

***o*-Benzenedisulfonimide and its chiral derivative as Brønsted acids catalysts for one-pot three-component Strecker reaction. Synthetic and mechanistic aspects.**

*Margherita Barbero, Silvano Cadamuro, Stefano Dughera, Giovanni Ghigo*

**Supplementary Information**

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## 2

### 1. General procedure for the preparation of Strecker adducts 5

TMSCN (**4**; 0.60 g, 6 mmol) was added to a mixture of OBS (**1**; 5 mol%; 55 mg, 0.25 mmol; in only three exceptions, Table 2 entries 13, 14, 17, the amount of **1** was 15 mol%; 165 mg, 0.75 mmol), ketone (**2**; 5 mmol) and amine (**3**; 5 mmol). The mixture was stirred at room temperature (or 40 °C in only two exceptions, Table 2 entries 13,17) until the GC and GC-MS analyses showed the complete disappearance of **2** and **3** and the complete formation of product **5**. It was also always detected the by-product bis(trimethylsilyl)ether, MS (EI) *m/z*: (%) 162 [M<sup>+</sup>](10), 147 (100). However, it was impossible to isolate it.

Cold H<sub>2</sub>O (20 ml) was added to the reaction mixture, under vigorous stirring. The resulting solid was filtered on a buchner funnel and washed with additional cold H<sub>2</sub>O (2 x 5 ml) and little amount of PE (5 ml). It was virtually pure (GC, GC-MS, <sup>1</sup>H NMR, <sup>13</sup>C NMR) title compound **5**. Whereas the adduct **5** was not solid (Table 2 entries 14, 16, 17, 18) the reaction mixture was poured into Et<sub>2</sub>O–H<sub>2</sub>O (50 ml, 1:1). The aqueous phase was separated and extracted with Et<sub>2</sub>O (2 x 50 ml). The combined organic extracts were washed with H<sub>2</sub>O (2 x 50 ml), dried over Na<sub>2</sub>SO<sub>4</sub>. After solvent removal under reduced pressure, the crude residue was the virtually pure (GC, GC-MS, <sup>1</sup>H NMR, <sup>13</sup>C NMR) compound **5**.

The aqueous washings were collected and evaporated under reduced pressure. After removal of the water, virtually pure (<sup>1</sup>H NMR) OBS (**1**) was recovered.

### 2. Spectral and physical data of known products 5

**2-Phenyl-2-phenylaminopropanenitrile (5a)**: white solid; 1.05 g (yield 95 %); mp 140–141 °C (EtOH; lit.<sup>12</sup> 139–140 °C ). <sup>1</sup>H NMR (200 MHz, CDCl<sub>3</sub>): δ = 1.97 (s, 3H), 3.55 (br s, 1 H), 6.57 (d, *J* = 8.2 Hz, 2H), 6.82 (t, *J* = 7.4 Hz, 1H), 7.09–7.17 (m, 2H), 7.35–7.42 (m, 3H), 7.64 (d, *J* = 8.2 Hz, 2H). <sup>13</sup>C NMR (50 MHz, CDCl<sub>3</sub>): δ = 33.0, 57.1, 115.8, 120.0, 120.4, 124.7, 128.5, 128.8, 129.0, 139.4, 142.9. MS (EI) *m/z*: (%) 222 [M<sup>+</sup>](10), 195 (50), 180 (100), 77 (45). IR (CHCl<sub>3</sub>) *v* (cm<sup>-1</sup>): 3419 (NH), 2254 (CN).

**2-(4-Methoxyphenylamino)-2-phenylpropanenitrile (5b)**: pale brown solid; 1.16 g (yield 92 %); mp 102–103 °C (EtOH; lit.<sup>8</sup> 101–102 °C ). <sup>1</sup>H NMR (200 MHz, CDCl<sub>3</sub>): δ = 1.94 (s, 3H), 3.65 (s, 3H), 6.46–6.51 (m, 2H), 6.62–6.67 (m, 2H), 7.31–7.36 (m, 3H), 7.56 (m, 2H). <sup>13</sup>C NMR (50 MHz, CDCl<sub>3</sub>): δ 32.8, 55.3, 58.0, 114.6, 118.1, 120.9, 124.9, 128.4, 129.0, 137.1, 140.0, 153.8. MS (EI) *m/z*: (%) 225 [M<sup>+</sup> -HCN] (65), 210 (100). IR (CHCl<sub>3</sub>) *v* (cm<sup>-1</sup>): 3425 (NH), 2251 (CN).

**2-(4-Bromophenylamino)-2-phenylpropanenitrile (5d):** brown solid; 1.10 g (yield 73 %); mp 122–123 °C (EtOH).  $^1\text{H}$  NMR (200 MHz,  $\text{CDCl}_3$ ):  $\delta$  = 1.96 (s, 3H), 4.31 (br s 1H), 6.36 (d,  $J$  = 8.4 Hz, 2H), 7.18 (d,  $J$  = 8.4 Hz, 2H), 7.31–7.40 (m, 3H), 7.49–7.52 (m, 2H).  $^{13}\text{C}$  NMR  $\delta$  (50 MHz,  $\text{CDCl}_3$ ):  $\delta$  = 33.4, 57.3, 112.3, 117.5, 120.6, 125.0, 129.0, 129.5, 132.0, 139.5, 142.7. MS (EI)  $m/z$ : (%) 273 [ $\text{M}^+ + 2 - \text{HCN}$ ] (65), 273 [ $\text{M}^+ - \text{HCN}$ ] (65), 260 (100), 258 (100). IR ( $\text{CHCl}_3$ )  $\nu$  ( $\text{cm}^{-1}$ ): 3433 (NH), 2254 (CN).

**2-(3-Methoxyphenylamino)-2-phenylpropanenitrile (5g):** pale brown solid; 1.06 g (yield 84 %); mp 105 °C (EtOH; lit.<sup>8</sup> 102–105 °C).  $^1\text{H}$  NMR (200 MHz,  $\text{CDCl}_3$ ):  $\delta$  = 1.92 (s, 3H), 3.58 (s, 3H), 6.01–6.11 (m, 2H), 6.27–6.31 (m, 1H), 6.96 (t,  $J$  = 7.7 Hz, 1H), 7.28–7.35 (m, 3H), 7.58–7.60 (m, 2H).  $^{13}\text{C}$  NMR (50 MHz,  $\text{CDCl}_3$ ):  $\delta$  = 33.5, 55.2, 57.3, 102.0, 105.5, 108.7, 121.0, 125.0, 128.8, 129.4, 130.0, 140.2, 145.1, 160.4. MS (EI)  $m/z$ : (%) 225 [ $\text{M}^+ - \text{HCN}$ ] (60), 210 (100). IR ( $\text{CHCl}_3$ )  $\nu$  ( $\text{cm}^{-1}$ ): 3440 (NH), 2251 (CN).

**2-(4-Methylphenyl)-2-phenylaminopropanenitrile (5h):** pale grey solid; 1.04 g (yield 88 %); mp 129–130 °C (EtOH; lit.<sup>11b</sup> 126–128 °C).  $^1\text{H}$  NMR (200 MHz,  $\text{CDCl}_3$ ):  $\delta$  = 1.92 (s, 3H), 2.31 (s, 3H), 6.48 (d,  $J$  = 8.4 Hz, 2H), 7.06 (t,  $J$  = 7.7 Hz, 1H), 7.11–7.20 (m, 4H), 7.45 (d,  $J$  = 8.4 Hz, 2H).  $^{13}\text{C}$  NMR (50 MHz, DMSO-d6):  $\delta$  = 25.9, 38.1, 61.6, 115.2, 119.3, 121.4, 129.6, 133.3, 133.6, 134.7, 143.0, 149.4. MS (EI)  $m/z$ : (%) [ $\text{M}^+ - \text{HCN}$ ] (85), 194 (100), 77 (35). IR ( $\text{CHCl}_3$ )  $\nu$  ( $\text{cm}^{-1}$ ): 3428 (NH), 2242 (CN).

**2-(4-Nitrophenyl)-2-phenylaminopropanenitrile (5i):** yellow solid; 1.08 g (yield 81 %); mp 162–164 °C (EtOH; lit.<sup>4e</sup> 164–166 °C).  $^1\text{H}$  NMR (200 MHz,  $\text{CDCl}_3$ ):  $\delta$  = 1.92 (s, 3H), 4.32 (br s, 1H), 6.41 (d,  $J$  = 8.4 Hz, 2H), 6.78–6.82 (m, 1H), 7.08 (t,  $J$  = 7.7 Hz, 1H), 7.78 (d,  $J$  = 8.4 Hz, 2H), 8.21 (d,  $J$  = 8.4 Hz, 2H).  $^{13}\text{C}$  NMR (50 MHz, DMSO-d6):  $\delta$  = 32.3, 56.8, 115.4, 119.2, 121.0, 124.4, 125.1, 126.7, 129.4, 144.7, 148.5. MS (EI)  $m/z$ : (%) 240 [ $\text{M}^+ - \text{HCN}$ ] (80), 225 (100), 179 (40), 77 (35). IR ( $\text{CHCl}_3$ )  $\nu$  ( $\text{cm}^{-1}$ ): 3432 (NH), 2251 (CN).

**2-(4-Methoxyphenylamino)-2-(4-nitrophenyl)propanenitrile (5l):** pale yellow solid; 1.25 g (yield 84 %); mp 109–111 °C (EtOH; lit.<sup>8</sup> 107–109 °C).  $^1\text{H}$  NMR (200 MHz,  $\text{CDCl}_3$ ):  $\delta$  = 1.97 (s, 3H), 3.74 (s, 3H), 4.08 (br s, 1H), 6.45 (d,  $J$  = 8.4 Hz, 2H), 6.68 (d,  $J$  = 8.4 Hz, 2H), 7.79 (d,  $J$  = 8.4 Hz, 2H), 8.22 (d,  $J$  = 8.4 Hz, 2H).  $^{13}\text{C}$  NMR (50 MHz,  $\text{CDCl}_3$ ):  $\delta$  = 32.3, 55.7, 58.0, 114.8, 118.4, 120.3, 124.7, 126.6, 136.6, 147.5, 148.2, 154.5. MS (EI)  $m/z$ : (%) 270 [ $\text{M}^+ - \text{HCN}$ ] (100), 255 (100), 209 (40). IR ( $\text{CHCl}_3$ )  $\nu$  ( $\text{cm}^{-1}$ ): 3424 (NH), 2251 (CN).

**2,2-Diphenyl-2-phenylaminoacetonitrile (5m):** pale grey solid; 1.07 g (yield 75 %); mp 114–116 °C (EtOH).  $^1\text{H}$  NMR (200 MHz,  $\text{CDCl}_3$ ):  $\delta$  = 4.39 (br s, 1H), 6.55–6.59 (m, 2H), 6.80–7.10 (m, 2H), 7.32–7.40 (m, 3H), 7.43–7.47 (m, 4H), 7.52–7.60 (m, 3H), 7.74–7.75 (m, 1H).  $^{13}\text{C}$  NMR (50 MHz,  $\text{CDCl}_3$ ):  $\delta$  = 65.3, 116.2, 119.9, 120.1, 126.3, 128.8, 128.9, 129.1, 139.9, 143.8. MS (EI)  $m/z$ : (%) 257 [ $\text{M}^+ - \text{HCN}$ ] (100), 180 (100), 165 (35), 77 (32). IR ( $\text{CHCl}_3$ )  $\nu$  ( $\text{cm}^{-1}$ ): 3429 (NH), 2245 (CN).

**2-Methyl-2-phenylaminopropanenitrile (5o):** white solid; 0.68 g (yield 85 %); mp 95–96 °C (EtOH; lit. 94–95 °C).  $^1\text{H}$  NMR (200 MHz,  $\text{CDCl}_3$ ):  $\delta$  = 1.64 (s, 3H), 3.20 (br s, 1H), 6.83–6.90 (m, 3H), 7.17–7.24 (m, 2H).  $^{13}\text{C}$  NMR (50 MHz,  $\text{CDCl}_3$ ):  $\delta$  = 28.4, 49.2, 117.7, 121.0, 122.3, 129.5, 143.9. MS (EI)  $m/z$ : (%) 160 [ $\text{M}^+$ ] (15), 133 (30), 118 (100), 77 (55). IR ( $\text{CHCl}_3$ )  $\nu$  ( $\text{cm}^{-1}$ ): 3418 (NH), 2255 (CN).

**1-Phenylaminocyclopentan-1-carbonitrile (5p):** viscous oil; 0.79 g (yield 85 %);  $^1\text{H}$  NMR (200 MHz,  $\text{CDCl}_3$ ):  $\delta$  = 1.65–1.88 (m, 4H), 2.02–2.14 (m, 2H), 2.26–2.37 (m, 2H), 3.86 (br s, 1H), 6.61–6.87 (m, 3H), 7.15–7.23 (m, 2H).  $^{13}\text{C}$  NMR (50 MHz,  $\text{CDCl}_3$ ):  $\delta$  = 23.9, 40.3, 57.6, 115.7, 119.9, 129.5, 144.4. MS (EI)  $m/z$ : (%) 186 [ $\text{M}^+$ ] (15), 185 (25), 159 (45), 130 (100), 77 (25). IR ( $\text{CHCl}_3$ )  $\nu$  ( $\text{cm}^{-1}$ ): 3428 (NH), 2244 (CN).

**2-Phenylamino-2-trifluoromethylpropanenitrile (5q):** viscous oil; 0.77 g (yield 72 %);  $^1\text{H}$  NMR (200 MHz,  $\text{CDCl}_3$ ):  $\delta$  = 1.69 (s, 3H), 3.45 (br s, 1H), 6.63–6.76 (m, 3H), 7.08–7.37 (m, 2H).  $^{13}\text{C}$  NMR (50 MHz,  $\text{CDCl}_3$ ):  $\delta$  = 29.9, 69.0, 115.3, 118.8, 120.0, 129.0, 141.7, 148.8 (d,  $J_I$  = 276.5 Hz). MS (EI)  $m/z$ : (%) 187 [ $\text{M}^+ - \text{HCN}$ ] (45), 118 (100), 77 (75). IR ( $\text{CHCl}_3$ )  $\nu$  ( $\text{cm}^{-1}$ ): 3432 (NH), 2240 (CN).

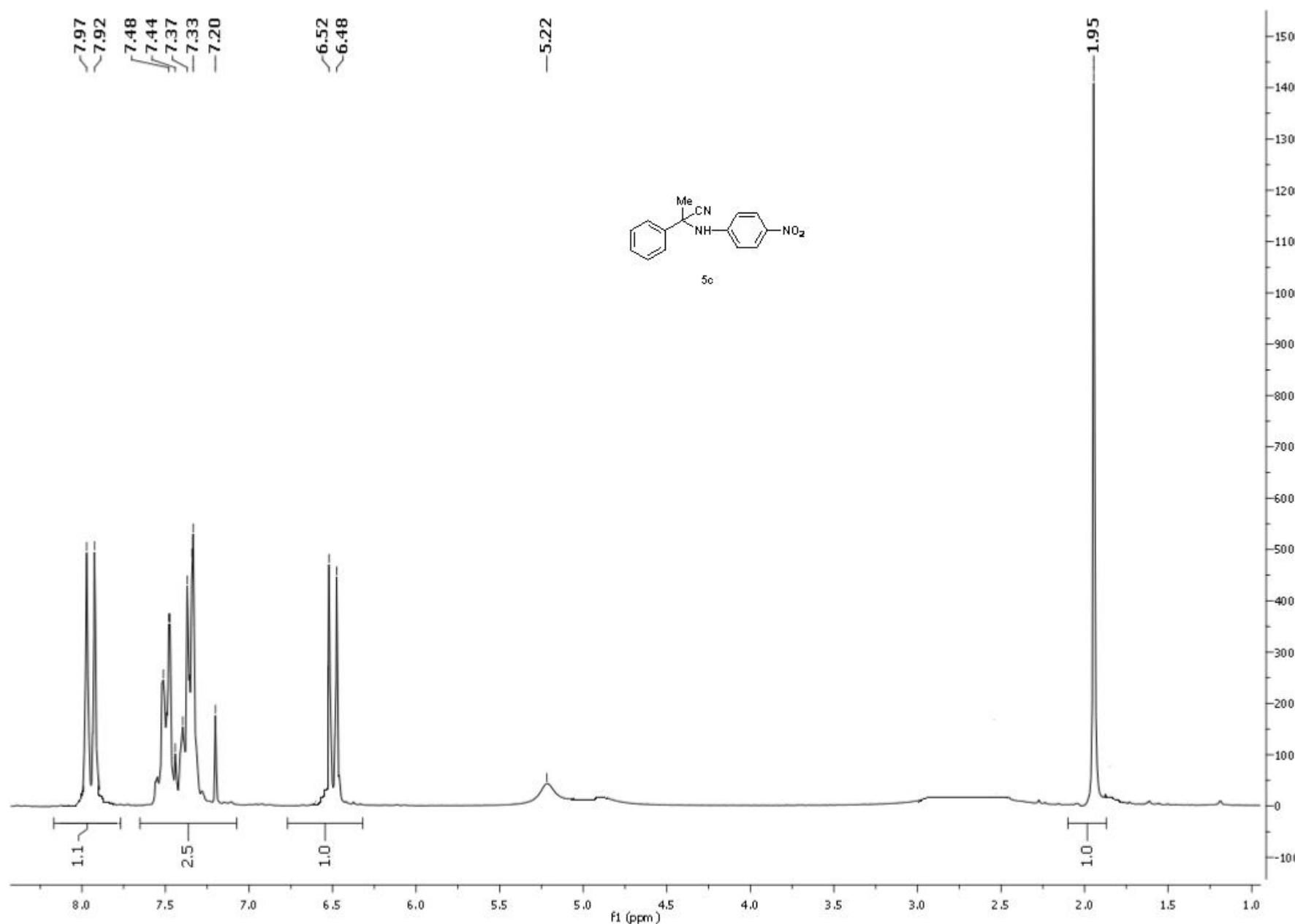
**2-Benzylamino-2-phenylpropanenitrile (5r):** viscous oil; 0.88 g (yield 75 %);  $^1\text{H}$  NMR (200 MHz,  $\text{CDCl}_3$ ):  $\delta$  = 1.79 (s, 3H), 3.82 (s, 2H), 7.20–7.92 (m, 10H).  $^{13}\text{C}$  NMR (50 MHz,  $\text{CDCl}_3$ ):  $\delta$  = 31.4, 49.7, 60.7, 121.3, 125.5, 127.6, 127.8, 128.4, 128.6, 129.1, 139.0, 139.9. MS (EI)  $m/z$ : (%) 209 [ $\text{M}^+ - \text{HCN}$ ] (45), 208 (74), 91 (100). IR ( $\text{CHCl}_3$ )  $\nu$  ( $\text{cm}^{-1}$ ): 3427 (NH), 2252 (CN).

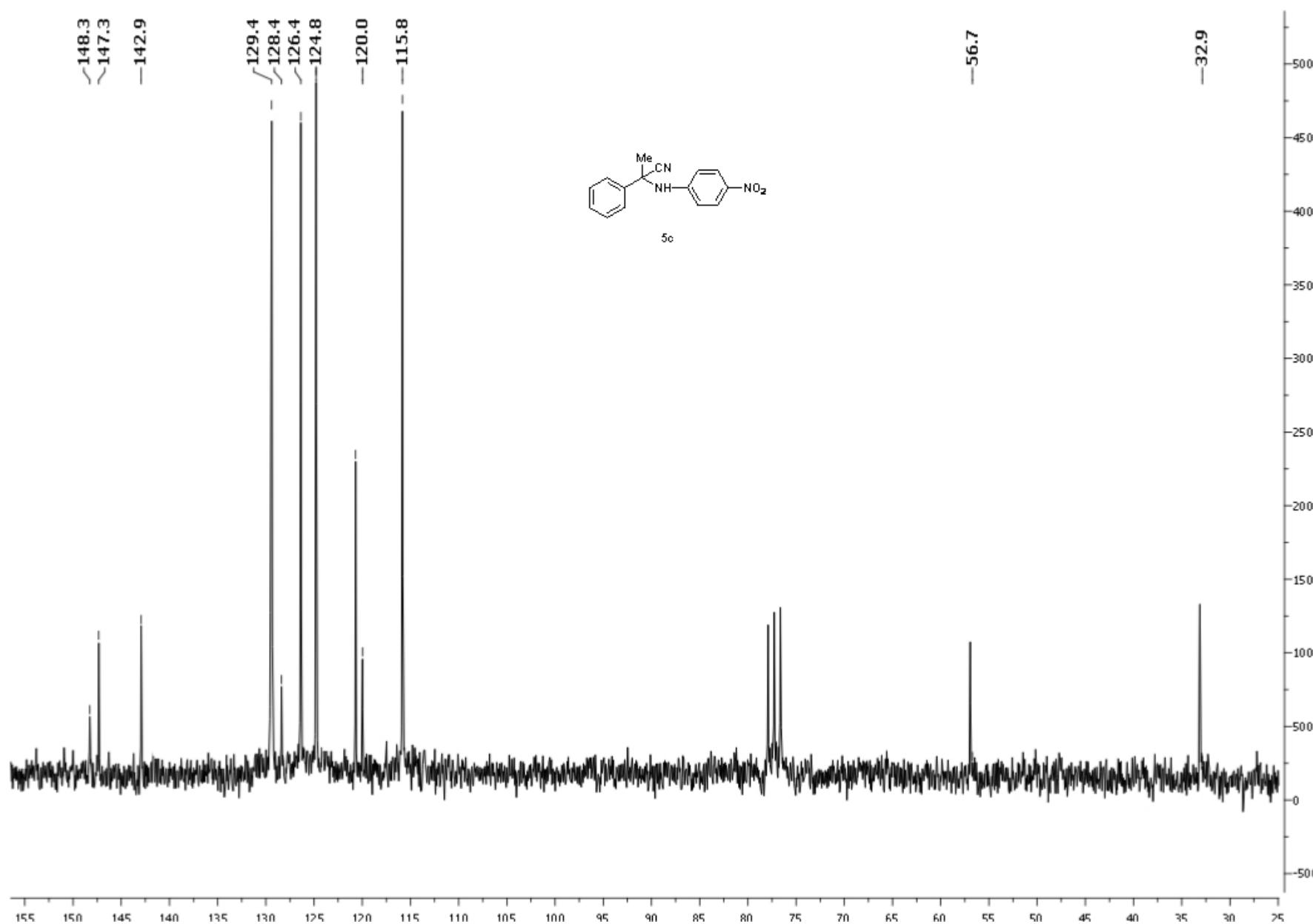
**2-Phenyl-2-phenylaminoacetonitrile (5t):** white solid; 0.99 g (yield 95 %); mp 79 °C (EtOH; lit. 76–78 °C).  $^1\text{H}$  NMR (200 MHz,  $\text{CDCl}_3$ ):  $\delta$  = 4.09 (br s, 1H), 5.37 (s, 1H), 6.65–6.75 (m, 2H), 6.85 (t,  $J$  = 7.7 Hz, 1H), 7.18–7.29 (m, 2H), 7.34–7.46 (m, 3H), 7.51–7.57 (m, 2H).  $^{13}\text{C}$  NMR (50 MHz,  $\text{CDCl}_3$ ):  $\delta$  = 50.9, 113.7, 118.4, 126.7, 127.8, 128.2, 128.3, 129.4, 130.2, 143.5. MS (EI)  $m/z$ : (%) 208 [ $\text{M}^+$ ] (15), 181 (90), 180 (100), 116 (15), 77 (20). IR ( $\text{CHCl}_3$ )  $\nu$  ( $\text{cm}^{-1}$ ): 3415 (NH), 2240 (CN).

