

Supplementary Materials

Dimethyl-2-((benzo[d]thiazol-2-ylamino)(benzofuran-2-yl)methyl) (5a)

Figure S1. The High Resolution Mass Spectra of 5a.

Monoisotopic Mass, Odd and Even Electron Ions

16 formula(e) evaluated with 1 results within limits (up to 51 closest results for each mass)

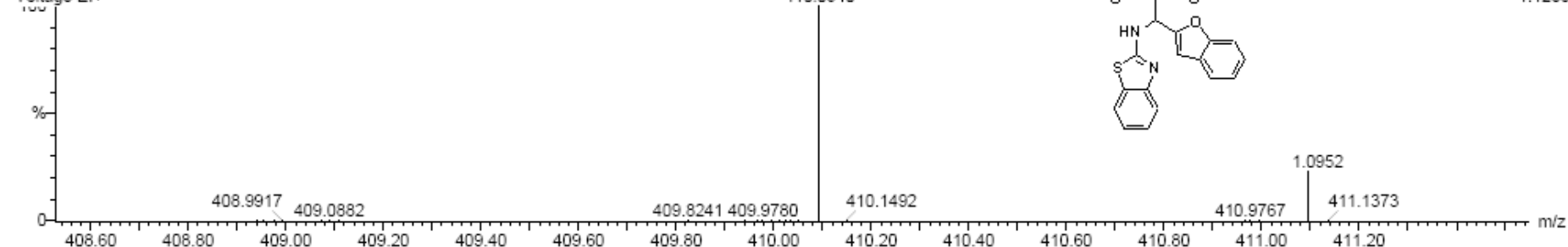
Elements Used:

C: 0-200 H: 0-400 N: 2-2 O: 4-6 S: 1-1

Ty/c23

10:48:09 08-Jun-2013

Voltage EI+



Minimum: -10.0

Maximum: 80.0 10.0 120.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
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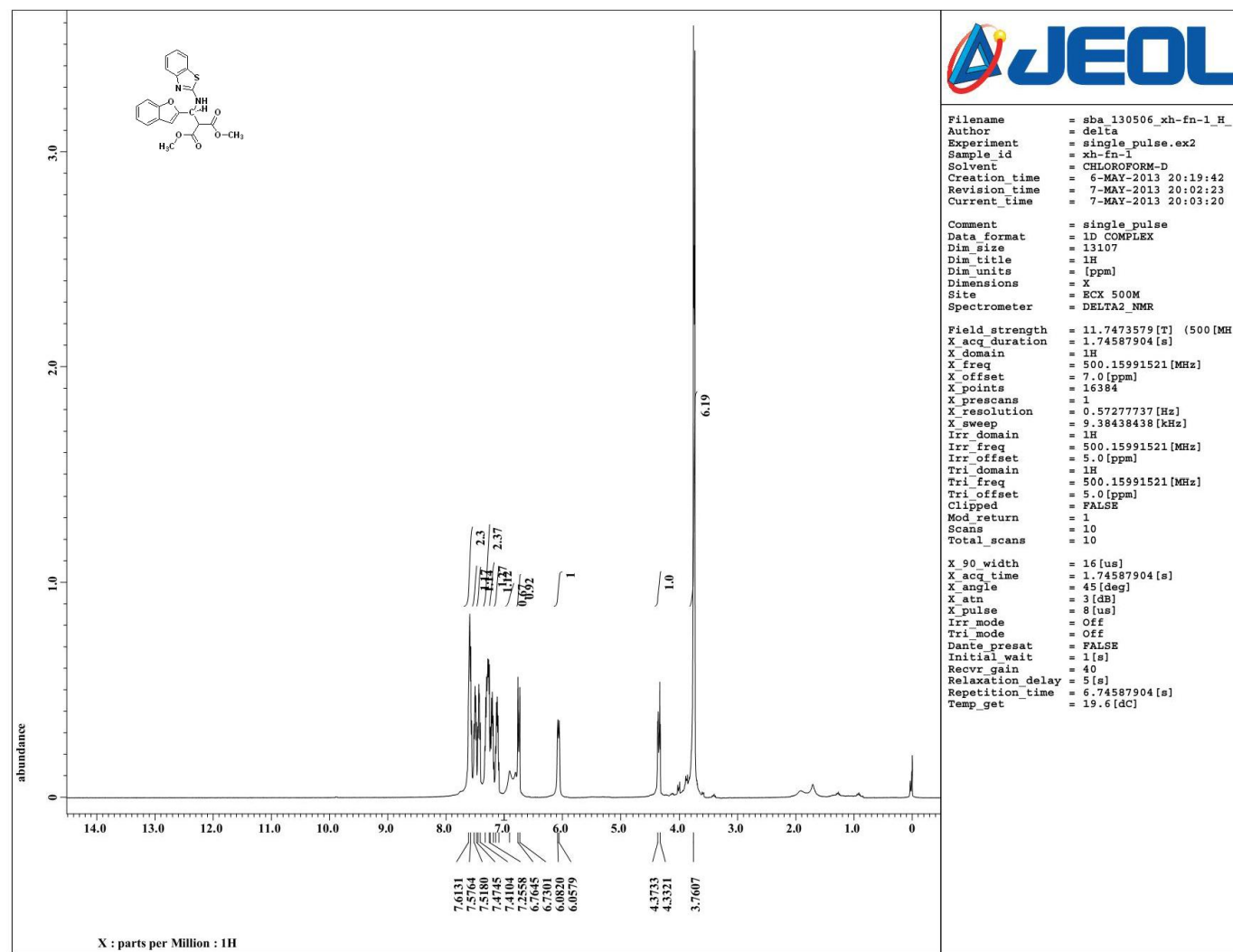
Figure S2. The ^1H -NMR Spectra of 5a.

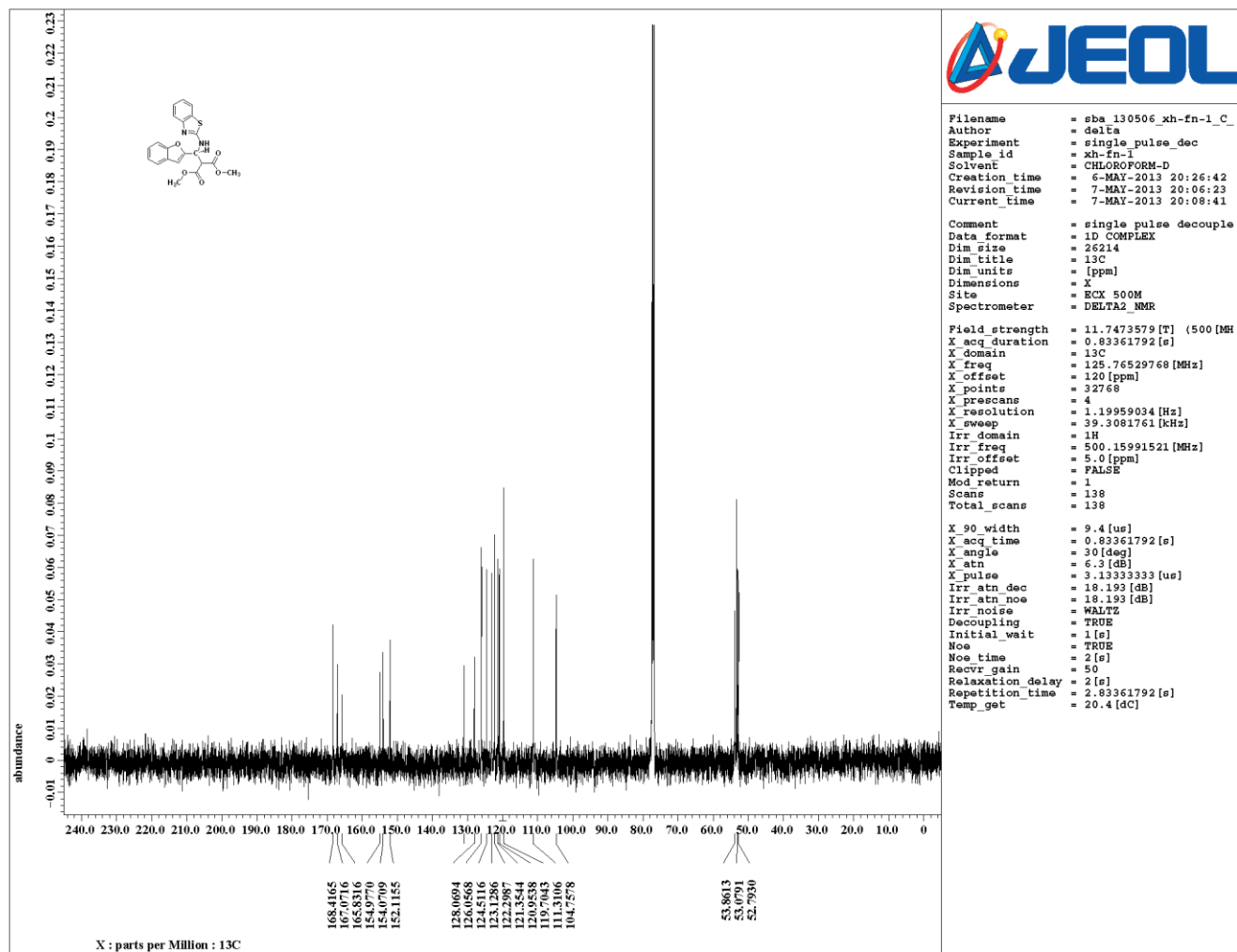
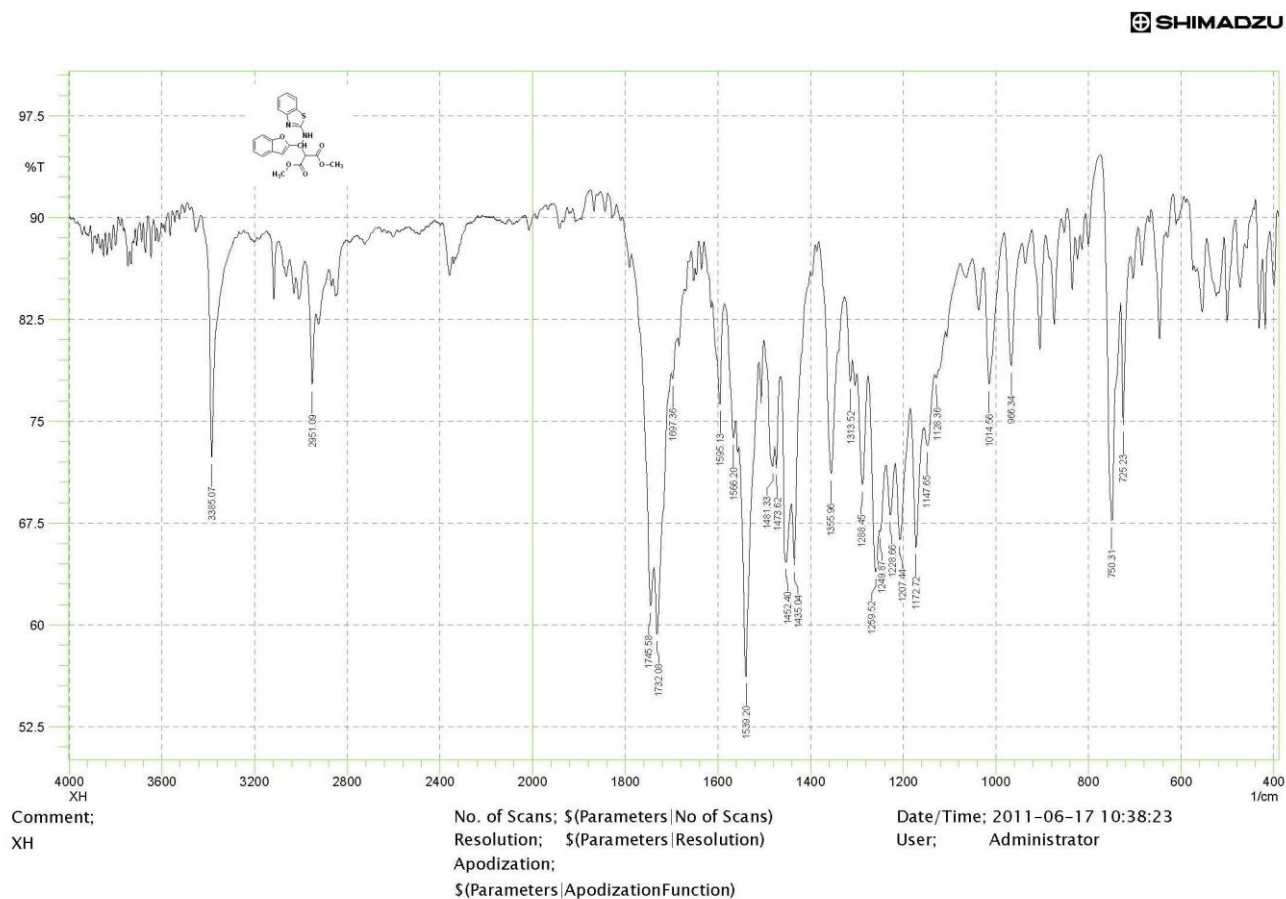
Figure S3. The ^{13}C -NMR Spectra of 5a.

Figure S4. The IR spectra of 5a.



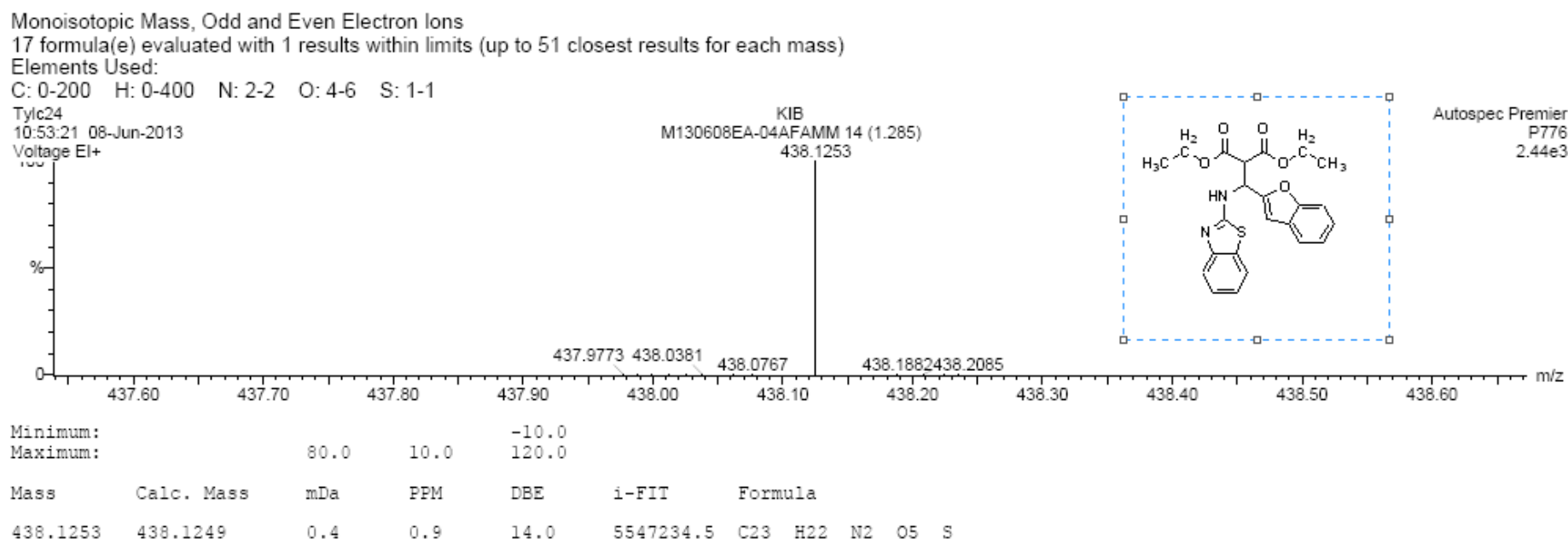
Diethyl 2-((benzo[d]thiazol-2-ylamino)(benzofuran-2-yl)methyl) malonate (**5b**)**Figure S5.** The High Resolution Mass Spectra of **5b**.

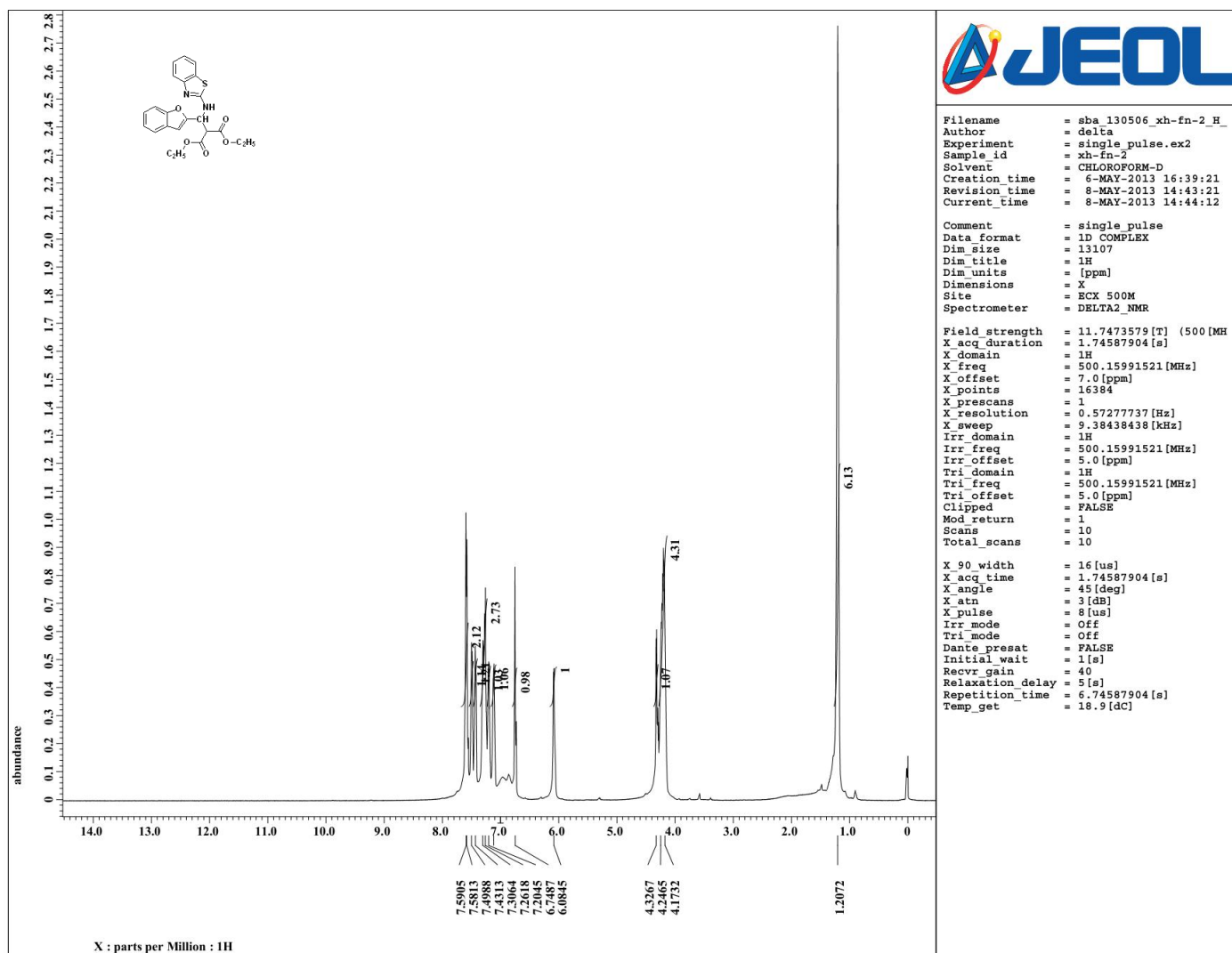
Figure S6. The ^1H -NMR Spectra of 5b.

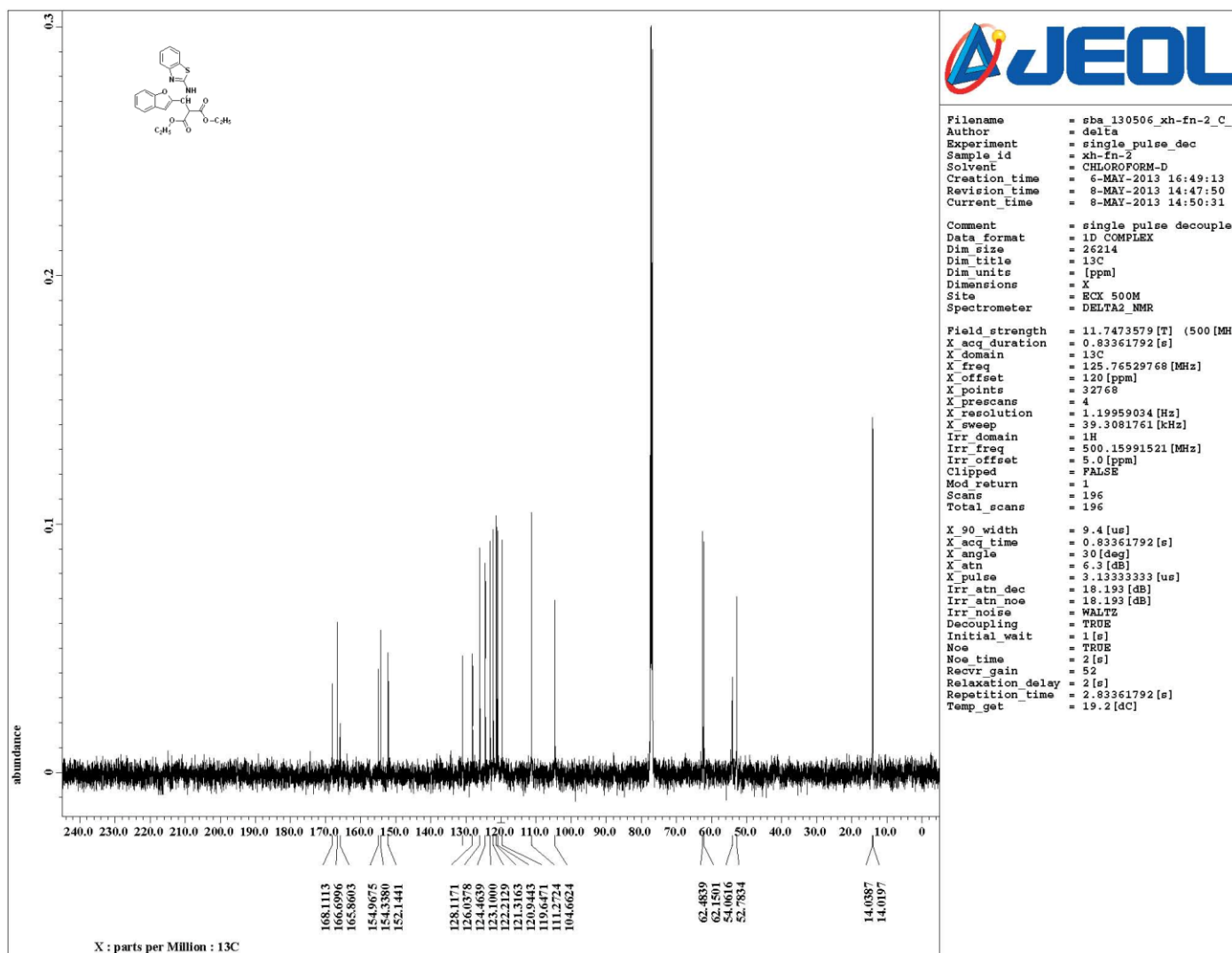
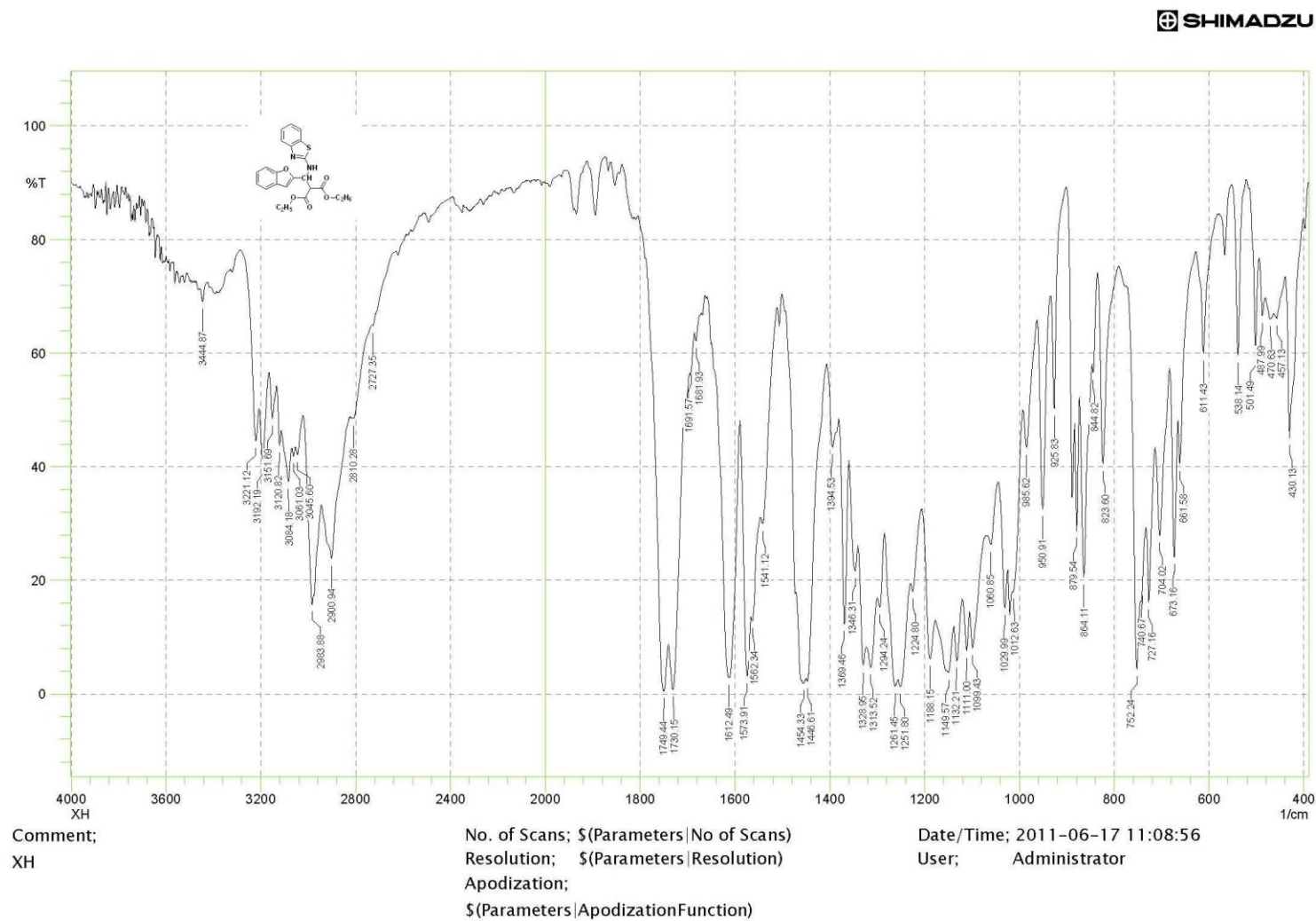
Figure S7. The ^{13}C -NMR Spectra of 5b.

