

Supplementary Information

A Conversion of Aromatic Thiocyanates into Sulfothioates: New Synthetic Route to Aromatic Bunte Salts

Petr Jansa, Lucie Čechová, Martin Dračínský and Zlatko Janeba*

Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, v.v.i., Flemingovo nám. 2, CZ-16610 Prague 6, Czech Republic. Fax: +420 220183560; Tel: +420 220183143; E-mail: janeba@uochb.cas.cz

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^1H NMR and ^{13}C NMR spectra of compounds 2a-2l.

Fig. S1. and S2. ^1H NMR and ^{13}C NMR spectra (DMSO- d_6) of sodium *S*-(2-methoxy-4-nitrophenyl) sulfthioate (**2a**).

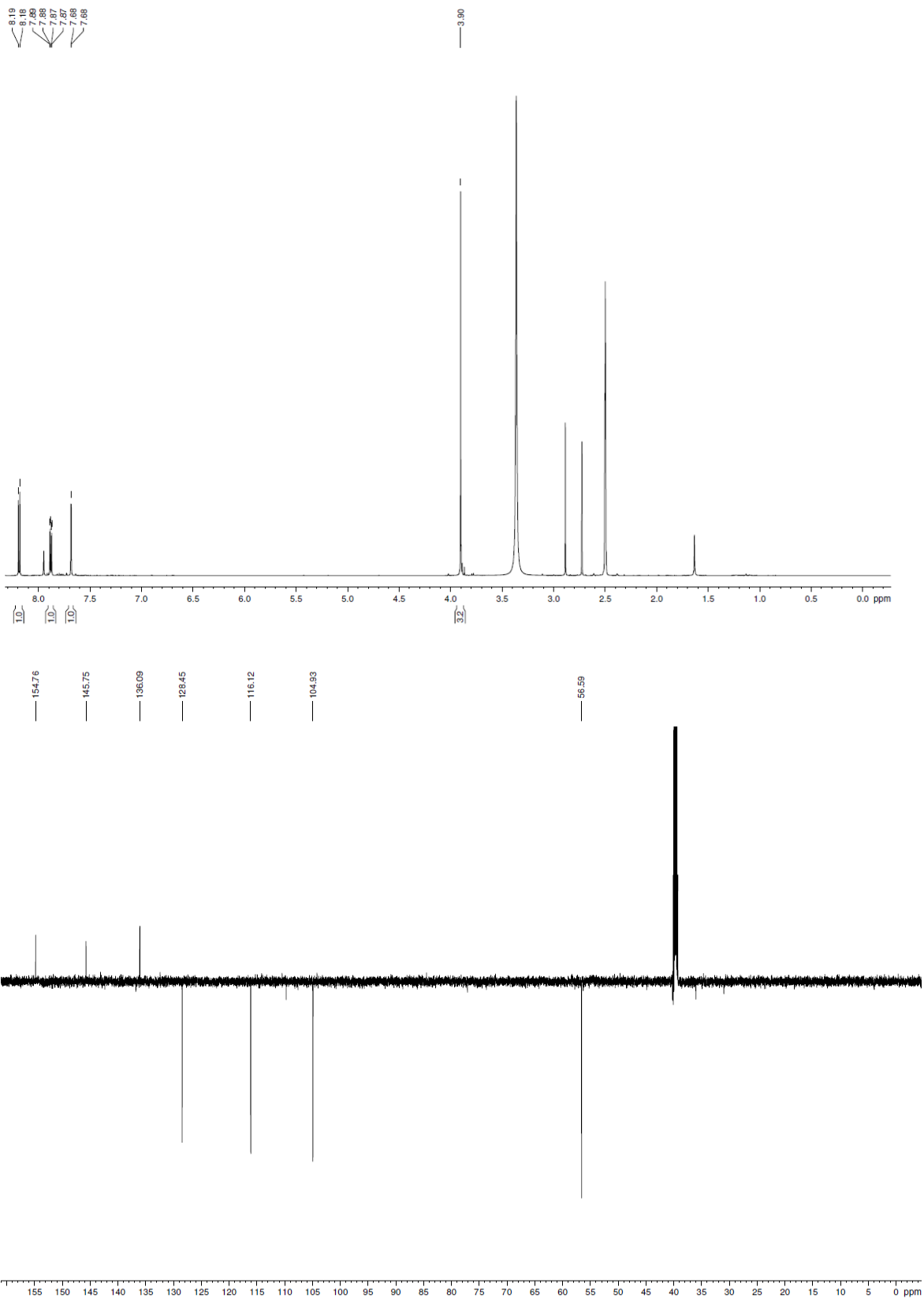


Fig. S3. and S4. ^1H NMR and ^{13}C NMR spectra (DMSO- d_6) of sodium *S*-(4-methyl-2-nitrophenyl) sulfothioate (**2b**).

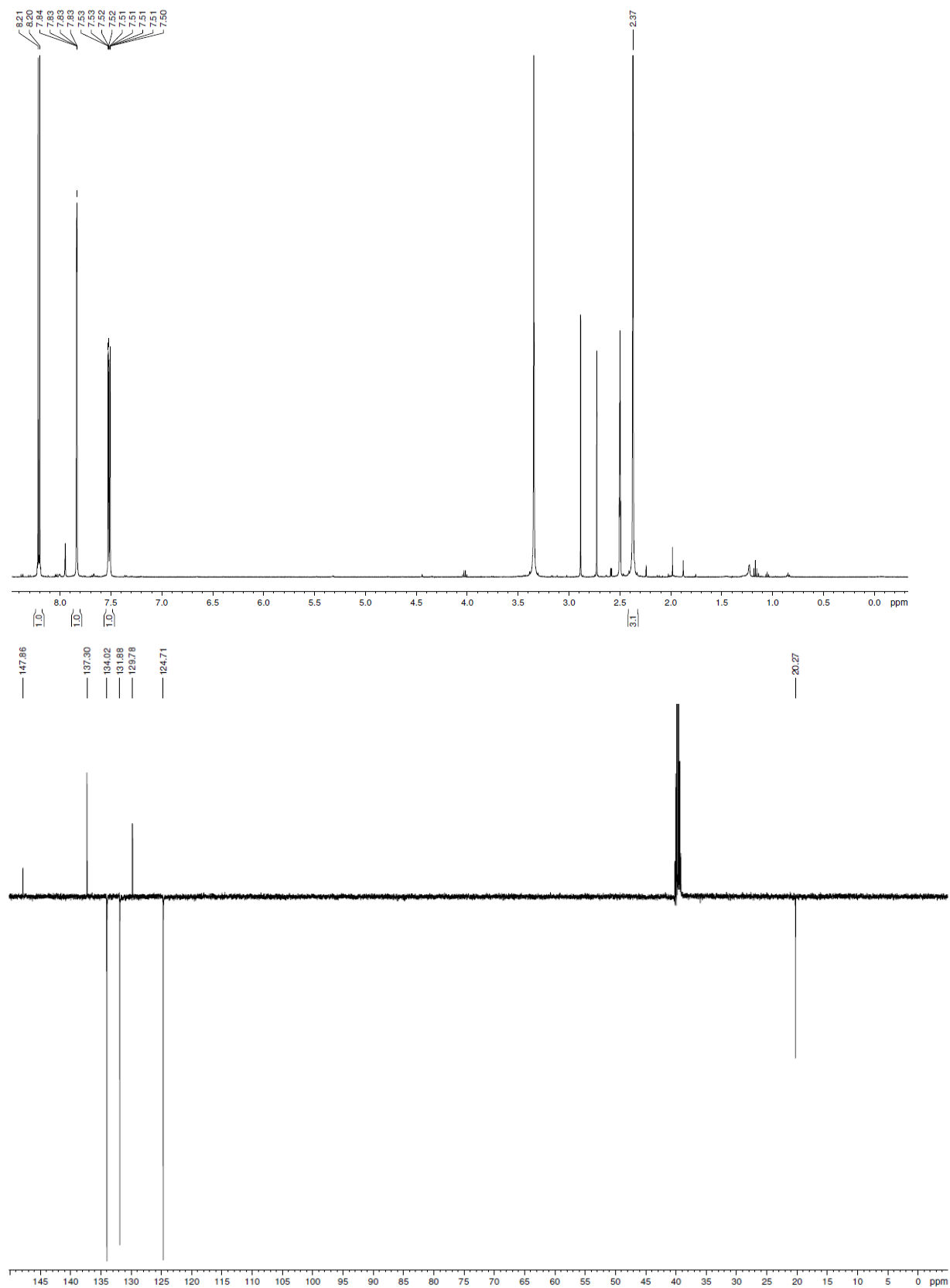


Fig. S5. and S6. ^1H NMR and ^{13}C NMR spectra (D_2O) of sodium *S*-(4-amino-3-nitrophenyl) sulfothioate (**2c**).

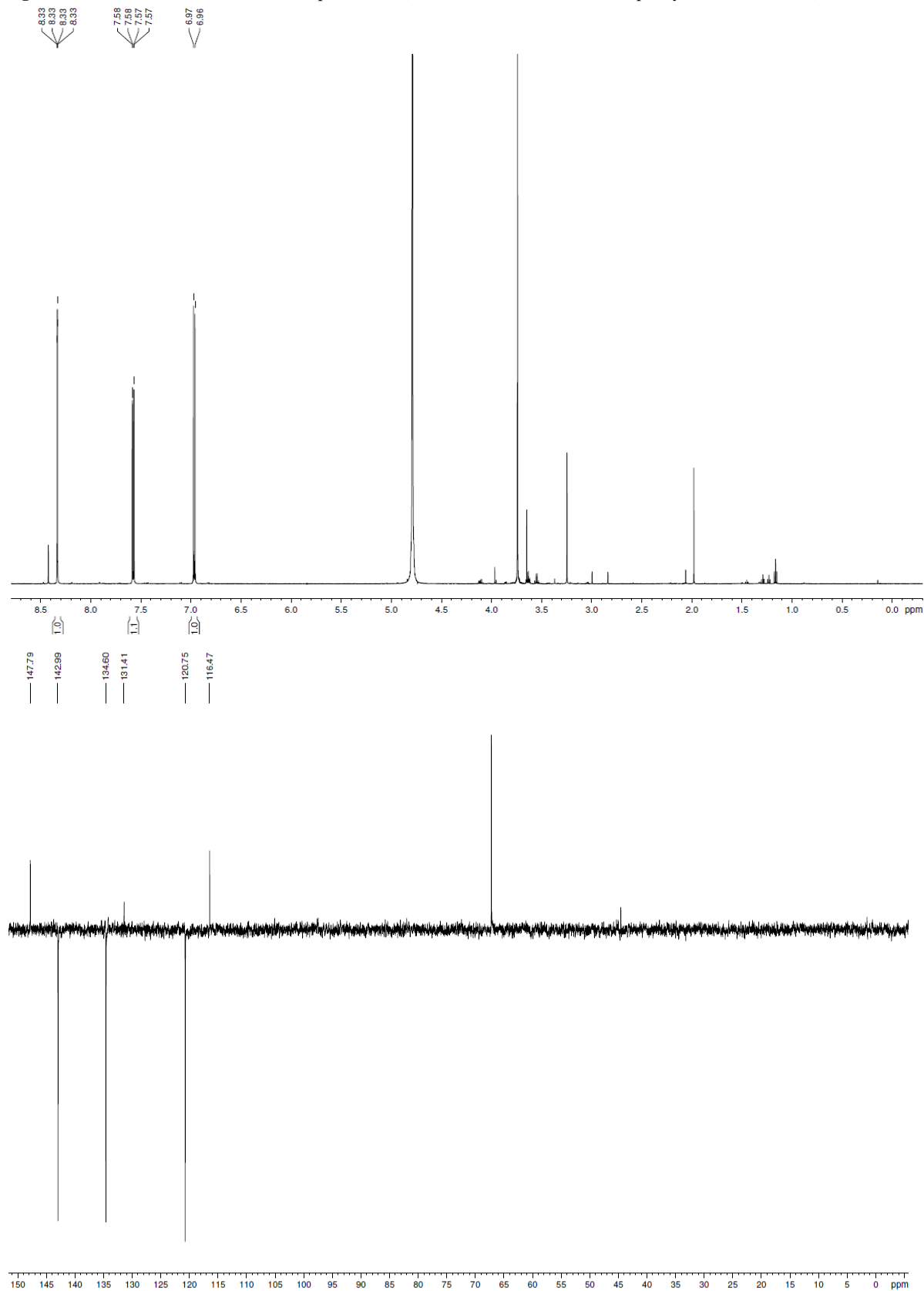


Fig. S7. and S8. ^1H NMR and ^{13}C NMR spectra (DMSO- d_6) of sodium *S*-(4-amino-3-methoxyphenyl) sulfothioate (**2d**).