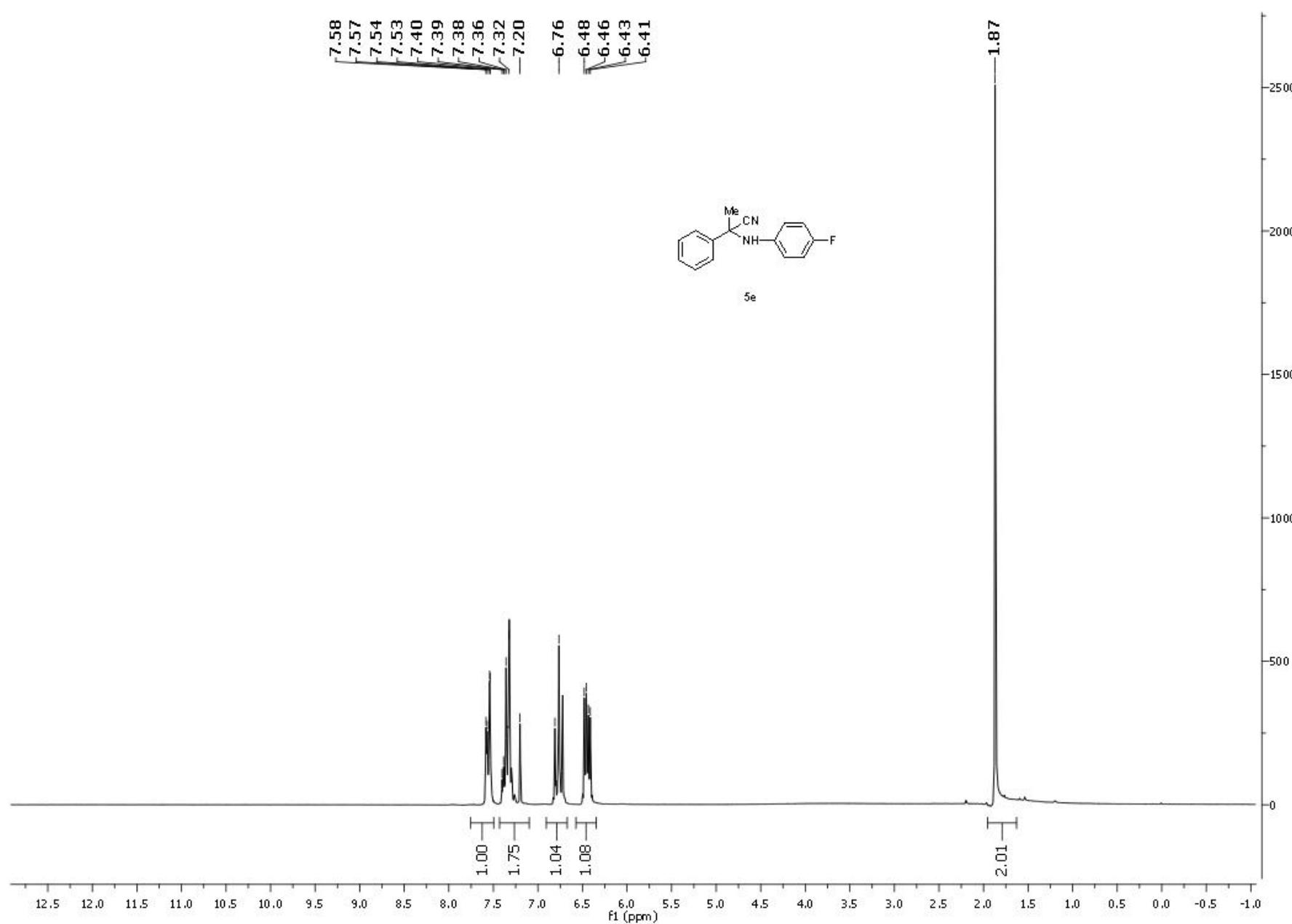
**2,2'-(1,4-Phenylenediamino)bis(2-phenylpropanenitrile) (5u):** white solid; 1.60 g (yield 87 %); mp 144 °C (EtOH; lit.<sup>12</sup> 140–142 °C). <sup>1</sup>H NMR (200 MHz, DMSO-d6): δ = 1.74 (s, 6H), 6.15–6.66 (m, 6H), 7.23–7.64 (m, 8H). <sup>13</sup>C NMR (50 MHz, DMSO-d6): δ = 32.9, 57.6, 115.8, 116.6, 125.2, 125.4, 128.4, 129.0, 129.3, 137.8, 141.6. MS (EI) *m/z*: (%) 312 [M<sup>+</sup> - 2HCN](100), 297 (100). IR (CHCl<sub>3</sub>)  $\nu$  (cm<sup>-1</sup>): 3428 (NH), 2252 (CN).

**2,2'-(1,4-Phenylene)bis[2-(phenylamino)propanenitrile] (5w):** white solid; 1.74 g (yield 95 %); mp 212 °C (EtOH; lit.<sup>12</sup> 208–210 °C). <sup>1</sup>H NMR (200 MHz, CDCl<sub>3</sub>): δ = 1.89 (s, 6H), 4.20 (br s, 2H), 6.45 (d, *J* = 7.8 Hz, 4H), 6.71–6.84 (m, 2H), 7.01–7.13 (m, 4H), 7.60 (s, 4H). <sup>13</sup>C NMR (50 MHz, DMSO-d6): δ = 32.6, 56.8, 115.4, 118.8, 121.6, 126.2, 129.2, 141.3, 145.0. MS (EI) *m/z*: (%) 312 [M<sup>+</sup> - 2HCN] (65), 297 (100), 77 (35). IR (CHCl<sub>3</sub>)  $\nu$  (cm<sup>-1</sup>): 3423 (NH), 2249 (CN).

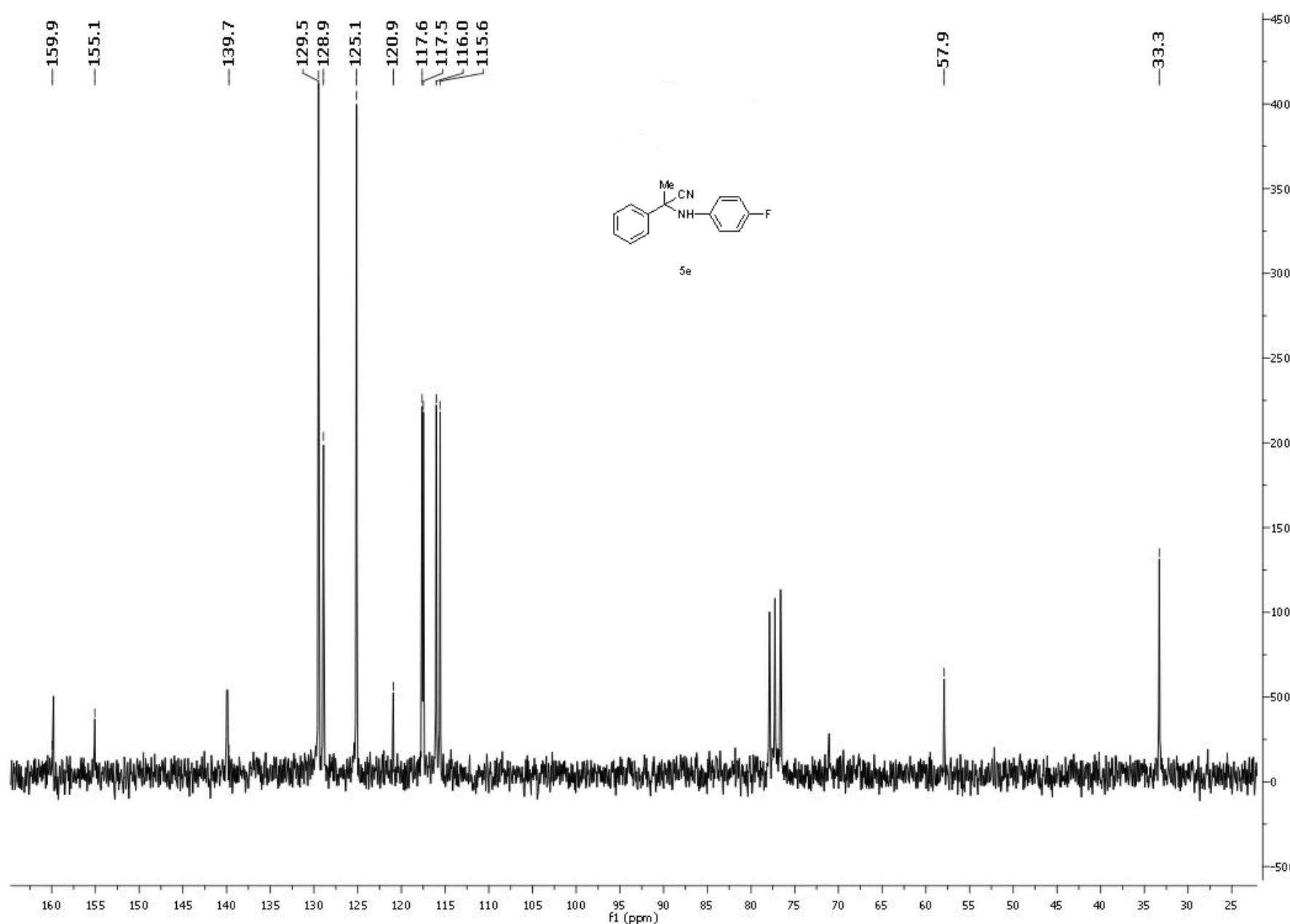
### 3. <sup>1</sup>H-NMR and <sup>13</sup>C-NMR spectra of unknown products 5