Figure S8. The IR spectra of 5b.



Dipropyl 2-((benzo[d]thiazol-2-ylamino)(benzofuran-2-yl)methyl) malonate (5c)

Figure S9. The High Resolution Mass Spectra of 5c.

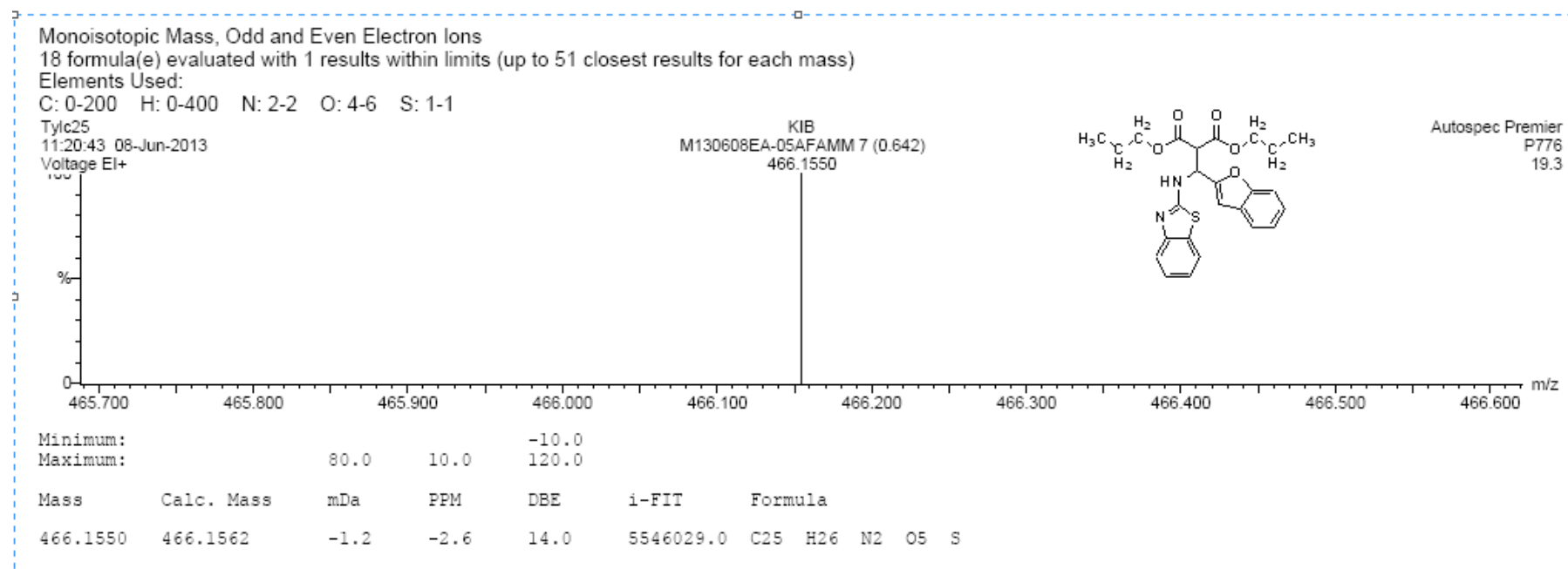


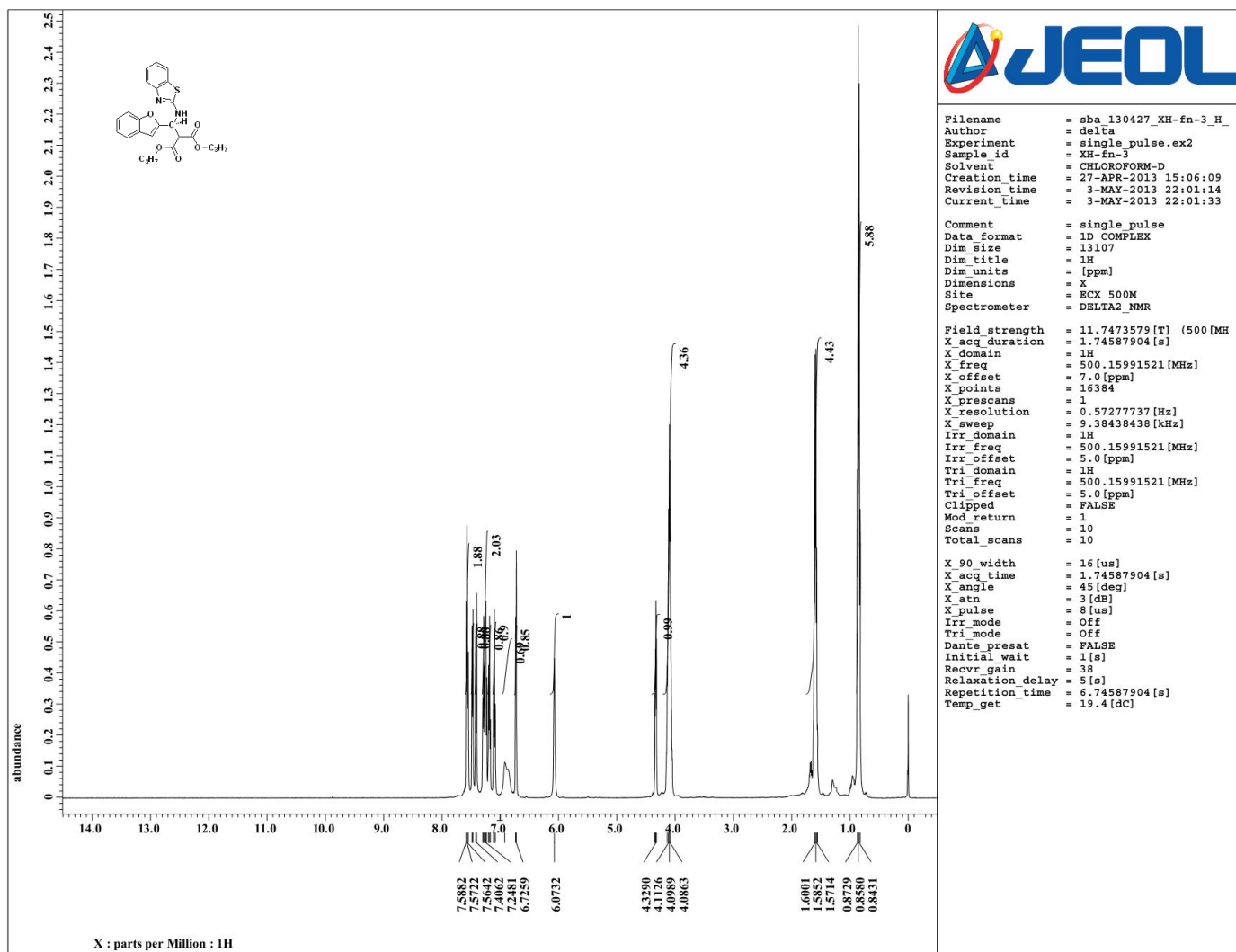
Figure S10. The ^1H -NMR Spectra of 5c.

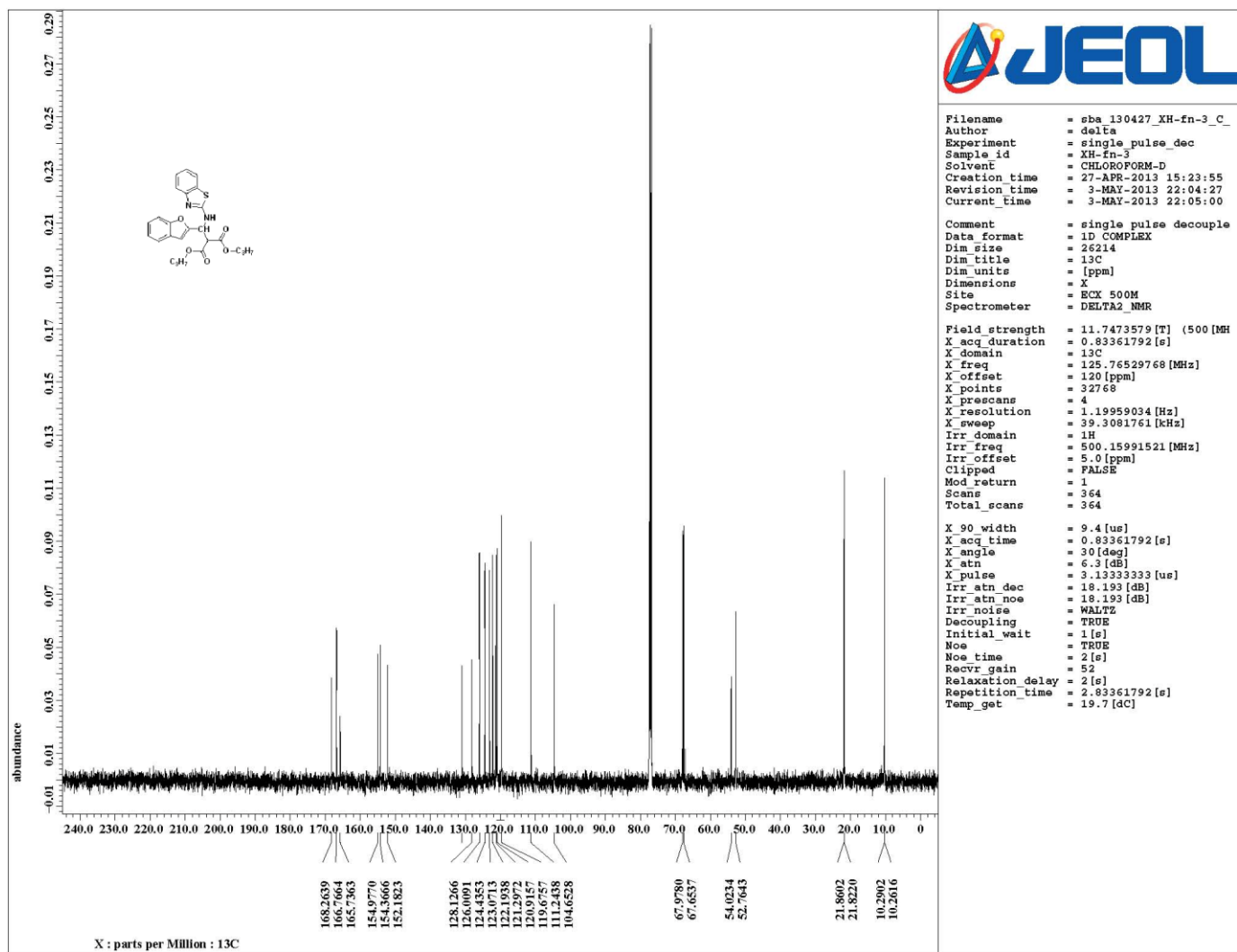
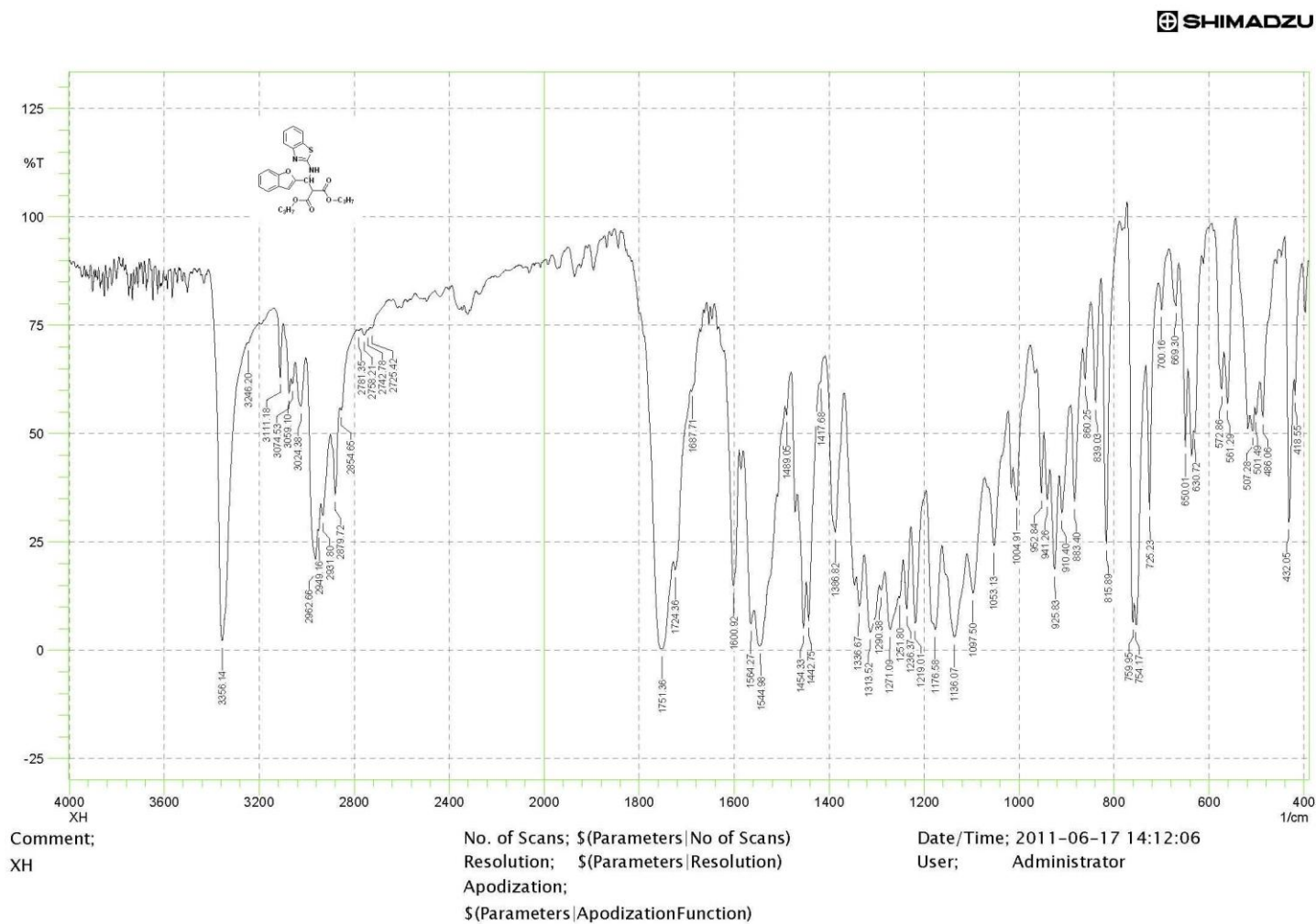
Figure S11. The ^{13}C -NMR Spectra of 5c.

Figure S12. The IR spectra of 5c.



Dibenzyl 2-((benzo[d]thiazol-2-ylamino)(benzofuran-2-yl)methyl) malonate (5d)

Figure S13. The High Resolution Mass Spectra of 5d.

Monoisotopic Mass, Odd and Even Electron Ions

22 formula(e) evaluated with 1 results within limits (up to 51 closest results for each mass)

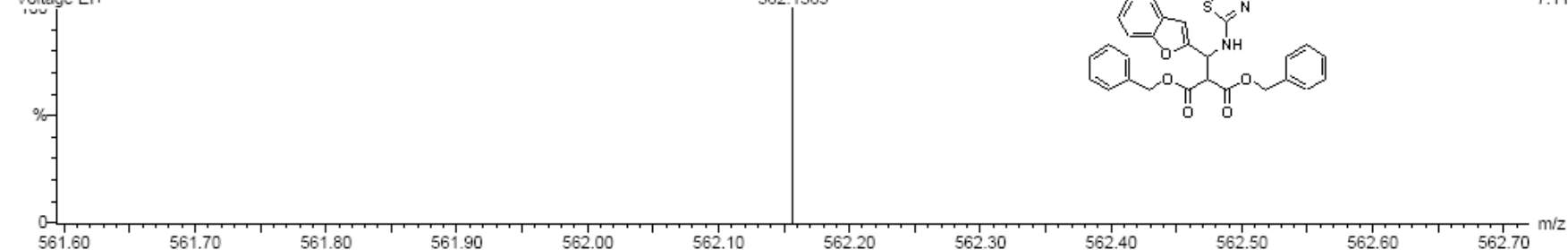
Elements Used:

C: 0-200 H: 0-400 N: 2-2 O: 4-6 S: 1-1

Tylc26

10:30:56 09-Jun-2013

Voltage EI+



Minimum: -10.0
Maximum: 10.0 10.0 120.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
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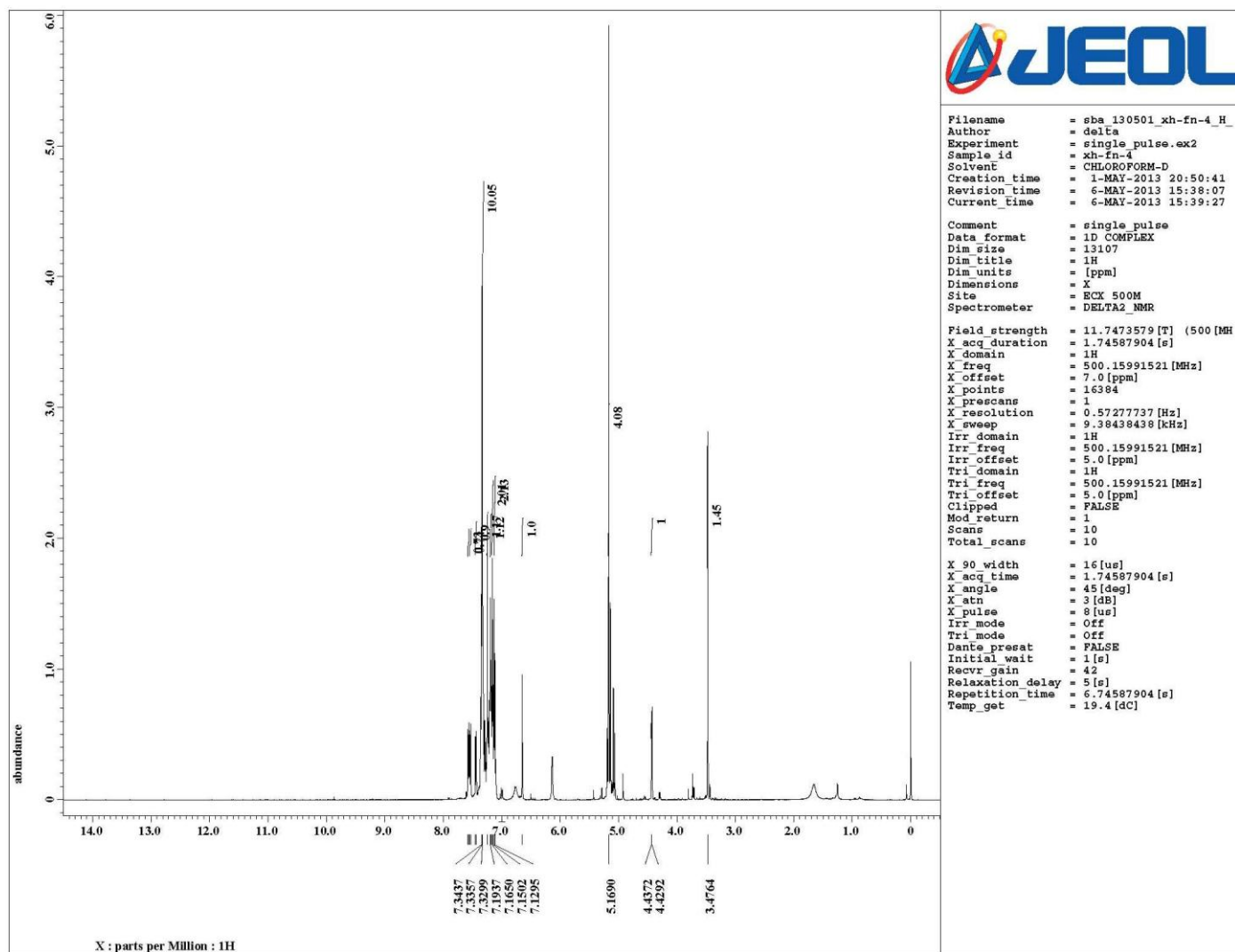
Figure S14. The ^1H -NMR Spectra of 5d.

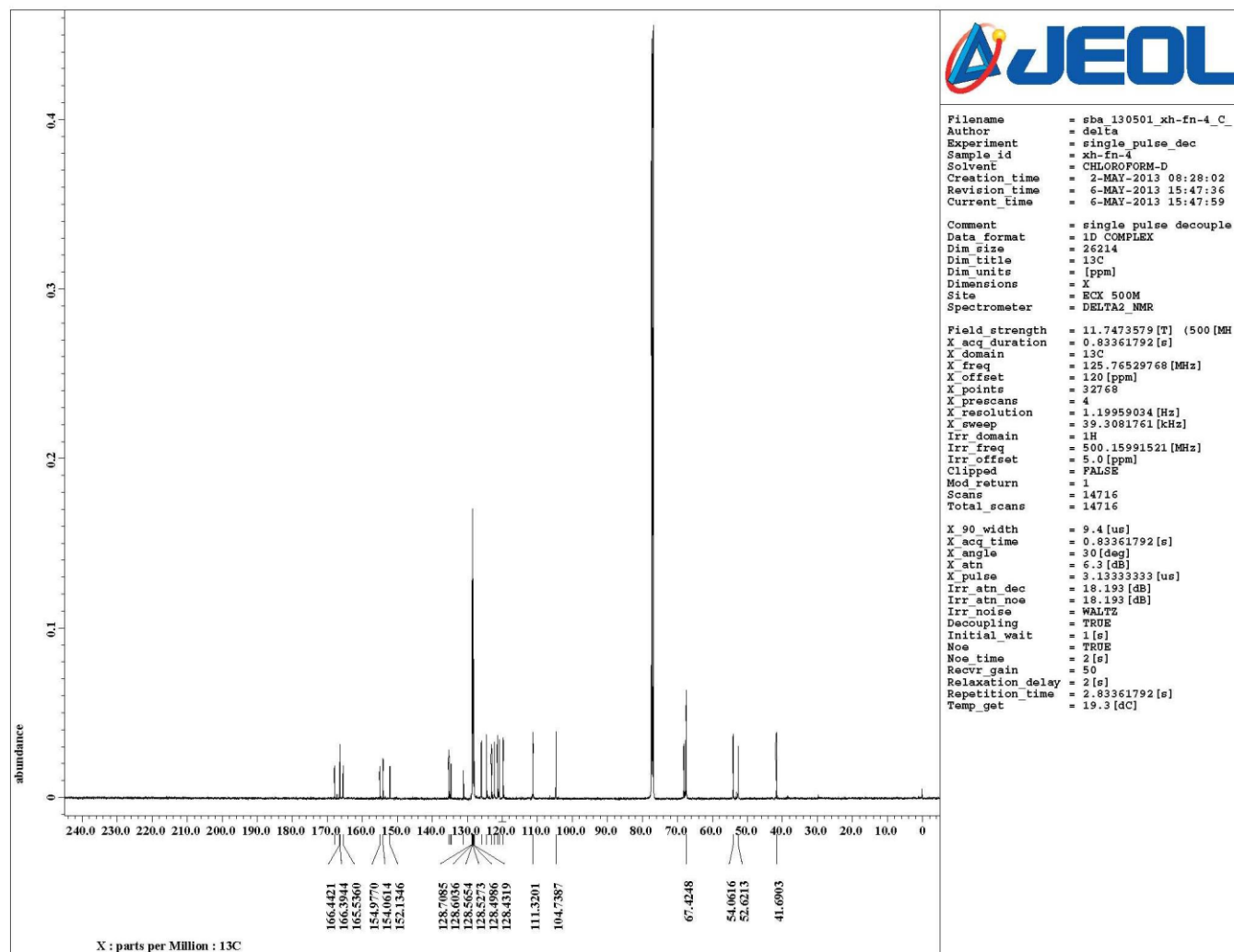
Figure S15. The ^{13}C -NMR Spectra of 5d.

Figure S16. The IR spectra of 5d.

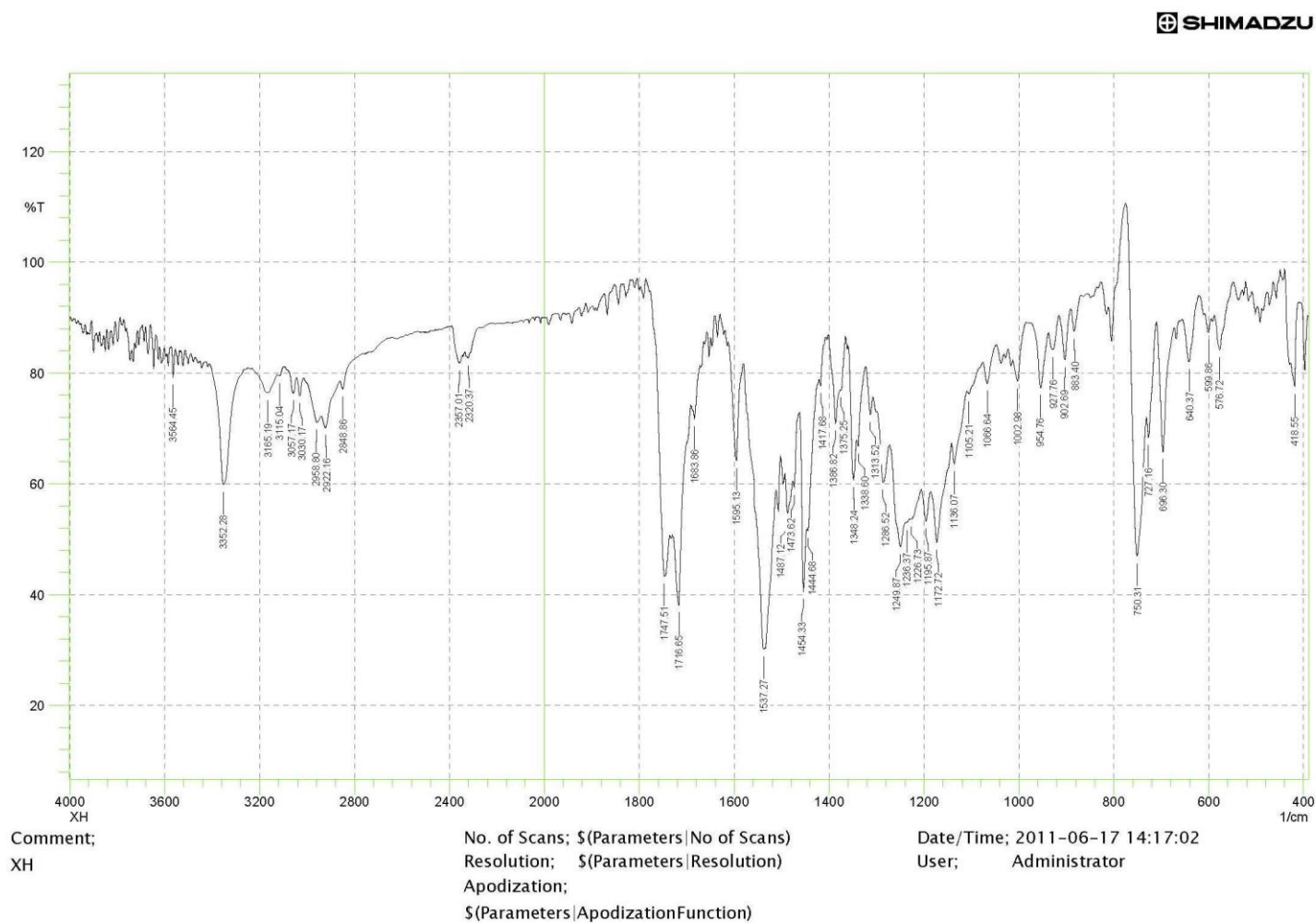


Figure S17. The High Resolution Mass Spectra of **5e**.

