269.5
2b	H	H1	9.95	6.78
2b	C	C2	150.7	155.6
2b	*N*	*N*3	–191.6	–200.0
2b	H	H3	.	.
2b	C	C4	161.9	170.0
2b	C	C5	110.5	116.9
2b	H	H5	.	.
2b	C	C6	135.9	145.6
2b	H	H6	7.04	7.26
2b	C	CH_3atC5	12.3	15.9
2b	H	HMeatC5	1.91	1.86
2b	C	CH_3atC6	.	.
2b	H	HMeatC6	.	.
2b	C	$COOCMe_3atN1$	.	.
2b	C	$COOCMe_3atN3$	147.8	159.7
2b	C	$CMe_3COOatN1$	.	.
2b	C	$CMe_3COOatN3$	87.0	97.4
2b	C	$CH_3CCOOatN1$	.	.
2b	C	$CH_3CCOOatN3$	27.5	28.3
2b	H	HMe_3atN1	.	.
2b	H	HMe_3atN3	1.60	1.60
3b	*N*	*N*1	–253.4	–266.4
3b	H	H1	10.04	6.92
3b	C	C2	150.5	155.9
3b	*N*	*N*3	–189.7	–198.1
3b	H	H3	.	.
3b	C	C4	161.0	168.9
3b	C	C5	102.0	105.3
3b	H	H5	5.76	5.52
3b	C	C6	140.1	149.9
3b	H	H6	.	7.43
3b	C	CH_3atC5	.	.
3b	H	HMeatC5	.	.
3b	C	CH_3atC6	.	.
3b	H	HMeatC6	.	.
3b	C	$COOCMe_3atN1$	.	.
3b	C	$COOCMe_3atN3$	147.6	159.6
3b	C	$CMe_3COOatN1$	.	.
3b	C	$CMe_3COOatN3$	87.1	97.5
3b	C	$CH_3CCOOatN1$	.	.
3b	C	$CH_3CCOOatN3$	27.5	28.3

3b	H	HMe$_3$at*N*1	.	.
3b	H	HMe$_3$at*N*3	1.61	1.60
1c	*N*	*N*1	–216.4	–221.0
1c	H	H1	.	.
1c	C	C2	147.8	156.4
1c	*N*	*N*3	–194.0	–201.6
1c	H	H3	.	.
1c	C	C4	159.5	166.9
1c	C	C5	101.2	106.2
1c	H	H5	5.54	5.52
1c	C	C6	148.9	163.1
1c	H	H6	.	.
1c	C	CH$_3$atC5	.	.
1c	H	HMeatC5	.	.
1c	C	CH$_3$atC6	18.6	21.7
1c	H	HMeatC6	2.18	2.20
1c	C	COOCMe$_3$at*N*1	147.3	158.6
1c	C	COOCMe$_3$at*N*3	147.1	158.8
1c	C	CMe$_3$COOat*N*1	88.1	99.8
1c	C	CMe$_3$COOat*N*3	87.1	98.0
1c	C	CH$_3$CCOOat*N*1	27.4	28.3
1c	C	CH$_3$CCOOat*N*3	27.3	28.3
1c	H	HMe$_3$at*N*1	1.60	1.63
1c	H	HMe$_3$at*N*3	1.59	1.60
2c	*N*	*N*1	–226.5	–229.0
2c	H	H1	.	.
2c	C	C2	145.7	154.2
2c	*N*	*N*3	.	–199.3
2c	H	H3	.	.
2c	C	C4	161.1	169.3
2c	C	C5	111.7	119.6
2c	H	H5	.	.
2c	C	C6	134.6	144.8
2c	H	H6	7.68	7.68
2c	C	CH$_3$atC5	12.5	16.2
2c	H	HMeatC5	1.95	1.92
2c	C	CH$_3$atC6	.	.
2c	H	HMeatC6	.	.
2c	C	COOCMe$_3$at*N*1	148.4	158.9
2c	C	COOCMe$_3$at*N*3	147.4	158.8
2c	C	CMe$_3$COOat*N*1	87.3	98.5
2c	C	CMe$_3$COOat*N*3	87.0	98.1
2c	C	CH$_3$CCOOat*N*1	27.8	28.7
2c	C	CH$_3$CCOOat*N*3	27.4	28.3
2c	H	HMe$_3$at*N*1	1.59	1.65
2c	H	HMe$_3$at*N*3	1.59	1.61

3c	*N*	*N*1	–224.8	–227.2
3c	H	H1	.	.
3c	C	C2	148.0	154.2
3c	*N*	*N*3	–190.0	–197.8
3c	H	H3	.	.
3c	C	C4	159.9	168.0
3c	C	C5	103.4	108.0
3c	H	H5	5.81	5.72
3c	C	C6	138.9	149.3
3c	H	H6	7.87	7.90
3c	C	CH_3atC5	.	.
3c	H	HMeatC5	.	.
3c	C	CH_3atC6	.	.
3c	H	HMeatC6	.	.
3c	C	COOCMe_3at*N*1	147.2	158.3
3c	C	COOCMe_3at*N*3	145.5	158.8
3c	C	CMe_3COOat*N*1	87.1	99.0
3c	C	CMe_3COOat*N*3	87.6	98.2
3c	C	CH_3CCOOat*N*1	27.7	28.7
3c	C	CH_3CCOOat*N*3	27.4	28.3
3c	H	HMe_3at*N*1	1.61	1.66
3c	H	HMe_3at*N*3	1.60	1.60
1d	*N*	*N*1	–114.8	–146.8
1d	H	H1	.	.
1d	C	C2	160.0	170.6
1d	*N*	*N*3	–136.3	–169.0
1d	H	H3	.	.
1d	C	C4	166.7	177.4
1d	C	C5	108.7	110.6
1d	H	H5	7.01	6.68
1d	C	C6	173.4	184.1
1d	H	H6	.	.
1d	C	CH_3atC5	.	.
1d	H	HMeatC5	.	.
1d	C	CH_3atC6	24.1	26.5
1d	H	HMeatC6	2.56	2.52
1d	C	COOCMe_3atO2	149.4	157.5
1d	C	COOCMe_3atO4	148.7	156.3
1d	C	CMe_3COOatO2	85.4	97.5
1d	C	CMe_3COOatO4	84.7	97.9
1d	C	CH_3CCOOatO2	27.6	28.3
1d	C	CH_3CCOOatO4	27.5	28.2
1d	H	HMe_3atO2	1.54	1.64
1d	H	HMe_3atO4	1.55	1.55

Table S2 Input data for the regression lines using *N*MR signals of the Table 4 and the corresponding DFT calculations.

Code of the molecule	*N*ucleus	Location in the molecule	*N*MR signal	DFT predicted signal
1	*N*	*N*1	–243.5	–261.1
1	H	H1	10.48	6.60
1	C	C2	151.6	155.5
1	*N*	*N*3	–225.0	–243.1
1	H	H3	9.58	6.52
1	C	C4	164.3	167.9
1	C	C5	99.1	103.7
1	H	H5	5.21	5.20
1	C	C6	152.4	163.4
1	H	H6	.	.
1	C	CH_3atC5	.	.
1	C	CH_3atC6	18.4	21.76
1	H	HMeatC6	1.94	2.14
1	C	COOCMe_3at*N*1	.	.
1	C	COOCMe_3at*N*3	.	.
1	C	CMe_3COOat *N*1	.	.
1	C	CMe_3COOat *N*3	.	.
1	H	HMe_3at*N*1	.	.
1	H	HMe_3at*N*1	.	.
2	*N*	*N*1	–252.2	–269.7
2	H	H1	10.16	6.58
2	C	C2	151.4	155.3
2	*N*	*N*3	–223.5	–241.3
2	H	H3	9.74	6.70
2	C	C4	164.9	169.5
2	C	C5	111.7	116.4
2	H	H5	.	.
2	C	C6	136.5	145.2
2	H	H6	6.74	7.22
2	C	CH_3atC5	11.6	15.9
2	H	HMeatC5	1.61	1.81
2	C	CH_3atC6	.	.
2	H	HMeatC6	.	.
2	C	COOCMe_3at*N*1	.	.
2	C	COOCMe_3at*N*3	.	.
2	C	CMe_3COOat *N*1	.	.
2	C	CMe_3COOat *N*3	.	.
2	H	HMe_3at*N*1	.	.
2	H	HMe_3at*N*1	.	.
3	*N*	*N*1	–249.7	–266.6
3	H	H1	10.40	6.74
3	C	C2	151.3	155.5

3	*N*	*N*3	–221.3	–239.5
3	H	H3	10.16	6.65
3	C	C4	164.3	168.2
3	C	C5	100.4	104.9
3	H	H5	5.28	5.36
3	C	C6	140.6	149.7
3	H	H6	6.87	7.39
3	C	CH_3atC5	.	.
3	H	HMeatC5	.	.
3	C	CH_3atC6	.	.
3	H	HMeatC6	.	.
3	C	$COOCMe_3$at*N*1	.	.
3	C	$COOCMe_3$at*N*3	.	.
3	C	CMe_3COOat*N*1	.	.
3	C	CMe_3COOat*N*3	.	.
3	H	HMe_3at*N*1	.	.
3	H	HMe_3at*N*1	.	.
1i	*N*	*N*1	–246.0	–261.5
1i	H	H1	9.83	6.72
1i	C	C2	152.9	157.4
1i	*N*	*N*3	–213.4	–225.1
1i	H	H3	.	.
1i	C	C4	163.1	169.3
1i	C	C5	100.4	103.8
1i	H	H5	5.56	5.31
1i	C	C6	149.4	160.9
1i	H	H6	.	.
1i	C	CH_3atC5	.	.
1i	H	HMeatC5	.	.
1i	C	CH_3atC6	18.7	21.4
1i	H	HMeatC6	2.15	2.13
1i	C	CH_2Meat*N*1	.	.
1i	C	CH_2Meat*N*3	35.5	39.9
1i	H	HCH_2Meat*N*1	.	.
1i	H	HCH_2Meat*N*3	3.96	3.71
1i	C	CH_3CH_2at*N*1	.	.
1i	C	CH_3CH_2at*N*3	12.9	14.8
1i	H	HMeat*N*1	.	.
1i	H	HMeat*N*3	1.22	1.12
1j	*N*	*N*1	–237.7	–244.1
1j	H	H1	.	.
1j	C	C2	151.6	159.8
1j	*N*	*N*3	–212.8	–223.7
1j	H	H3	.	.
1j	C	C4	162.1	167.8
1j	C	C5	101.7	105.4

1j	H	H5	5.55	5.40
1j	C	C6	150.9	163.8
1j	H	H6	.	.
1j	C	CH_3atC5	.	.
1j	H	HMeatC5	.	.
1j	C	CH_3atC6	19.5	22.3
1j	H	HMeatC6	2.22	2.23
1j	C	CH_2Meat*N*1	40.1	45.4
1j	C	CH_2Meat*N*3	36.3	40.8
1j	H	HCH_2Meat*N*1	3.87	3.82
1j	H	HCH_2Meat*N*3	3.96	3.76
1j	C	CH_3CH_2at*N*1	14.1	15.5
1j	C	CH_3CH_2at*N*3	12.8	14.6
1j	H	HMeat*N*1	1.26	1.22
1j	H	HMeat*N*3	1.19	1.14
1l	*N*	*N*1	–179.0	–194.9
1l	H	H1	.	.
1l	C	C2	155.6	164.9
1l	*N*	*N*3	–215.8	–226.2
1l	H	H3	.	.
1l	C	C4	163.1	167.9
1l	C	C5	105.9	110.3
1l	H	H5	5.95	5.80
1l	C	C6	162.5	172.7
1l	H	H6	.	.
1l	C	CH_3atC5	.	.
1l	H	HMeatC5	.	.
1l	C	CH_3atC6	23.6	26.4
1l	H	HMeatC6	2.16	2.19
1l	C	CH_2MeatO2	64.7	71.6
1l	C	CH_2Meat*N*3	36.1	40.9
1l	H	HCH_2MeatO2	4.45	4.34
1l	H	HCH_2Meat*N*3	4.03	3.84
1l	C	CH_3CH_2atO2	14.2	16.3
1l	C	CH_3CH_2at*N*3	13.3	15.1
1l	H	HMeatO2	1.41	1.51
1l	H	HMeat*N*3	1.23	1.19
2h	*N*	*N*1	–244.3	–249.9
2h	H	H1	.	.
2h	C	C2	150.8	156.9
2h	*N*	*N*3	–225.0	–241.1
2h	H	H3	9.17	6.81
2h	C	C4	164.3	169.1
2h	C	C5	110.9	116.8
2h	H	H5	.	.
2h	C	C6	140.0	149.6

2h	H	H6	7.00	7.29
2h	C	CH_3atC5	12.4	16.1
2h	H	HMeatC5	1.93	1.83
2h	C	CH_3atC6	.	.
2h	H	HMeatC6	.	.
2h	C	CH_2Meat*N*1	43.6	49.2
2h	C	CH_2Meat*N*3	.	.
2h	H	HCH_2Meat*N*1	3.78	3.67
2h	H	HCH_2Meat*N*3	.	.
2h	C	CH_3CH_2at*N*1	14.4	16.8
2h	C	CH_3CH_2at*N*3	.	.
2h	H	HMeat*N*1	1.29	1.21
2h	H	HMeat*N*3	.	.
2j	*N*	*N*1	–245.5	–250.9
2j	H	H1	.	.
2j	C	C2	151.0	158.7
2j	*N*	*N*3	–212.1	–222.7
2j	H	H3	.	.
2j	C	C4	163.6	170.3
2j	C	C5	109.9	116.2
2j	H	H5	.	.
2j	C	C6	137.8	147.7
2j	H	H6	6.98	7.30
2j	C	CH_3atC5	13.0	16.8
2j	H	HMeatC5	1.93	1.86
2j	C	CH_3atC6	.	.
2j	H	HMeatC6	.	.
2j	C	CH_2Meat*N*1	44.4	50.1
2j	C	CH_2Meat*N*3	36.5	40.9
2j	H	HCH_2Meat*N*1	3.78	3.72
2j	H	HCH_2Meat*N*3	4.03	3.83
2j	C	CH_3CH_2at*N*1	14.3	16.7
2j	C	CH_3CH_2at*N*3	12.8	14.7
2j	H	HMeat*N*1	1.31	1.23
2j	H	HMeat*N*3	1.22	1.15
3h	*N*	*N*1	–241.2	–246.5
3h	H	H1	.	.
3h	C	C2	150.9	157.2
3h	*N*	*N*3	–222.9	–239.2
3h	H	H3	.	6.77
3h	C	C4	164.1	167.8
3h	C	C5	102.4	105.2
3h	H	H5	5.72	5.38
3h	C	C6	144.0	153.9
3h	H	H6	7.19	7.47
3h	C	CH_3atC5	.	.

3h	H	HMeatC5	.	.
3h	C	CH_3atC6	.	.
3h	H	HMeatC6	.	.
3h	C	CH_2Meat*N*1	43.9	49.9
3h	C	CH_2Meat*N*3	.	.
3h	H	HCH_2Meat*N*1	3.80	3.70
3h	H	HCH_2Meat*N*3	.	.
3h	C	CH_3CH_2at*N*1	14.4	16.8
3h	C	CH_3CH_2at*N*3	.	.
3h	H	HMeat*N*1	1.32	1.22
3h	H	HMeat*N*3	.	.
3i	*N*	*N*1	–253.4	–267.0
3i	H	H1	9.78	6.83
3i	C	C2	152.8	157.5
3i	*N*	*N*3	–209.8	–220.6
3i	H	H3	.	.
3i	C	C4	163.0	169.7
3i	C	C5	102.3	105.1
3i	H	H5	5.77	5.45
3i	C	C6	138.1	147.4
3i	H	H6	7.16	7.35
3i	C	CH_3atC5	.	.
3i	H	HMeatC5	.	.
3i	C	CH_3atC6	.	.
3i	H	HMeatC6	.	.
3i	C	CH_2Meat*N*1	.	.
3i	C	CH_2Meat*N*3	35.8	40.2
3i	H	HCH_2Meat*N*1	.	.
3i	H	HCH_2Meat*N*3	3.99	3.74
3i	C	CH_3CH_2at*N*1	.	.
3i	C	CH_3CH_2at*N*3	12.8	14.8
3i	H	HMeat*N*1	.	.
3i	H	HMeat*N*3	1.24	1.14
3j	*N*	*N*1	–242.3	–247.3
3j	H	H1	.	.
3j	C	C2	151.0	159.2
3j	*N*	*N*3	–210.0	–220.6
3j	H	H3	.	.
3j	C	C4	163.0	169.2
3j	C	C5	101.8	105.0
3j	H	H5	5.70	5.48
3j	C	C6	141.7	151.6
3j	H	H6	7.13	7.43
3j	C	CH_3atC5	.	.
3j	H	HMeatC5	.	.
3j	C	CH_3atC6	.	.

3j	H	HMeatC6	.	.
3j	C	CH_2Meat*N*1	44.7	50.9
3j	C	CH_2Meat*N*3	36.2	40.8
3j	H	HCH_2Meat*N*1	3.79	3.73
3j	H	HCH_2Meat*N*3	3.98	3.77
3j	C	CH_3CH_2at*N*1	14.3	16.6
3j	C	CH_3CH_2at*N*3	12.8	14.7
3j	H	HMeat*N*1	1.30	1.25
3j	H	HMeat*N*3	1.20	1.15
3m	*N*	*N*1	–224.4	–224.3
3m	H	H1	.	.
3m	C	C2	156.5	161.6
3m	*N*	*N*3	.	–169.2
3m	H	H3	.	.
3m	C	C4	171.3	179.7
3m	C	C5	95.8	92.5
3m	H	H5	5.85	5.78
3m	C	C6	146.1	158.3
3m	H	H6	7.40	7.83
3m	C	CH_3atC5	.	.
3m	H	HMeatC5	.	.
3m	C	CH_3atC6	.	.
3m	H	HMeatC6	.	.
3m	C	CH_2Meat*N*1	45.4	51.5
3m	C	CH_2MeatO4	63.0	69.9
3m	H	HCH_2Meat*N*1	3.90	3.76
3m	H	HCH_2MeatO4	4.43	4.42
3m	C	CH_3CH_2at*N*1	14.5	16.7
3m	C	CH_3CH_2atO4	14.2	16.2
3m	H	HMeat*N*1	1.35	1.24
3m	H	HMeatO4	1.36	1.31

Table S3 Linear regression parameters [1]for the correspondence between the *N*MR chemical shifts[2] and the DFT[3] predicted chemical shifts[4] in ppm.

*N*MR source data	Regression line	*n*	R^2
Table 2 (Boc_2O)			
^{15}N	*N*MR = 23.23 + 1.046 DFT	25	0.9454
^{1}H	*N*MR = –0.4812 + 1.2667 DFT	51	0.8807
^{13}C	*N*MR = –1.986 + 0.9559 DFT	103	0.9962
Table 4 (EtI)			
^{15}N	*N*MR = –1.791 + 0.9426 DFT	23	0.9181
^{1}H	*N*MR = –2.427 + 0.9716 DFT	83	0.9986
^{13}C	*N*MR = –0.3466 + 1.2027 DFT	61	0.8657

[1] *n* is the number of data included, R^2 is the determination coefficient

[2] *N*MR data are given in the Table 2 and Table 4

[3] DFT data are given in the Table S8A and Table S8B

[4] Based on the calculated linear regression line the lacking value for the ^{15}N chemical shift for the *N*3 nitrogen atom in the **2c** compound was – 185 ppm with the 95 % confidence interval of [–202;–168] ppm and for the *N*3 nitrogen atom in the **3m** compound was –161 ppm with the 95 % confidence interval of [–176; –147] ppm.

Table S4 $(Boc)_2O$ reaction with uracil (**3**), thymine (**2**) and 6–methyluracil (**3**)[1)]. The B3LYP/6–311G(d) theoretical estimation of ΔG including acetonitrile as solvent.

Reaction product	ΔG Uracil (**3**) kcal/mole (kJ/mol)	ΔG Thymine (**2**) kcal/mole (kJ/mol)	ΔG 6–methyluracil (**1**) kcal/mole (kJ/mol)
N^1–Boc	–11.03 (–46.16) **3a**	–10.89 (–45.58) **2a**	+2.11 (+8.81) **1a**
O^2–Boc	+2.26 (+9.45)	+3.10 (+12.96)	+2.77 (+11.59)
N^3–Boc	–10.96 (–45.84) **3b**	–10.13 (–42.37) **2b**	–10.49 (–43.87) **1b**
O^4–Boc	–0.68 (–2.86)	+0.18 (+0.77)	–0.72 (–3.00)
C^5–Boc	–19.18 (–80.24)	–	–15.23(–63.71)
C^6–Boc	–18.92 (–79.15)	–14.67 (–61.38)	–
N^1,O^2–diBoc	–3.98 (–16.66)	–5.49 (–22.98)	–1.45 (–6.06)
N^1,N^3–diBoc	–21.08 (–88.19) **3c**	–21.00 (–87.89) **2c**	–18.86 (–78.91) **1c**
N^1,O^4–diBoc	–10.91 (–45.64) **3f**	–10.79 (–45.17) **2f**	–10.25 (–42.90) **1f**
N^1,C^5–diBoc	–29.05 (–121.57)	–	–22.73 (–95.11)
N^1,C^6–diBoc	–24.21 (–101.30)	–22.30 (–93.29)	–
O^2,N^3–diBoc	–3.42 (–14.32) **3e**	–7.98 (–33.37) **2e**	–3.40 (–14.23) **1e**
O^2,O^4–diBoc	–6.36 (–26.61) **3d**	–6.94 (–29.03) **2d**	–6.71 (–28.06) **1d**
O^2,C^5–diBoc	–15.83 (–66.22)	–	–13.29 (–55.61)
O^2,C^6–diBoc	–16.09 (–67.33)	–12.36 (–51.70)	–
N^3,O^4–diBoc	–2.18 (–9.14)	–0.77 (–3.24)	–2.97 (–12.42)
N^3,C^5–diBoc	–29.07 (–121.62)	–	–25.36 (–106.11)
N^3,C^6–diBoc	–28.95 (–121.14)	–25.24 (–105.60)	–
O^4,C^5–diBoc	–11.76 (–49.19)	–	–9.42 (–39.40)
O^4,C^6–diBoc	–18.52 (–77.47)	–13.96 (–58.41)	–
C^5,C^6–diBoc	–29.85 (–124.90)	–	–

[1)] Models of the $(Boc)_2O$ reaction with **3**, **2**, **1**:

3/**2**/**1** + *n**Boc_2O → product + *n***tert*–Butanol + *n**CO_2

where *n*=1 for mono–substitutions, and *n*=2 for di–substitutions.

