

Naturally Occurring Homoisoflavonoids Function as Potent Protein Tyrosine Kinase Inhibitors by c-Src-based High-Throughput Screening

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Supporting Information

Page 3–21, spectroscopic data of haematoxylol (1), epihaematoxylol (2), 4-*O*-methylhaematoxylol (3), 4-*O*-methylepihaematoxylol (4), haematoxylene (6), haematoxylone (7), isohematoxylin (10), sappanone B (11), sappanchalcone (20), hematoxylol (25) and hematoxylin (26).

Figure S1. ¹H NMR spectrum of haematoxylol (1) in CD₃OD.

Figure S2. ¹³C NMR and DEPT spectra of haematoxylol (1) in CD₃OD.

Figure S3. LC-MS spectrum of haematoxylol (1).

Figure S4. ¹H NMR spectrum of epihaematoxylol (2) in CD₃OD.

Figure S5. LC-MS spectrum of epihaematoxylol (2).

Figure S6. ¹H NMR spectrum of 4-*O*-methylhaematoxylol (3) in CD₃OD.

Figure S7. ¹³C NMR and DEPT spectra of 4-*O*-methylhaematoxylol (3) in CD₃OD.

Figure S8. LC-MS spectrum of 4-*O*-methylhaematoxylol (3).

Figure S9. ¹H NMR spectrum of 4-*O*-methylepihaematoxylol (4) in CD₃OD.

Figure S10. ¹³C NMR and DEPT spectra of 4-*O*-methylepihaematoxylol (4) in CD₃OD.

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Figure S11. LC-MS spectrum of 4-*O*-methylepihaematoxylol (**4**).

Figure S12. ^1H NMR spectrum of haematoxylene (**6**) in CD_3OD .

Figure S13. ^{13}C NMR and DEPT spectrum of haematoxylene (**6**) in CD_3OD .

Figure S14. LC-MS spectrum of haematoxylene (**6**).

Figure S15. ^1H NMR spectrum of haematoxylone (**7**) in CD_3OD .

Figure S16. ^{13}C NMR and DEPT spectrum of haematoxylone (**7**) in CD_3OD .

Figure S17. LC-MS spectrum of haematoxylone (**7**).

Figure S18. ^1H NMR spectrum of isohematoxylin (**10**) in CD_3COCD_3 .

Figure S19. ^{13}C NMR and DEPT spectrum of isohematoxylin (**10**) in CD_3COCD_3 .

Figure S20. LC-MS spectrum of isohematoxylin (**10**).

Figure S21. ^1H NMR spectrum of sappanone B (**11**) in CD_3COCD_3 .

Figure S22. LC-MS spectrum of sappanone B (**11**).

Figure S23. ^1H NMR spectrum of sappanchalcone (**20**) in CD_3COCD_3 .

Figure S24. LC-MS spectrum of sappanchalcone (**20**).

Figure S25. ^1H NMR spectrum of hematoxylol (**25**) in CD_3OD .

Figure S26. LC-MS spectrum of hematoxylol (**25**).

Figure S27. ^1H NMR spectrum of hematoxylin (**26**) in CD_3COCD_3 .

Figure S28. LC-MS spectrum of hematoxylin (**26**).

Page 22–32: Purity checks for the potent protein tyrosine kinase inhibitors 1–4, 6, 7, 10, 11, 20, 25 and 26 by HPLC with two different mobile phases ($\text{CH}_3\text{CN}-\text{H}_2\text{O}$, 2%~25% in 9 min / $\text{CH}_3\text{OH}-\text{H}_2\text{O}$, 5%~40% in 15 min).

Figure S29. HPLC purity checks of compound **1**.

Figure S30. HPLC purity checks of compound **2**.

Figure S31. HPLC purity checks of compound **3**.

Figure S32. HPLC purity checks of compound **4**.

Figure S33. HPLC purity checks of compound **6**.

Figure S34. HPLC purity checks of compound **7**.

Figure S35. HPLC purity checks of compound **10**.

Figure S36. HPLC purity checks of compound **11**.

Figure S37. HPLC purity checks of compound **20**.

Figure S38. HPLC purity checks of compound **25**.

Figure S39. HPLC purity checks of compound **26**.

Figure S1. ^1H NMR spectrum of haematoxylol (**1**) in CD_3OD .

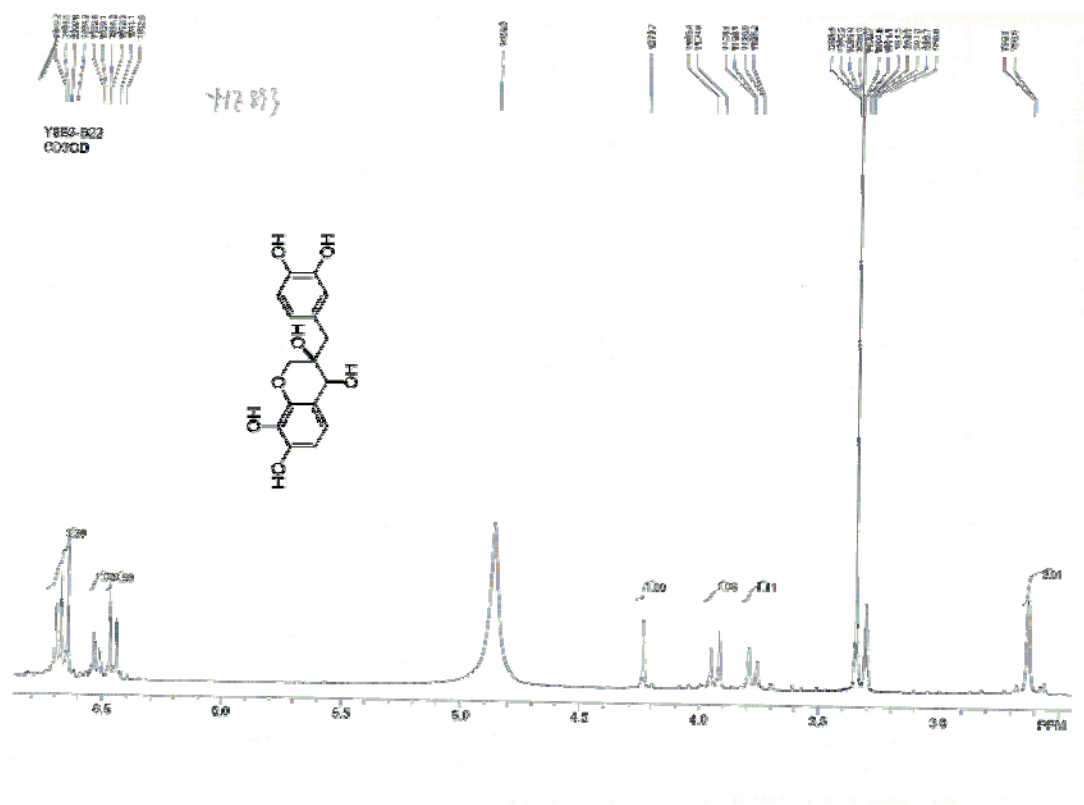


Figure S2. ^{13}C NMR and DEPT spectra of haematoxylol (**1**) in CD_3OD .

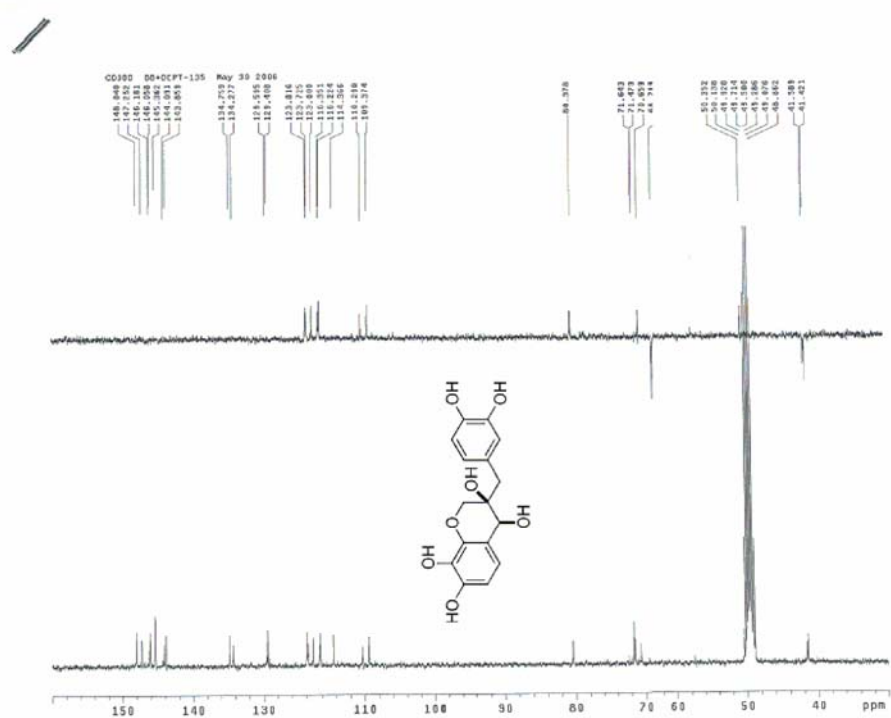


Figure S3. LC-MS spectrum of haematoxylol (1).

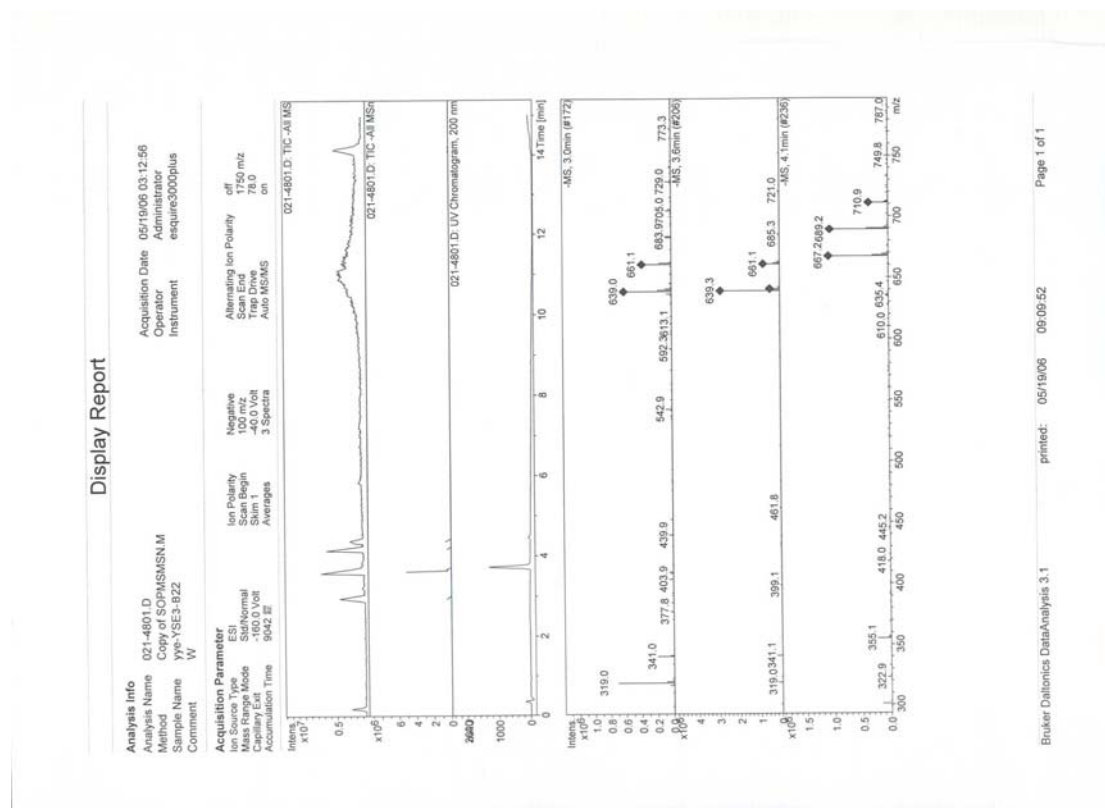
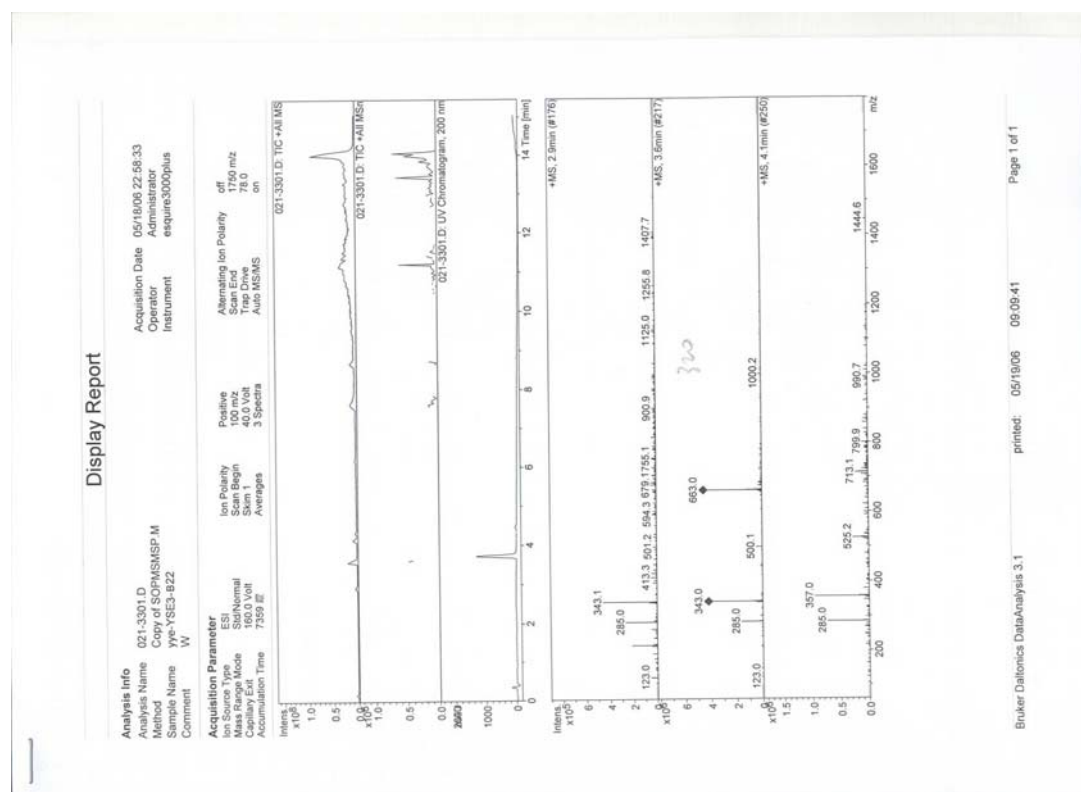


Figure S4. ^1H NMR spectrum of epihaematoxylol (2) in CD_3OD .