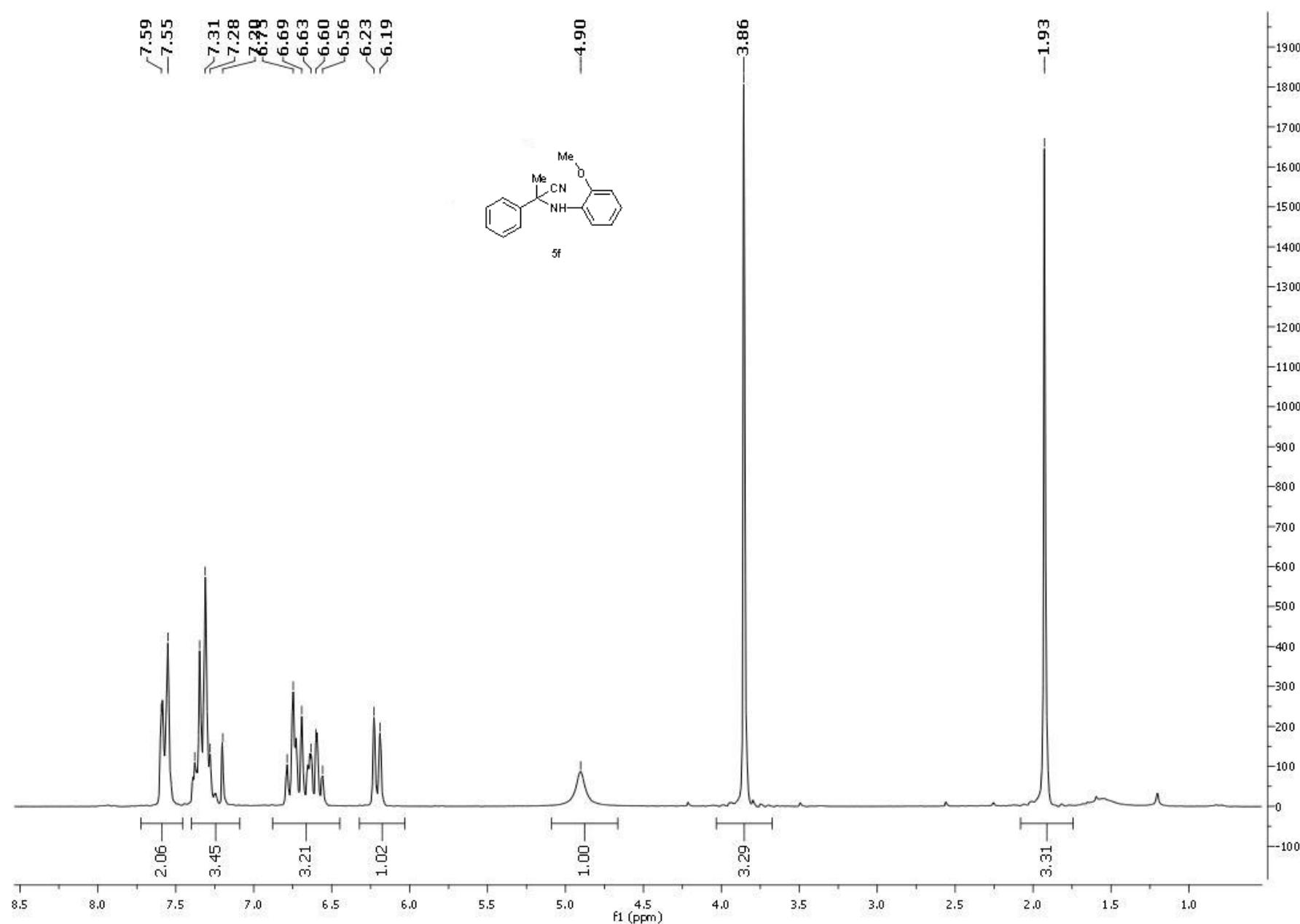


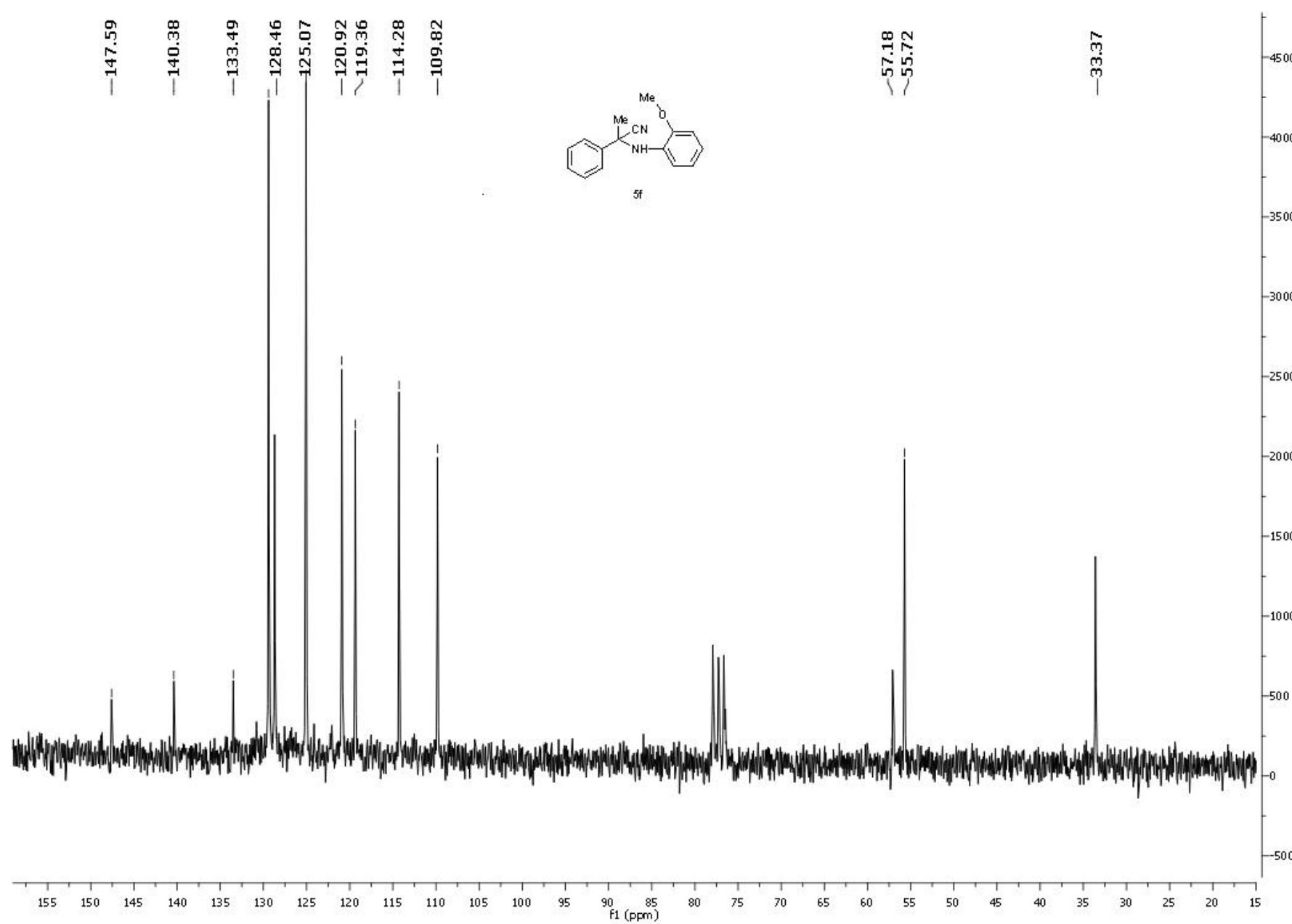


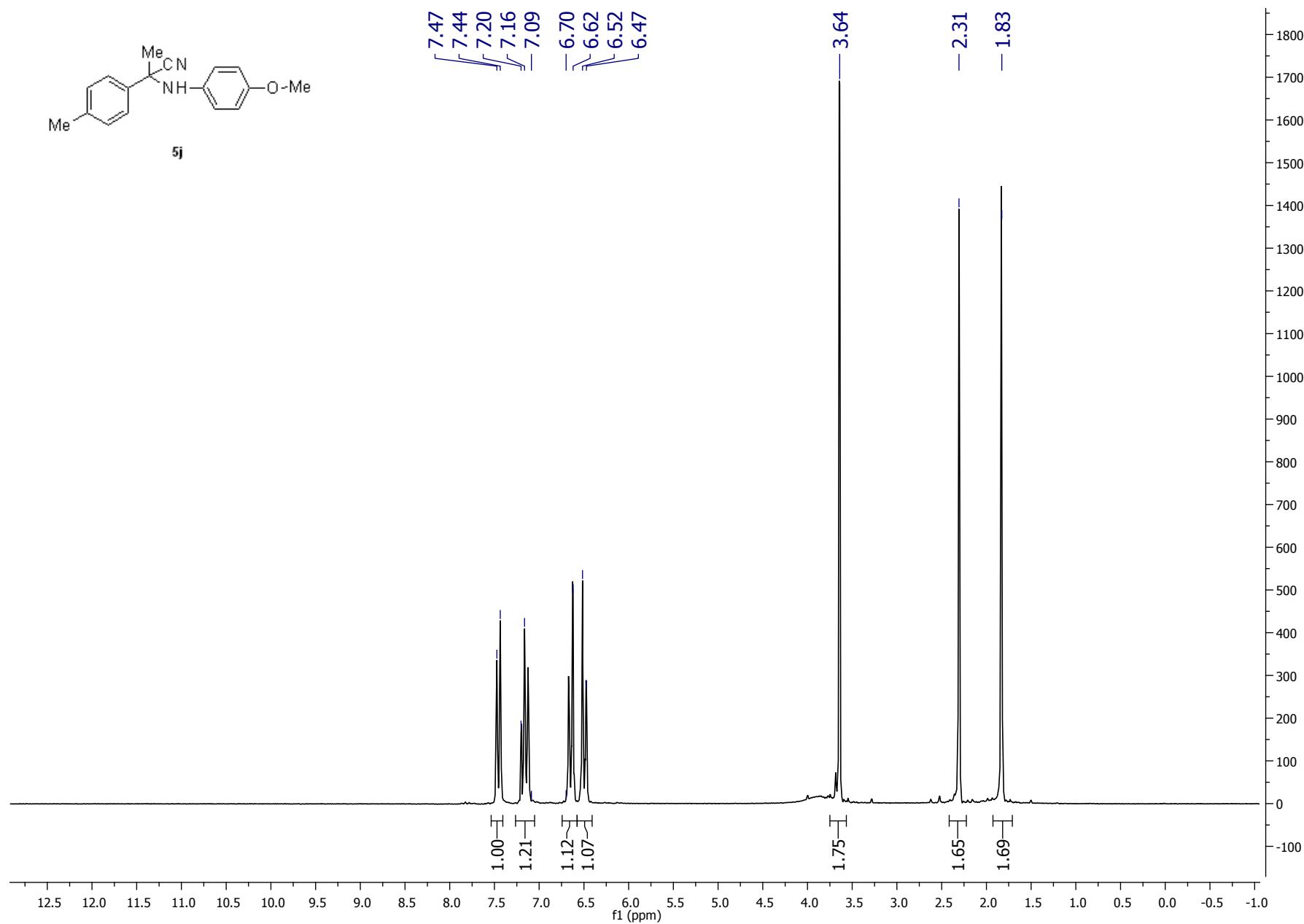


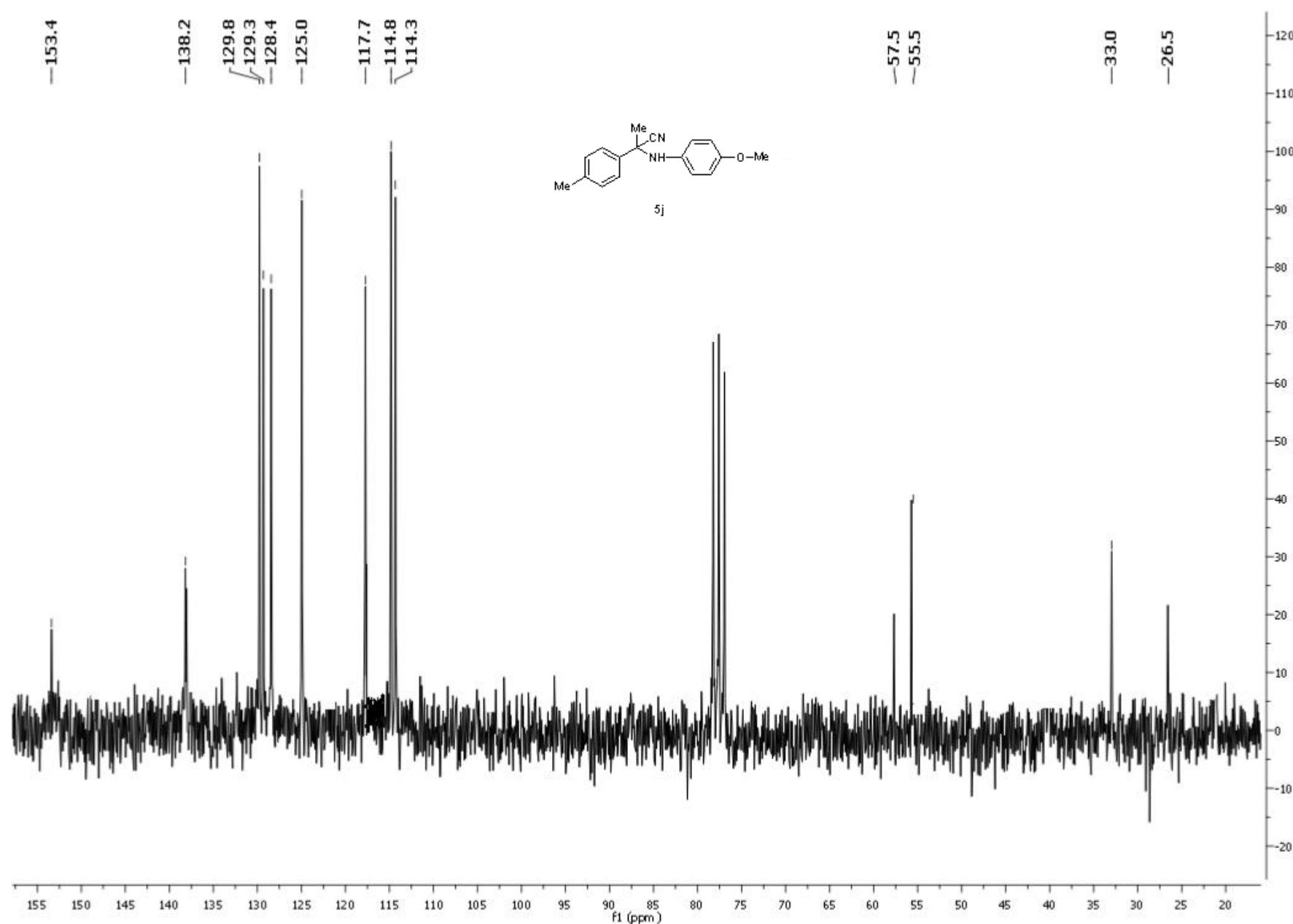
9

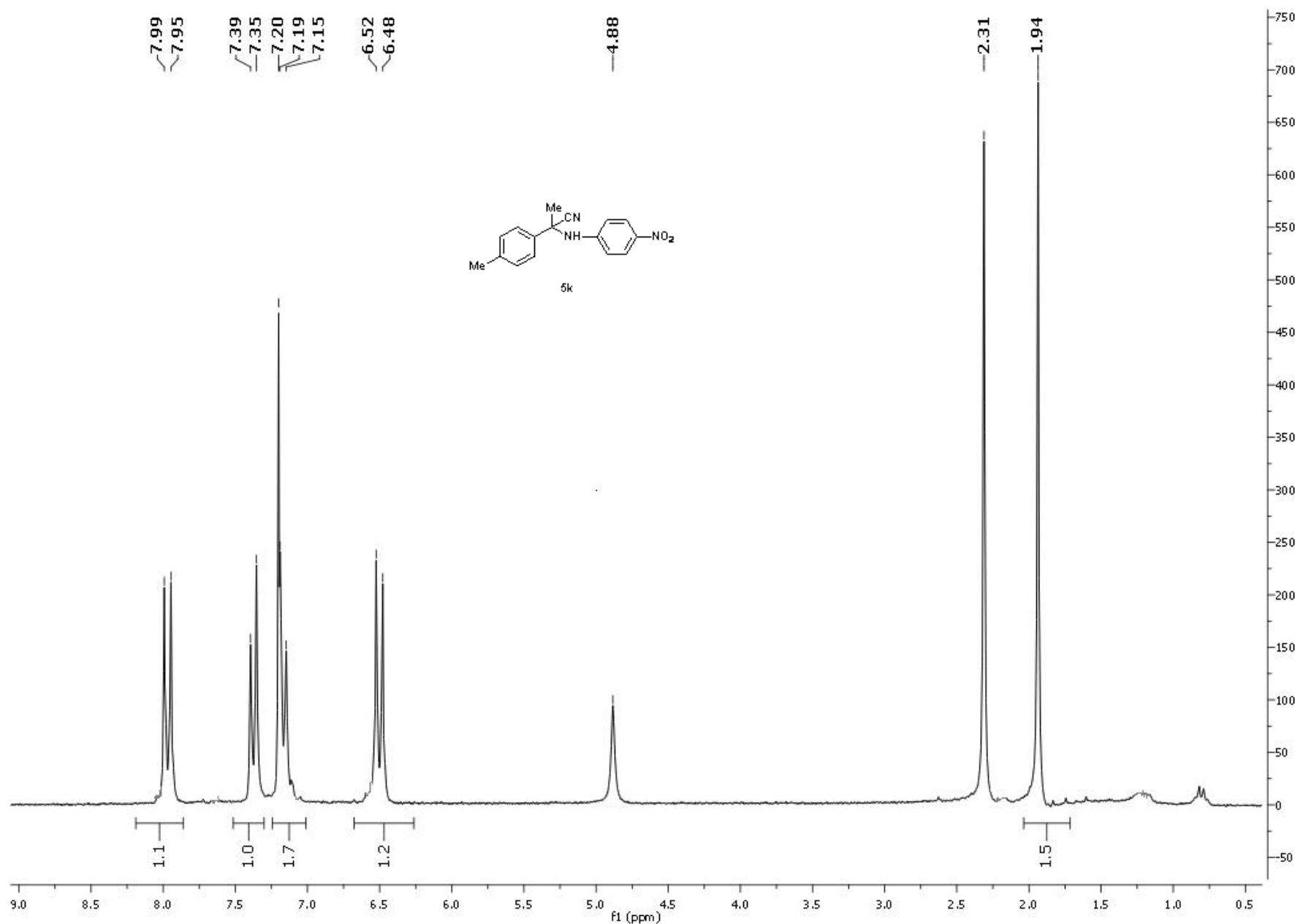


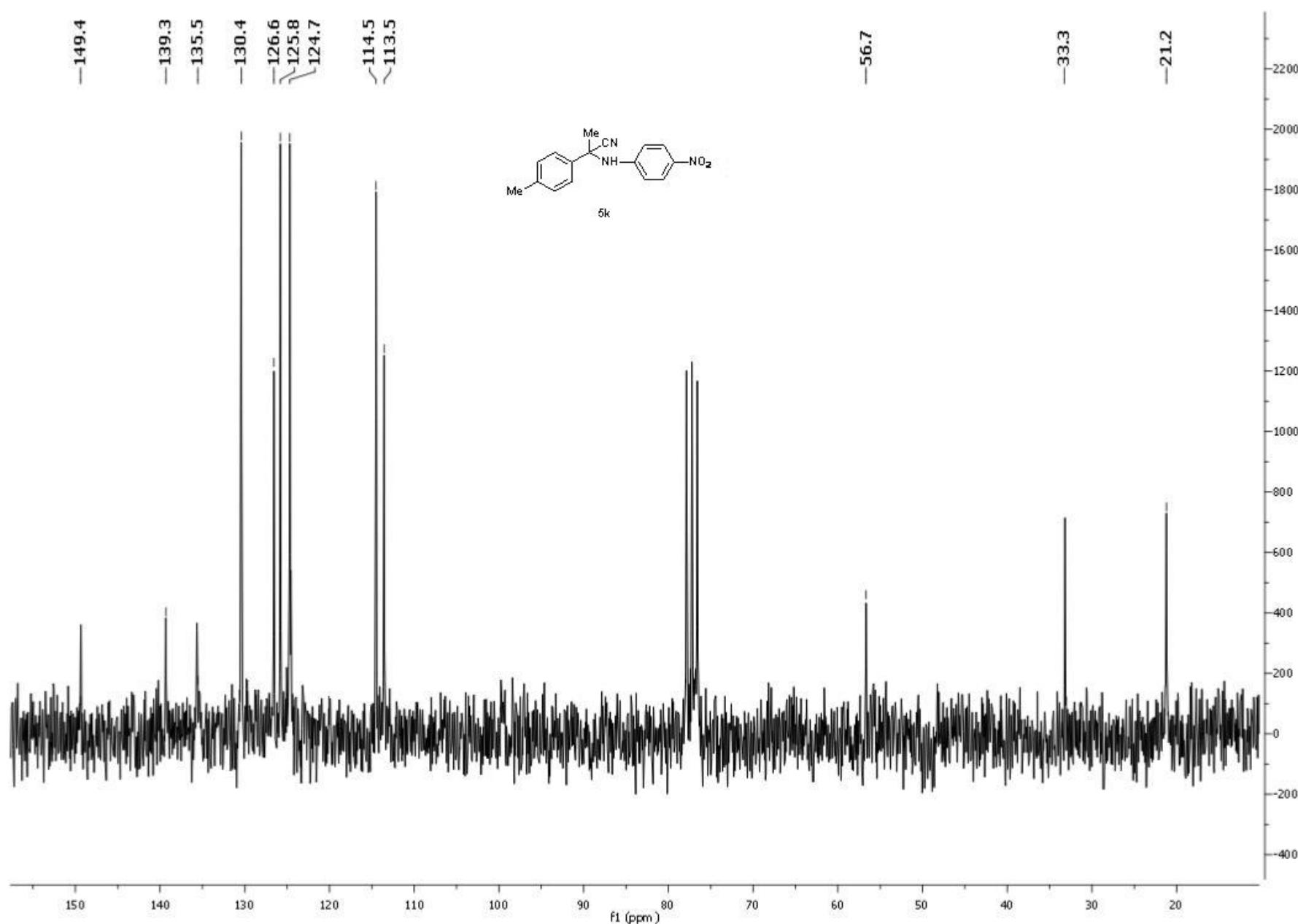


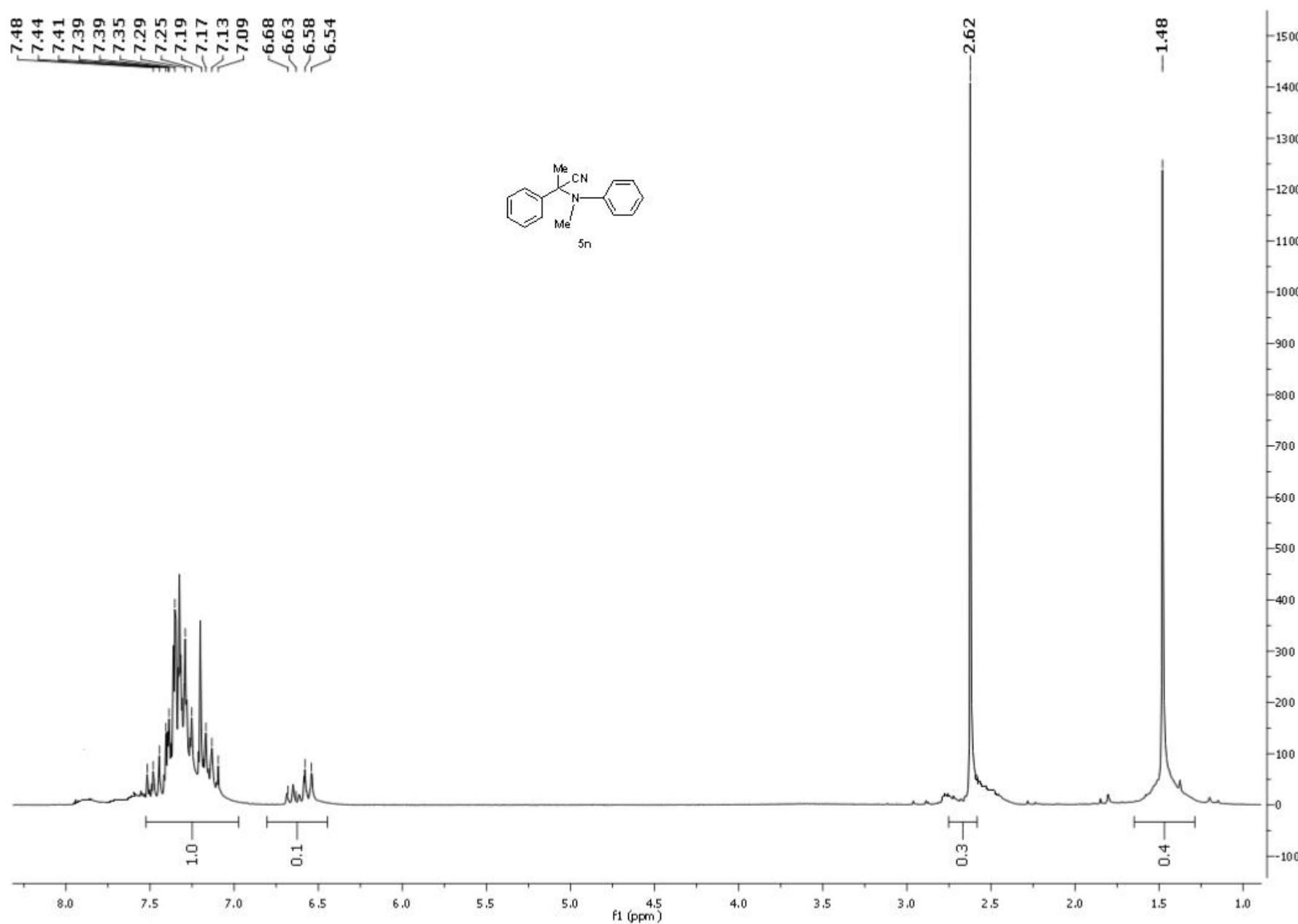


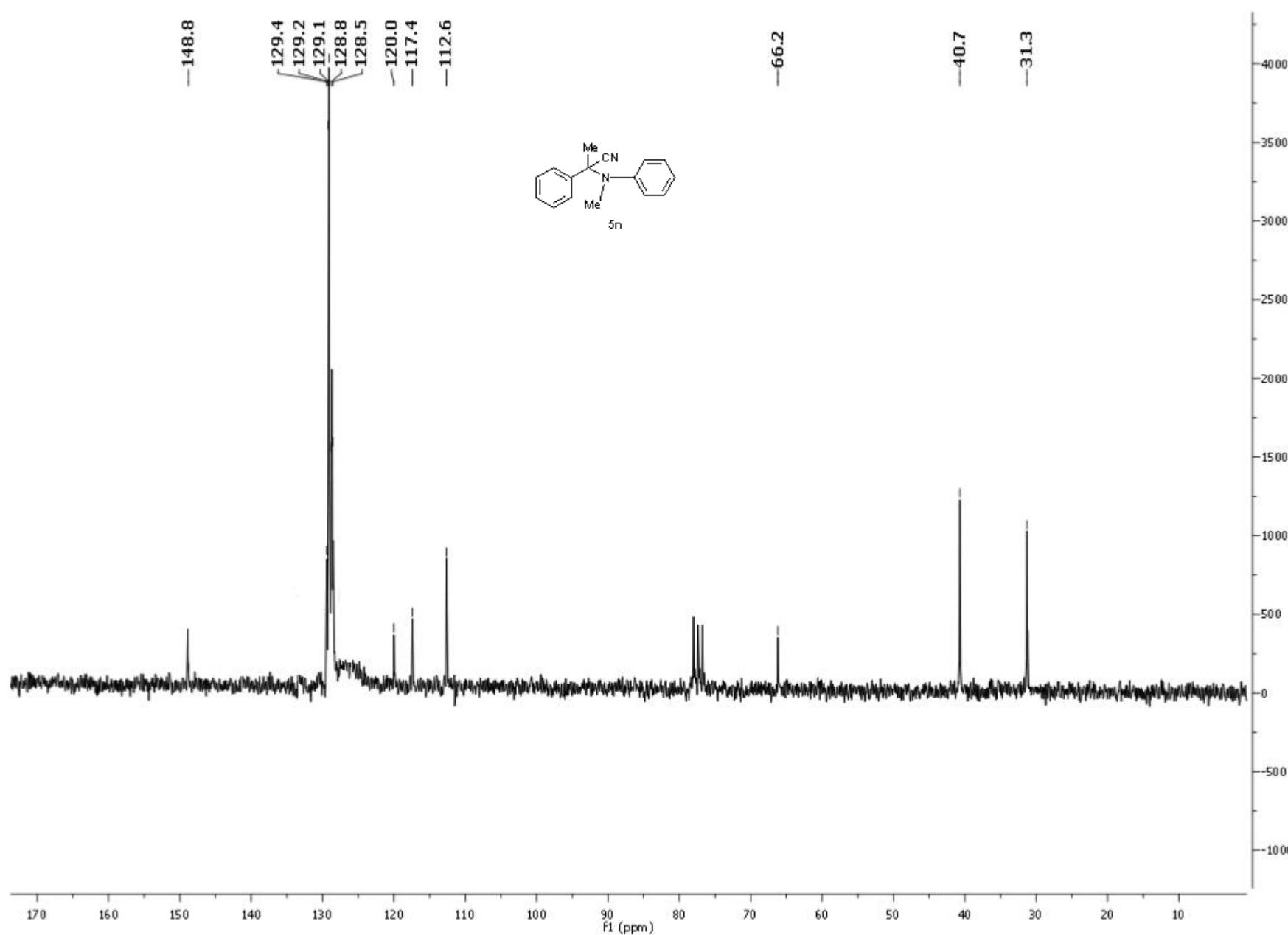


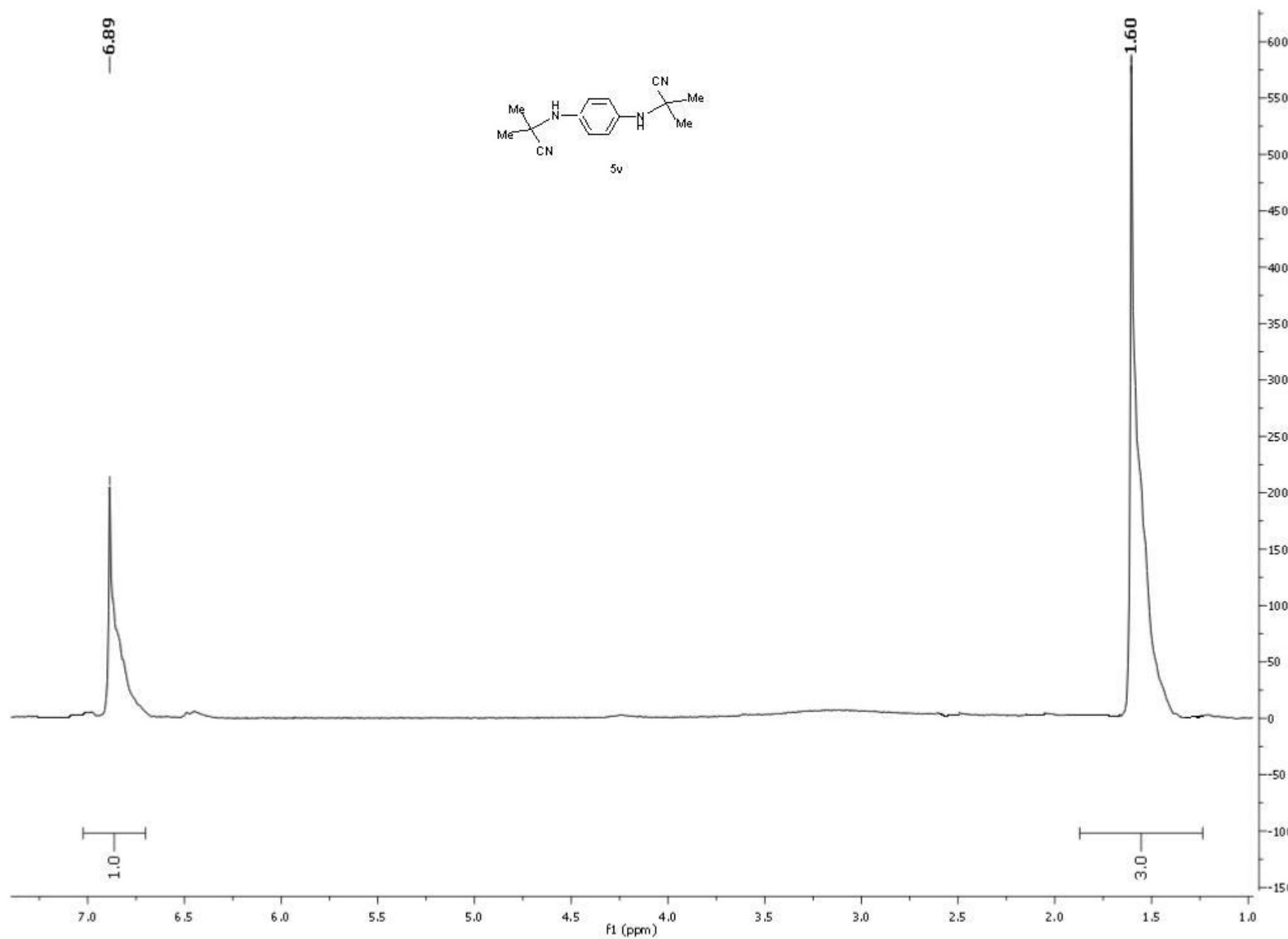


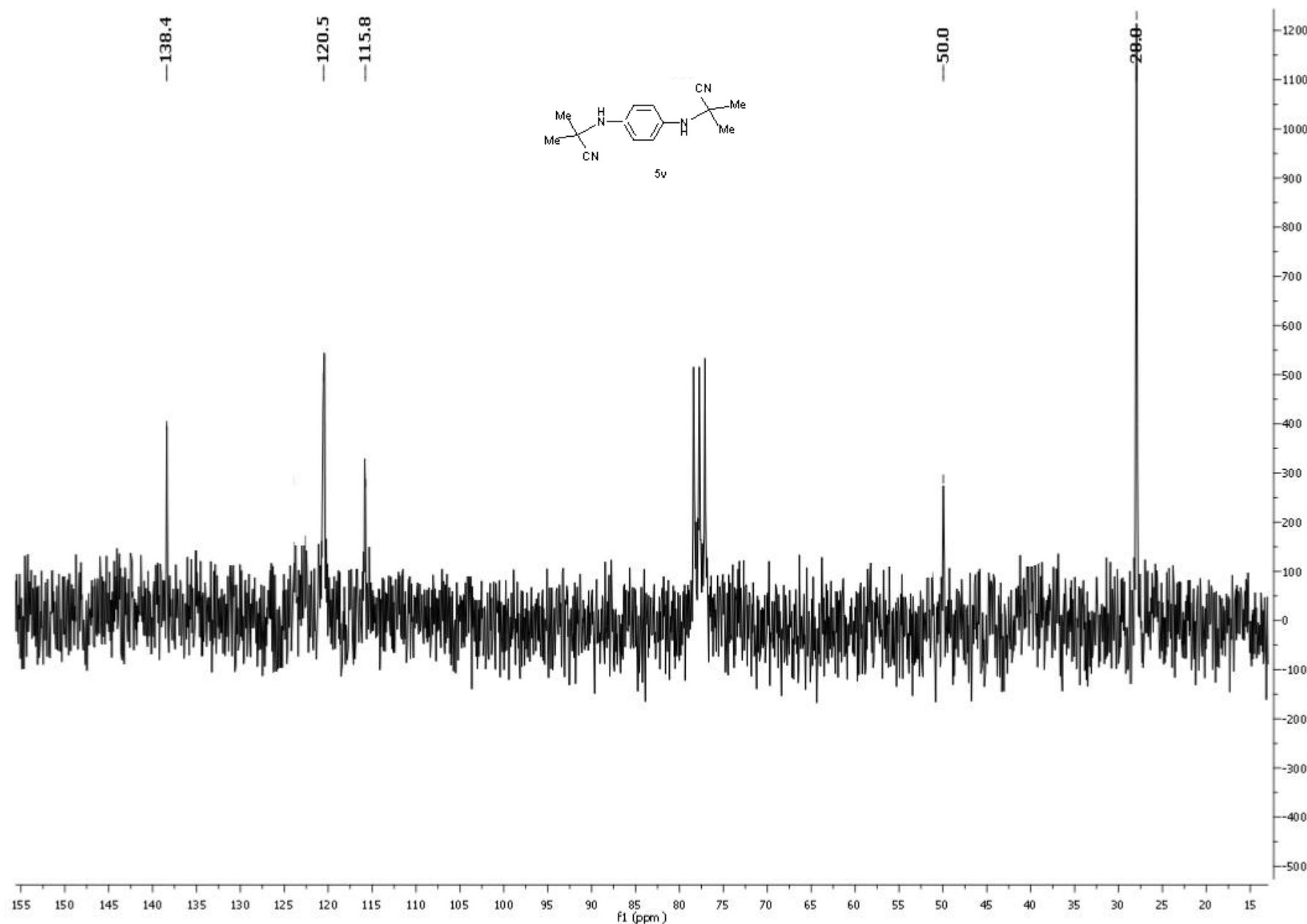


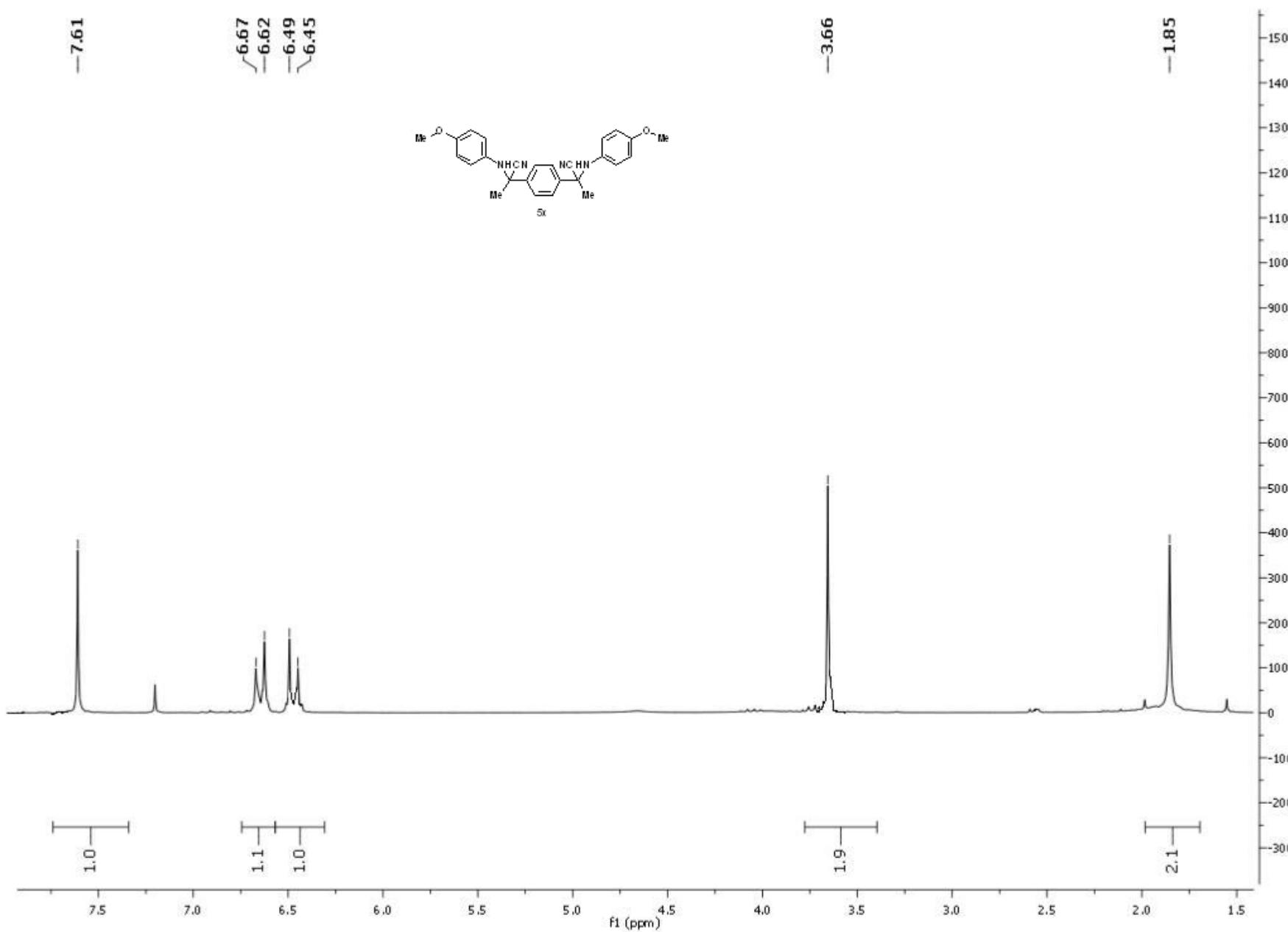


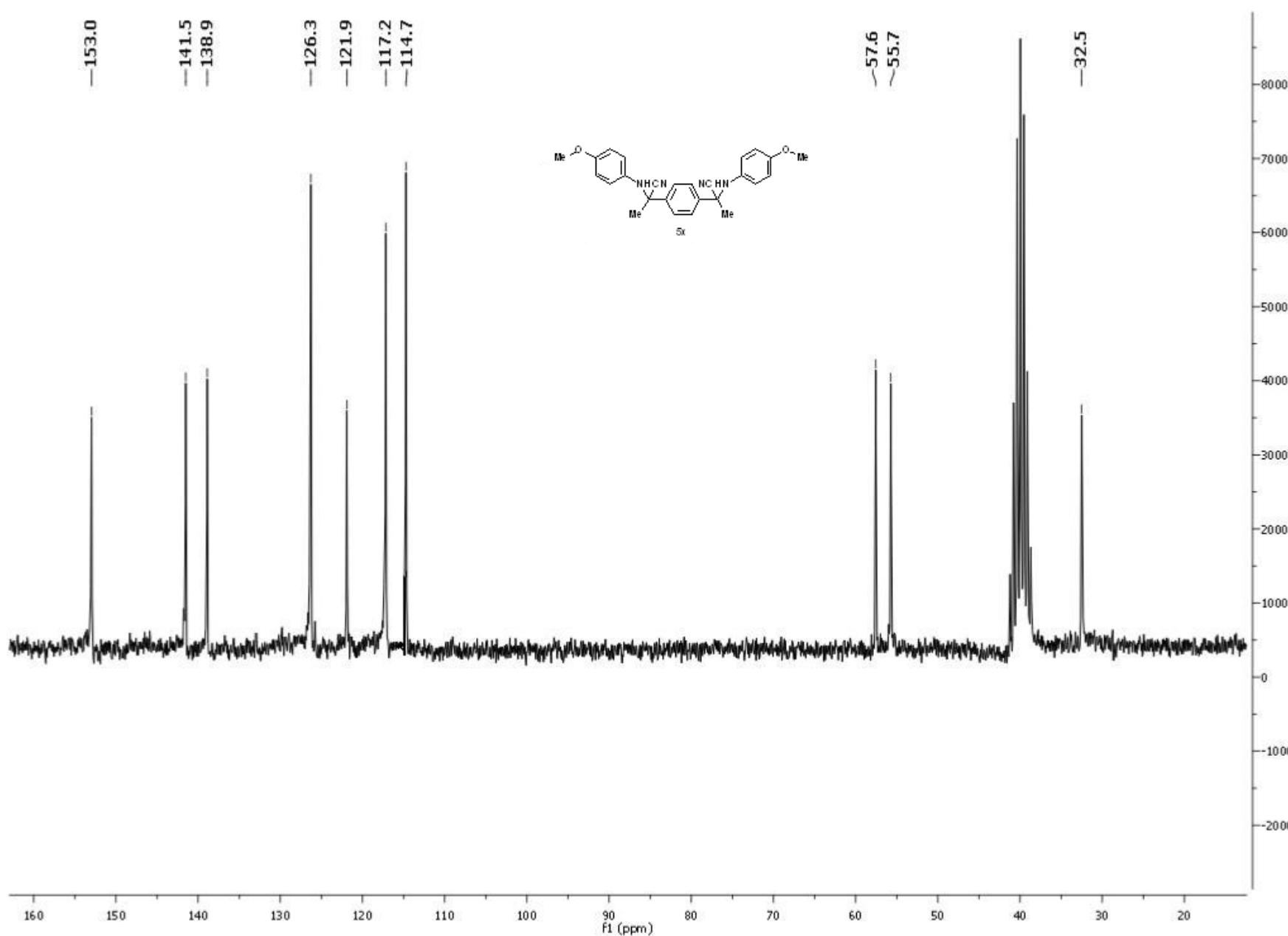






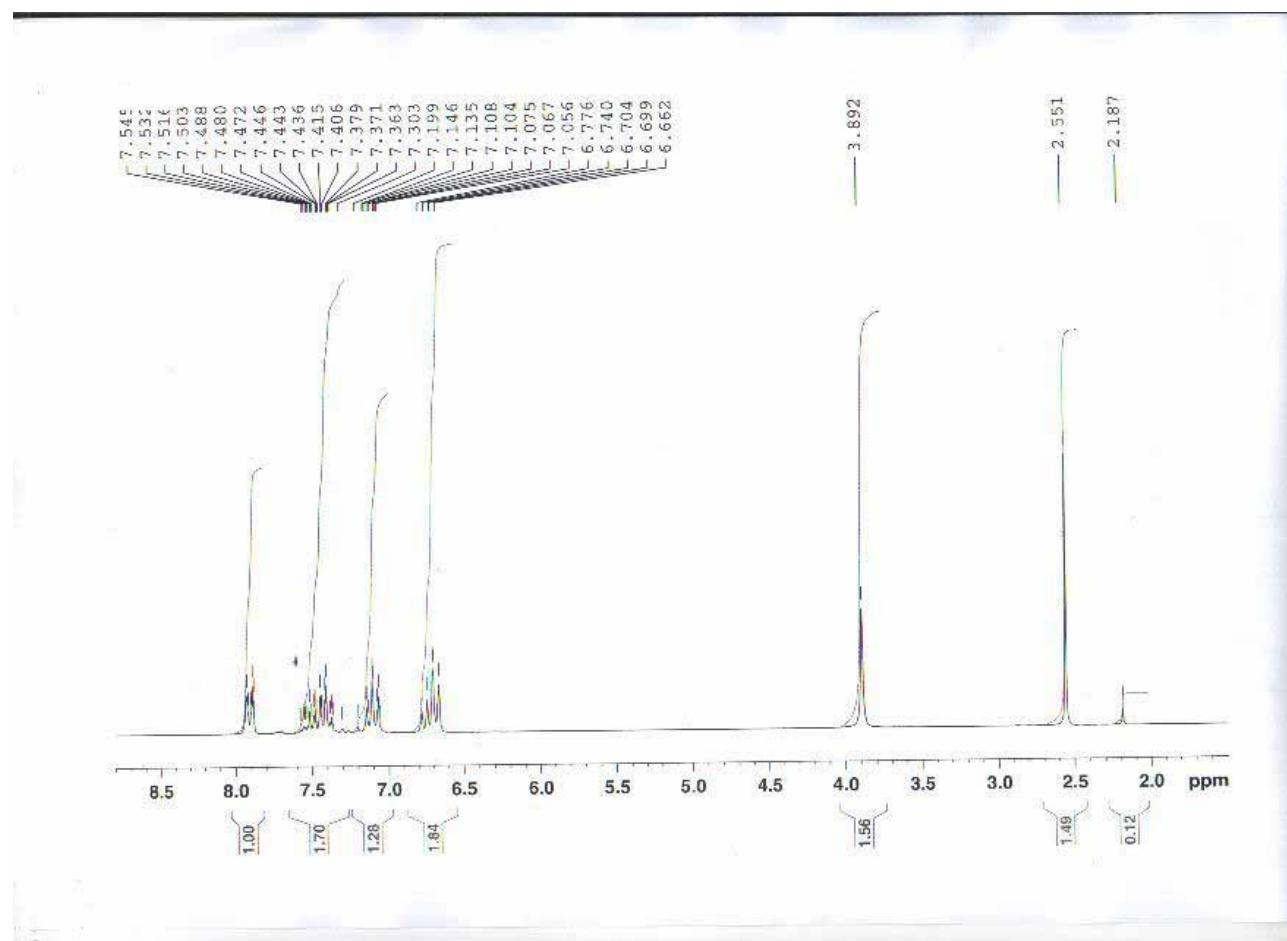






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**4  $^1\text{H}$  NMR spectrum of the crude residue of the reaction described in the second collateral proof**



At  $\delta = 2.18$  the peak of Me of 13a; at  $\delta = 2.55$  the peak of Me of starting 2a

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## 5. Gas-chromatography performed with chiral column.

