Compound identification using liquid chromatography and high-resolution non-contact fraction collection with a solenoid valve

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Supplementary information

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Supplementary information 1. Fraction collection stability

**H₂O: MeOH 98/2**

| TIME (SECONDS) | SINGLET | DUPLO |
|----------------|---------|-------|
| 30             |         |       |
| 130            |         |       |
| 230            |         |       |
| 330            |         |       |
| 430            |         |       |
| 530            |         |       |
| 630            |         |       |
| 730            |         |       |

**H₂O: MeOH 50/50**

| TIME (SECONDS) | SINGLET | DUPLO |
|----------------|---------|-------|
| 30             |         |       |
| 130            |         |       |
| 230            |         |       |
| 330            |         |       |
| 430            |         |       |
| 530            |         |       |
| 630            |         |       |
| 730            |         |       |

Flow: 0.1 ml/min
Freq.: 1 Hz Int.: 6 sec

|             | SINGLET | DUPLO |
|-------------|---------|-------|
| Average     | 169.0   | 172.2 |
| SD          | 27.9    | 25.5  |
| RSD         | 16.5%   | 14.8% |

| Average     | 170.6   | 173.2 |
| SD          | 20.0    | 19.5  |
| RSD         | 11.7%   | 11.2% |
H₂O: MeOH 98/2

Flow: 0.1 ml/min
Freq.: 3 Hz Int.: 6 sec

|          | SINGLET | DUPLO |
|----------|---------|-------|
| Average  | 167.0   | 169.4 |
| SD       | 6.5     | 6.2   |
| RSD      | 3.91%   | 3.66% |

H₂O: MeOH 50/50

|          | SINGLET | DUPLO |
|----------|---------|-------|
| Average  | 168.7   | 171.9 |
| SD       | 5.8     | 7.3   |
| RSD      | 3.5%    | 4.3%  |
H₂O: MeOH 98/2

Flow: 0.1 ml/min
Freq.: 3 Hz Int.: 6 sec

|       | SINGLET | DUPLO |
|-------|---------|-------|
| Average | 172.9   | 174.6 |
| SD     | 9.1     | 8.3   |
| RSD    | 5.2%    | 4.8%  |

H₂O: MeOH 50/50

Flow: 0.1 ml/min
Freq.: 3 Hz Int.: 6 sec

|       | SINGLET | DUPLO |
|-------|---------|-------|
| Average | 176.5   | 174.8 |
| SD     | 7.5     | 8.4   |
| RSD    | 4.2%    | 4.8%  |
Flow: 0.3 ml/min
Freq.: 10 Hz Int.: 2 sec

H₂O: MeOH 98/2

|          | SINGLET | DUPLO |
|----------|---------|-------|
| Average  | 176.0   | 178.4 |
| SD       | 4.9     | 4.8   |
| RSD      | 2.8%    | 2.7%  |

H₂O: MeOH 50/50

|          | SINGLET | DUPLO |
|----------|---------|-------|
| Average  | 171.2   | 175.6 |
| SD       | 5.1     | 6.3   |
| RSD      | 3.0%    | 3.6%  |
H₂O: MeOH 98/2

Flow: 0,6 ml/min
Freq.: 10 Hz Int.: 1 sec

|          | SINGLET | DUPLO |
|----------|---------|-------|
| Average  | 176,8   | 178,6 |
| SD       | 6,6     | 6,1   |
| RSD      | 3,7%    | 3,4%  |

H₂O: MeOH 50/50

|          | SINGLET | DUPLO |
|----------|---------|-------|
| Average  | 175,2   | 175,8 |
| SD       | 6,6     | 7,9   |
| RSD      | 3,8%    | 4,5%  |
H$_2$O: MeOH 98/2

Flow: 0.6 ml/min
Freq.: 20 Hz Int.: 1 sec

|          | SINGLET | DUPLO |
|----------|---------|-------|
| Average  | 176.2   | 178.6 |
| SD       | 6.0     | 5.2   |
| RSD      | 3.4%    | 2.9%  |

H$_2$O: MeOH 50/50

|          | SINGLET | DUPLO |
|----------|---------|-------|
| Average  | 176.7   | 177.3 |
| SD       | 7.0     | 5.9   |
| RSD      | 4.0%    | 3.3%  |
**H$_2$O: MeOH 98/2**

|       | SINGLET | DUPLO |
|-------|---------|-------|
| Average | 279,4   | 285,2 |
| SD     | 13,5    | 10,5  |
| RSD    | 4,8%    | 3,7%  |

**H$_2$O: MeOH 50/50**

|       | SINGLET | DUPLO |
|-------|---------|-------|
| Average | 280,3   | 291,4 |
| SD     | 14,3    | 11,6  |
| RSD    | 5,1%    | 4,0%  |
Flow: 1.0 ml/min
Freq.: 20 Hz Int.: 1 sec