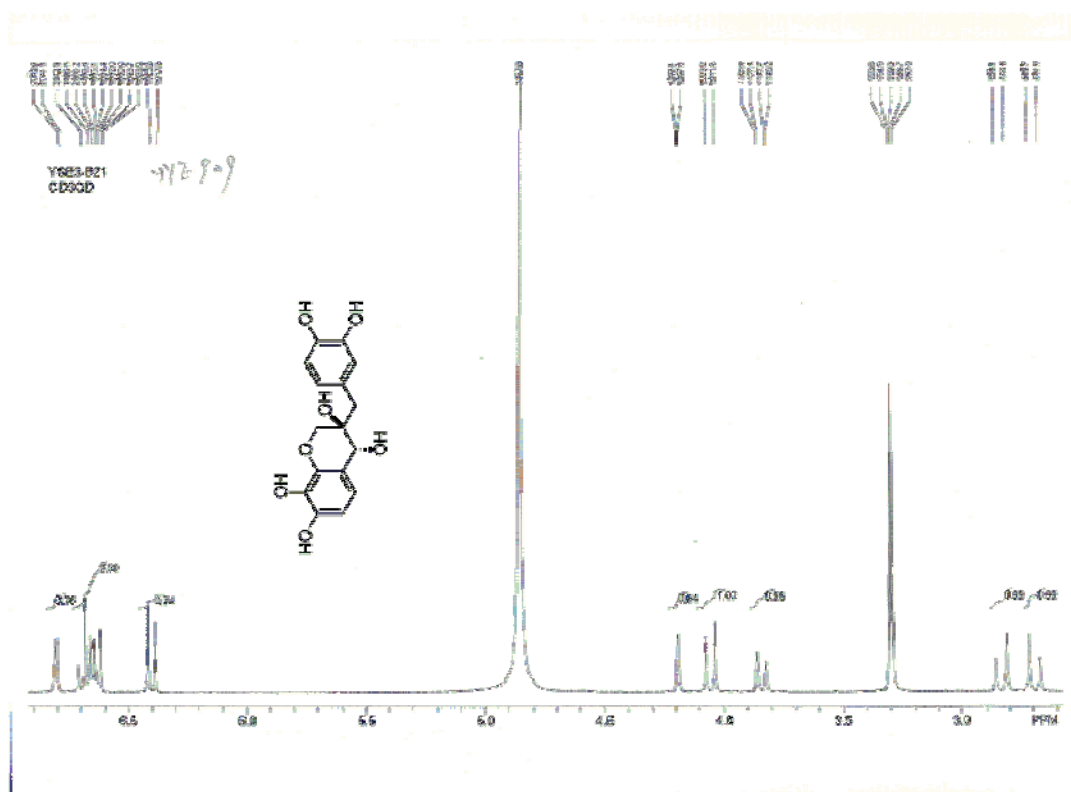
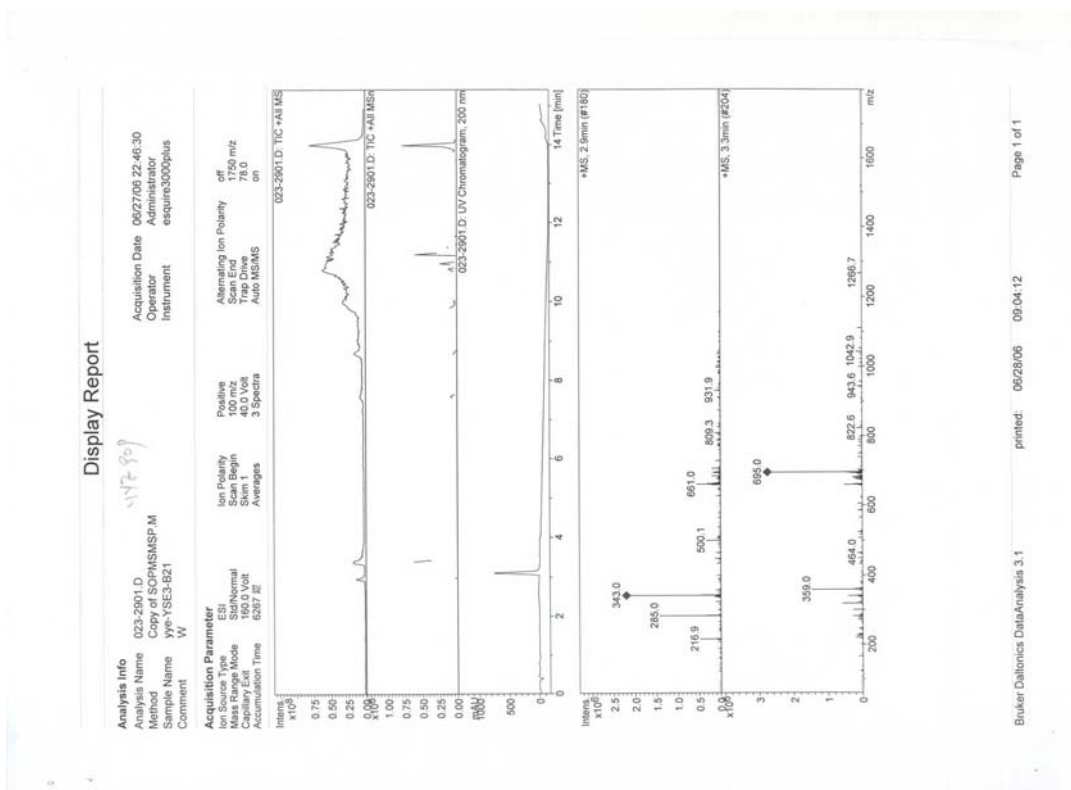
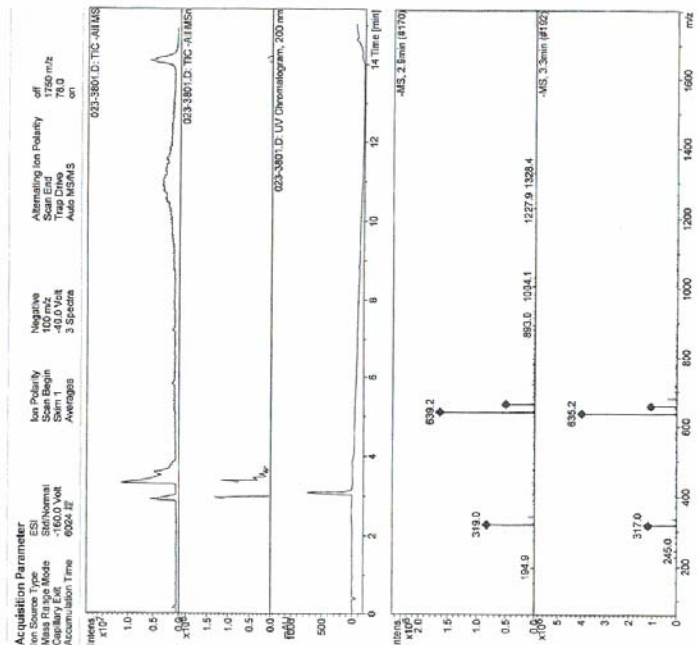


Figure S5. LC-MS spectrum of epihaematoxylol (2).



| | | | |
|---------------|--------------------|------------------|-------------------|
| Analysis Info | 023-3801.D | Acquisition Date | 06/23/05 01:16:35 |
| Analysis Name | Copy of SOP\NMSM.M | Operator | Administrator |
| Method | yje-YSE3-B21 | Instrument | esquire300plus |
| Sample Name | | | |
| Comment | | | |



Bruker Daltonics DataAnalysis 3.1 printed: 06/28/06 09:04:20 Page 1 of 1

Figure S6. ^1H NMR spectrum of 4-*O*-methylhaematoxylol (**3**) in CD_3OD .

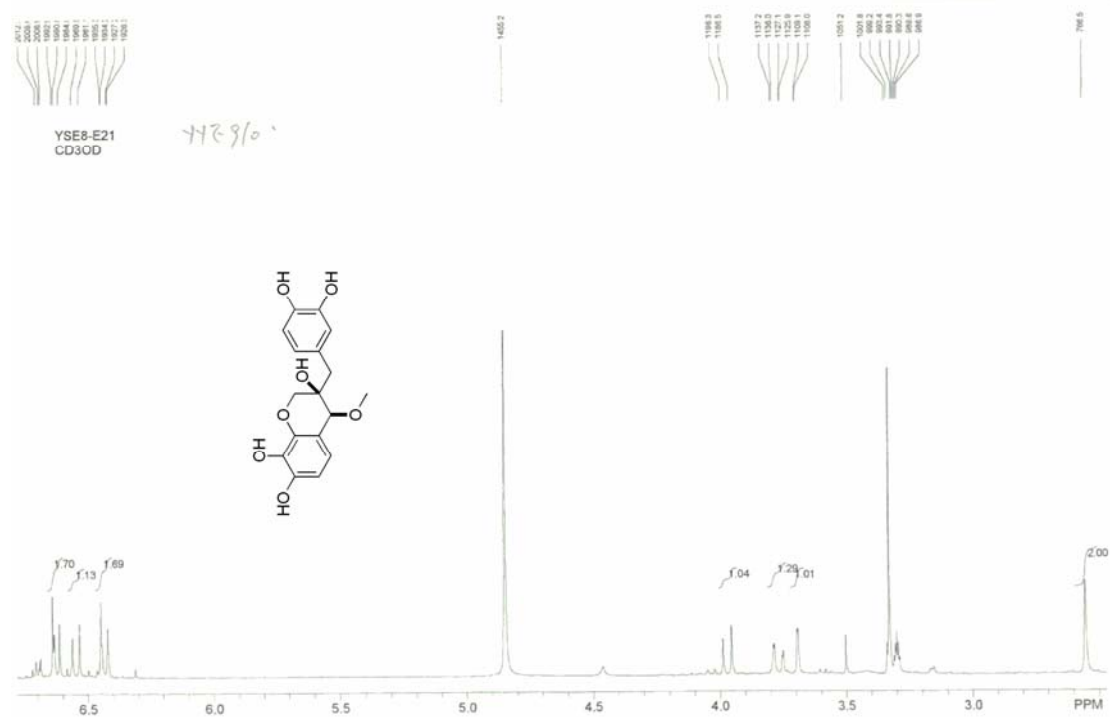


Figure S7. ^{13}C NMR and DEPT spectra of 4-*O*-methylhaematoxylol (**3**) in CD_3OD .

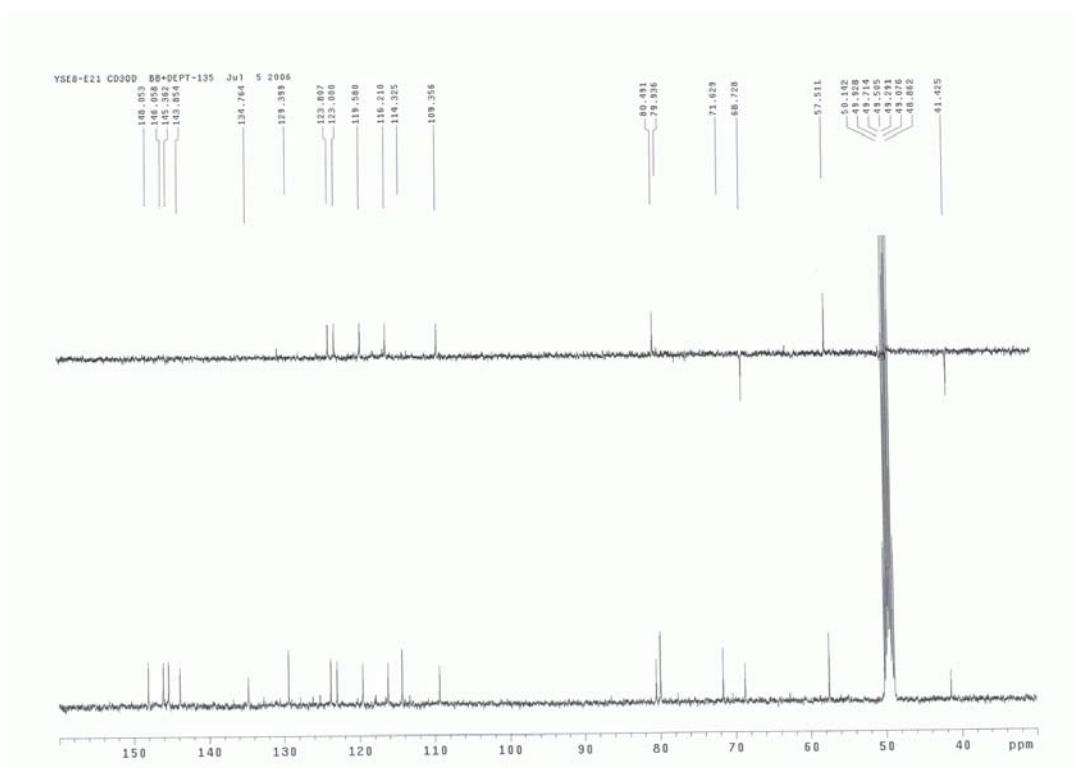
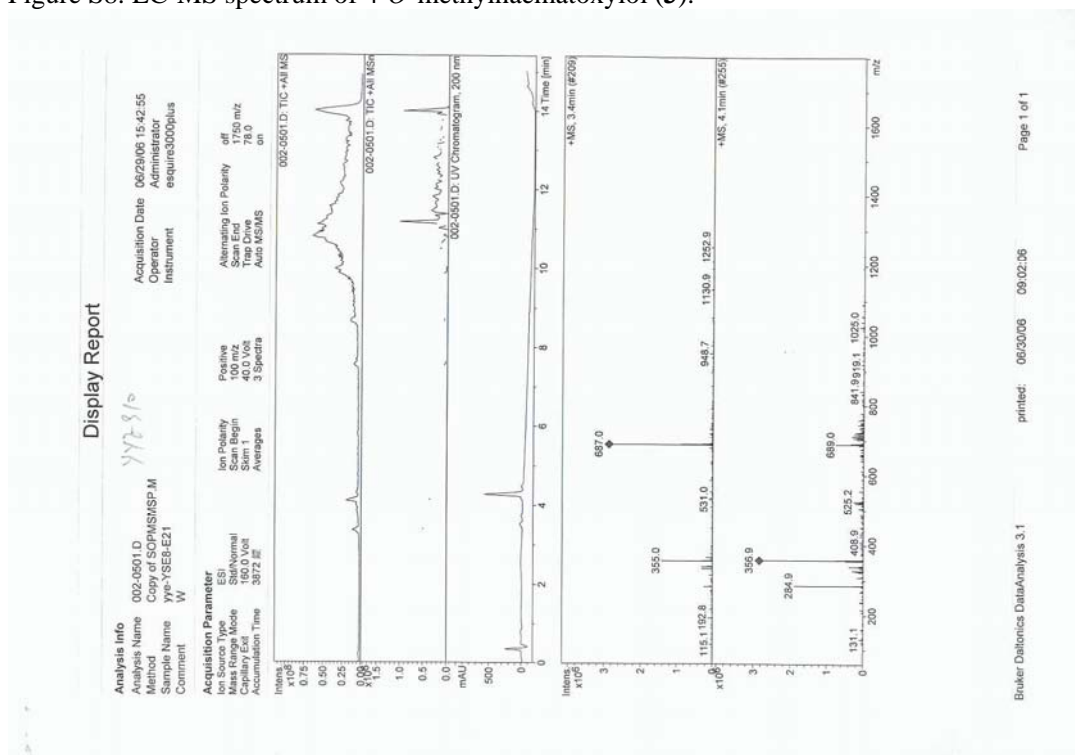


Figure S8. LC-MS spectrum of 4-*O*-methylhaematoxylol (**3**).



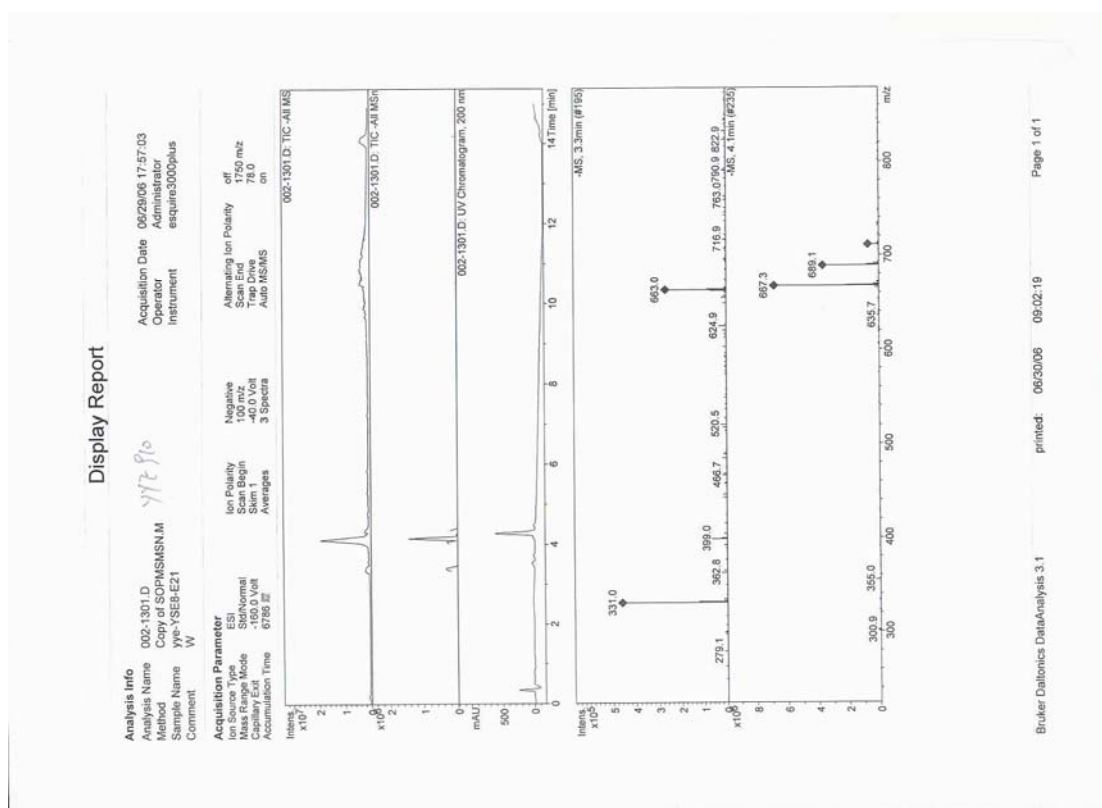


Figure S9. ^1H NMR spectrum of 4-*O*-methylepiphaematoxylol (**4**) in CD_3OD .