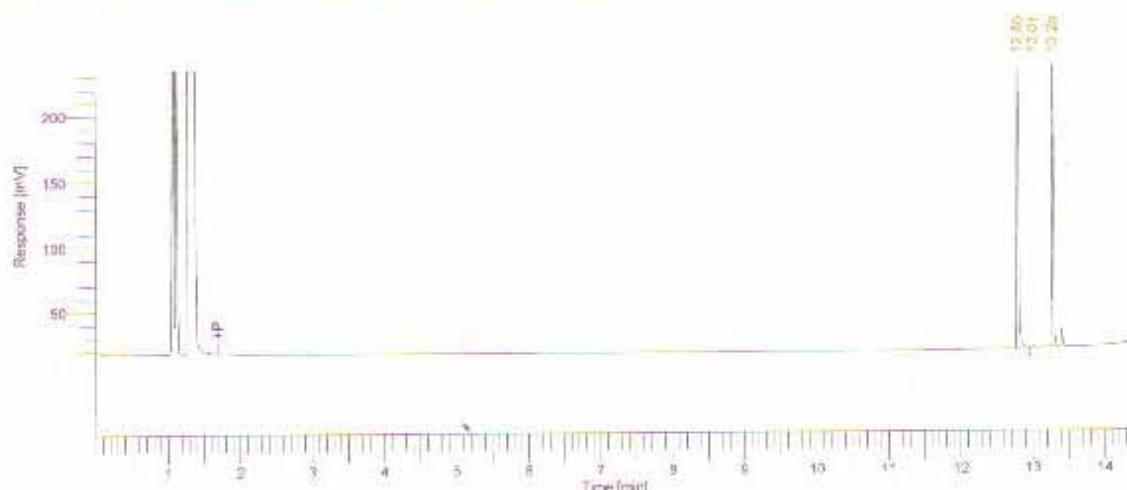
### 5.1 Gas-chromatography of 5a obtained using 1 as a catalyst

Page 1 of 1

Software Version	: 6.2.1.0.104:0104	Date	: 05/07/2011 9.51.00
Reprocess Number	: chpc-lab-e11: 157	Data Acquisition Time	: 05/07/2011 9.36.29
Sample Name	:	Channel	: A
Instrument Name	: autosystemxl	Operator	: Chimica Organica
Rack/Vial	: 0/0	Dilution Factor	: 1,000000
Sample Amount	: 1,000000		
Cycle	: 3		

Result File : D:\DATI\_TC\Chrom\data003-20110705-095059.rst

Sequence File : D:\DATI\_TC\Sequenzer\sequenza2.seq



### DEFAULT REPORT

Peak #	Component Name	Time [min]	Area [ $\mu$ V*sec]	Height [ $\mu$ V]	Area [%]
1		12,797	439394,30	180127,72	50,58
2		13,015	3302,30	1002,52	0,38
3		13,283	425997,88	192681,44	49,04
			868694,48	373811,68	100,00

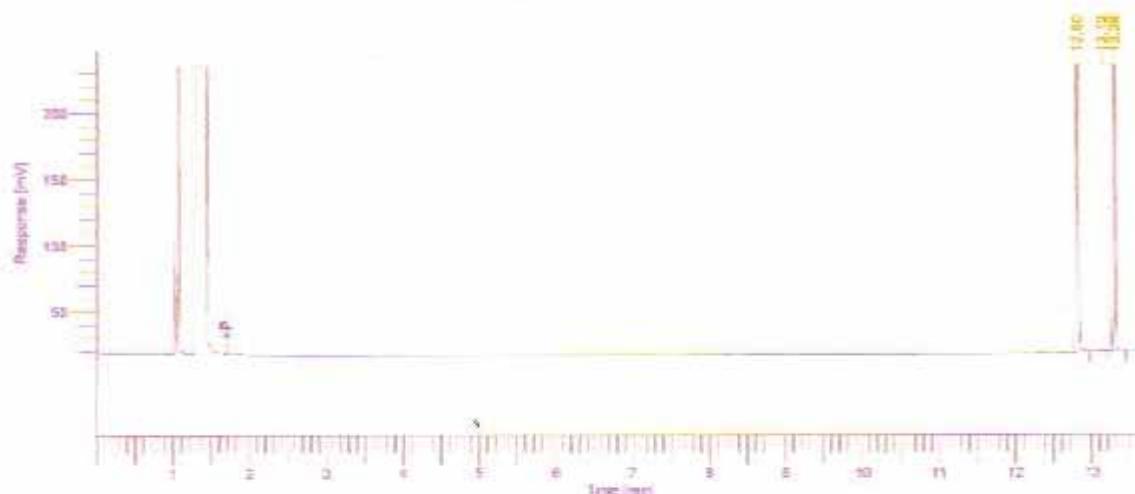
5.2 Gas-chromatography of 5a obtained using chiral 19 as a catalyst at r.t.