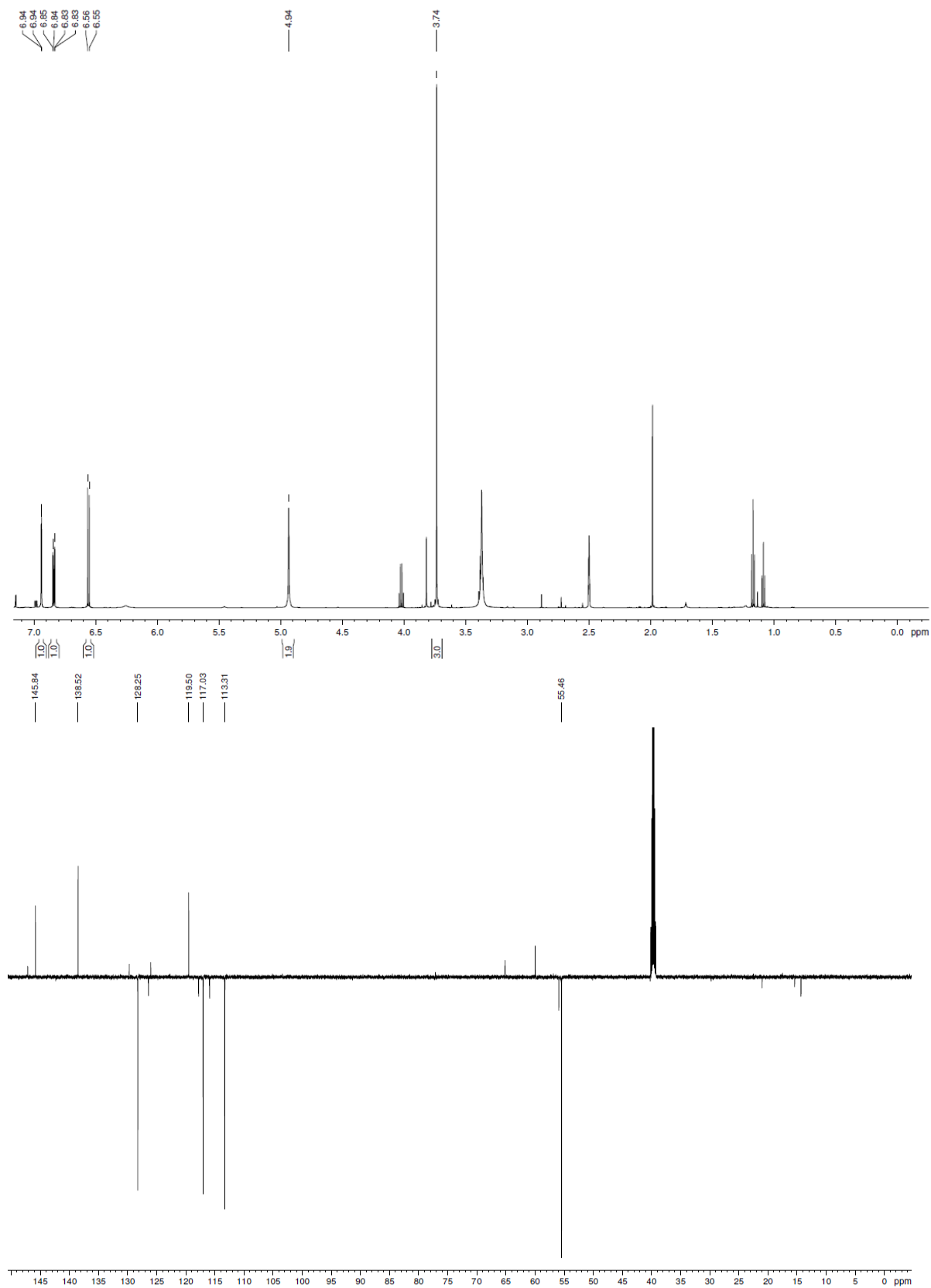


Fig. S9. and S10. ^1H NMR and ^{13}C NMR spectra (DMSO- d_6) of sodium *S*-(3,4-dimethoxyphenyl) sulfthioate (**2e**).

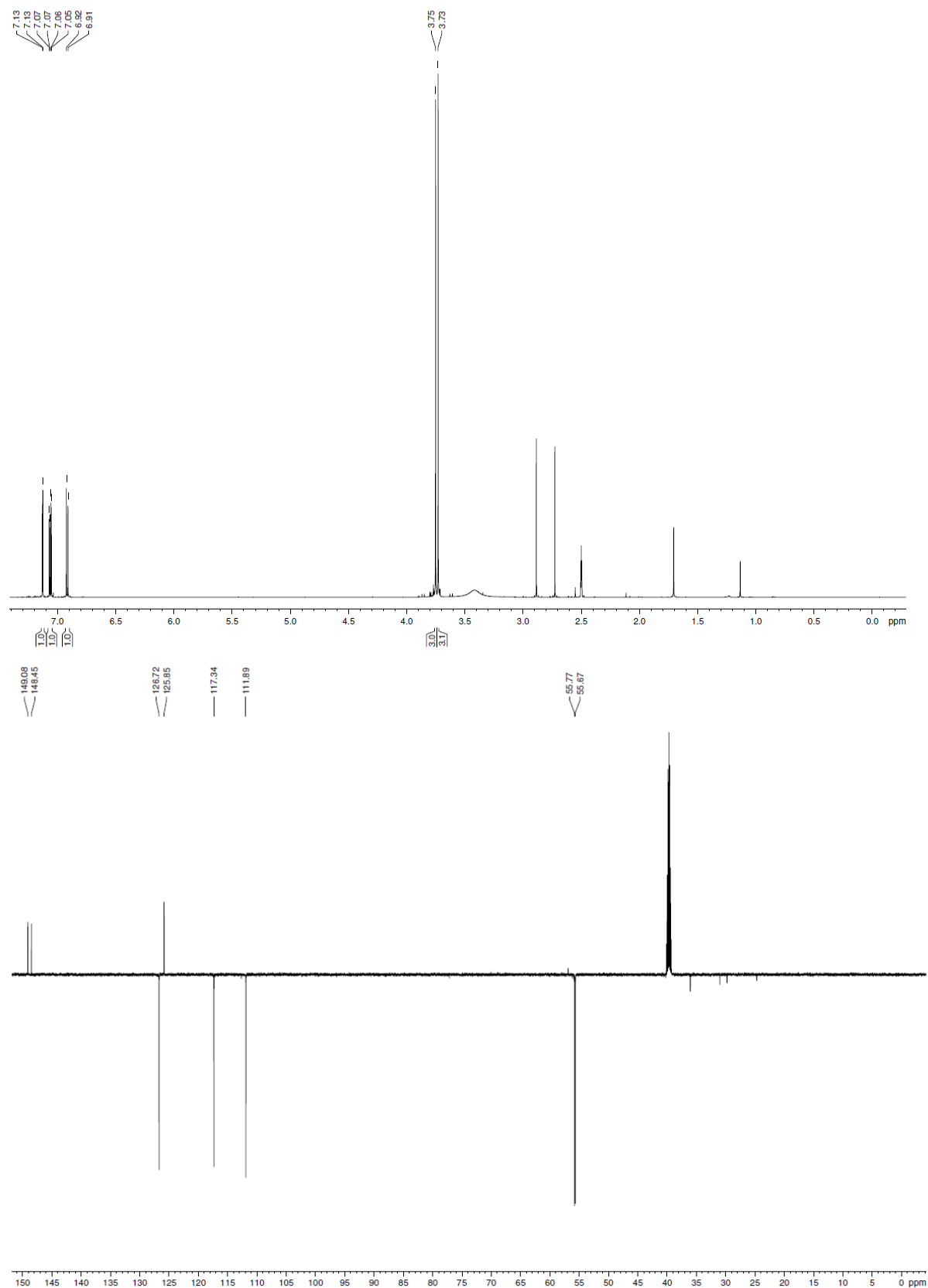


Fig. S11. and S12. ^1H and ^{13}C NMR spectra (DMSO- d_6) of sodium *S*-(4-acetamido-3-methoxyphenyl) sulfothioate (**2f**).

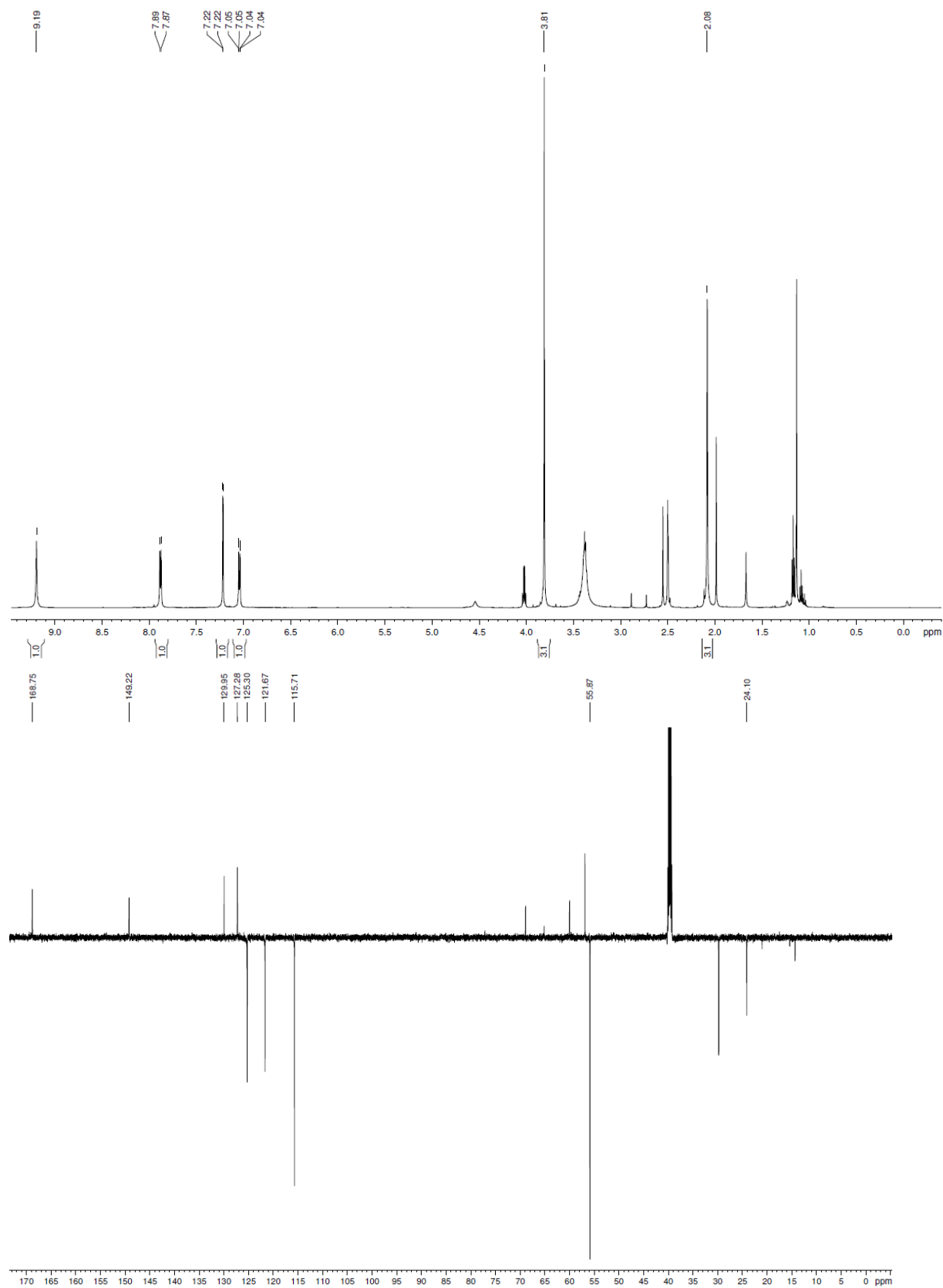


Fig. S13. and S14. ^1H and ^{13}C NMR spectra (DMSO- d_6) of sodium *S*-(3-carboxy-4-nitrophenyl) sulfothioate (**2g**).