Table S5 Ethylation of uracil, thymine and 6–methyluracil [1)]. The B3LYP/6–311G(d) theoretical estimation of ΔG including DMF as solvent.

Reaction product	ΔG Uracil (**3**) kcal/mole (kJ/mol)	ΔG Thymine (**2**) kcal/mole (kJ/mol)	ΔG 6–methyluracil (**3**) kcal/mole (kJ/mol)
N^1–Et	–39.03 (–163.32) **3h**	–27.99 (–117.11)**2h**	–23.73 (–99.30) **1h**
O^2–Et	–20.85 (–87.25)	–6.77 (–28.34)	–9.20 (–38.51)
N^3–Et	–38.64 (–161.69) **3i**	–27.56 (–115.33) **2i**	–27.20 (–113.80) **1i**
O^4–Et	–22.59 (–94.52)	–10.88 (–45.51)	–11.35 (–47.48)
C^5–Et	–44.39 (–185.75)	–	–30.47 (–127.50)
C6–Et	–46.99 (–196.59)	–33.59 (–140.55)	–
N^1,O^2–diEt	–55.21 (–231.00)	–34.87 (–145.91)	–29.51 (–123.46)
N^1,N^3–diEt	–77.39 (–323.81) **3j**	–55.74 (–233.23) **2j**	–52.06 (–217.83) **1j**
N^1,O^4–diEt	–57.63 (–241.13) **3m**	–40.56 (–169.73) **2m**	–36.24 (–151.62) **1m**
N^1,C^5–diEt	–82.88 (–346.76)	–	–53.71 (–224.71)

N^1,C^6–diEt	–80.60 (–337.25)	–56.10 (–234.72)	–
O^2,N^3–diEt	–59.82 (–250.27) **3l**	–37.48 (–156.82) **2l**	–37.93 (–158.72) **1l**
O^2,O^4–diEt	–46.35 (–193.93) **3k**	–28.06 (–117.39) **2k**	–24.27 (–101.53) **1k**
O^2,C^5–diEt	–61.86 (–258.81)	–	–37.90 (–158.56)
O^2,C^6–diEt	–62.93 (–263.31)	–40.16 (–168.03)	–
N^3,O^4–diEt	–53.68 (–224.61)	–25.50 (–106.71)	–32.24 (–134.91)
N^3,C^5–diEt	–82.19 (–343.87)	–	–58.60 (–245.17)
N^3,C^6–diEt	–85.03 (–355.76)	–61.25 (–256.28)	–
O^4,C^5–diEt	–65.35 (–273.42)	–	–41.14 (–172.14)
O^4,C^6–diEt	–69.38 (–290.28)	–44.88 (–187.78)	–
C^5,C^6–diEt	–88.73 (–371.23)	–	–

1) Models of the EtI reaction with **1**, **2**, **3**:

(**3**/**2**/**1**) + *n**EtI + (*n*/2)*K_2CO_3→product + *n**KI + (*n*/2)*H_2O + (*n*/2)*CO_2

where *n*=1 for mono–substitutions, and *n*=2 for di–substitutions

Table S6 Comparison of experimental yields of di–Boc and di–Et products with theoretical ones based on ΔG calculations.

	Experimental yield of the reactions[1]			Theoretical, ΔG [kcal/mol]		
	U	T	6–MeU	U	T	6–MeU
di–Boc	N^1,N^3 (**3c**)	N^1,N^3 (**2c**)	N^1,N^3 (**1c**)	N^1,N^3	N^1,N^3	N^1,N^3
	—	—	5% 1.5 eq D	–21.1	–21.0	–18.9
	42 % 3.0 eq D	39 % 3.0 eq D	11 % 3.0 eq D			
	77 % 3.0 eq P	89 % 3.0 eq P	20 % 3.0 eq P			
	O^2,O^4	O^2,O^4	O^2,O^4 (**1d**)	O^2,O^4	O^2,O^4	O^2,O^4
	—	—	12 % 1.5 eq D	–6.4	–6.9	–6.7
	—	—	32 % 3.0 eq D			
	O^2,N^3	O^2,N^3	O^2,N^3	O^2,N^3	O^2,N^3	O^2,N^3
	—	—	—	–3.4	–8.0	–3.4
di–Et	N^1,N^3 (**3j**)	N^1,N^3 (**2j**)	N^1,N^3 (**1j**)	N^1,N^3	N^1,N^3	N^1,N^3
	—	26 % 1.0 eq	30 % 1.0 eq	–39.0	–28.0	–23.7
	31 % 1.5 eq	30 % 1.5 eq	75 % 1.5 eq			
	29 % 3.0 eq	32 % 1.5 eq	99 % 3.0 eq			
	O^2,O^4	O^2,O^4	O^2,O^4	O^2,O^4	O^2,O^4	O^2,O^4
	–	–	–	–46.4	–28.1	–24.3
	O^2,N^3	O^2,N^3	O^2,N^3 (**1l**)	O^2,N^3	O^2,N^3	O^2,N^3
	—	—	3 % 1.5 eq	–59.8	–37.5	–37.9
	N^1,O^4 (**3m**)	N^1,O^4	N^1,O^4	N^1,O^4	N^1,O^4	N^1,O^4
	1 % 1.5 eq	—	—	–57.6	–40.6	–36.2
	1 % 3.0 eq	—	—			

Table S7 Comparison of experimental yields of mono–Boc and mono–Et products with theoretical ones based on ΔG calculations.

	Experimental yield of the reactions[1]			Theoretical, ΔG [kcal/mol]		
	U	T	6–MeU	U	T	6–MeU
mono–Boc	N^1 (**3a**)	N^1 (**2a**)	N^1 (**1a**)	N^1	N^1	N^1

	—	33 % 1.5eq D	5 % 1.5eq D	–11.0	–10.9	2.1
	12 % 3.0eq D	59 % 3.0eq D	3 % 3.0eq D			
	—	—	9 % 3.0eq P			
	N^3 (**3b**)	*N*^{3} (**2b**)	*N*^{3} (**1b**)	*N*^{3}	*N*^{3}	*N*^{3}
	—	4 % 3.0eq P	5 % 1.5eq D	–11.0	–10.1	–10.5
	12 % 3.0eq D	—	3 % 3.0eq D			
	23 % 3.0eq P	—	15 % 3.0eq P			
mono–Et	*N*^{1} (**3h**)	*N*^{1} (**2h**)	*N*^{1}	*N*^{1}	*N*^{1}	*N*^{1}
	—	19 % 1.0eq	—	–39.0	–28.0	–23.7
	12 % 1,5 eq	22 % 1.5eq	—			
	16 % 3,0 eq	33 % 3.0 eq	—			
	N^3 (**3i**)	*N*^{3}	*N*^{3} (**1i**)	*N*^{3}	*N*^{3}	*N*^{3}
	—	—	17 % 1.0eq	–38.6	–27.6	–27.2
	1 % 1.5eq	—	5 % 1.5eq			
	1 % 3.0eq	—	—			

Table S8 The molecular structure of the **1g** product for the reaction of pyridine (**4**) and Boc_2O with 3–Boc–6–methyluracil (**1b**) according to the B3LYP/6–31G(d,p) calculations. Geometry readable by the JMol software.

C	1.916592	4.482851	0.867407
C	2.1090113	049713	0.453690
C	1.098484	2.177506	0.163332
C	1.430283	0.814915	–0.223707
N	2.817325	0.515411	–0.259345
C	3.854049	1.382709	0.36960
N	3.424213	2.643926	0.381503
H	4.158033	3.305004	0.602001
O	5.028663	1.059453	–0.002887
C	3.190759	–0.836639	–0.677551
O	3.403014	–1.102829	–1.826657
O	3.235844	–1.612180	0.382780
C	3.573083	–3.073560	0.281969
C	2.523637	–3.772164	–0.576935
H	2.687517	–4.851820	–0.534051
H	1.518519	–3.566617	–0.200493
H	2.577864	–3.460616	–1.619517
C	4.990615	–3.224458	–0.261231
H	5.289474	–4.273720	–0.196132
H	5.062336	–2.913831	–1.303090
H	5.694761	–2.634564	0.331075
C	3.486398	–3.522896	1.735761
H	3.708901	–4.589926	1.805864
H	4.204598	–2.980985	2.355704
H	2.484331	–3.354644	2.137266
O	0.640658	–0.070817	–0.515087
C	–0.373713	2.582748	0. 234069
C	–1.076924	2.486177	–1.103463
C	–2.162030	1.741981	–1.317759
N	–2.768708	0.974909	–0.303285
C	–3.882537	0.202925	–0.626181
O	–4.331432	–0.461996	0.444265
C	–5.523353	–1.350930	0.373016

C	–5.257565	–2.498327	–0.599357
H	–5.185497	–2.146288	–1.627342
H	–4.330577	–3.016567	–0.339165
H	–6.075294	–3.221329	–0.538771
C	–5.631120	–1.866439	1.805189
H	–4.729015	–2.411742	2.093146
H	–5.775548	–1.041278	2.506940
H	–6.483860	–2.543529	1.893083
C	–6.756150	–0.531731	–0.003177
H	–6.694590	–0.156240	–1.023699
H	–7.647603	–1.158961	0.080039
H	–6.876634	0.315775	0.677048
O	–4.350846	0.165633	–1.747268
C	–2.230695	1.066863	0.996942
C	–1.148237	1.796805	1.270686
H	–0.800719	1.833206	2.297999
H	–2.767054	0.516592	1.753976
H	–2.657314	1.681083	–2.275649
H	–0.673230	3.059377	–1.931675
H	–0.378593	3.634815	0.538884
H	2.872507	4.971975	1.059777
H	1.400185	5.048429	0.088536
H	1.315955	4.550299	1.776993

Table S9 ΔG free energy, kcal/mol, of the reactions leading to the formation of the **1g** product according to the B3LYP/6–31G(d) calculations.

Reaction	Substrates	Products	ΔG
R1	**4** + $(Boc)_2O$	$\mathbf{5}^{(+)}$ + $Boc^{(-)}$	21.8
R2	$\mathbf{5}^{(+)}$ **+** $Boc^{(-)}$ + **1b**	**6**[1]	40.7
R3	**6**	**1g** + CO_2 + *tert*–Butanol	–48.2
		Sum of ΔG	14.3[1)]

[1)] The geometry of **6** is given in the Table S7.

Table S10 The molecular structure of the transition complex (**6**) for the reaction of pyridine (**4**) and Boc_2O with 3–Boc–6–methyluracil (**1b**), Scheme 2, according to the B3LYP/6–31G(d) calculations. Geometry readable by the JMol software.

C	–2.257480	0.519040	3.476540
C	–1.510368	1.182451	2.374032
C	–1.142166	0.462009	1.166957
C	–0.413417	1.261447	0.128385
N	–0.166848	2.620945	0.426448
C	–0.556162	3.284099	1.563966
N	–1.256270	2.477031	2.493697
O	–0.347490	4.456894	1.790249
C	0.501958	3.427685	–0.612803
O	–0.138861	4.034428	–1.430716
O	1.798625	3.330414	–0.439698
C	2.772631	4.027442	–1.354044

C	2.588994	3.496897	–2.773897
C	2.563884	5.535684	–1.241548
C	4.116157	3.603407	–0.767969
O	–0.051380	0.829067	–0.948667
C	–0.501558	–0.979471	1.437985
C	–0.518818	–1.871254	0.225366
C	0.574117	–2.470304	–0.259551
N	1.854312	–2.295264	0.303786
C	2.939359	–2.959692	–0.274852
O	4.073914	–2.679735	0.377708
C	5.377008	–3.263277	–0.035311
C	5.724776	–2.801928	–1.451403
C	6.341172	–2.660202	0.986015
C	5.326178	–4.786062	0.096640
O	2.815046	–3.688055	–1.246603
C	1.962063	–1.463205	1.429204
C	0.899747	–0.858031	1.978828
O	–3.739426	0.069263	0.489936
C	–4.220333	–0.869204	–0.233047
O	–5.597109	–0.757821	–0.308351
C	–6.410709	–1.702109	–1.068767
C	–7.834490	–1.178843	–0.848736
C	–6.054098	–1.647202	–2.559132
C	–6.276047	–3.118332	–0.496229
O	–3.609295	–1.778502	–0.814871
H	–1.575451	2.983576	3.320116
H	3.390105	3.895589	–3.405483
H	2.654108	2.403715	–2.788234
H	1.631127	3.801909	–3.200924
H	3.355715	6.044563	–1.801624
H	1.600129	5.844052	–1.652751
H	2.625232	5.856356	–0.195997
H	4.924839	4.053922	–1.352078
H	4.212157	3.937303	0.270516
H	4.230435	2.514901	–0.800033
H	5.040147	–3.222672	–2.190308
H	5.691270	–1.708604	–1.517635
H	6.742607	–3.125926	–1.695057
H	6.341061	–1.566646	0.923847
H	6.063013	–2.952346	2.004351
H	7.357385	–3.017266	0.789940
H	4.635385	–5.228454	–0.623659
H	6.326273	–5.195965	–0.082565
H	5.017359	–5.073230	1.108074
H	1.065557	–0.240512	2.857885
H	2.959649	–1.361043	1.831462
H	0.556542	–3.130721	–1.115871
H	–1.477309	–2.035008	–0.261491
H	–1.167527	–1.411560	2.196452
H	–2.677182	1.243139	4.180403
H	–3.059222	–0.088470	3.045220
H	–1.584132	–0.155094	4.021192
H	–2.234622	0.205759	0.724309
H	–8.559834	–1.808182	–1.376435
H	–8.087487	–1.181141	0.217662

H	–7.932212	–0.153039	–1.222006
H	–6.747161	–2.271538	–3.135609
H	–6.135737	–0.618625	–2.931077
H	–5.035451	–2.000217	–2.729040
H	–6.977651	–3.795629	–0.997652
H	–5.261386	–3.497501	–0.629879
H	–6.512673	–3.118267	0.574800

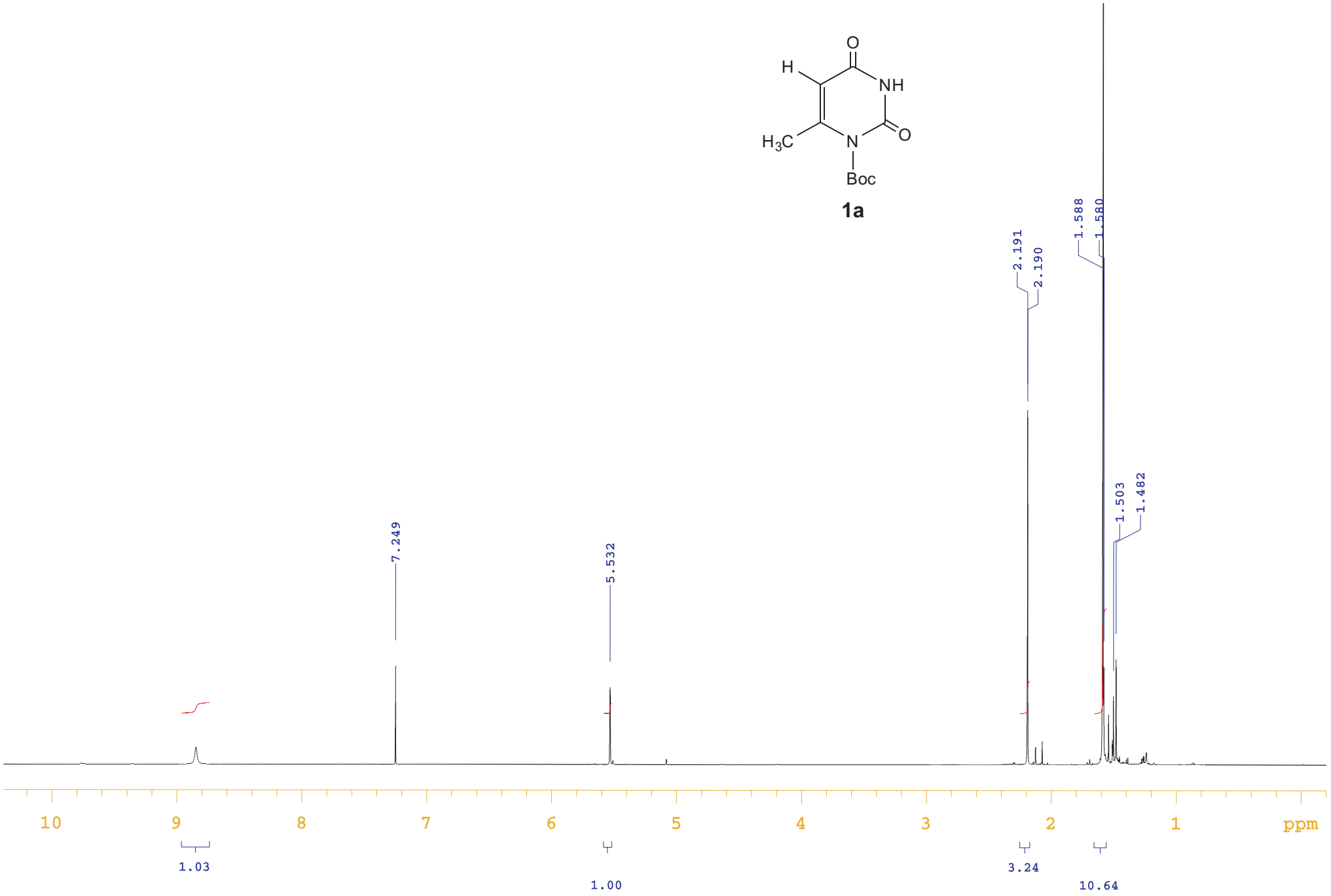
Table S11 The Fukui's condensed function, f^-, calculated with the DFT/B3LYP/6–31G(d,p) method and using the Mulliken net charges.

Position in the molecule	Uracil (**3**)	Thymine (**2**)	6–methyluracil (**1**)	N^3–Boc–6–methyluracil (**1b**)	N^1–Boc–6–methyluracil (**1a**)
*N*1	–0.092	–0.077	–0.081	–0.078	0.050
*N*3	0.000	0.003	0.001	0.011	–0.002
O2	–0.098	–0.096	–0.089	–0.089	–0.080
O4	–0.106	–0.089	–0.106	–0.104	–0.103
C5	–0.165	–0.097	–0.186	–0.187	–0.173
C6	–0.111	–0.133	–0.069	–0.069	–0.067

Table S12 The effect of H–bonded pyridine (**4**) and DMAP on the predicted ΔG, in kcal/mol, of reaction of $(Boc)_2O$ with 6–methyluracil.

Product	*N*o explicite solvent B3LYP/6–31G(d,p)	H–bonded Pyridine B3LYP/6–31G(d,p)	H–bonded DMAP B3LYP/6–31G(d,p)
N^1–Boc **3a**	5.1	5.2	2.3
N^3–Boc **3b**	–7.1	–7.2	–10.9
N^1,N^3–di–Boc **3c**	–12.1	–11.7	–21.2
O^2,O^4–di–Boc **3d**	–2.7	–2.3	–11.8
O^2,N^3–di–Boc **3e**	2.4	2.8	–6.7

Copies of the ^{1}H and ^{13}C NMR spectra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N
O
Boc
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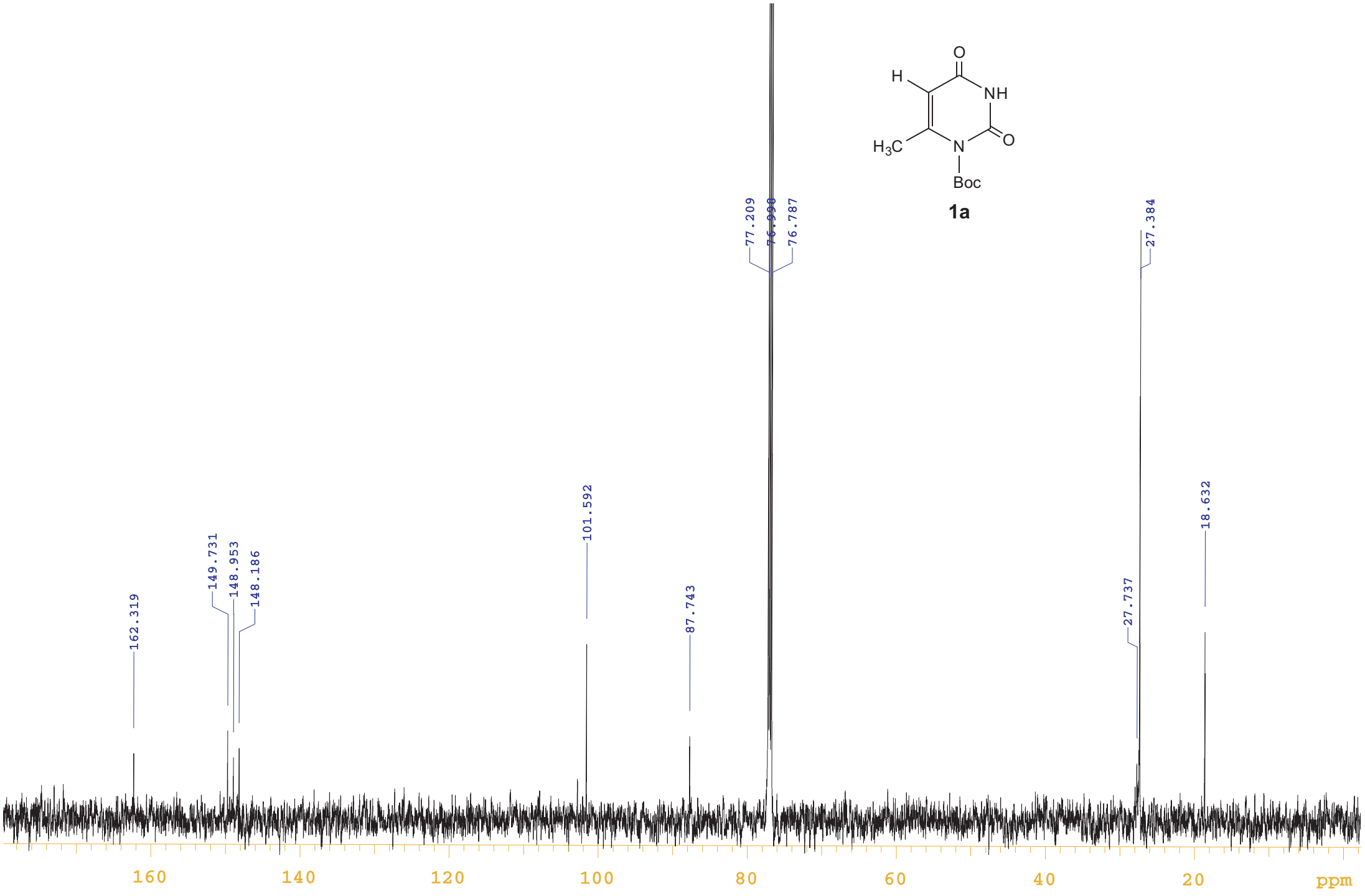
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H
NH
H3C
N
O
Boc
1a
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76.998
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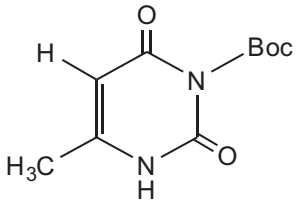
40
20
ppm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Boc
N
H_3C
N
H
O