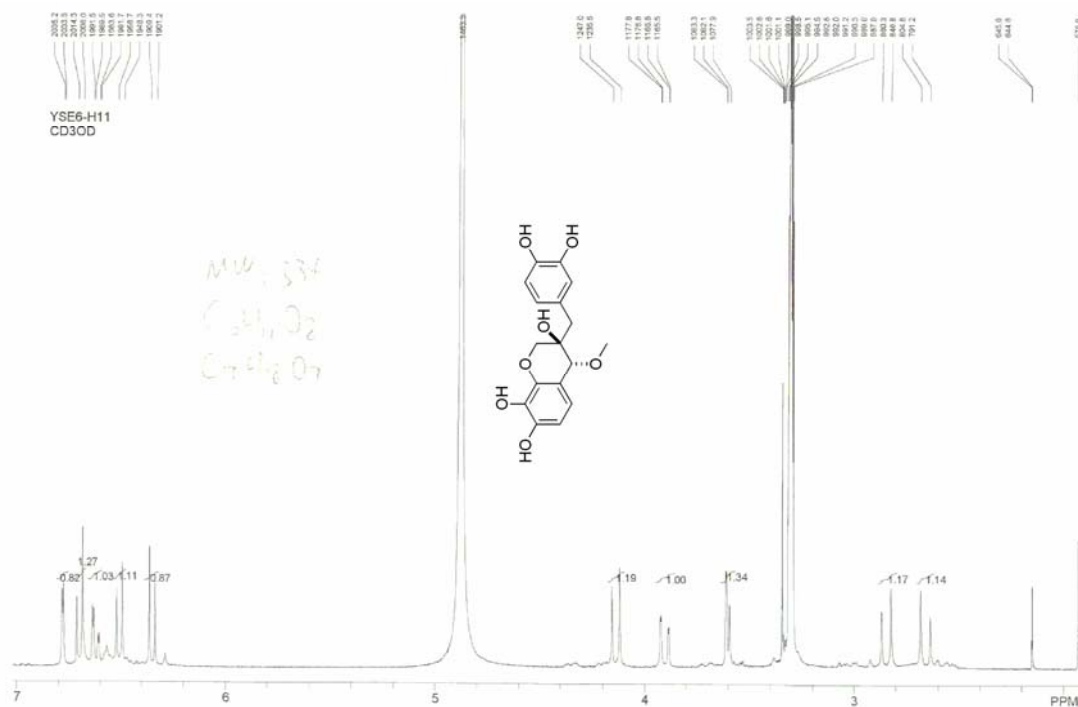


Figure S10. ^{13}C NMR and DEPT spectra of 4-*O*-methylepihaematoxylol (**4**) in CD_3OD .

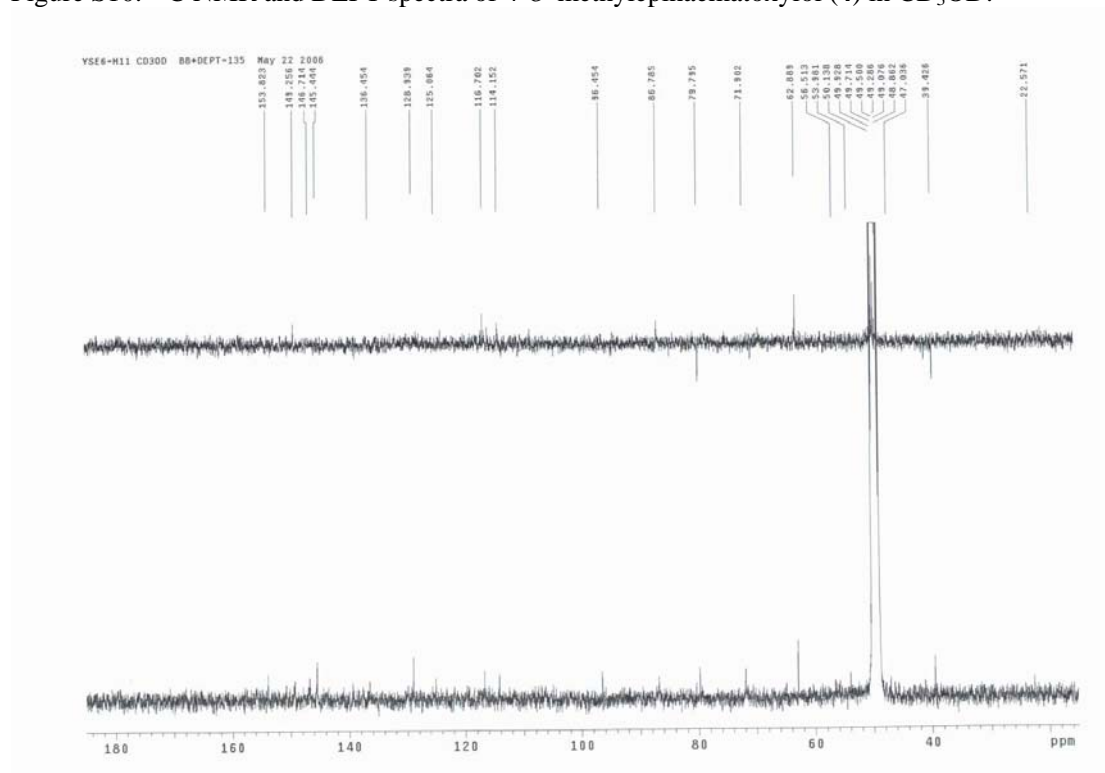


Figure S11. LC-MS spectrum of 4-*O*-methylepihaematoxylol (**4**).

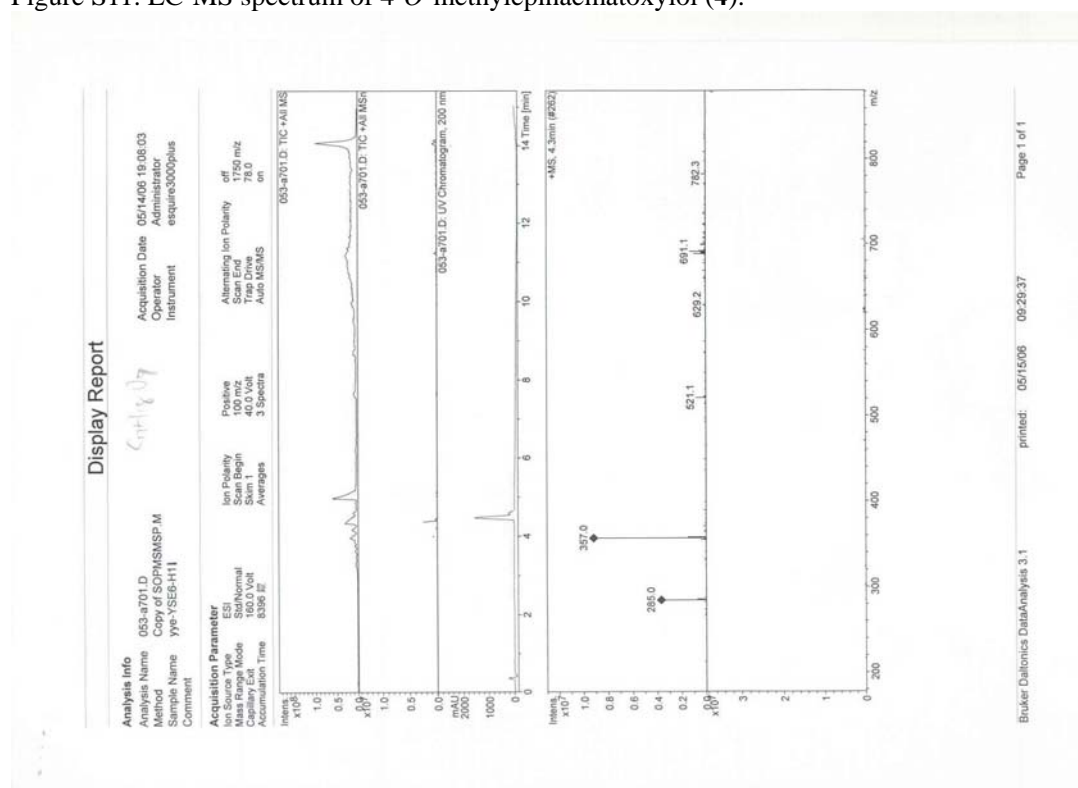


Figure S12. ^1H NMR spectrum of haematoxylene (**6**) in CD_3OD .

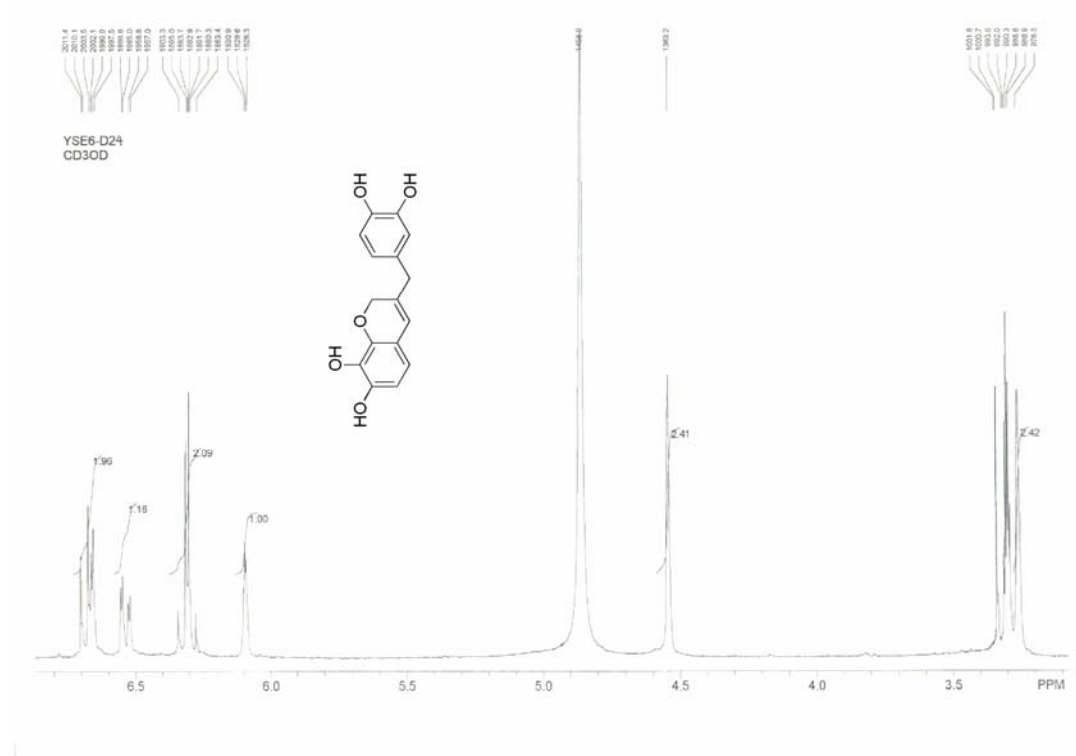


Figure S13. ^{13}C NMR and DEPT spectrum of haematoxylene (**6**) in CD_3OD .

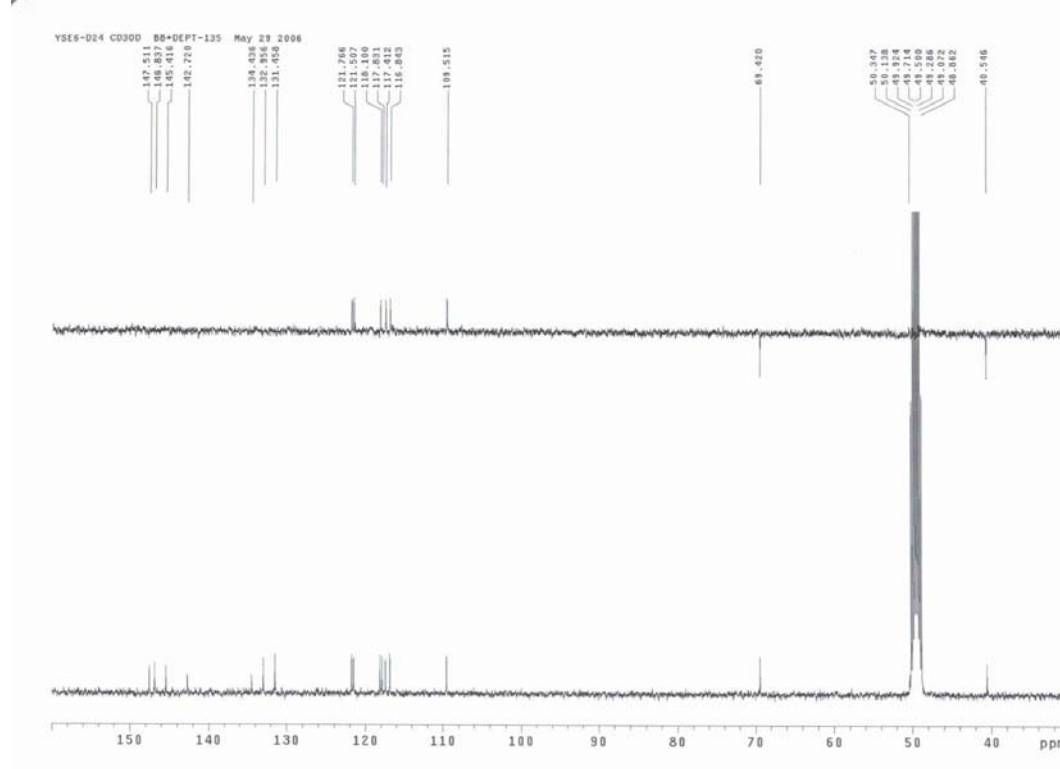


Figure S14. LC-MS spectrum of haematoxylene (6).