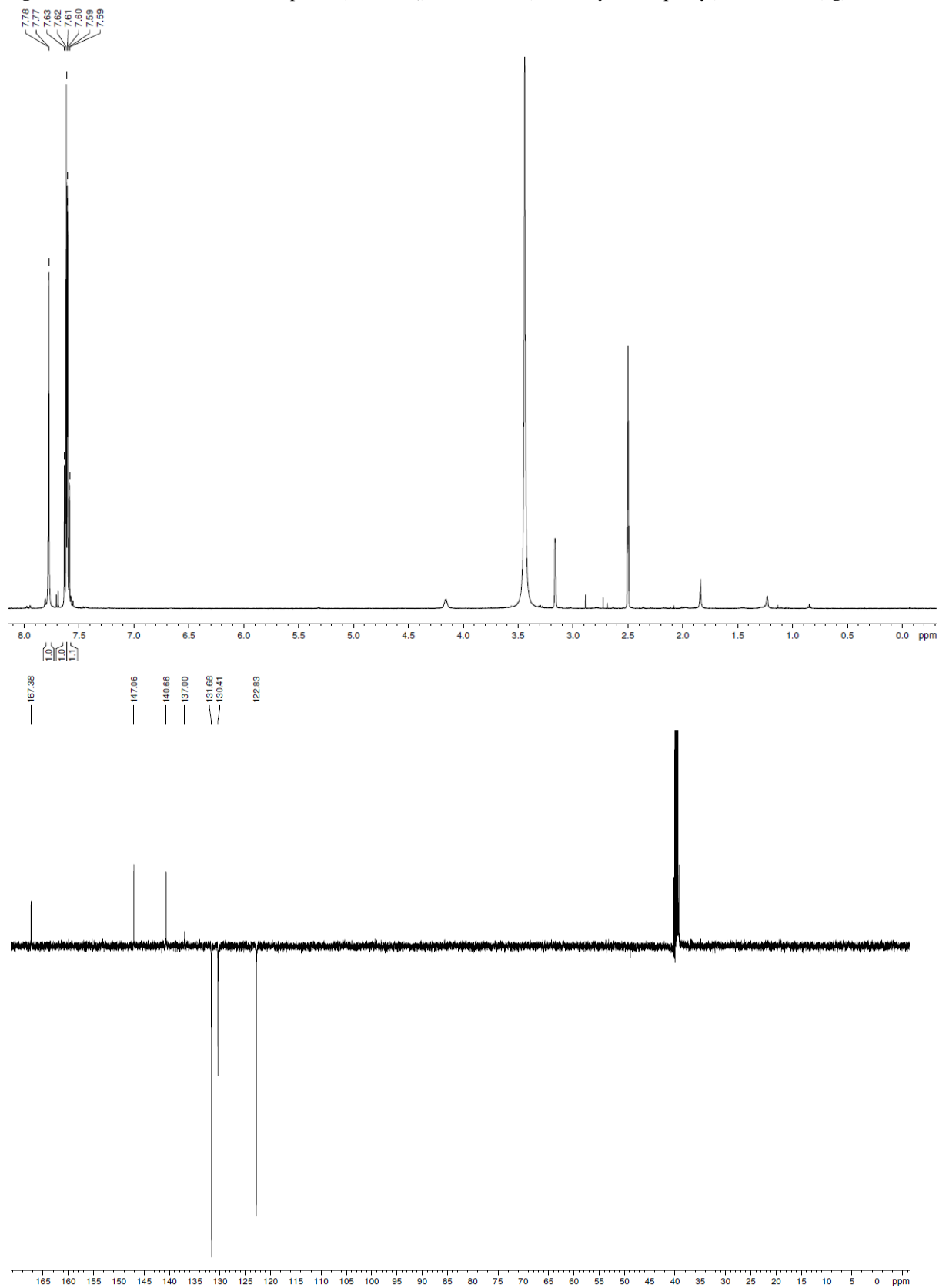


Fig. S17. and S18. ^1H and ^{13}C NMR spectra (DMSO- d_6) of sodium *S*-(2,4-diamino-6-chloropyrimidin-5-yl) sulfathioate (**2i**).

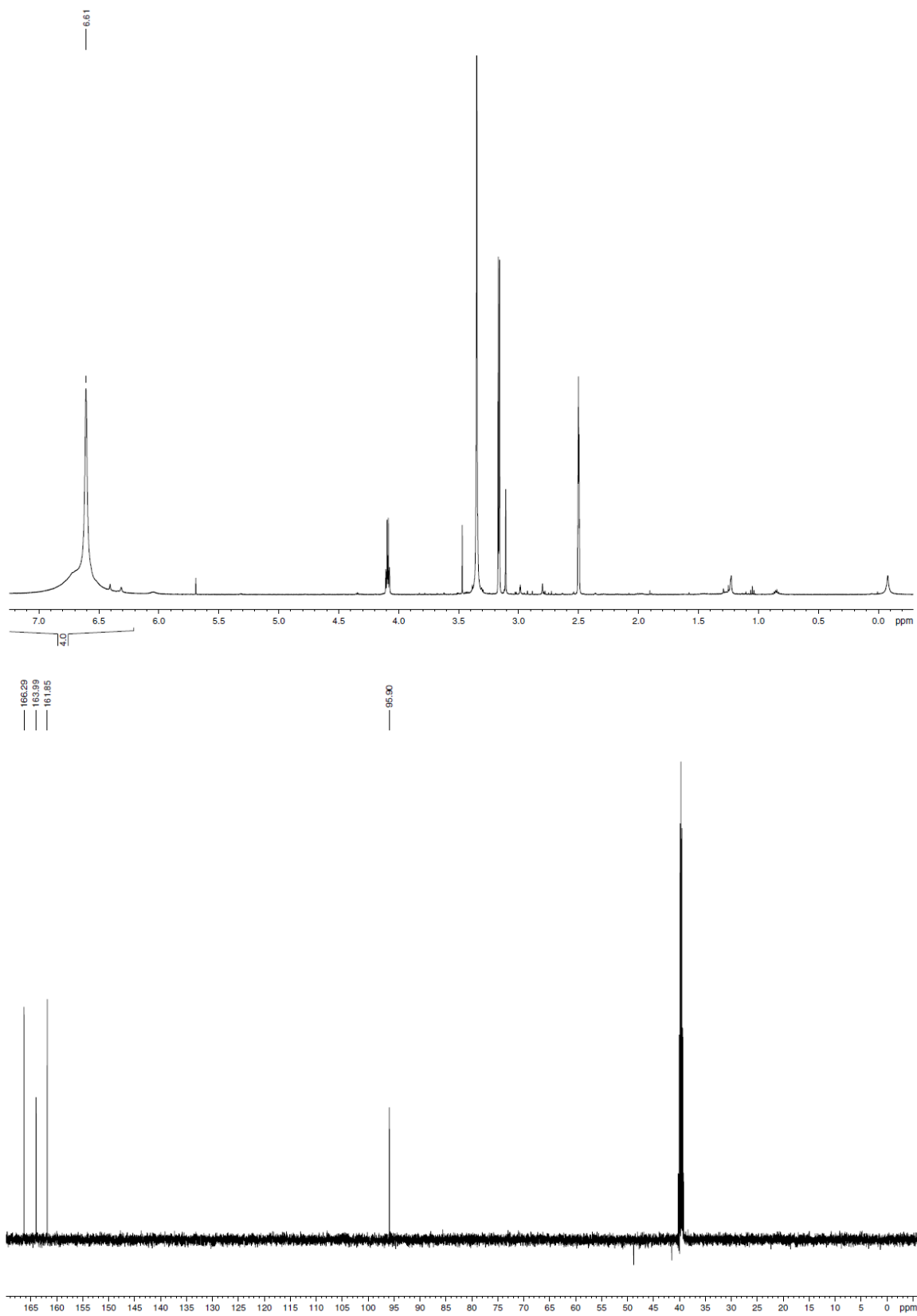


Fig. S19. and S20. ^1H and ^{13}C NMR spectra (DMSO- d_6) of sodium *S*-(2-amino-4,6-dimethoxypyrimidin-5-yl) sulfathioate (**2j**).

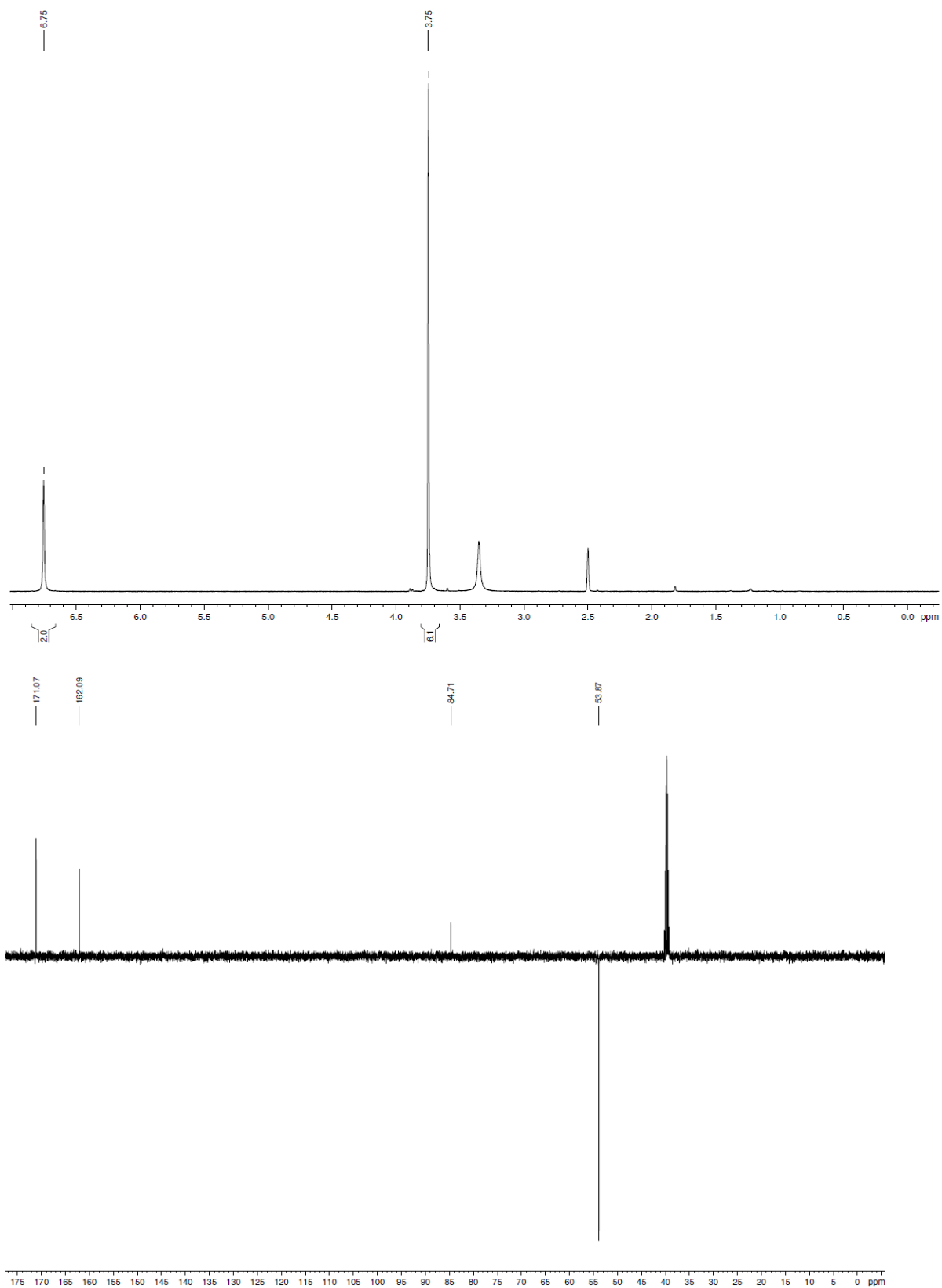


Fig. S21. and S22. ^1H and ^{13}C NMR spectra (DMSO- d_6) of sodium *S*-(2,4-diamino-6-hydroxypyrimidin-5-yl) sulfthioate (**2k**).