1b

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8
7
6
5
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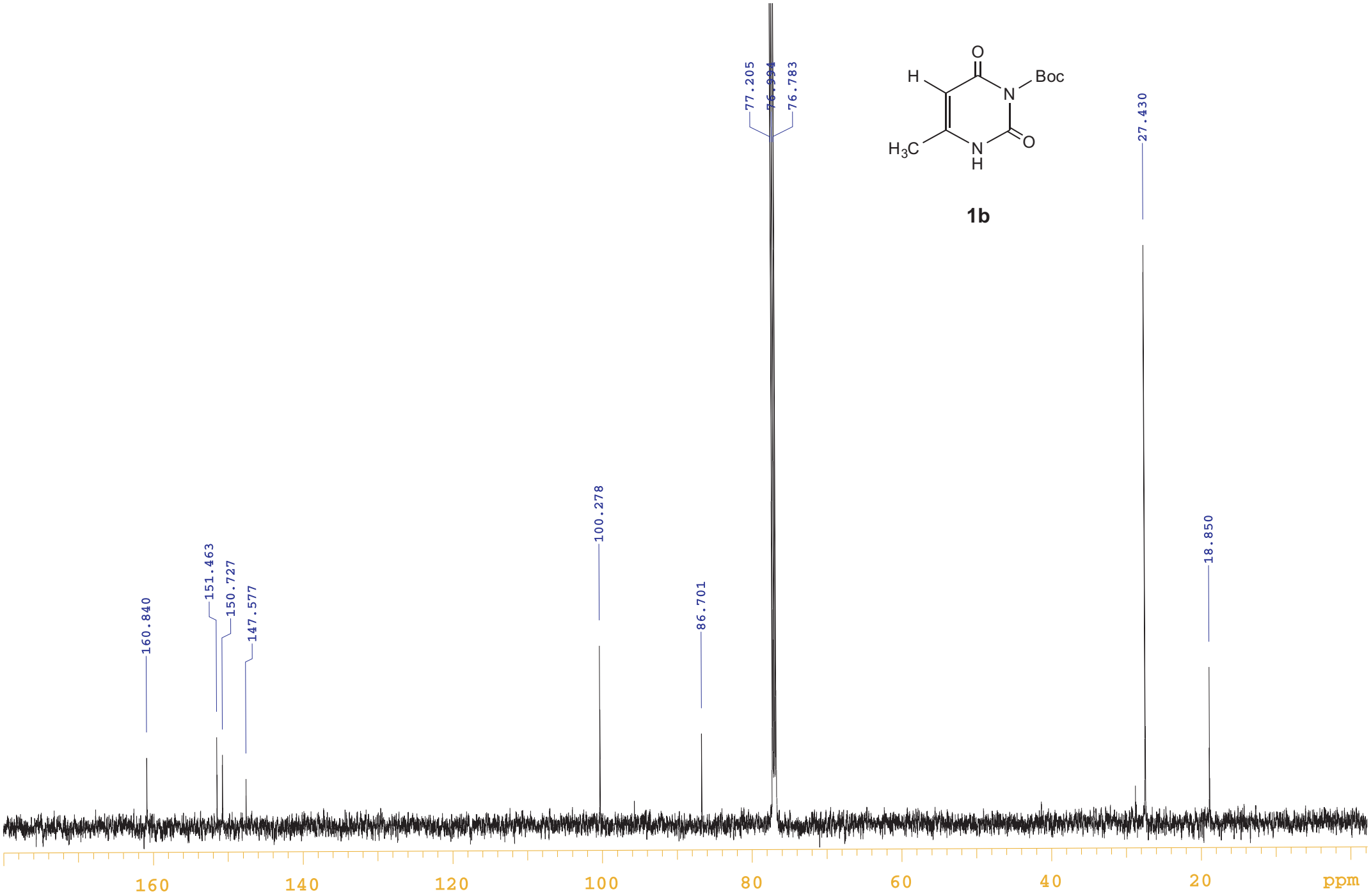
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N
H_3C
N
H
O
1b
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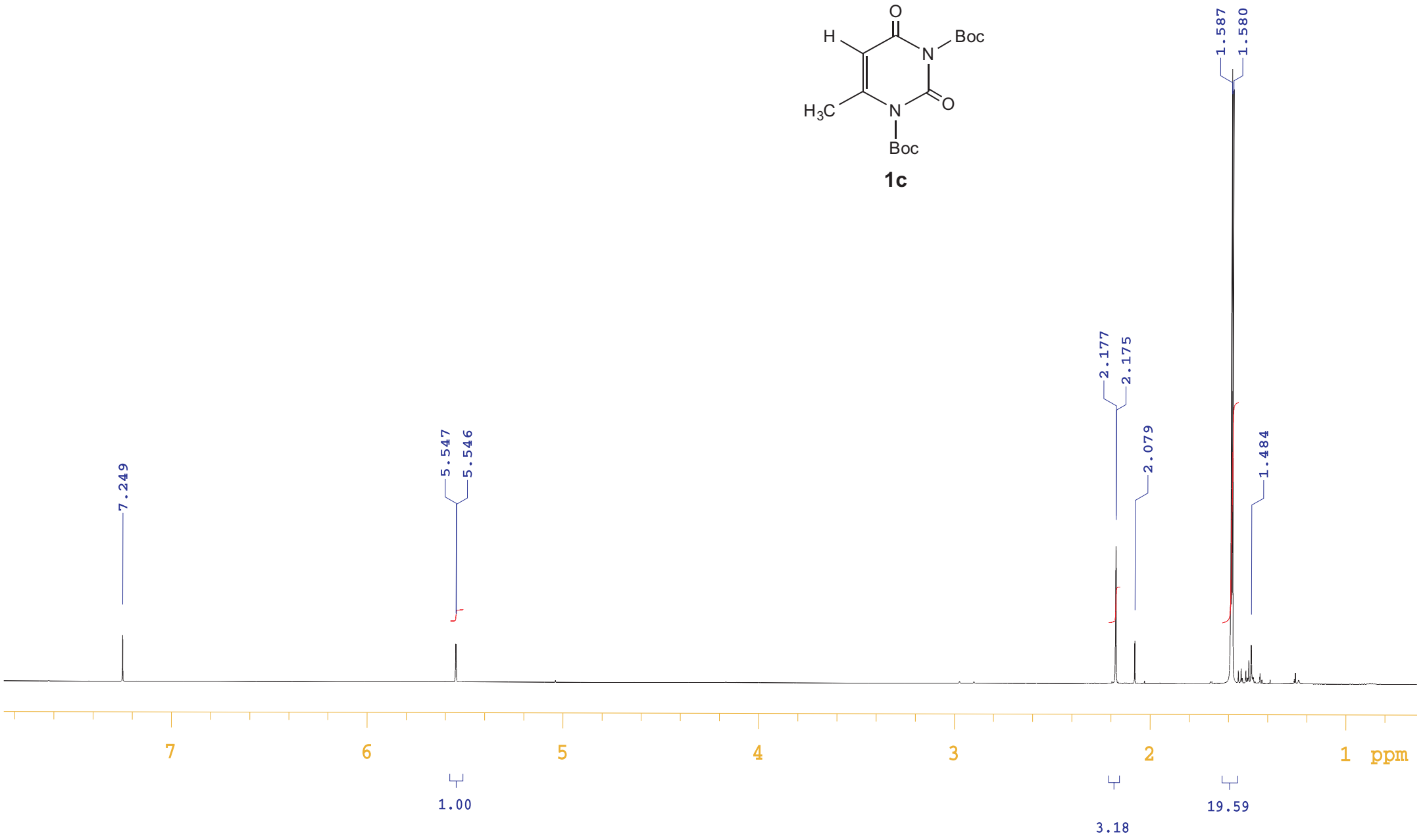
120
100
80
60
40
20
ppm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Boc
N
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O
Boc
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2
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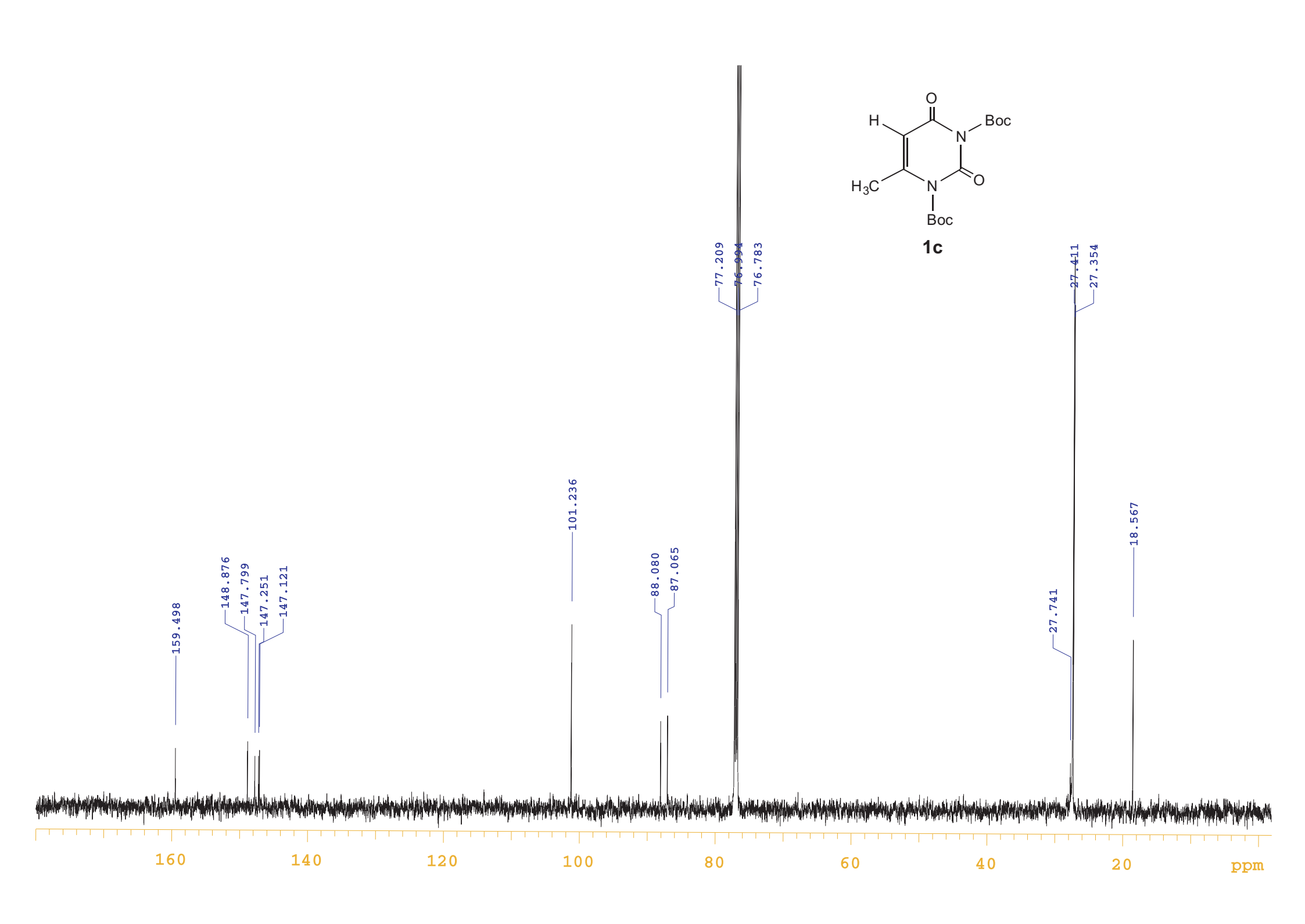
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N
H3C
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O
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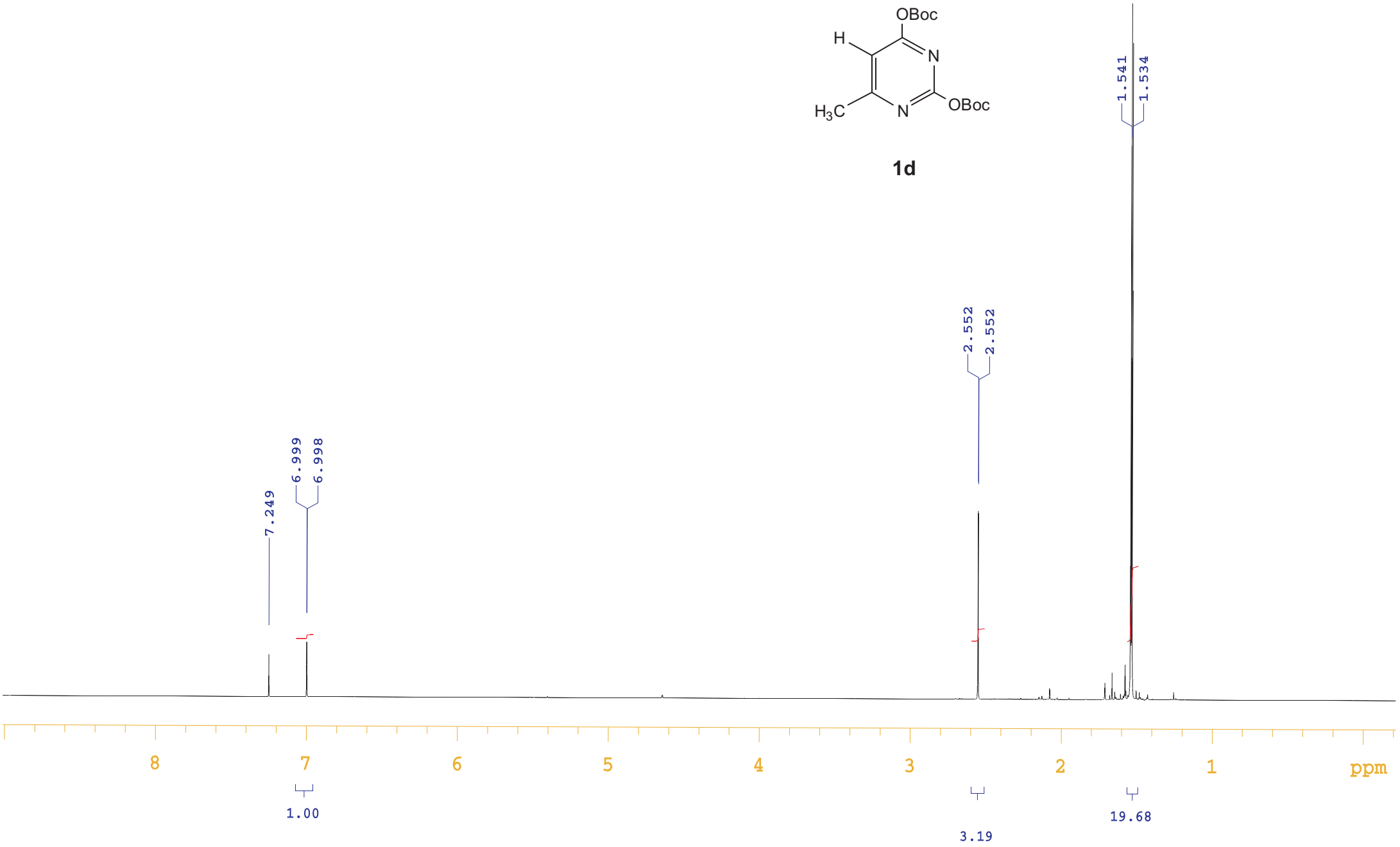
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H3C
N
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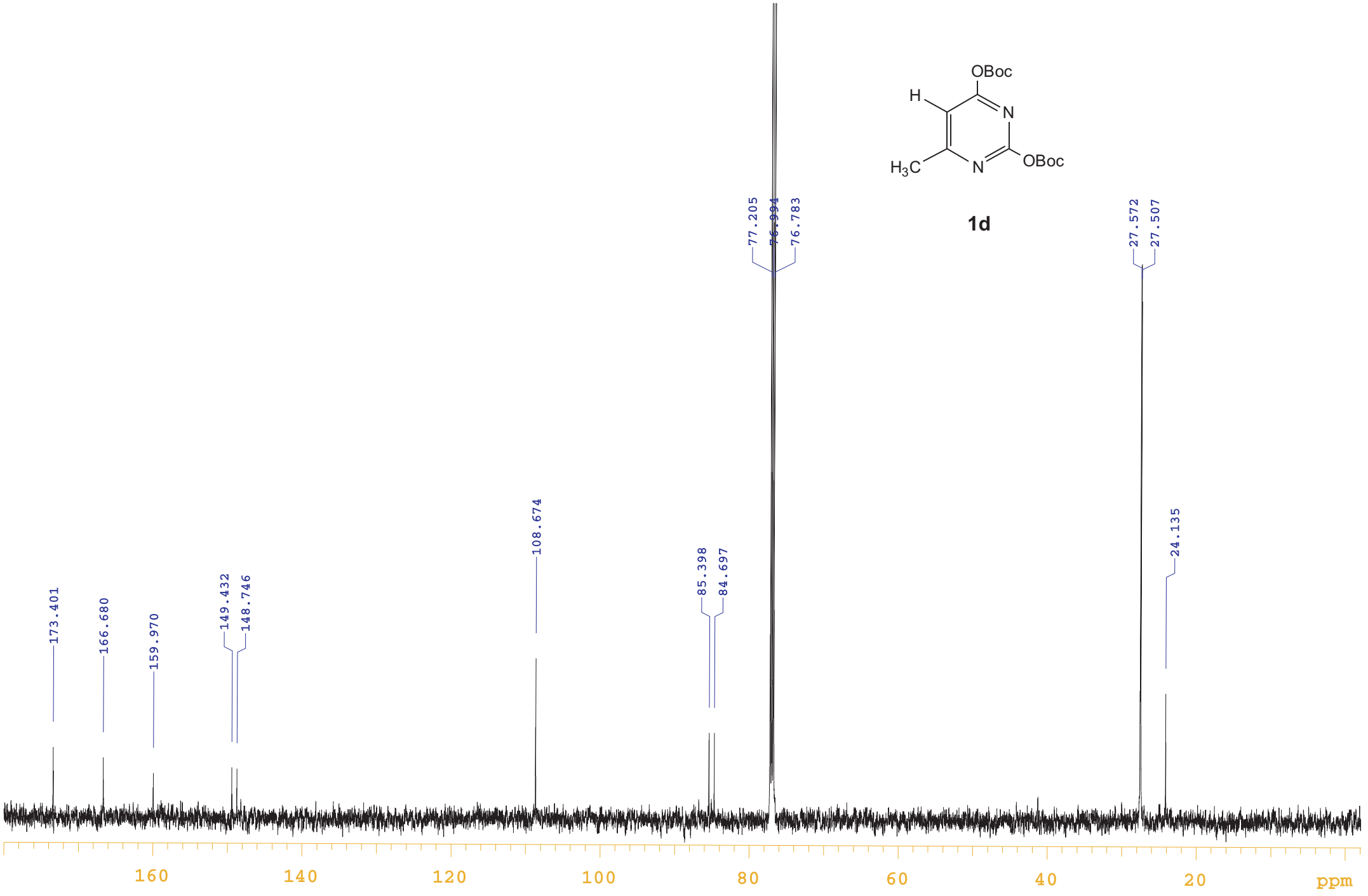
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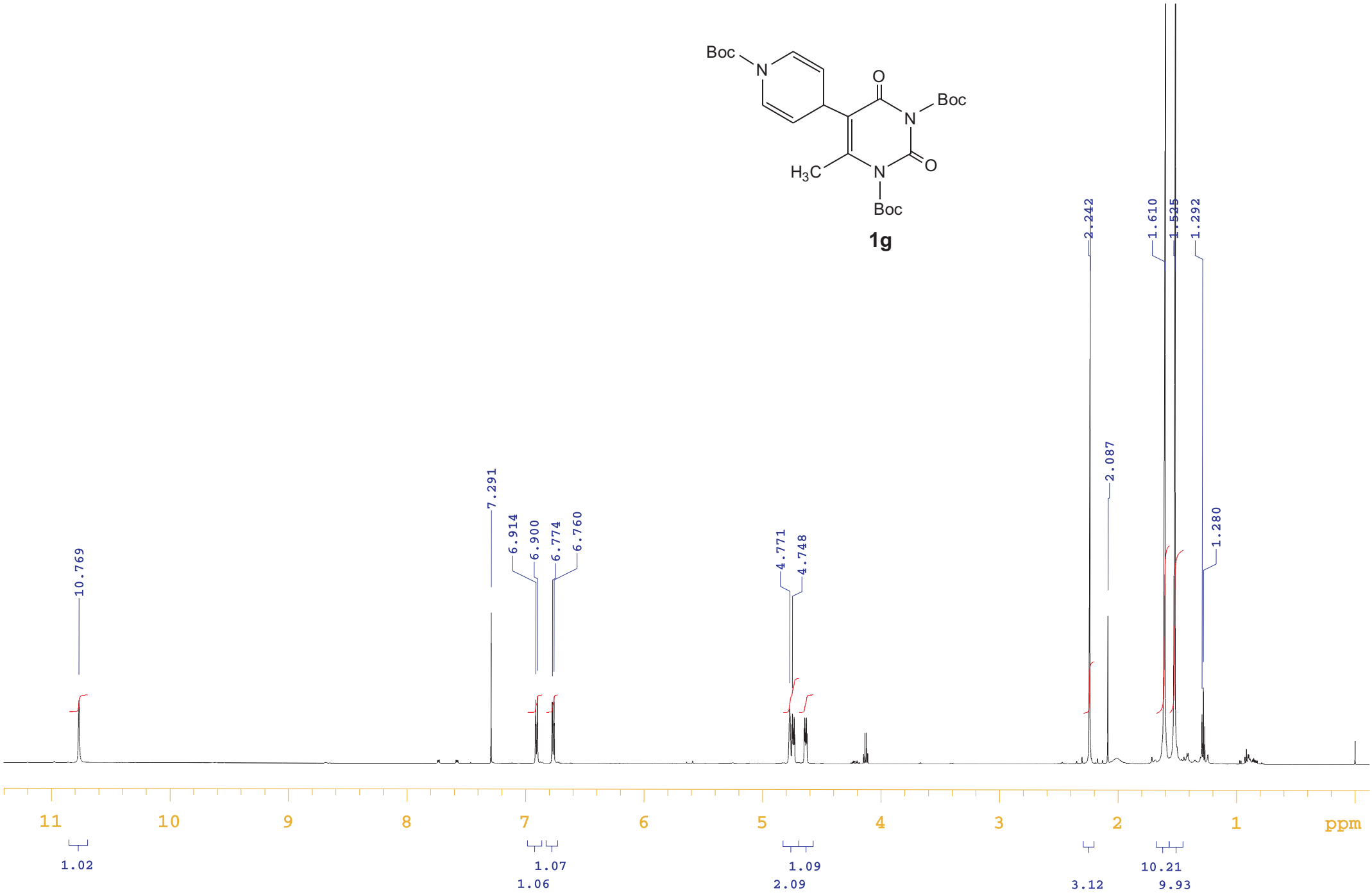
60
40
20
ppm