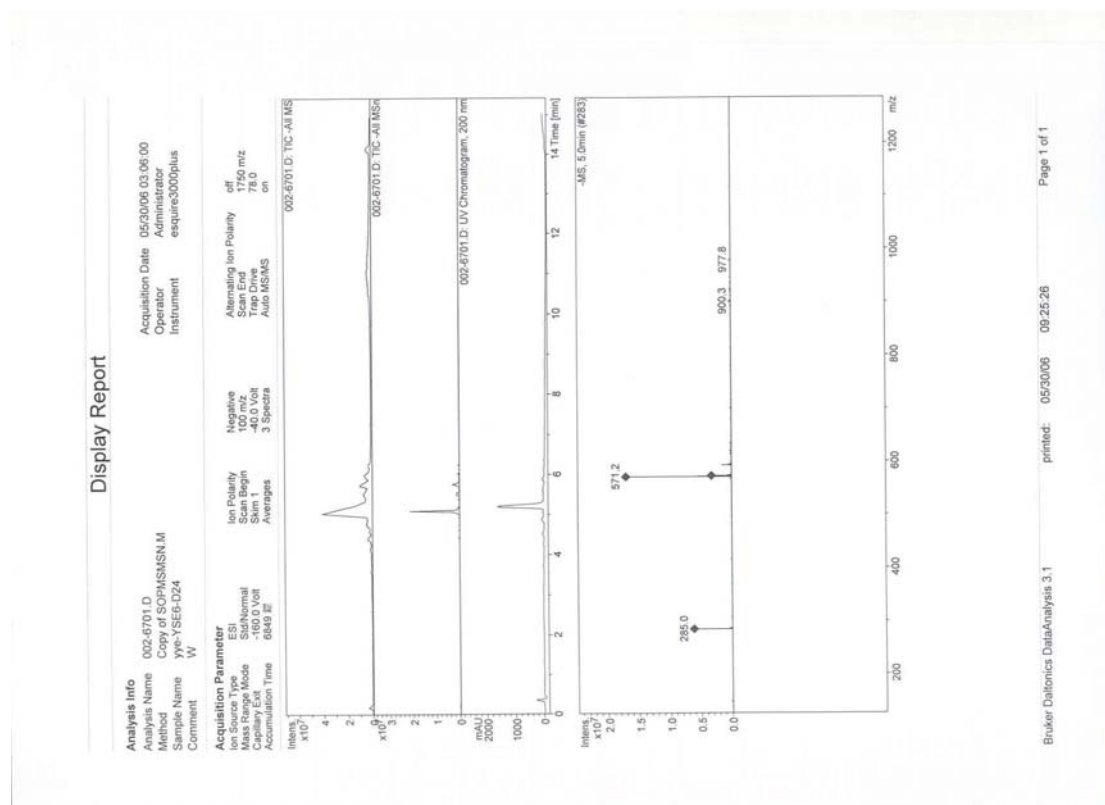
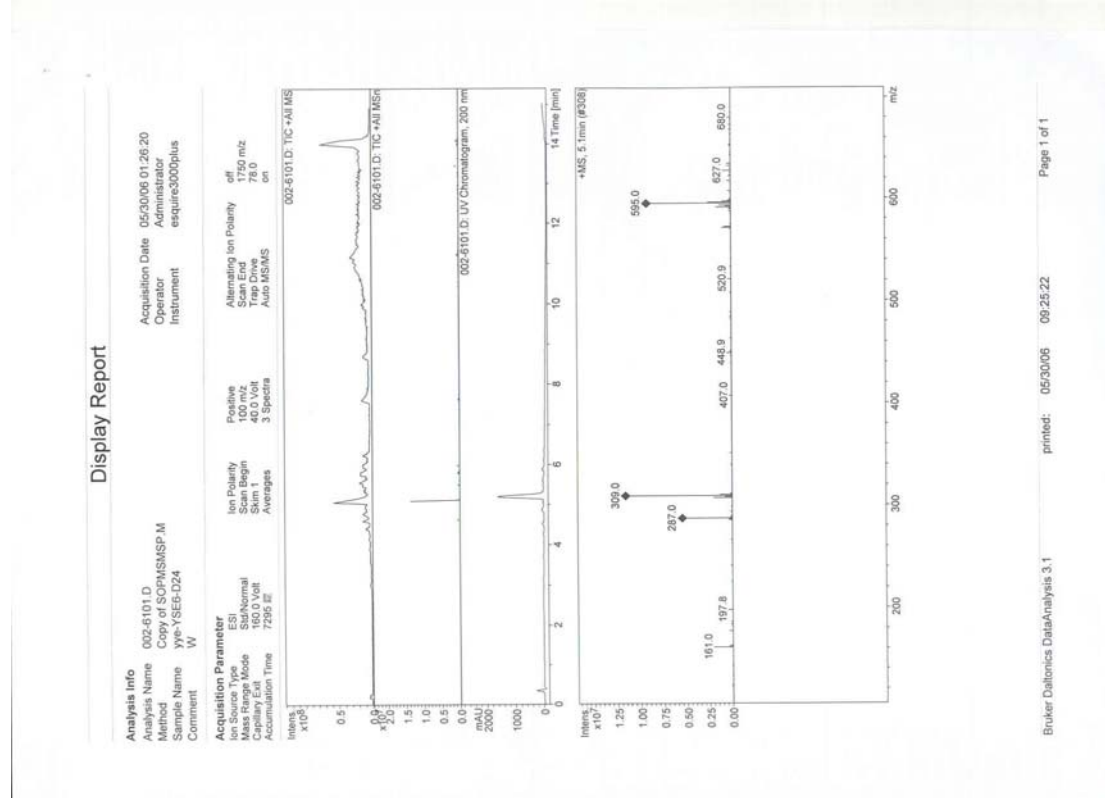


Figure S15. ^1H NMR spectrum of haematoxylone (7) in CD_3OD .

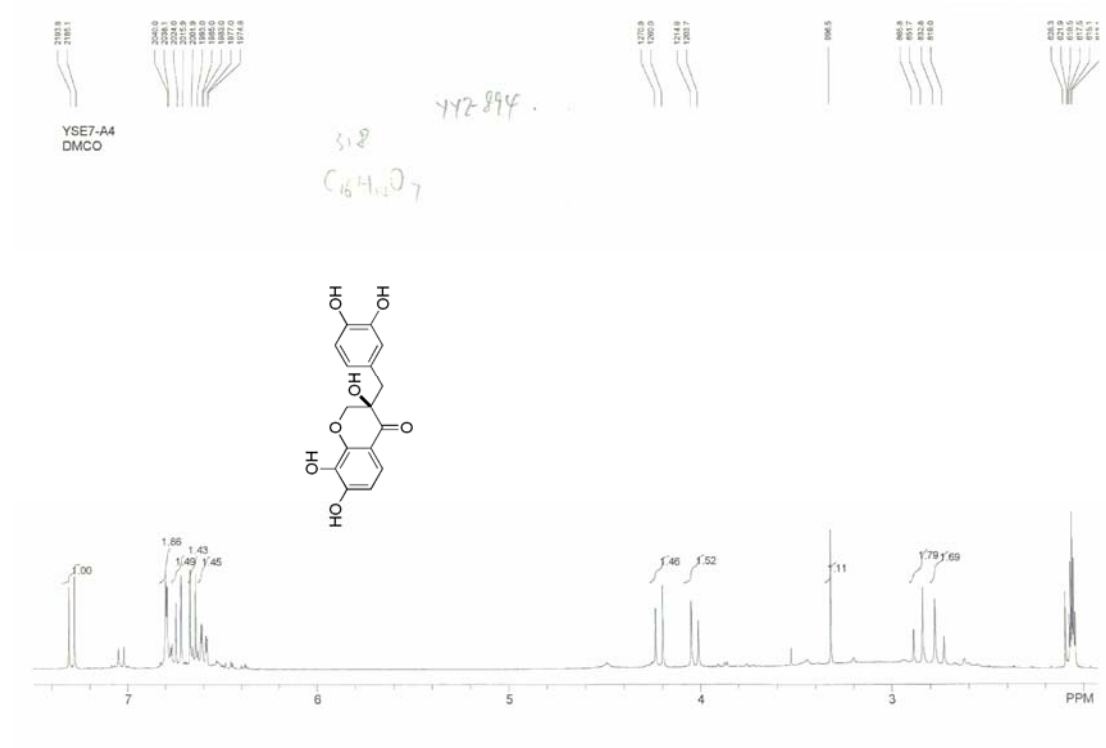


Figure S16. ^{13}C NMR and DEPT spectrum of haematoxylone (7) in CD_3OD .

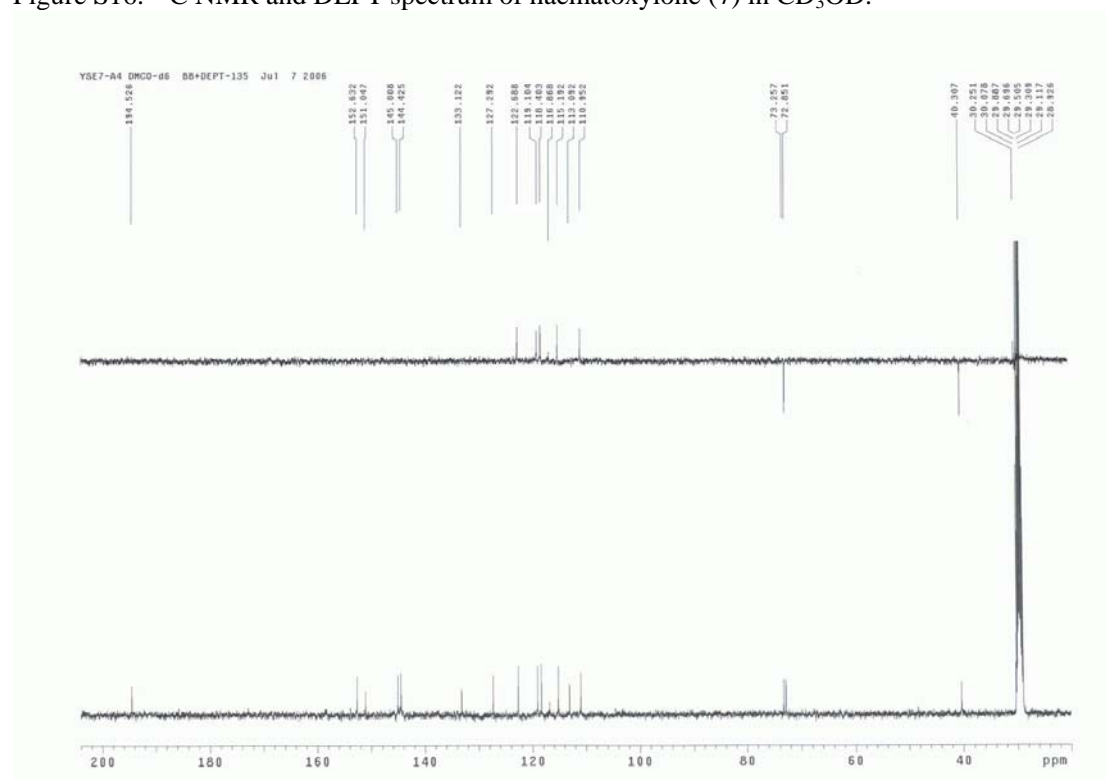


Figure S17. LC-MS spectrum of haematoxylone (7).



Figure S18. ^1H NMR spectrum of isohematoxylin (**10**) in CD_3COCD_3 .

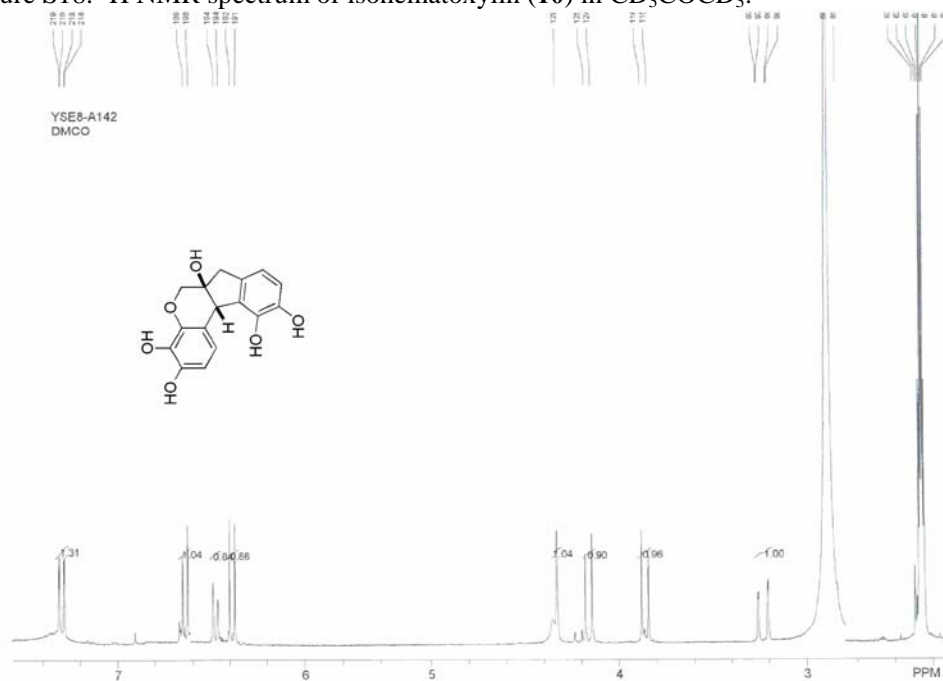


Figure S19. ^{13}C NMR and DEPT spectrum of isohematoxylin (**10**) in CD_3COCD_3 .

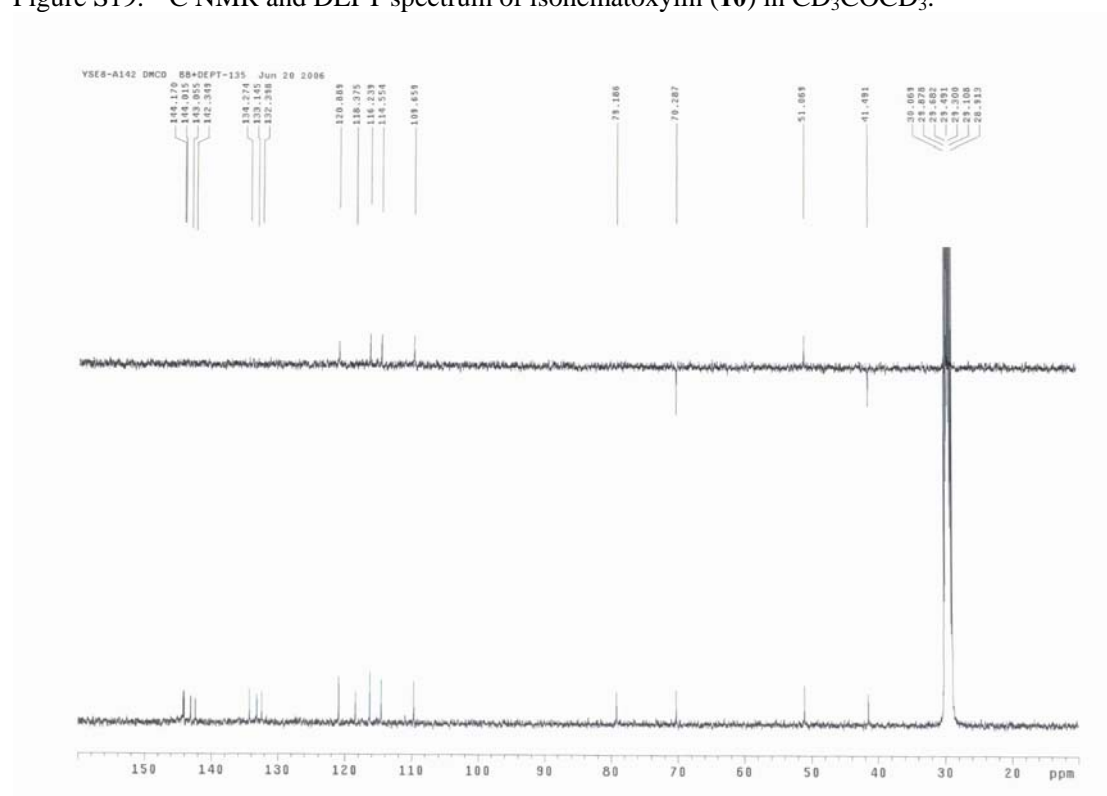


Figure S20. LC-MS spectrum of isohematoxylin (**10**).

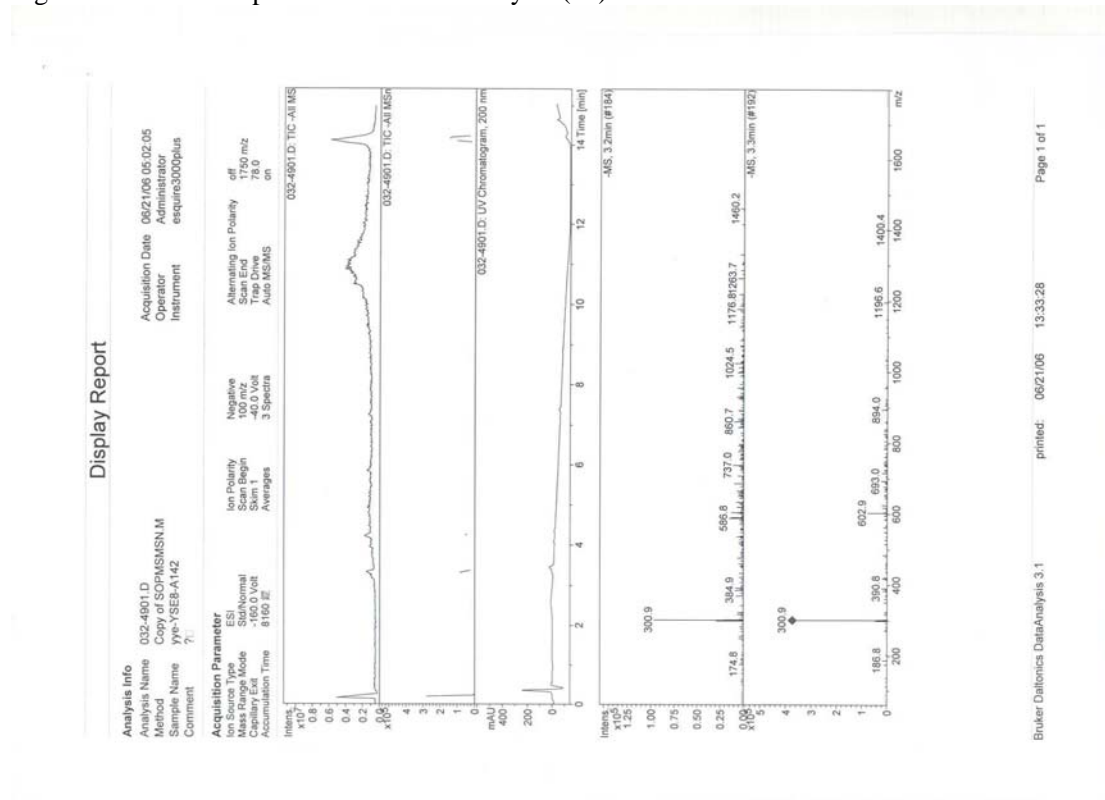


Figure S21. ¹H NMR spectrum of sappanone B (**11**) in CD₃COCD₃.