**H₂O: MeOH 98/2**

![Graph 1](image1)

**H₂O: MeOH 50/50**

![Graph 2](image2)

|          | SINGLET | DUPLO |
|----------|---------|-------|
| **Average** | 284,6   | 288,4 |
| **SD**    | 8,9     | 9,3   |
| **RSD**   | 3,1%    | 3,2%  |

|          | SINGLET | DUPLO |
|----------|---------|-------|
| **Average** | 291,8   | 294,7 |
| **SD**    | 10,2    | 10,9  |
| **RSD**   | 3,5%    | 3,7%  |
H₂O: MeOH 2/98

Flow: 0.1 ml/min
Freq.: 1 Hz Int.: 6 sec

|       | SINGLET | DUPLO |
|-------|---------|-------|
| Average | 183.2   | 216.2 |
| SD     | 11.4    | 12.4  |
| RSD    | 6.2%    | 5.7%  |

H₂O: ACN 98/2

|       | SINGLET | DUPLO |
|-------|---------|-------|
| Average | 171.9   | 176.4 |
| SD     | 13.7    | 14.1  |
| RSD    | 8.0%    | 8.0%  |
H₂O: MeOH 2/98

Flow: 0.1 ml/min
Freq.: 3 Hz Int.: 6 sec

H₂O: ACN 98/2

|       | SINGLET | DUPLO |
|-------|---------|-------|
| Average | 169.8   | 166.7 |
| SD     | 7.7     | 8.0   |
| RSD    | 4.5%    | 4.8%  |

|       | SINGLET | DUPLO |
|-------|---------|-------|
| Average | 175.7   | 176.8 |
| SD     | 4.5     | 4.9   |
| RSD    | 2.6%    | 2.7%  |
**H₂O: MeOH 2/98**

- Flow: 0.1 ml/min
- Freq.: 3 Hz
- Int.: 6 sec

**H₂O: ACN 98/2**

- Flow: 0.1 ml/min
- Freq.: 3 Hz
- Int.: 6 sec

**Graphs showing RFU over time for Singlet and Duplo samples.**

**Table: Average RFU**

|       | SINGLET | DUPLO  |
|-------|---------|--------|
| Average | 174.5   | 180.9  |
| SD     | 7.9     | 8.9    |
| RSD    | 4.5%    | 4.9%   |

**Table: Average RFU**

|       | SINGLET | DUPLO  |
|-------|---------|--------|
| Average | 196.0   | 195.4  |
| SD     | 7.3     | 7.9    |
| RSD    | 3.7%    | 4.0%   |
H₂O: MeOH 2/98

- Flow: 0.3 ml/min
- Freq.: 10 Hz
- Int.: 2 sec

|          | SINGLET | DUPLO  |
|----------|---------|--------|
| Average  | 162.4   | 167.1  |
| SD       | 7.1     | 6.5    |
| RSD      | 4.4%    | 3.9%   |

H₂O: ACN 98/2

- Flow: 0.3 ml/min
- Freq.: 10 Hz
- Int.: 2 sec

|          | SINGLET | DUPLO  |
|----------|---------|--------|
| Average  | 193.9   | 194.2  |
| SD       | 4.7     | 5.8    |
| RSD      | 2.4%    | 3.0%   |
Flow: 0.6 ml/min
Freq.: 10 Hz Int.: 1 sec

**H₂O: MeOH 2/98**

|       | SINGLET | DUPLO |
|-------|---------|-------|
| Average | 169.2   | 171.5 |
| SD     | 7.9     | 7.8   |
| RSD    | 4.7%    | 4.6%  |

**H₂O: ACN 98/2**

|       | SINGLET | DUPLO |
|-------|---------|-------|
| Average | 196.4   | 195.5 |
| SD     | 6.5     | 7.5   |
| RSD    | 3.3%    | 3.8%  |
Flow: 0,6 ml/min
Freq.: 20 Hz Int.: 1 sec

|          | SINGLET | DUPLO |
|----------|---------|-------|
| Average  | 168,0   | 168,8 |
| SD       | 8,1     | 7,1   |
| RSD      | 4,8%    | 4,2%  |

|          | SINGLET | DUPLO |
|----------|---------|-------|
| Average  | 191,8   | 195,5 |
| SD       | 7,8     | 5,8   |
| RSD      | 4,1%    | 3,0%  |
Flow: 1.0 ml/min  
Freq.: 15 Hz Int.: 1 sec

|            | SINGLET | DUPLO |
|------------|---------|-------|
| Average    | 259.5   | 265.8 |
| SD         | 10.9    | 11.0  |
| RSD        | 4.2%    | 4.2%  |

|            | SINGLET | DUPLO |
|------------|---------|-------|
| Average    | 287.3   | 291.5 |
| SD         | 11.6    | 11.6  |
| RSD        | 4.1%    | 4.0%  |
H_2O: MeOH 2/98