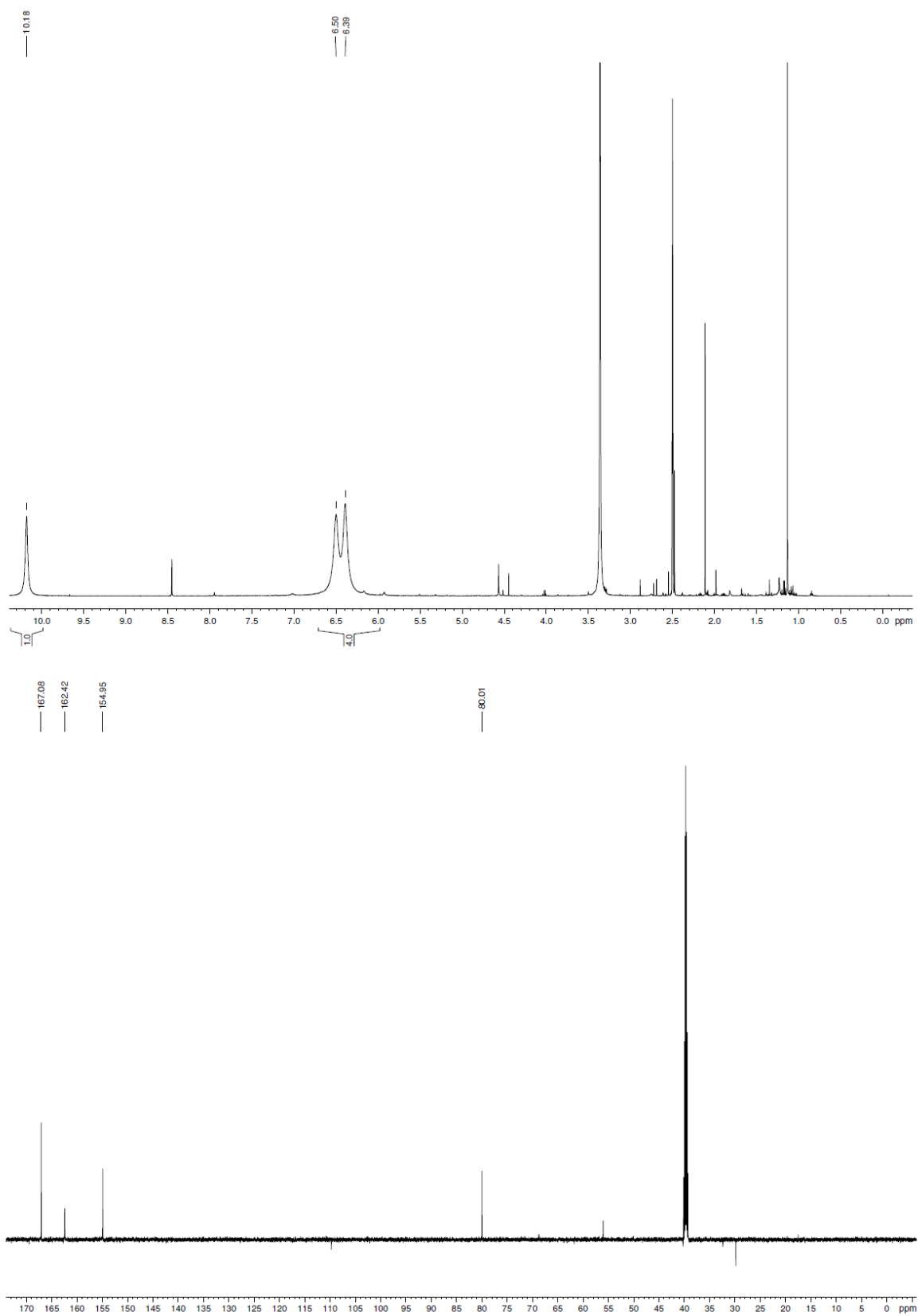


Fig. S23. and S24. ^1H and ^{13}C NMR spectra (DMSO- d_6) of sodium *S*-(4,6-dimethylpyrimidin-2-yl) sulfathioate (**21**).

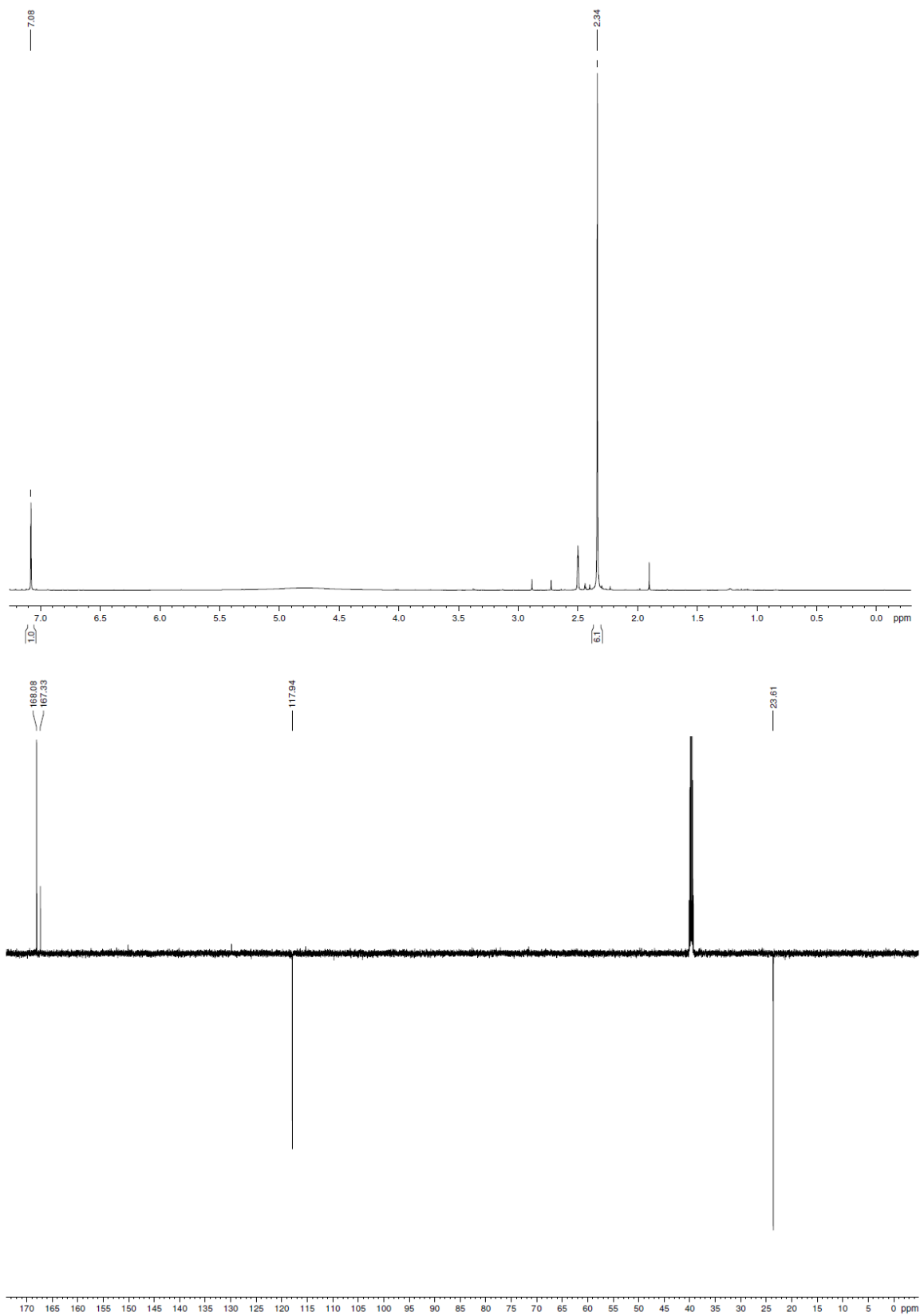


Fig. S25. HR MS spectrum (ESI) of sodium *S*-(2-methoxy-4-nitrophenyl) sulfathioate (**2a**).

280411servis_07-

4/28/2011 5:52:35 PM

Jansa, LC95

280411servis_07-#63-67 RT: 1.81-1.92 AV: 5 NL: 2.20E6
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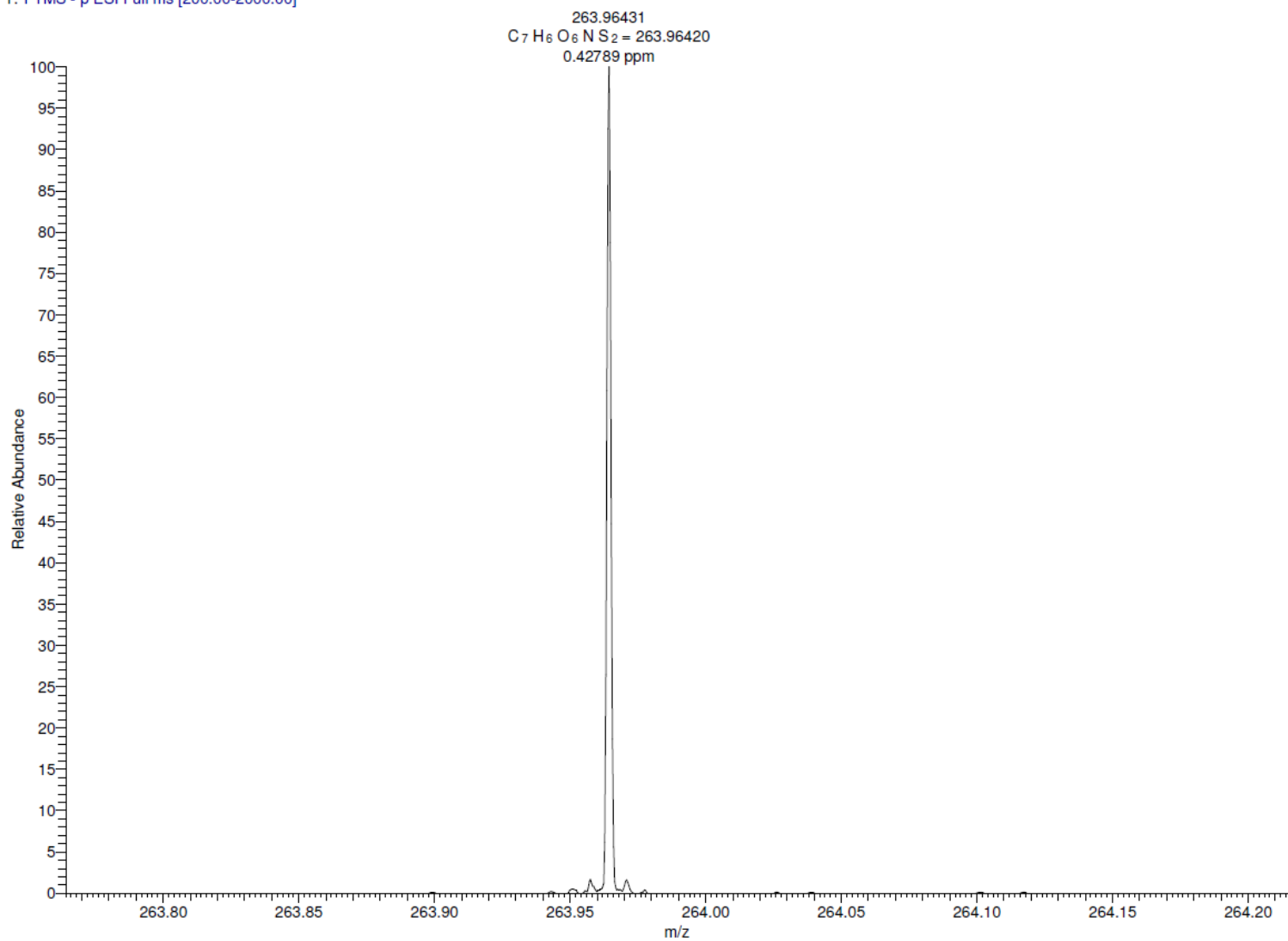


Fig. S26. HR MS spectrum (ESI) of sodium *S*-(4-methyl-2-nitrophenyl) sulfothioate (**2b**).

