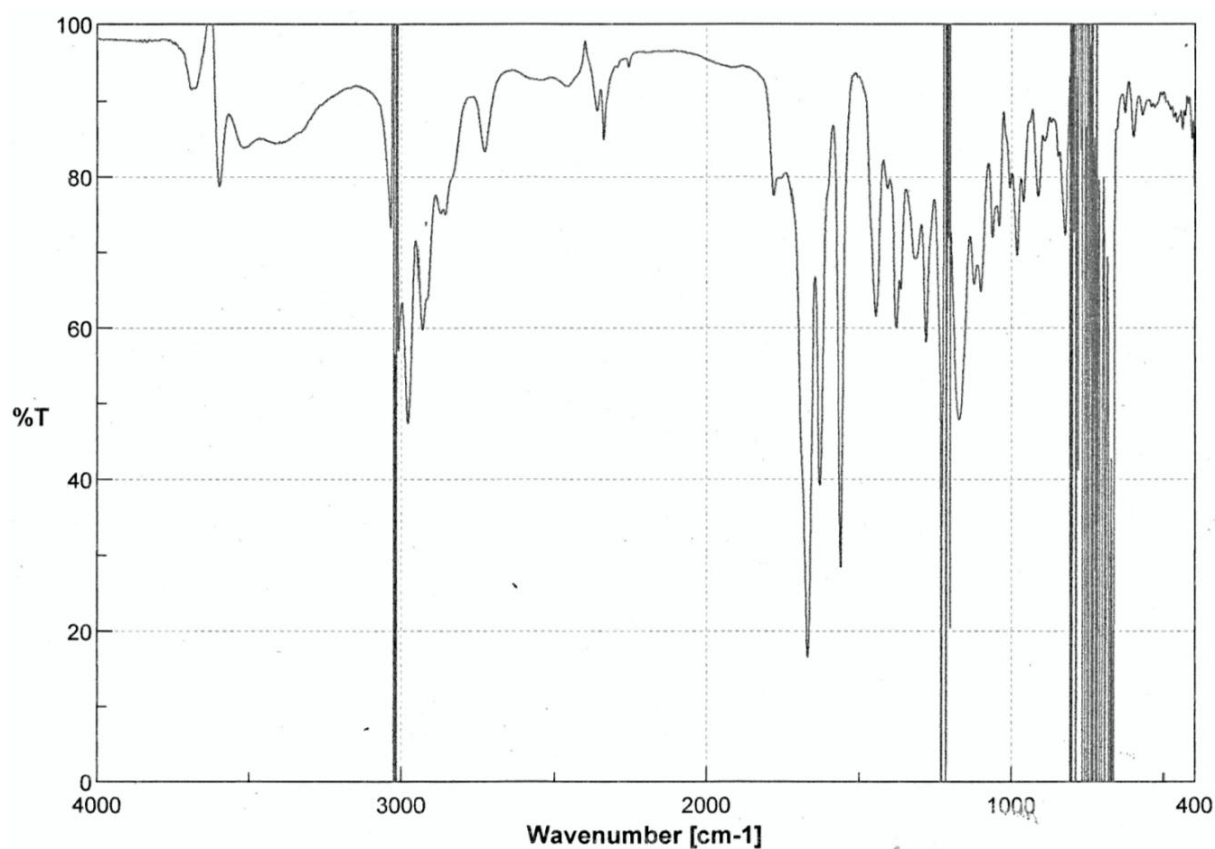


# Supplementary Materials

Figure S1. IR spectrum of cubelin.



Accumulation: 4  
Resolution: 4 cm<sup>-1</sup>  
Zero Filling: ON  
Apodization: Cosine  
Gain: Auto (2)  
Aperture: Auto (7.1 mm)  
Scan Speed: Auto (2 mm/sec)  
User:  
Acquisition Date: 2013/11/16 17:42  
Modify Date: 2013/11/25 19:31  
File Name: C1-4mg.jws  
Sample Name:  
Comment:

Figure S2. HRESIMS spectrum of cubelin.