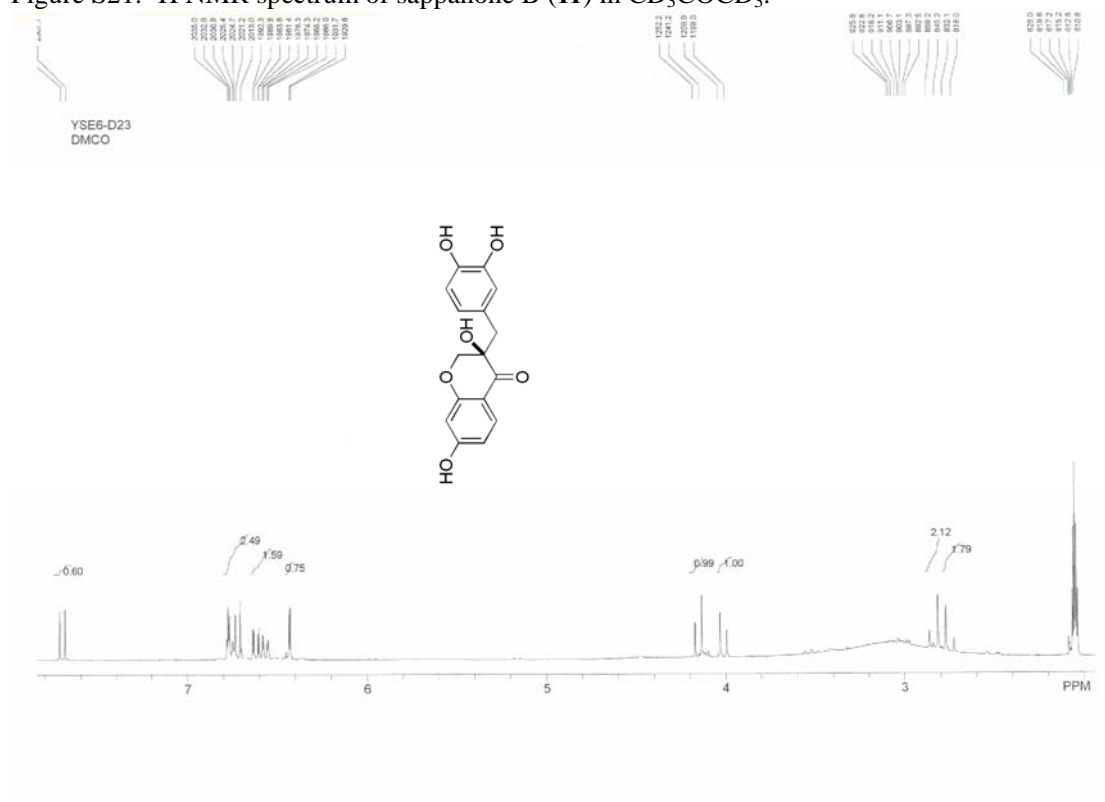
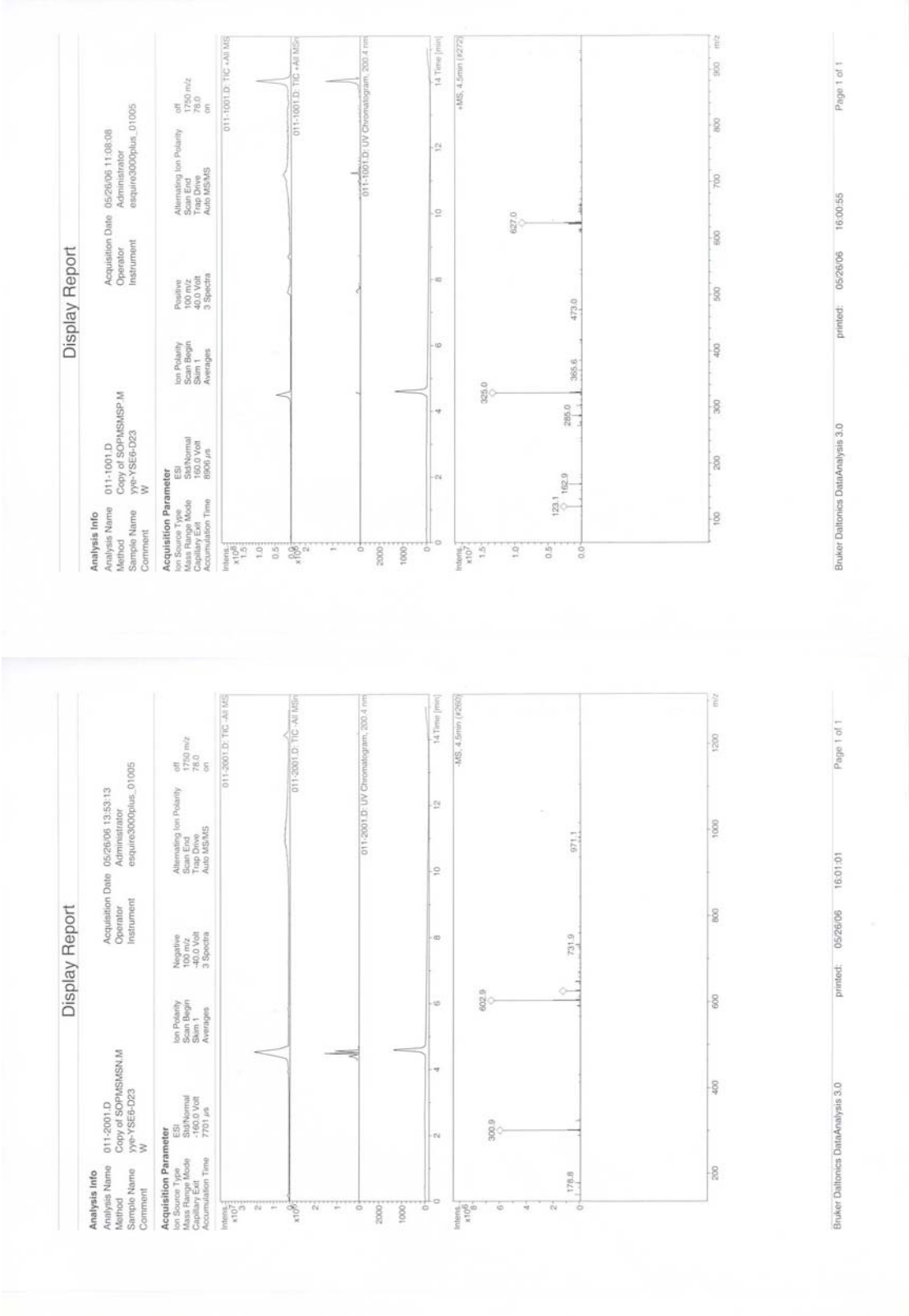


Figure S22. LC-MS spectrum of sappanone B (11).



YSD11-B2
DMCO

Oc1ccc(cc1OC(=O)/C=C/c2ccc(O)c(O)c2)O

Chemical structure of YSD11-B2 is shown above the spectrum.

Integration values for the peaks are listed below the spectrum:

- 8.00: 1.11
- 7.40: 0.08
- 7.20: 0.98
- 7.00: 1.00
- 6.80: 1.00
- 6.30: 0.95
- 6.10: 0.01
- 3.80: 0.45
- 1.50: 1.54

Display Report

Analysis Info

| | | | |
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| Analysis Name | 026-8201.D | Acquisition Date | 05/11/06 12:59:03 |
| Method | Copy of SQP.MS.MSP.M | Operator | Administrator |
| Sample Name | lys-1SD11-EZ | Instrument | esquire3000plus |
| Comment | | | |

Acquisition Parameter

| | | | |
|-------------------|------------|--------------|----------|
| Ion Source Type | ESI | Ion Polarity | Positive |
| Mass Range Mode | StdNormal | Scan End | 1750 m/z |
| Capillary Exit | 160.0 Volt | Trap Drive | 78.0 cm |
| Accumulation Time | 2994.00 | Auto MS/MS | off |

026-8201.D: TIC - All MS

026-8201.D: UV Chromatogram, 200 nm

*MS, 4.8min (#293)

Analysis Info

| | | | |
|---------------|----------------------|------------------|-------------------|
| Analysis Name | 026-8201.D | Acquisition Date | 05/11/06 12:59:03 |
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| Sample Name | lys-1SD11-EZ | Instrument | esquire3000plus |
| Comment | | | |

Acquisition Parameter

| | | | |
|-------------------|------------|--------------|----------|
| Ion Source Type | ESI | Ion Polarity | Positive |
| Mass Range Mode | StdNormal | Scan End | 1750 m/z |
| Capillary Exit | 160.0 Volt | Trap Drive | 78.0 cm |
| Accumulation Time | 2994.00 | Auto MS/MS | off |

026-8201.D: TIC - All MS

026-8201.D: UV Chromatogram, 200 nm

*MS, 4.8min (#293)

Analysis Info

| | | | |
|---------------|----------------------|------------------|-------------------|
| Analysis Name | 026-8201.D | Acquisition Date | 05/11/06 12:59:03 |
| Method | Copy of SQP.MS.MSP.M | Operator | Administrator |
| Sample Name | lys-1SD11-EZ | Instrument | esquire3000plus |
| Comment | | | |

Acquisition Parameter

| | | | |
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| Ion Source Type | ESI | Ion Polarity | Positive |
| Mass Range Mode | StdNormal | Scan End | 1750 m/z |
| Capillary Exit | 160.0 Volt | Trap Drive | 78.0 cm |
| Accumulation Time | 2994.00 | Auto MS/MS | off |

026-8201.D: TIC - All MS

026-8201.D: UV Chromatogram, 200 nm

*MS, 4.8min (#293)

Analysis Info

| | | | |
|---------------|----------------------|------------------|-------------------|
| Analysis Name | 026-8201.D | Acquisition Date | 05/11/06 12:59:03 |
| Method | Copy of SQP.MS.MSP.M | Operator | Administrator |
| Sample Name | lys-1SD11-EZ | Instrument | esquire3000plus |
| Comment | | | |

Acquisition Parameter

| | | | |
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| Capillary Exit | 160.0 Volt | Trap Drive | 78.0 cm |
| Accumulation Time | 2994.00 | Auto MS/MS | off |

026-8201.D: TIC - All MS

026-8201.D: UV Chromatogram, 200 nm

*MS, 4.8min (#293)

Analysis Info

| | |
|---------------|------------|
| Analysis Name | 026-8201.D |
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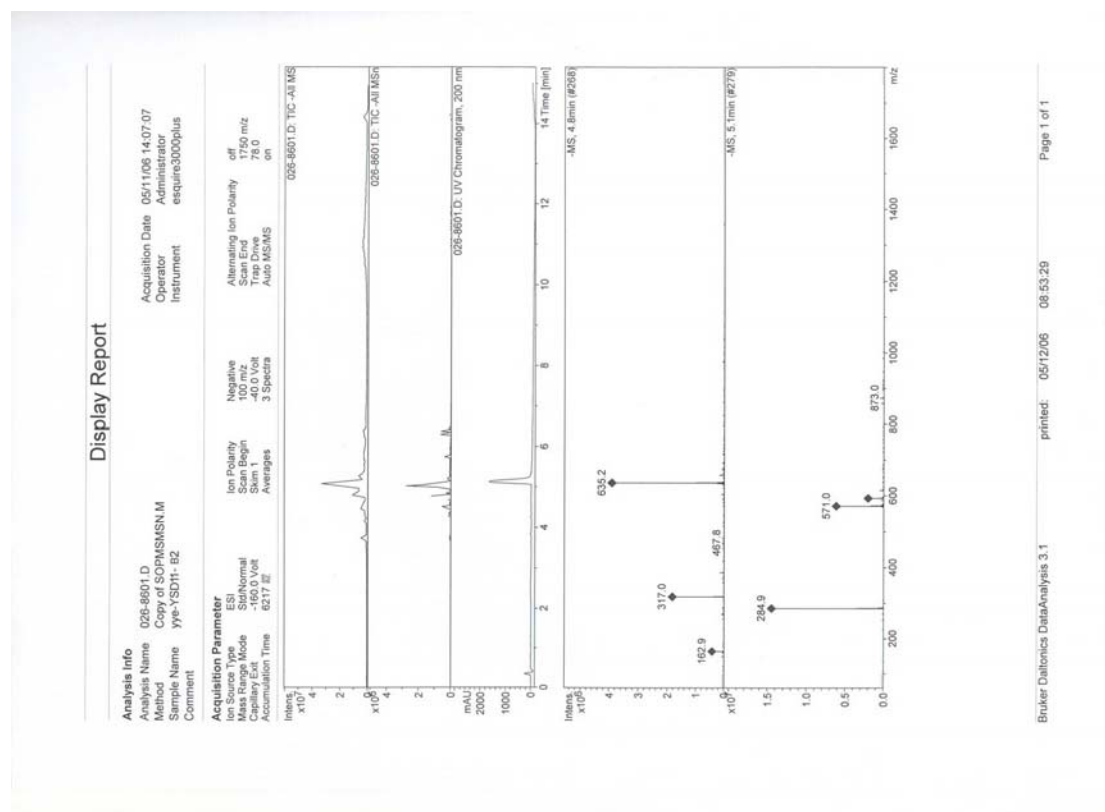


Figure S25. ^1H NMR spectrum of hematoxylol (**25**) in CD_3OD .

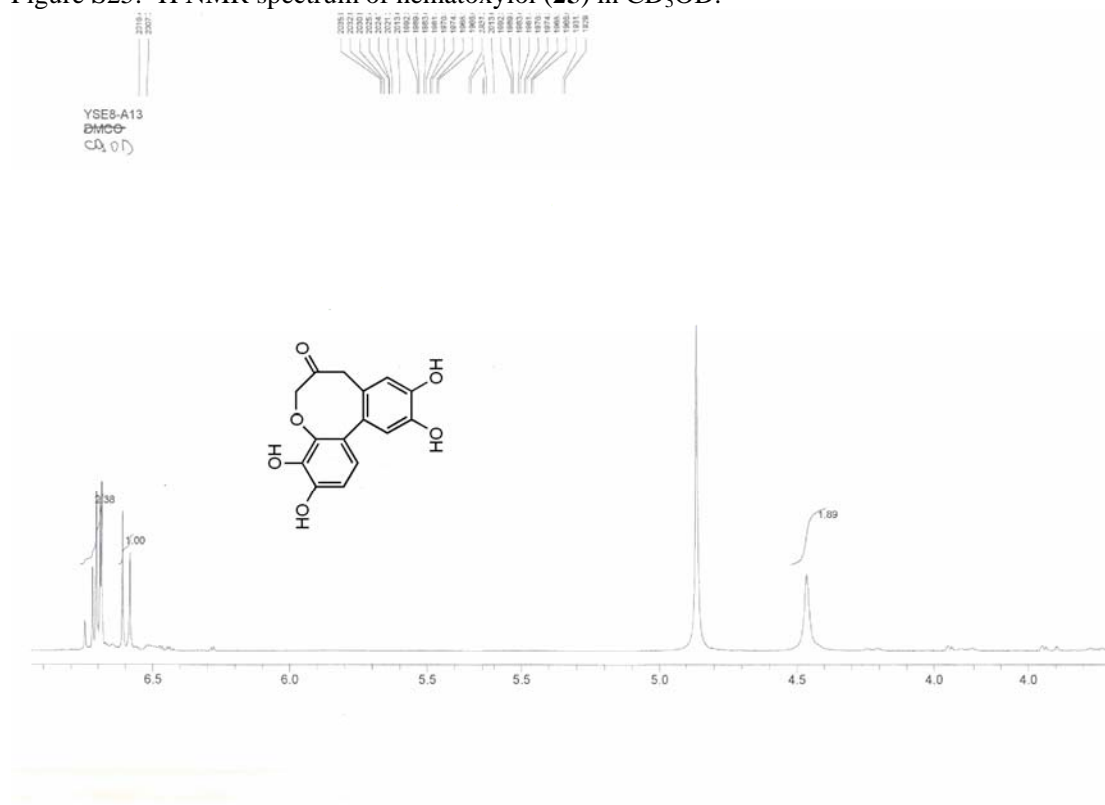


Figure S26. LC-MS spectrum of hematoxylol (25).