H_2O: ACN 98/2

Flow: 1.0 ml/min
Freq.: 20 Hz Int.: 1 sec

|        | SINGLET | DUPLO |
|--------|---------|-------|
| Average| 268.0   | 273.2 |
| SD     | 11.8    | 12.6  |
| RSD    | 4.4%    | 4.6%  |

|        | SINGLET | DUPLO |
|--------|---------|-------|
| Average| 282.7   | 286.4 |
| SD     | 12.2    | 11.2  |
| RSD    | 4.3%    | 3.9%  |
Flow: 1.0 ml/min
Freq.: 20 Hz Int.: 1 sec

H$_2$O: ACN 50/50

H$_2$O: ACN 2/98

|       | SINGLET | DUPLO |
|-------|---------|-------|
| Average | 163.5   | 167.3 |
| SD     | 12.6    | 12.7  |
| RSD    | 7.7%    | 7.6%  |

|       | SINGLET | DUPLO |
|-------|---------|-------|
| Average | 187.7   | 189.2 |
| SD     | 20.0    | 15.1  |
| RSD    | 10.6%   | 8.0%  |
**H₂O: ACN 50/50**

- **Flow**: 0.1 ml/min
- **Freq.**: 3 Hz
- **Int.**: 6 sec

**H₂O: ACN 2/98**

- **Flow**: 0.1 ml/min
- **Freq.**: 3 Hz
- **Int.**: 6 sec

|            | SINGLET | DUPLO |
|------------|---------|-------|
| **Average**  | 162.6   | 160.1 |
| **SD**      | 5.8     | 6.1   |
| **RSD**     | 3.6%    | 3.8%  |
**H$_2$O: ACN 50/50**

- Flow: 0.1 ml/min
- Freq.: 3 Hz
- Int.: 6 sec

**H$_2$O: ACN 2/98**

- Flow: 0.1 ml/min
- Freq.: 3 Hz
- Int.: 6 sec

|                | SINGLET | DUPLO |
|----------------|---------|-------|
| **Average**    | 161,0   | 159,9 |
| **SD**         | 7,0     | 7,2   |
| **RSD**        | 4,3%    | 4,5%  |

|                | SINGLET | DUPLO |
|----------------|---------|-------|
| **Average**    | 163,2   | 162,6 |
| **SD**         | 6,5     | 6,4   |
| **RSD**        | 4,0%    | 3,9%  |
Flow: 0.3 ml/min
Freq.: 10 Hz Int.: 2 sec

|        | SINGLET | DUPLO |
|--------|---------|-------|
| Average| 152.9   | 153.4 |
| SD     | 5.6     | 5.3   |
| RSD    | 3.7%    | 3.5%  |

|        | SINGLET | DUPLO |
|--------|---------|-------|
| Average| 165.6   | 166.0 |
| SD     | 5.0     | 5.9   |
| RSD    | 3.0%    | 3.5%  |
Flow: 0.6 ml/min
Freq.: 10 Hz Int.: 1 sec

|        | SINGLET | DUPLO |
|--------|---------|-------|
| Average| 187.5   | 188.3 |
| SD     | 7.7     | 6.0   |
| RSD    | 4.1%    | 3.2%  |

|        | SINGLET | DUPLO |
|--------|---------|-------|
| Average| 167.2   | 166.1 |
| SD     | 6.7     | 6.1   |
| RSD    | 4.0%    | 3.6%  |
H$_2$O: ACN 50/50

Flow: 0.6 ml/min
Freq.: 20 Hz Int.: 1 sec

|          | SINGLET | DUPLO  |
|----------|---------|--------|
| Average  | 308.5   | 308.8  |
| SD       | 15.7    | 14.3   |
| RSD      | 5.1%    | 4.6%   |

H$_2$O: ACN 2/98

|          | SINGLET | DUPLO  |
|----------|---------|--------|
| Average  | 169.5   | 167.6  |
| SD       | 5.1     | 5.3    |
| RSD      | 3.0%    | 3.2%   |
**Flow:** 1,0 ml/min  
**Freq.:** 15 Hz Int.: 1 sec

### H₂O: ACN 50/50

|          | SINGLET | DUPLO  |
|----------|---------|--------|
| **Average** | 264,7   | 271,3  |
| **SD**    | 15,2    | 11,7   |
| **RSD**   | 5,7%    | 4,3%   |

### H₂O: ACN 2/98

|          | SINGLET | DUPLO  |
|----------|---------|--------|
| **Average** | 260,8   | 259,6  |
| **SD**    | 6,7     | 6,2    |
| **RSD**   | 2,6%    | 2,4%   |
Flow: 1.0 ml/min
Freq.: 20 Hz Int.: 1 sec