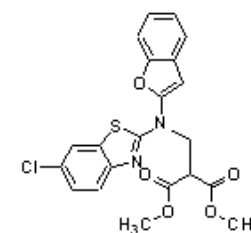
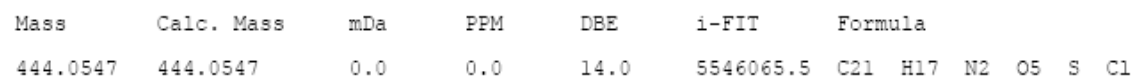


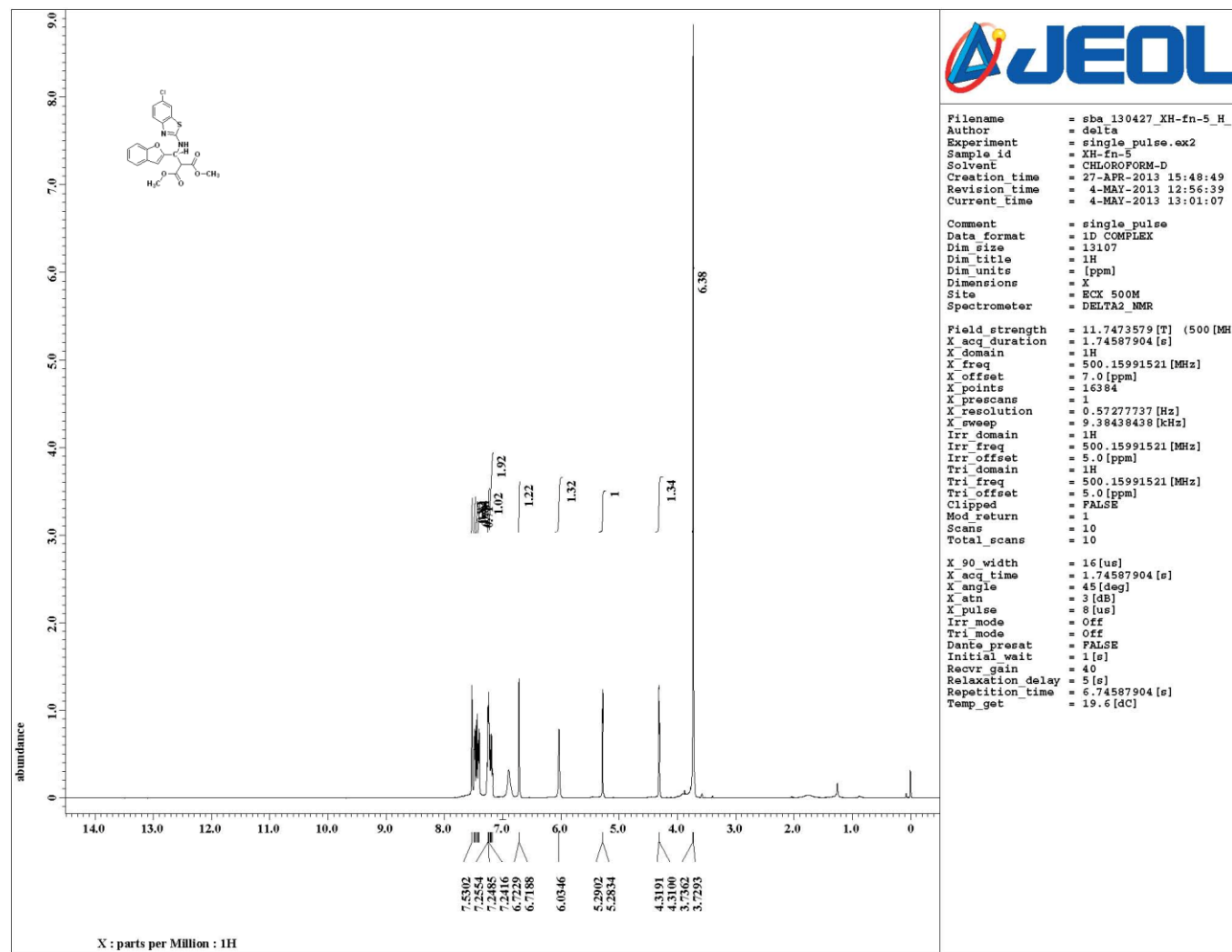
Figure S18. The ^1H -NMR Spectra of 5e.

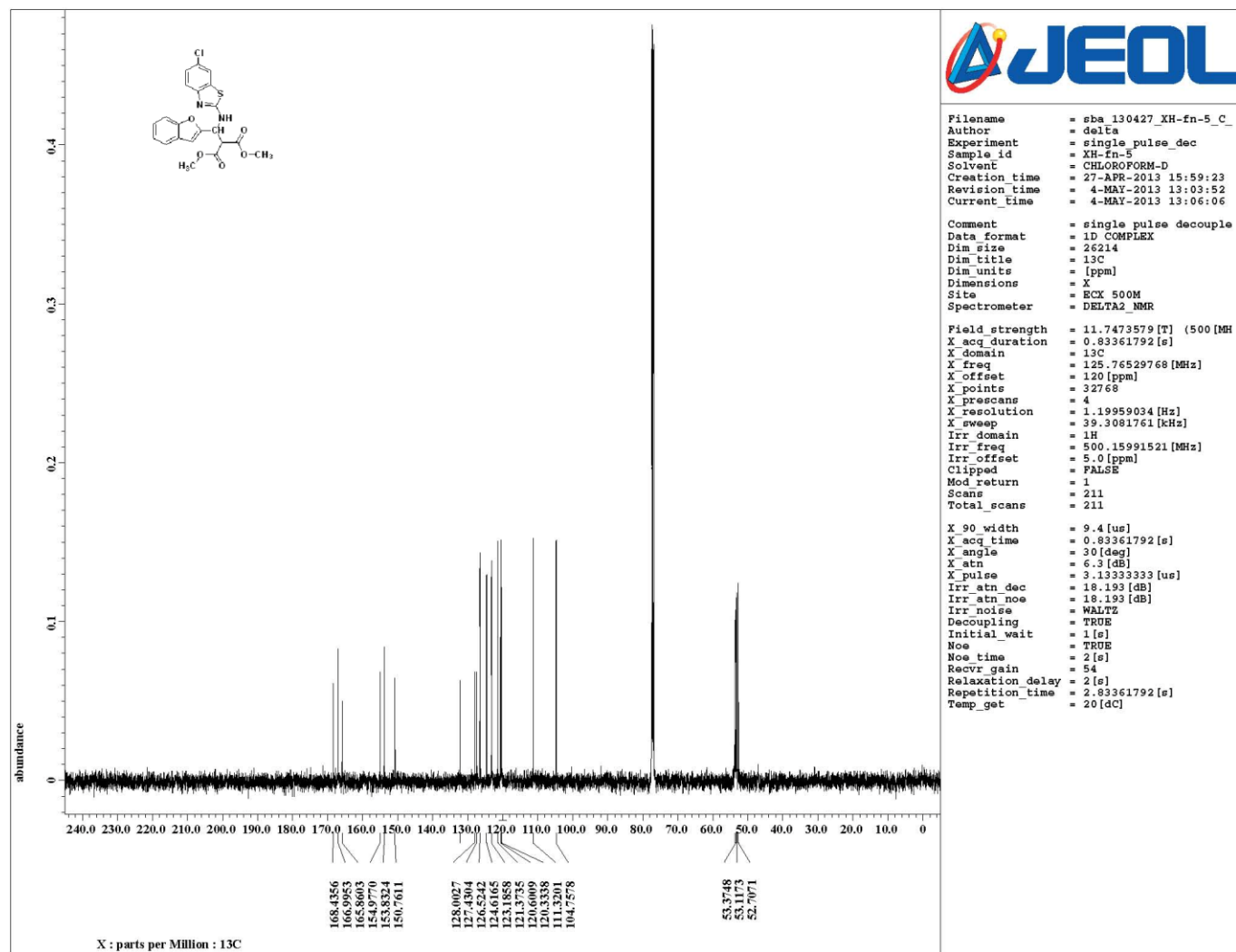
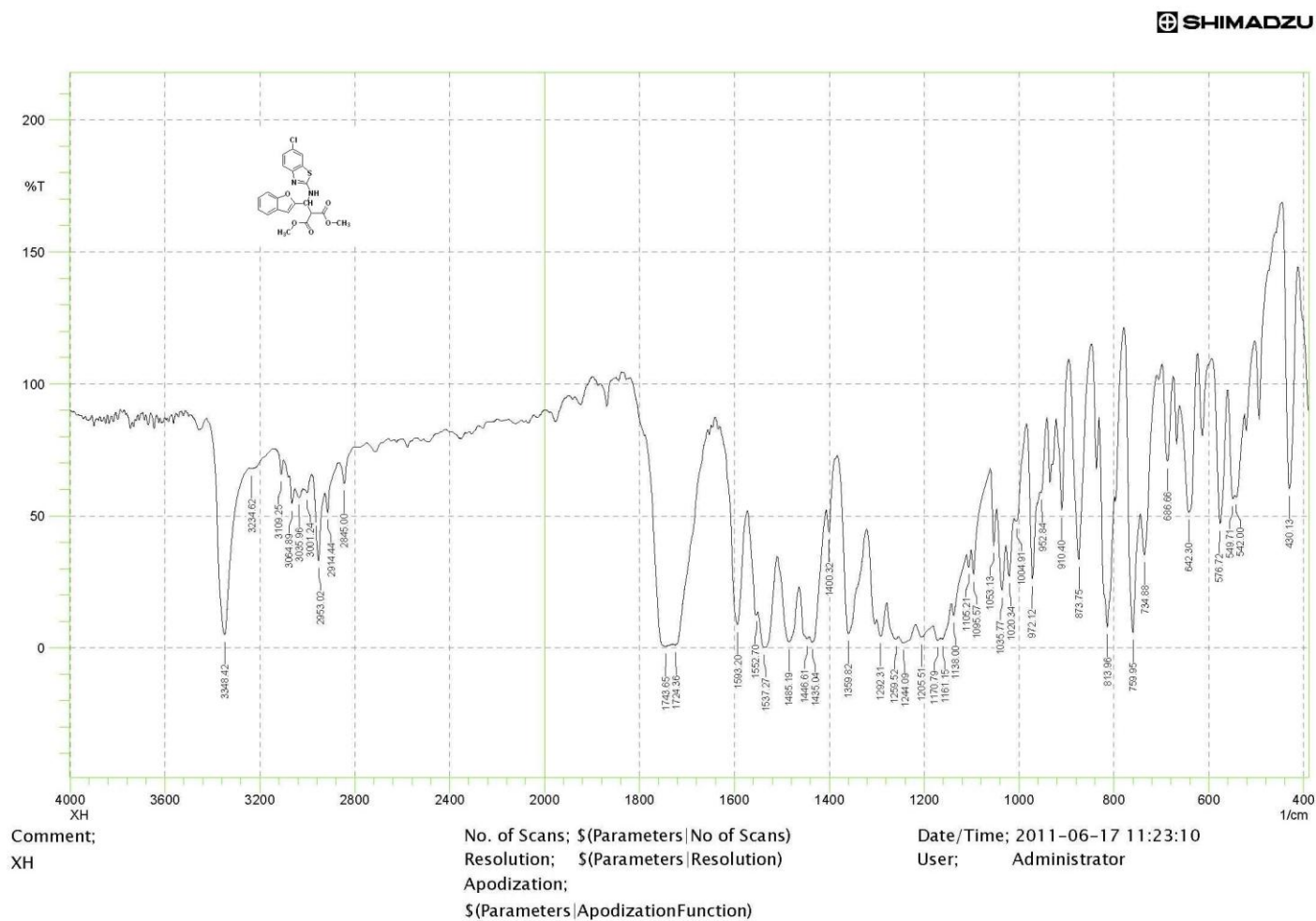
Figure S19. The ^{13}C -NMR Spectra of 5e.

Figure S20. The IR spectra of 5e.



Diethyl 2-(benzofuran-2-yl)((6-chlorobenzo[d]thiazol-2-yl)amino)methyl)malonate (5f)

Figure S21. The High Resolution Mass Spectra of 5f.

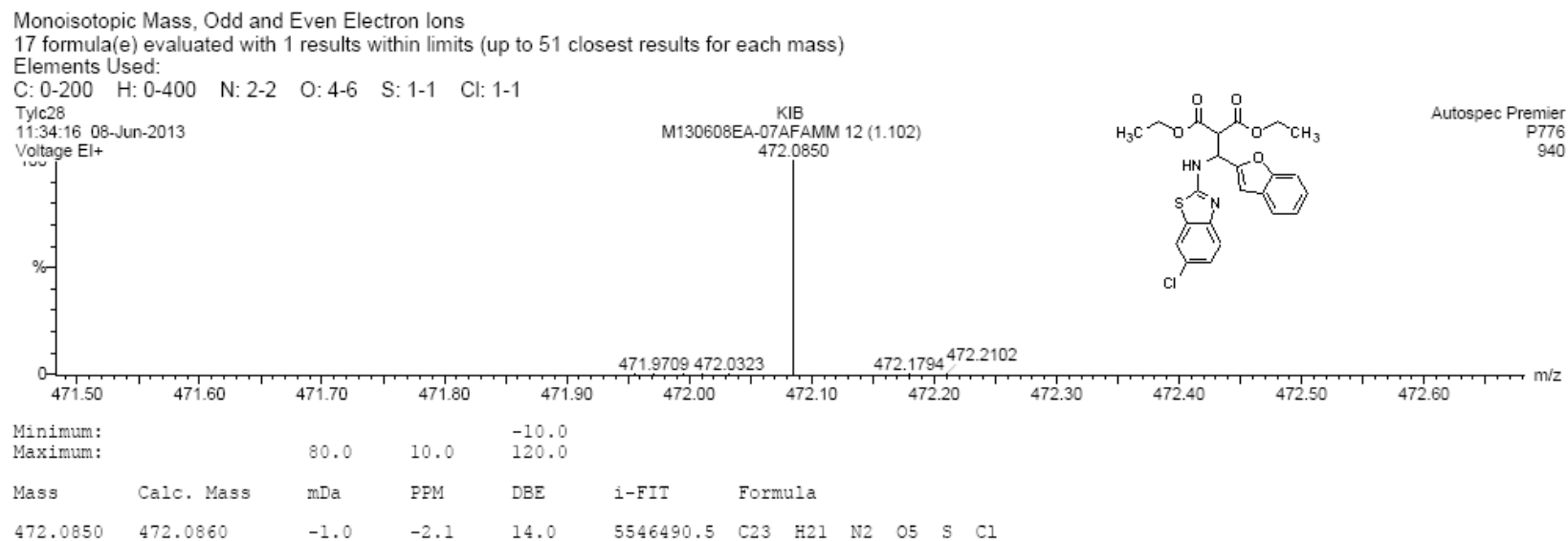


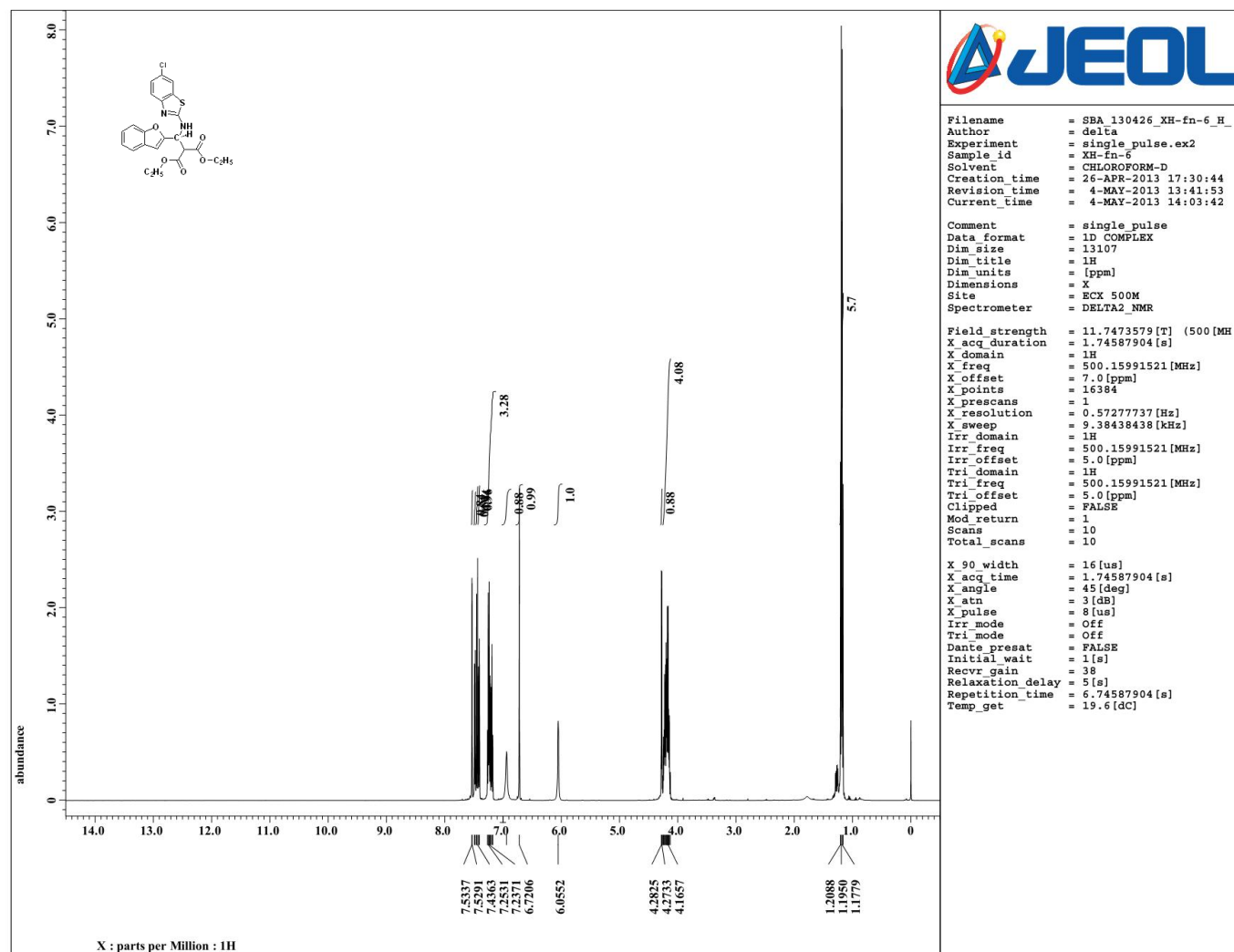
Figure S22. The ^1H -NMR Spectra of 5f.

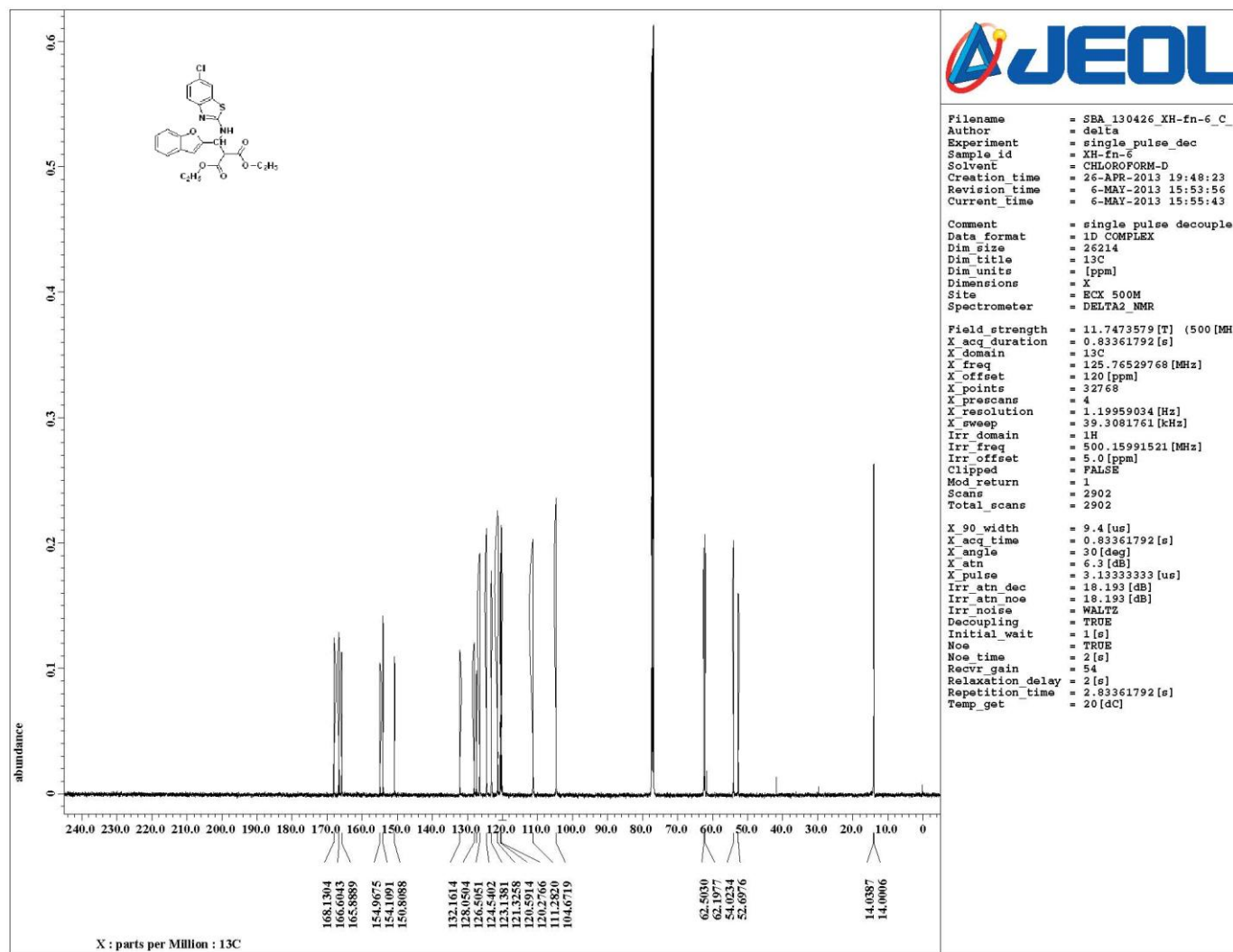
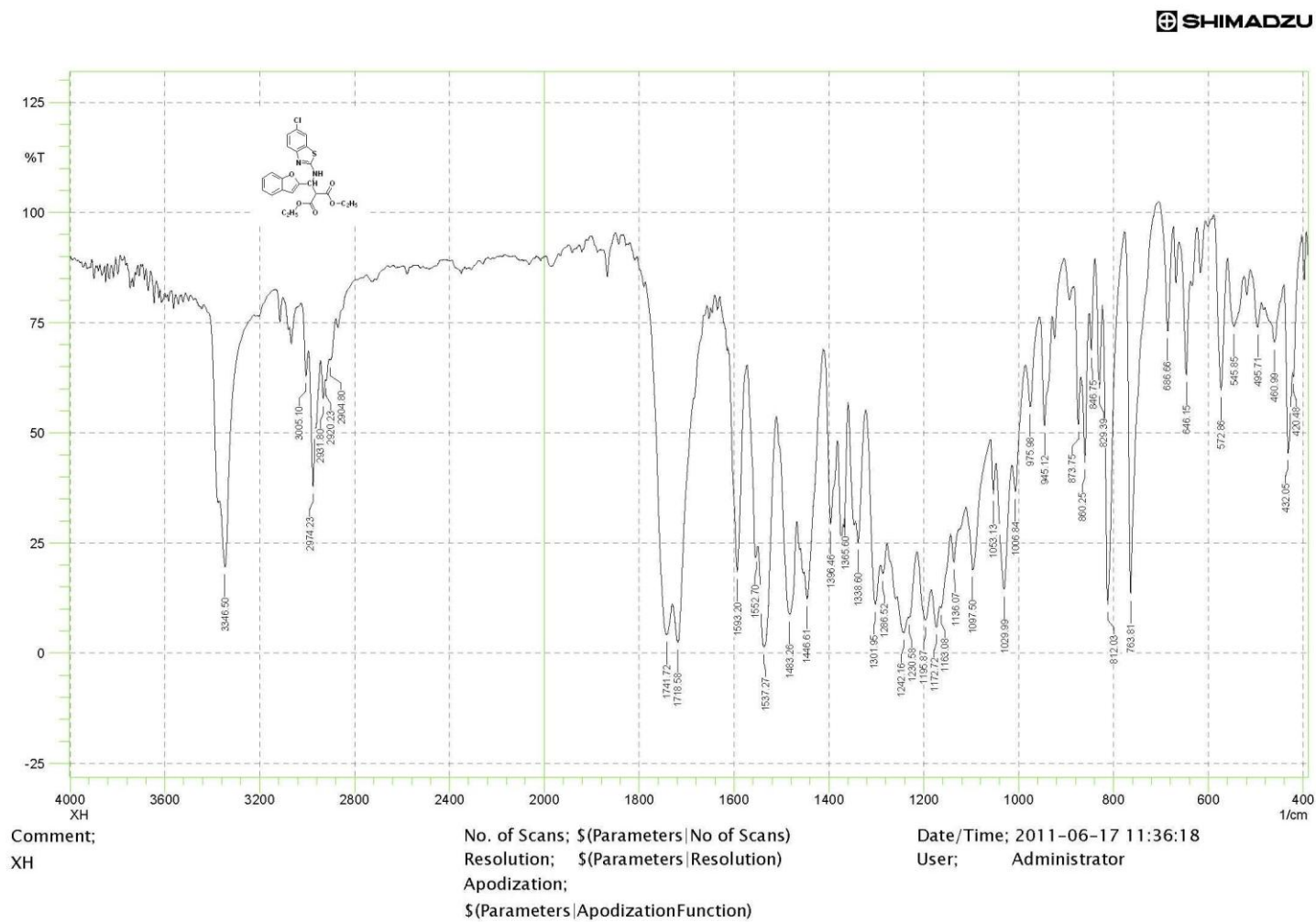
Figure S23. The ^{13}C -NMR Spectra of 5f.