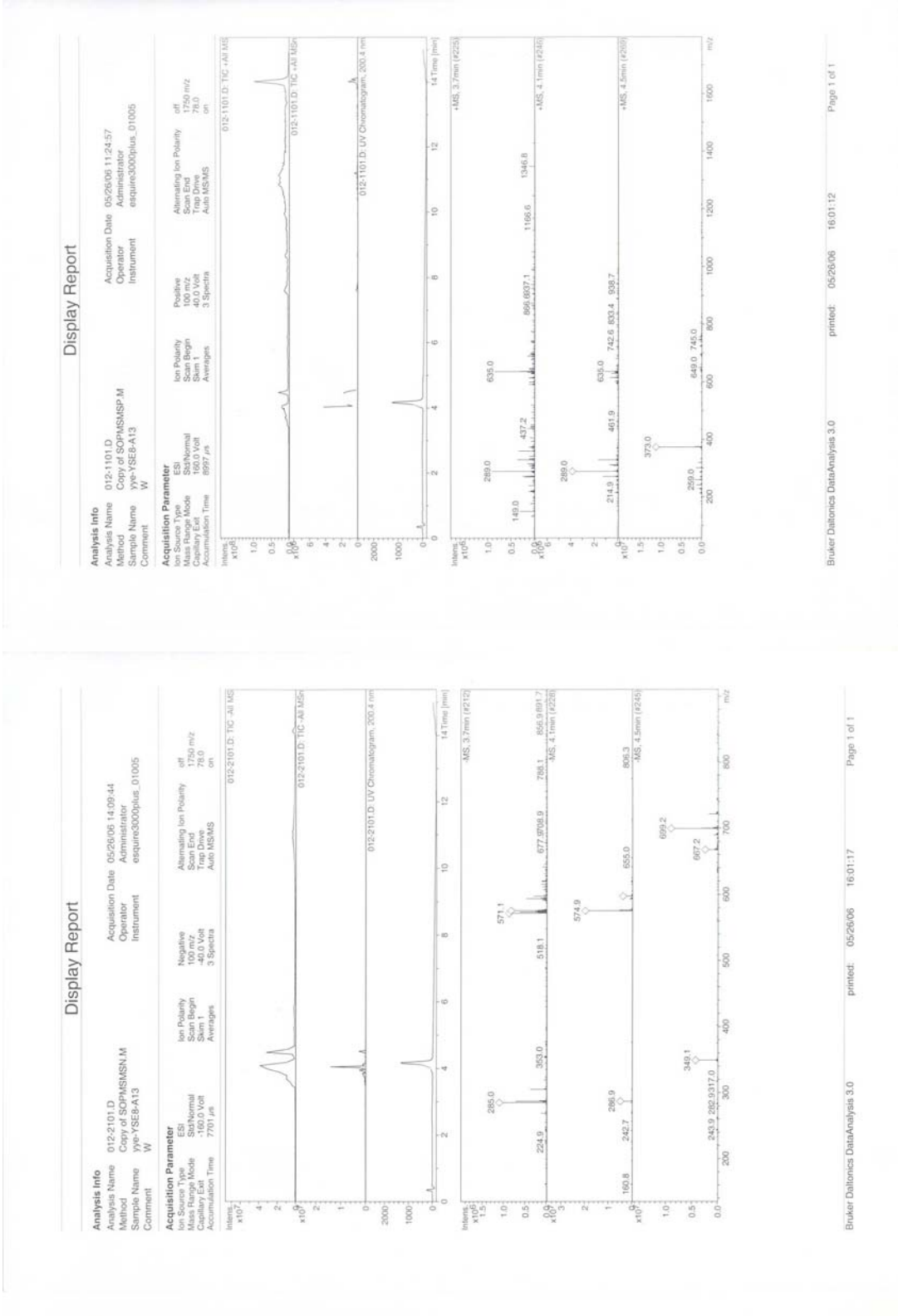


Figure S27. ^1H NMR spectrum of hematoxylin (**26**) in CD_3COCD_3 .

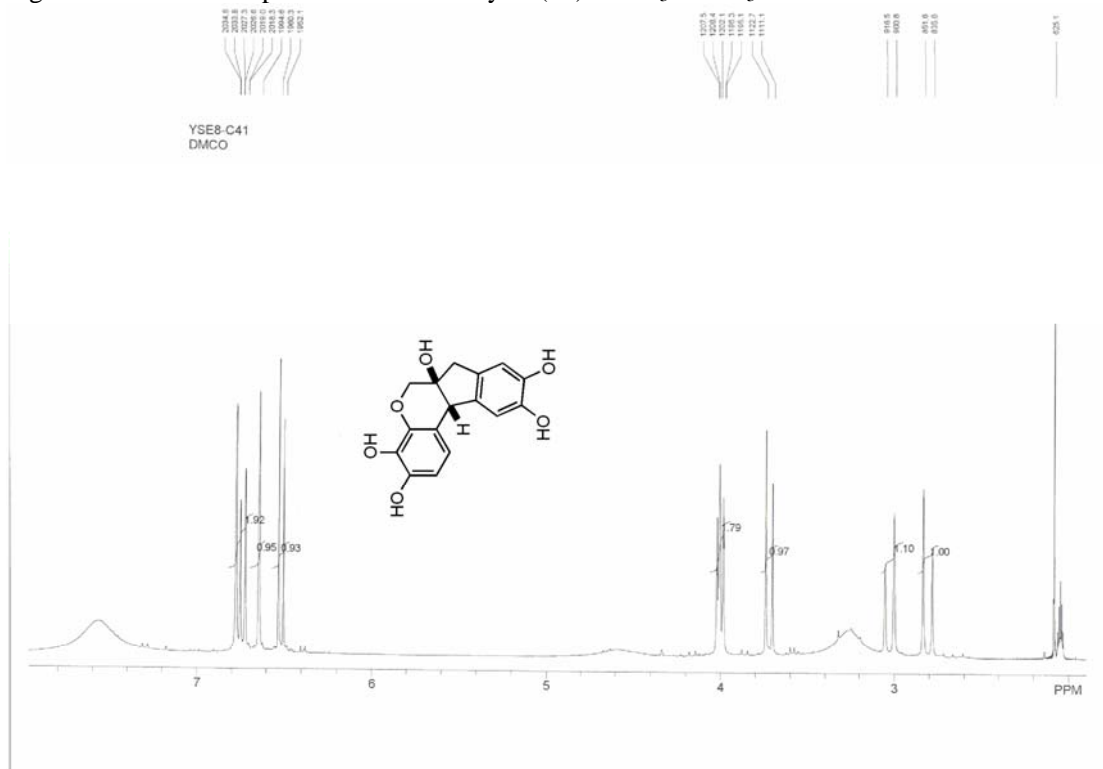
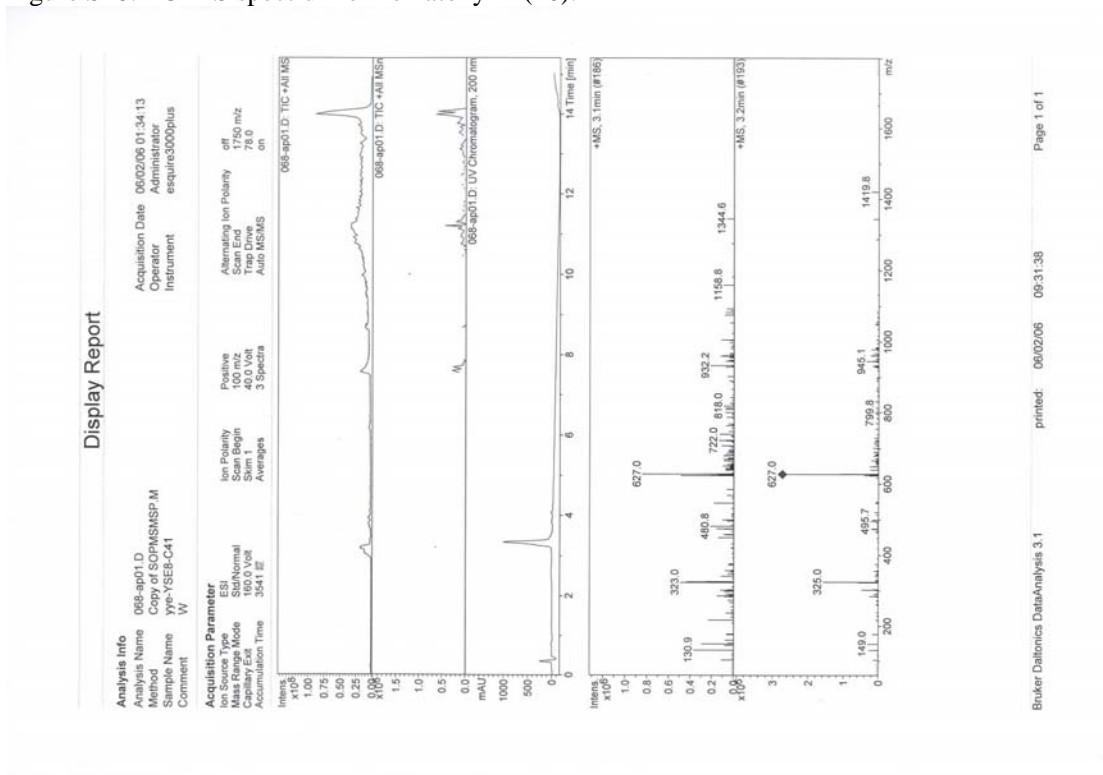


Figure S28. LC-MS spectrum of hematoxylin (**26**).



Display Report

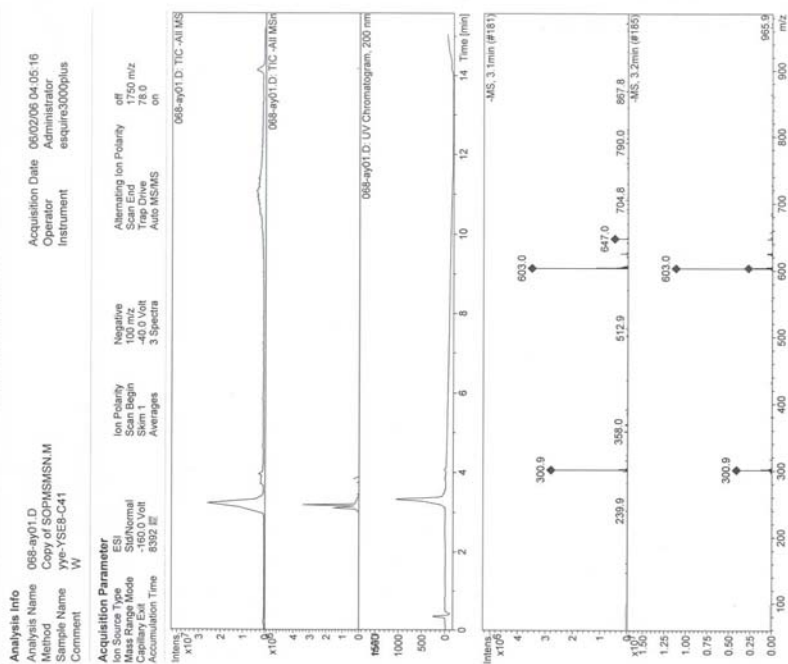


Figure S29. HPLC purity checks of compound 1.

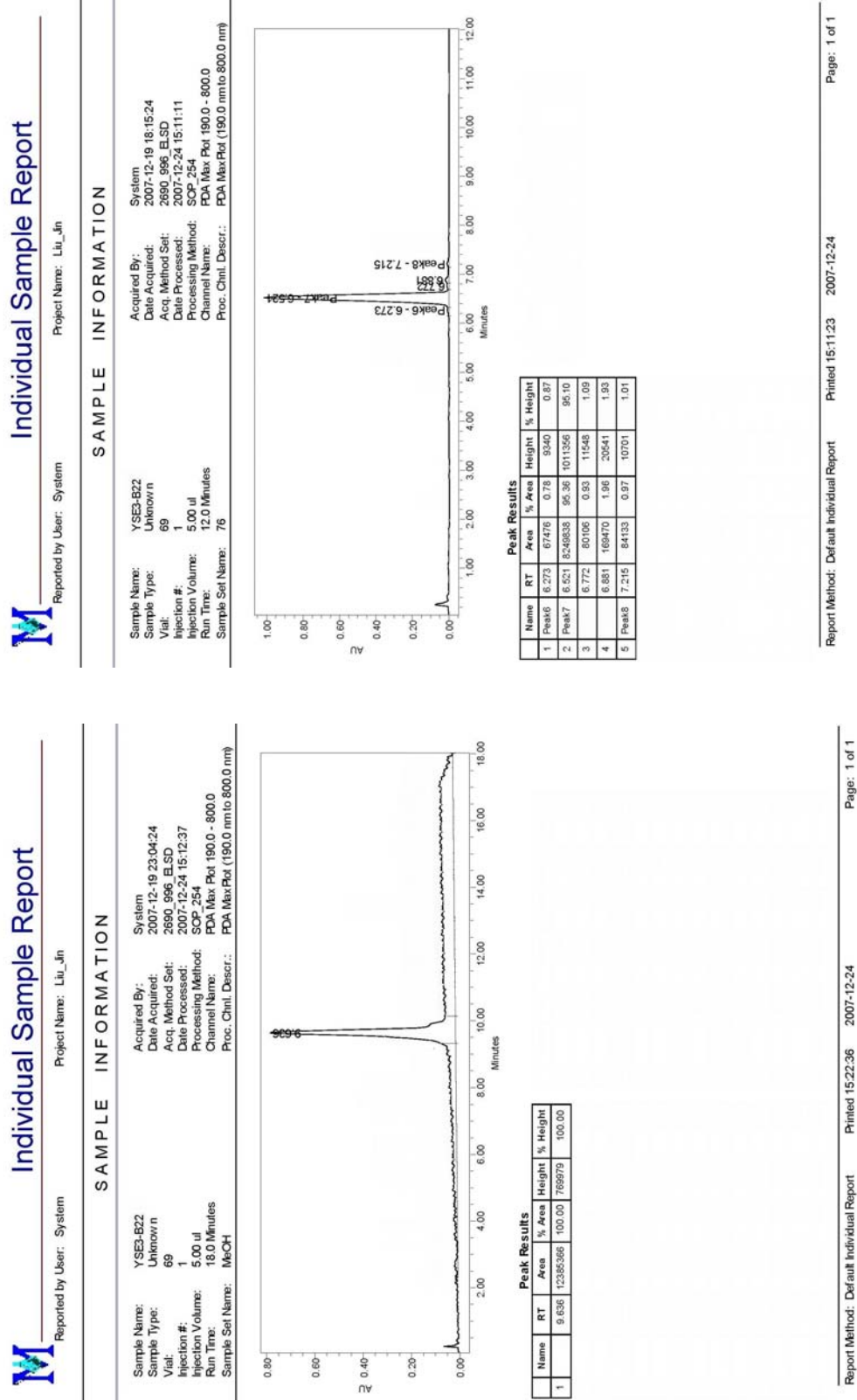


Figure S30. HPLC purity checks of compound 2.