Page 1 of 1

Software Version	: 6.2.1.0.104:0104	Date	: 05/07/2011 10.47.31
Reprocess Number	: chpo-lab-e11: 160		
Sample Name	:	Data Acquisition Time	: 05/07/2011 10.33.42
Instrument Name	: autosystemxd	Channel	: A
Rack/Vial	: 0/0	Operator	: Chimica Organica
Sample Amount	: 1,000000	Dilution Factor	: 1,000000
Cycle	: 6		

Result File : D:\DATI\_TC\Chrom\data006-20110705-104730.rst

Sequence File : D:\DATI\_TC\Sequenze\sequenza2.seq



DEFAULT REPORT

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3		13,283	494820,85	226284,50	33,80

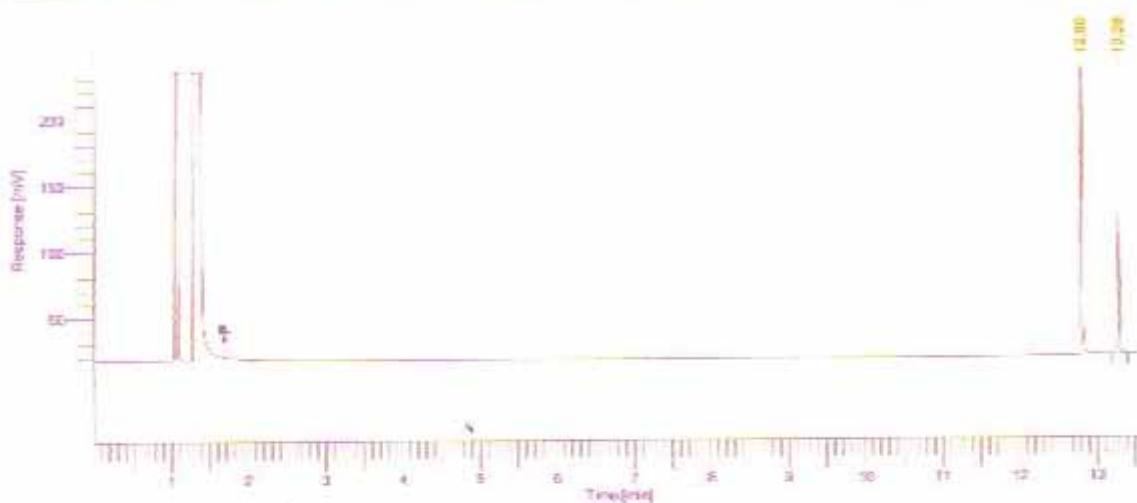
### 5.3 Gas-chromatography of 5a obtained using chiral 19 as a catalyst at 0 °C

Page 1 of 1

Software Version	: 6.2.1.0.104:0104	Date	: 05/07/2011 11.10.57
Reprocess Number	: chpc-lab-e11: 161	Data Acquisition Time	: 05/07/2011 10.57.13
Sample Name	:	Channel	: A
Instrument Name	: autosystemxl	Operator	: Chimica Organica
Rack/Vial	: 0/0	Dilution Factor	: 1,000000
Sample Amount	: 1,000000		
Cycle	: 7		

Result File : D:\DATI\_TC\Chrom\data007-20110705-111056.rst

Sequence File : D:\DATI\_TC\Sequenze\sequenza2.seq



### DEFAULT REPORT

Peak #	Component Name	Time [min]	Area [uV*sec]	Height [uV]	Area [%]
1		12,798	589629,66	246773,69	78,23
2		13,281	164049,40	69880,34	21,77
			753679,05	316654,03	100,00

Missing Component Report

Uncatalyzed	Opt. 6-31+G(d)		SP 6-311+G(2df,p)		H(298K)*		G(298K)*		G* <sub>298K</sub>	<i>n</i>
	E/au	kcal/mol	E/au	kcal/mol	E/au	kcal/mol	E/au	kcal/mol		
<b>3a*2a*3a</b>	-959.757586	<b>0.00</b>	-960.048464	<b>0.00</b>	0.401288	<b>0.00</b>	0.322068	<b>0.00</b>	<b>0.00</b>	3
<b>TS''<sub>Add</sub></b>	-959.716966	<b>25.49</b>	-960.004919	<b>27.33</b>	0.398350	<b>25.48</b>	0.327032	<b>30.44</b>	<b>30.44</b>	3
<b>7a*3a</b>	-959.755261	<b>1.46</b>	-960.043995	<b>2.80</b>	0.403403	<b>4.13</b>	0.329076	<b>7.20</b>	<b>7.20</b>	3
<b>7a*4</b>	-1174.24453102	<b>1.46</b>	-1174.546868	<b>2.80</b>	0.409123	<b>4.13</b>	0.326415	<b>7.20</b>	<b>7.20</b>	3
<b>TS<sub>Exch</sub></b>	-1174.19620412	<b>31.78</b>	-1174.499633	<b>32.44</b>	0.406498	<b>32.12</b>	0.327272	<b>37.38</b>	<b>37.38</b>	3
<b>5a*15</b>	-1174.269580	<b>-14.26</b>	-1174.577393	<b>-16.35</b>	0.408048	<b>-23.96</b>	0.323677	<b>-28.07</b>	<b>-28.07</b>	3
<b>2a*3a</b>	-672.254256	<b>0.00</b>	-672.457300	<b>0.00</b>	0.274358	<b>0.00</b>	0.214524	<b>0.00</b>	<b>0.00</b>	2
<b>TS'''<sub>Add</sub></b>	-672.191188	<b>39.58</b>	-672.392569	<b>40.62</b>	0.270871	<b>38.43</b>	0.214290	<b>40.47</b>	<b>40.47</b>	2
<b>7a</b>	-672.246854	<b>4.65</b>	-672.448880	<b>5.28</b>	0.276151	<b>6.41</b>	0.220089	<b>8.78</b>	<b>8.78</b>	2

Phase 1	Opt. 6-31+G(d)		SP 6-311+G(2df,p)		H <sub>298K</sub>		G <sub>298K</sub>		G* <sub>298K</sub>	<i>n</i> <sup>a</sup>
	E/au	kcal/mol	E/au	kcal/mol	E/au	kcal/mol	E/au	kcal/mol		
<b>2a</b>	-384.750110		-384.864249		0.147975		0.106548			
<b>3a</b>	-287.495792		-287.584252		0.124677		0.088845			
<b>HZ</b>	-1229.655049		-1229.946052		0.078615		0.036559			
<b>2a + 3a + HZ</b>	-1901.900950	<b>0.00</b>	-1902.394553	<b>0.00</b>	0.351267	<b>0.00</b>	0.231952	<b>0.00</b>	<b>0.00</b>	4
<b>2a*3a</b>	-672.254256		-672.457300		0.274358		0.214524			
<b>2a*3a + HZ</b>	-1901.909305	<b>-5.24</b>	-1902.403353	<b>-5.52</b>	0.352973	<b>-4.45</b>	0.251083	<b>6.48</b>	<b>4.59</b>	3
<b>9a*3a</b>	-1901.920884	<b>-12.51</b>	-1902.414035	<b>-12.23</b>	0.354151	<b>-10.42</b>	0.273992	<b>14.16</b>	<b>10.37</b>	2
<b>TS<sub>Add</sub></b>	-1901.920773	<b>-12.44</b>	-1902.413126	<b>-11.65</b>	0.353576	<b>-10.21</b>	0.274978	<b>15.34</b>	<b>11.56</b>	2
<b>10a</b>	-1901.939906	<b>-24.44</b>	-1902.428734	<b>-21.45</b>	0.358620	<b>-16.83</b>	0.279343	<b>8.29</b>	<b>4.50</b>	2
<b>TS<sub>HZ disp</sub></b>	-1901.915970	<b>-9.42</b>	-1902.406186	<b>-7.30</b>	0.355995	<b>-4.33</b>	0.278324	<b>21.80</b>	<b>18.01</b>	2
<b>11a</b>	-1901.918709	<b>-11.14</b>	-1902.409442	<b>-9.34</b>	0.356439	<b>-6.10</b>	0.276925	<b>18.88</b>	<b>15.09</b>	2
<b>TS<sub>H/CO</sub></b>	-1901.904854	<b>-2.45</b>	-1902.396131	<b>-0.99</b>	0.353646	<b>0.50</b>	0.275912	<b>26.60</b>	<b>22.81</b>	2
<b>12a</b>	-1901.927312	<b>-16.54</b>	-1902.422232	<b>-17.37</b>	0.355197	<b>-14.90</b>	0.270751	<b>6.98</b>	<b>3.19</b>	2
<b>13a</b>	-1825.522313		-1825.980679		0.327708		0.249108			
<b>H<sub>2</sub>O</b>	-76.393611		-76.431619		0.024904		0.002803			
<b>13a + H<sub>2</sub>O</b>	-1901.915924	<b>-9.40</b>	-1902.412298	<b>-11.13</b>	0.352612	<b>-10.29</b>	0.251911	<b>1.39</b>	<b>-0.50</b>	3
<b>TS<sub>HZ loss</sub></b>	-1901.909664	<b>-5.47</b>	-1902.402375	<b>-4.91</b>	0.355640	<b>-2.16</b>	0.276246	<b>22.89</b>	<b>19.10</b>	2
<b>7a</b>	-672.253205		-672.455901		0.275638		0.219831			
<b>7a + HZ</b>	-1901.908253	<b>-4.58</b>	-1902.401953	<b>-4.64</b>	0.354253	<b>-2.77</b>	0.256390	<b>10.69</b>	<b>8.80</b>	3

**G\* = G - TS**    **TS = RT ln(1/24.465) = -1.89 kcal mol<sup>-1</sup>**    <sup>a</sup> 4 is the fourth specie

Phase 2	Opt. 6-31+G(d)		SP 6-311+G(2df,p)		H(298K)*		G(298K)*		G* <sub>298K</sub>	<i>n</i> <sup>b</sup>
	E/au	kcal/mol	E/au	kcal/mol	E/au	kcal/mol	E/au	kcal/mol		
<b>8a</b>	-595.835709		-596.004498		0.246147		0.192570			
<b>4</b>	-501.991982		-502.092358		0.130945		0.087530			
<b>HZ</b>	-1229.655049		-1229.946052		0.078615		0.036559			
<b>H<sub>2</sub>O</b>	-76.393611		-76.431619		0.024904		0.002803			
<b>13a</b>	-1825.522313		-1825.980679		0.327708		0.249108			
<b>13a + 4</b>	-2327.514294	<b>-9.40</b>	-2328.073036	<b>-11.13</b>	0.458653	<b>-10.29</b>	0.336638	<b>1.39</b>	<b>-0.50</b>	<b>3</b>
<b>13a*4</b>	-2327.525372	<b>-16.35</b>	-2328.082966	<b>-17.37</b>	0.460456	<b>-15.39</b>	0.357153	<b>8.03</b>	<b>4.24</b>	<b>2</b>
<b>TS' Add</b>	-2327.489771	<b>5.99</b>	-2328.049673	<b>3.53</b>	0.459447	<b>4.87</b>	0.356875	<b>28.75</b>	<b>24.96</b>	<b>2</b>
<b>5a*14</b>	-2327.531707	<b>-20.32</b>	-2328.091630	<b>-22.80</b>	0.461487	<b>-20.18</b>	0.362478	<b>5.94</b>	<b>2.15</b>	<b>2</b>
<b>5a</b>	-689.256906		-689.456266		0.271314		0.213948			
<b>14</b>	-1638.264177		-1638.624116		0.188329		0.128336			
<b>5a + 14 + H<sub>2</sub>O</b>	-2403.914694	<b>-13.66</b>	-2404.512001	<b>-15.74</b>	0.484547	<b>-14.28</b>	0.345087	<b>0.32</b>	<b>-1.57</b>	<b>3</b>
<b>15</b>	-485.003842		-485.111866		0.135075		0.093520			
<b>5a + 15 + HZ</b>	-2403.915797	<b>-14.35</b>	-2404.514184	<b>-17.11</b>	0.485004	<b>-15.36</b>	0.344027	<b>-1.71</b>	<b>-3.61</b>	<b>3</b>
<b>8a + 4 + HZ</b>	-4655.021478	<b>10.40</b>	-4656.141304	<b>7.77</b>	0.920934	<b>6.77</b>	0.719353	<b>7.76</b>	<b>7.76</b>	<b>4</b>
<b>8a*4</b>	-1097.838599	<b>3.56</b>	-1098.107736	<b>0.94</b>	0.379287	<b>1.32</b>	0.300396	<b>13.67</b>	<b>11.77</b>	<b>3</b>
<b>TS<sub>SI</sub> Add</b>	-1097.802589	<b>26.16</b>	-1098.071083	<b>23.94</b>	0.377851	<b>23.42</b>	0.299910	<b>36.36</b>	<b>34.47</b>	<b>3</b>
<b>16</b>	-1097.804630	<b>24.88</b>	-1098.073523	<b>22.41</b>	0.379182	<b>22.72</b>	0.302120	<b>36.22</b>	<b>34.32</b>	<b>3</b>
<b>TS<sub>CN</sub> det</b>	-1097.804509	<b>24.95</b>	-1098.073690	<b>22.31</b>	0.378431	<b>22.14</b>	0.303034	<b>36.69</b>	<b>34.79</b>	<b>3</b>
<b>17</b>	-1097.818121	<b>16.41</b>	-1098.088029	<b>13.31</b>	0.379235	<b>13.65</b>	0.300280	<b>25.96</b>	<b>24.07</b>	<b>3</b>
<b>TS<sub>CN</sub> Aadd</b>	-1097.809915	<b>21.56</b>	-1098.079266	<b>18.81</b>	0.378088	<b>18.43</b>	0.303204	<b>33.29</b>	<b>31.40</b>	<b>3</b>
<b>18</b>	-1097.849754	<b>-3.44</b>	-1098.119104	<b>-6.19</b>	0.379626	<b>-5.60</b>	0.305153	<b>9.52</b>	<b>7.62</b>	<b>3</b>

**G\* = G - T ΔS**    **T ΔS = RT ln(1/24.465) = -1.89 kcal mol<sup>-1</sup>**    <sup>b</sup> H<sub>2</sub>O is the fourth molecule

7. Cartesian coordinates (Gaussian format).

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Cartesian coordinates of optimized structures

M06-2X/6-31+G(d) in acetonitrile (PCM)

Data in Angstroms

For labels see Manuscript Schemes 2-4

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HZ (model for 1)

1	7	0	-0.026811	0.130432	-0.027759
2	16	0	-0.053989	-0.097965	1.660105
3	16	0	1.526869	-0.096702	-0.688116
4	6	0	1.698853	0.083382	1.931674
5	6	0	2.437135	0.083827	0.834401
6	8	0	-0.815269	0.996215	2.231790
7	8	0	-0.415961	-1.470528	1.953533
8	8	0	1.773539	0.997260	-1.607816
9	8	0	1.661158	-1.469562	-1.133613
10	1	0	2.050193	0.111867	2.960448
11	1	0	3.522290	0.113627	0.773473
12	1	0	-0.402414	1.054624	-0.277634

2a

1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.400058
3	6	0	1.206045	0.000000	2.100488
4	6	0	2.416585	0.000013	1.407259
5	6	0	2.422436	0.000030	0.009721
6	6	0	1.219673	0.000014	-0.689620
7	1	0	-0.936027	-0.000011	1.950901
8	1	0	1.199558	-0.000020	3.186823
9	1	0	3.355479	0.000011	1.954277
10	1	0	3.364733	0.000051	-0.530937
11	1	0	1.211571	0.000019	-1.775755
12	6	0	-1.275765	-0.000053	-0.789038
13	8	0	-1.244042	-0.000319	-2.009849
14	6	0	-2.587383	0.000233	-0.046828
15	1	0	-2.665147	-0.883391	0.596144

29

	16	1	0	-2.664939	0.884093	0.595850
17	1	0	-3.406706	0.000203	-0.767611	

3a

1	6	0	-0.004287	-0.004101	-0.001975
2	6	0	-0.004406	-0.001384	1.402093
3	6	0	1.197600	-0.000771	2.106379
4	6	0	2.421151	-0.003810	1.432738
5	6	0	2.422569	-0.005704	0.036027
6	6	0	1.226485	-0.006189	-0.677880
7	7	0	-1.203997	-0.070366	-0.712907
8	1	0	-1.153288	0.299453	-1.657191
9	1	0	-2.006733	0.305916	-0.217835
10	1	0	-0.953677	0.000502	1.933444
11	1	0	1.175309	0.003698	3.193299
12	1	0	3.355751	-0.002705	1.985630
13	1	0	3.364187	-0.005059	-0.507220
14	1	0	1.235295	-0.007671	-1.765670

4

1	14	0	0.001585	0.001161	-0.001867
2	6	0	0.002266	0.002504	1.904989
3	6	0	1.801709	-0.001562	-0.493635
4	1	0	1.887284	-0.002426	-1.586813
5	1	0	2.317162	0.886737	-0.112878
6	1	0	2.314768	-0.890757	-0.111715
7	6	0	-0.903225	-1.556121	-0.488784
8	1	0	-0.944671	-1.633507	-1.581801
9	1	0	-0.395661	-2.447517	-0.104846
10	1	0	-1.930734	-1.551276	-0.109399
11	6	0	-0.899483	1.559961	-0.490780
12	1	0	-0.940961	1.635988	-1.583888
13	1	0	-1.926908	1.558049	-0.111135
14	1	0	-0.389715	2.450654	-0.108136
15	7	0	0.002427	0.003338	3.064663

**5a**

1	6	0	-0.024501	-0.045691	0.055261
2	6	0	0.015112	-0.441278	1.393789
3	6	0	1.224152	-0.437384	2.094428
4	6	0	2.402034	-0.042495	1.464164
5	6	0	2.369088	0.350453	0.124265
6	6	0	1.163513	0.350233	-0.572001
7	1	0	-0.889045	-0.754542	1.906190
8	1	0	1.239129	-0.746024	3.135930
9	1	0	3.341062	-0.042316	2.010369
10	1	0	3.281802	0.656963	-0.378951
11	1	0	1.147931	0.667897	-1.613557
12	6	0	-1.350211	0.068623	-0.712871
13	6	0	-2.497546	-0.726790	-0.081200
14	1	0	-2.723459	-0.351671	0.918199
15	1	0	-3.392192	-0.631442	-0.701299
16	1	0	-2.222087	-1.781960	-0.004572
17	7	0	-1.741095	1.491588	-0.930423
18	6	0	-1.951651	2.257027	0.261745
19	6	0	-0.939589	3.076698	0.775447
20	6	0	-1.169024	3.850484	1.913227
21	6	0	-2.404589	3.798993	2.559185
22	6	0	-3.416286	2.983922	2.047697
23	6	0	-3.197519	2.226108	0.898088
24	1	0	0.026608	3.106793	0.275846
25	1	0	-0.377255	4.487857	2.297397
26	1	0	-2.582039	4.396066	3.449153
27	1	0	-4.387113	2.950145	2.534392
28	1	0	-3.995734	1.620294	0.478486
29	6	0	-1.156197	-0.487514	-2.076078
30	7	0	-1.018411	-0.931158	-3.134800
31	1	0	-0.992513	1.932850	-1.466716

**2a\*3a**

1	6	0	-0.095800	0.461162	-0.237969
2	6	0	-0.485170	-0.027057	1.126010
3	8	0	1.082144	0.545675	-0.549857
4	6	0	0.495426	-0.602482	1.942843

31

	5	6	0	0.166388	-1.076883	3.209886
6	6	0	-1.147092	-0.971724	3.674940	
7	6	0	-2.128498	-0.394399	2.868313	
8	6	0	-1.800845	0.071660	1.595026	
9	1	0	1.513006	-0.680410	1.570377	
10	1	0	0.930602	-1.530129	3.835162	
11	1	0	-1.405443	-1.342520	4.663195	
12	1	0	-3.151067	-0.312792	3.226391	
13	1	0	-2.575153	0.514337	0.974784	
14	6	0	-1.185484	0.885732	-1.188331	
15	1	0	-1.619956	1.833665	-0.847406	
16	1	0	-0.759921	1.027543	-2.183571	
17	1	0	-1.990172	0.145752	-1.228156	
18	7	0	-0.750460	-2.363499	-1.207598	
19	6	0	-1.770765	-2.791169	-0.365908	
20	6	0	-3.107994	-2.448937	-0.630481	
21	6	0	-4.116696	-2.804993	0.262594	
22	6	0	-3.820907	-3.507296	1.433060	
23	6	0	-2.492751	-3.856138	1.693278	
24	6	0	-1.476400	-3.504671	0.808865	
25	1	0	-3.346504	-1.902369	-1.540484	
26	1	0	-5.144334	-2.530350	0.037913	
27	1	0	-4.610064	-3.782087	2.126614	
28	1	0	-2.241773	-4.405158	2.597740	
29	1	0	-0.443741	-3.774235	1.020956	
30	1	0	0.109905	-2.898942	-1.151832	
31	1	0	-1.024316	-2.188354	-2.169209	

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9a\*3a

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1	6	0	0.273171	-0.855380	0.168283
2	6	0	0.126071	-0.411085	1.613495
3	8	0	1.442205	-0.331563	-0.348125
4	6	0	1.281506	-0.189613	2.371828
5	6	0	1.184266	0.166939	3.715033
6	6	0	-0.069282	0.307303	4.313085
7	6	0	-1.222232	0.090959	3.560307
8	6	0	-1.126565	-0.268778	2.215014
9	1	0	2.258311	-0.294906	1.908734
10	1	0	2.087832	0.337468	4.293419

32

	11	1	0	-0.145962	0.586110	5.360319
12	1	0	-2.201639	0.199888	4.017234	
13	1	0	-2.037669	-0.439425	1.649723	
14	6	0	-0.932042	-0.604446	-0.718066	
15	1	0	-1.100584	0.473816	-0.771687	
16	1	0	-0.742928	-0.978216	-1.729385	
17	1	0	-1.833936	-1.087017	-0.338662	
18	1	0	1.455934	-0.400047	-1.335136	
19	7	0	1.648805	-0.667166	-3.134472	
20	16	0	0.975151	0.511418	-4.039396	
21	16	0	1.320307	-2.147225	-3.695751	
22	6	0	-0.092154	-1.767759	-4.730408	
23	6	0	-0.261194	-0.467642	-4.896224	
24	8	0	1.878168	1.053577	-5.058325	
25	8	0	0.339262	1.484096	-3.149955	
26	8	0	2.360975	-2.727484	-4.545858	
27	8	0	0.895668	-3.001786	-2.567229	
28	1	0	-0.650781	-2.586423	-5.174732	
29	1	0	-0.996467	0.041330	-5.512998	
30	7	0	0.537266	-2.407954	0.192548	
31	6	0	-0.484641	-3.278823	0.767630	
32	6	0	-1.481281	-3.783811	-0.061005	
33	6	0	-2.466333	-4.598593	0.495188	
34	6	0	-2.441838	-4.897912	1.857740	
35	6	0	-1.428137	-4.388350	2.670776	
36	6	0	-0.438300	-3.571927	2.127139	
37	1	0	-1.487248	-3.546458	-1.122139	
38	1	0	-3.249282	-5.001059	-0.140222	
39	1	0	-3.210524	-5.534486	2.285868	
40	1	0	-1.403449	-4.626886	3.729665	
41	1	0	0.359843	-3.169298	2.746554	
42	1	0	1.426095	-2.533926	0.695399	
43	1	0	0.723087	-2.681366	-0.792577	

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1	6	0	-0.115991	-0.021542	-0.143075
2	6	0	-0.256524	-0.071096	1.315052
3	8	0	1.080294	-0.067601	-0.597035
4	6	0	0.851308	-0.417148	2.104951