Boc
N
O
Boc
N
H3C
N
O
Boc
1g
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6.914
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6.774
6.760
4.771
4.748
2.242
2.087
1.610
1.525
1.292
1.280
11
10
9
8
7
6
5
4
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2
1
ppm
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1.06
1.09
2.09
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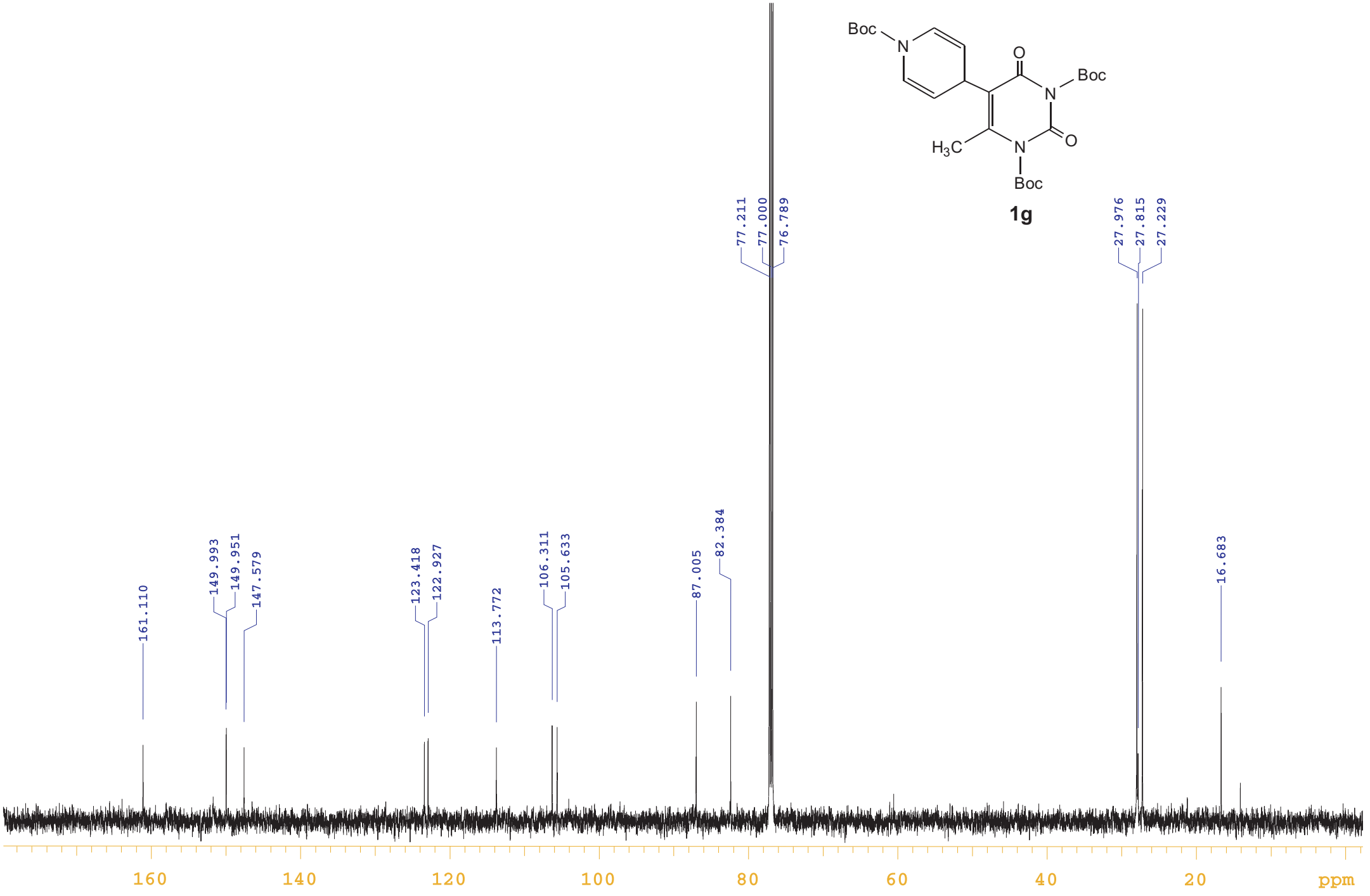
10.21
9.93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O
Boc
N
O
H3C
N
Boc
1g
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27.815
27.229
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149.993
149.951
147.579
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20
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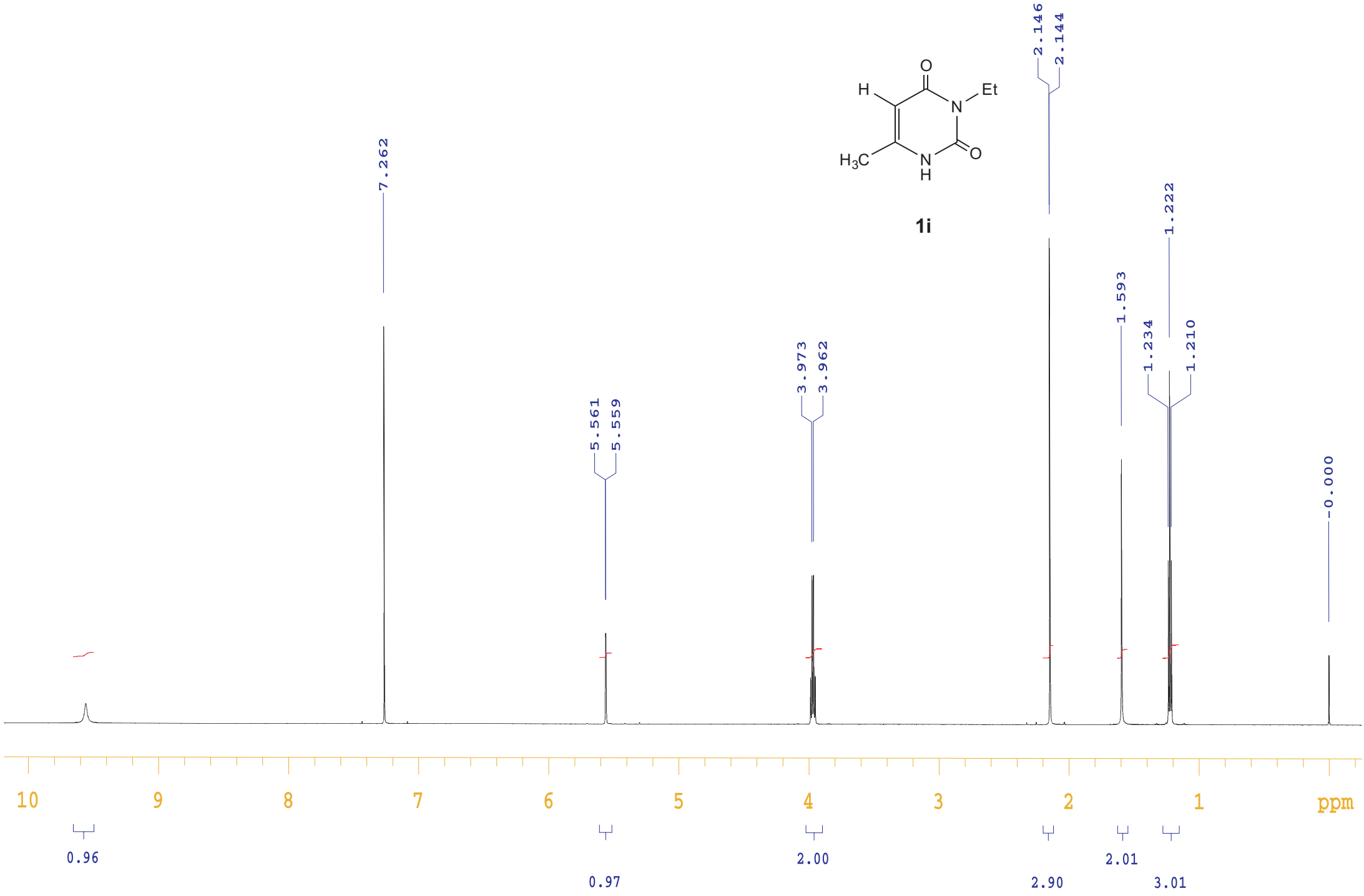
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9
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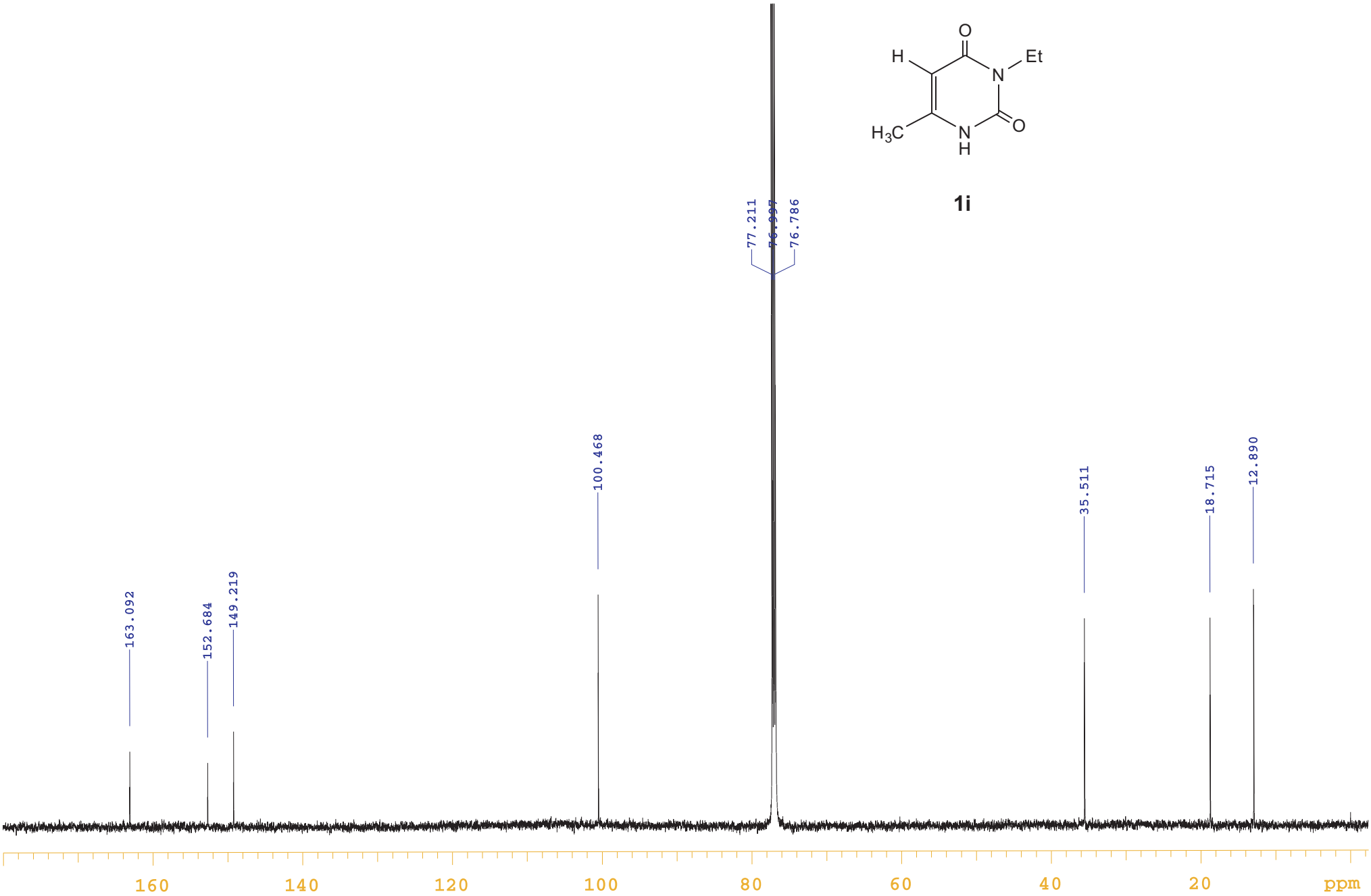
3.01

1i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H
O
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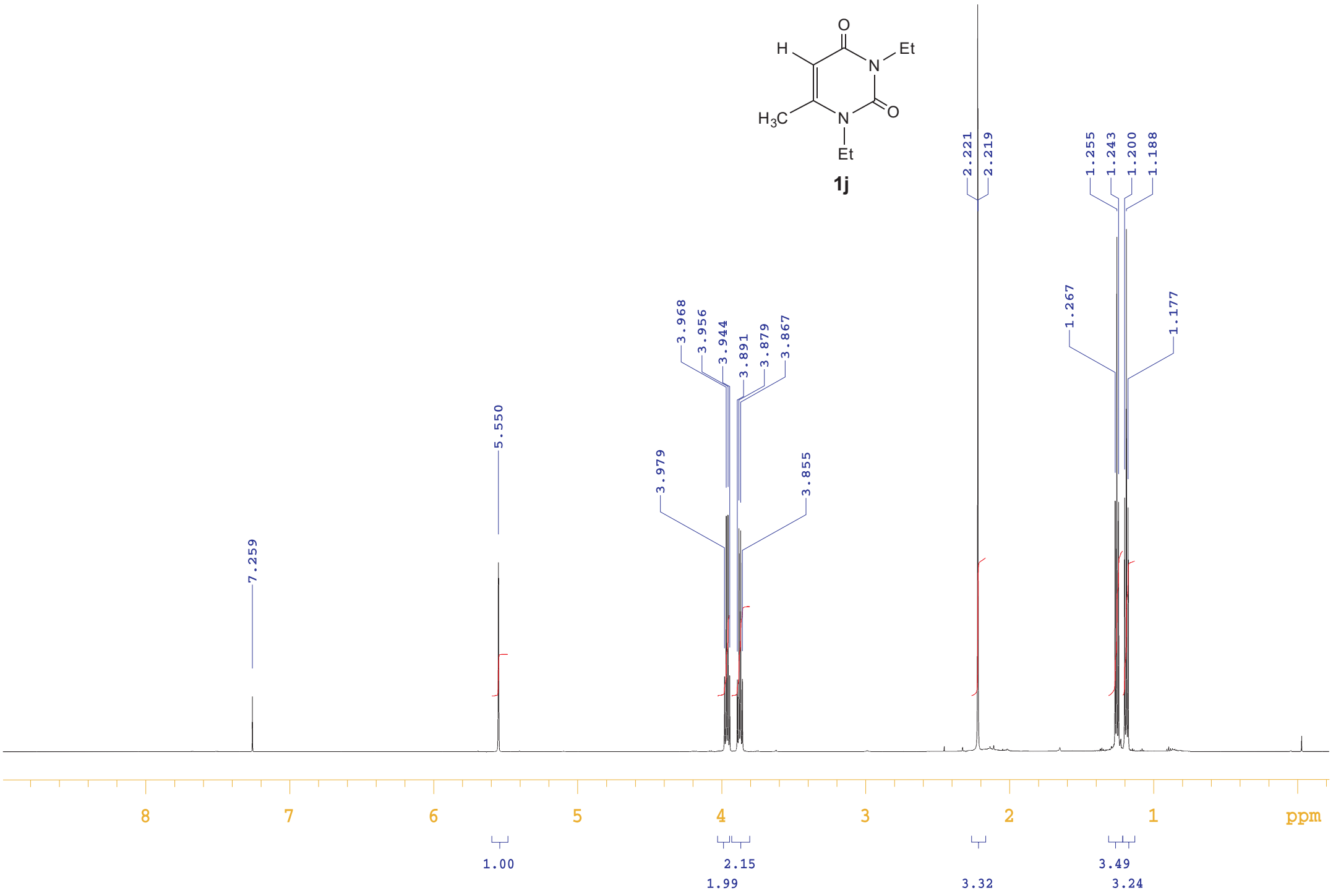
60
40
20
ppm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Et
N
H3C
N
O
Et
1j
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3.879
3.867
3.855
2.221
2.219
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1.255
1.243
1.200
1.188
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5
4
3
2
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2.15
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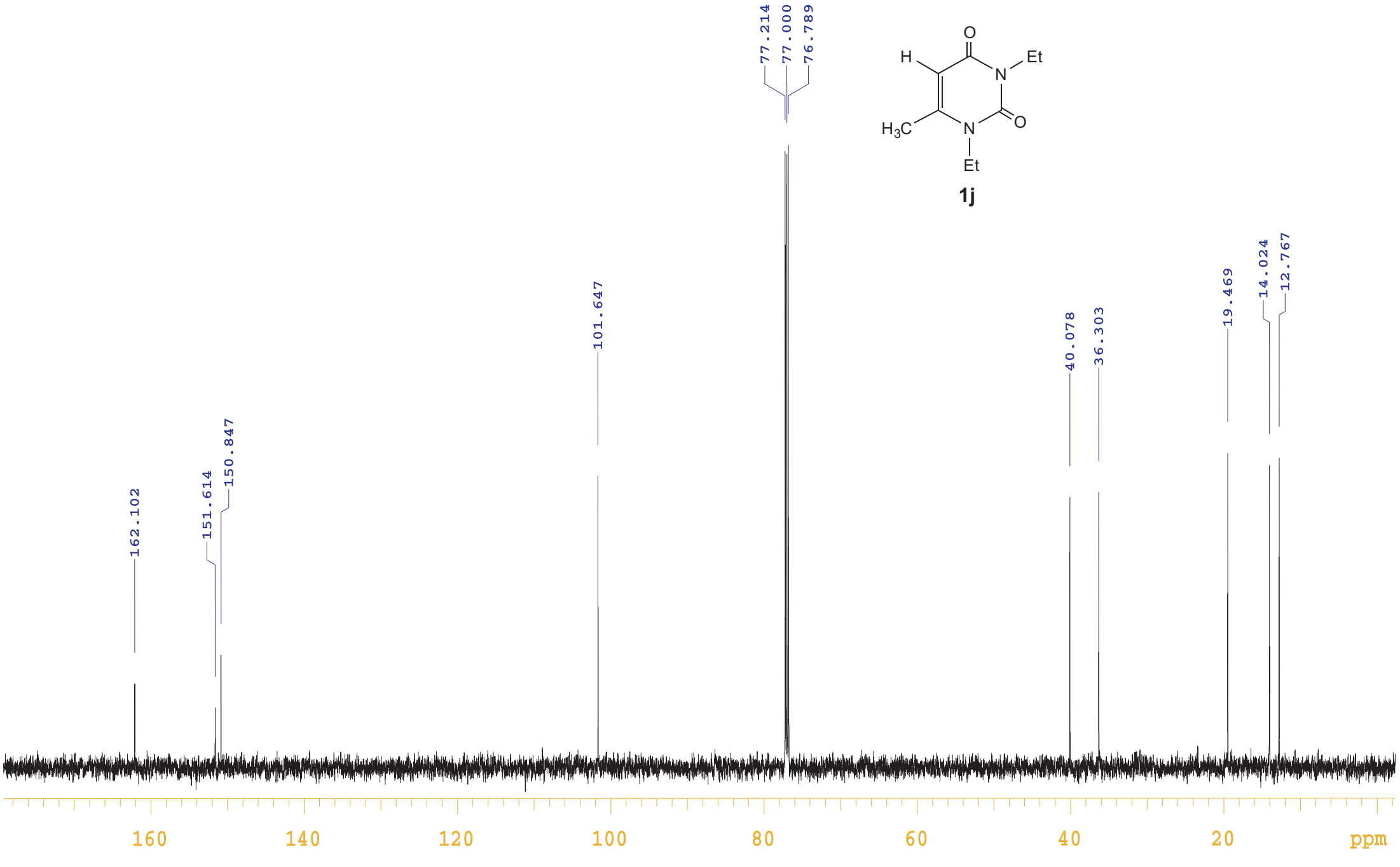
3.49
3.24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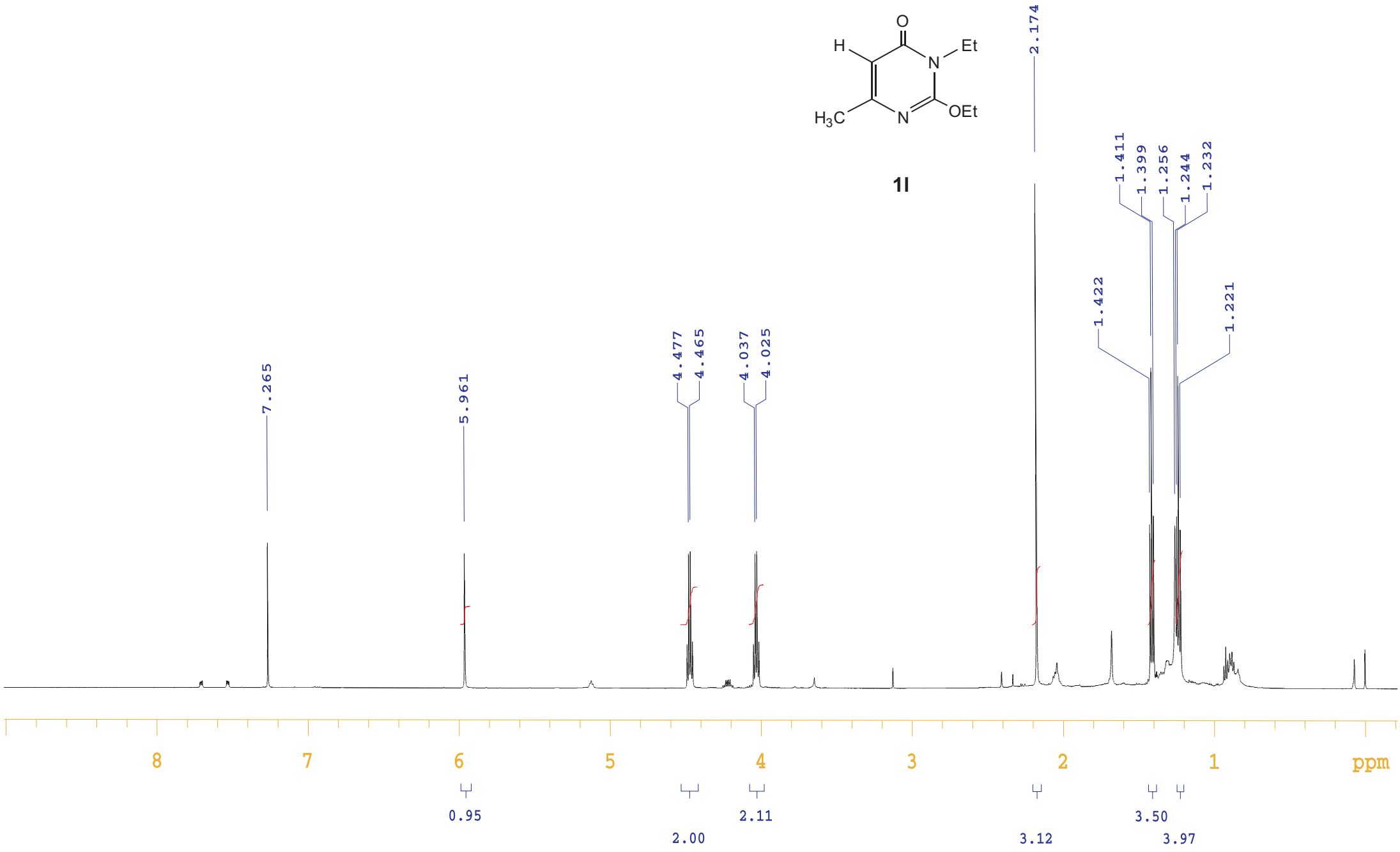
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Et
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1.422
1.411
1.399
1.256
1.244
1.232
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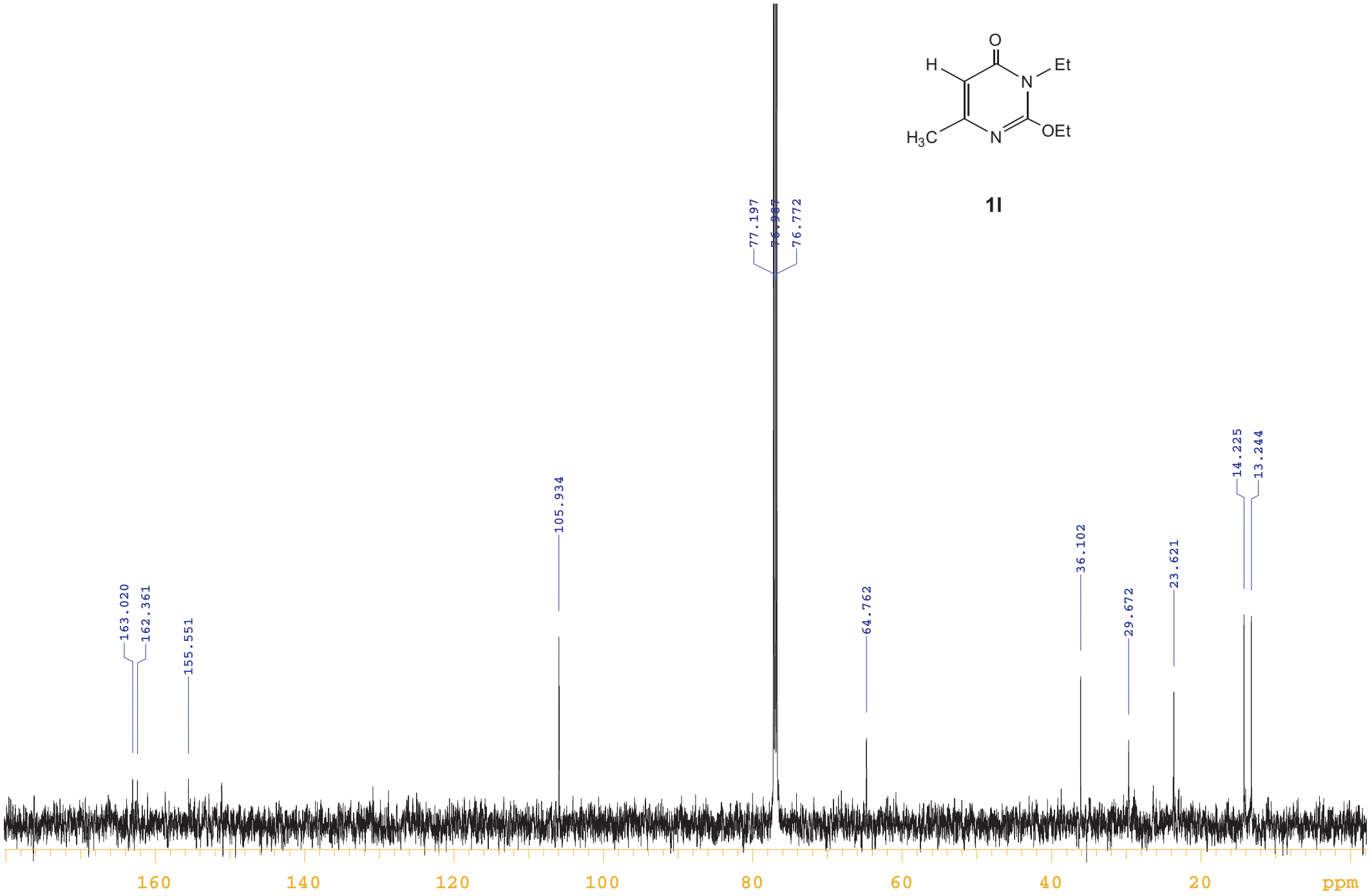
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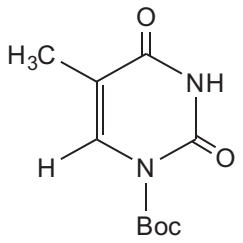
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NH
H
N
O
Boc