Figure S24. The IR spectra of 5f.



Dipropyl-2-(benzofuran-2-yl)((6-chlorobenzo[d]thiazol-2-yl)amino) methyl)malonate (5g)

Figure S25. The High Resolution Mass Spectra of 5g.

Monoisotopic Mass, Odd and Even Electron Ions

18 formula(e) evaluated with 1 results within limits (up to 51 closest results for each mass)

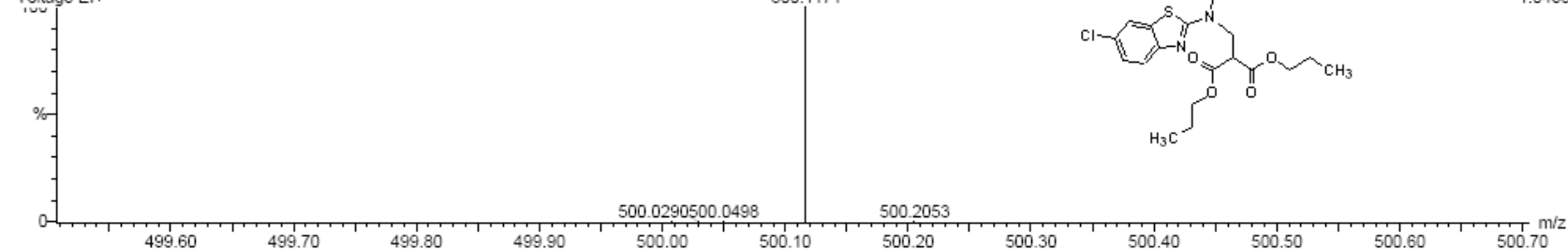
Elements Used:

C: 0-200 H: 0-400 N: 2-2 O: 4-6 S: 1-1 Cl: 1-1

Tyle29

11:51:27 08-Jun-2013

Voltage EI+

Autospec Premier
P776
1.04e3

Minimum: -10.0
Maximum: 80.0 10.0 120.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
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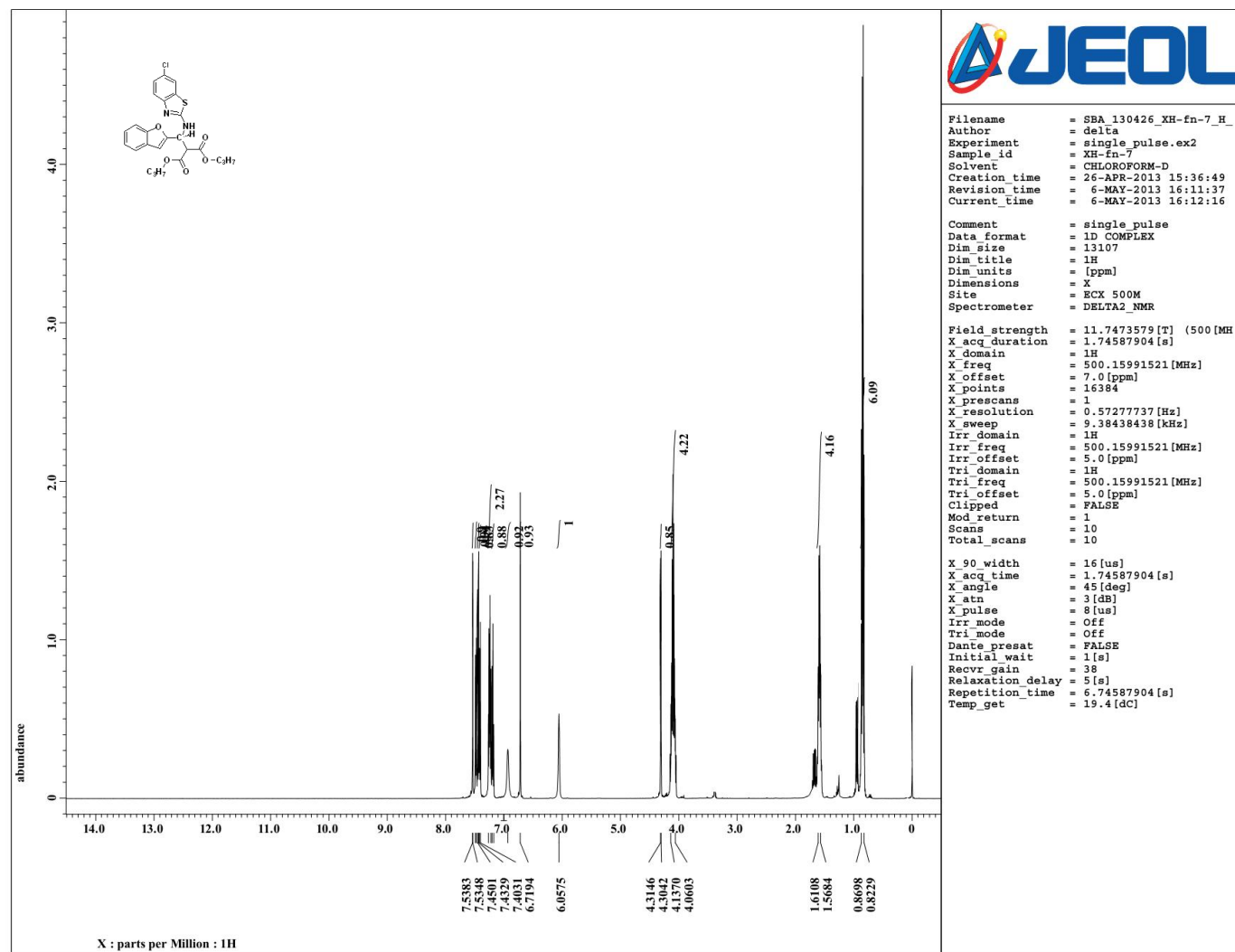
Figure S26. The ^1H -NMR Spectra of 5g.

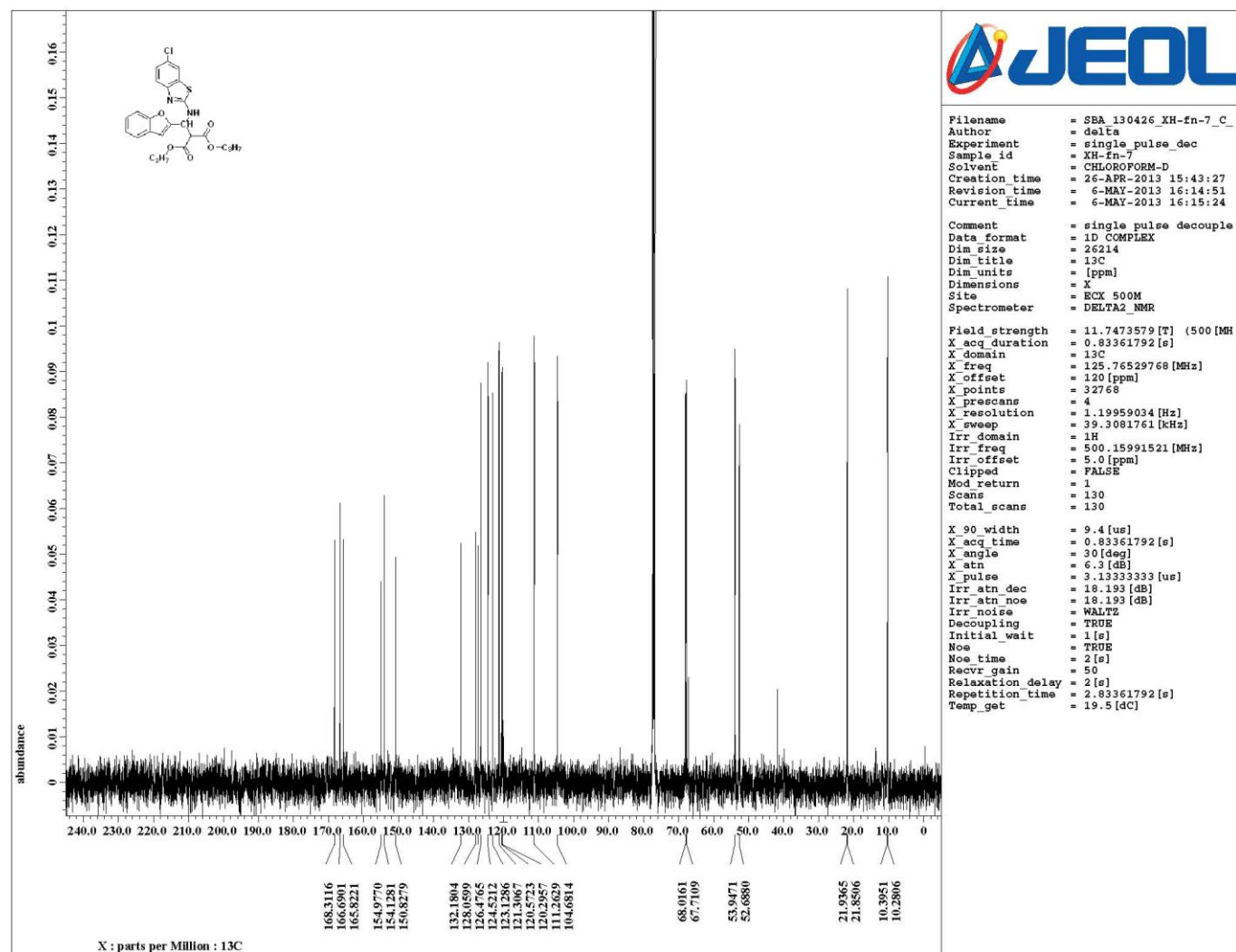
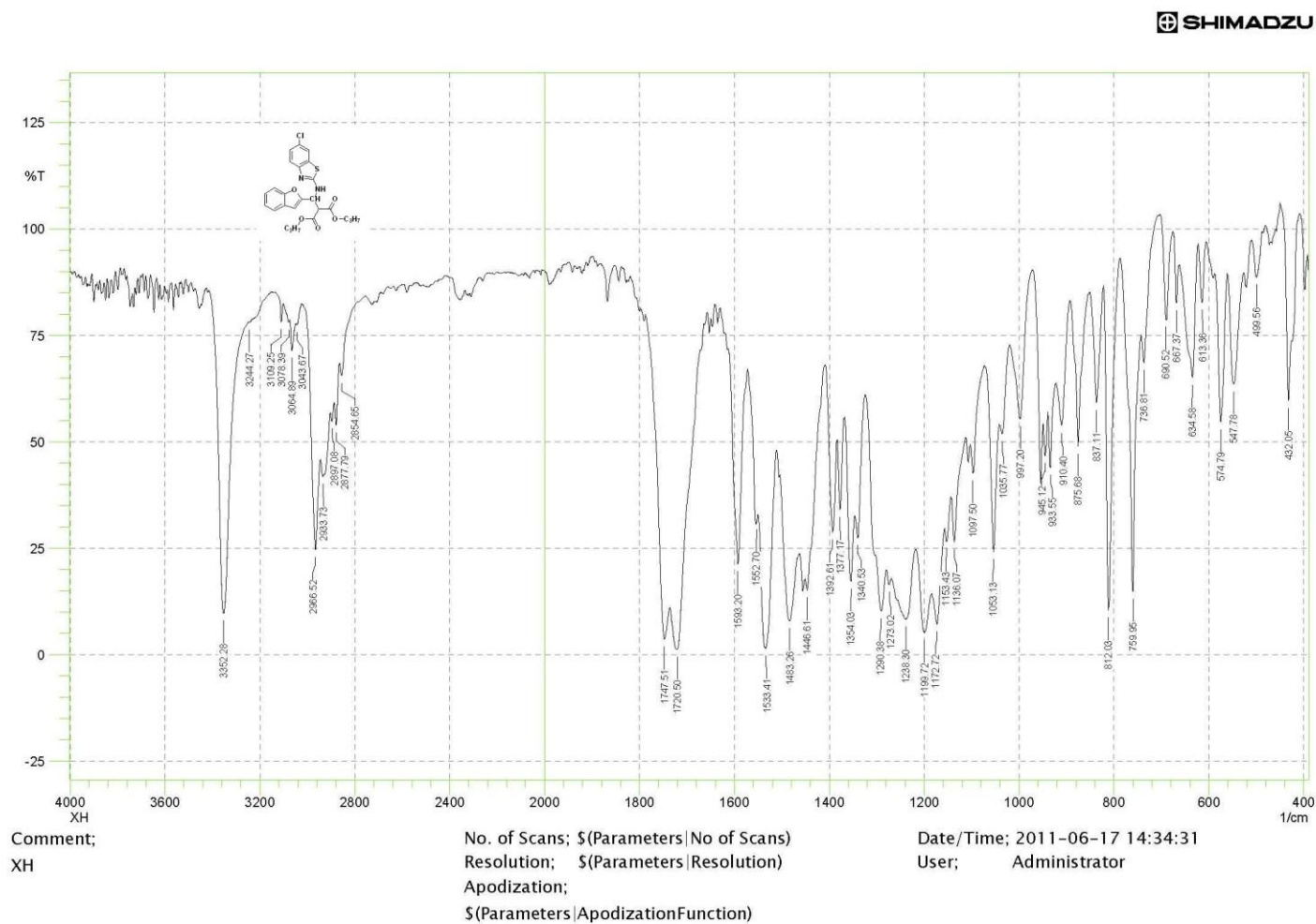
Figure S27. The ^{13}C -NMR Spectra of 5g.

Figure S28. The IR spectra of 5g.



Dibenzyl2-(benzofuran-2-yl((6-chlorobenzo[d]thiazol-2-yl)amino)methyl)malonate (5h)

Figure S29. The High Resolution Mass Spectra of 5h.

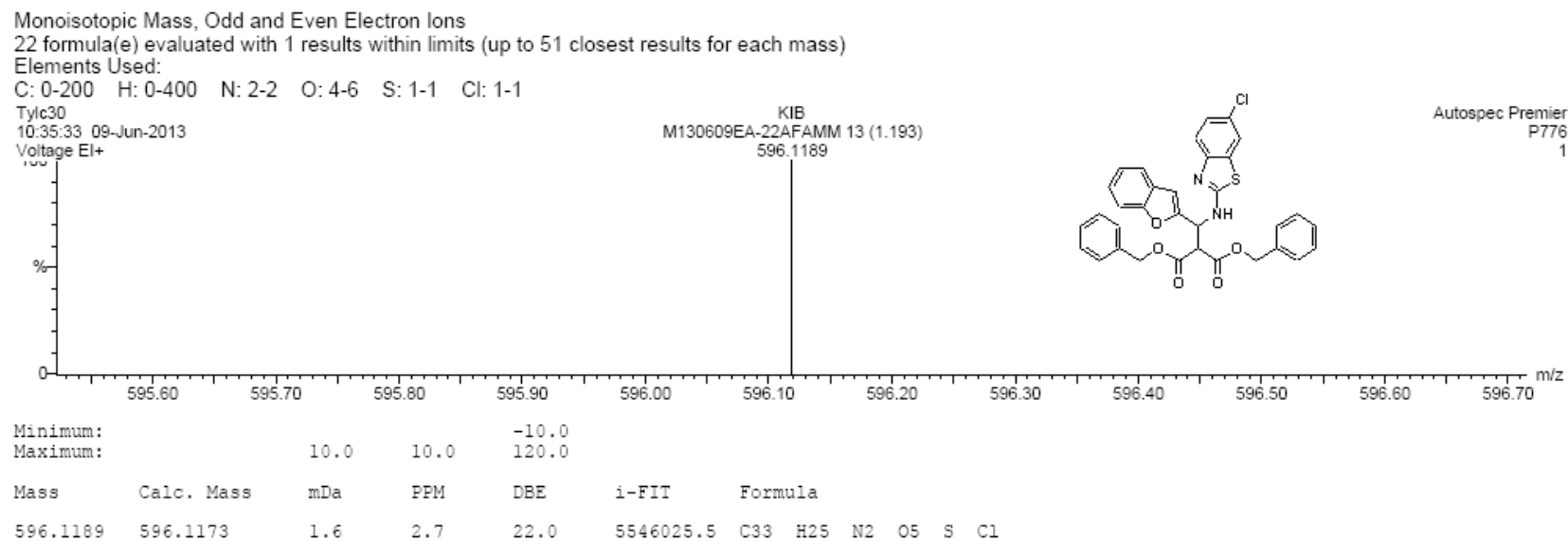


Figure S30. The ^1H -NMR Spectra of **5h**.

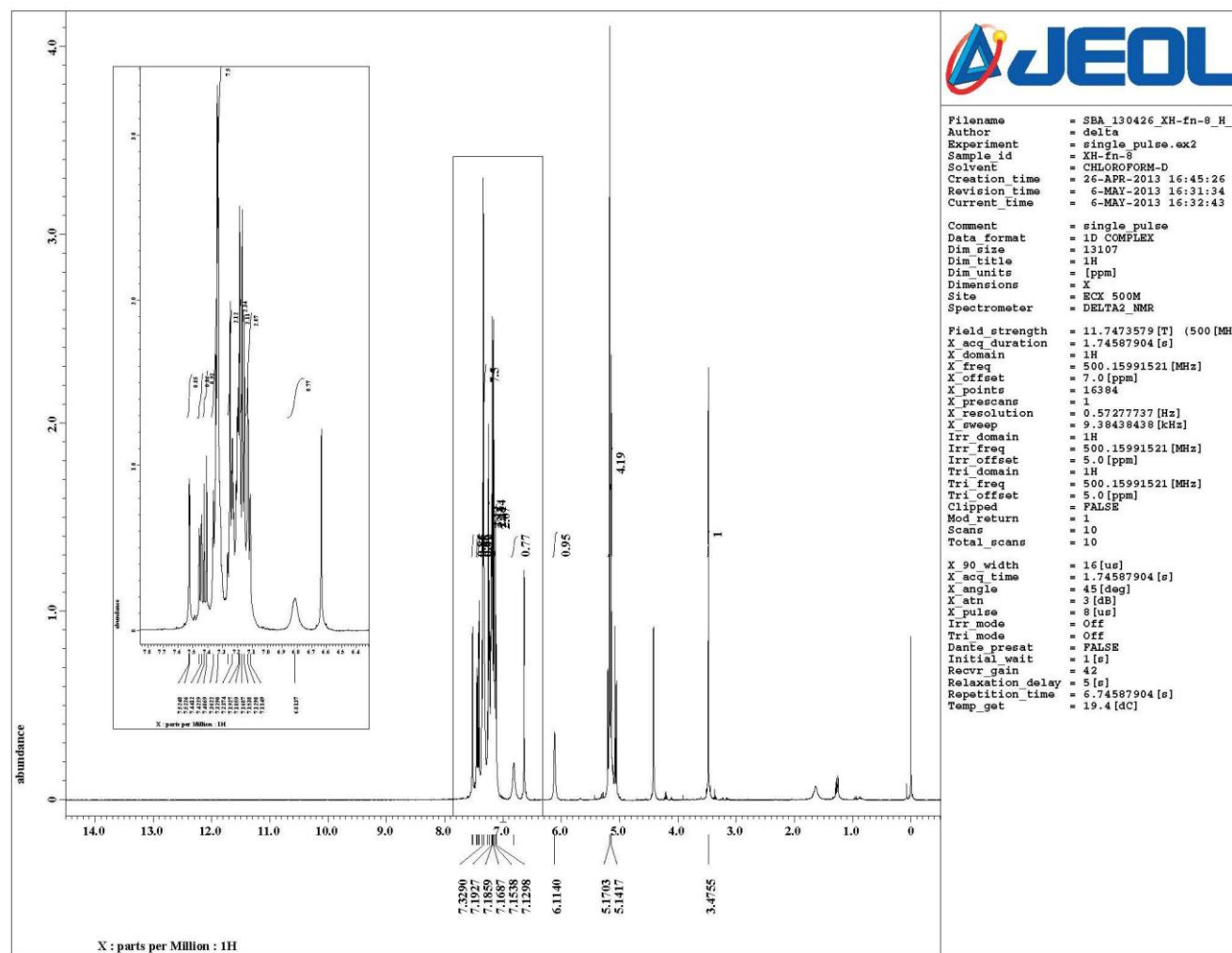


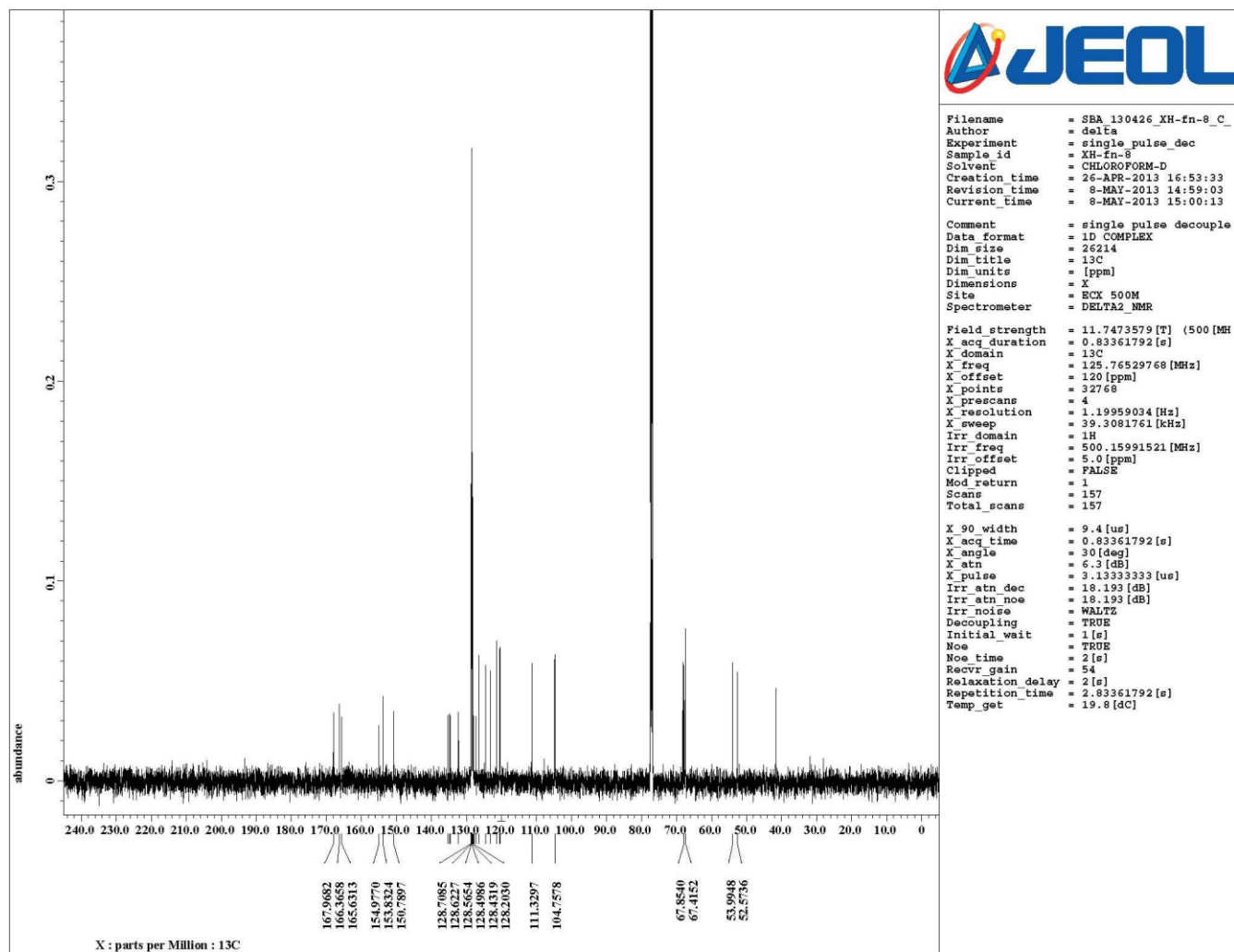
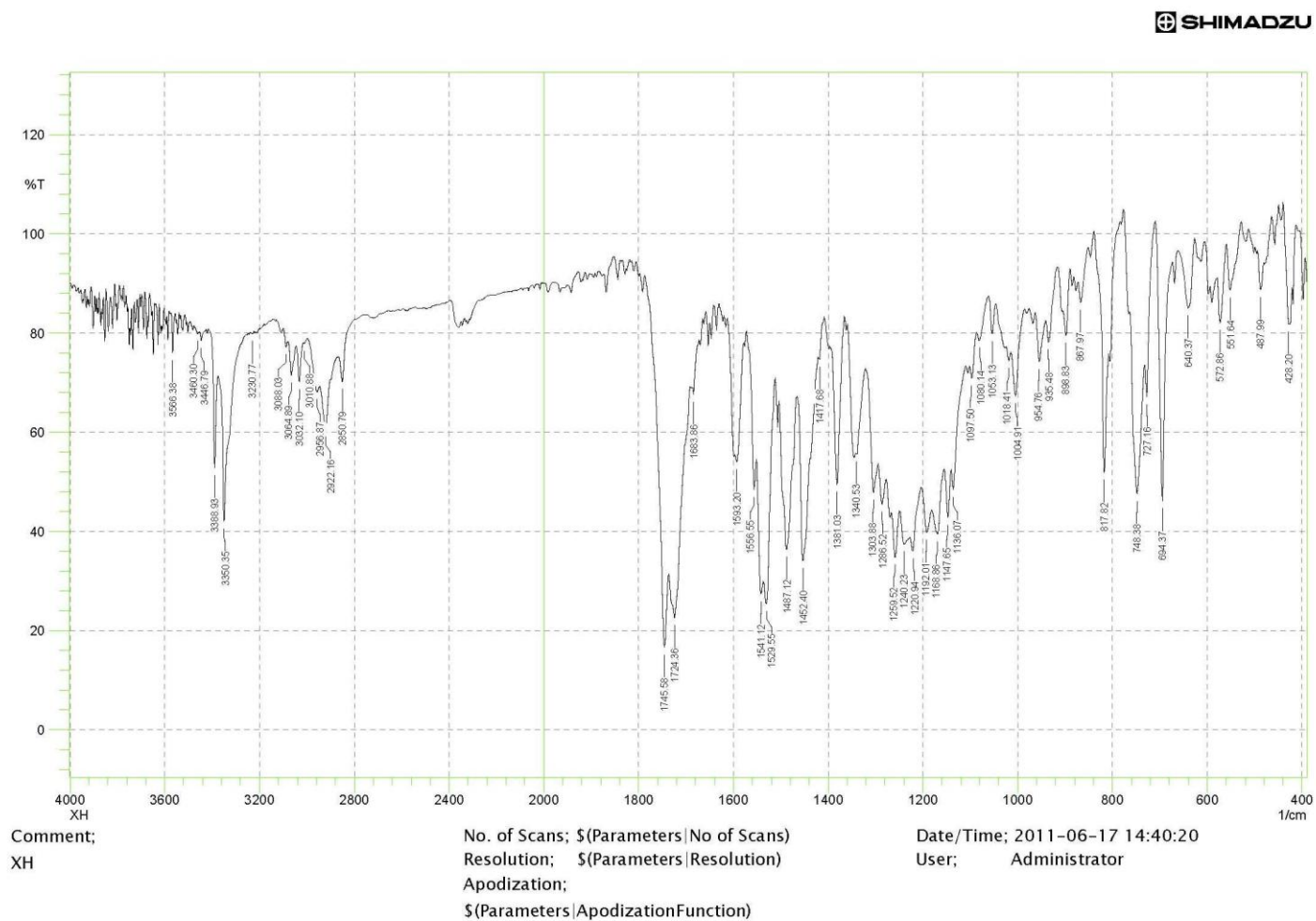
Figure S31. The ^{13}C -NMR Spectra of 5h.