33

	5	6	0	0.721782	-0.495676	3.486227
6	6	0	-0.511771	-0.232496	4.088497	
7	6	0	-1.615430	0.113215	3.307978	
8	6	0	-1.492651	0.192209	1.923115	
9	1	0	1.804682	-0.632417	1.632439	
10	1	0	1.579469	-0.765998	4.094749	
11	1	0	-0.611935	-0.298582	5.168299	
12	1	0	-2.573350	0.318997	3.776161	
13	1	0	-2.357644	0.466512	1.328003	
14	6	0	-1.240583	0.384692	-1.031053	
15	1	0	-1.336177	1.476498	-0.965467	
16	1	0	-1.041807	0.114508	-2.069099	
17	1	0	-2.181580	-0.066812	-0.715227	
18	1	0	1.170724	0.018473	-1.630639	
19	7	0	1.479608	0.137955	-3.161316	
20	16	0	1.159377	1.624492	-3.768509	
21	16	0	0.868103	-1.067963	-4.077448	
22	6	0	-0.339659	-0.122095	-5.003309	
23	6	0	-0.199159	1.183711	-4.852116	
24	8	0	2.231433	2.156639	-4.610076	
25	8	0	0.700170	2.473322	-2.668177	
26	8	0	1.822778	-1.625040	-5.035404	
27	8	0	0.205660	-2.024826	-3.184504	
28	1	0	-1.038006	-0.652953	-5.644135	
29	1	0	-0.755606	1.978858	-5.340250	
30	7	0	-0.664750	-2.360481	-0.395129	
31	6	0	-1.560958	-2.794125	0.586280	
32	6	0	-2.942336	-2.636564	0.401161	
33	6	0	-3.825287	-2.951336	1.432866	
34	6	0	-3.348952	-3.423345	2.657652	
35	6	0	-1.973017	-3.590680	2.836208	
36	6	0	-1.082691	-3.282303	1.811183	
37	1	0	-3.314695	-2.264905	-0.550994	
38	1	0	-4.893348	-2.825308	1.275917	
39	1	0	-4.039954	-3.664173	3.460047	
40	1	0	-1.587800	-3.963460	3.781848	
41	1	0	-0.011433	-3.408837	1.951872	
42	1	0	0.260307	-2.781735	-0.338204	
43	1	0	-1.010289	-2.394563	-1.352011	

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1	6	0	0.273171	-0.855380	0.168283
2	6	0	0.126071	-0.411085	1.613495
3	8	0	1.442205	-0.331563	-0.348125
4	6	0	1.281506	-0.189613	2.371828
5	6	0	1.184266	0.166939	3.715033
6	6	0	-0.069282	0.307303	4.313085
7	6	0	-1.222232	0.090959	3.560307
8	6	0	-1.126565	-0.268778	2.215014
9	1	0	2.258311	-0.294906	1.908734
10	1	0	2.087832	0.337468	4.293419
11	1	0	-0.145962	0.586110	5.360319
12	1	0	-2.201639	0.199888	4.017234
13	1	0	-2.037669	-0.439425	1.649723
14	6	0	-0.932042	-0.604446	-0.718066
15	1	0	-1.100584	0.473816	-0.771687
16	1	0	-0.742928	-0.978216	-1.729385
17	1	0	-1.833936	-1.087017	-0.338662
18	1	0	1.455934	-0.400047	-1.335136
19	7	0	1.648805	-0.667166	-3.134472
20	16	0	0.975151	0.511418	-4.039396
21	16	0	1.320307	-2.147225	-3.695751
22	6	0	-0.092154	-1.767759	-4.730408
23	6	0	-0.261194	-0.467642	-4.896224
24	8	0	1.878168	1.053577	-5.058325
25	8	0	0.339262	1.484096	-3.149955
26	8	0	2.360975	-2.727484	-4.545858
27	8	0	0.895668	-3.001786	-2.567229
28	1	0	-0.650781	-2.586423	-5.174732
29	1	0	-0.996467	0.041330	-5.512998
30	7	0	0.537266	-2.407954	0.192548
31	6	0	-0.484641	-3.278823	0.767630
32	6	0	-1.481281	-3.783811	-0.061005
33	6	0	-2.466333	-4.598593	0.495188
34	6	0	-2.441838	-4.897912	1.857740
35	6	0	-1.428137	-4.388350	2.670776
36	6	0	-0.438300	-3.571927	2.127139
37	1	0	-1.487248	-3.546458	-1.122139
38	1	0	-3.249282	-5.001059	-0.140222
39	1	0	-3.210524	-5.534486	2.285868
40	1	0	-1.403449	-4.626886	3.729665

35

	41	1	0	0.359843	-3.169298	2.746554
42	1	0	1.426095	-2.533926	0.695399	
43	1	0	0.723087	-2.681366	-0.792577	

TS\_HZ-disp

1	6	0	0.472726	0.499191	-0.349924
2	6	0	0.029262	0.092196	1.058516
3	8	0	1.857629	0.831850	-0.366317
4	6	0	0.970640	-0.389074	1.976188
5	6	0	0.571672	-0.837344	3.235350
6	6	0	-0.776961	-0.818175	3.592611
7	6	0	-1.722330	-0.348842	2.680933
8	6	0	-1.322608	0.103311	1.422438
9	1	0	2.021957	-0.413645	1.703439
10	1	0	1.316629	-1.202076	3.937399
11	1	0	-1.088820	-1.166210	4.573459
12	1	0	-2.775728	-0.331860	2.947062
13	1	0	-2.077049	0.460604	0.727436
14	6	0	-0.326975	1.660755	-0.919670
15	1	0	-0.200619	2.528875	-0.263677
16	1	0	0.057859	1.903528	-1.913736
17	1	0	-1.394502	1.446997	-0.995750
18	1	0	2.033593	-0.161650	-2.366596
19	7	0	2.660572	-0.341501	-3.186139
20	16	0	1.804413	0.143534	-4.573351
21	16	0	2.949095	-2.018882	-3.228839
22	6	0	1.579595	-2.456404	-4.290531
23	6	0	1.028740	-1.430592	-4.920159
24	8	0	2.737779	0.432975	-5.645526
25	8	0	0.848469	1.151430	-4.153038
26	8	0	4.185937	-2.280216	-3.939973
27	8	0	2.770372	-2.524343	-1.879055
28	1	0	1.332016	-3.509345	-4.400342
29	1	0	0.231593	-1.461204	-5.658956
30	7	0	0.469248	-0.681542	-1.243069
31	6	0	-0.772922	-1.254201	-1.645886
32	6	0	-1.544731	-0.652931	-2.648780
33	6	0	-2.731317	-1.250531	-3.069602
34	6	0	-3.150006	-2.463776	-2.518338

36

	35	6	0	-2.371707	-3.075627	-1.535911
36	6	0	-1.194343	-2.470415	-1.094943	
37	1	0	-1.199451	0.266706	-3.110925	
38	1	0	-3.321620	-0.773249	-3.847206	
39	1	0	-4.069844	-2.930637	-2.858608	
40	1	0	-2.682561	-4.022605	-1.103156	
41	1	0	-0.591065	-2.940524	-0.320360	
42	1	0	1.013794	-1.400051	-0.760718	
43	1	0	2.003246	1.611754	0.197877	

11a

1	6	0	-0.290928	0.260500	0.327635
2	6	0	-0.012786	-0.033636	1.804260
3	8	0	0.933048	0.368651	-0.397395
4	6	0	1.292690	-0.090063	2.294381
5	6	0	1.528968	-0.342017	3.648029
6	6	0	0.463049	-0.535756	4.524095
7	6	0	-0.845599	-0.471835	4.040900
8	6	0	-1.081008	-0.219419	2.691075
9	1	0	2.130169	0.069150	1.622871
10	1	0	2.550970	-0.385215	4.014335
11	1	0	0.647962	-0.732227	5.576421
12	1	0	-1.684832	-0.615966	4.715624
13	1	0	-2.106618	-0.162474	2.331055
14	6	0	-0.981008	1.615791	0.180626
15	1	0	-0.342684	2.401688	0.596296
16	1	0	-1.175083	1.845107	-0.869562
17	1	0	-1.929645	1.608012	0.724588
18	1	0	1.627787	1.528893	-1.558907
19	7	0	2.200972	1.911924	-2.343616
20	16	0	1.315731	3.018266	-3.277349
21	16	0	2.825164	0.633967	-3.268037
22	6	0	1.757407	0.837467	-4.681552
23	6	0	1.055282	1.958642	-4.688290
24	8	0	2.173666	4.113395	-3.687049
25	8	0	0.081481	3.290107	-2.563185
26	8	0	4.182690	0.934000	-3.679452
27	8	0	2.547175	-0.595166	-2.542662
28	1	0	1.798216	0.083604	-5.464277
29	1	0	0.403142	2.319820	-5.479623
30	7	0	-1.051022	-0.864423	-0.209843

37

31	6	0	-1.722518	-0.811951	-1.442246
32	6	0	-1.170132	-0.187879	-2.572480
33	6	0	-1.844416	-0.207003	-3.791384
34	6	0	-3.070112	-0.861421	-3.920185
35	6	0	-3.616689	-1.495784	-2.802909
36	6	0	-2.956684	-1.468139	-1.576982
37	1	0	-0.206586	0.301558	-2.493902
38	1	0	-1.395803	0.286044	-4.650452
39	1	0	-3.588418	-0.879487	-4.874160
40	1	0	-4.569890	-2.012079	-2.880677
41	1	0	-3.394369	-1.956330	-0.708795
42	1	0	-1.593209	-1.342965	0.502963
43	1	0	1.291699	-0.525146	-0.552723

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1	6	0	0.178674	-0.067575	0.024304
2	6	0	0.070410	-0.053901	1.540958
3	8	0	1.776859	-0.118675	-0.233829
4	6	0	1.060892	0.534861	2.333912
5	6	0	0.900849	0.604493	3.716508
6	6	0	-0.250819	0.097443	4.319191
7	6	0	-1.247661	-0.472891	3.529677
8	6	0	-1.091274	-0.545581	2.145380
9	1	0	1.960262	0.934460	1.877230
10	1	0	1.680976	1.056076	4.322590
11	1	0	-0.372032	0.151676	5.397309
12	1	0	-2.153028	-0.861764	3.986582
13	1	0	-1.884584	-0.975336	1.539772
14	6	0	-0.213887	1.265670	-0.584696
15	1	0	0.378077	2.064779	-0.129898
16	1	0	-0.083674	1.301510	-1.666694
17	1	0	-1.268081	1.435409	-0.346176
18	1	0	2.150481	0.436684	-1.033310
19	7	0	3.101878	0.883764	-2.237713
20	16	0	2.682641	1.827864	-3.510819
21	16	0	3.932596	-0.449139	-2.693668
22	6	0	3.436457	-0.510410	-4.412309
23	6	0	2.842869	0.601793	-4.810268
24	8	0	3.650179	2.890165	-3.783359
25	8	0	1.285425	2.233291	-3.359158

38

	26	8	0	5.385704	-0.298685	-2.659228
27	8	0	3.379234	-1.584504	-1.937475	
28	1	0	3.702600	-1.381729	-5.003898	
29	1	0	2.505287	0.859253	-5.810367	
30	7	0	-0.399774	-1.197660	-0.518276	
31	6	0	-0.751891	-1.436521	-1.867234	
32	6	0	-0.010682	-0.936845	-2.941458	
33	6	0	-0.402601	-1.213772	-4.250708	
34	6	0	-1.514051	-2.017186	-4.501550	
35	6	0	-2.236551	-2.541209	-3.427386	
36	6	0	-1.865392	-2.247701	-2.117972	
37	1	0	0.875050	-0.336856	-2.766318	
38	1	0	0.179888	-0.809367	-5.074548	
39	1	0	-1.811306	-2.238084	-5.522346	
40	1	0	-3.102152	-3.172430	-3.607819	
41	1	0	-2.435724	-2.639783	-1.279300	
42	1	0	-0.510544	-1.991276	0.105207	
43	1	0	2.056155	-1.044897	-0.424531	

12a

1	6	0	-0.371648	0.006656	0.091305
2	6	0	-0.399436	0.474356	1.410022
3	6	0	0.796072	0.677262	2.095628
4	6	0	2.016505	0.446985	1.460027
5	6	0	2.044548	0.006151	0.135430
6	6	0	0.854841	-0.225047	-0.547569
7	1	0	-1.348196	0.646772	1.908767
8	1	0	0.772764	1.019663	3.125774
9	1	0	2.946795	0.616023	1.994827
10	1	0	2.993010	-0.159735	-0.366618
11	1	0	0.877746	-0.564095	-1.579753
12	6	0	-1.631895	-0.175905	-0.657353
13	6	0	-2.638079	0.920754	-0.663458
14	1	0	-2.823241	1.251535	0.361636
15	1	0	-3.582043	0.617000	-1.119634
16	1	0	-2.220551	1.770831	-1.215638
17	7	0	-1.853901	-1.226879	-1.380887
18	6	0	-1.096333	-2.443934	-1.435563
19	6	0	-0.789529	-2.962917	-2.690936
20	6	0	-0.085323	-4.163327	-2.769438
21	6	0	0.292652	-4.830655	-1.603526

39

	22	6	0	-0.041584	-4.304438	-0.353810
23	6	0	-0.746601	-3.106609	-0.260355	
24	1	0	-1.089761	-2.425998	-3.587230	
25	1	0	0.166702	-4.574873	-3.742139	
26	1	0	0.840633	-5.766100	-1.668383	
27	1	0	0.237624	-4.832657	0.553032	
28	1	0	-1.040751	-2.692436	0.699842	
29	1	0	-2.717234	-1.246012	-1.964606	
30	7	0	-4.206407	-1.553642	-2.977108	
31	16	0	-4.298278	-0.332011	-4.050542	
32	16	0	-5.537025	-1.700709	-2.065336	
33	8	0	-3.068251	0.459958	-3.950497	
34	8	0	-4.689819	-0.753908	-5.397453	
35	8	0	-5.135948	-1.796674	-0.651110	
36	8	0	-6.468436	-2.734571	-2.520170	
37	6	0	-5.682949	0.564024	-3.345350	
38	6	0	-6.288704	-0.102871	-2.378565	
39	1	0	-7.174576	0.178076	-1.816152	
40	1	0	-5.952536	1.526997	-3.769184	
41	8	0	-3.095690	-1.416545	1.316015	
42	1	0	-3.817479	-1.577961	0.679879	
43	1	0	-3.530046	-1.311256	2.177570	

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1	8	0	0.001037	0.000000	0.000939
2	1	0	0.002134	0.000000	0.971002
3	1	0	0.938607	0.000000	-0.249289

13a

1	6	0	0.000063	-0.008203	-0.012469
2	6	0	-0.018281	0.047863	1.389051
3	6	0	1.179391	0.048539	2.095756
4	6	0	2.395778	-0.027372	1.413418
5	6	0	2.414842	-0.081641	0.019831
6	6	0	1.220756	-0.053616	-0.696946
7	1	0	-0.963305	0.112044	1.921356
8	1	0	1.163352	0.107364	3.179867

40

	9	1	0	3.328872	-0.038021	1.969335
10	1	0	3.359422	-0.139419	-0.512467	
11	1	0	1.241216	-0.094208	-1.781875	
12	6	0	-1.264876	0.054212	-0.771870	
13	6	0	-1.368521	0.977234	-1.936092	
14	1	0	-1.080149	1.986347	-1.626292	
15	1	0	-2.371128	0.989390	-2.364589	
16	1	0	-0.660954	0.653708	-2.708292	
17	7	0	-2.306924	-0.639563	-0.439230	
18	6	0	-2.411077	-1.680483	0.542292	
19	6	0	-1.508496	-2.742568	0.546445	
20	6	0	-1.664347	-3.750102	1.495152	
21	6	0	-2.714984	-3.696872	2.413741	
22	6	0	-3.621876	-2.637192	2.380491	
23	6	0	-3.476979	-1.621688	1.436662	
24	1	0	-0.703788	-2.779963	-0.182631	
25	1	0	-0.967072	-4.582423	1.509996	
26	1	0	-2.830451	-4.486437	3.150448	
27	1	0	-4.443850	-2.597140	3.088862	
28	1	0	-4.170605	-0.785744	1.399255	
29	1	0	-3.199282	-0.458834	-0.953718	
30	7	0	-4.839785	-0.296178	-1.690896	
31	16	0	-4.783684	-0.780375	-3.241560	
32	16	0	-5.359991	1.233313	-1.511324	
33	8	0	-3.466955	-1.375537	-3.496883	
34	8	0	-5.942241	-1.576755	-3.656305	
35	8	0	-4.417563	1.946833	-0.641704	
36	8	0	-6.776542	1.339535	-1.149911	
37	6	0	-4.912702	0.817307	-4.048113	
38	6	0	-5.193133	1.796911	-3.206348	
39	1	0	-5.369151	2.845752	-3.426684	
40	1	0	-4.802454	0.866496	-5.127720	

TS\_HZ-loss

1	6	0	0.174243	-0.071285	-0.252274
2	6	0	0.192624	0.143976	1.266117
3	8	0	1.455441	-0.437243	-0.735679
4	6	0	1.389726	0.090197	1.981947
5	6	0	1.401891	0.319411	3.360198
6	6	0	0.218212	0.610202	4.035370

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	7	6	0	-0.981259	0.677042	3.323374
8	6	0	-0.992258	0.450083	1.948621	
9	1	0	2.319470	-0.122758	1.463660	
10	1	0	2.341868	0.271207	3.903212	
11	1	0	0.228182	0.788767	5.106958	
12	1	0	-1.909410	0.910762	3.837722	
13	1	0	-1.933446	0.521987	1.406315	
14	6	0	-0.162786	1.253548	-0.941775	
15	1	0	0.571176	2.006166	-0.637574	
16	1	0	-0.137682	1.147471	-2.029482	
17	1	0	-1.157758	1.595177	-0.642045	
18	1	0	2.548425	1.936771	-2.582147	
19	7	0	2.549204	2.844299	-3.066914	
20	16	0	2.435316	4.124508	-1.949741	
21	16	0	1.312180	2.903790	-4.236965	
22	6	0	0.190953	3.938382	-3.311359	
23	6	0	0.717835	4.511942	-2.241767	
24	8	0	3.236266	5.238975	-2.415772	
25	8	0	2.658830	3.565349	-0.629782	
26	8	0	1.777102	3.657290	-5.384614	
27	8	0	0.810399	1.553427	-4.403262	
28	1	0	-0.809714	4.085797	-3.710638	
29	1	0	0.240442	5.228547	-1.577728	
30	7	0	-0.767490	-1.153055	-0.530241	
31	6	0	-1.257341	-1.444512	-1.808870	
32	6	0	-0.505584	-1.241131	-2.978477	
33	6	0	-1.033170	-1.595363	-4.219818	
34	6	0	-2.297995	-2.173789	-4.329111	
35	6	0	-3.040891	-2.390650	-3.166138	
36	6	0	-2.532908	-2.026052	-1.923133	
37	1	0	0.488389	-0.812777	-2.916997	
38	1	0	-0.436630	-1.420585	-5.111732	
39	1	0	-2.696679	-2.452637	-5.299979	
40	1	0	-4.028936	-2.839946	-3.224382	
41	1	0	-3.121241	-2.190062	-1.022608	
42	1	0	-1.467148	-1.279186	0.193561	
43	1	0	1.629365	-1.350456	-0.445228	

7a

1	6	0	-0.003626	0.005718	0.003873
2	6	0	-0.013826	0.076039	1.400774
3	6	0	1.180602	0.078120	2.119227
4	6	0	2.402697	0.010806	1.446789
5	6	0	2.418400	-0.056082	0.054145
6	6	0	1.220836	-0.056544	-0.665026
7	1	0	-0.962883	0.121605	1.931296
8	1	0	1.156888	0.128559	3.204452
9	1	0	3.334427	0.009114	2.005632
10	1	0	3.364477	-0.109985	-0.477909
11	1	0	1.237944	-0.112538	-1.748839
12	6	0	-1.327075	0.069301	-0.760981
13	8	0	-1.077743	-0.441232	-2.062323
14	6	0	-1.794187	1.523088	-0.854076
15	1	0	-2.734116	1.576896	-1.415663
16	1	0	-1.950815	1.949118	0.142046
17	1	0	-1.034217	2.112500	-1.373459
18	1	0	-1.922395	-0.412993	-2.544754
19	7	0	-2.397051	-0.691665	-0.132277
20	6	0	-2.237661	-1.998256	0.332627
21	6	0	-1.268075	-2.872475	-0.188326
22	6	0	-1.175027	-4.179156	0.291410
23	6	0	-2.036700	-4.647322	1.283444
24	6	0	-3.003313	-3.780152	1.799233
25	6	0	-3.102421	-2.472101	1.335409
26	1	0	-0.599635	-2.532397	-0.971787
27	1	0	-0.416685	-4.837989	-0.124209
28	1	0	-1.957832	-5.667007	1.648494
29	1	0	-3.684037	-4.120946	2.575144
30	1	0	-3.852460	-1.799798	1.747449
31	1	0	-3.015867	-0.127751	0.442020

13a\*4

1	6	0	0.337838	0.880353	-0.181572
2	7	0	0.293961	0.292683	0.974758
3	6	0	1.615844	0.851988	-0.917107
4	6	0	-0.834990	1.584793	-0.772170
5	1	0	-1.518298	1.944610	-0.000933
6	1	0	-1.383980	0.892924	-1.423048

43

	7	1	0	-0.487912	2.420138	-1.382325
8	1	0	1.145684	-0.218363	1.298466	
9	6	0	-0.801381	0.227455	1.895111	
10	6	0	-0.761557	-5.568028	2.093003	
11	7	0	0.139258	-6.284635	1.949224	
12	7	0	2.391069	-1.449619	1.867705	
13	6	0	1.602146	0.749842	-2.315710	
14	6	0	2.802475	0.703164	-3.017712	
15	6	0	4.016733	0.791730	-2.334031	
16	6	0	4.032099	0.926223	-0.945100	
17	6	0	2.836472	0.951341	-0.233699	
18	1	0	0.658388	0.683515	-2.849838	
19	1	0	2.790060	0.603201	-4.098783	
20	1	0	4.951930	0.767096	-2.886008	
21	1	0	4.974948	1.018820	-0.414423	
22	1	0	2.852988	1.087218	0.844111	
23	6	0	-0.514111	0.486287	3.235549	
24	6	0	-1.549711	0.451542	4.167697	
25	6	0	-2.849364	0.148378	3.761080	
26	6	0	-3.111885	-0.150613	2.423395	
27	6	0	-2.086071	-0.121079	1.480308	
28	1	0	0.505495	0.718869	3.533908	
29	1	0	-1.337560	0.664273	5.211311	
30	1	0	-3.654355	0.123190	4.489989	
31	1	0	-4.116952	-0.417502	2.109837	
32	1	0	-2.279648	-0.378380	0.443472	
33	16	0	1.730820	-2.930788	1.755586	
34	16	0	3.139602	-1.198873	3.285031	
35	6	0	1.687654	-3.355492	3.500317	
36	6	0	2.372607	-2.506093	4.246664	
37	1	0	2.567916	-2.553526	5.314140	
38	1	0	1.190410	-4.270591	3.808927	
39	8	0	4.579937	-1.478900	3.254505	
40	8	0	2.762380	0.122253	3.800898	
41	8	0	0.373042	-2.789847	1.215809	
42	8	0	2.591946	-3.911000	1.087921	
43	14	0	-2.271242	-4.446649	2.395448	
44	6	0	-3.576984	-5.629829	3.024663	
45	6	0	-1.768245	-3.216600	3.706440	
46	6	0	-2.728706	-3.695047	0.750547	
47	1	0	-4.502870	-5.082655	3.239208	
48	1	0	-3.804039	-6.404424	2.283957	