2a

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7
6
5
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ppm
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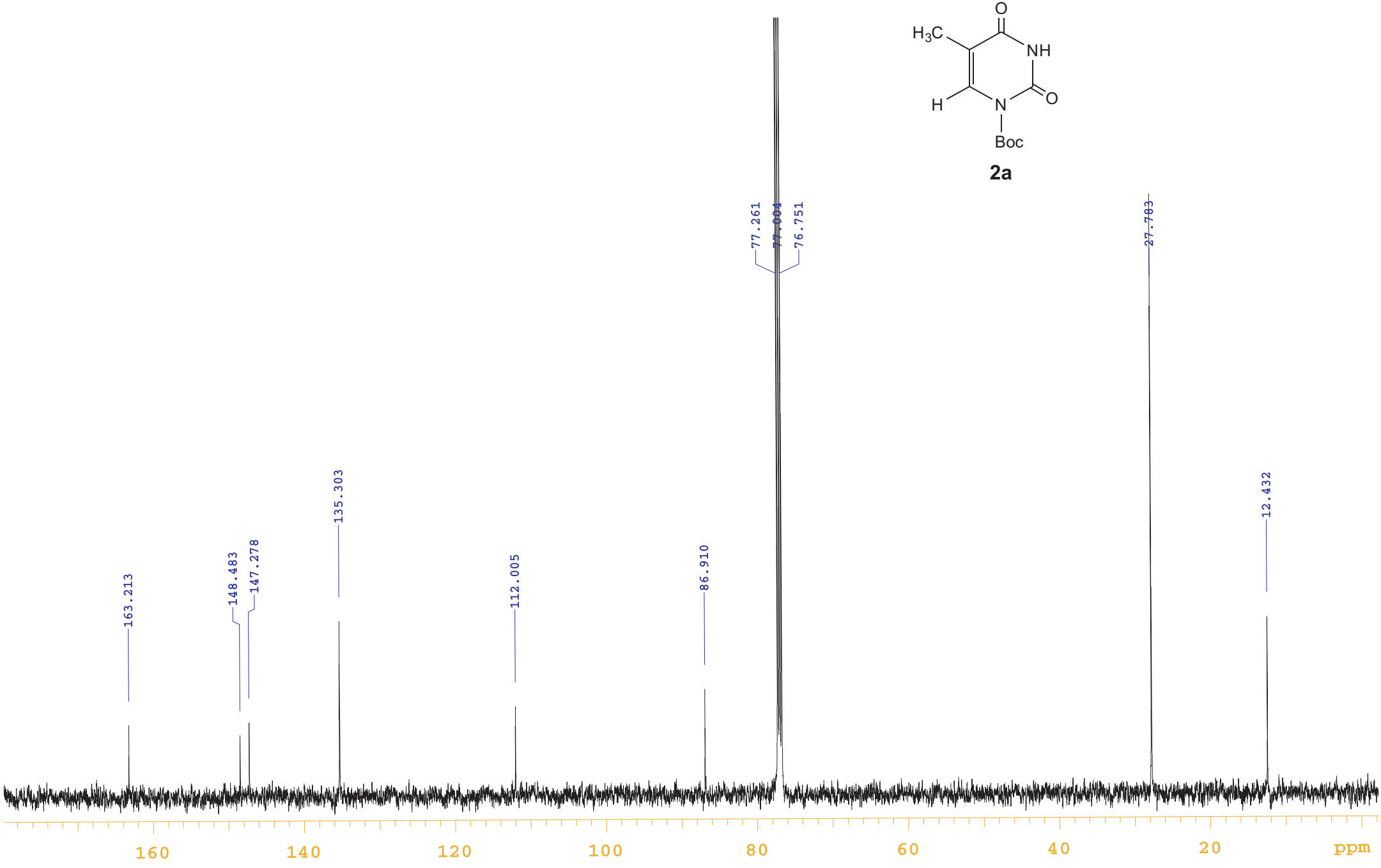
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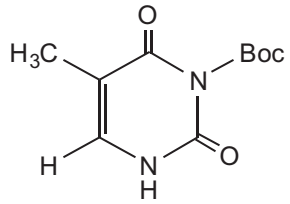
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H3C
Boc
N
H
N
H
O