Figure S32. The IR spectra of 5h.



Dimethyl 2-(benzofuran-2-yl)((6-methoxybenzo[d]thiazol-2-yl)amino)methyl)malonate (5i)

Figure S33. The High Resolution Mass Spectra of 5i.

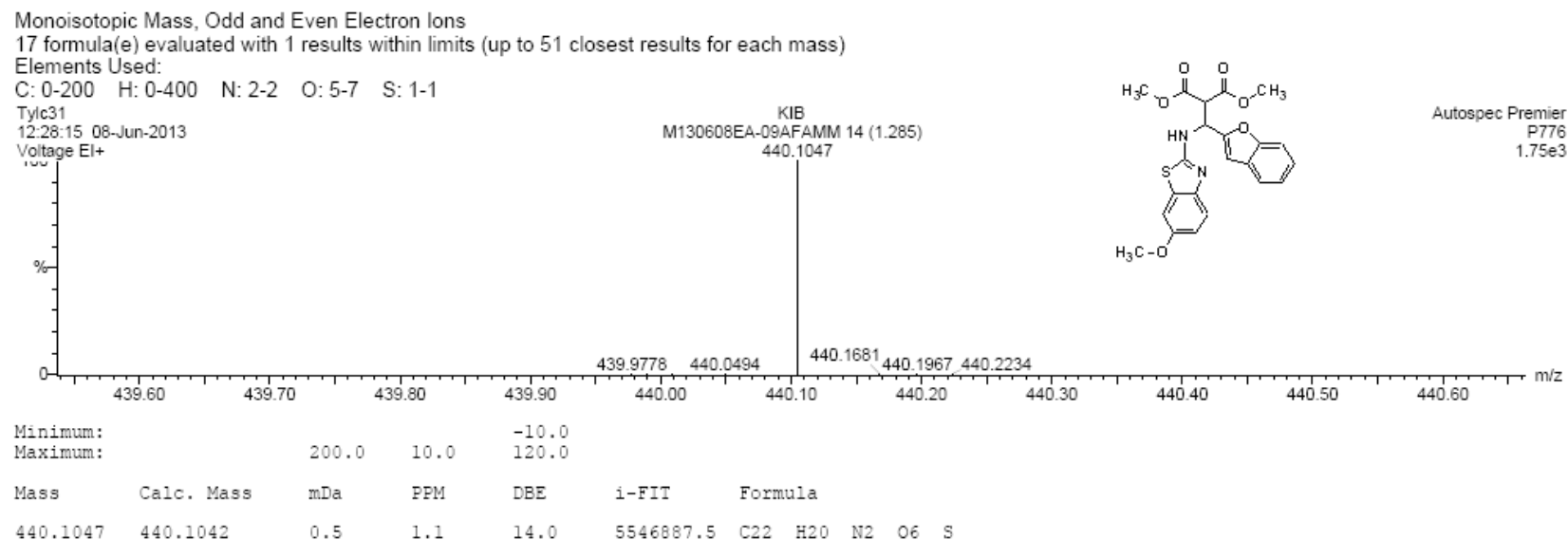


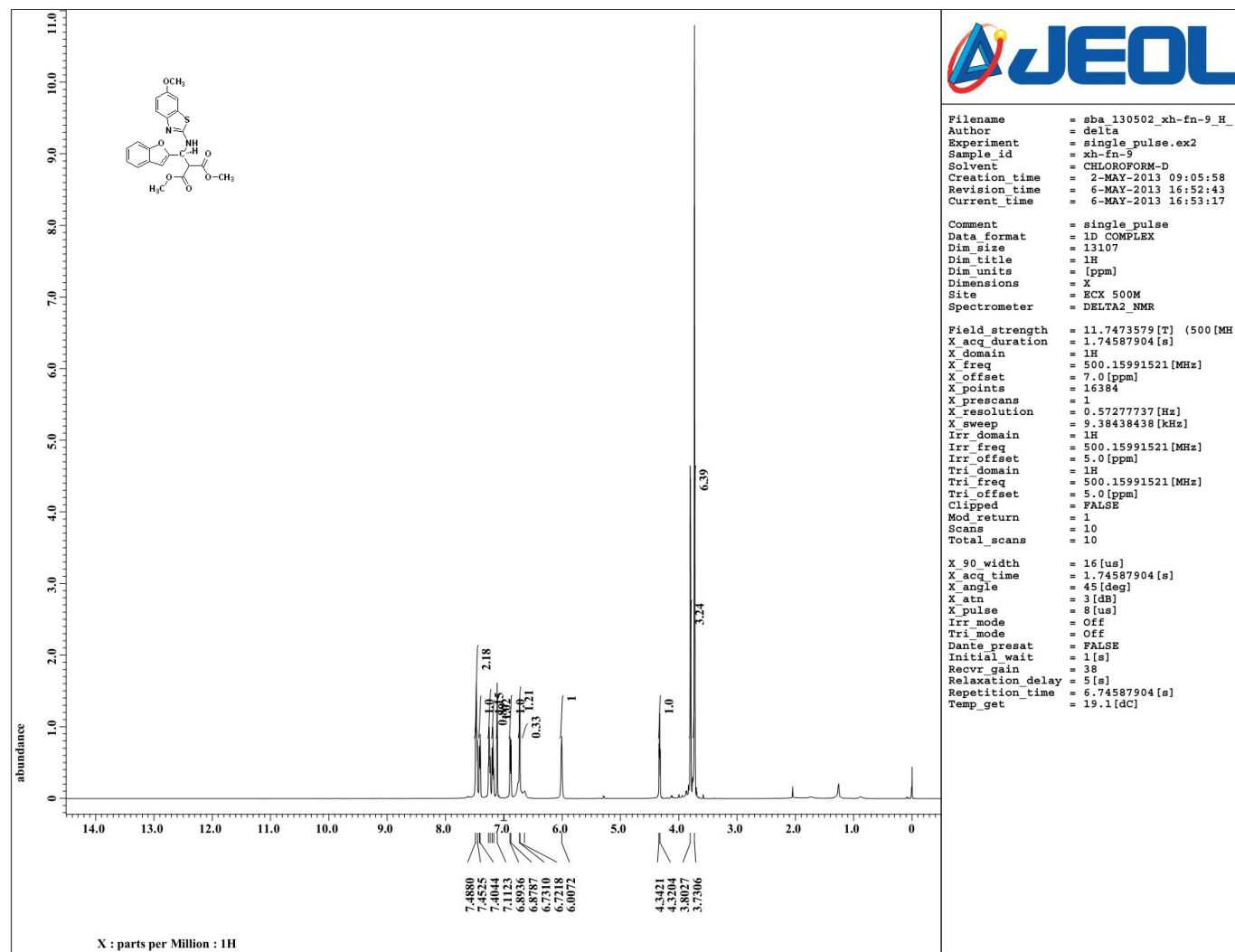
Figure S34. The ^1H -NMR Spectra of **5i**.

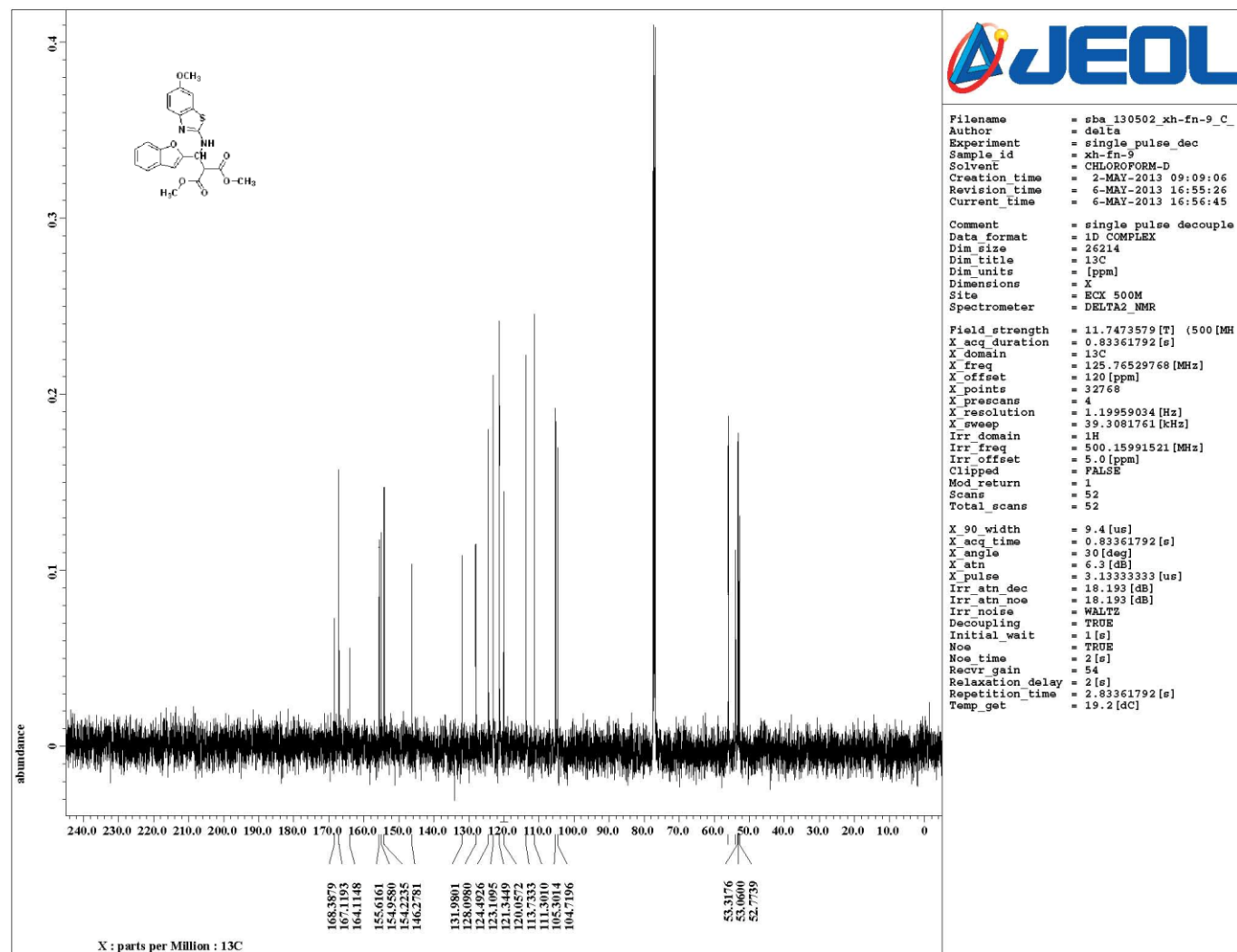
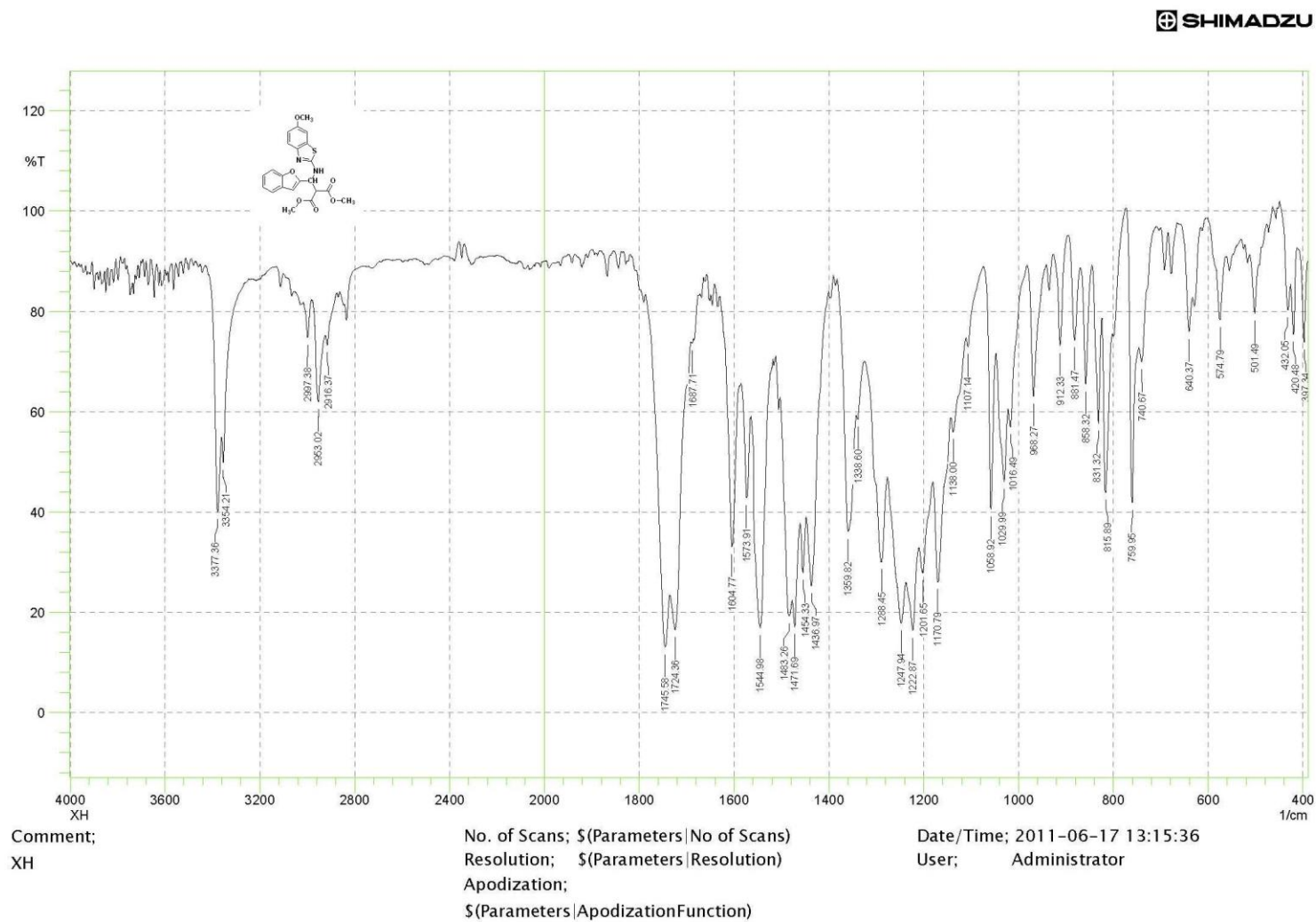
Figure S35. The ^{13}C -NMR Spectra of **5i**.

Figure S36. The IR spectra of 5i.



Diethyl 2-((benzofuran-2-yl)((6-methoxybenzo[d]thiazol-2-yl)amino)methyl)malonate (5j)

Figure S37. The High Resolution Mass Spectra of 5j.

Monoisotopic Mass, Odd and Even Electron Ions

18 formula(e) evaluated with 1 results within limits (up to 51 closest results for each mass)

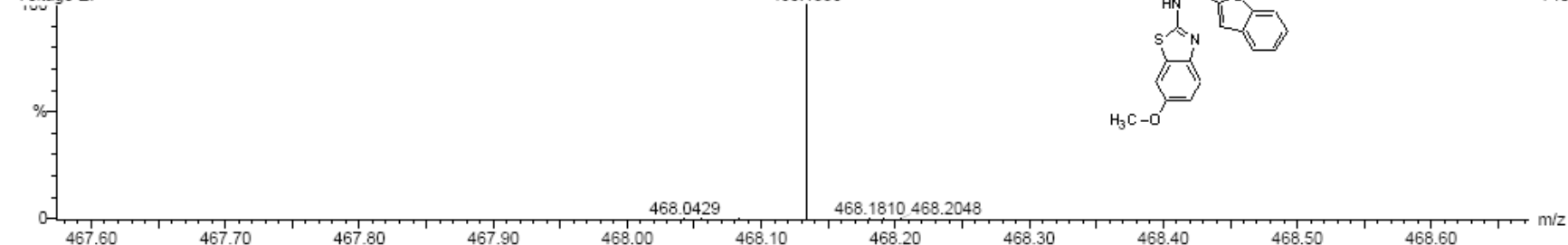
Elements Used:

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Tylc32

12:32:48 08-Jun-2013

Voltage EI+



Minimum: -10.0
Maximum: 200.0 10.0 120.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
468.1336	468.1355	-1.9	-4.1	14.0	5546370.5	C ₂₄ H ₂₄ N ₂ O ₆ S

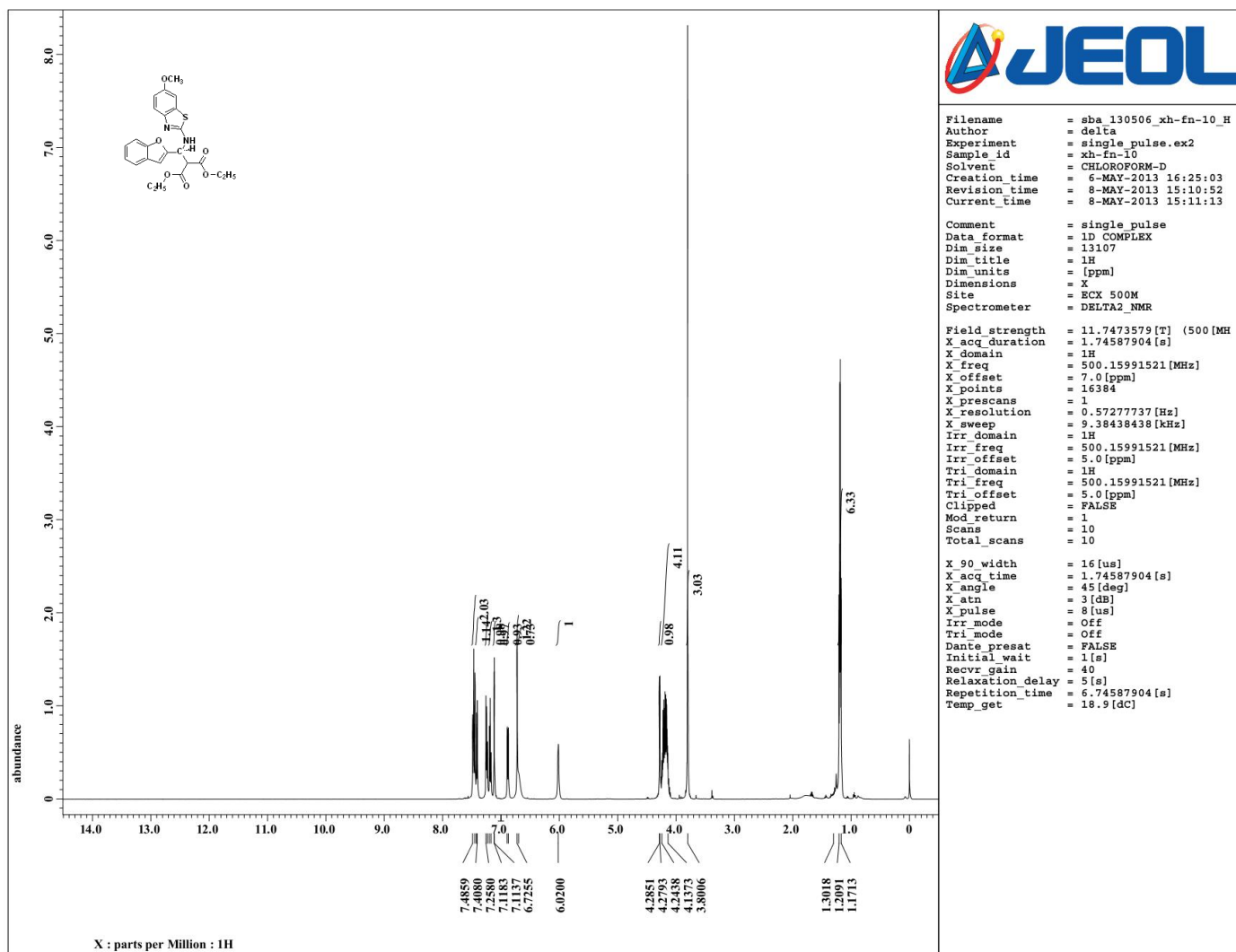
Figure S38. The ^1H -NMR Spectra of 5j.

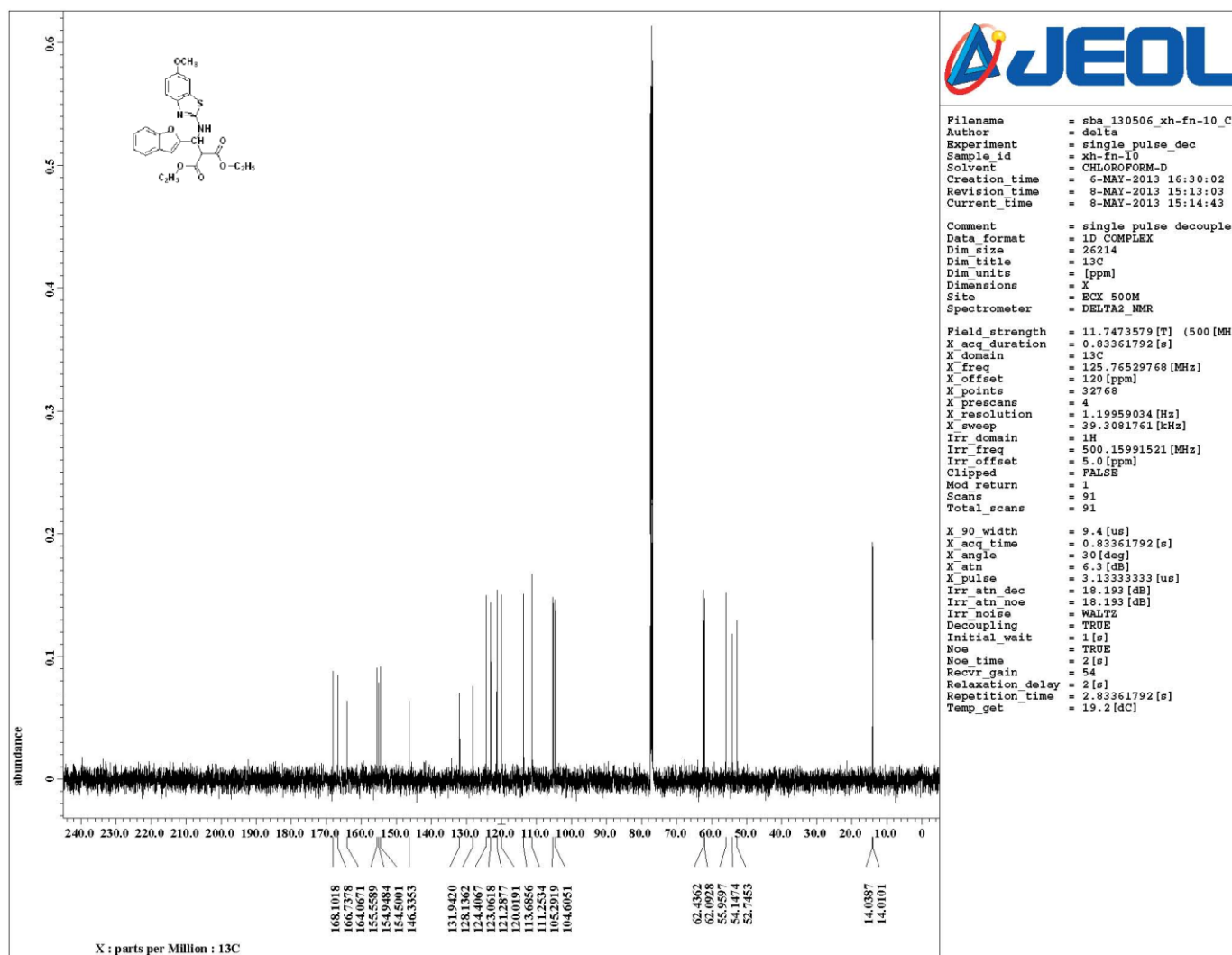
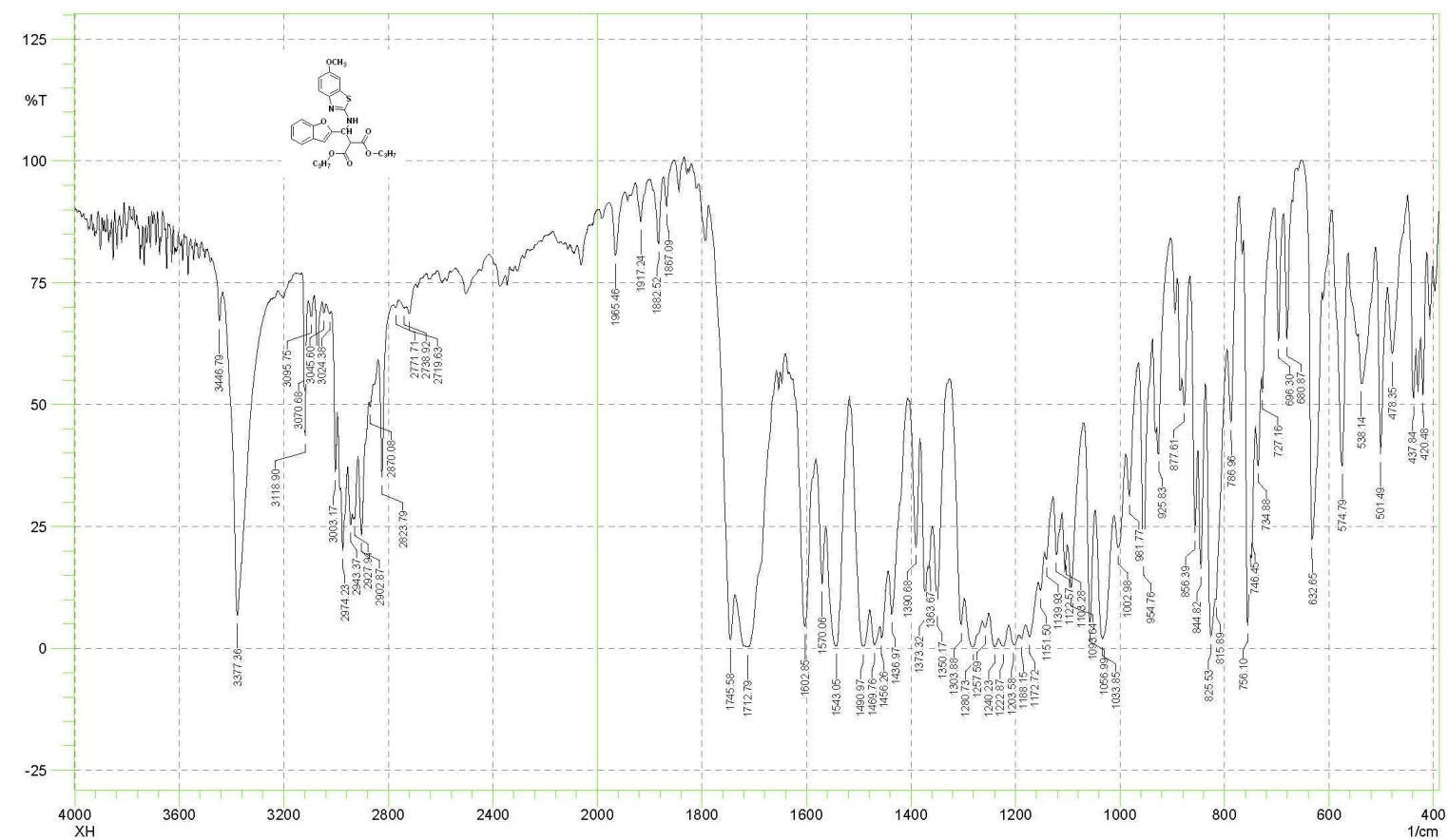
Figure S39. The ^{13}C -NMR Spectra of **5j**.