## Elemental Composition Report

Page 1

## Single Mass Analysis

Tolerance = 50.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

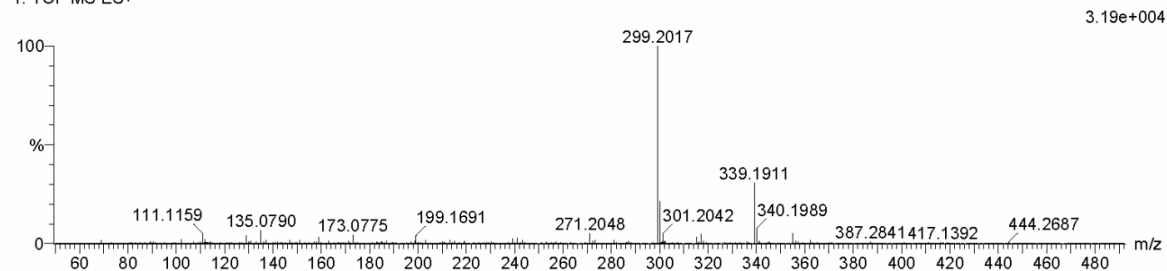
56 formula(e) evaluated with 8 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-30 H: 0-1000 O: 0-200

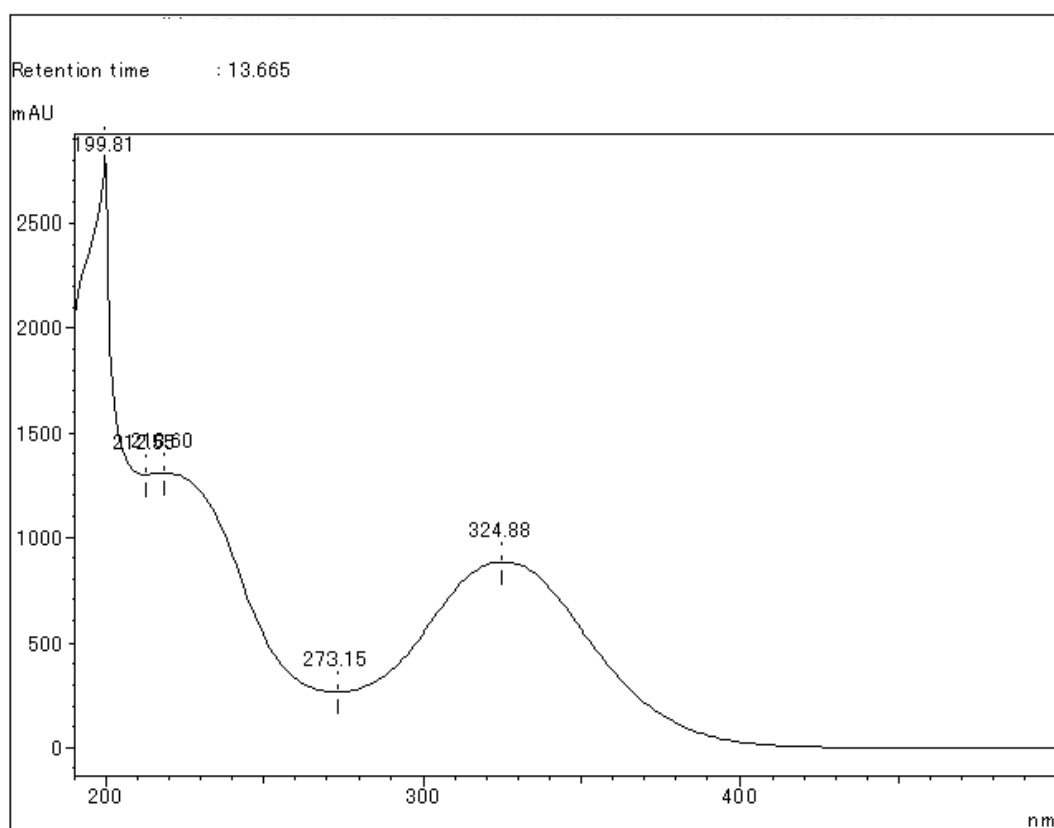
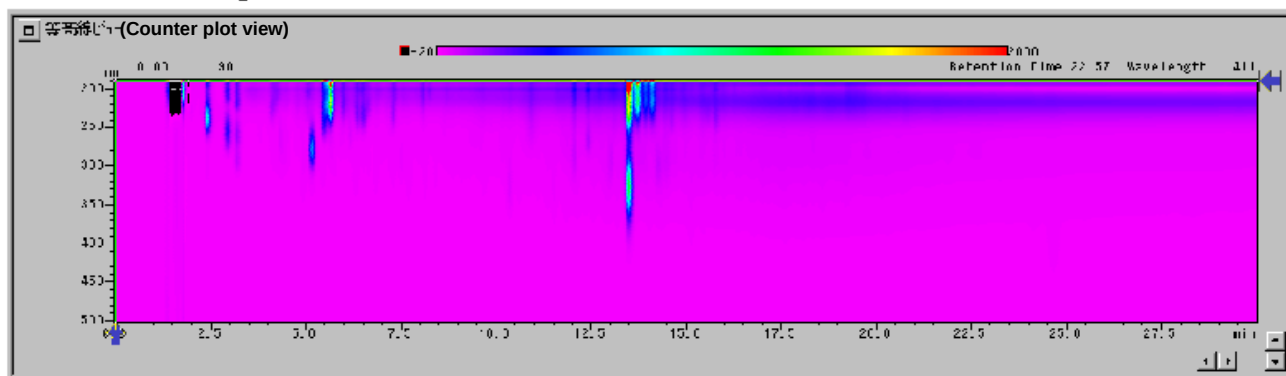
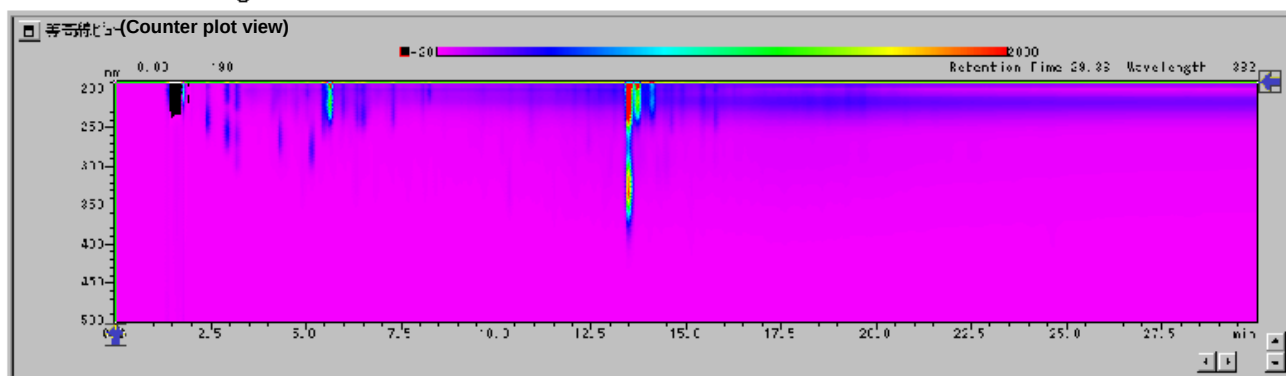
131118\_1\_2 619 (4.769)