2b

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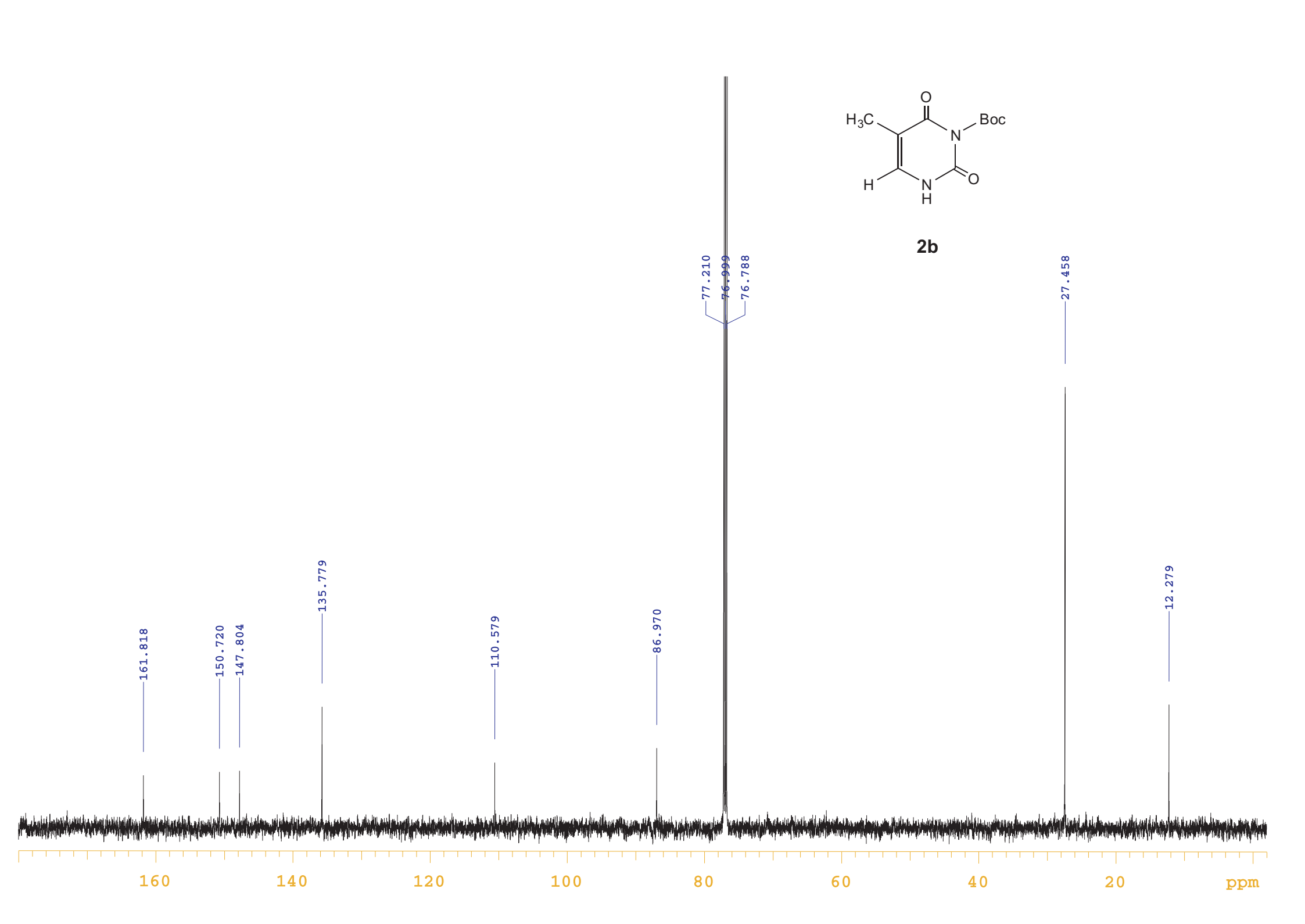
8.93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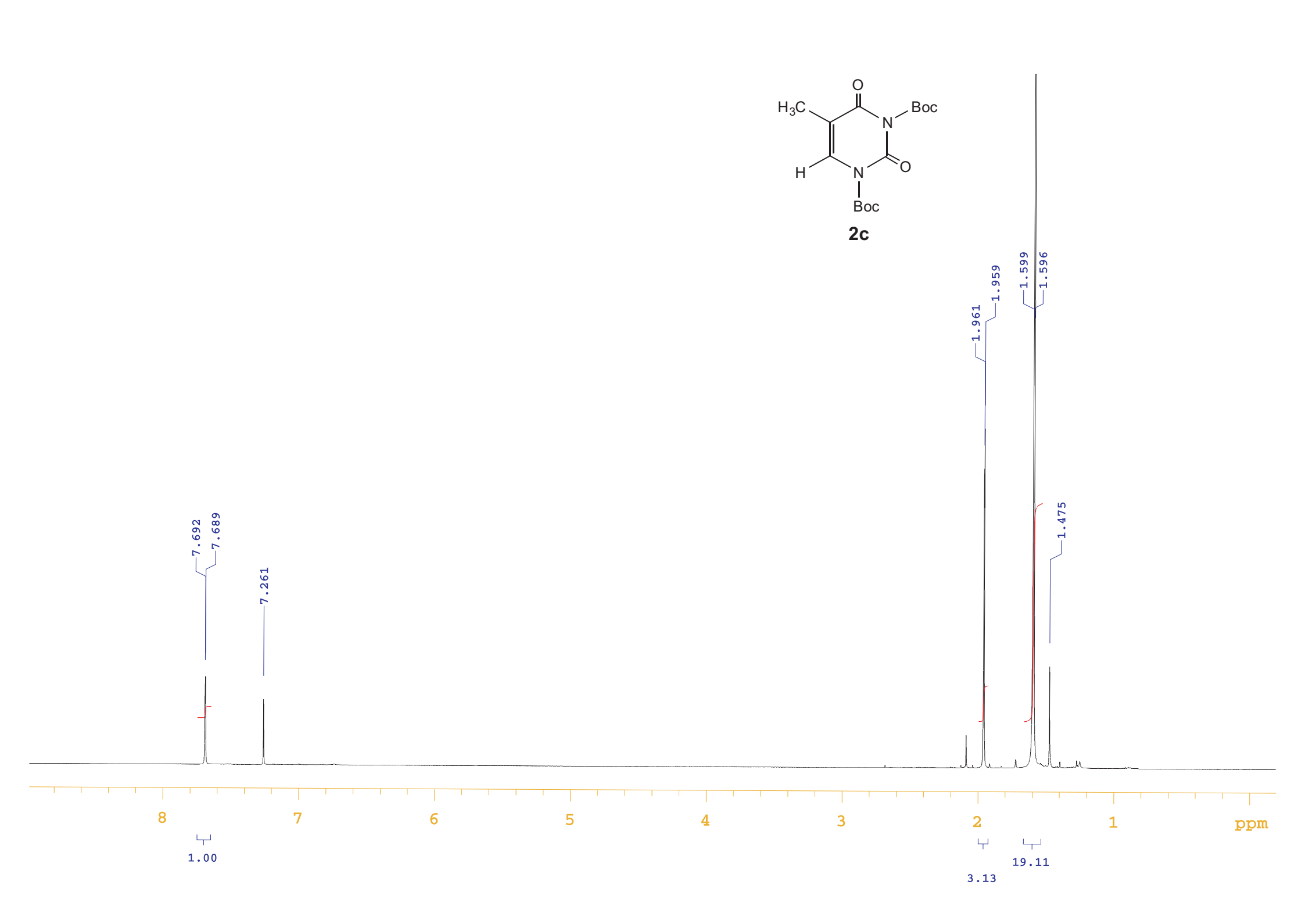
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N
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7
6
5
4
3
2
1
ppm
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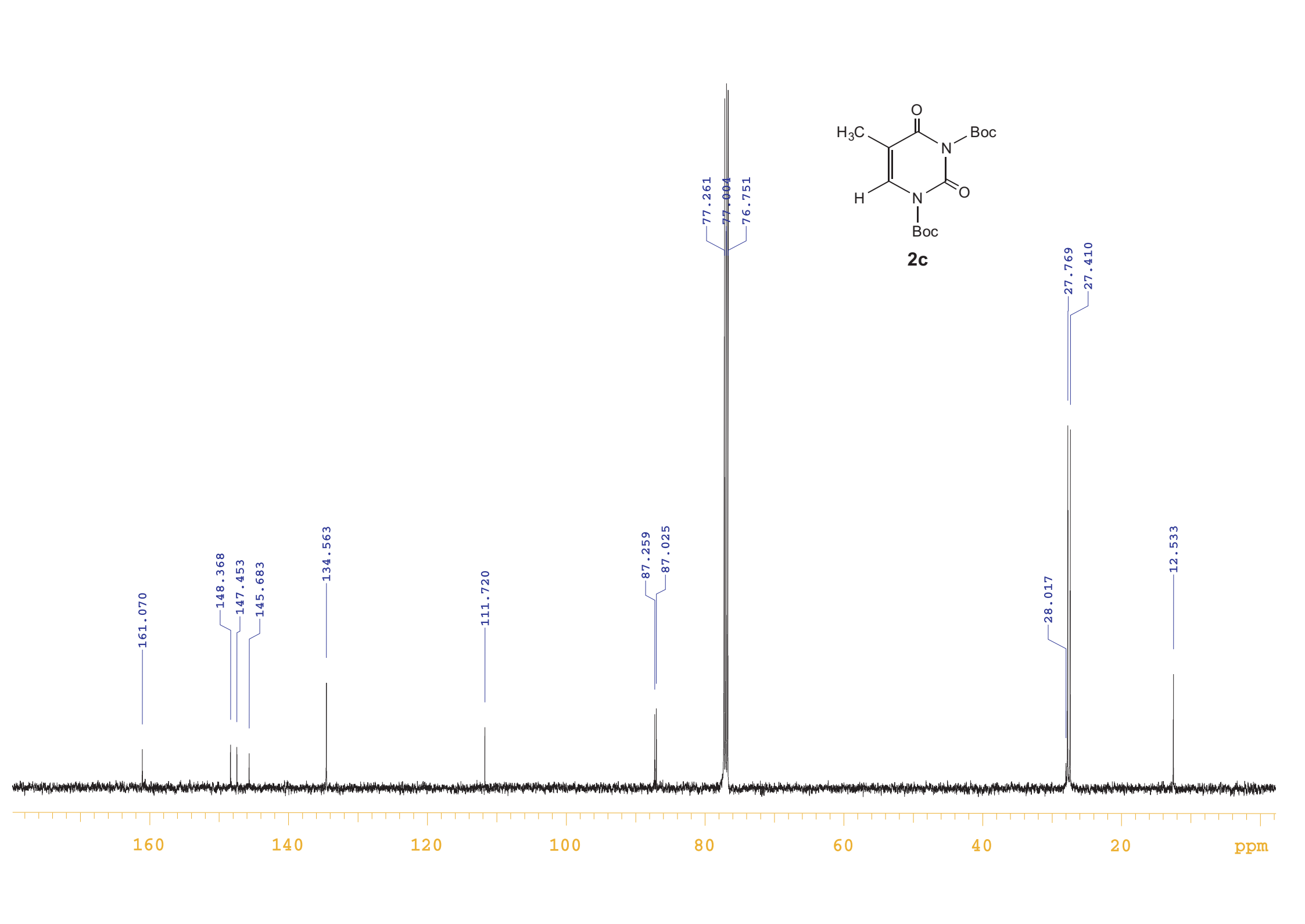
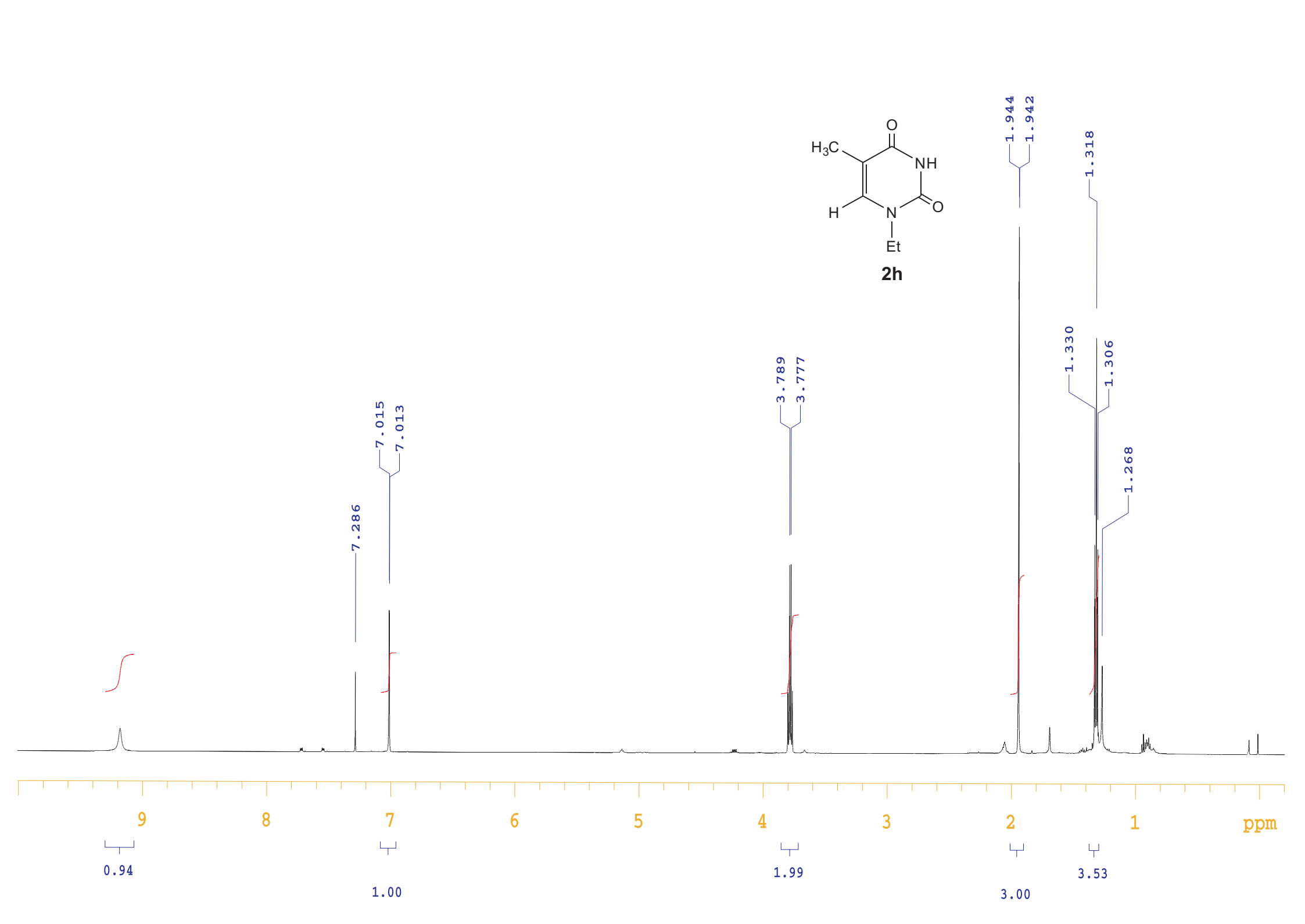
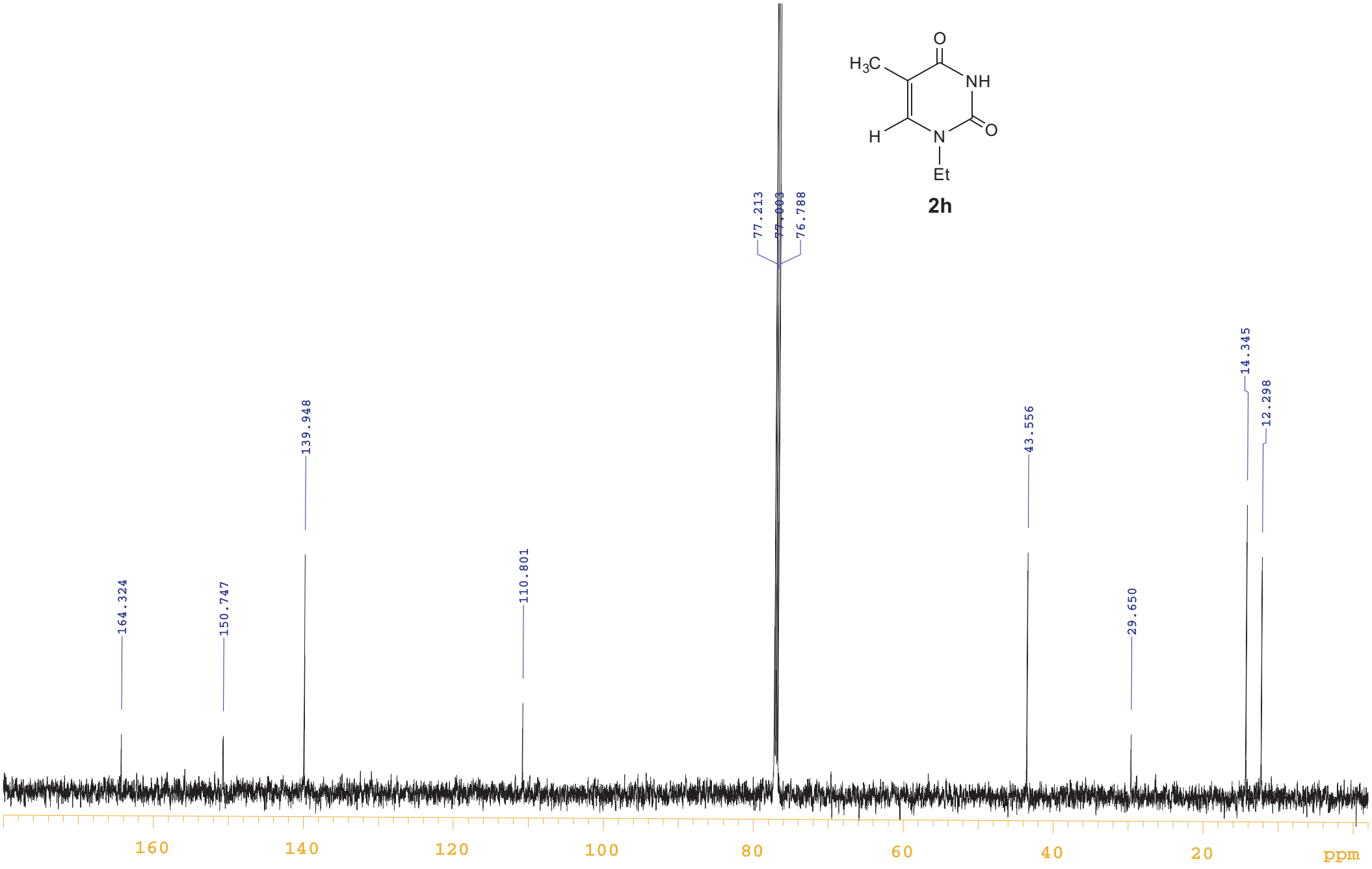
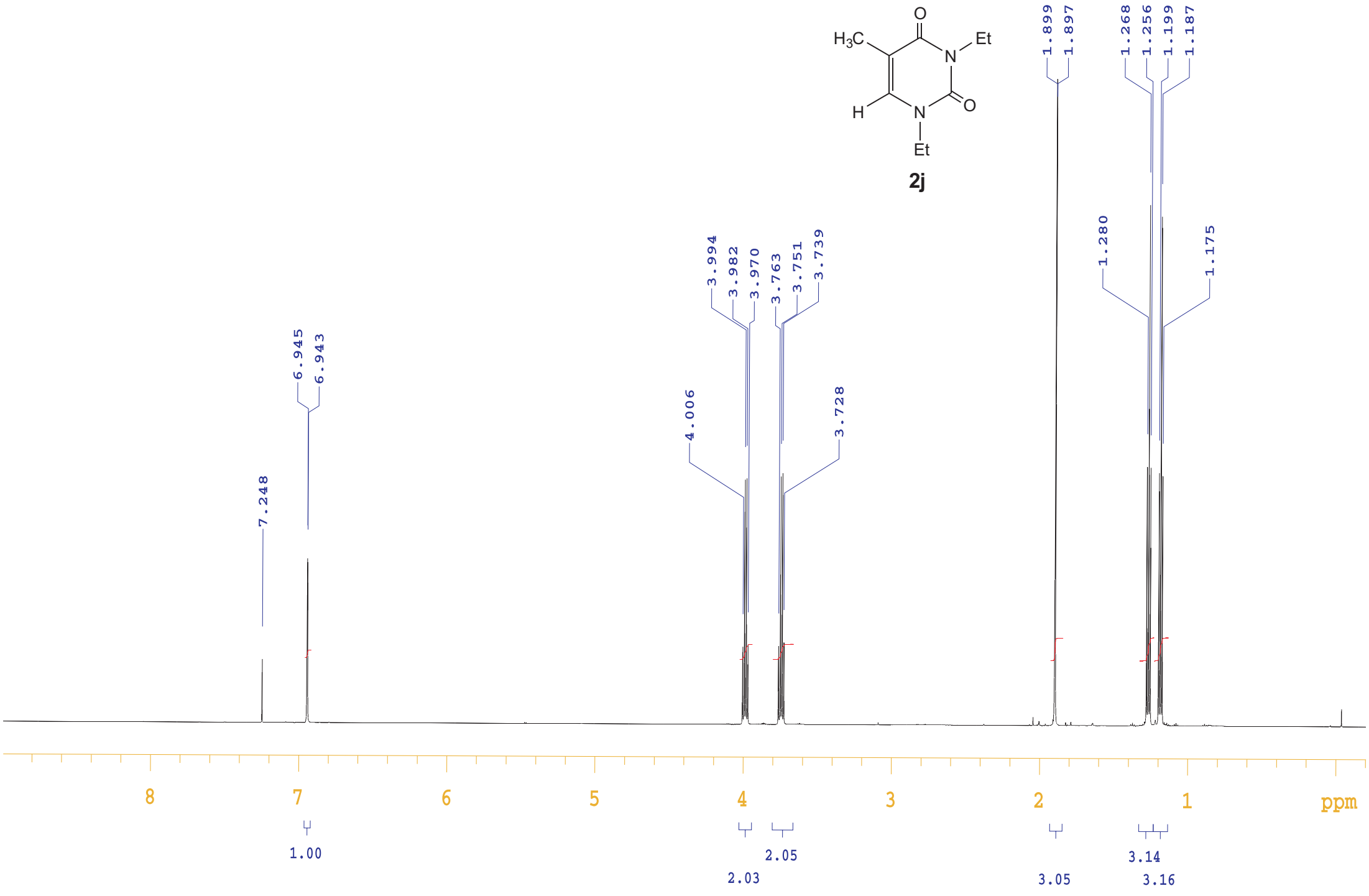
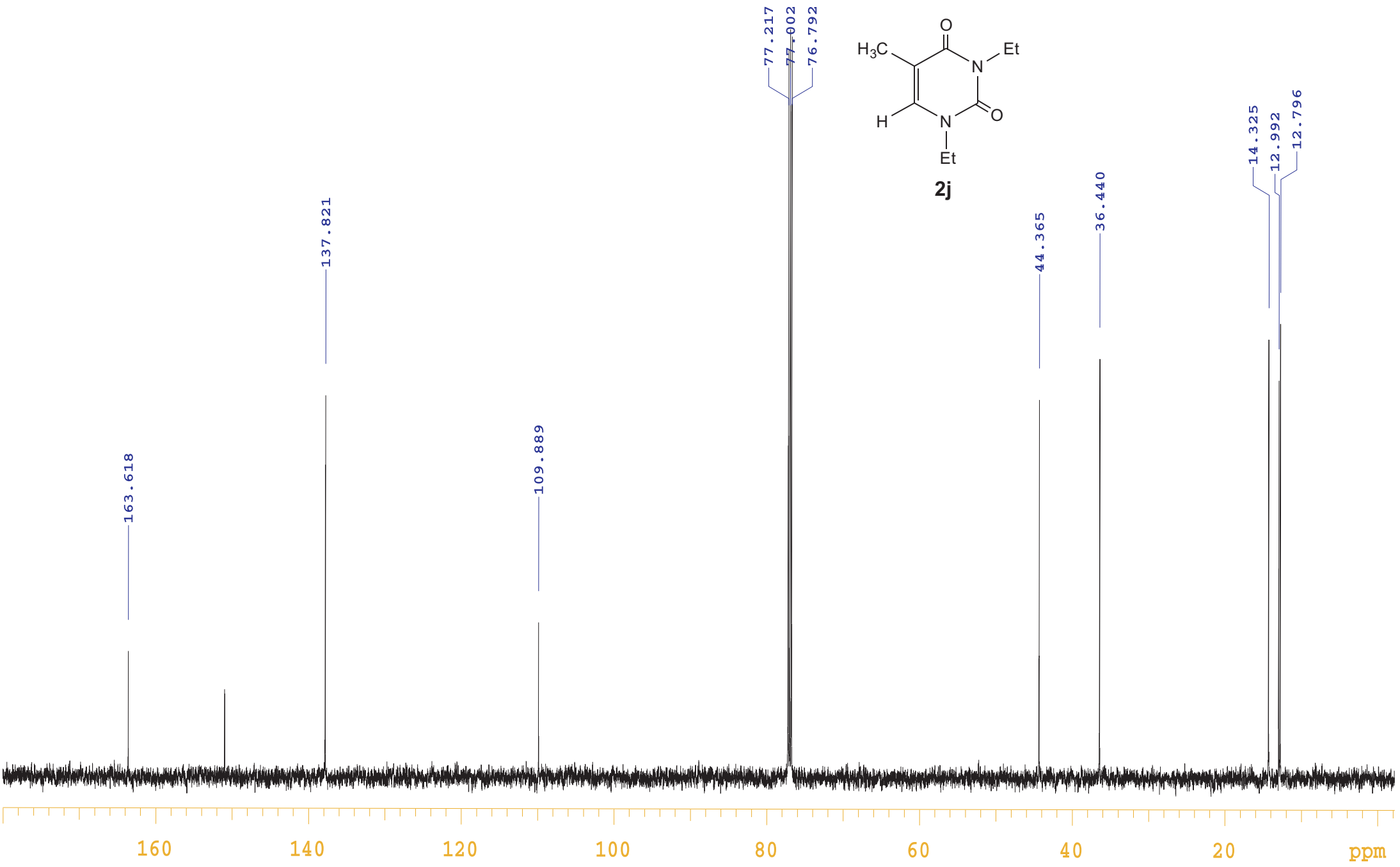
3.13
19.11

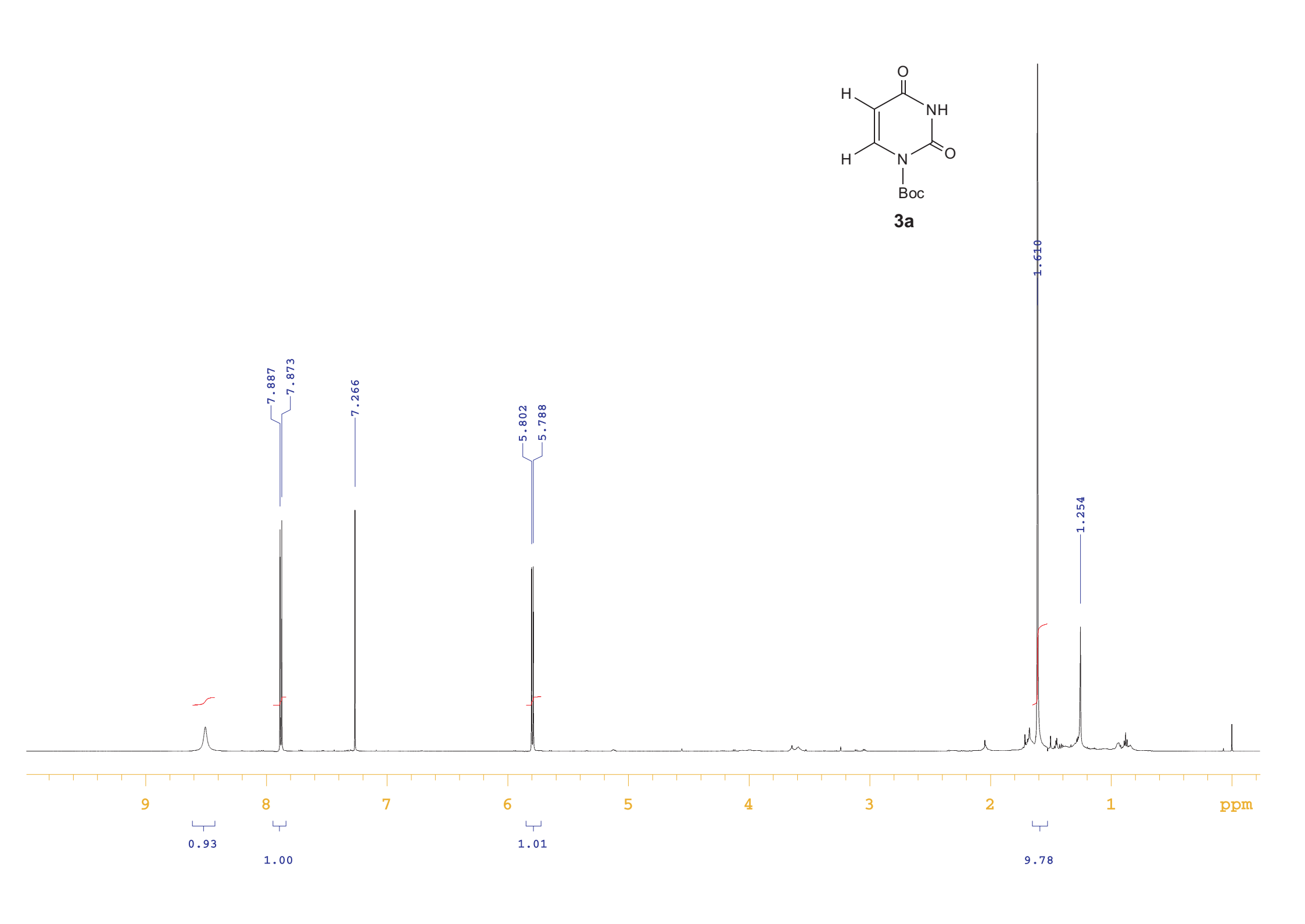

O
H3C
Boc
N
H
N
O
Boc
2c
77.261
77.004
76.751
27.769
27.410
161.070
148.368
147.453
145.683
134.563
111.720
87.259
87.025
28.017
12.533
160
140
120
100
80
60
40
20
ppm

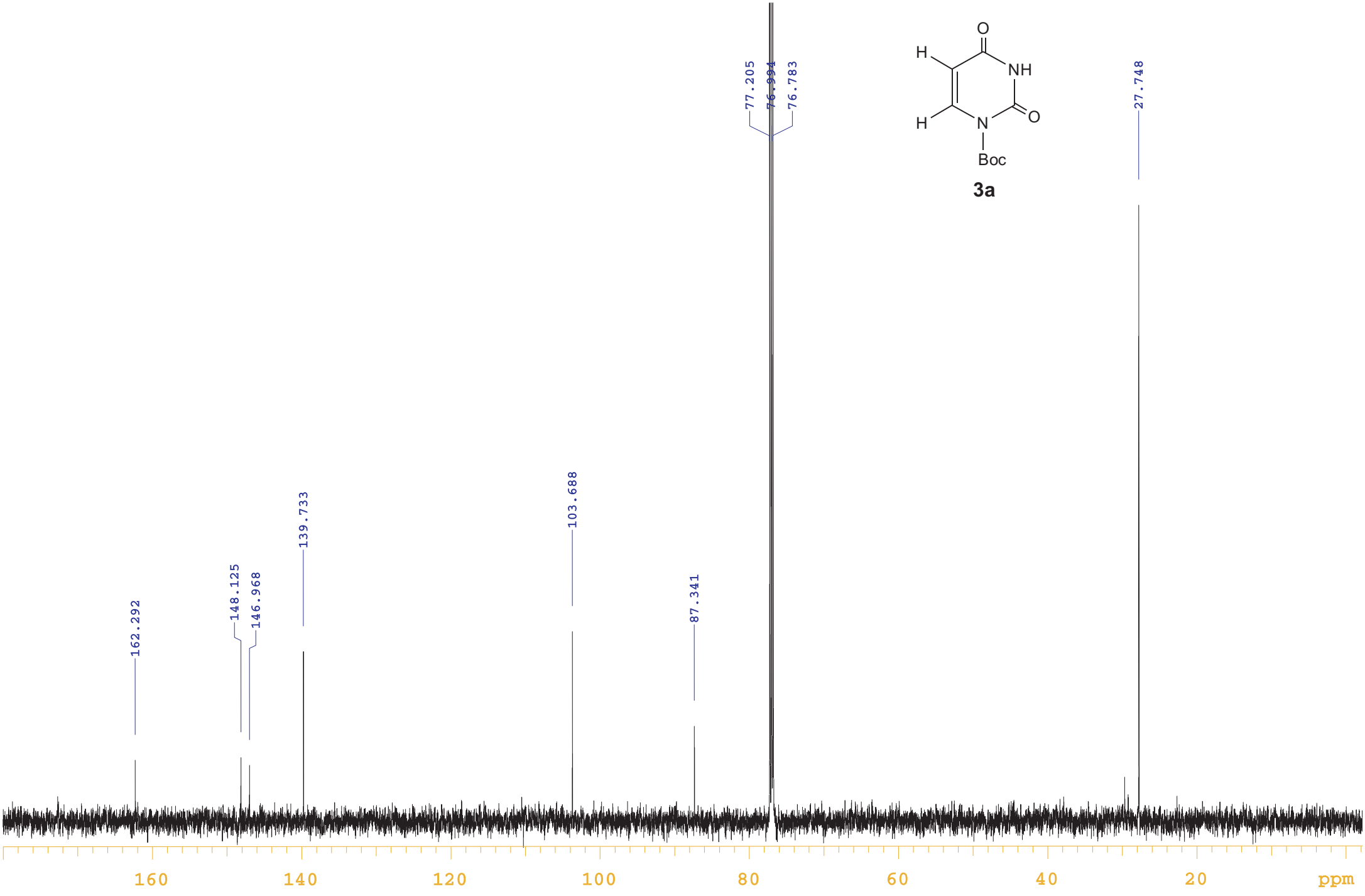

O
H3C
NH
H
N
O
Et
2h
1.944
1.942
1.318
1.330
1.306
1.268
3.789
3.777
7.286
7.015
7.013
9
8
7
6
5
4
3
2
1
ppm
0.94
1.00
1.99
3.00
3.53