Figure S40. The IR spectra of 5j.

SHIMADZU



Comment;
XH

No. of Scans; \$(Parameters|No of Scans)
Resolution; \$(Parameters|Resolution)
Apodization;
\$(Parameters|ApodizationFunction)

Date/Time; 2011-06-17 14:52:40
User; Administrator

Dipropyl 2-(benzofuran-2-yl)((6-methoxybenzo[d]thiazol-2-yl)amino)methyl)malonate (5k)

Figure S41. The High Resolution Mass Spectra of 5k.

Monoisotopic Mass, Odd and Even Electron Ions

19 formula(e) evaluated with 1 results within limits (up to 51 closest results for each mass)

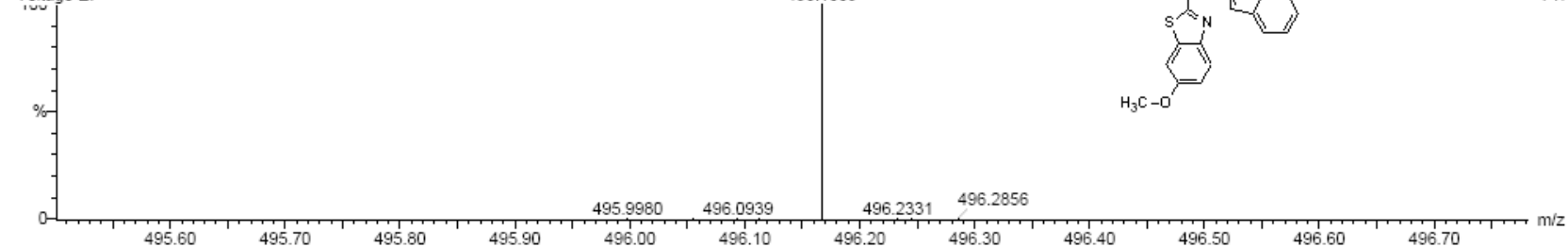
Elements Used:

C: 0-200 H: 0-400 N: 2-2 O: 5-7 S: 1-1

Tylc33

12:37:57 08-Jun-2013

Voltage El+



Minimum: -10.0
Maximum: 200.0 10.0 120.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
496.1669	496.1668	0.1	0.2	14.0	5546375.0	C26 H28 N2 O6 S

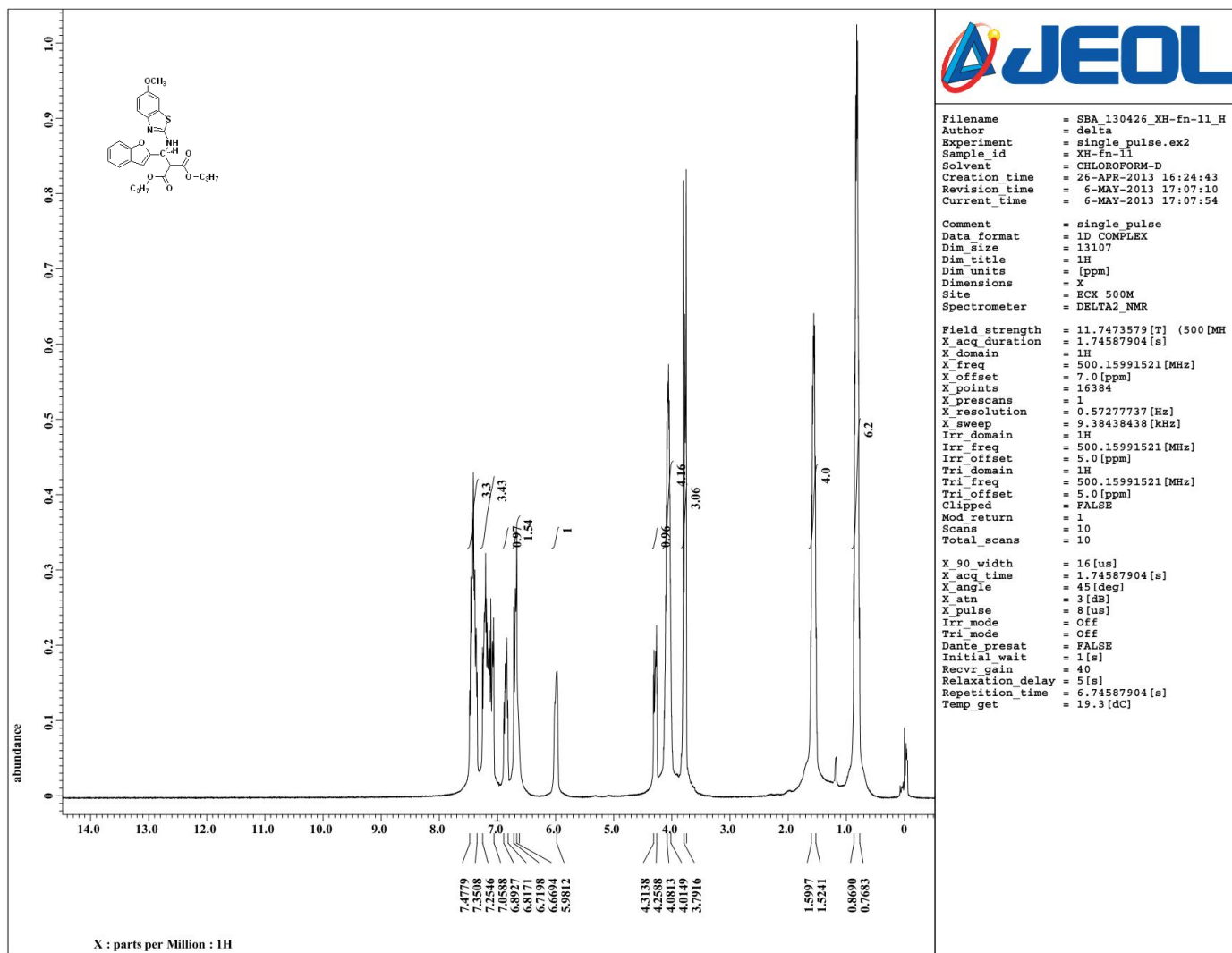
Figure S42. The ^1H -NMR Spectra of 5k.

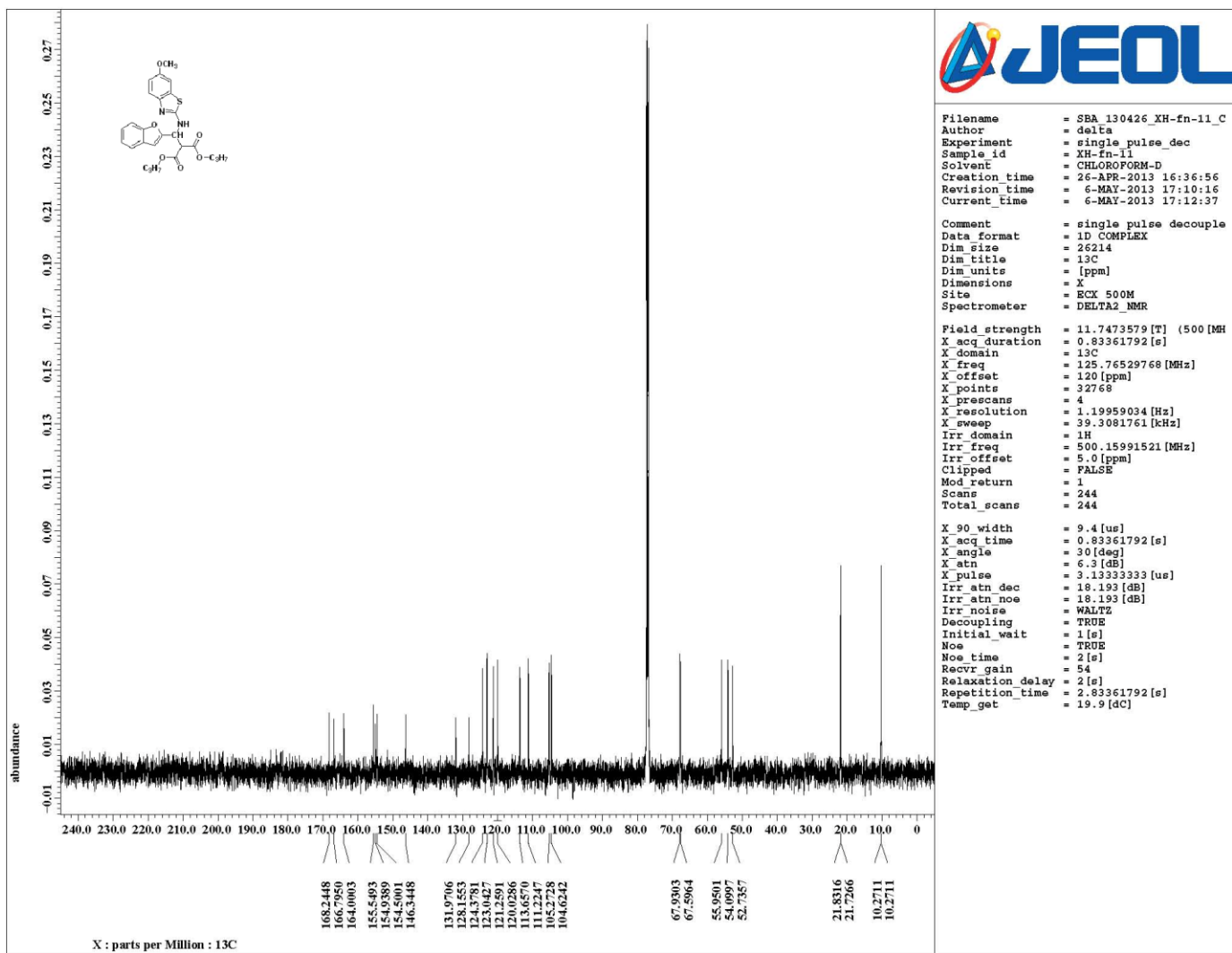
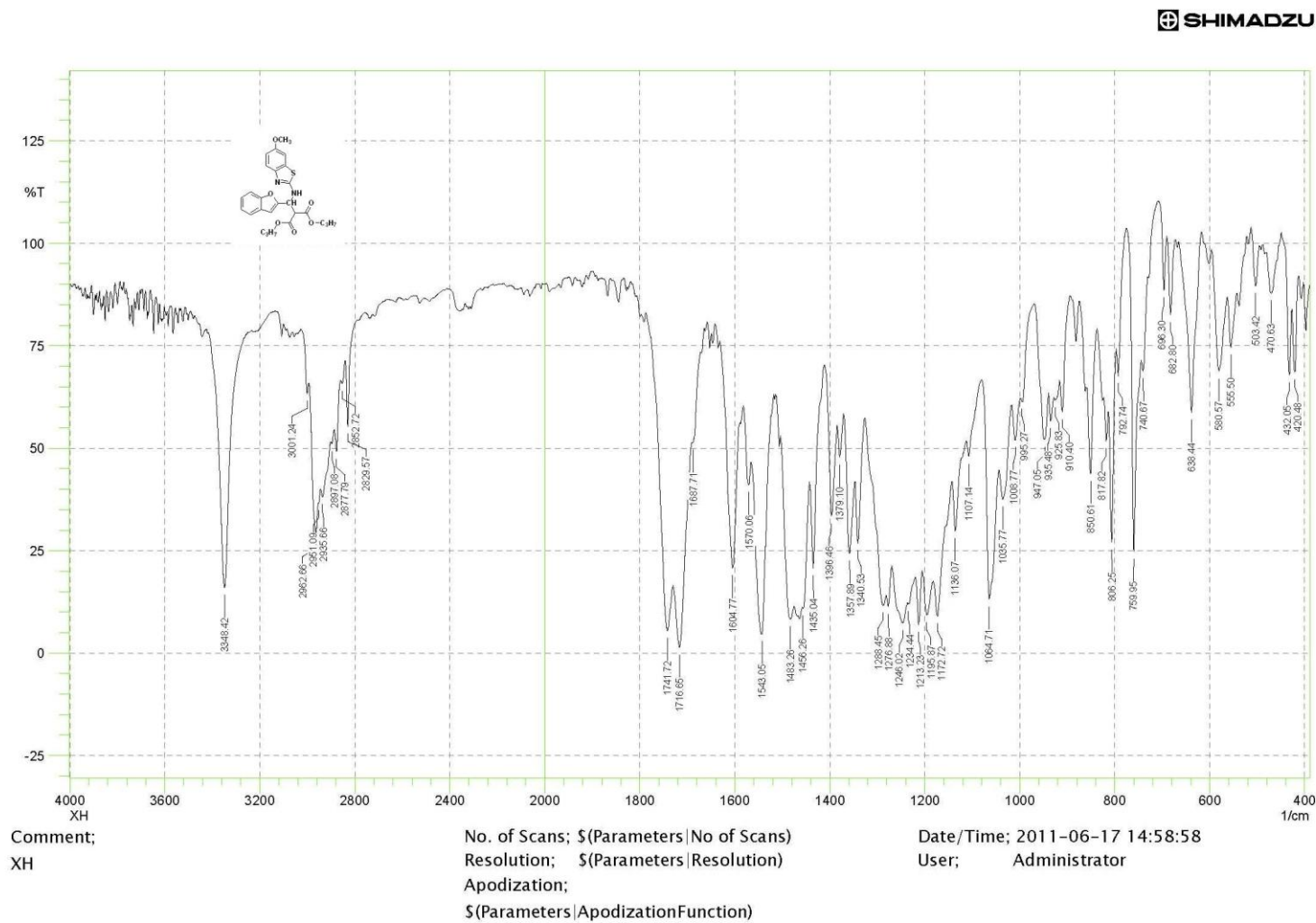
Figure S43. The ^{13}C -NMR Spectra of 5k.

Figure S44. The IR spectra of 5k.



Dibenzyl 2-(benzofuran-2-yl)((6-methoxybenzo[d]thiazol-2-yl)amino)methyl)malonate (5I)

Figure S45. The High Resolution Mass Spectra of 5I.

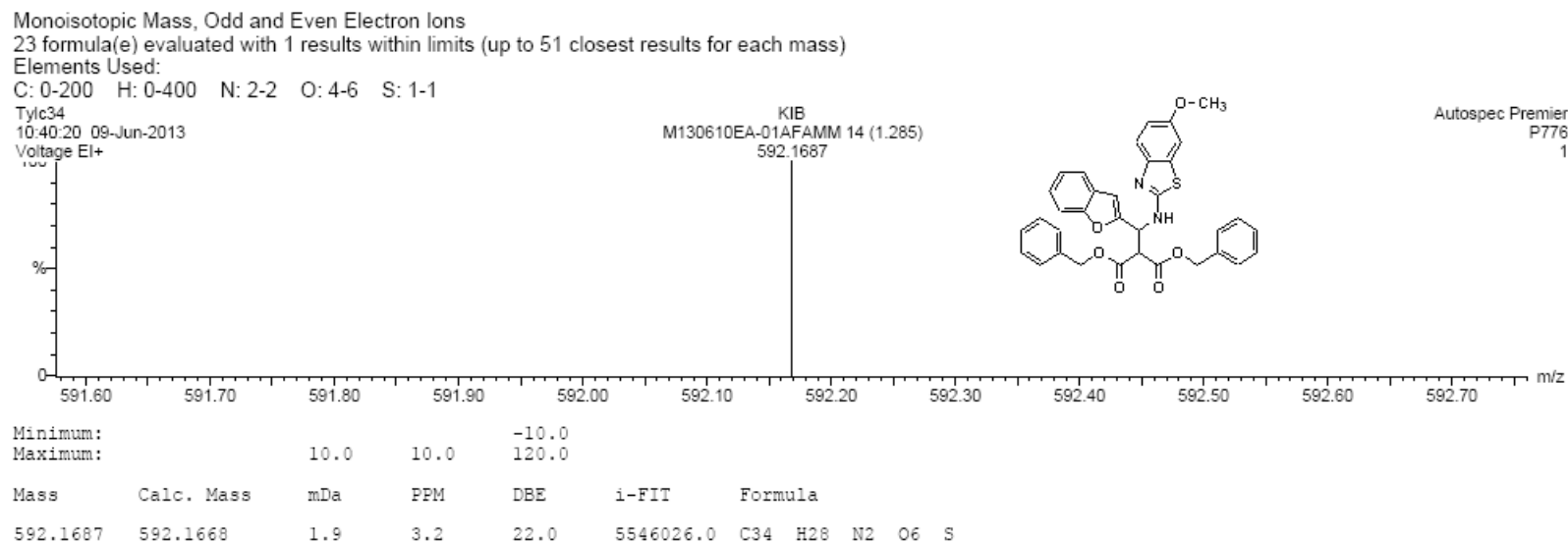


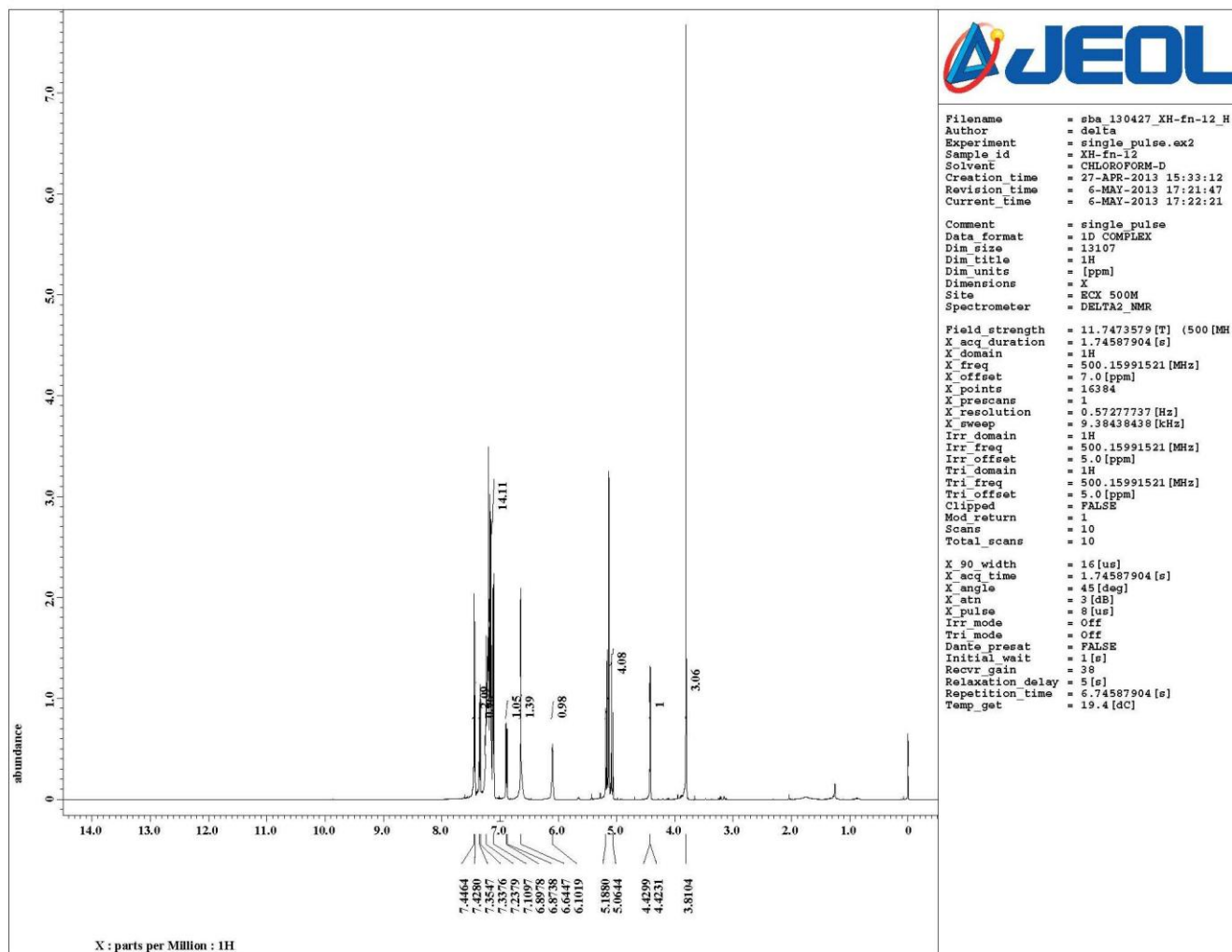
Figure S46. The ^1H -NMR Spectra of 5l.

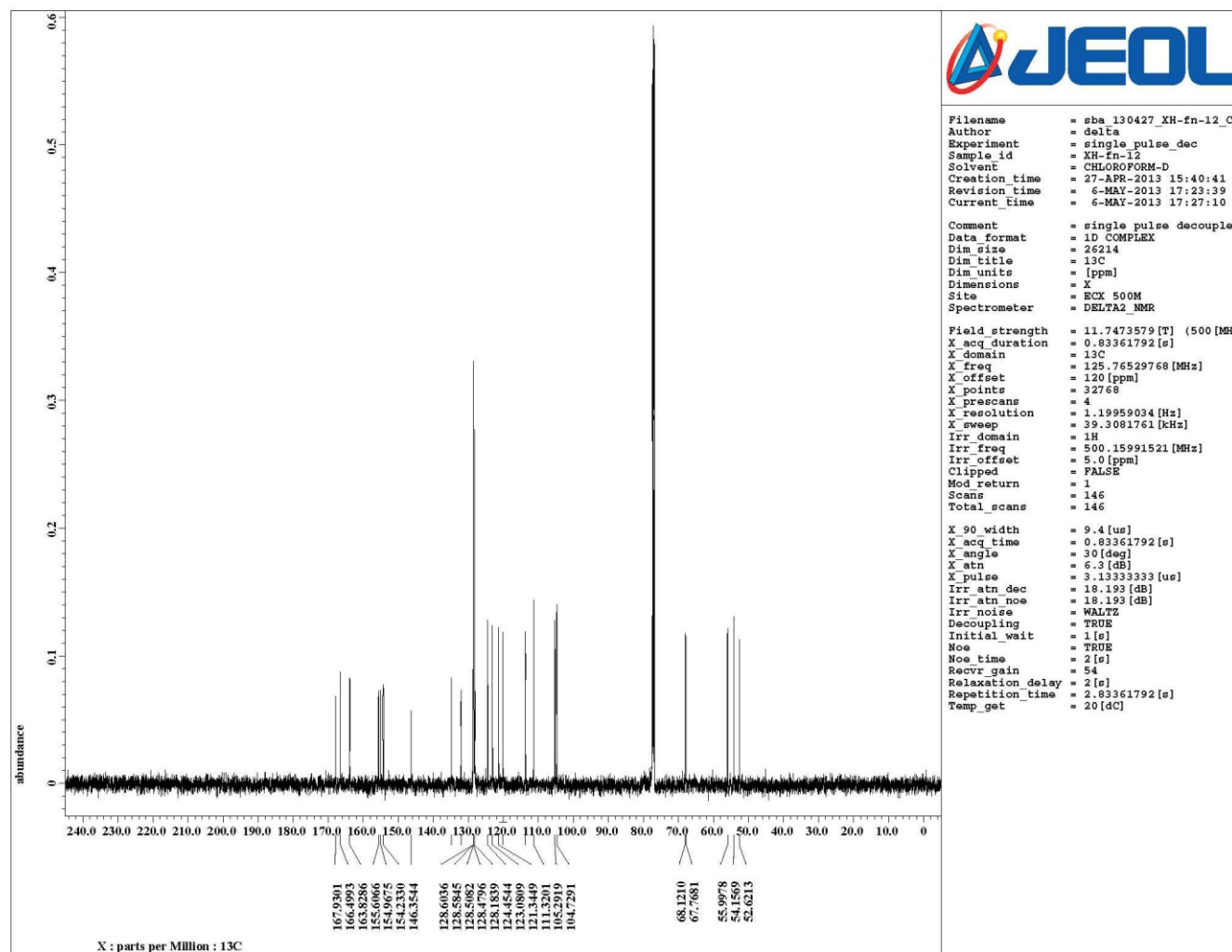
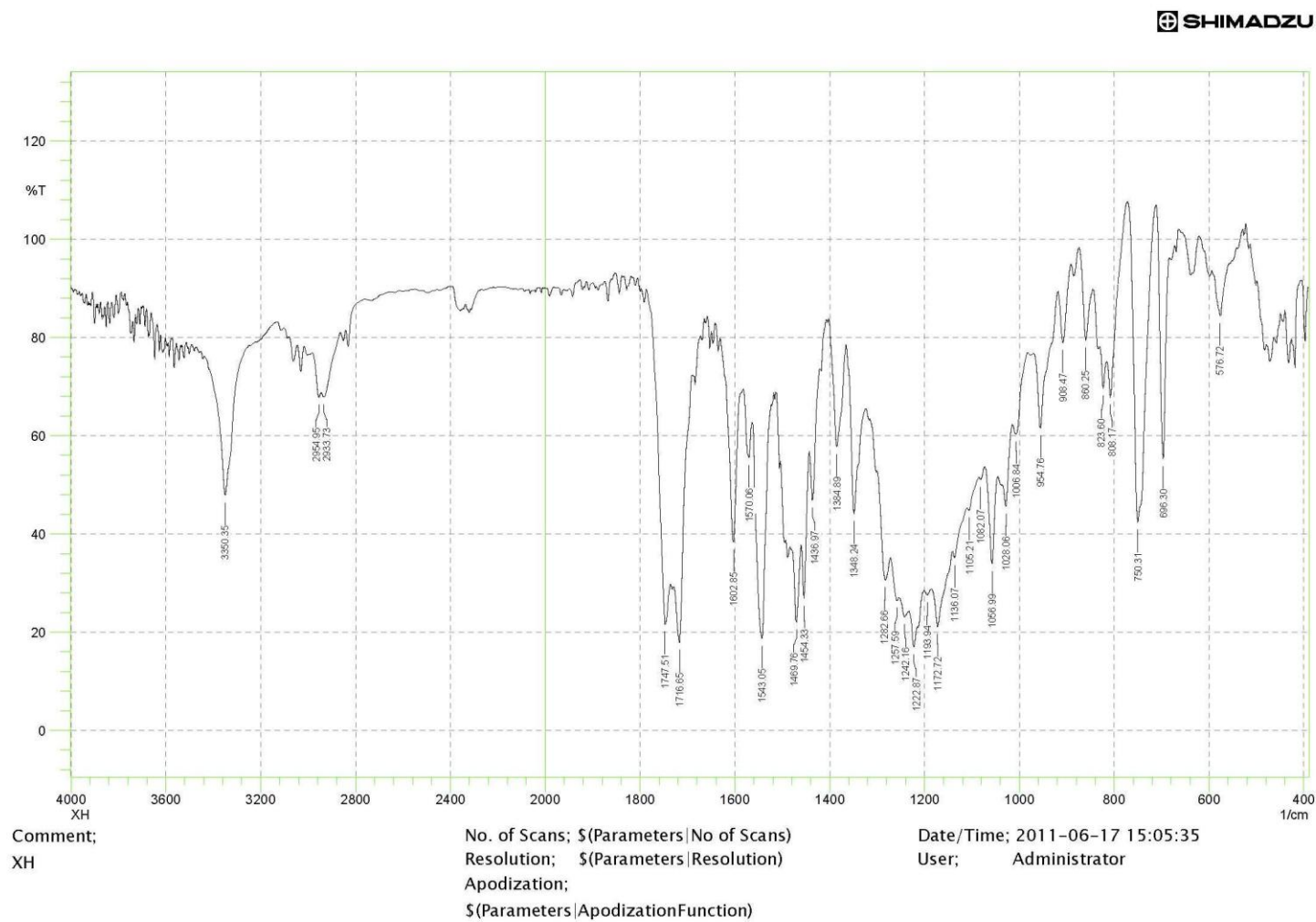
Figure S47. The ^{13}C -NMR Spectra of 5l.