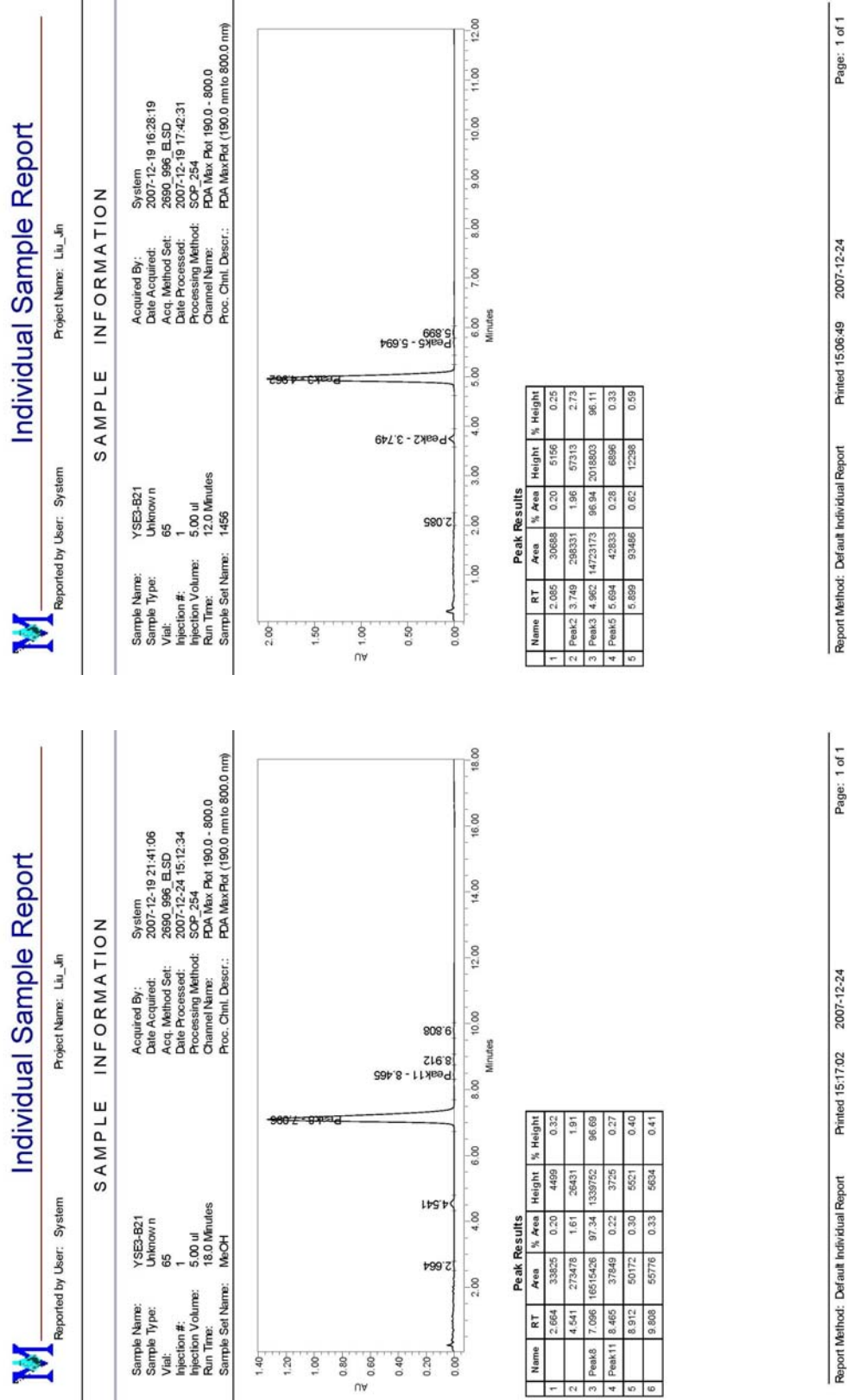


Figure S31. HPLC purity checks of compound 3.

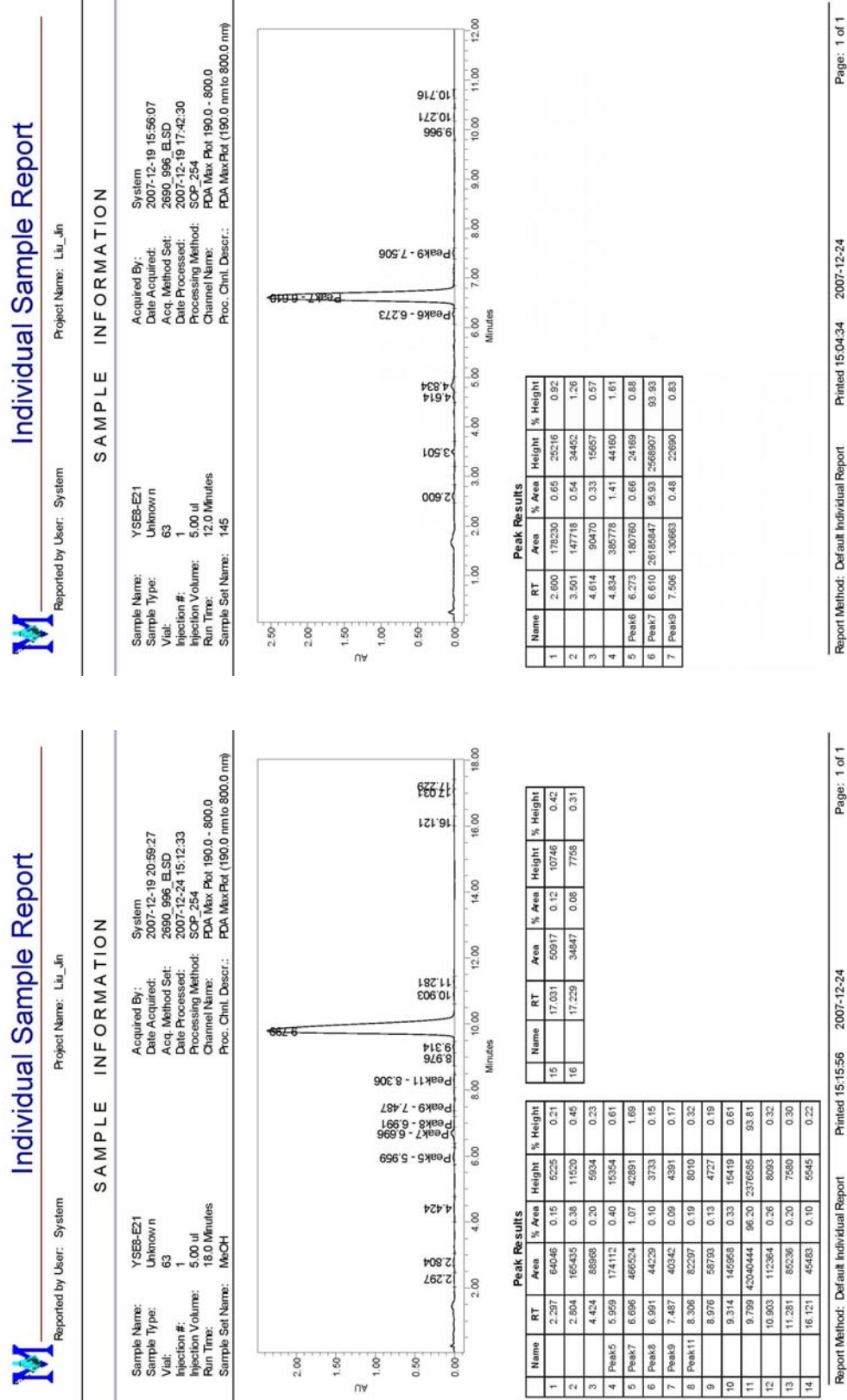


Figure S32. HPLC purity checks of compound 4.

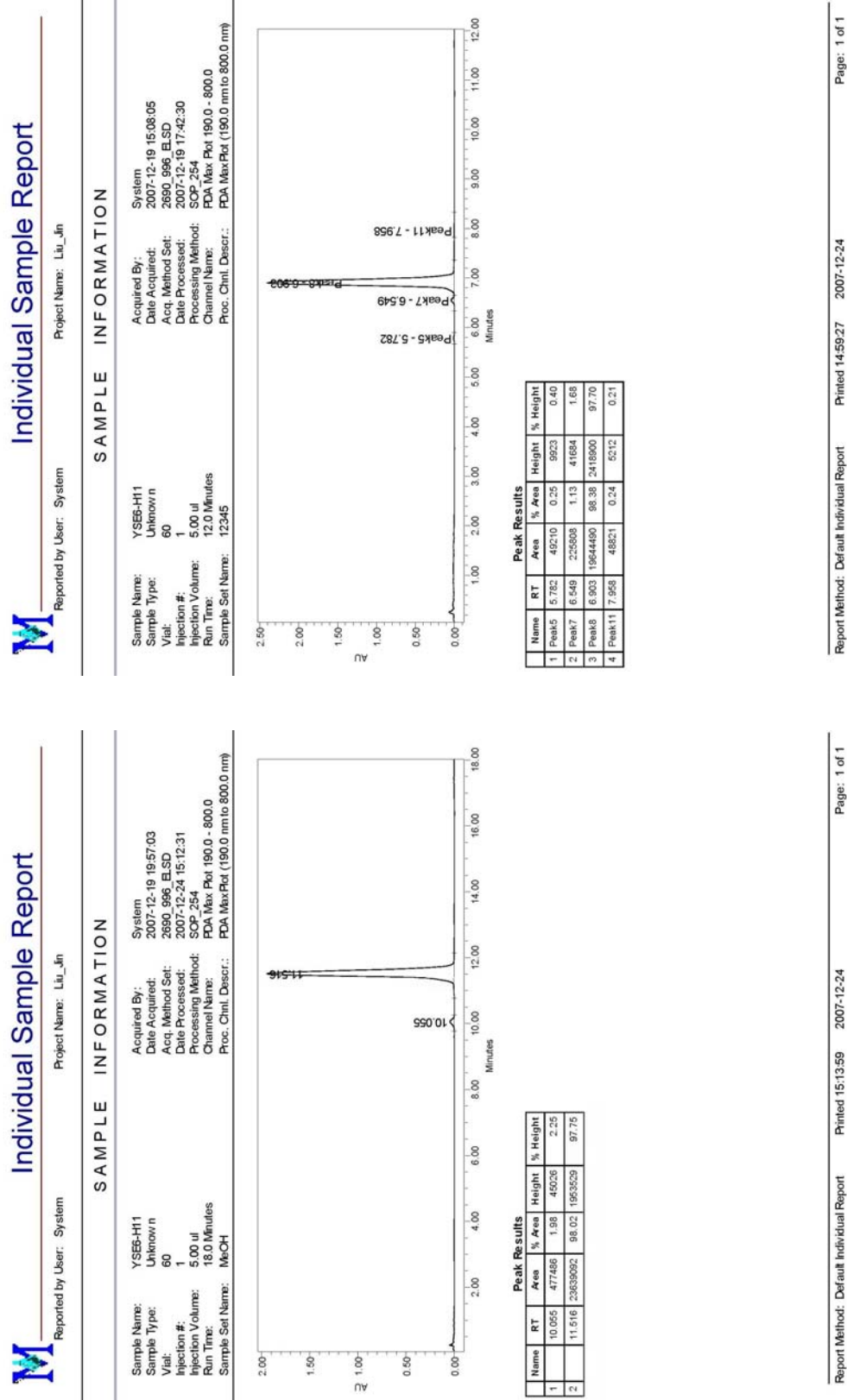


Figure S33. HPLC purity checks of compound 6.

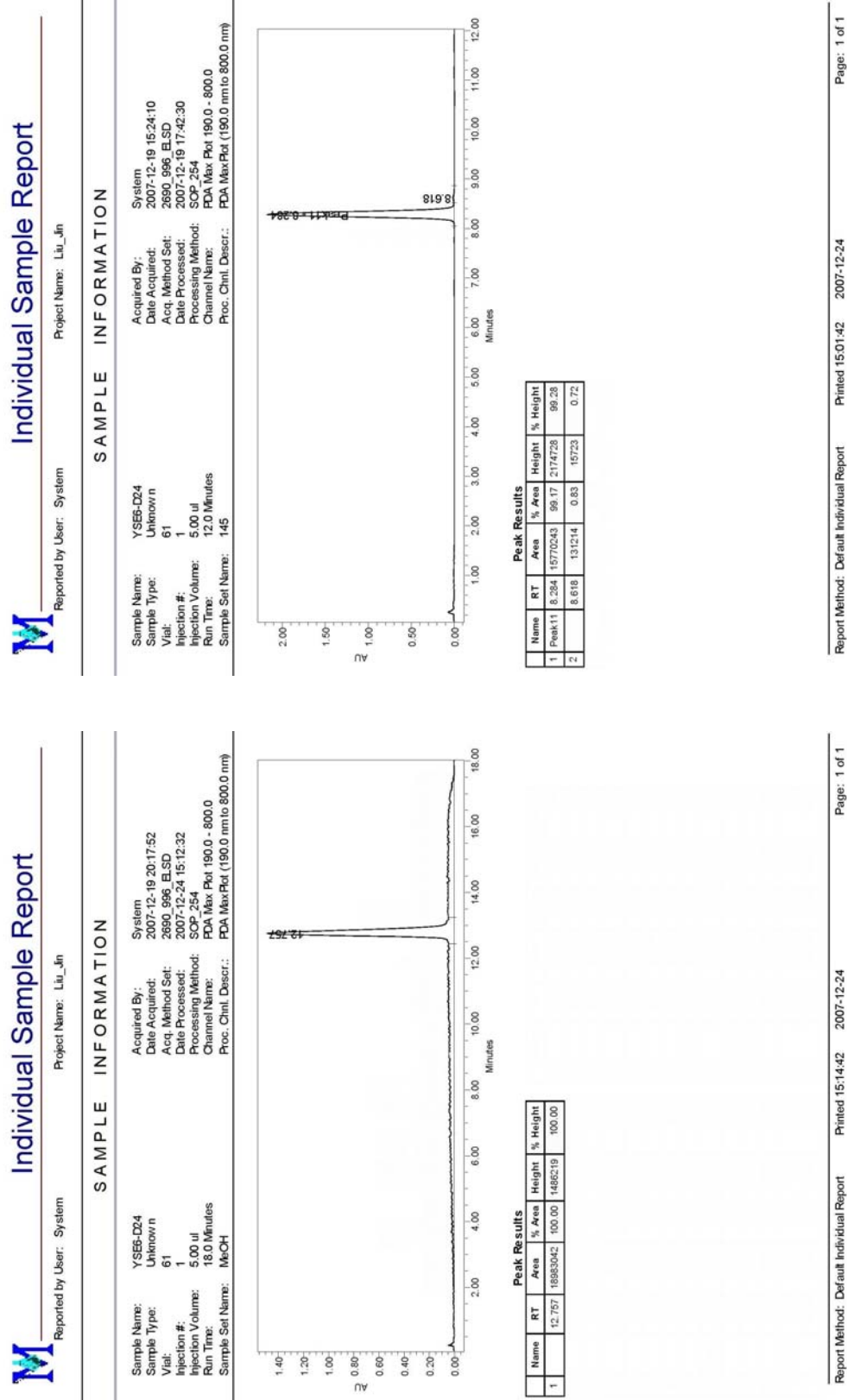


Figure S34. HPLC purity checks of compound 7.

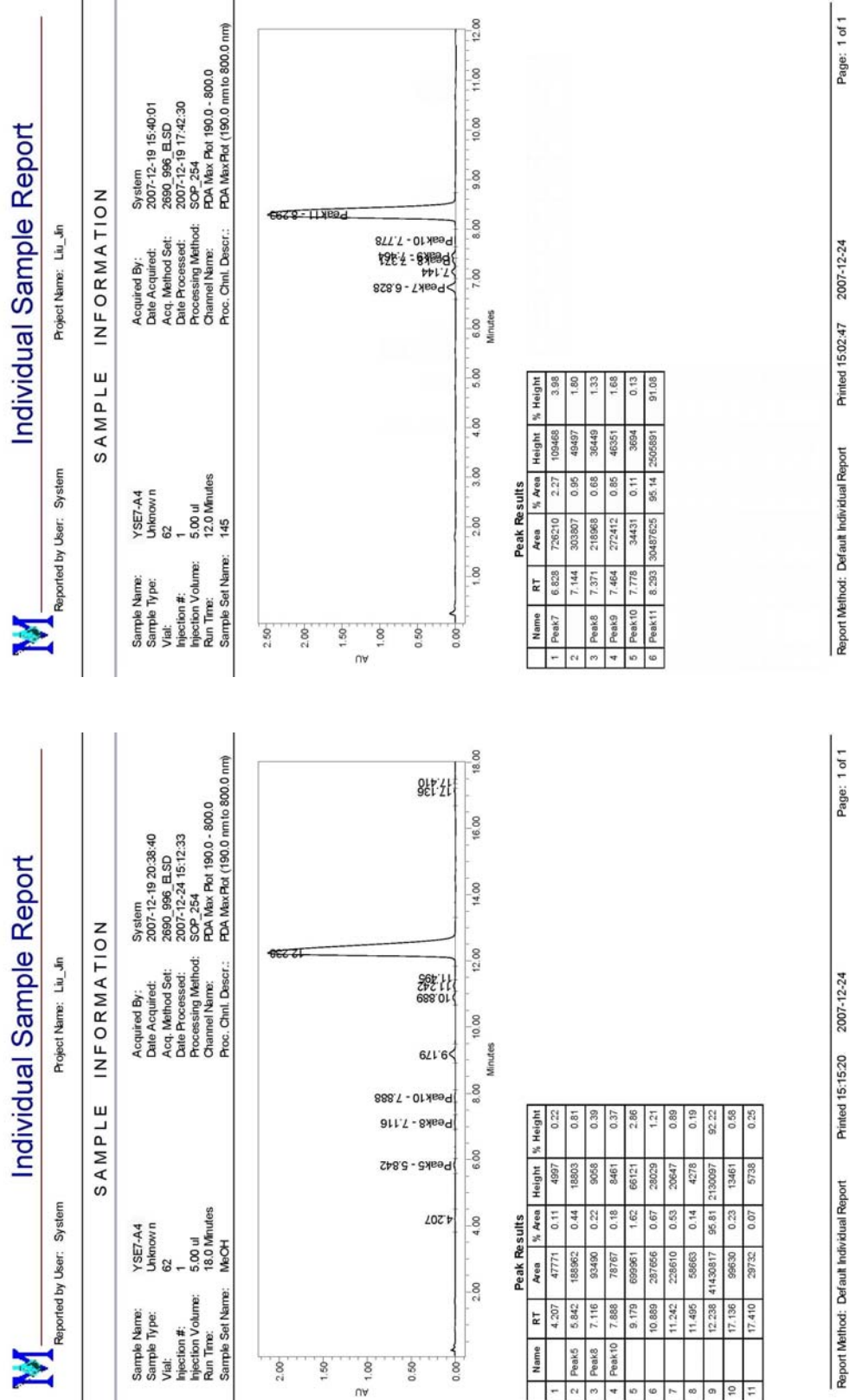


Figure S35. HPLC purity checks of compound **10**.