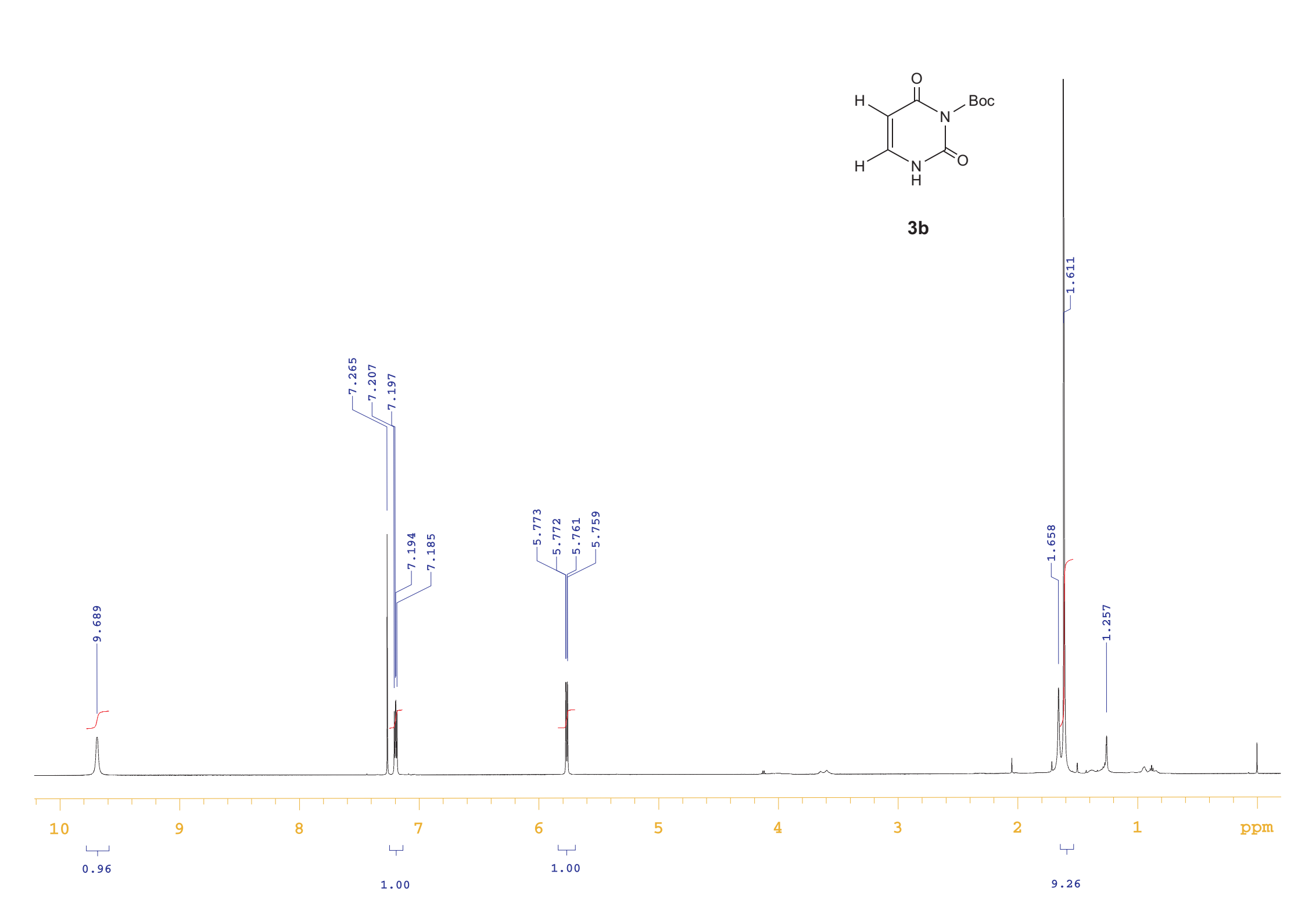

O
H3C
NH
H
N
O
Et
2h
77.213
77.003
76.788
164.324
150.747
139.948
110.801
43.556
29.650
14.345
12.298
160
140
120
100
80
60
40
20
ppm

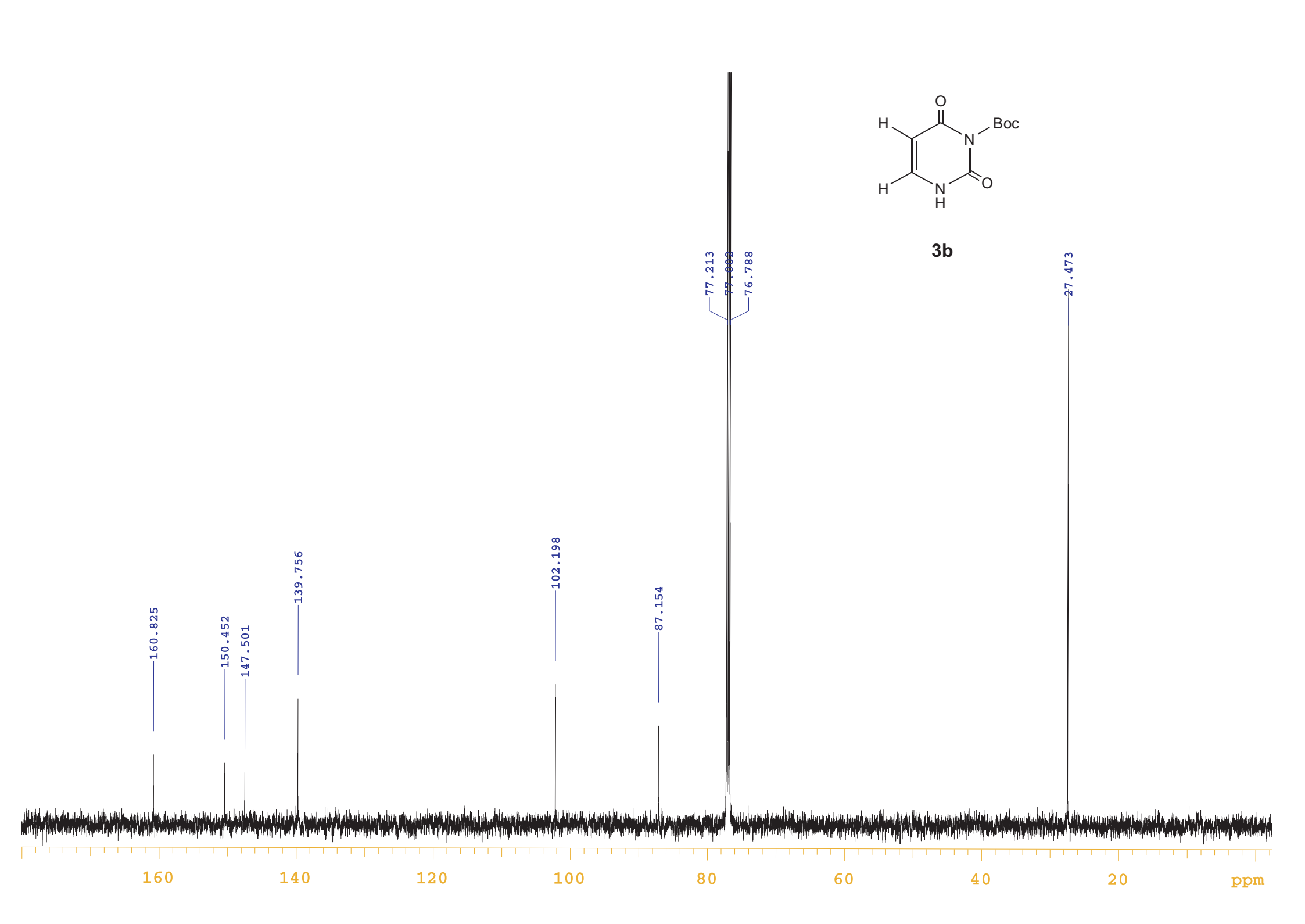

O
H3C
Et
N
H
N
O
Et
2j
7.248
6.945
6.943
4.006
3.994
3.982
3.970
3.763
3.751
3.739
3.728
1.899
1.897
1.280
1.268
1.256
1.199
1.187
1.175
8
7
6
5
4
3
2
1
ppm
1.00
2.03
2.05
3.05
3.14
3.16

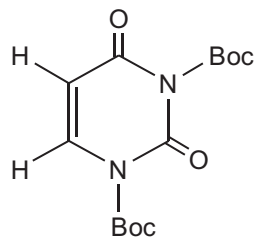

77.217
77.002
76.792
163.618
137.821
109.889
44.365
36.440
14.325
12.992
12.796
O
H3C
Et
N
H
N
O
Et
2j
160
140
120
100
80
60
40
20
ppm


O
H
NH
H
N
O
Boc
3a
7.887
7.873
7.266
5.802
5.788
1.610
1.254
9
8
7
6
5
4
3
2
1
ppm
0.93
1.00
1.01
9.78


77.205
76.994
76.783
27.748
162.292
148.125
146.968
139.733
103.688
87.341
O
H
NH
H
N
O
Boc
3a
160
140
120
100
80
60
40
20
ppm

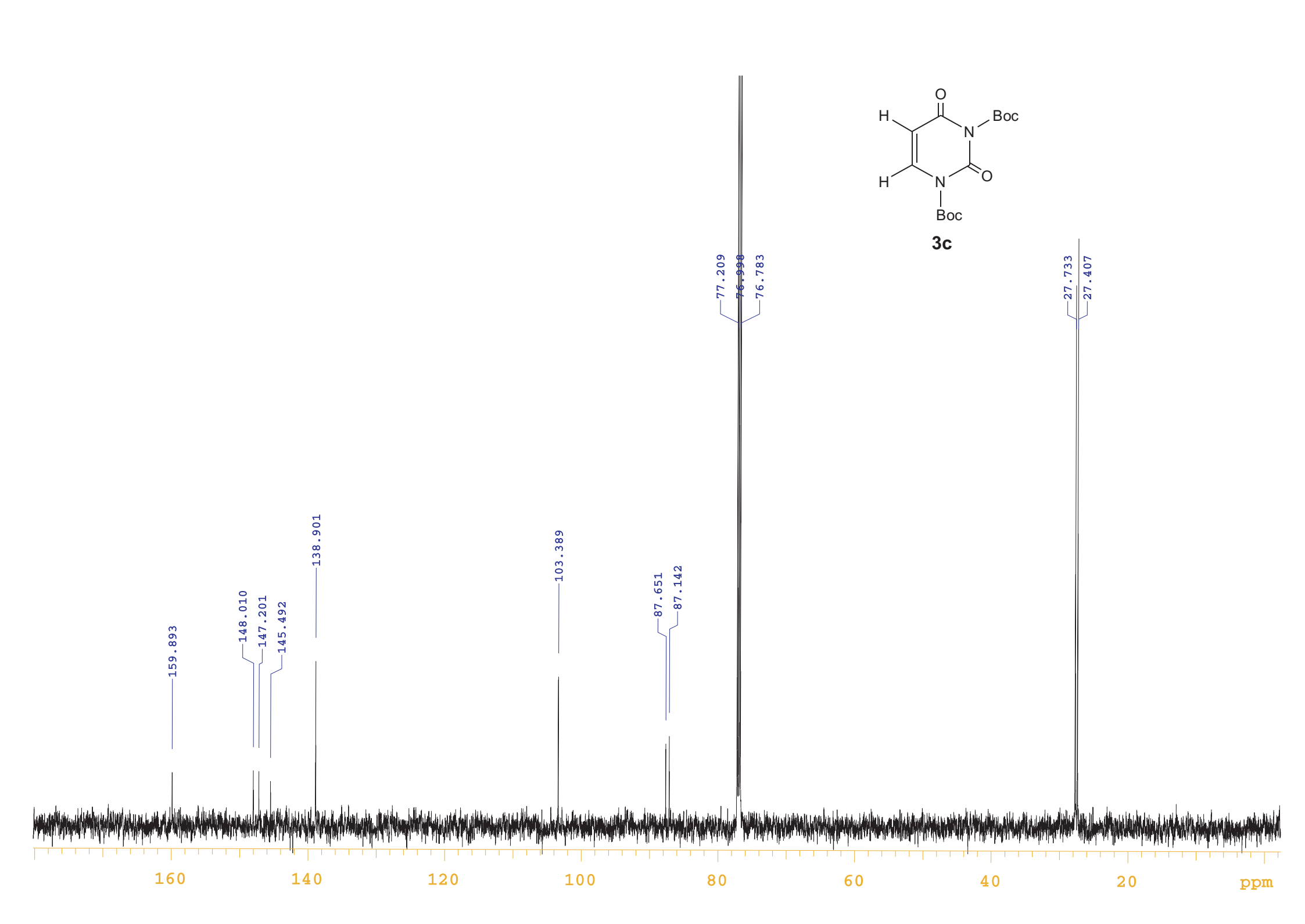

O
H
Boc
N
H
N
H
O
3b
9.689
7.265
7.207
7.197
7.194
7.185
5.773
5.772
5.761
5.759
1.658
1.611
1.257
10
9
8
7
6
5
4
3
2
1
ppm
0.96
1.00
1.00
9.26

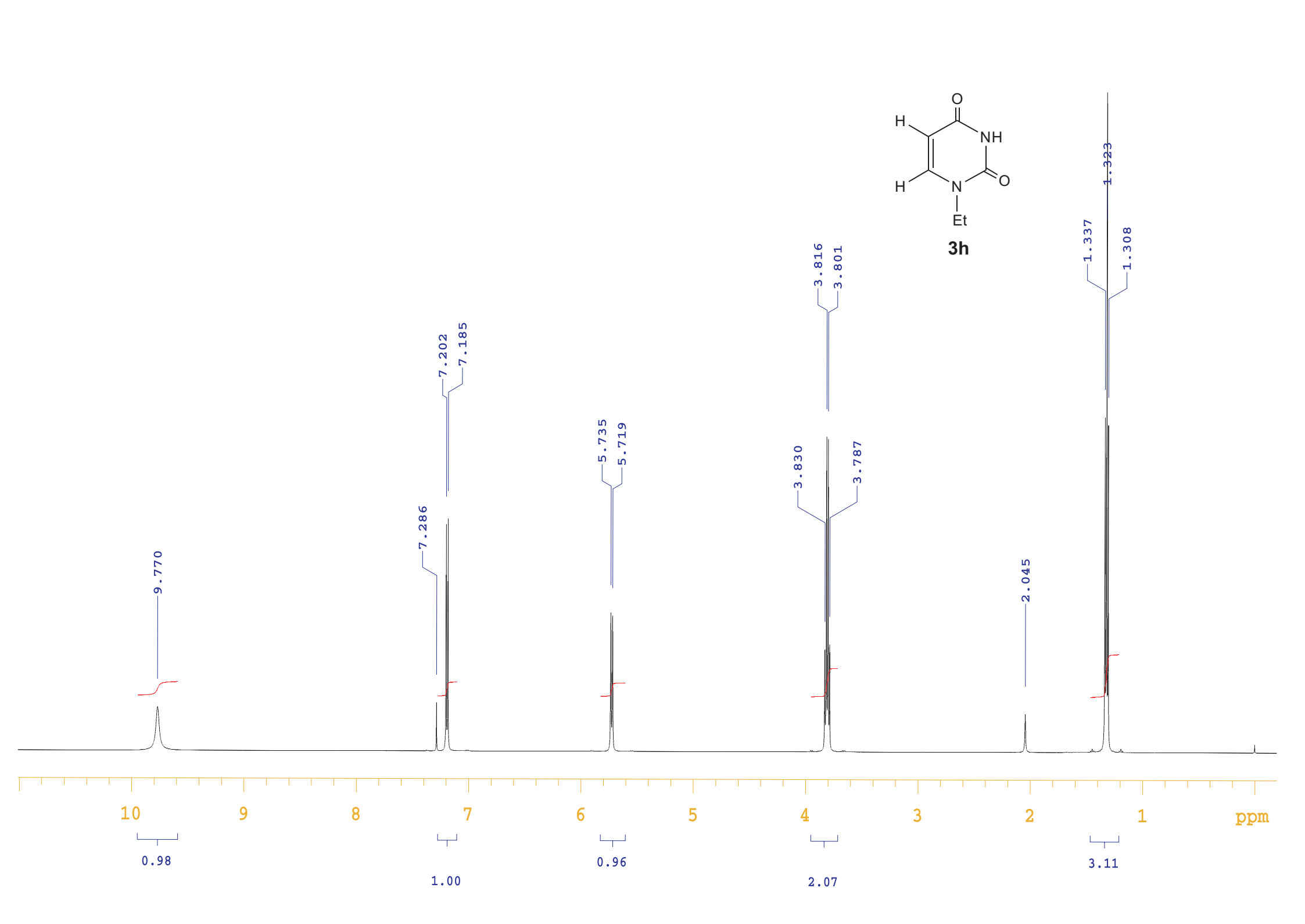

O
H
Boc
N
H
N
O
H
3b
77.213
77.000
76.788
27.473
160.825
150.452
147.501
139.756
102.198
87.154
160
140
120
100
80
60
40
20
ppm

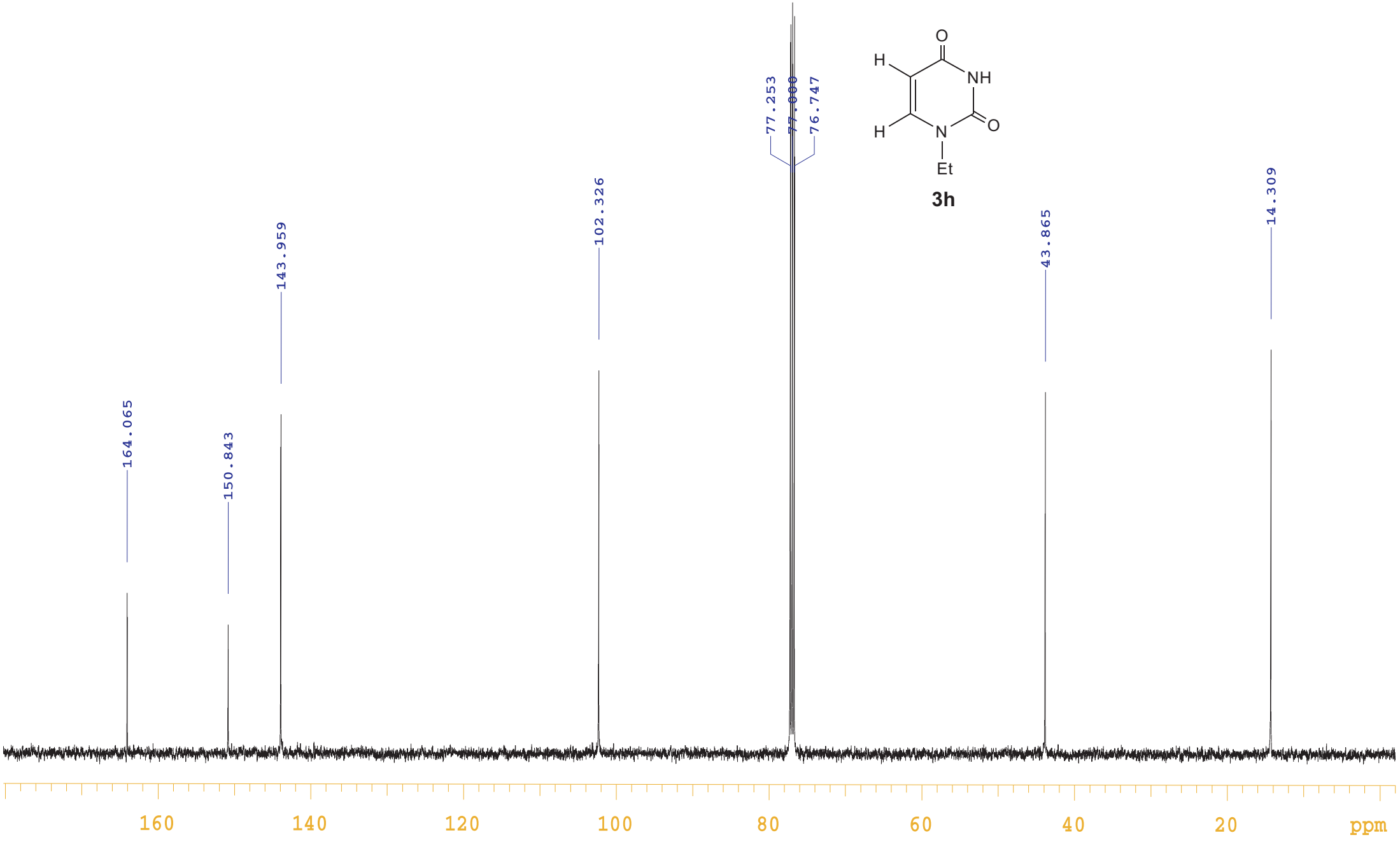

O
H
Boc
N
H
N
O
Boc

3c

1.606
1.604
7.868
7.854
5.820
5.806
8
7
6
5
4
3
2
1
ppm
1.00
0.99
19.26

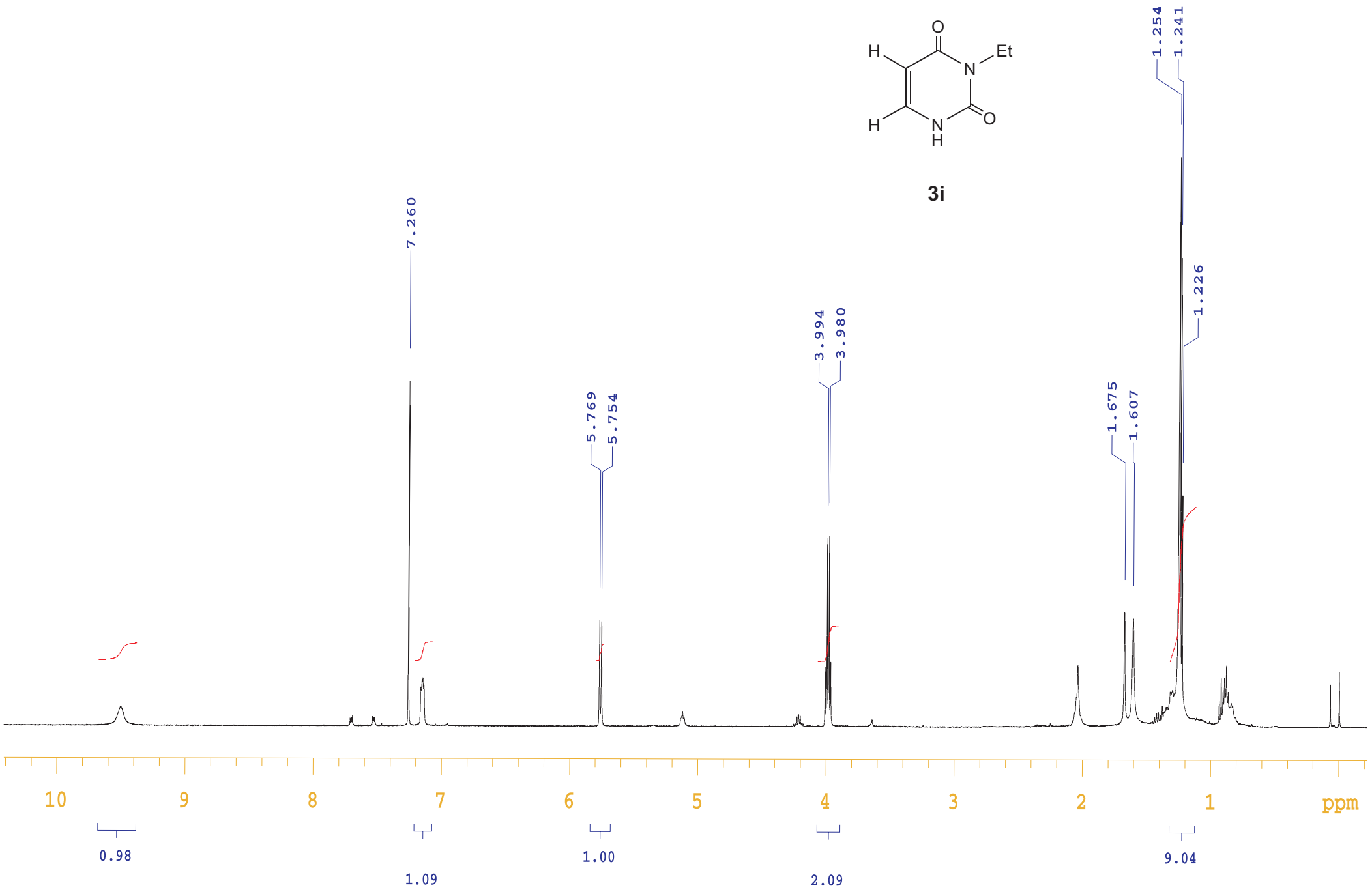

O
H
Boc
N
H
N
O
Boc
3c
159.893
148.010
147.201
145.492
138.901
103.389
87.651
87.142
77.209
76.998
76.783
27.733
27.407
160
140
120
100
80
60
40
20
ppm