1: TOF MS ES+



Minimum: -1.5  
Maximum: 50.0 10.0 50.0

| Mass     | Calc. Mass | mDa   | PPM    | DBE  | i-FIT | i-FIT (Norm) | Formula    |
|----------|------------|-------|--------|------|-------|--------------|------------|
| 299.2017 | 299.2011   | 0.6   | 2.0    | 7.5  | 159.2 | 1.6          | C20 H27 O2 |
|          | 299.2070   | -5.3  | -17.7  | -1.5 | 160.3 | 2.6          | C13 H31 O7 |
|          | 299.1858   | 15.9  | 53.1   | 3.5  | 159.6 | 1.9          | C16 H27 O5 |
|          | 299.2222   | -20.5 | -68.5  | 2.5  | 159.2 | 1.6          | C17 H31 O4 |
|          | 299.1800   | 21.7  | 72.5   | 12.5 | 160.7 | 3.1          | C23 H23    |
|          | 299.1706   | 31.1  | 103.9  | -0.5 | 161.1 | 3.5          | C12 H27 O8 |
|          | 299.2375   | -35.8 | -119.7 | 6.5  | 159.8 | 2.1          | C21 H31 O  |
|          | 299.1647   | 37.0  | 123.7  | 8.5  | 159.3 | 1.7          | C19 H23 O3 |