230311servis_07-

3/23/2011 7:10:40 PM

Jansa, LC83-B

230311servis_07- #59-62 RT: 1.71-1.80 AV: 4 NL: 6.07E6
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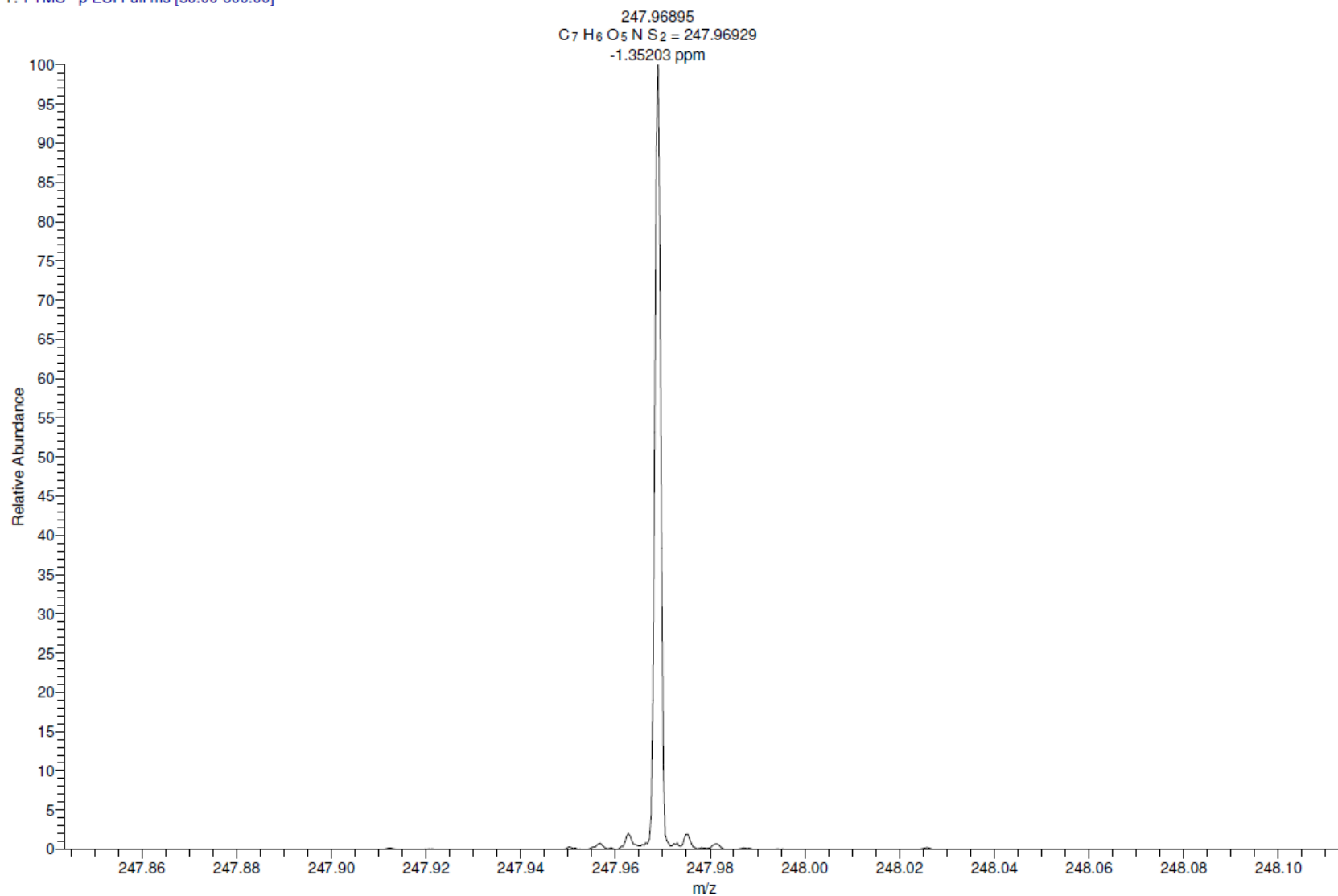


Fig. S27. HR MS spectrum (ESI) of sodium *S*-(4-amino-3-nitrophenyl) sulfothioate (**2c**).

210510servis_13--

5/21/2010 10:56:35 AM

Jansa, PJ 626

210510servis_13-- #59-64 RT: 1.69-1.84 AV: 6 NL: 5.37E6
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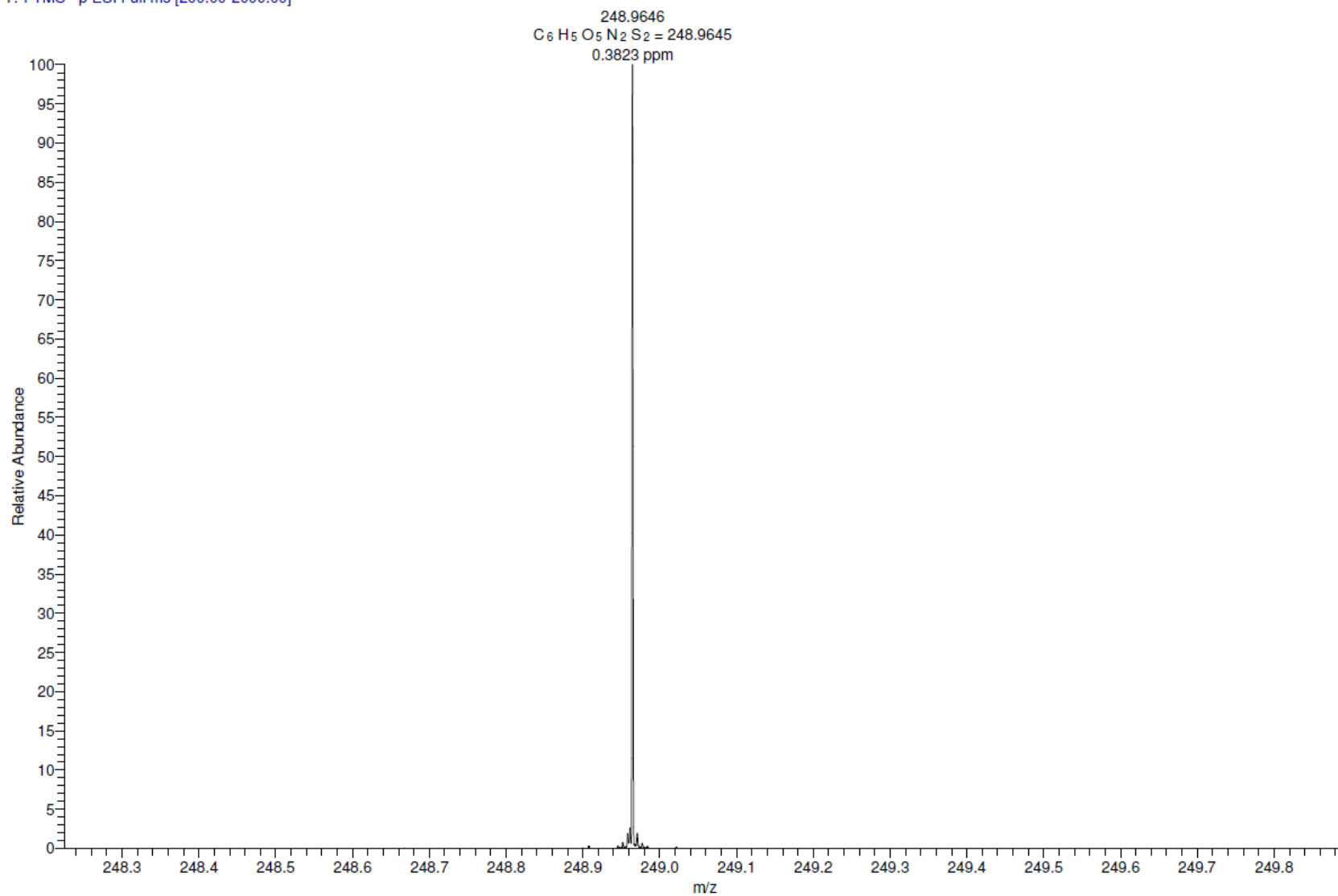


Fig. S28. HR MS spectrum (ESI) of sodium *S*-(4-amino-3-methoxyphenyl) sulfothioate (**2d**).

280411servis_10-

4/28/2011 6:04:49 PM

Jansa, LC93

280411servis 10- #61-64 RT: 1.75-1.83 AV: 4 NL: 3.94E6
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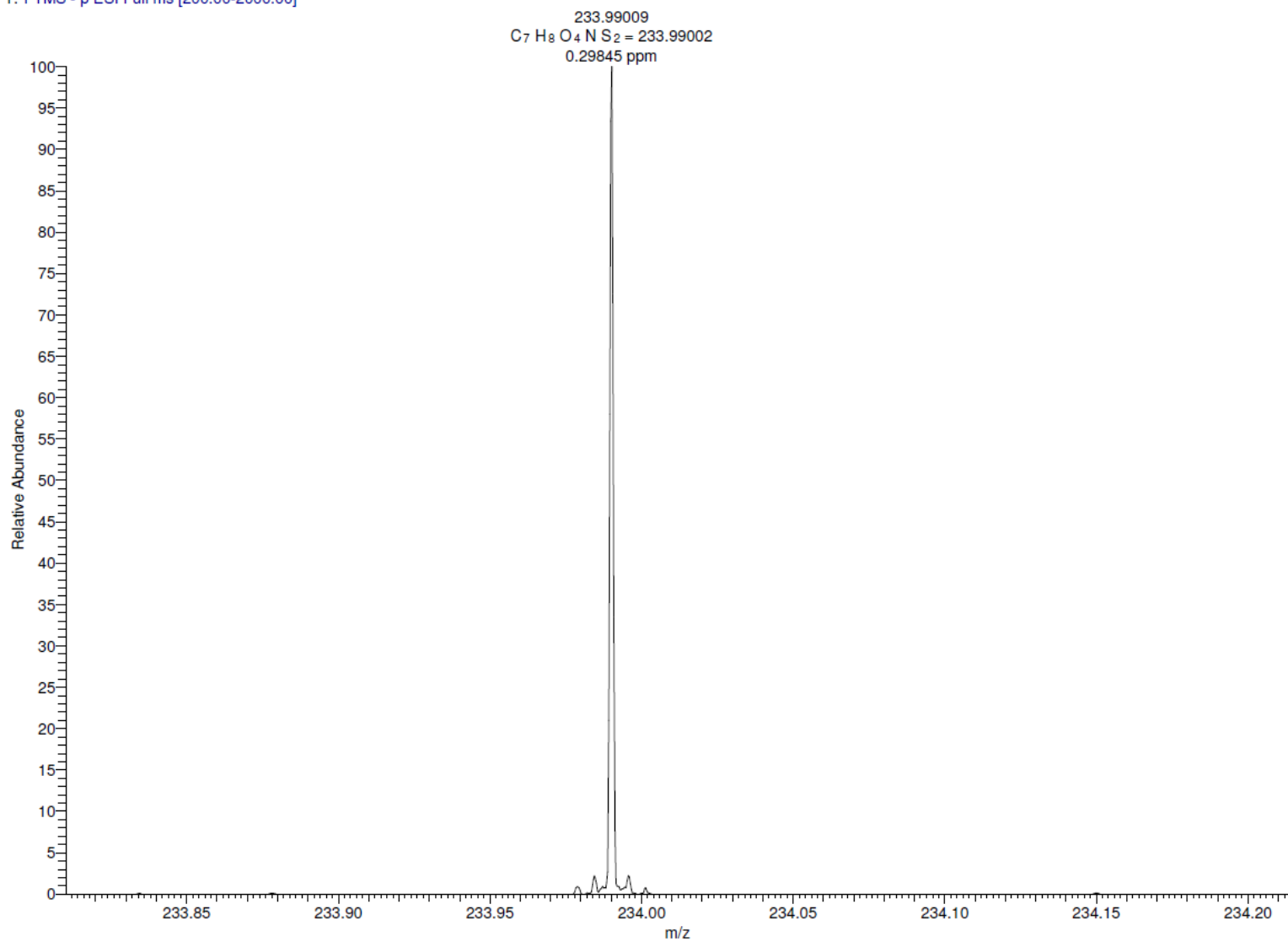


Fig. S29. HR MS spectrum (ESI) of sodium *S*-(3,4-dimethoxyphenyl) sulfathioate (**2e**).