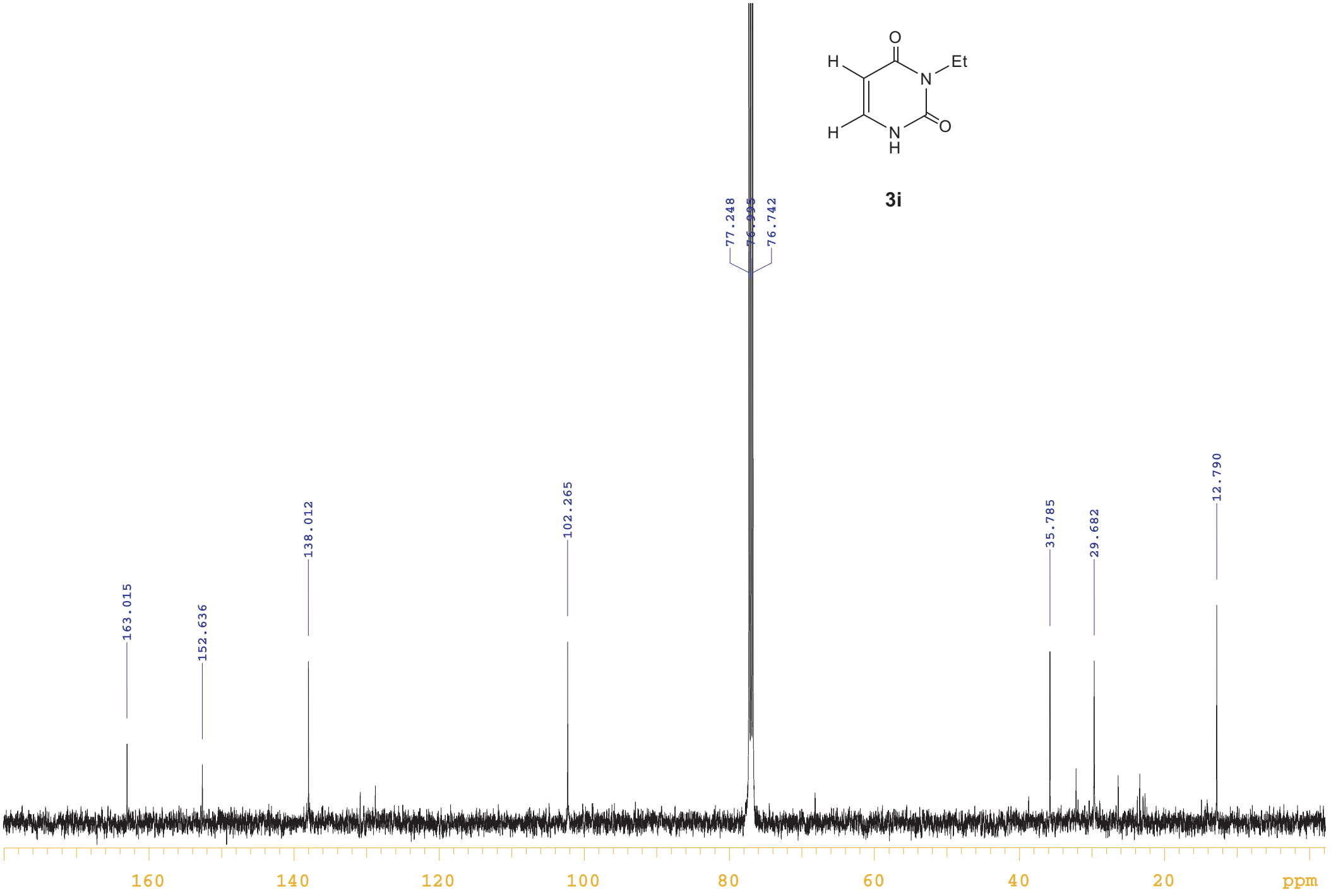

O
H
NH
H
N
O
Et
3h
9.770
7.286
7.202
7.185
5.735
5.719
3.830
3.816
3.801
3.787
2.045
1.337
1.323
1.308
10
9
8
7
6
5
4
3
2
1
ppm
0.98
1.00
0.96
2.07
3.11

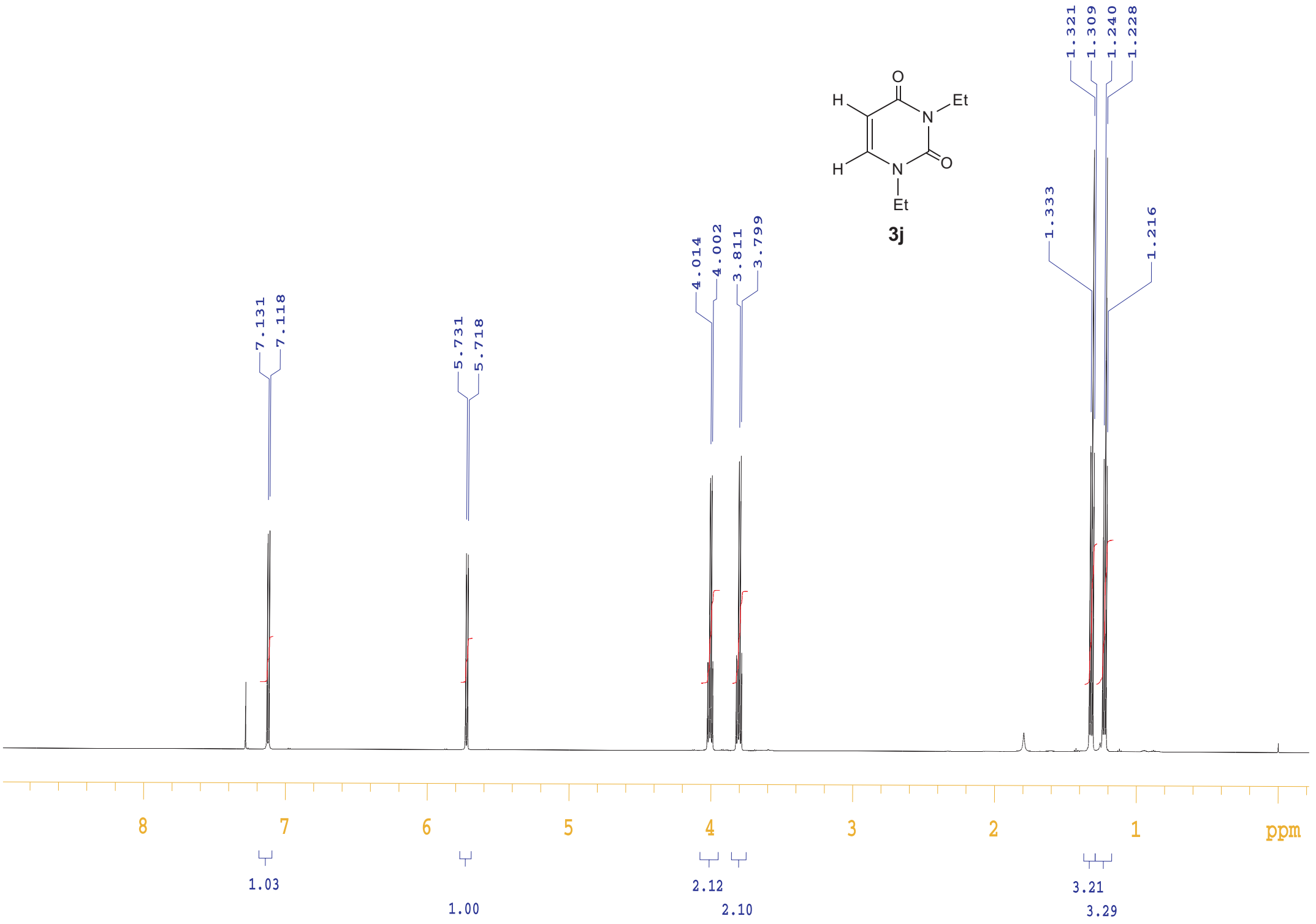

164.065
150.843
143.959
102.326
77.253
77.000
76.747
43.865
14.309
160
140
120
100
80
60
40
20
ppm

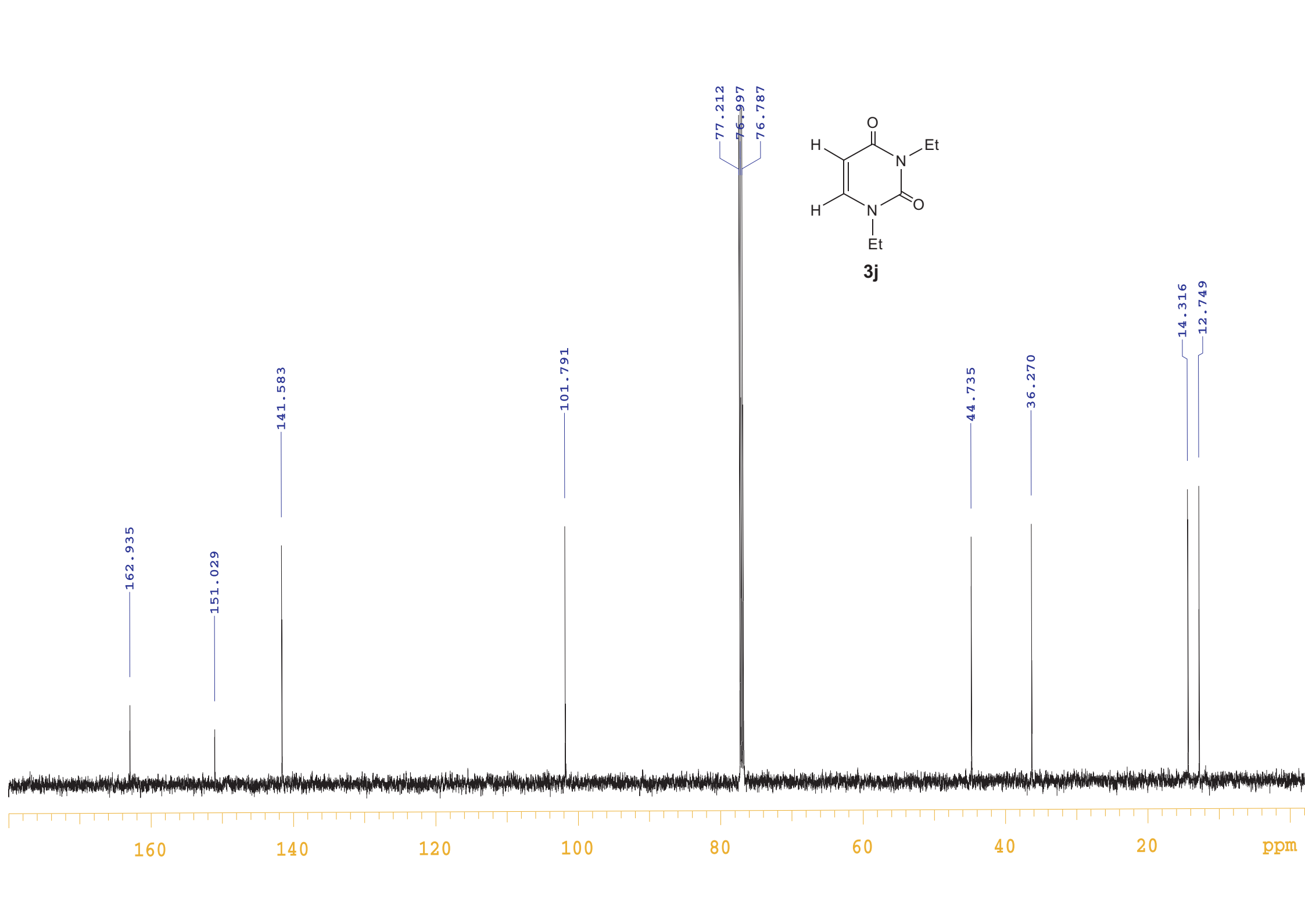
O
H
NH
H
N
O
Et

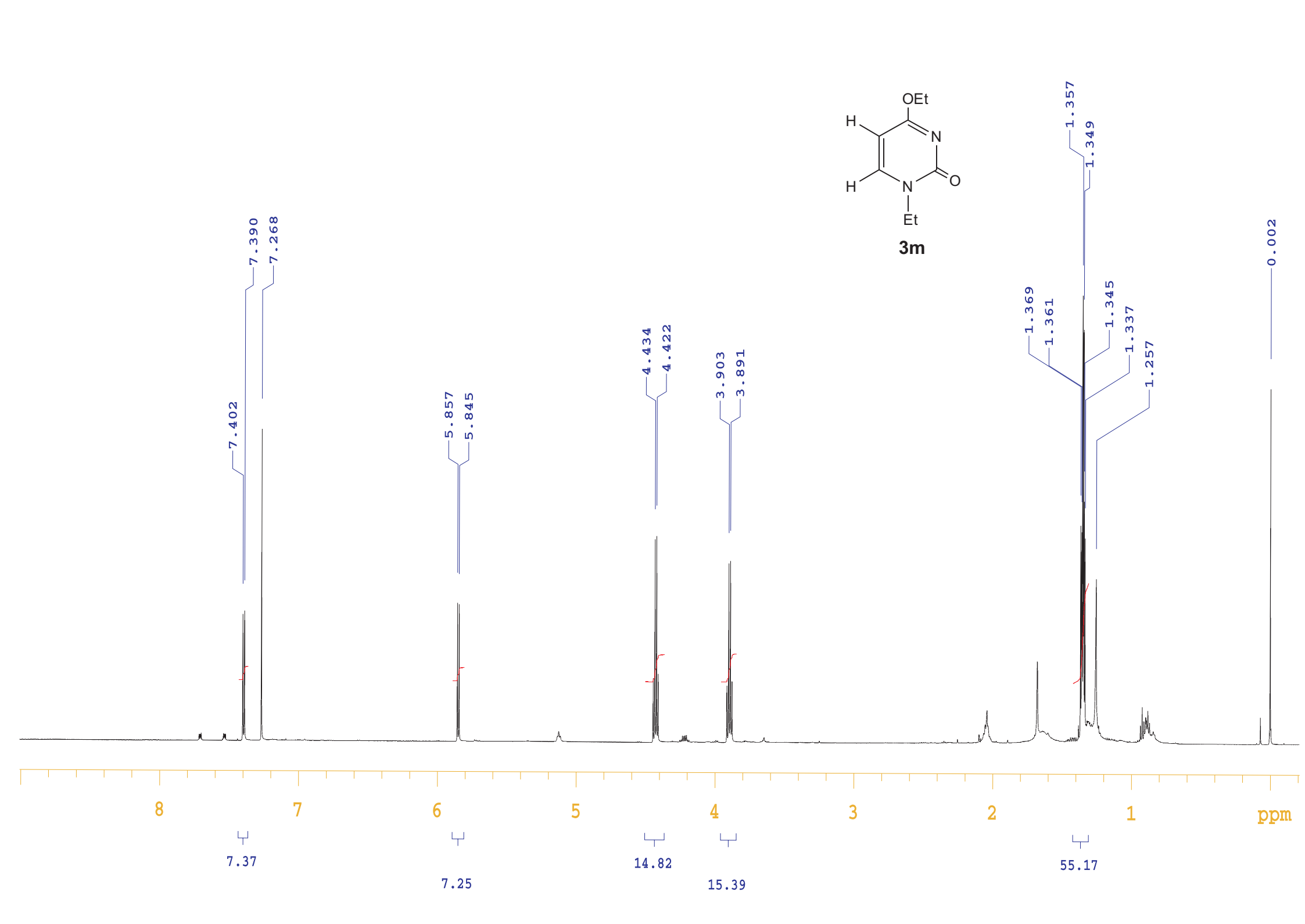
3h

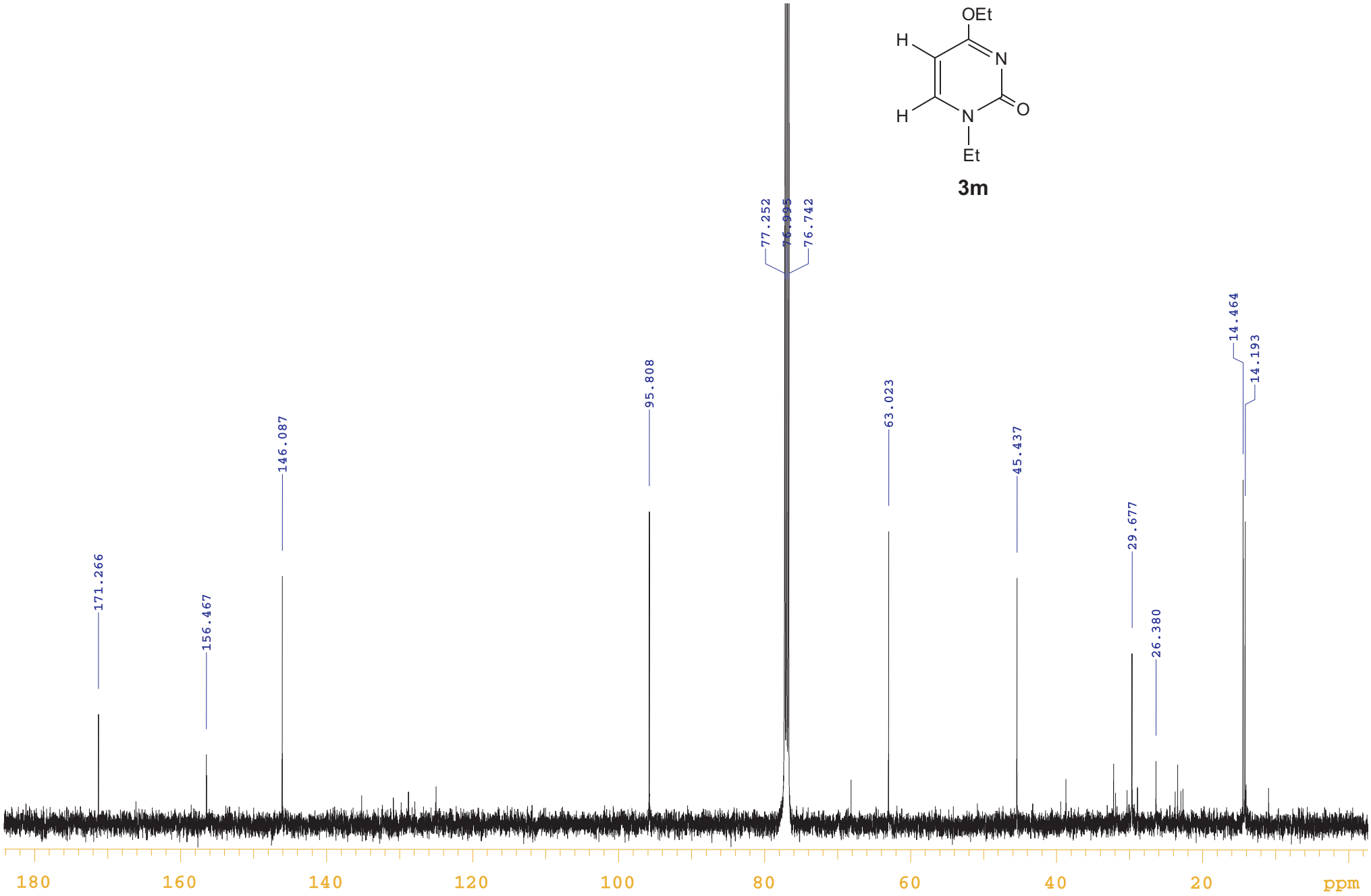

O
H
Et
N
H
N
H
O
3i
1.254
1.241
7.260
1.226
3.994
3.980
5.769
5.754
1.675
1.607
10
9
8
7
6
5
4
3
2
1
ppm
0.98
1.09
1.00
2.09
9.04


O
H
Et
N
H
H
N
O
3i
77.248
76.995
76.742
163.015
152.636
138.012
102.265
35.785
29.682
12.790
160
140
120
100
80
60
40
20
ppm


7.131
7.118
5.731
5.718
4.014
4.002
3.811
3.799
1.333
1.321
1.309
1.240
1.228
1.216
O
H
Et
N
H
N
O
Et
3j
8
7
6
5
4
3
2
1
ppm
1.03
1.00
2.12
2.10
3.21
3.29


77.212
76.997
76.787
O
H
Et
N
H
N
O
Et
3j
162.935
151.029
141.583
101.791
44.735
36.270
14.316
12.749
160
140
120
100
80
60
40
20
ppm


OEt
H
N
H
N
O
Et
3m
7.402
7.390
7.268
5.857
5.845
4.434
4.422
3.903
3.891
1.369
1.361
1.357
1.349
1.345
1.337
1.257
0.002
8
7
6
5
4
3
2
1
ppm
7.37
7.25
14.82
15.39
55.17


OEt
H
N
H
N
O
Et
3m
171.266
156.467
146.087
95.808
77.252
76.742
63.023
45.437
29.677
26.380
14.464
14.193
180
160
140
120
100
80
60
40
20
ppm