**Figure S3.** UV-VIS spectrum of cubelin.**HPLC-DAD Chromatogram: Fraction 11****HPLC-DAD Chromatogram: Fraction 12**

**Figure S4.**  $^1\text{H}$ -NMR spectrum of cubelin.

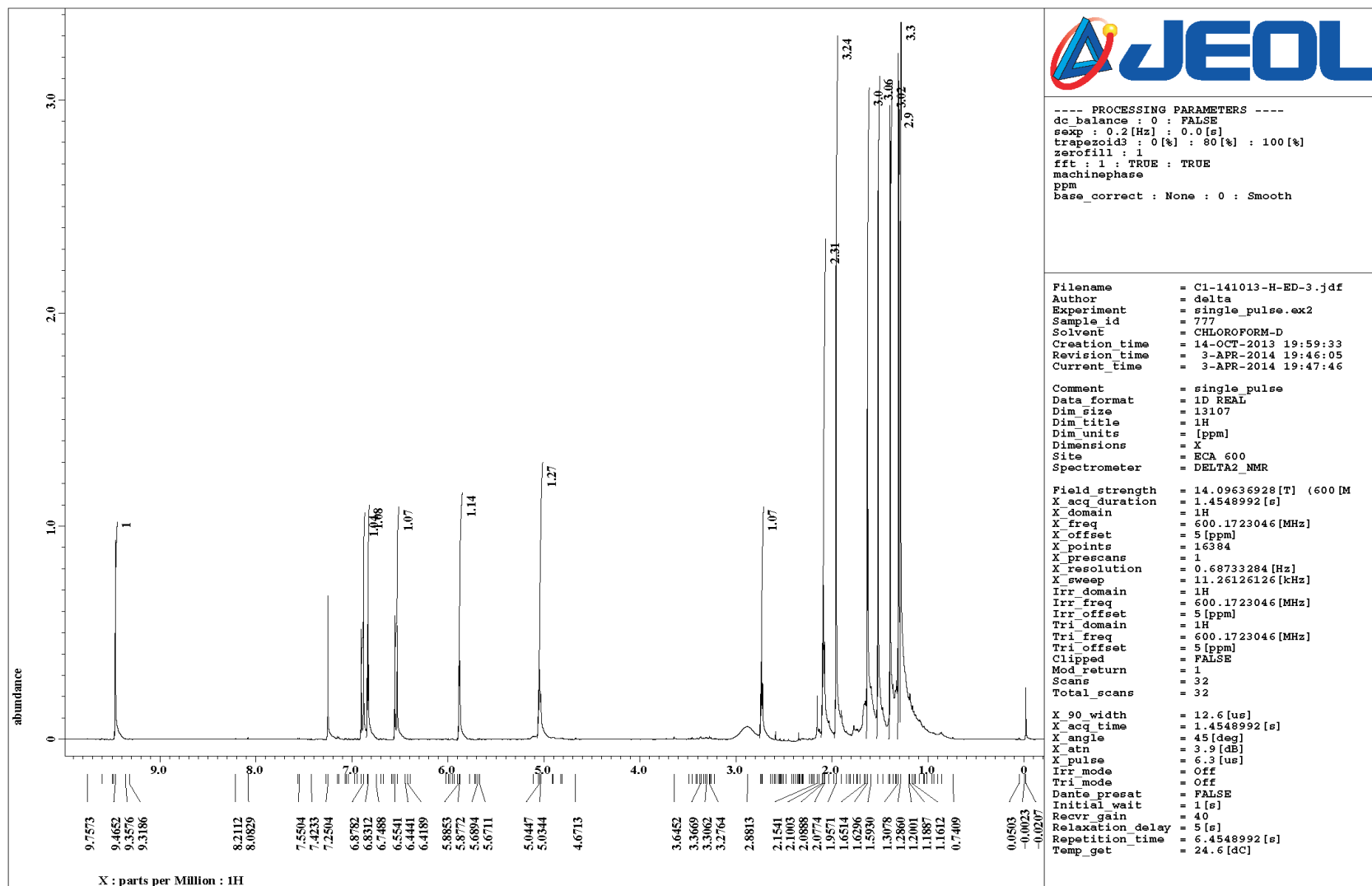


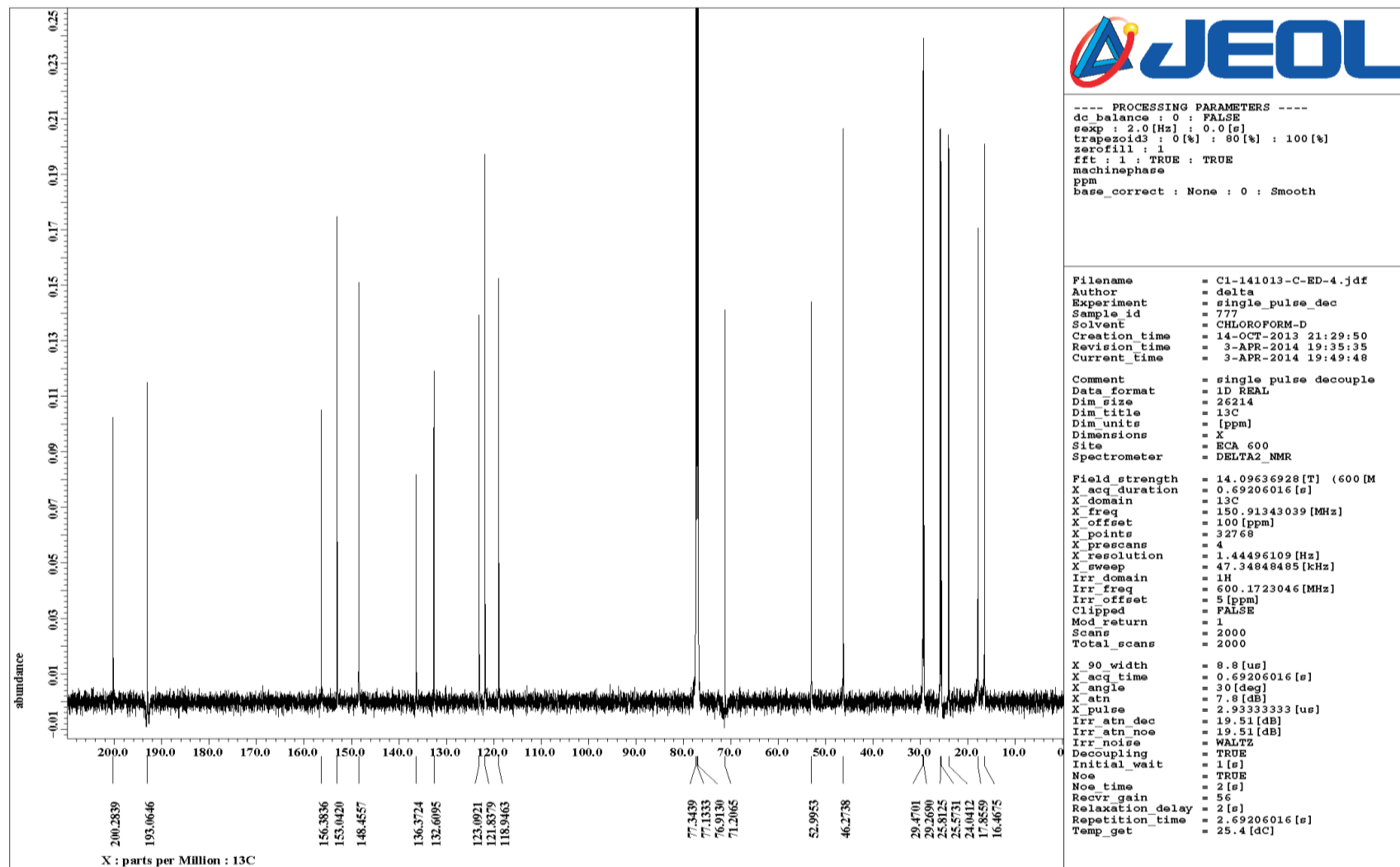
Figure S5.  $^{13}\text{C}$ -NMR spectrum of cubelin.

Figure S6. DEPT-45 NMR spectrum of cubelin.