280411servis_09-

4/28/2011 6:00:45 PM

Jansa, LC94

280411servis_09- #60-63 RT: 1.72-1.81 AV: 4 NL: 6.04E6
T: FTMS - p ESI Full ms [200.00-2000.00]

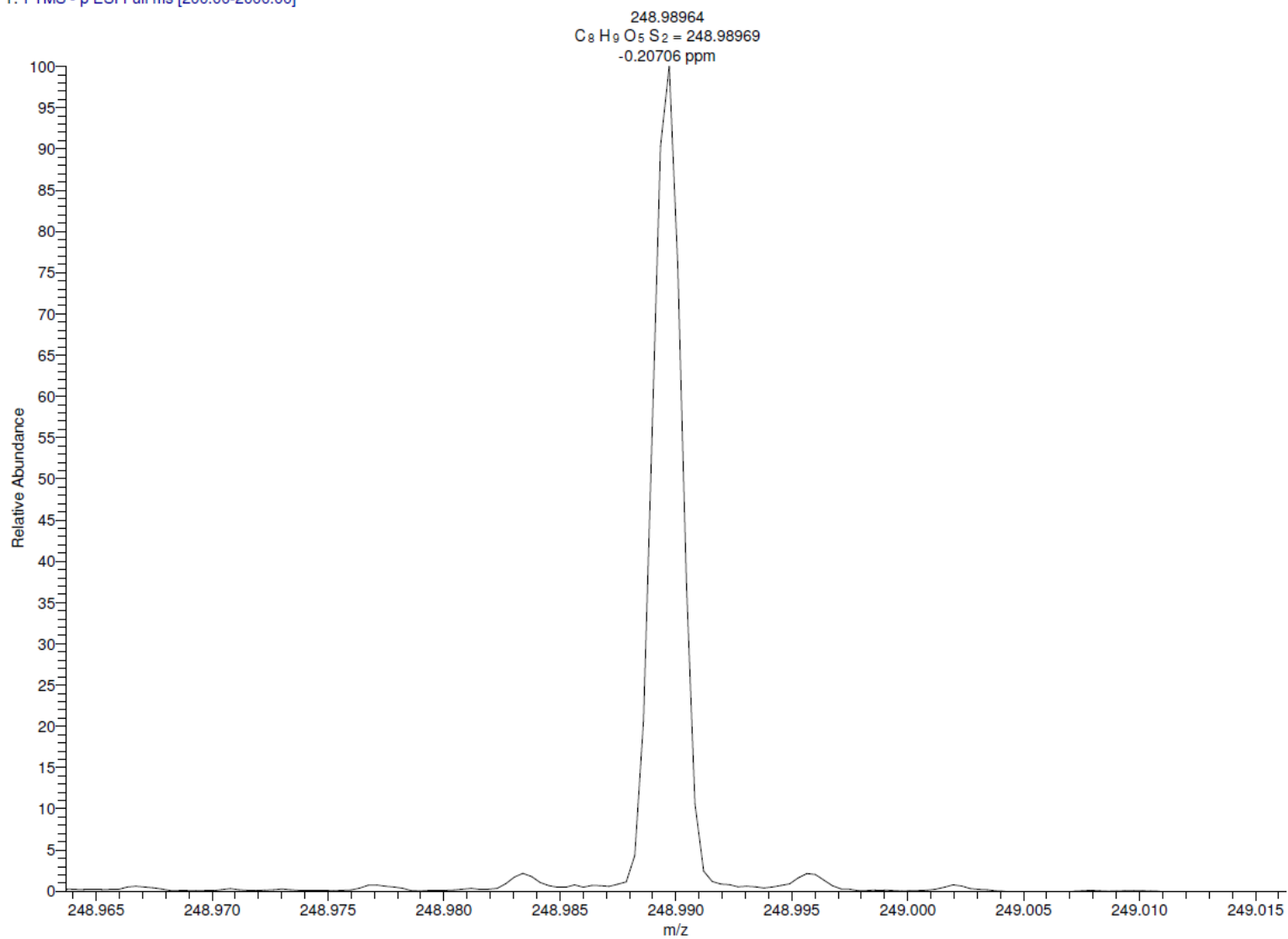


Fig. S30. HR MS spectrum (ESI) of sodium *S*-(4-acetamido-3-methoxyphenyl) sulfothioate (**2f**).

280411servis_08-

4/28/2011 5:56:40 PM

Jansa, LC96

280411servis_08- #61-63 RT: 1.75-1.81 AV: 3 NL: 9.58E6
T: FTMS - p ESI Full ms [200.00-2000.00]

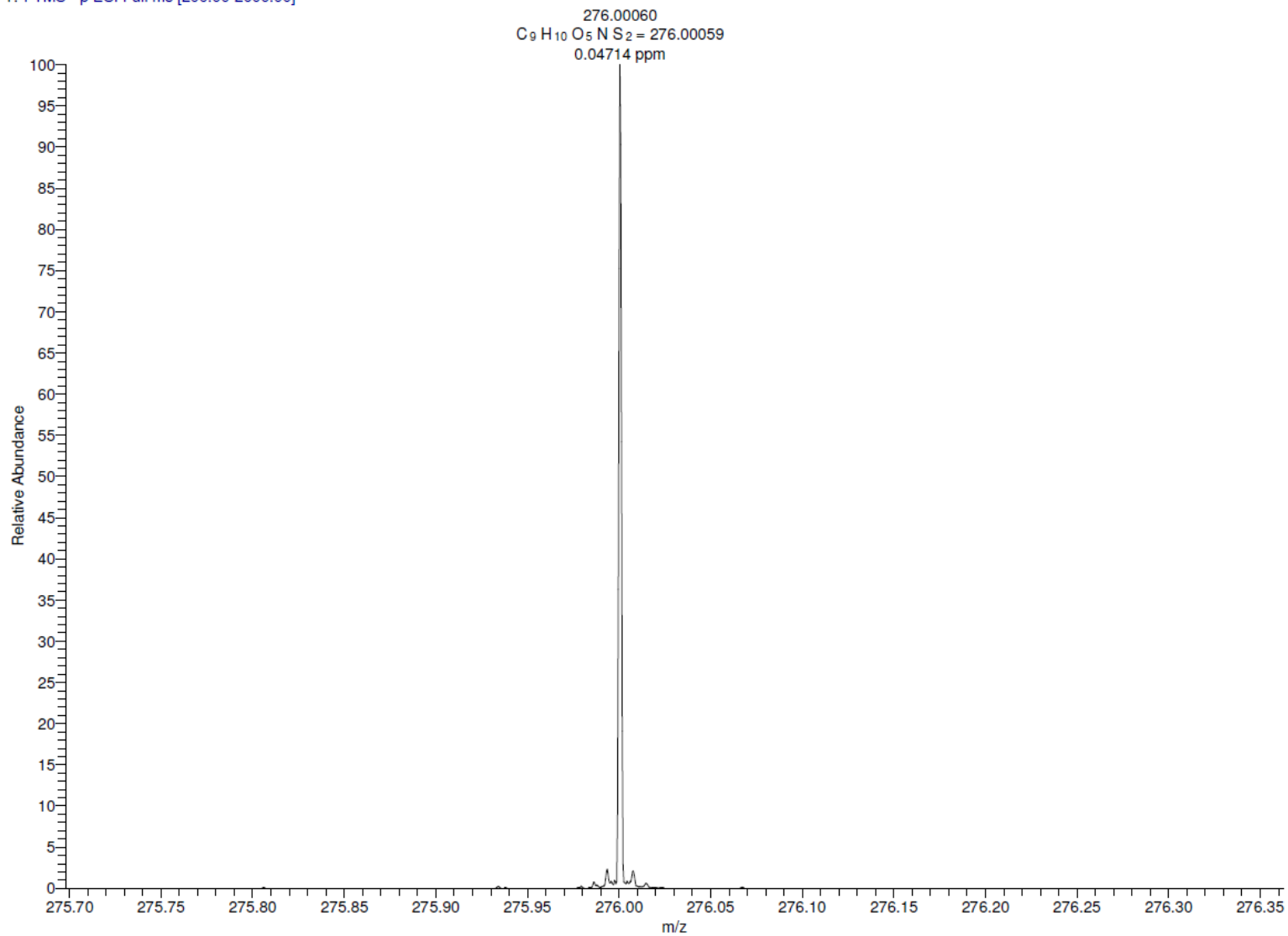


Fig. S31. HR MS spectrum (ESI) of sodium *S*-(3-carboxy-4-nitrophenyl) sulfathioate (**2g**).

230311servis_04-

3/23/2011 6:56:41 PM

Jansa, LC68-2

230311servis_04- #61-64 RT: 1.77-1.86 AV: 4 NL: 5.53E6
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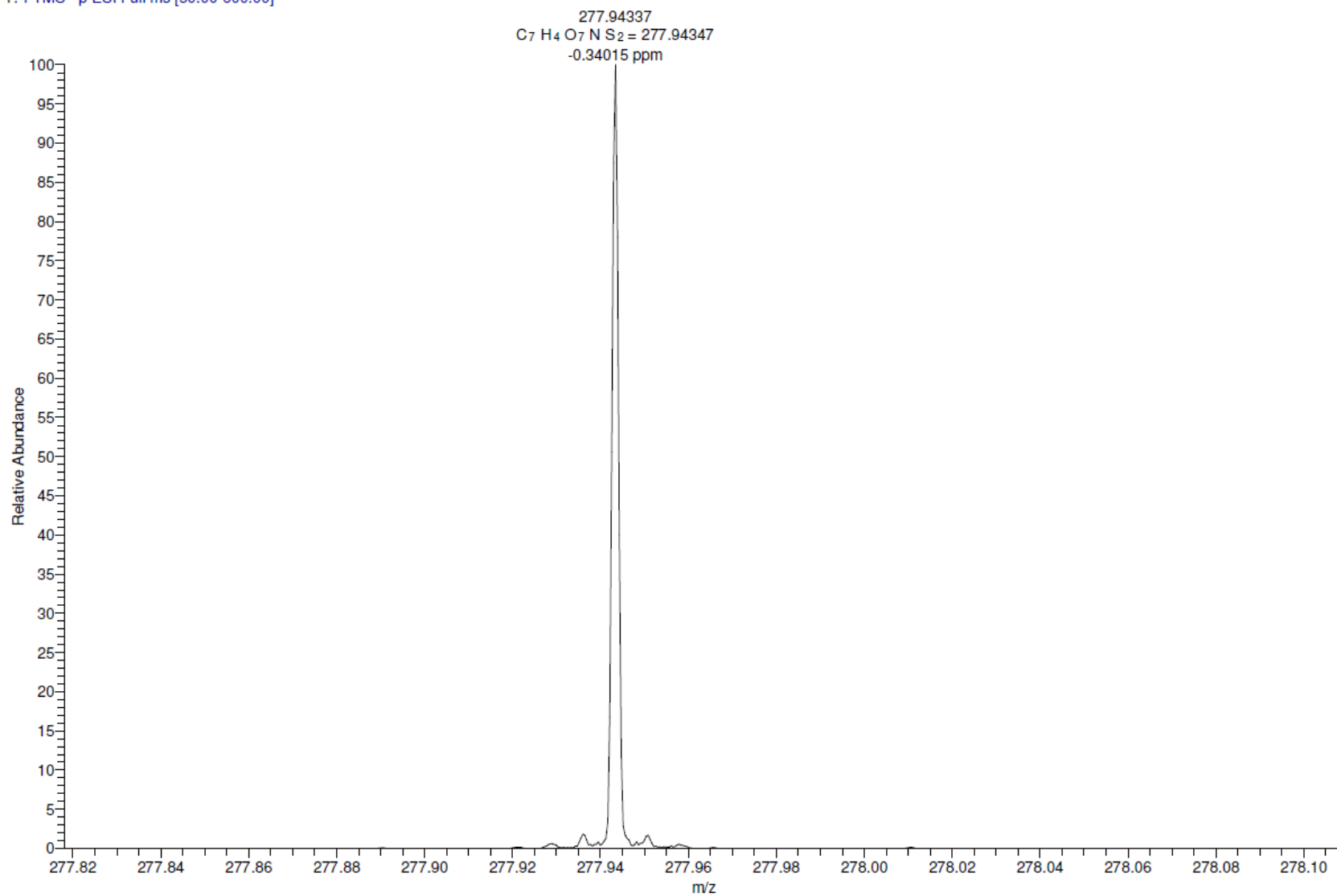


Fig. S32. HR MS spectrum (ESI) of sodium *S*-(2-aminobenzo[*d*]thiazol-6-yl) sulfthioate (**2h**).