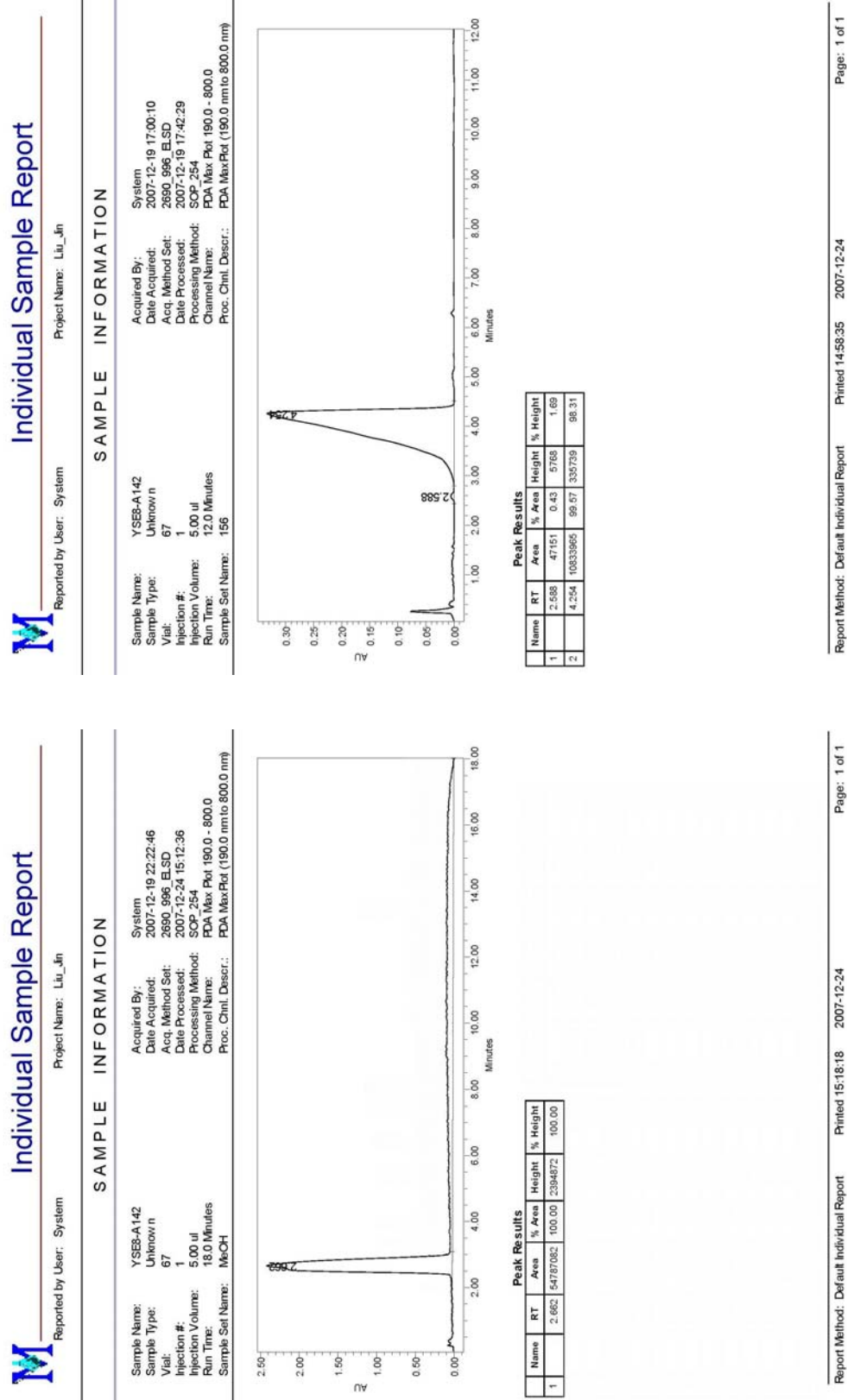


Figure S36. HPLC purity checks of compound **11**.

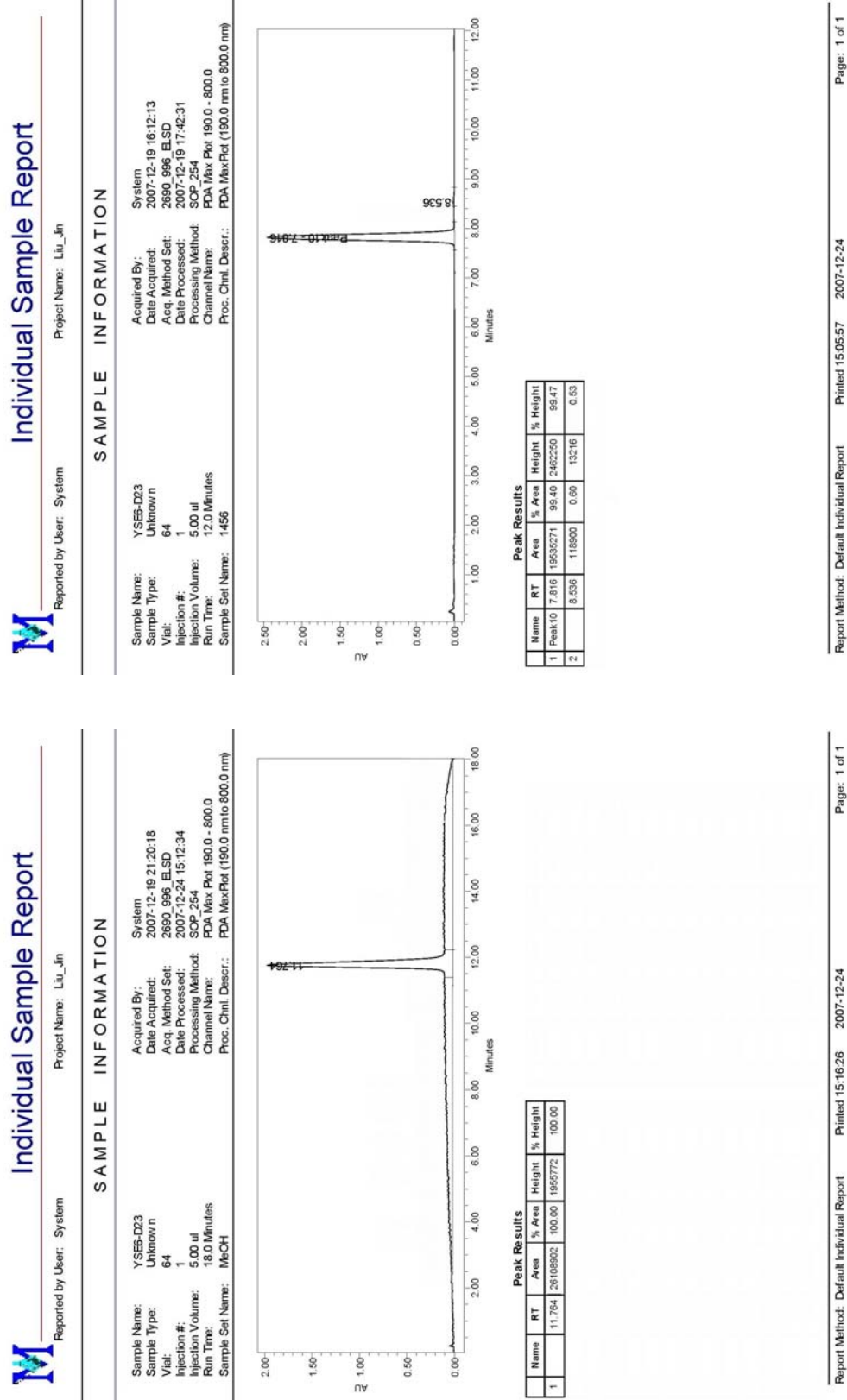


Figure S37. HPLC purity checks of compound **20**.

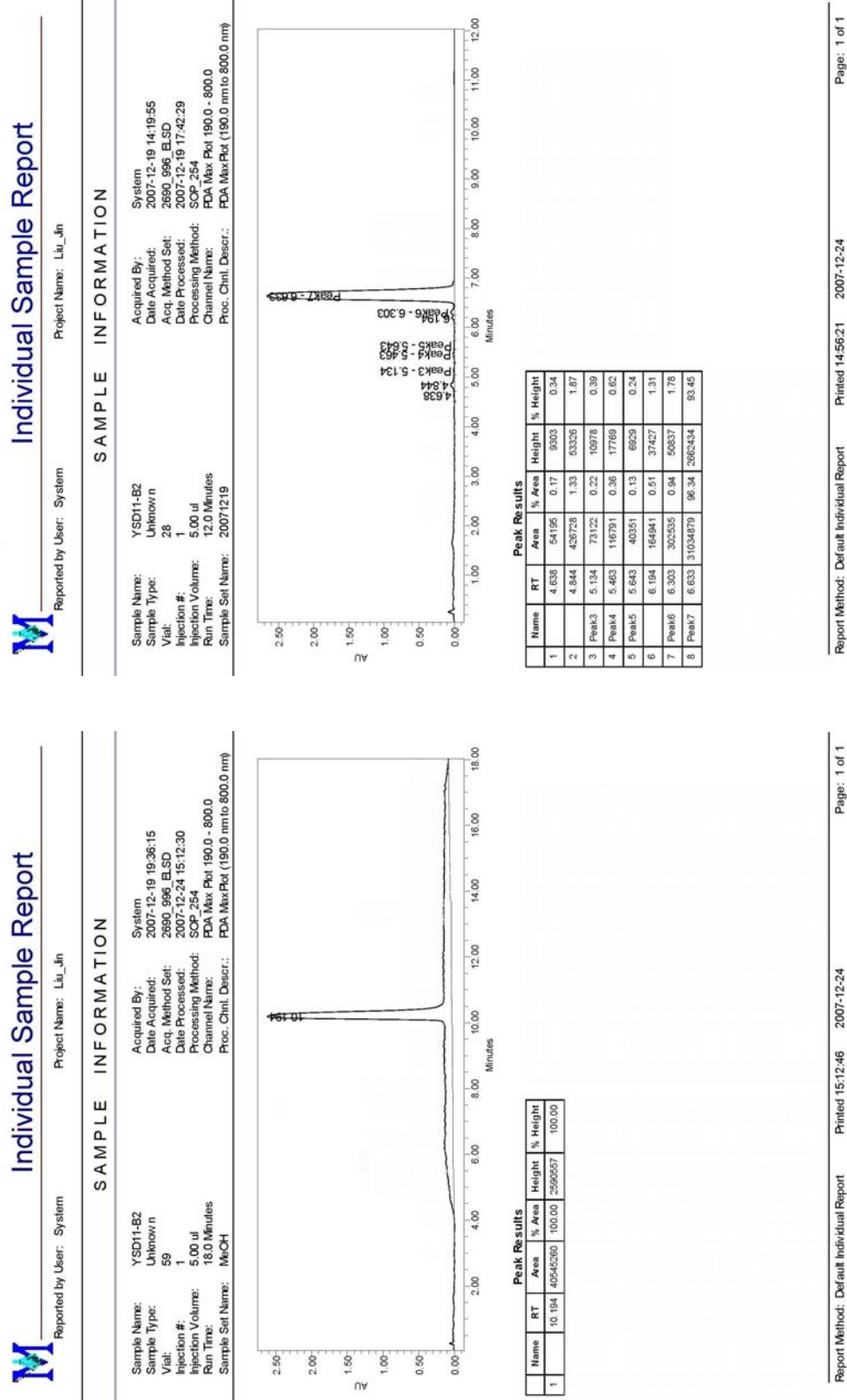


Figure S38. HPLC purity checks of compound **25**.

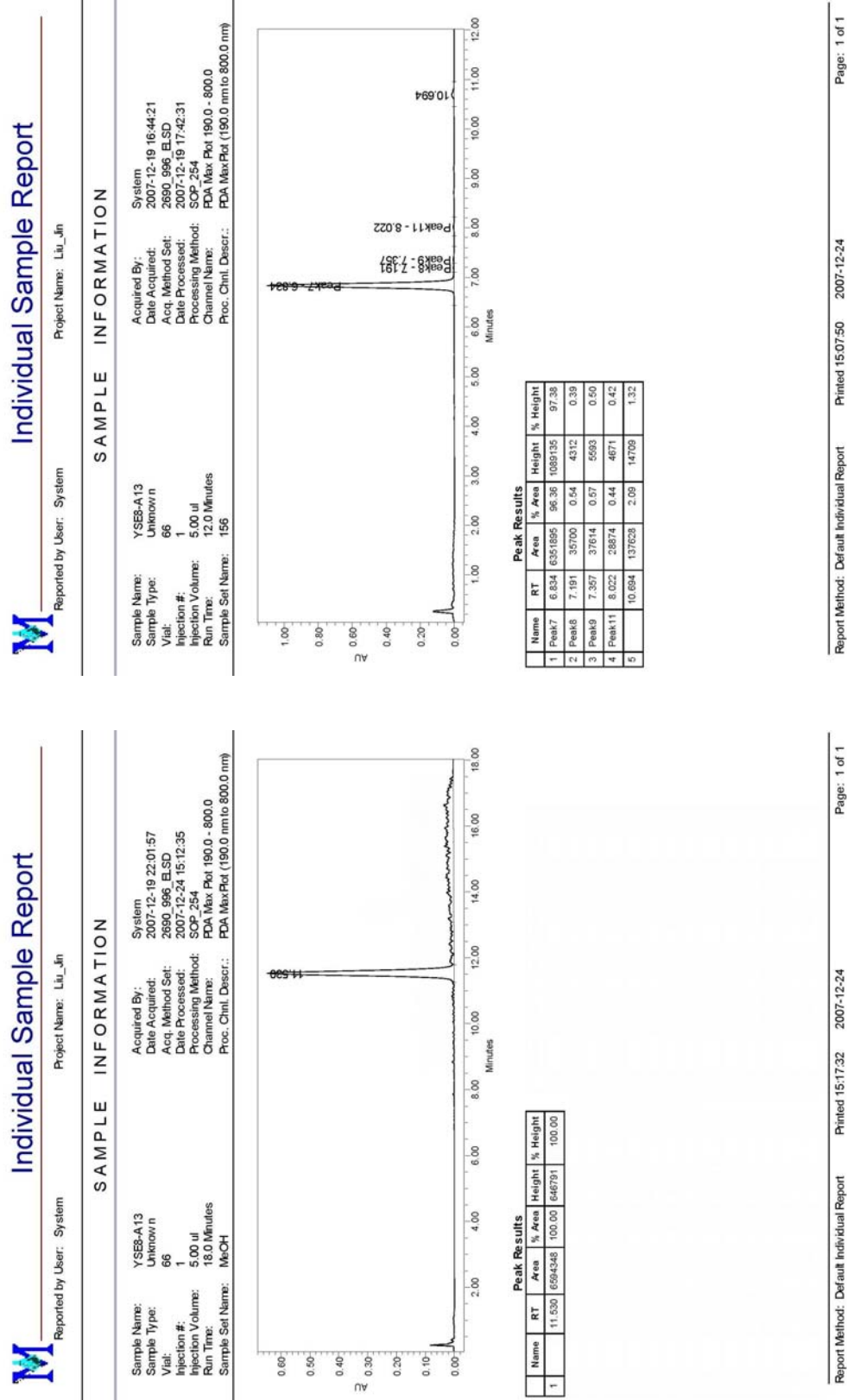


Figure S39. HPLC purity checks of compound **26**.