Figure S48. The IR spectra of 5l.



Dimethyl 2-(benzofuran-2-yl)((6-methylbenzo[d]thiazol-2-yl)amino)methyl)malonate (**5m**)**Figure S49.** The High Resolution Mass Spectra of **5m**.

Monoisotopic Mass, Odd and Even Electron Ions
17 formula(e) evaluated with 1 results within limits (up to 51 closest results for each mass)

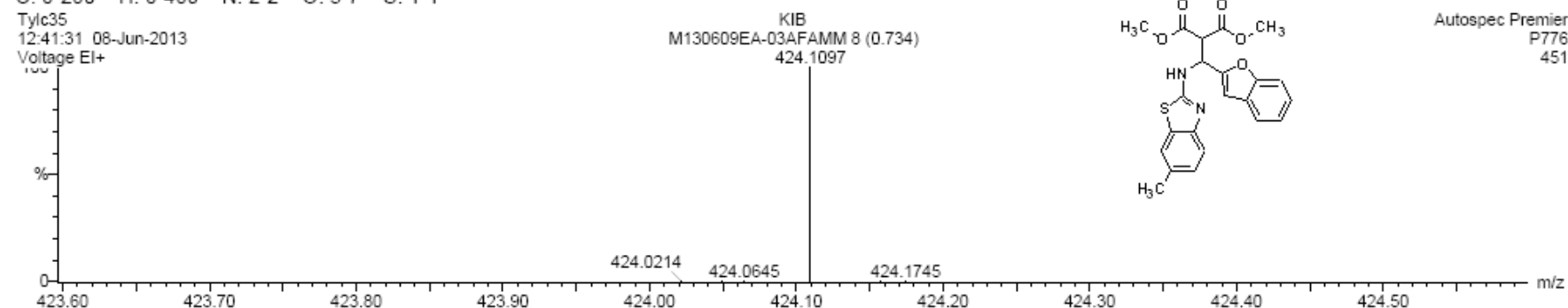
Elements Used:

C: 0-200 H: 0-400 N: 2-2 O: 5-7 S: 1-1

Tylo35

12:41:31 08-Jun-2013

Voltage EI+



Minimum: -10.0
Maximum: 200.0 10.0 120.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
424.1097	424.1093	0.4	0.9	14.0	5546240.0	C22 H20 N2 O5 S

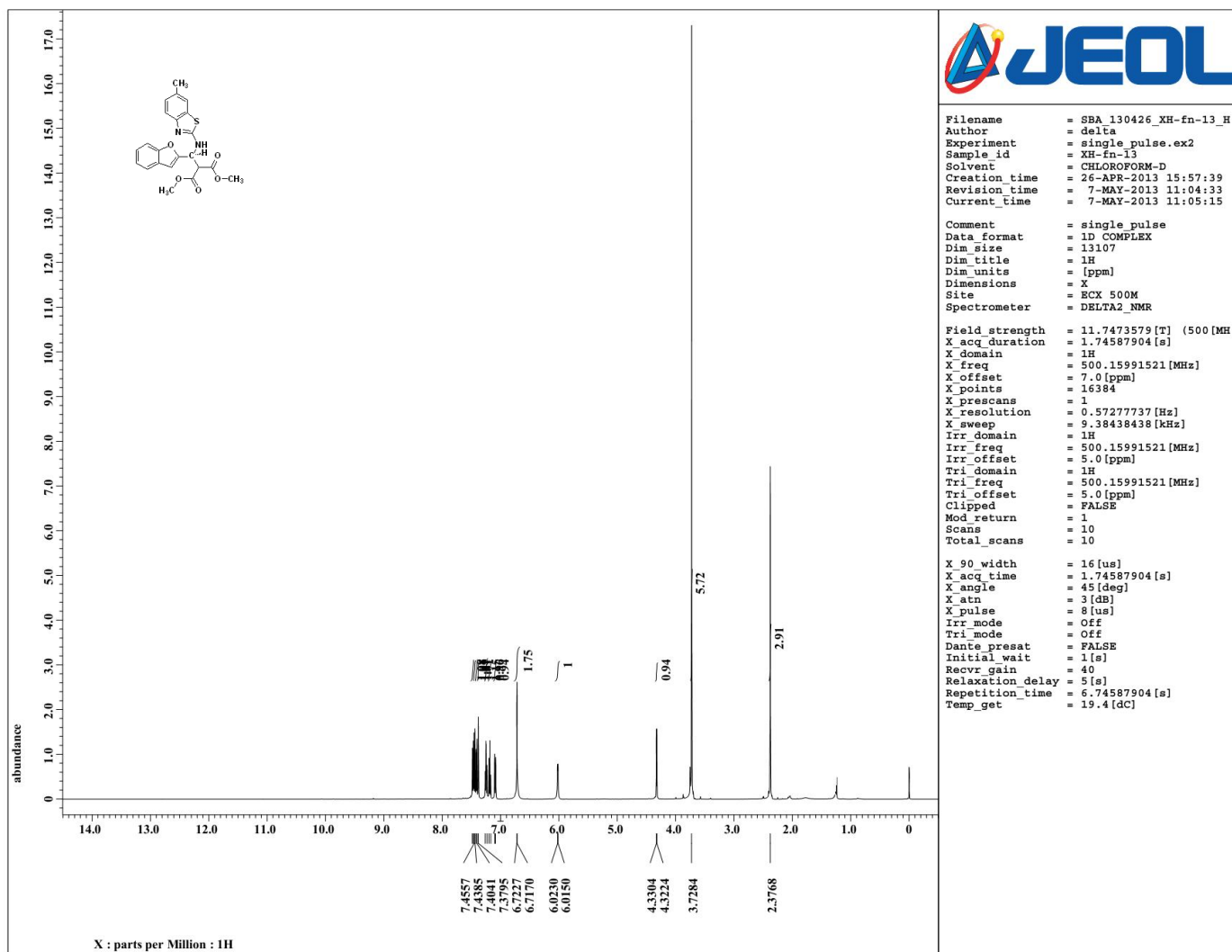
Figure S50. The ^1H -NMR Spectra of 5m.

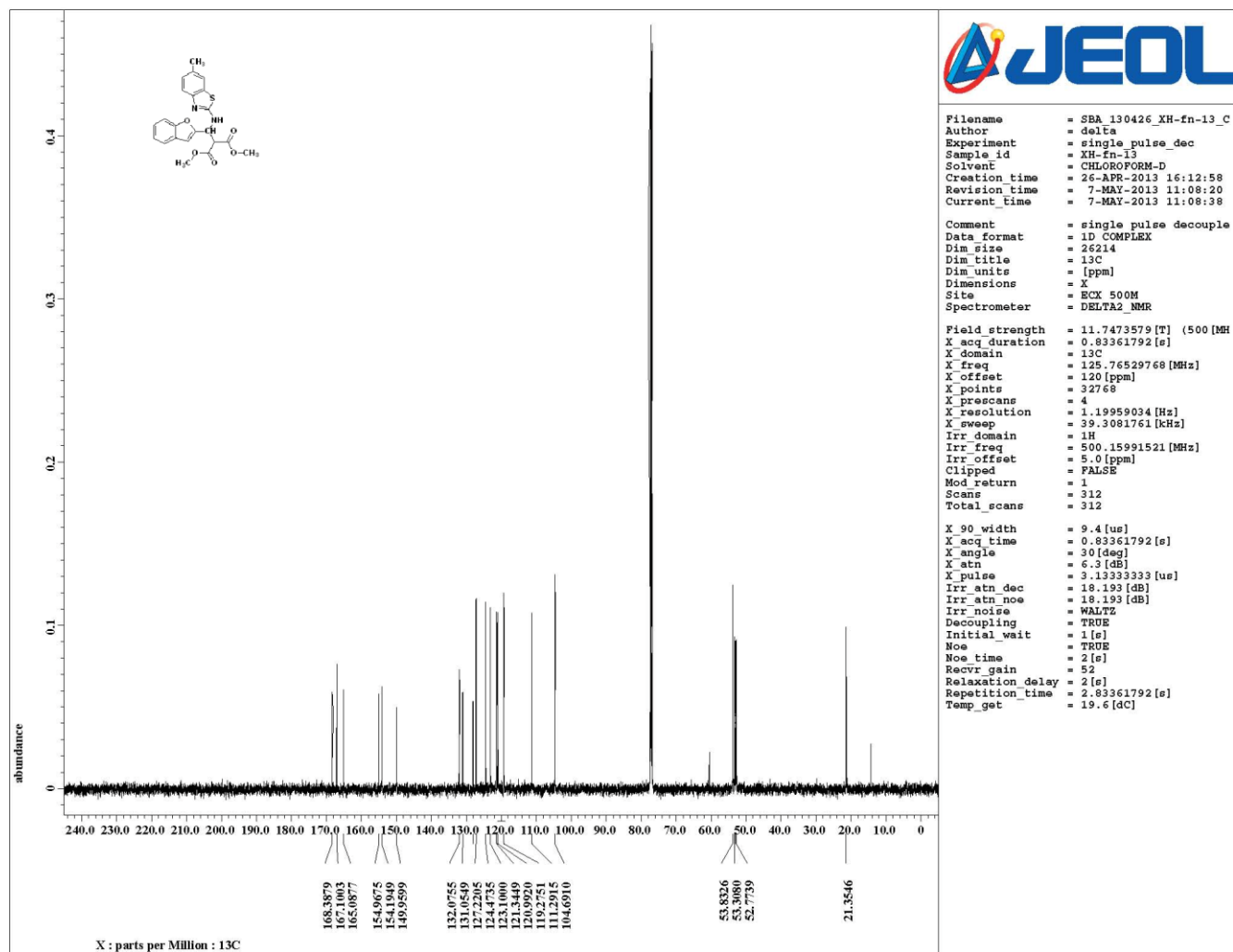
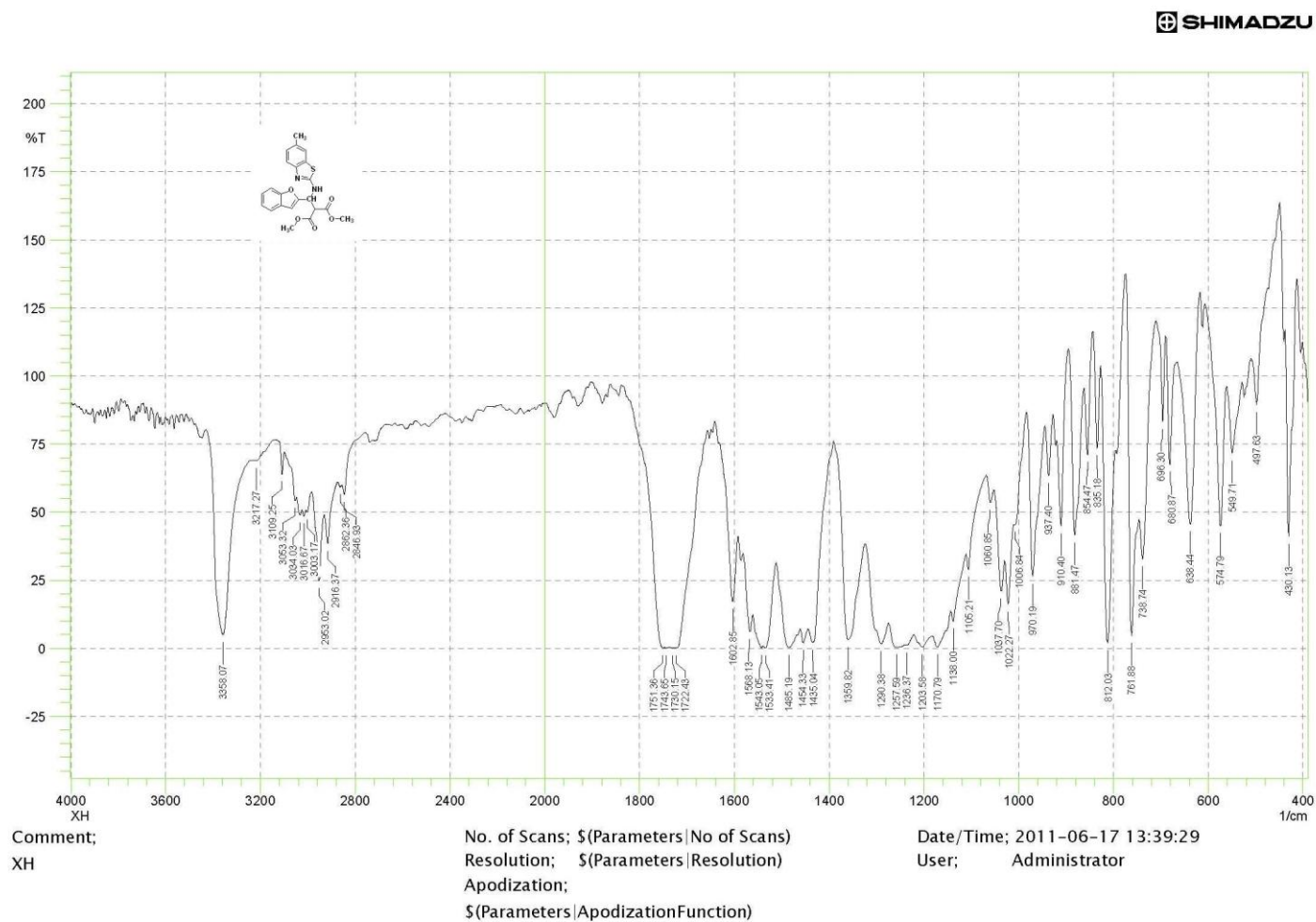
Figure S51. The ^{13}C -NMR Spectra of 5m.

Figure S52. The IR spectra of 5m.



Diethyl 2-(benzofuran-2-yl)((6-methylbenzo[d]thiazol-2-yl)amino)methyl)malonate (**5n**)**Figure S53.** The High Resolution Mass Spectra of **5n**.

Monoisotopic Mass, Odd and Even Electron Ions

18 formula(e) evaluated with 1 results within limits (up to 51 closest results for each mass)

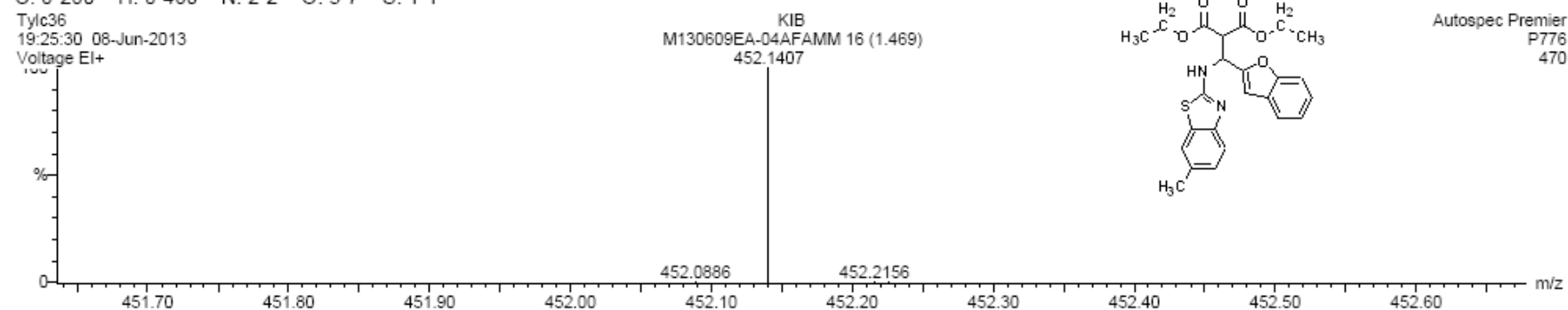
Elements Used:

C: 0-200 H: 0-400 N: 2-2 O: 5-7 S: 1-1

Tylc36

19:25:30 08-Jun-2013

Voltage EI+



Minimum: -10.0
Maximum: 200.0 10.0 120.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
452.1407	452.1406	0.1	0.2	14.0	5546251.0	C24 H24 N2 O5 S

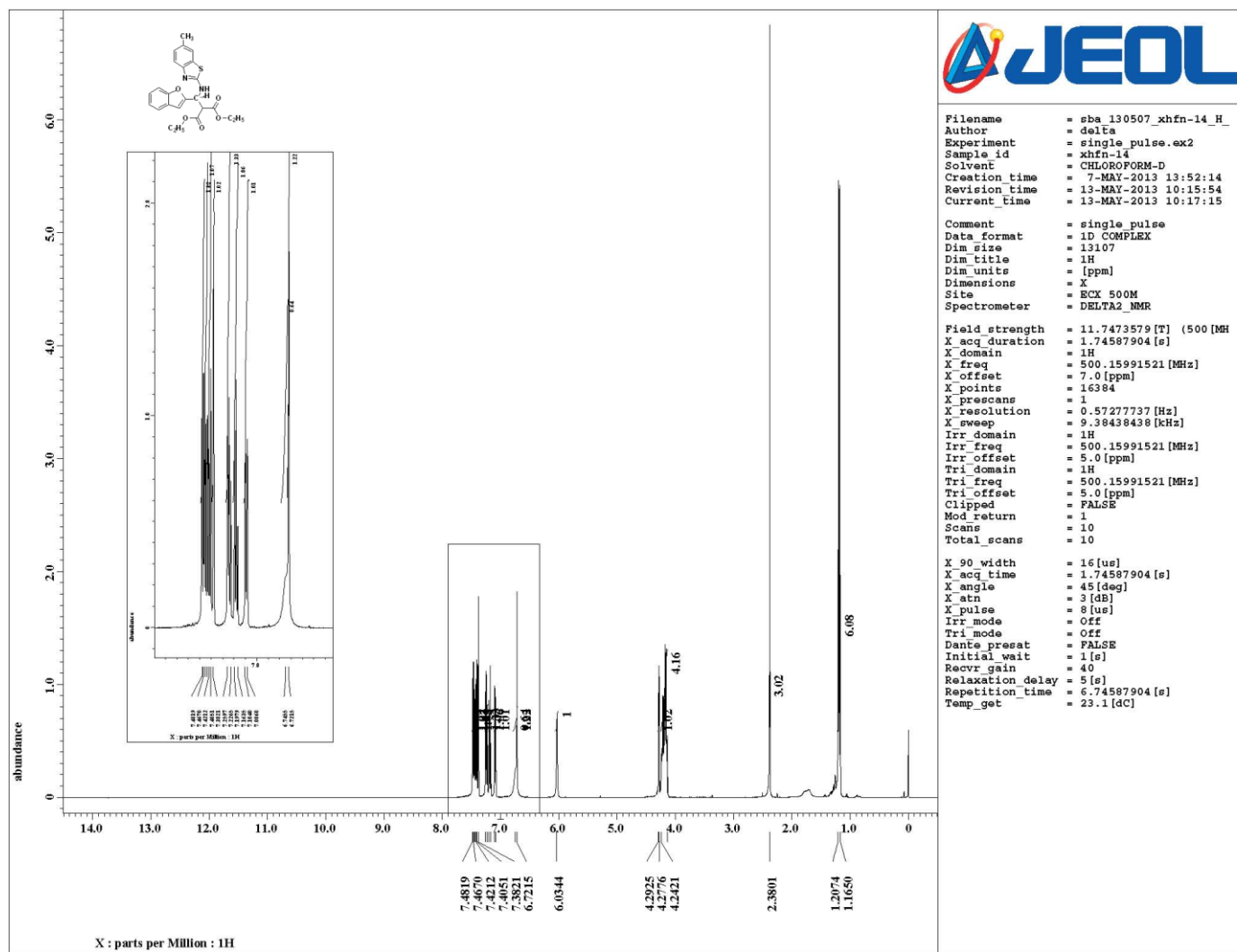
Figure S54. The ^1H -NMR Spectra of 5n.

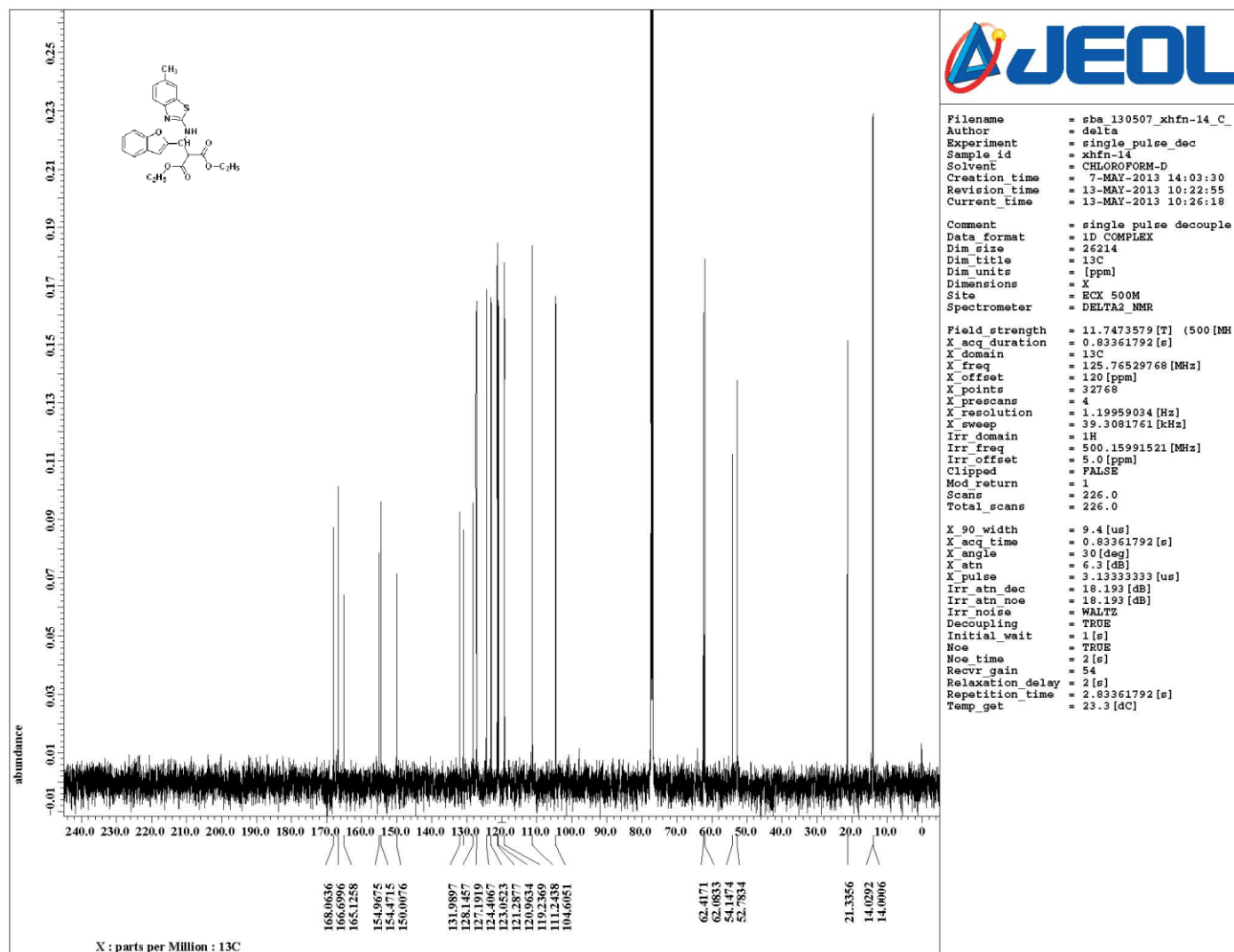
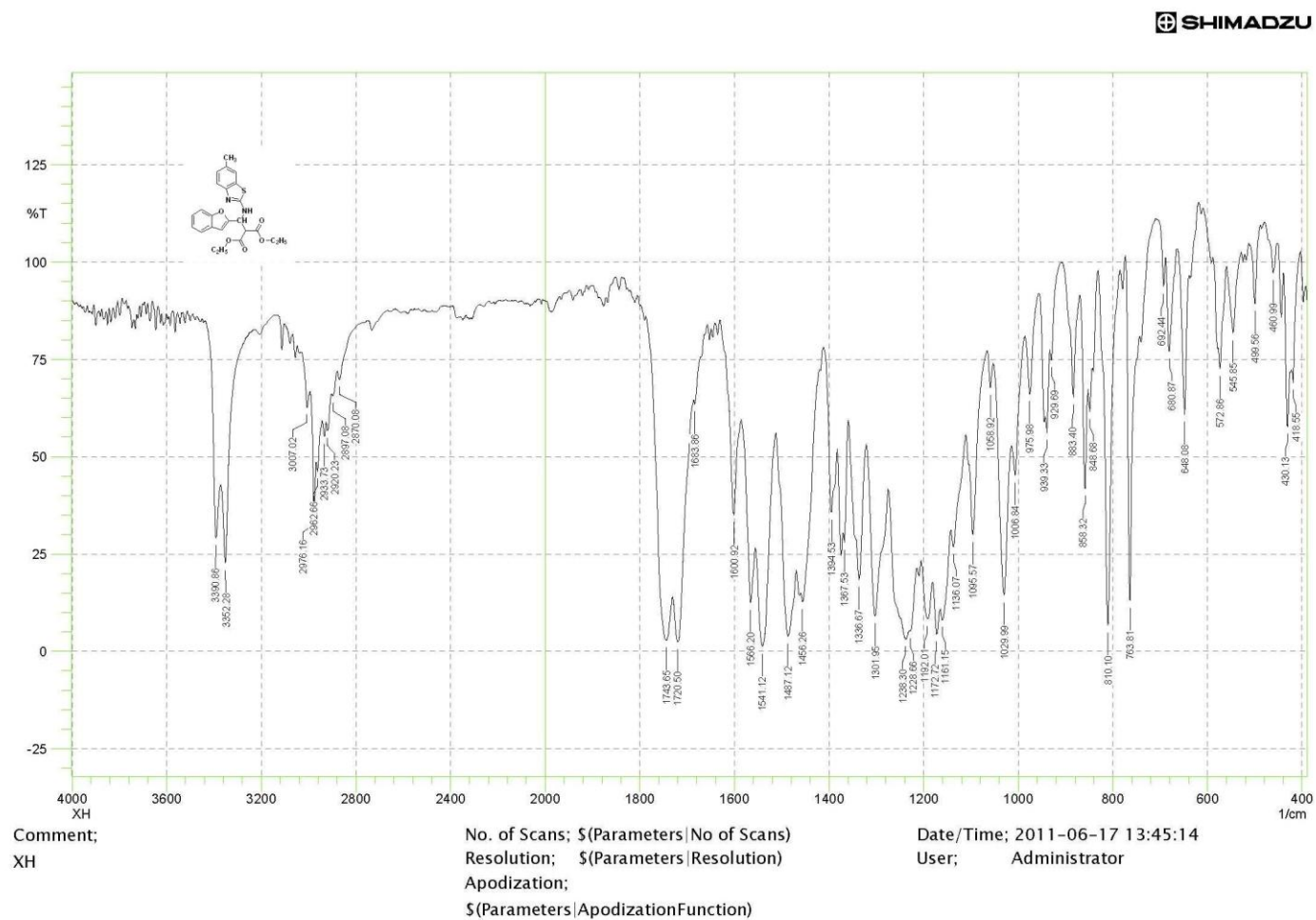
Figure S55. The ^{13}C -NMR Spectra of 5n.