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10/27/2010 9:29:04 AM

Jansa, LC 67-D

271010servis_4 #44-49 RT: 1.24-1.38 AV: 6 NL: 3.42E6

T: FTMS + p ESI Full ms [200.00-2000.00]

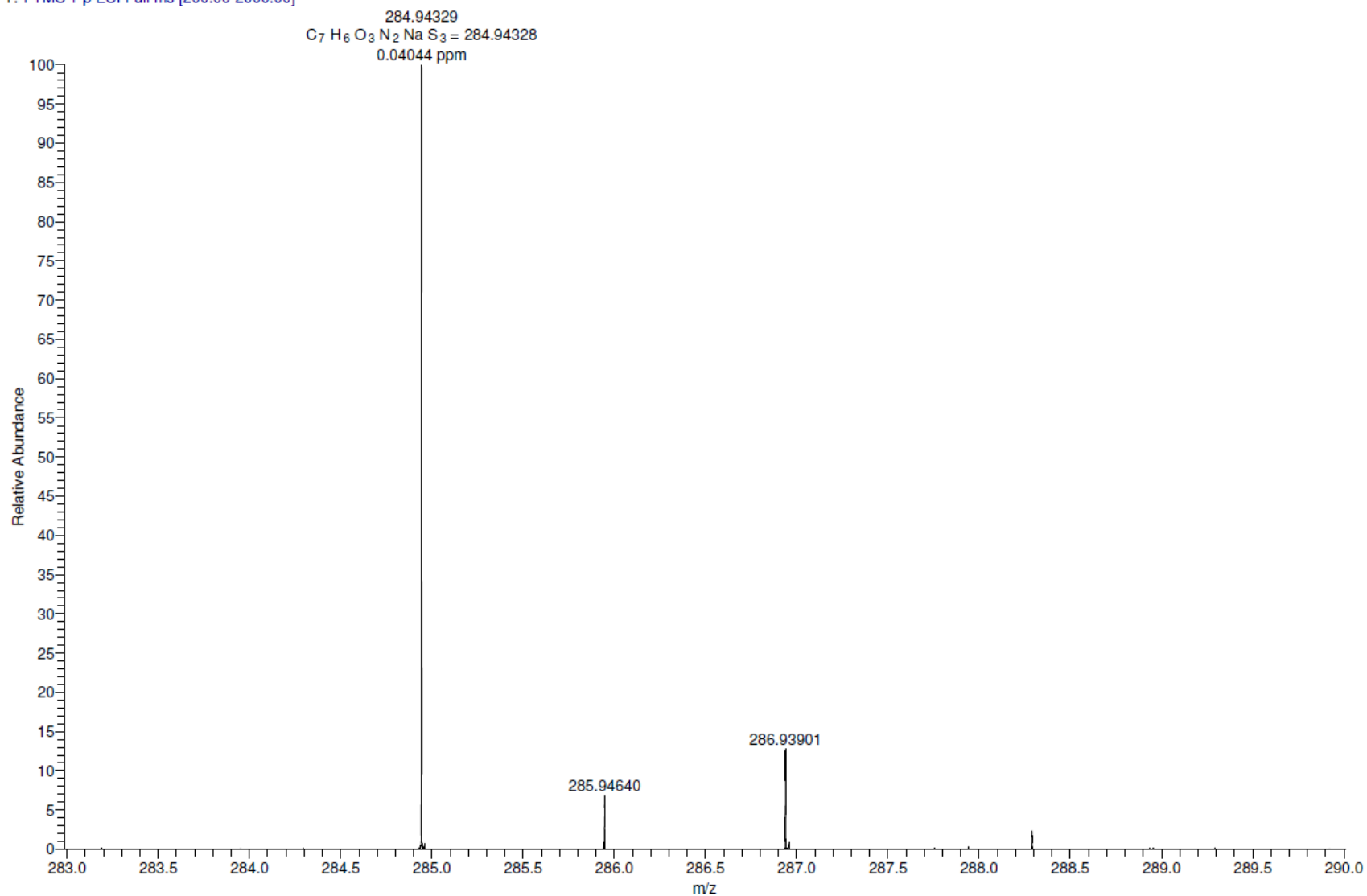


Fig. S33. HR MS spectrum (ESI) of sodium *S*-(2,4-diamino-6-chloropyrimidin-5-yl) sulfathioate (**2i**).

010411servis_10-

4/1/2011 1:34:47 PM

Jansa, LC 86

010411servis_10- #60-63 RT: 1.74-1.83 AV: 4 NL: 1.16E7
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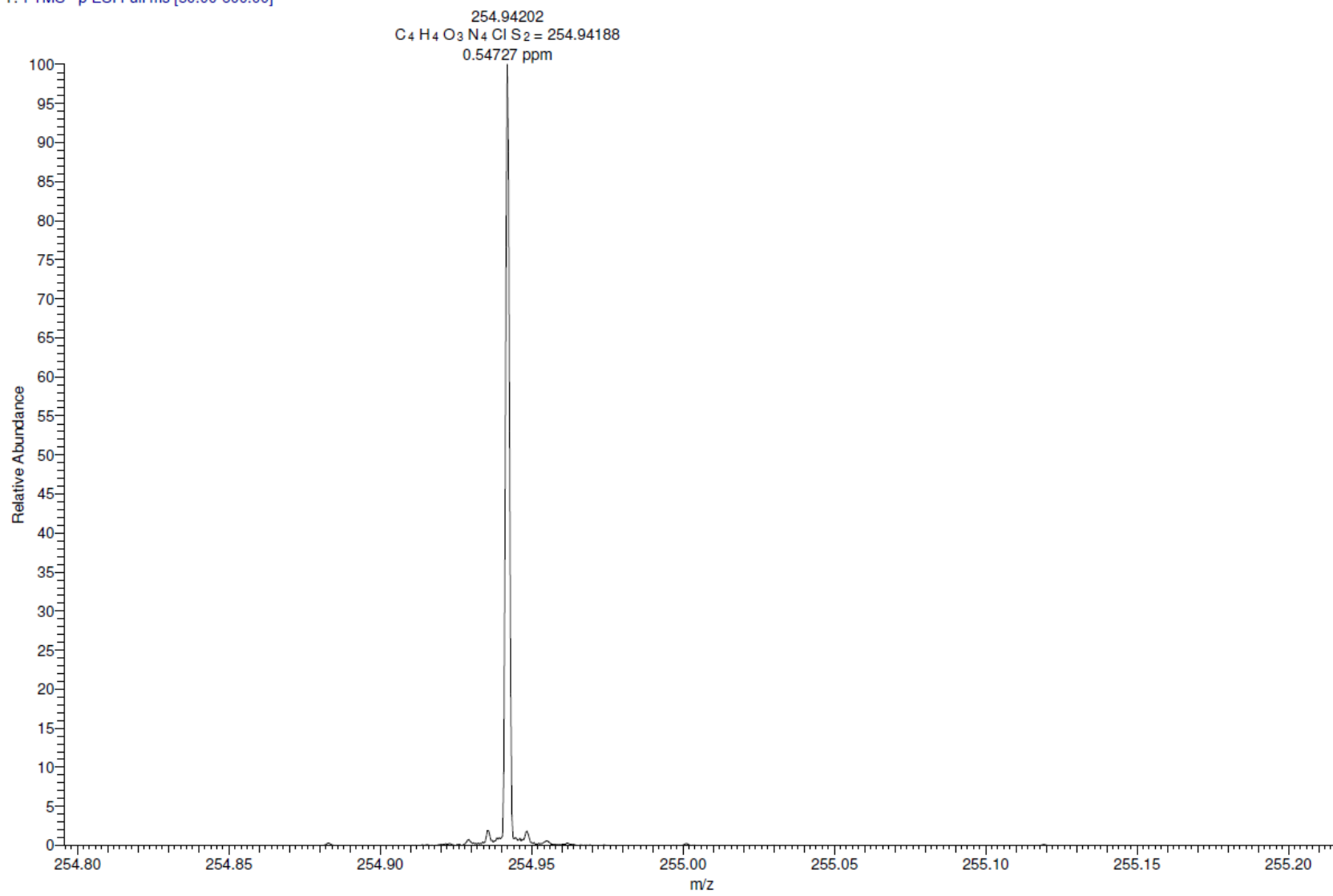


Fig. S34. HR MS spectrum (ESI) of sodium *S*-(2-amino-4,6-dimethoxypyrimidin-5-yl) sulfthioate (**2j**).

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4/14/2011 7:00:15 PM

Jansa, LC 92

140411servis_02- #64-70 RT: 1.73-1.89 AV: 7 NL: 3.69E7

T: FTMS - p ESI Full ms [200.00-2000.00]

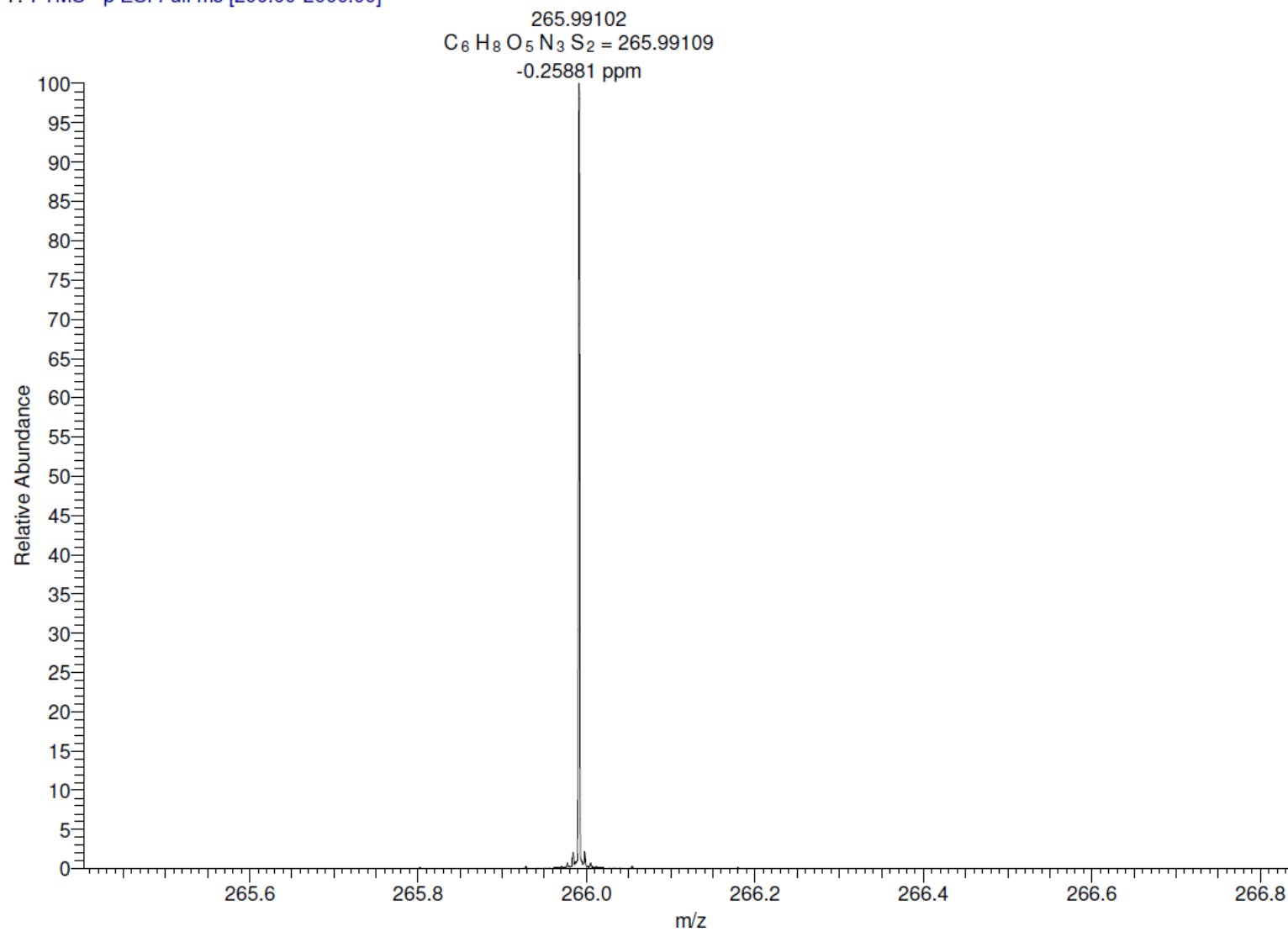


Fig. S35. HR MS spectrum (ESI) of sodium *S*-(2,4-diamino-6-hydroxypyrimidin-5-yl) sulfathioate (**2k**).