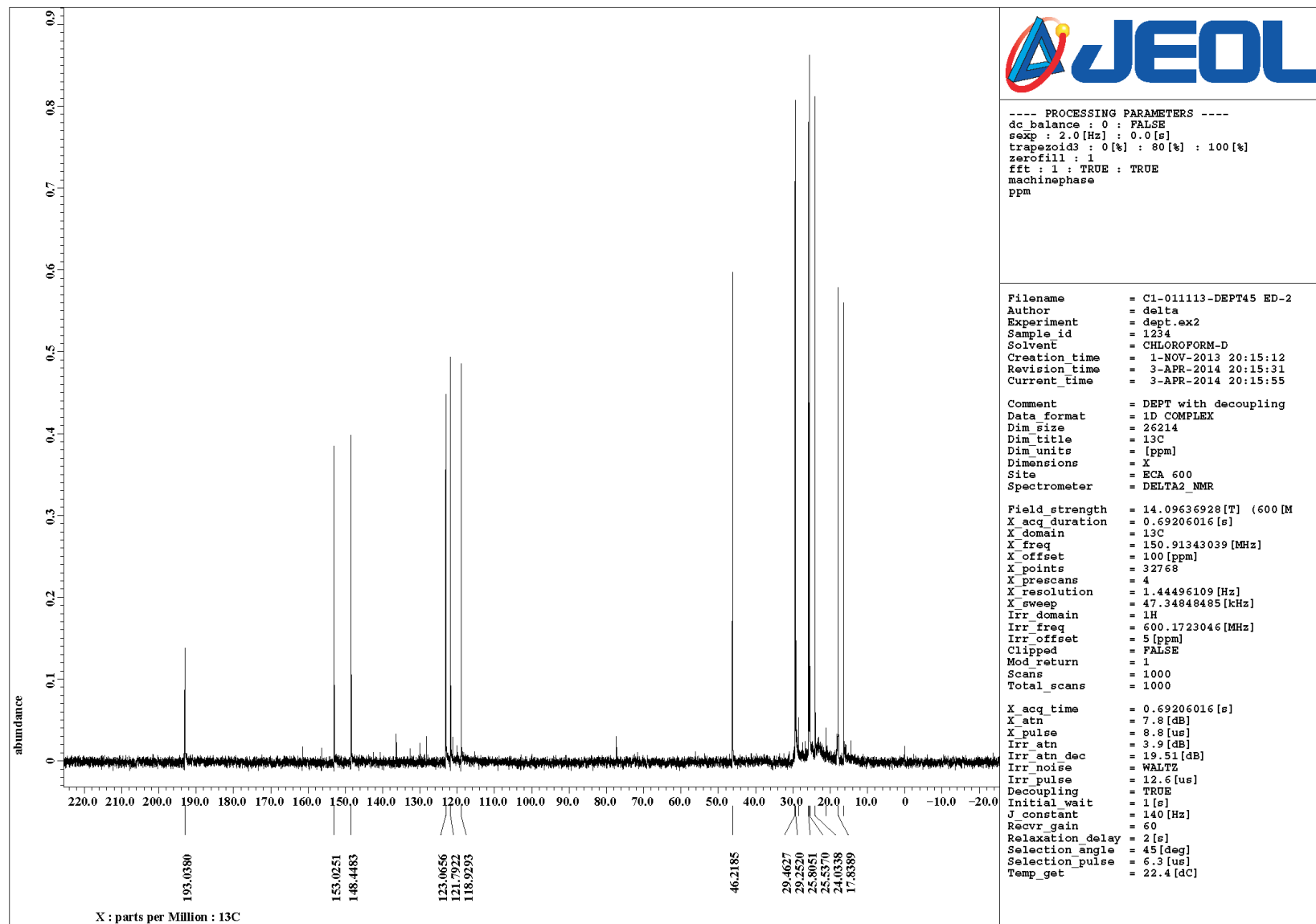


Figure S7. DEPT-90 NMR spectrum of cubelin

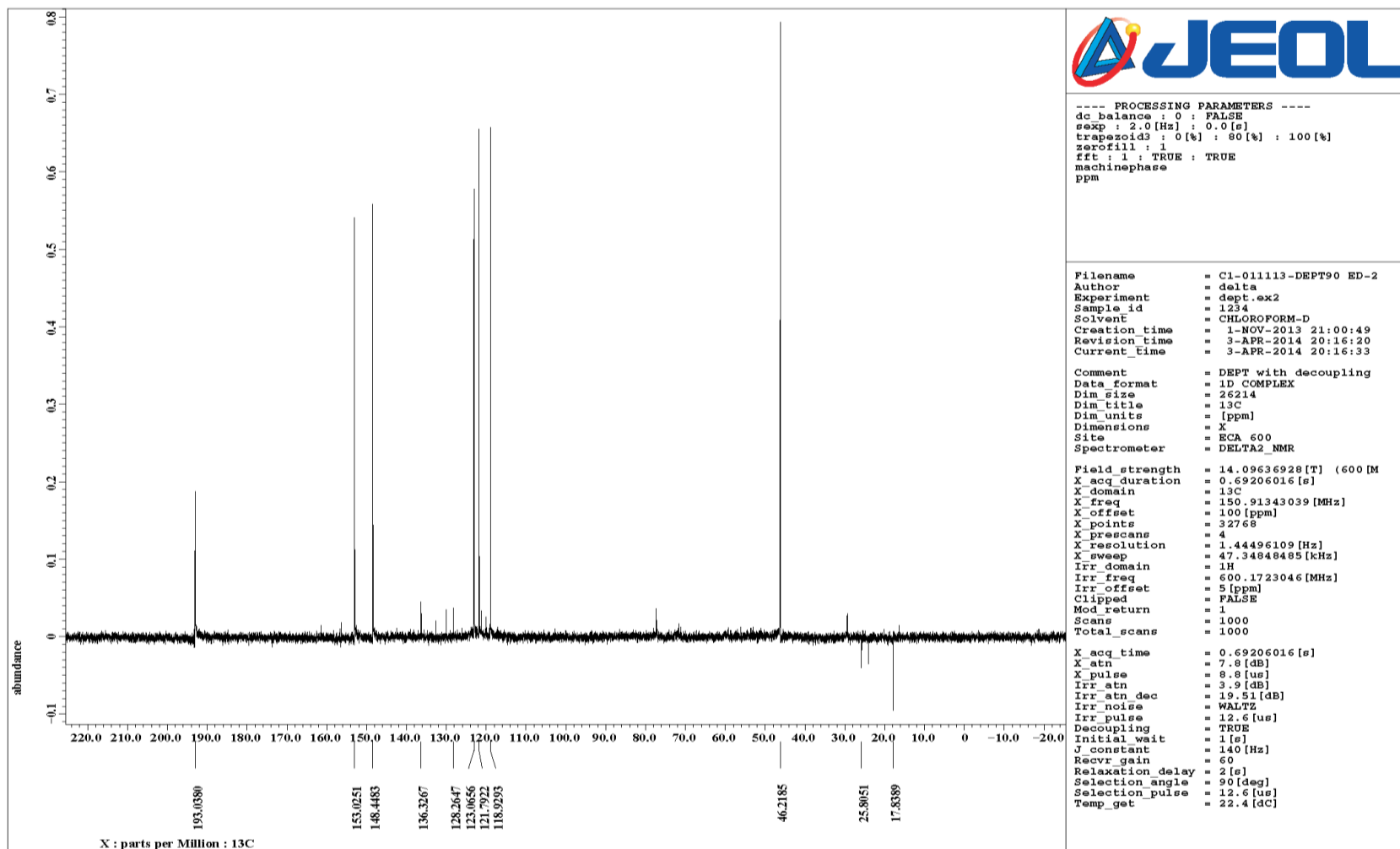


Figure S8. DEPT-135 NMR spectrum of cubelin.