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	49	1	0	-3.251734	-6.120252	3.948915
50	1	0	-2.668535	-2.735178	4.106447	
51	1	0	-1.257346	-3.711789	4.540291	
52	1	0	-1.112712	-2.440656	3.296957	
53	1	0	-3.604060	-3.045579	0.872876	
54	1	0	-1.902662	-3.101599	0.348188	
55	1	0	-2.988283	-4.475915	0.026611	

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1	6	0	-0.277315	0.148140	-0.262789
2	7	0	-0.569041	0.305753	1.013823
3	6	0	1.167113	-0.066121	-0.583395
4	6	0	-1.130216	0.771526	-1.324848
5	1	0	-2.197506	0.664296	-1.145860
6	1	0	-0.881582	0.353263	-2.299546
7	1	0	-0.877820	1.841106	-1.333642
8	1	0	0.138608	0.013834	1.689120
9	6	0	-1.815378	0.688720	1.599999
10	6	0	-1.014215	-2.032912	-0.655768
11	7	0	-1.319425	-3.161417	-0.567272
12	14	0	0.304451	-3.499131	2.793146
13	6	0	-1.194591	-2.428014	3.066796
14	1	0	-1.943340	-2.903365	3.709781
15	1	0	-0.921486	-1.458405	3.499478
16	1	0	-1.660761	-2.252638	2.089458
17	6	0	1.645146	-2.624404	1.839784
18	1	0	2.560423	-3.220750	1.753295
19	1	0	1.278383	-2.429333	0.824240
20	1	0	1.894118	-1.663361	2.304035
21	6	0	-0.080468	-5.214603	2.187032
22	1	0	0.827152	-5.826819	2.150909
23	1	0	-0.808033	-5.704270	2.843505
24	1	0	-0.504682	-5.162895	1.177654
25	7	0	1.034262	-3.674194	4.492018
26	6	0	1.552461	-0.753314	-1.741591
27	6	0	2.899612	-0.913195	-2.045514
28	6	0	3.879188	-0.376769	-1.205149
29	6	0	3.501462	0.331619	-0.067343
30	6	0	2.150550	0.491486	0.242140
31	1	0	0.796330	-1.193743	-2.384549
32	1	0	3.186543	-1.463403	-2.936810

45

	33	1	0	4.931117	-0.505950	-1.443450
34	1	0	4.253979	0.768171	0.582721	
35	1	0	1.875683	1.071692	1.119214	
36	6	0	-1.772119	1.595953	2.659170	
37	6	0	-2.953387	1.948846	3.307934	
38	6	0	-4.168722	1.397685	2.898971	
39	6	0	-4.197855	0.482008	1.846670	
40	6	0	-3.020695	0.115056	1.195694	
41	1	0	-0.817434	2.013934	2.968347	
42	1	0	-2.922100	2.656397	4.131282	
43	1	0	-5.089358	1.674797	3.404220	
44	1	0	-5.138589	0.037527	1.535285	
45	1	0	-3.038795	-0.626409	0.402587	
46	16	0	0.073660	-3.834572	5.855471	
47	16	0	2.652037	-4.047280	4.721036	
48	6	0	1.279221	-4.653180	6.874642	
49	6	0	2.483618	-4.755486	6.343536	
50	1	0	3.374306	-5.181174	6.798355	
51	1	0	0.960841	-4.976502	7.862342	
52	8	0	3.040191	-5.055299	3.743995	
53	8	0	3.463705	-2.842936	4.817712	
54	8	0	-0.233256	-2.537730	6.440828	
55	8	0	-1.037503	-4.722544	5.542336	

5a\*14

1	6	0	-0.077407	-0.254989	-0.152406
2	7	0	0.010274	0.049147	1.273641
3	6	0	1.352795	-0.446493	-0.679317
4	6	0	-0.747833	0.886420	-0.942961
5	1	0	-1.770447	1.075746	-0.613387
6	1	0	-0.759927	0.640149	-2.008393
7	1	0	-0.157082	1.793382	-0.791584
8	1	0	0.867786	-0.311085	1.683703
9	6	0	-1.062179	-0.016660	2.175205
10	6	0	-0.852403	-1.513526	-0.370850
11	7	0	-1.457117	-2.489399	-0.513192
12	14	0	-0.411017	-4.359555	2.609059
13	6	0	-2.069649	-3.536505	2.805721
14	1	0	-2.841934	-4.244930	3.125632
15	1	0	-2.024761	-2.712531	3.527165
16	1	0	-2.379288	-3.129157	1.836574

	17	6	0	0.997343	-3.182270	2.283063
18	1	0	1.971360	-3.679921	2.351463	
19	1	0	0.908995	-2.793890	1.260945	
20	1	0	0.985289	-2.336909	2.980206	
21	6	0	-0.429675	-5.816447	1.452017	
22	1	0	0.529987	-6.344098	1.471447	
23	1	0	-1.222533	-6.521783	1.724100	
24	1	0	-0.612843	-5.475643	0.425426	
25	7	0	-0.048647	-5.000825	4.310190	
26	6	0	1.732363	-1.545901	-1.450858	
27	6	0	3.039347	-1.649526	-1.932319	
28	6	0	3.975203	-0.658355	-1.645862	
29	6	0	3.598063	0.443440	-0.875742	
30	6	0	2.294370	0.551176	-0.397497	
31	1	0	1.019366	-2.332292	-1.682795	
32	1	0	3.320600	-2.512185	-2.529538	
33	1	0	4.992058	-0.741723	-2.018764	
34	1	0	4.318793	1.223415	-0.647432	
35	1	0	2.007862	1.414380	0.197662	
36	6	0	-0.740330	-0.003699	3.546693	
37	6	0	-1.736739	-0.027613	4.513775	
38	6	0	-3.085093	-0.064836	4.144158	
39	6	0	-3.408043	-0.084588	2.790256	
40	6	0	-2.414736	-0.063920	1.807398	
41	1	0	0.306888	0.028233	3.840227	
42	1	0	-1.457317	-0.018669	5.564105	
43	1	0	-3.864928	-0.083760	4.899606	
44	1	0	-4.448589	-0.123558	2.478835	
45	1	0	-2.718352	-0.099143	0.767759	
46	16	0	-1.259099	-5.587181	5.311443	
47	16	0	1.513657	-5.326858	4.822333	
48	6	0	-0.211910	-6.556842	6.371973	
49	6	0	1.082489	-6.440515	6.139558	
50	1	0	1.898605	-6.911609	6.681598	
51	1	0	-0.696315	-7.145774	7.147029	
52	8	0	2.219641	-6.021572	3.754472	
53	8	0	2.138539	-4.143794	5.395367	
54	8	0	-1.862029	-4.515203	6.089517	
55	8	0	-2.140763	-6.443739	4.530139	

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14

1	7	0	0.158193	0.679205	0.103580
2	16	0	0.038863	0.299696	1.732790
3	16	0	1.644941	0.341526	-0.594749
4	6	0	1.762429	-0.045599	2.000339
5	6	0	2.511514	-0.028752	0.913200
6	8	0	-0.378397	1.492230	2.456978
7	8	0	-0.722502	-0.923745	1.934907
8	8	0	2.157362	1.558495	-1.208773
9	8	0	1.581464	-0.861588	-1.410695
10	1	0	2.071664	-0.280478	3.015677
11	1	0	3.573367	-0.248349	0.837116
12	14	0	-1.094955	1.751225	-0.735523
13	6	0	-0.655963	3.522147	-0.370573
14	6	0	-0.948400	1.300738	-2.537278
15	6	0	-2.717676	1.209759	0.002269
16	1	0	-1.378927	4.194682	-0.848006
17	1	0	-0.671062	3.715254	0.707438
18	1	0	0.340563	3.763807	-0.755837
19	1	0	-1.732616	1.831358	-3.092059
20	1	0	0.015292	1.592342	-2.967481
21	1	0	-1.097537	0.226998	-2.694342
22	1	0	-3.526343	1.764641	-0.489944
23	1	0	-2.893356	0.141658	-0.165707
24	1	0	-2.783092	1.415381	1.075863

15

1	14	0	-0.001192	0.000000	-0.002855
2	8	0	-0.007154	0.000000	1.682973
3	6	0	1.809727	0.000000	-0.463496
4	1	0	1.935385	0.000000	-1.552862
5	1	0	2.317357	0.887318	-0.067106
6	1	0	2.317357	-0.887318	-0.067106
7	6	0	-0.867661	-1.531289	-0.650385
8	1	0	-0.860307	-1.546445	-1.747393
9	1	0	-0.377172	-2.446344	-0.297830
10	1	0	-1.914982	-1.562562	-0.325161
11	6	0	-0.867661	1.531289	-0.650385
12	1	0	-0.860307	1.546445	-1.747393

48

	13	1	0	-1.914982	1.562561	-0.325161
14	1	0	-0.377173	2.446344	-0.297830	
15	1	0	-0.878519	0.000000	2.109254	

8a

1	6	0	-0.031753	-0.040540	-0.051815
2	6	0	-0.121985	-0.404051	1.298139
3	6	0	1.023959	-0.461319	2.088667
4	6	0	2.272460	-0.169857	1.535337
5	6	0	2.367492	0.195108	0.192288
6	6	0	1.218873	0.272783	-0.595720
7	1	0	-1.092401	-0.634096	1.730767
8	1	0	0.942183	-0.735605	3.136693
9	1	0	3.166548	-0.222392	2.150192
10	1	0	3.335862	0.423790	-0.243917
11	1	0	1.300699	0.559043	-1.641083
12	6	0	-1.268726	0.049492	-0.893814
13	6	0	-1.489021	1.349860	-1.613863
14	1	0	-1.490123	2.181442	-0.900263
15	1	0	-2.435916	1.328493	-2.157190
16	1	0	-0.673380	1.535362	-2.322012
17	7	0	-2.147031	-0.874574	-1.008121
18	6	0	-1.961090	-2.157889	-0.444251
19	6	0	-0.886104	-2.974140	-0.820721
20	6	0	-0.770818	-4.261659	-0.298812
21	6	0	-1.721187	-4.748354	0.600633
22	6	0	-2.801178	-3.940202	0.962465
23	6	0	-2.931577	-2.658086	0.431803
24	1	0	-0.147412	-2.594640	-1.522432
25	1	0	0.067122	-4.886108	-0.597264
26	1	0	-1.626567	-5.750788	1.007997
27	1	0	-3.551536	-4.311881	1.655123
28	1	0	-3.775675	-2.028456	0.701761

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1	6	0	-0.132346	-0.157797	0.049460
2	6	0	-0.250710	-0.010572	1.534833
3	6	0	1.188744	-0.621804	-0.507305

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	4	1	0	1.122064	-0.826360	-1.576246
5	1	0	1.959930	0.139649	-0.341287	
6	1	0	1.510957	-1.536245	-0.001141	
7	7	0	-1.175402	0.102649	-0.647188	
8	6	0	-1.170897	0.055865	-2.054627	
9	6	0	-1.280044	-3.452483	0.048818	
10	7	0	-0.411846	-3.529906	-0.716859	
11	14	0	-2.714804	-3.337607	1.299901	
12	6	0	-3.774962	-1.915116	0.718291	
13	6	0	-3.587092	-4.985251	1.184027	
14	6	0	-1.897497	-3.071230	2.957042	
15	1	0	-4.455721	-1.607111	1.521502	
16	1	0	-3.166966	-1.050999	0.429744	
17	1	0	-4.382263	-2.213818	-0.143763	
18	1	0	-3.989994	-5.149189	0.178632	
19	1	0	-2.910114	-5.811733	1.426238	
20	1	0	-4.423216	-5.012743	1.893094	
21	1	0	-2.652872	-2.827546	3.713690	
22	1	0	-1.374075	-3.979214	3.277677	
23	1	0	-1.170808	-2.252933	2.921753	
24	6	0	-2.018633	-0.849833	-2.706013	
25	6	0	-2.083103	-0.870938	-4.098274	
26	6	0	-1.327036	0.026520	-4.855080	
27	6	0	-0.499506	0.944577	-4.205903	
28	6	0	-0.417263	0.961337	-2.814345	
29	1	0	-2.615063	-1.538555	-2.112536	
30	1	0	-2.733820	-1.587390	-4.592562	
31	1	0	-1.386510	0.014270	-5.939545	
32	1	0	0.088699	1.652108	-4.784293	
33	1	0	0.226011	1.675864	-2.306203	
34	6	0	-1.428125	0.506027	2.099467	
35	6	0	-1.559999	0.633206	3.478330	
36	6	0	-0.512070	0.254385	4.321904	
37	6	0	0.667436	-0.244829	3.772706	
38	6	0	0.798599	-0.375935	2.388928	
39	1	0	-2.238957	0.809579	1.445199	
40	1	0	-2.480057	1.031473	3.897183	
41	1	0	-0.614762	0.353035	5.399052	
42	1	0	1.490534	-0.536416	4.418953	
43	1	0	1.727072	-0.769049	1.987408	

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1	6	0	-0.009302	-0.021357	-0.054355	
2	6	0	-0.000751	-0.038475	1.341934	
3	6	0	1.204817	-0.017248	2.045857	
4	6	0	2.409279	0.021452	1.344229	
5	6	0	2.410801	0.040406	-0.051179	
6	6	0	1.200782	0.014444	-0.746217	
7	7	0	-1.243215	-0.012241	2.051532	
8	14	0	-2.181832	2.007429	2.200530	
9	6	0	-1.160757	2.076373	3.814615	
10	6	0	-1.712762	-1.072252	2.600371	
11	6	0	-1.075241	-2.427202	2.559873	
12	6	0	-3.009212	-0.982341	3.345513	
13	6	0	-3.005052	-0.797668	4.731776	
14	6	0	-4.211295	-0.719662	5.427104	
15	6	0	-5.422224	-0.846482	4.744929	
16	6	0	-5.425592	-1.064184	3.366712	
17	6	0	-4.221992	-1.136940	2.666008	
18	6	0	-3.137471	1.144682	0.651260	
19	7	0	-3.701398	0.745004	-0.285620	
20	6	0	-1.250571	3.212939	1.087591	
21	6	0	-3.836150	2.669353	2.857424	
22	1	0	-0.194857	-2.469716	1.918016	
23	1	0	-0.796504	-2.713157	3.581604	
24	1	0	-1.820845	-3.152677	2.216500	
25	1	0	-0.877146	4.052735	1.686082	
26	1	0	-0.384107	2.735337	0.613254	
27	1	0	-1.890263	3.607773	0.290144	
28	1	0	-3.672493	3.461027	3.598631	
29	1	0	-4.476128	3.058628	2.056644	
30	1	0	-4.389806	1.861732	3.358757	
31	1	0	-1.222054	3.109501	4.184938	
32	1	0	-1.545312	1.421002	4.602875	
33	1	0	-0.101638	1.841900	3.658056	
34	1	0	-2.060725	-0.711831	5.263757	
35	1	0	-4.203197	-0.563546	6.502067	
36	1	0	-6.361030	-0.784667	5.288090	
37	1	0	-6.365204	-1.177937	2.833528	
38	1	0	-4.223785	-1.309752	1.593748	
39	1	0	1.192470	-0.040905	3.132461	

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	40	1	0	3.347288	0.033523	1.891973
41	1	0	3.350726	0.071158	-0.594487	
42	1	0	1.194871	0.021275	-1.832550	
43	1	0	-0.955212	-0.043450	-0.587882	

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1	6	0	1.357418	-0.074988	0.130643
2	6	0	1.355762	-0.039872	1.619837
3	6	0	2.695602	-0.165767	-0.526264
4	1	0	2.645642	-0.366644	-1.595810
5	1	0	3.223848	0.780851	-0.354906
6	1	0	3.274082	-0.948377	-0.023977
7	7	0	0.236690	-0.022414	-0.505705
8	6	0	0.240353	-0.008038	-1.952067
9	6	0	-1.104014	-2.143912	0.446313
10	7	0	-0.945106	-3.295935	0.563062
11	14	0	-1.568467	0.040035	0.273778
12	6	0	-2.941340	-0.511805	-0.902787
13	6	0	-1.929512	-0.067529	2.129130
14	6	0	-1.650155	1.942106	-0.010059
15	1	0	-3.594630	0.329924	-1.161048
16	1	0	-2.543568	-0.928073	-1.835331
17	1	0	-3.544886	-1.295423	-0.429612
18	1	0	-2.105402	0.922992	2.563800
19	1	0	-2.845278	-0.664608	2.243431
20	1	0	-1.144019	-0.570194	2.700829
21	1	0	-2.613133	2.292335	0.390095
22	1	0	-0.860783	2.508679	0.499122
23	1	0	-1.629809	2.218352	-1.071774
24	6	0	1.125572	1.162622	2.292758
25	6	0	1.131316	1.184755	3.687140
26	6	0	1.357660	0.010250	4.404312
27	6	0	1.603408	-1.186736	3.728151
28	6	0	1.618390	-1.212488	2.335312
29	1	0	0.950758	2.075588	1.730546
30	1	0	0.954505	2.119907	4.210615
31	1	0	1.351482	0.027478	5.490526
32	1	0	1.787452	-2.100851	4.285176
33	1	0	1.812502	-2.140689	1.803638
34	6	0	0.429305	1.198878	-2.621791

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	35	6	0	0.414470	1.211133	-4.016188
36	6	0	0.213083	0.026993	-4.726466	
37	6	0	0.032844	-1.175792	-4.041793	
38	6	0	0.045712	-1.200004	-2.647896	
39	1	0	0.594739	2.110375	-2.053802	
40	1	0	0.564527	2.147791	-4.545110	
41	1	0	0.202379	0.040376	-5.812491	
42	1	0	-0.114623	-2.101001	-4.591199	
43	1	0	-0.084774	-2.130280	-2.102140	

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1	6	0	-0.048267	-0.074212	0.027390
2	6	0	-0.025836	-0.032806	1.514237
3	6	0	1.277647	-0.193429	-0.647659
4	1	0	1.211562	-0.391277	-1.716577
5	1	0	1.827635	0.741447	-0.480124
6	1	0	1.845672	-0.988496	-0.152856
7	7	0	-1.175357	0.003565	-0.598759
8	6	0	-1.177356	0.029983	-2.047719
9	6	0	-2.446020	-2.270615	0.339845
10	7	0	-2.281614	-3.424212	0.459249
11	14	0	-2.951207	0.090287	0.163595
12	6	0	-4.270886	-0.542887	-1.024436
13	6	0	-3.265058	-0.107241	2.013368
14	6	0	-3.102758	1.981214	-0.079827
15	1	0	-4.856055	0.288905	-1.433771
16	1	0	-3.855326	-1.113617	-1.859908
17	1	0	-4.946927	-1.212064	-0.478614
18	1	0	-3.419380	0.867309	2.490600
19	1	0	-4.188206	-0.694110	2.116308
20	1	0	-2.478262	-0.644208	2.548280
21	1	0	-4.078441	2.286778	0.325707
22	1	0	-2.335935	2.562459	0.445930
23	1	0	-3.089555	2.280182	-1.134675
24	6	0	-0.279650	1.166198	2.185034
25	6	0	-0.249942	1.195810	3.578721
26	6	0	0.020270	0.031361	4.297127
27	6	0	0.289608	-1.161550	3.622604
28	6	0	0.284528	-1.193616	2.229993
29	1	0	-0.488779	2.071128	1.621505

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	30	1	0	-0.443639	2.128338	4.100844
31	1	0	0.030986	0.053723	5.383190	
32	1	0	0.508386	-2.067142	4.180913	
33	1	0	0.498570	-2.117890	1.699358	
34	6	0	-1.021510	1.248594	-2.703568	
35	6	0	-1.034348	1.274151	-4.098178	
36	6	0	-1.199771	0.091796	-4.820079	
37	6	0	-1.346612	-1.122819	-4.147799	
38	6	0	-1.336295	-1.160385	-2.754566	
39	1	0	-0.881158	2.158378	-2.126293	
40	1	0	-0.909981	2.219807	-4.617577	
41	1	0	-1.208442	0.115432	-5.905941	
42	1	0	-1.466268	-2.046338	-4.706672	
43	1	0	-1.441989	-2.098280	-2.216626	

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1	6	0	-0.347441	0.046475	-0.101067
2	14	0	0.025044	-0.096229	1.719966
3	6	0	1.833859	-0.485266	1.962600
4	7	0	-0.867639	-1.580322	2.470197
5	6	0	-1.953687	-2.142861	2.028364
6	6	0	-2.445936	-3.460397	2.519260
7	6	0	-2.818679	-1.406383	1.080289
8	6	0	-0.460868	1.396640	2.731898
9	6	0	-0.385458	-4.452724	-0.150559
10	7	0	0.153243	-3.430978	0.064833
11	1	0	-1.652801	-4.094144	2.915290
12	1	0	-3.181643	-3.268726	3.312794
13	1	0	-2.971025	-3.970101	1.707298
14	6	0	-0.181242	-2.173196	3.604853
15	1	0	0.434770	0.686453	-0.531348
16	1	0	-0.284779	-0.932130	-0.588166
17	1	0	-1.316665	0.502246	-0.322712
18	1	0	0.341615	2.141349	2.658012
19	1	0	-1.385435	1.862064	2.376273
20	1	0	-0.582066	1.145586	3.791990
21	1	0	2.399081	0.329363	1.490460
22	1	0	2.128199	-0.527935	3.016204
23	1	0	2.126937	-1.420038	1.473081
24	6	0	-0.534921	-1.730712	4.876639

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	25	6	0	0.124845	-2.260900	5.986483
26	6	0	1.122624	-3.219533	5.813810	
27	6	0	1.462058	-3.654521	4.530447	
28	6	0	0.813479	-3.129965	3.414576	
29	1	0	-1.318975	-0.986457	4.990794	
30	1	0	-0.145526	-1.923928	6.982814	
31	1	0	1.634410	-3.631638	6.678634	
32	1	0	2.235300	-4.405238	4.396128	
33	1	0	1.057281	-3.456724	2.407721	
34	6	0	-3.175193	-1.956092	-0.155955	
35	6	0	-3.983815	-1.224635	-1.021163	
36	6	0	-4.471542	0.027602	-0.638321	
37	6	0	-4.153506	0.552105	0.614441	
38	6	0	-3.319910	-0.160305	1.473923	
39	1	0	-2.791216	-2.930000	-0.447722	
40	1	0	-4.239359	-1.634263	-1.993900	
41	1	0	-5.110010	0.588779	-1.314672	
42	1	0	-4.550174	1.514707	0.923378	
43	1	0	-3.077879	0.233366	2.458135	