060511servis_3-

5/6/2011 10:07:49 AM

Jansa, LC 91

060511servis 3- #62-63 RT: 1.71-1.74 AV: 2 NL: 2.95E6
T: FTMS - p ESI Full ms [50.00-600.00]

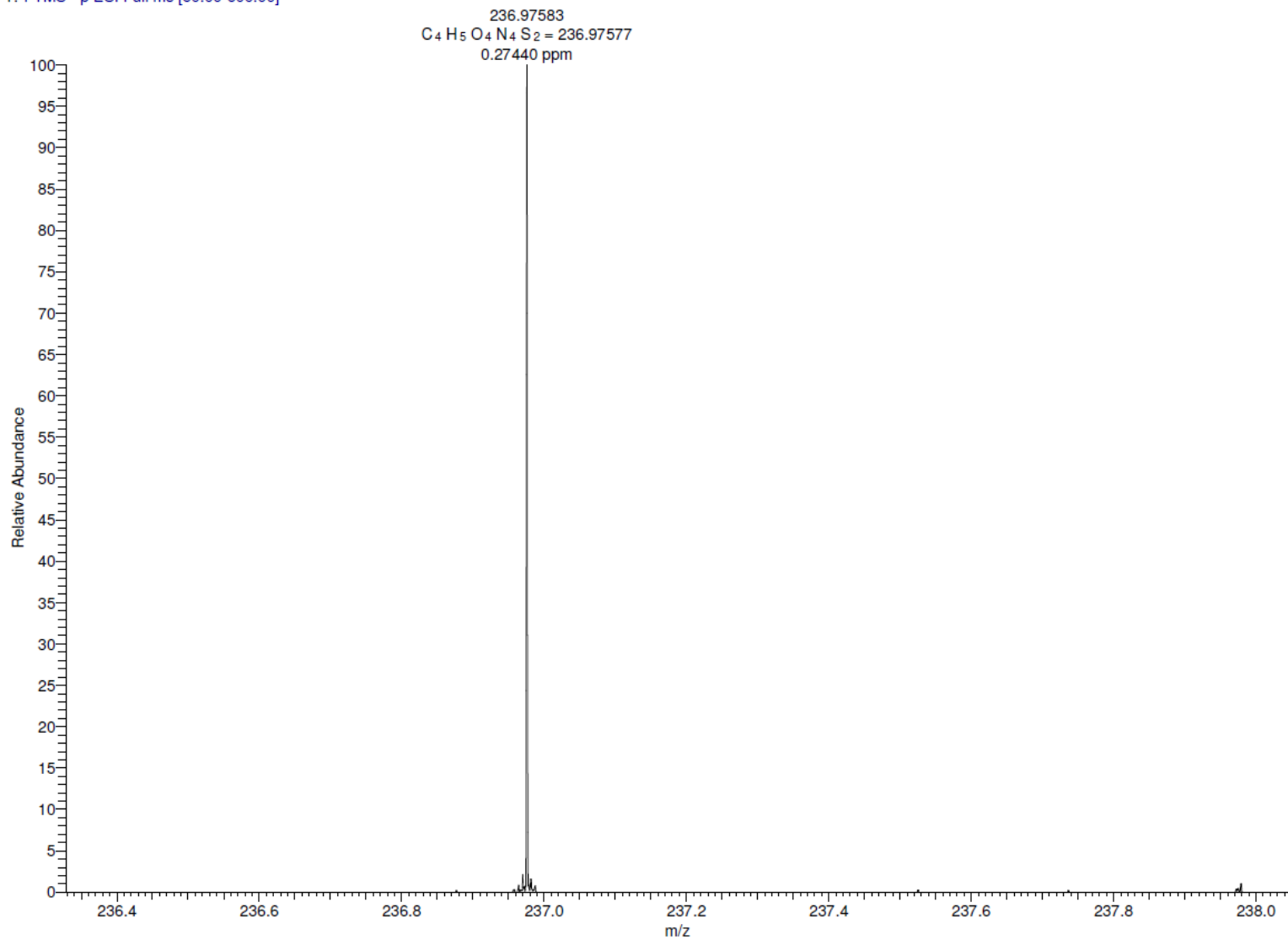


Fig. S36. ^1H and ^{13}C NMR spectra (DMSO- d_6) of sodium *S*-(4,6-dimethylpyrimidin-2-yl) sulfathioate (**21**).

060511servis_4-

5/6/2011 10:11:53 AM

Jansa, LC 100

060511servis 4- #66-68 RT: 1.83-1.88 AV: 3 NL: 3.40E5
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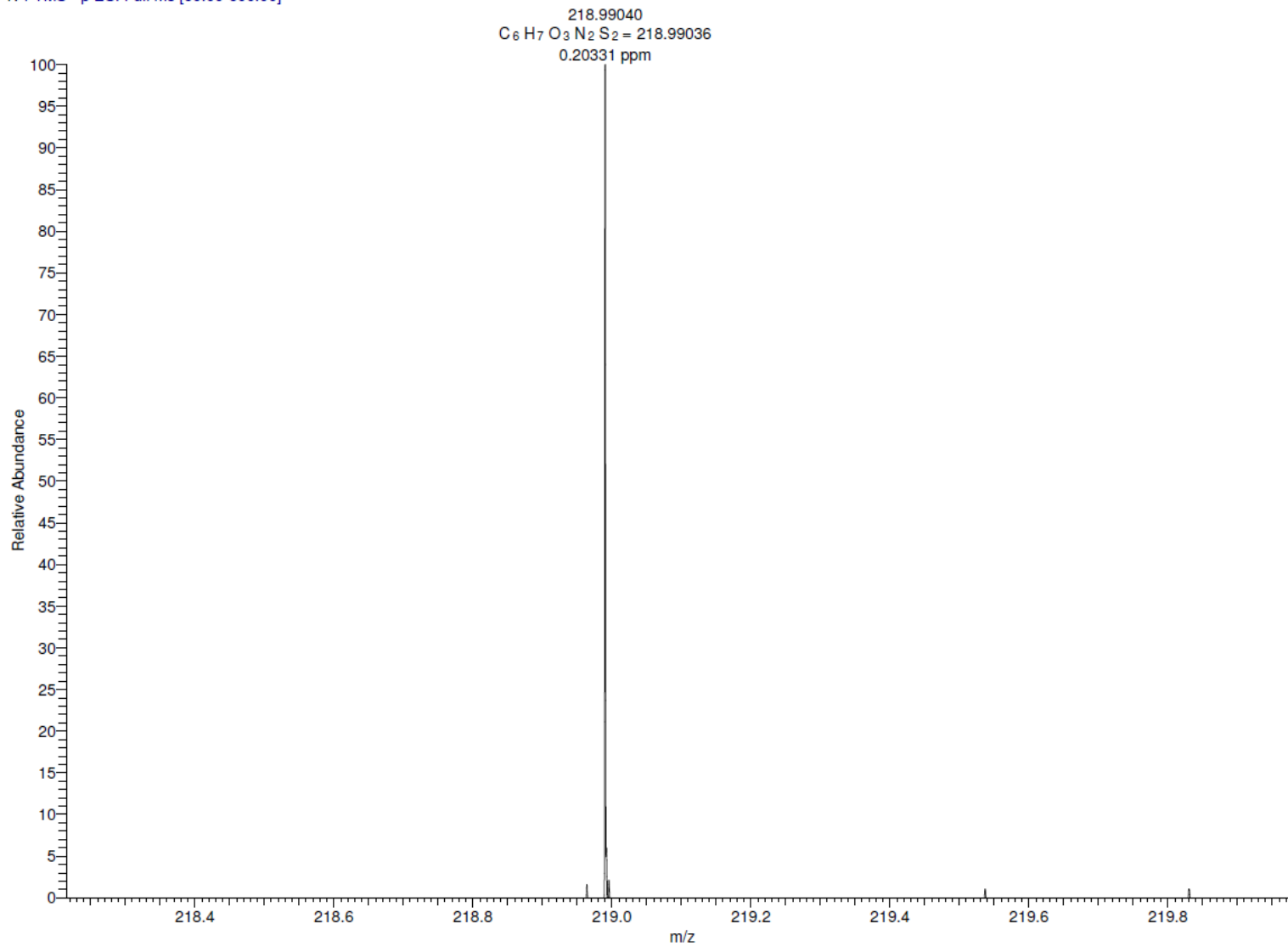


Fig. S37. UPLCs of conversion of **1c** to **2c**

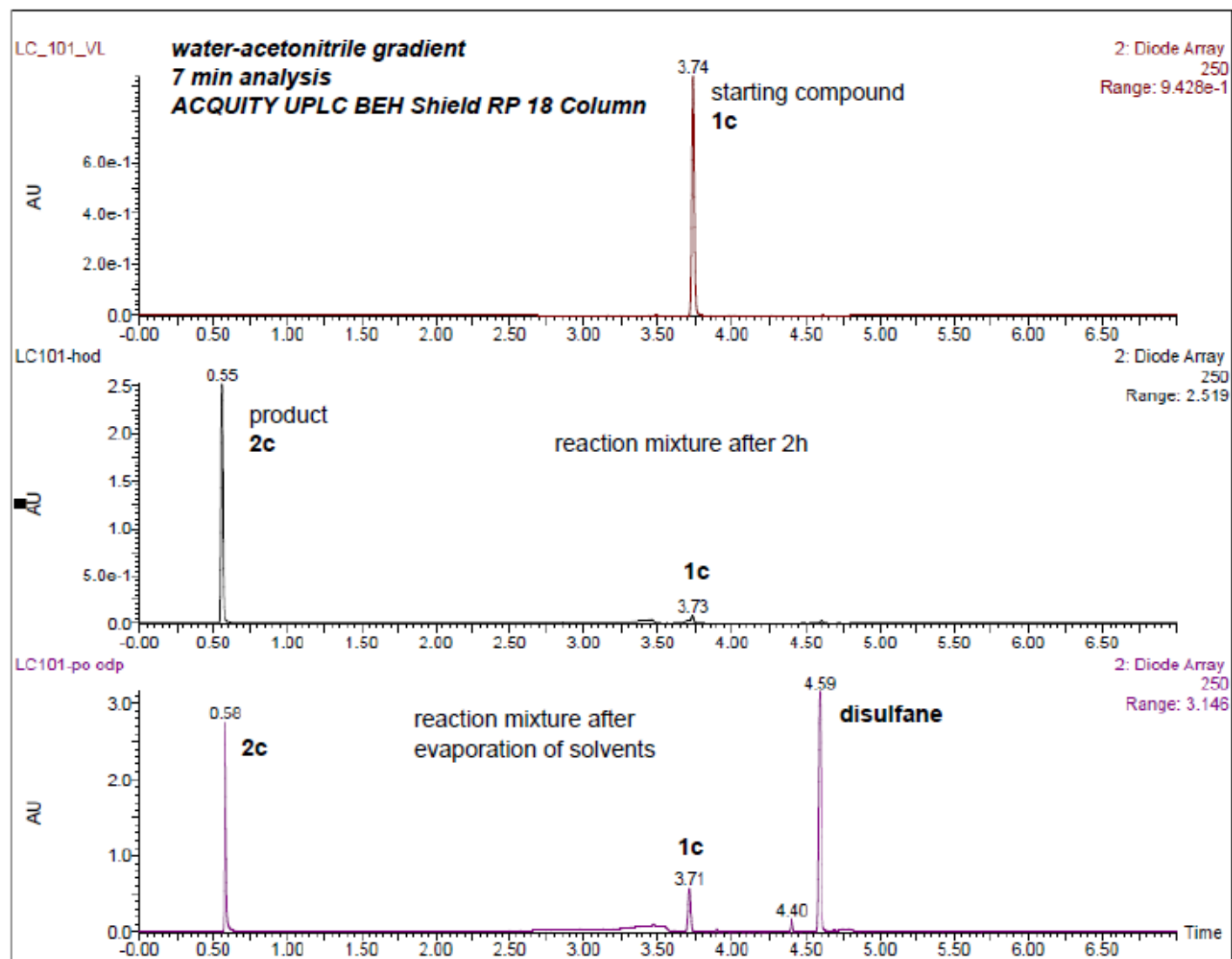


Fig. S38. UPLCs of conversion of **1h** to **2h**