Figure S56. The IR spectra of 5n.



Dipropyl 2-(benzofuran-2-yl((6-methylbenzo[d]thiazol-2-yl)amino)methyl)malonate (5o)

Figure S57. The High Resolution Mass Spectra of 5o.

Monoisotopic Mass, Odd and Even Electron Ions
 19 formula(e) evaluated with 1 results within limits (up to 51 closest results for each mass)

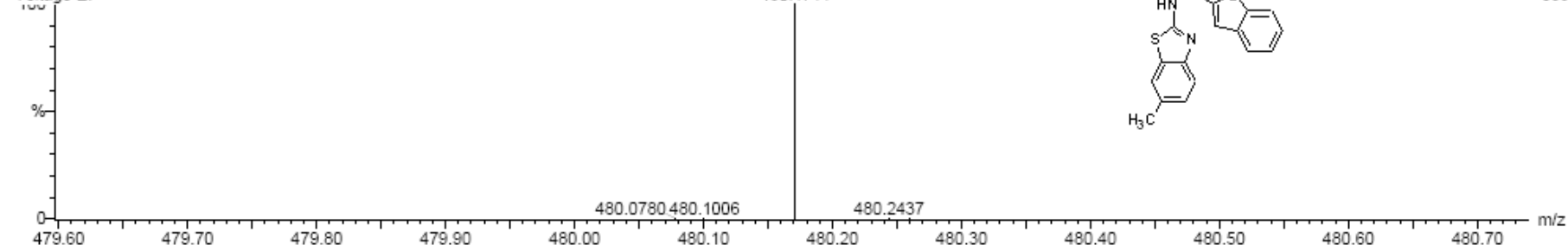
Elements Used:

C: 0-200 H: 0-400 N: 2-2 O: 5-7 S: 1-1

Tyler37

19:29:51 08-Jun-2013

Voltage EI+



Autospec Premier
 P776
 399

Minimum: -10.0
 Maximum: 200.0 10.0 120.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
480.1711	480.1719	-0.8	-1.7	14.0	5546216.5	C26 H28 N2 O5 S

Figure S58. The ^1H -NMR Spectra of **50**.

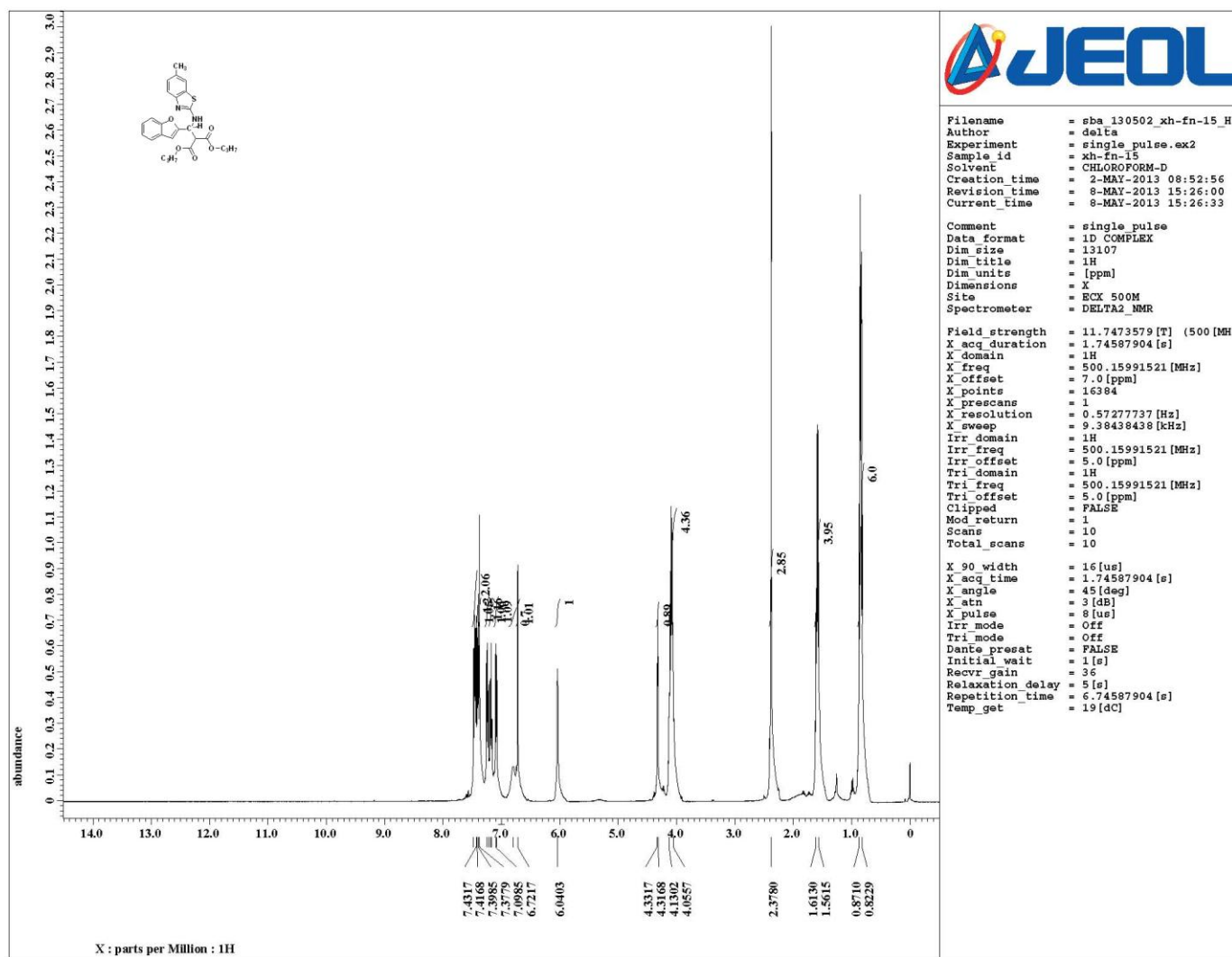


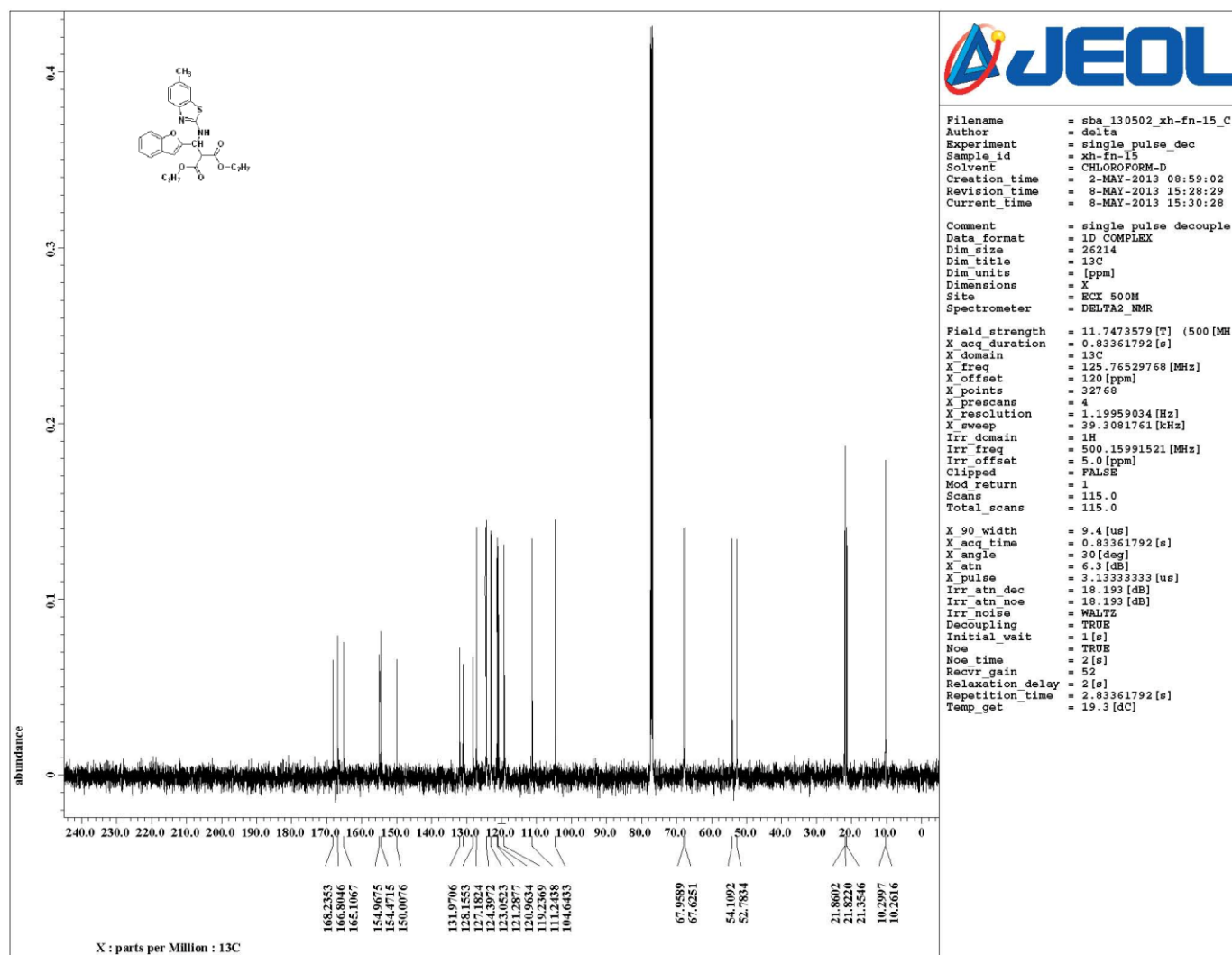
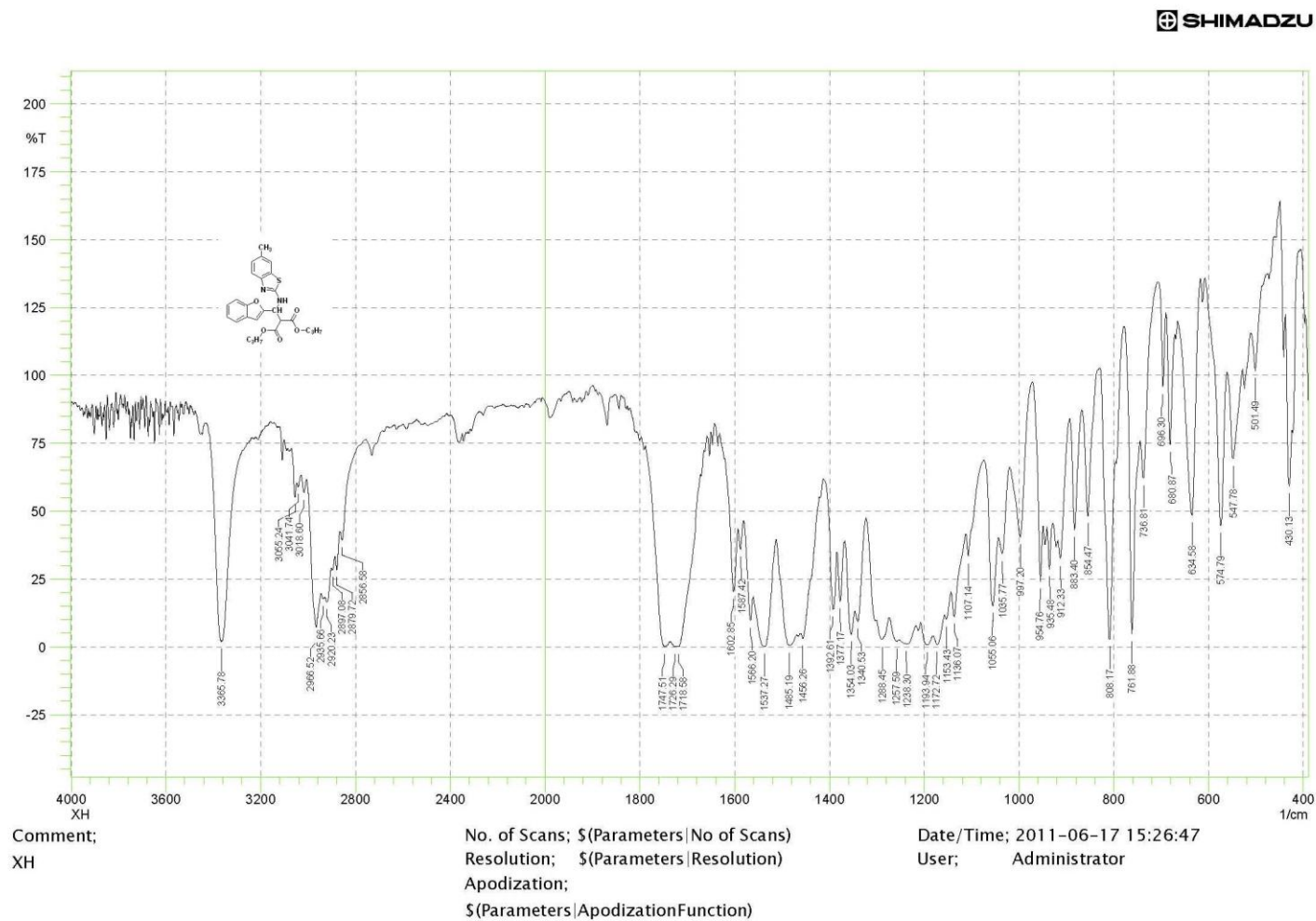
Figure S59. The ^{13}C -NMR Spectra of 5o.

Figure S60. The IR spectra of 50.



Dibenzyl 2-(benzofuran-2-yl)((6-methylbenzo[d]thiazol-2-yl)amino)methyl) malonate (5p)

Figure S61. The High Resolution Mass Spectra of 5p.

Monoisotopic Mass, Odd and Even Electron Ions

23 formula(e) evaluated with 1 results within limits (up to 51 closest results for each mass)

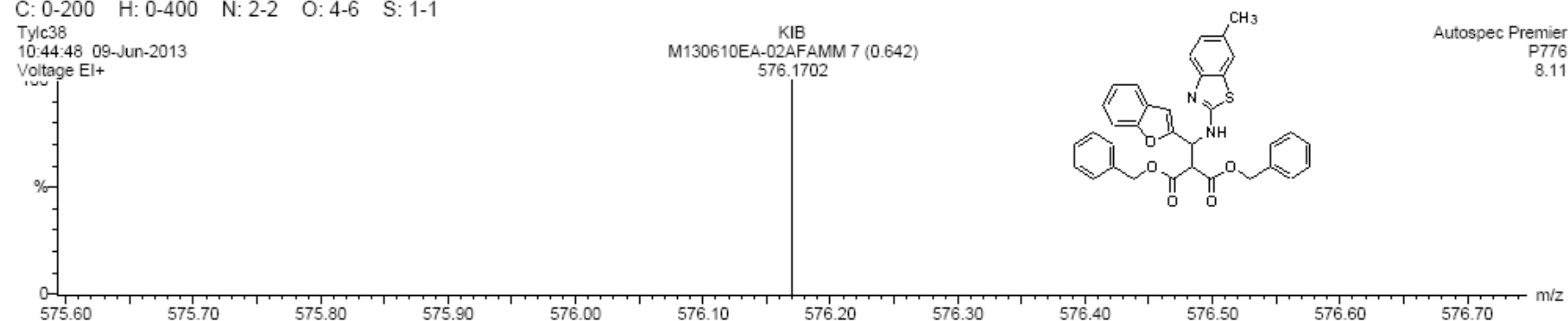
Elements Used:

C: 0-200 H: 0-400 N: 2-2 O: 4-6 S: 1-1

Tylc38

10:44:48 09-Jun-2013

Voltage EI+



Minimum: -10.0
Maximum: 10.0 10.0 120.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
576.1702	576.1719	-1.7	-3.0	22.0	5546026.0	C34 H28 N2 O5 S

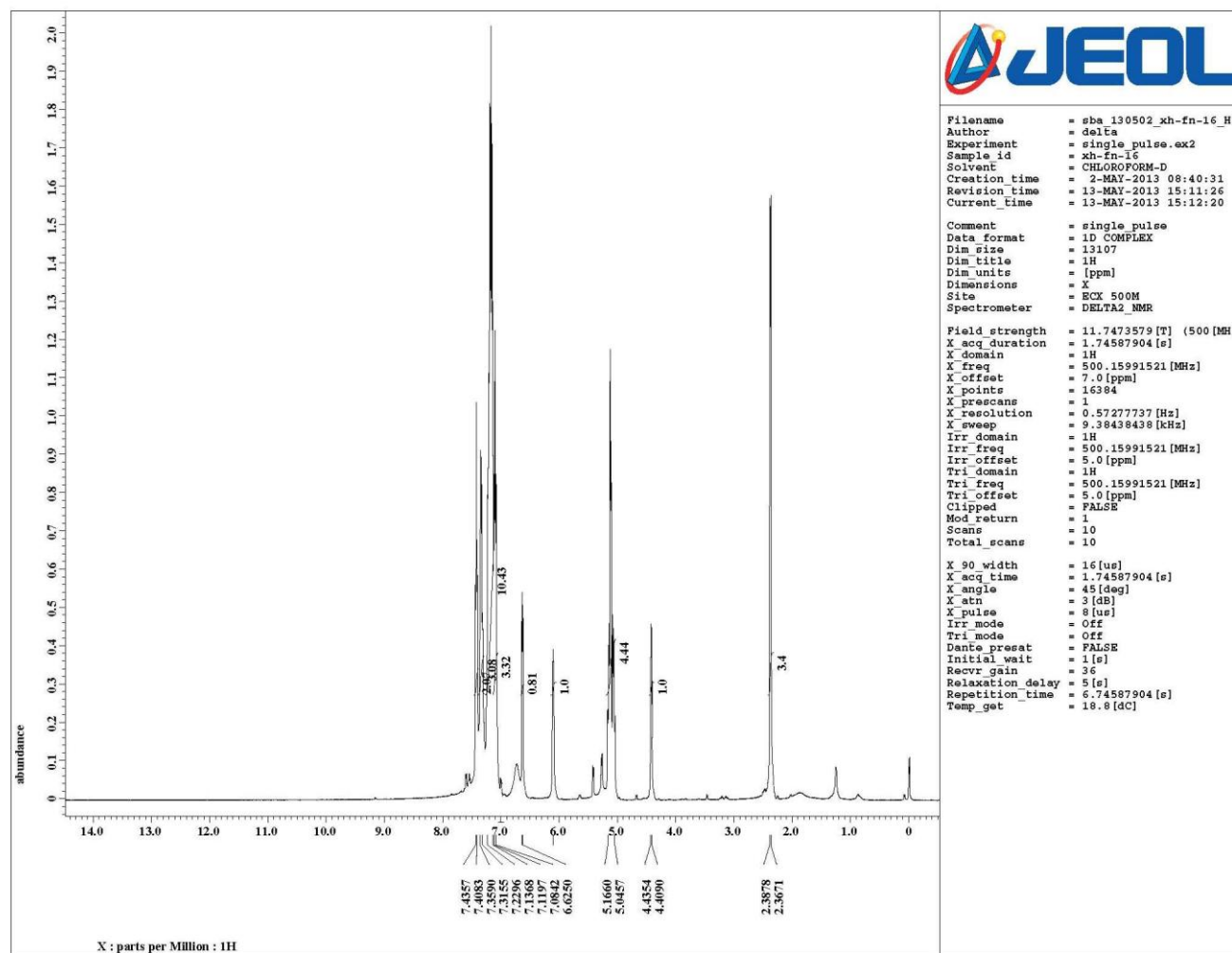
Figure S62. The ^1H -NMR Spectra of 5p.

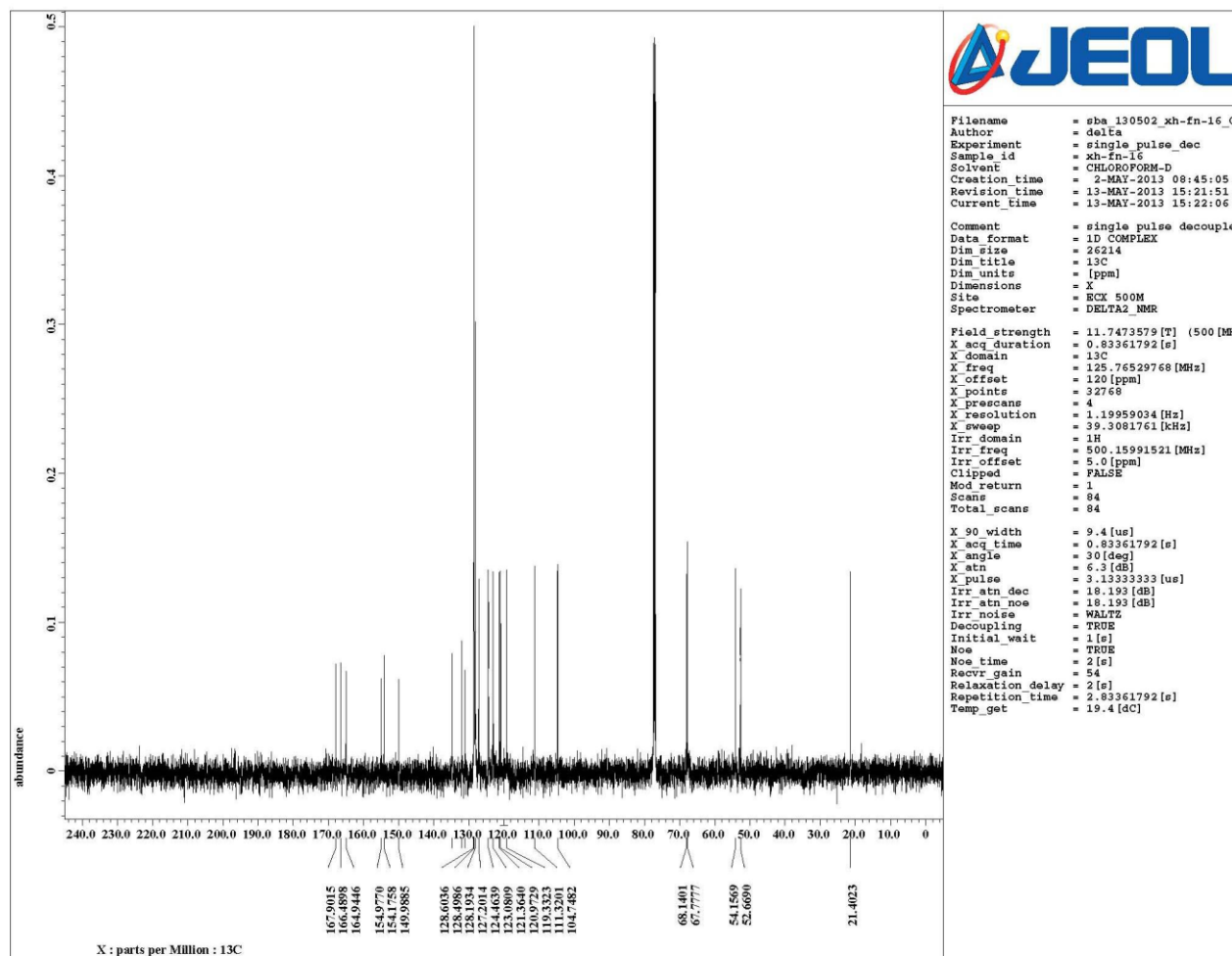
Figure S63. The ^{13}C -NMR Spectra of 5p.

Figure S64. The IR spectra of 5p.