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1	6	0	-0.017678	0.078980	0.006007
2	14	0	0.069796	-0.034340	1.868922
3	6	0	1.865244	-0.135810	2.381000
4	7	0	-0.690717	-1.603425	2.497206
5	6	0	-1.369684	-2.483504	1.777609
6	6	0	-1.840157	-3.775537	2.381268
7	6	0	-2.219868	-1.961785	0.660601
8	6	0	-0.784645	1.383159	2.732648
9	6	0	0.368533	-3.474176	0.566703
10	7	0	1.455605	-3.692118	0.185054
11	1	0	-1.070776	-4.270129	2.973800
12	1	0	-2.693671	-3.537972	3.031850
13	1	0	-2.186325	-4.441513	1.589874
14	6	0	-0.250707	-1.975377	3.824645
15	1	0	0.703273	0.852054	-0.292203
16	1	0	0.284983	-0.857647	-0.474650
17	1	0	-1.001600	0.370578	-0.372420
18	1	0	-0.259800	2.313852	2.481212

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	19	1	0	-1.829063	1.493118	2.422524
20	1	0	-0.753811	1.269697	3.822187	
21	1	0	2.383471	0.735156	1.959323	
22	1	0	2.003868	-0.115213	3.466763	
23	1	0	2.350591	-1.035153	1.983978	
24	6	0	-0.990551	-1.521585	4.914184	
25	6	0	-0.574871	-1.843510	6.207316	
26	6	0	0.572078	-2.612766	6.400976	
27	6	0	1.305583	-3.063790	5.300817	
28	6	0	0.898980	-2.744192	4.007075	
29	1	0	-1.884688	-0.926970	4.742996	
30	1	0	-1.149669	-1.492987	7.059617	
31	1	0	0.894785	-2.862737	7.407573	
32	1	0	2.198281	-3.664379	5.449717	
33	1	0	1.459753	-3.090451	3.143001	
34	6	0	-2.298352	-2.548272	-0.605420	
35	6	0	-3.188373	-2.045750	-1.550632	
36	6	0	-4.024306	-0.971647	-1.234955	
37	6	0	-3.975531	-0.409178	0.038878	
38	6	0	-3.078451	-0.903931	0.985210	
39	1	0	-1.641938	-3.375241	-0.855381	
40	1	0	-3.227382	-2.493339	-2.539578	
41	1	0	-4.714343	-0.581897	-1.977924	
42	1	0	-4.632593	0.414852	0.301768	
43	1	0	-3.056437	-0.477395	1.985029	

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1	6	0	-0.273817	0.054609	0.114535
2	14	0	0.171232	-0.140276	1.930535
3	6	0	2.031888	-0.323635	2.085777
4	7	0	-0.619733	-1.613938	2.557045
5	6	0	-1.655031	-1.614523	3.593410
6	6	0	-2.047193	-3.041517	4.027608
7	6	0	-1.168363	-0.869392	4.845043
8	6	0	-0.394836	1.395873	2.849284
9	6	0	-2.893231	-0.960706	3.061405
10	7	0	-3.829621	-0.468865	2.590996
11	1	0	-2.501892	-3.605779	3.210538
12	1	0	-1.147114	-3.561755	4.368870

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	13	1	0	-2.760026	-2.980578	4.854177
14	6	0	-0.551693	-2.737438	1.670493	
15	1	0	0.153484	0.989542	-0.270153	
16	1	0	0.116107	-0.765458	-0.499674	
17	1	0	-1.360755	0.099699	-0.029379	
18	1	0	-0.029513	2.262124	2.281341	
19	1	0	-1.485854	1.482242	2.910934	
20	1	0	0.016884	1.464234	3.861614	
21	1	0	2.523599	0.597973	1.748120	
22	1	0	2.333976	-0.506934	3.123814	
23	1	0	2.412035	-1.145750	1.468298	
24	6	0	0.587498	-3.548358	1.687570	
25	6	0	0.706629	-4.622010	0.802445	
26	6	0	-0.319089	-4.902450	-0.099622	
27	6	0	-1.462747	-4.099678	-0.117466	
28	6	0	-1.574031	-3.017718	0.753122	
29	1	0	1.375642	-3.330699	2.404738	
30	1	0	1.598502	-5.242290	0.825634	
31	1	0	-0.230174	-5.740180	-0.785511	
32	1	0	-2.265142	-4.309920	-0.819422	
33	1	0	-2.456968	-2.382859	0.725910	
34	6	0	-1.992733	-0.009332	5.571008	
35	6	0	-1.516102	0.616043	6.724770	
36	6	0	-0.214370	0.380930	7.164475	
37	6	0	0.606229	-0.494146	6.449711	
38	6	0	0.130785	-1.117751	5.297990	
39	1	0	-3.007188	0.195170	5.236805	
40	1	0	-2.164927	1.292675	7.273910	
41	1	0	0.158713	0.873487	8.058007	
42	1	0	1.620739	-0.689147	6.786474	
43	1	0	0.773689	-1.790845	4.736943	

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1	6	0	0.026496	-0.545353	-0.822676
2	7	0	-0.176137	-0.957791	2.111854
3	8	0	1.243861	-0.631435	-0.926065
4	7	0	1.987228	-2.881405	1.017494
5	6	0	-0.852945	-1.753797	-1.004122
6	6	0	-0.619498	0.778208	-0.555232
7	1	0	-0.124450	-1.968201	2.031849

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	8	6	0	-1.380703	-0.397119	2.500035
9	1	0	0.658357	-0.559244	2.529360	
10	1	0	1.809433	-2.340939	0.172540	
11	1	0	2.154720	-3.861798	0.812696	
12	6	0	2.917466	-2.302267	1.880582	
13	6	0	0.187050	1.866851	-0.202424	
14	6	0	-0.386470	3.104674	0.075300	
15	6	0	-1.772475	3.265698	-0.004323	
16	6	0	-2.581523	2.185750	-0.358968	
17	6	0	-2.007817	0.943304	-0.629171	
18	1	0	1.263135	1.729254	-0.140219	
19	1	0	0.243666	3.944014	0.355782	
20	1	0	-2.220828	4.231187	0.213895	
21	1	0	-3.659394	2.307610	-0.419588	
22	1	0	-2.647783	0.108036	-0.898595	
23	1	0	-1.421927	-1.654858	-1.936771	
24	1	0	-0.235889	-2.652908	-1.060754	
25	1	0	-1.573252	-1.845566	-0.185493	
26	6	0	-2.592335	-1.090070	2.326611	
27	6	0	-3.806351	-0.471048	2.618525	
28	6	0	-3.846037	0.841573	3.094255	
29	6	0	-2.641882	1.525402	3.285995	
30	6	0	-1.423258	0.919116	2.995619	
31	1	0	-2.571970	-2.113695	1.958774	
32	1	0	-4.730805	-1.024569	2.473137	
33	1	0	-4.794715	1.320160	3.318336	
34	1	0	-2.649803	2.545990	3.661228	
35	1	0	-0.490522	1.461353	3.138369	
36	6	0	3.577435	-3.076508	2.849590	
37	6	0	4.452449	-2.478960	3.753652	
38	6	0	4.688807	-1.102451	3.717833	
39	6	0	4.036035	-0.330981	2.754077	
40	6	0	3.160494	-0.918084	1.842521	
41	1	0	3.396307	-4.148510	2.886236	
42	1	0	4.954054	-3.097261	4.493865	
43	1	0	5.371512	-0.641062	4.425141	
44	1	0	4.210851	0.741024	2.705618	
45	1	0	2.659049	-0.313724	1.088712	

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1	6	0	-0.289898	-0.410261	0.253269
2	7	0	-0.108047	-0.554345	1.830749
3	8	0	0.959216	-0.644601	-0.242645
4	7	0	1.589884	-2.658752	1.123931
5	6	0	-1.296685	-1.471241	-0.168097
6	6	0	-0.721367	1.026914	0.003627
7	1	0	0.401177	-1.481622	1.913196
8	6	0	-1.279308	-0.479509	2.685009
9	1	0	0.573284	0.166654	2.099010
10	1	0	1.308179	-1.598690	0.231141
11	1	0	1.271360	-3.597644	0.886709
12	6	0	2.819096	-2.688069	1.734449
13	6	0	0.245900	2.035168	0.093928
14	6	0	-0.107076	3.371816	-0.074665
15	6	0	-1.434405	3.716303	-0.341436
16	6	0	-2.400359	2.716625	-0.439867
17	6	0	-2.046401	1.376543	-0.264820
18	1	0	1.278850	1.763406	0.295696
19	1	0	0.652859	4.144915	-0.000796
20	1	0	-1.711601	4.758336	-0.475048
21	1	0	-3.434256	2.975217	-0.651004
22	1	0	-2.815626	0.613985	-0.339943
23	1	0	-1.421092	-1.405620	-1.252773
24	1	0	-0.899833	-2.461896	0.075917
25	1	0	-2.274681	-1.358799	0.304493
26	6	0	-1.941452	-1.655628	3.027938
27	6	0	-3.079898	-1.583284	3.828572
28	6	0	-3.543255	-0.345854	4.278526
29	6	0	-2.864623	0.823353	3.932365
30	6	0	-1.725810	0.762436	3.130303
31	1	0	-1.566548	-2.612154	2.671836
32	1	0	-3.601522	-2.495458	4.102355
33	1	0	-4.429720	-0.293334	4.903784
34	1	0	-3.218331	1.786687	4.287404
35	1	0	-1.185402	1.666164	2.858162
36	6	0	3.496369	-3.886765	2.074472
37	6	0	4.740194	-3.867418	2.699322
38	6	0	5.371609	-2.660194	3.014530
39	6	0	4.719040	-1.466188	2.687920
40	6	0	3.475695	-1.473188	2.064085

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	41	1	0	3.022723	-4.837638	1.835324
42	1	0	5.225076	-4.811063	2.941209	
43	1	0	6.342696	-2.649402	3.500458	
44	1	0	5.188228	-0.512442	2.920764	
45	1	0	2.988256	-0.532051	1.813575	

7a\*3a

1	6	0	0.130778	-0.074129	-0.210793
2	7	0	0.076369	-0.297378	1.262671
3	8	0	1.495213	0.081488	-0.511720
4	7	0	3.049045	-2.086958	0.578593
5	6	0	-0.438749	-1.261556	-0.981390
6	6	0	-0.570790	1.236674	-0.575866
7	1	0	3.937065	-2.076232	0.081558
8	6	0	-1.174934	-0.477877	1.908375
9	1	0	0.552015	0.504395	1.678469
10	1	0	1.985173	-0.687461	-0.130990
11	1	0	3.199093	-1.863695	1.559881
12	6	0	2.311813	-3.269523	0.381675
13	6	0	0.165344	2.411982	-0.762619
14	6	0	-0.478632	3.621154	-1.030924
15	6	0	-1.870063	3.674968	-1.112023
16	6	0	-2.612754	2.509246	-0.921787
17	6	0	-1.968490	1.300487	-0.656821
18	1	0	1.248155	2.375271	-0.703335
19	1	0	0.110566	4.522287	-1.179947
20	1	0	-2.371860	4.615537	-1.322284
21	1	0	-3.697568	2.537303	-0.980600
22	1	0	-2.568748	0.406870	-0.507482
23	1	0	-0.259216	-1.094033	-2.047885
24	1	0	0.075285	-2.179482	-0.675515
25	1	0	-1.511353	-1.398297	-0.831210
26	6	0	-1.874753	-1.688225	1.795172
27	6	0	-3.090989	-1.862399	2.453211
28	6	0	-3.615984	-0.848733	3.258135
29	6	0	-2.909437	0.346170	3.398343
30	6	0	-1.704315	0.533716	2.722091
31	1	0	-1.454842	-2.497696	1.204971
32	1	0	-3.621660	-2.805343	2.350443
33	1	0	-4.559131	-0.993421	3.777248

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	34	1	0	-3.300566	1.141918	4.026895
35	1	0	-1.163340	1.473458	2.816882	
36	6	0	1.412448	-3.716351	1.358682	
37	6	0	0.602980	-4.823897	1.111282	
38	6	0	0.677371	-5.502371	-0.106741	
39	6	0	1.580589	-5.060552	-1.076461	
40	6	0	2.392044	-3.953125	-0.839255	
41	1	0	1.344385	-3.184457	2.305518	
42	1	0	-0.092296	-5.155484	1.878402	
43	1	0	0.044540	-6.364246	-0.296588	
44	1	0	1.654568	-5.579788	-2.028434	
45	1	0	3.085863	-3.604230	-1.600945	

7a\*4

1	14	0	0.015153	0.663205	-0.642446
2	6	0	0.301428	0.323269	1.173113
3	6	0	1.187682	-0.281698	-1.742664
4	6	0	-1.778368	0.508450	-1.134635
5	1	0	-0.341473	0.948574	1.802237
6	1	0	0.077210	-0.727079	1.394251
7	1	0	1.344565	0.512962	1.448870
8	1	0	0.958865	-0.098202	-2.796722
9	1	0	2.229952	-0.004671	-1.548575
10	1	0	1.081738	-1.355707	-1.545526
11	1	0	-1.920765	0.761996	-2.190117
12	1	0	-2.113870	-0.525001	-0.983713
13	1	0	-2.413956	1.162185	-0.527111
14	8	0	-0.338298	1.289628	-4.329726
15	1	0	-1.137857	0.833595	-4.648262
16	6	0	0.448415	2.510478	-0.830231
17	7	0	0.713588	3.638556	-0.884970
18	6	0	-0.423798	2.632101	-4.769417
19	6	0	0.888579	3.306352	-4.374668
20	6	0	-1.640001	3.290566	-4.131155
21	1	0	-1.772092	4.331300	-4.431835
22	1	0	-2.540978	2.733145	-4.410256
23	1	0	-1.522869	3.258527	-3.043040
24	7	0	-0.558110	2.548675	-6.249420
25	6	0	-0.581002	3.758935	-6.999798
26	1	0	0.235087	1.986727	-6.562452

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	27	6	0	2.035168	2.541111	-4.133476
28	6	0	3.242493	3.155408	-3.798719	
29	6	0	3.323696	4.545542	-3.711122	
30	6	0	2.190354	5.316177	-3.971361	
31	6	0	0.982242	4.701073	-4.301853	
32	1	0	1.979595	1.458957	-4.194053	
33	1	0	4.119466	2.544500	-3.600987	
34	1	0	4.262082	5.024641	-3.445631	
35	1	0	2.242078	6.400092	-3.913517	
36	1	0	0.112614	5.322521	-4.498025	
37	6	0	0.551384	4.172468	-7.714106	
38	6	0	0.521089	5.338116	-8.479158	
39	6	0	-0.634786	6.118236	-8.525254	
40	6	0	-1.767244	5.707801	-7.818578	
41	6	0	-1.748407	4.529924	-7.073224	
42	1	0	1.459281	3.574489	-7.661265	
43	1	0	1.407482	5.640976	-9.030195	
44	1	0	-0.657203	7.031434	-9.113008	
45	1	0	-2.679185	6.297118	-7.862436	
46	1	0	-2.644983	4.194668	-6.560030	

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1	14	0	0.000546	0.001830	0.017100
2	6	0	-0.022832	0.001234	1.978393
3	6	0	1.904726	0.008820	-0.140002
4	6	0	-1.045104	-1.564152	-0.234841
5	1	0	-1.043755	0.058685	2.384703
6	1	0	0.430170	-0.926521	2.360688
7	1	0	0.548346	0.841294	2.402082
8	1	0	2.264845	-0.602211	-0.976845
9	1	0	2.254895	1.036311	-0.314507
10	1	0	2.387057	-0.348111	0.776475
11	1	0	-0.451762	-2.303122	-0.789804
12	1	0	-1.367429	-2.021506	0.706853
13	1	0	-1.933060	-1.352472	-0.841493
14	8	0	-0.090035	0.287031	-1.882063
15	1	0	0.800781	0.415151	-2.245403
16	6	0	-0.955238	1.707883	0.103143
17	7	0	-1.511984	2.715450	0.272791

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	18	6	0	-1.239170	1.103800	-3.452074
19	6	0	-0.912839	2.541115	-3.236442	
20	6	0	-2.524595	0.561816	-2.915549	
21	1	0	-3.331774	0.929310	-3.562543	
22	1	0	-2.550236	-0.525219	-2.921527	
23	1	0	-2.690636	0.926215	-1.901142	
24	7	0	-0.664435	0.546838	-4.506261	
25	6	0	-0.823353	-0.790908	-4.982883	
26	1	0	0.017383	1.106286	-5.016903	
27	6	0	0.410518	2.994670	-3.318366	
28	6	0	0.700340	4.343847	-3.141841	
29	6	0	-0.329457	5.254803	-2.894322	
30	6	0	-1.647387	4.808264	-2.820332	
31	6	0	-1.940248	3.454394	-2.982767	
32	1	0	1.224198	2.294508	-3.495001	
33	1	0	1.730803	4.683038	-3.191758	
34	1	0	-0.101960	6.308011	-2.756365	
35	1	0	-2.452948	5.510992	-2.628637	
36	1	0	-2.970580	3.119539	-2.913483	
37	6	0	-0.974075	-0.980062	-6.356770	
38	6	0	-1.092848	-2.274554	-6.859266	
39	6	0	-1.063685	-3.368769	-5.993354	
40	6	0	-0.901929	-3.166156	-4.621759	
41	6	0	-0.771054	-1.877065	-4.108007	
42	1	0	-0.999700	-0.118559	-7.018967	
43	1	0	-1.212415	-2.425650	-7.928070	
44	1	0	-1.160058	-4.376476	-6.386771	
45	1	0	-0.865006	-4.015315	-3.945244	
46	1	0	-0.614792	-1.698510	-3.047848	

5a\*15

1	14	0	-0.260043	0.181940	-0.077450
2	6	0	-1.580080	-0.134576	1.219865
3	6	0	1.192653	1.056658	0.725842
4	6	0	0.271698	-1.421024	-0.879492
5	1	0	-2.449114	-0.654202	0.797850
6	1	0	-1.174768	-0.763696	2.023187
7	1	0	-1.925647	0.800881	1.676350
8	1	0	1.995487	1.242780	0.002312
9	1	0	0.884490	2.023733	1.143277

63

	10	1	0	1.609490	0.457530	1.544929
11	1	0	1.023639	-1.246065	-1.658136	
12	1	0	0.706331	-2.104429	-0.139987	
13	1	0	-0.582463	-1.928902	-1.343628	
14	8	0	-0.865353	1.118627	-1.336332	
15	1	0	-1.256778	1.961461	-1.050461	
16	6	0	-3.089065	3.360301	0.775401	
17	7	0	-2.041053	3.342870	0.285538	
18	6	0	-4.456593	3.359207	1.391644	
19	6	0	-4.627738	4.731912	2.066773	
20	6	0	-4.536655	2.193761	2.386576	
21	1	0	-5.527198	2.201695	2.847704	
22	1	0	-4.404007	1.235748	1.883170	
23	1	0	-3.770727	2.289291	3.161097	
24	7	0	-5.482423	3.244115	0.360089	
25	6	0	-5.450775	2.341283	-0.710673	
26	1	0	-5.895871	4.137049	0.109663	
27	6	0	-4.435812	5.886906	1.297279	
28	6	0	-4.610876	7.148363	1.859368	
29	6	0	-4.977308	7.270186	3.201340	
30	6	0	-5.164429	6.124659	3.970865	
31	6	0	-4.989632	4.857766	3.408270	
32	1	0	-4.144261	5.803551	0.251392	
33	1	0	-4.455974	8.034823	1.251190	
34	1	0	-5.112191	8.253313	3.643238	
35	1	0	-5.446840	6.208681	5.016387	
36	1	0	-5.138157	3.982252	4.030457	
37	6	0	-6.394156	2.530137	-1.739152	
38	6	0	-6.452863	1.660746	-2.820311	
39	6	0	-5.575485	0.575210	-2.910625	
40	6	0	-4.637666	0.388201	-1.899651	
41	6	0	-4.565050	1.258065	-0.808503	
42	1	0	-7.082754	3.369579	-1.673486	
43	1	0	-7.191436	1.832495	-3.598803	
44	1	0	-5.622898	-0.105773	-3.754927	
45	1	0	-3.938402	-0.442765	-1.950032	
46	1	0	-3.810088	1.071288	-0.053933	

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1	6	0	-0.490063	0.206514	0.205270
2	6	0	-0.088587	0.102263	1.673262
3	8	0	0.553354	0.386901	-0.667287
4	6	0	1.214735	0.421215	2.054480
5	6	0	1.595635	0.349253	3.396815
6	6	0	0.676068	-0.051347	4.365400
7	6	0	-0.629502	-0.377116	3.987892
8	6	0	-1.010180	-0.295945	2.649663
9	1	0	1.920827	0.723293	1.286982
10	1	0	2.612560	0.603611	3.683913
11	1	0	0.972099	-0.111249	5.409179
12	1	0	-1.350293	-0.694121	4.736818
13	1	0	-2.028252	-0.552094	2.362060
14	6	0	-1.645560	1.177353	0.007096
15	1	0	-1.305232	2.166473	0.330663
16	1	0	-1.912807	1.235877	-1.051554
17	1	0	-2.531897	0.906593	0.590302
18	7	0	-0.856234	-1.240739	-0.314971
19	6	0	-2.151702	-1.548842	-0.858100
20	6	0	-2.438293	-1.196757	-2.176986
21	6	0	-3.700868	-1.467866	-2.701975
22	6	0	-4.668466	-2.096058	-1.915907
23	6	0	-4.370505	-2.455301	-0.600681
24	6	0	-3.111544	-2.180703	-0.067333
25	1	0	-1.673779	-0.718439	-2.783938
26	1	0	-3.925093	-1.194318	-3.728906
27	1	0	-5.649643	-2.310668	-2.329460
28	1	0	-5.117243	-2.950584	0.013252
29	1	0	-2.869334	-2.456804	0.956087
30	1	0	-0.564613	-1.947823	0.365414
31	1	0	0.071842	-0.829240	-0.998868