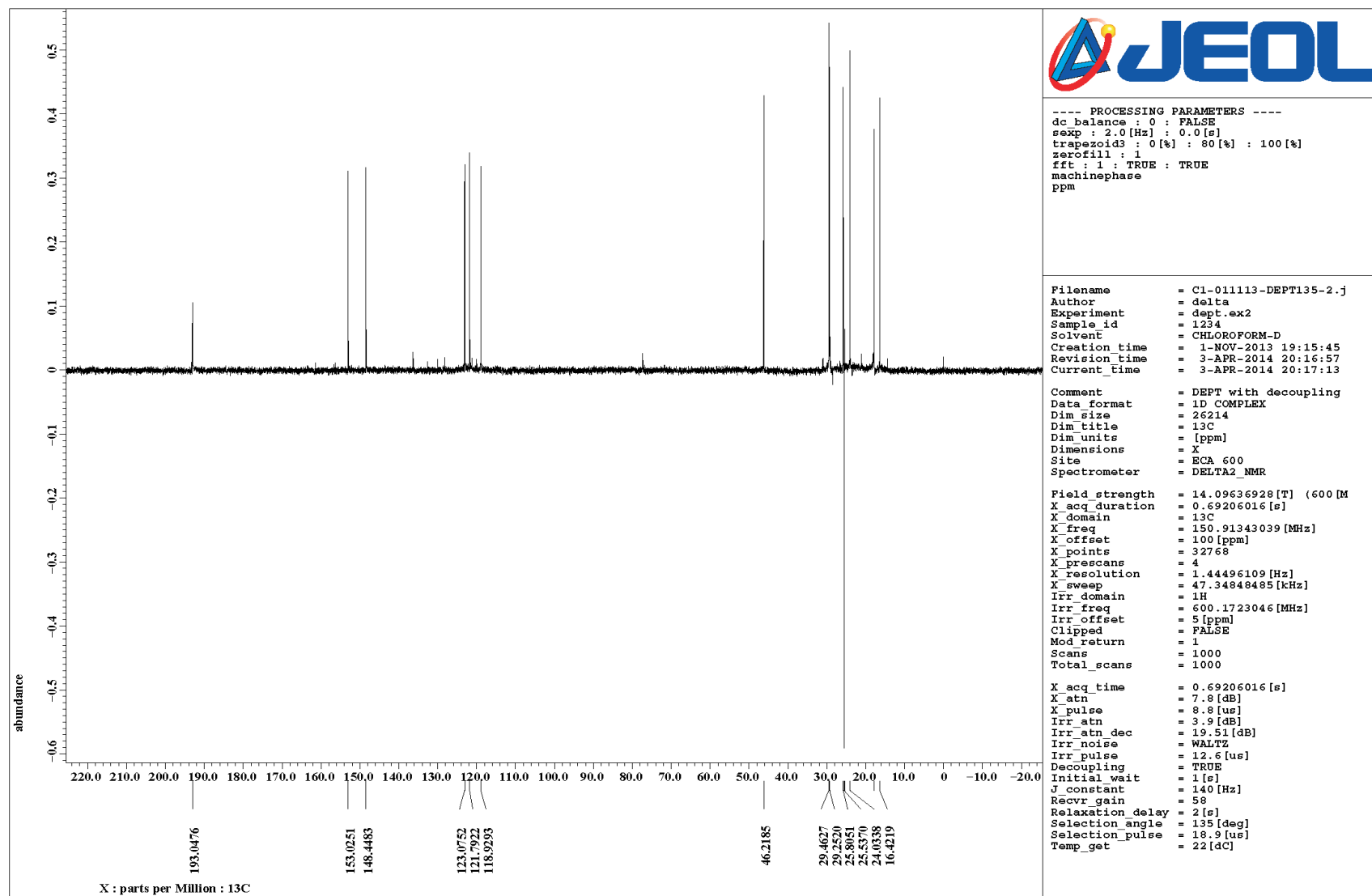


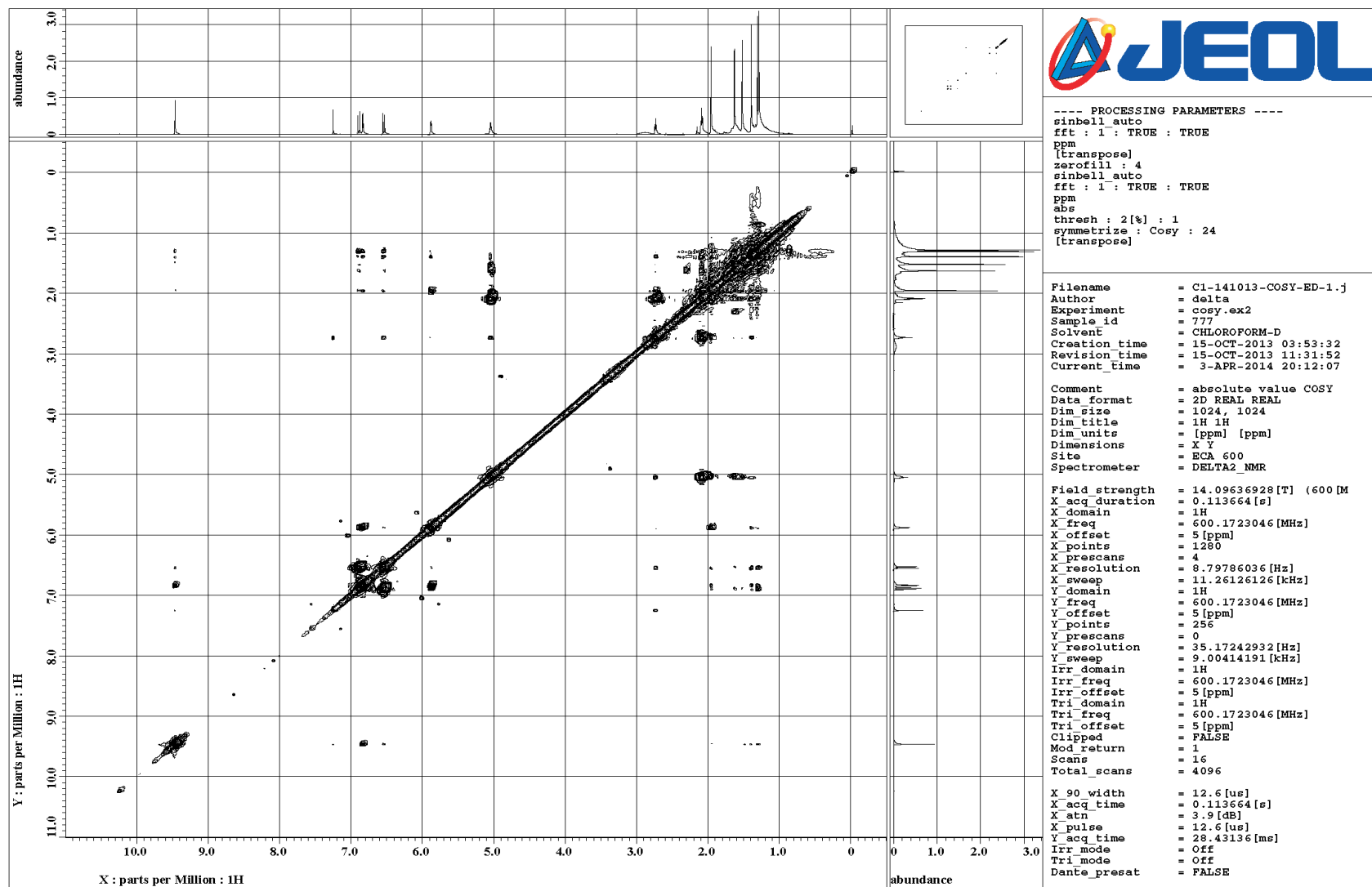
Figure S9.  $^1\text{H}$ - $^1\text{H}$  COSY NMR spectrum of cubelin

Figure S10. HETCOR NMR spectrum of cubelin

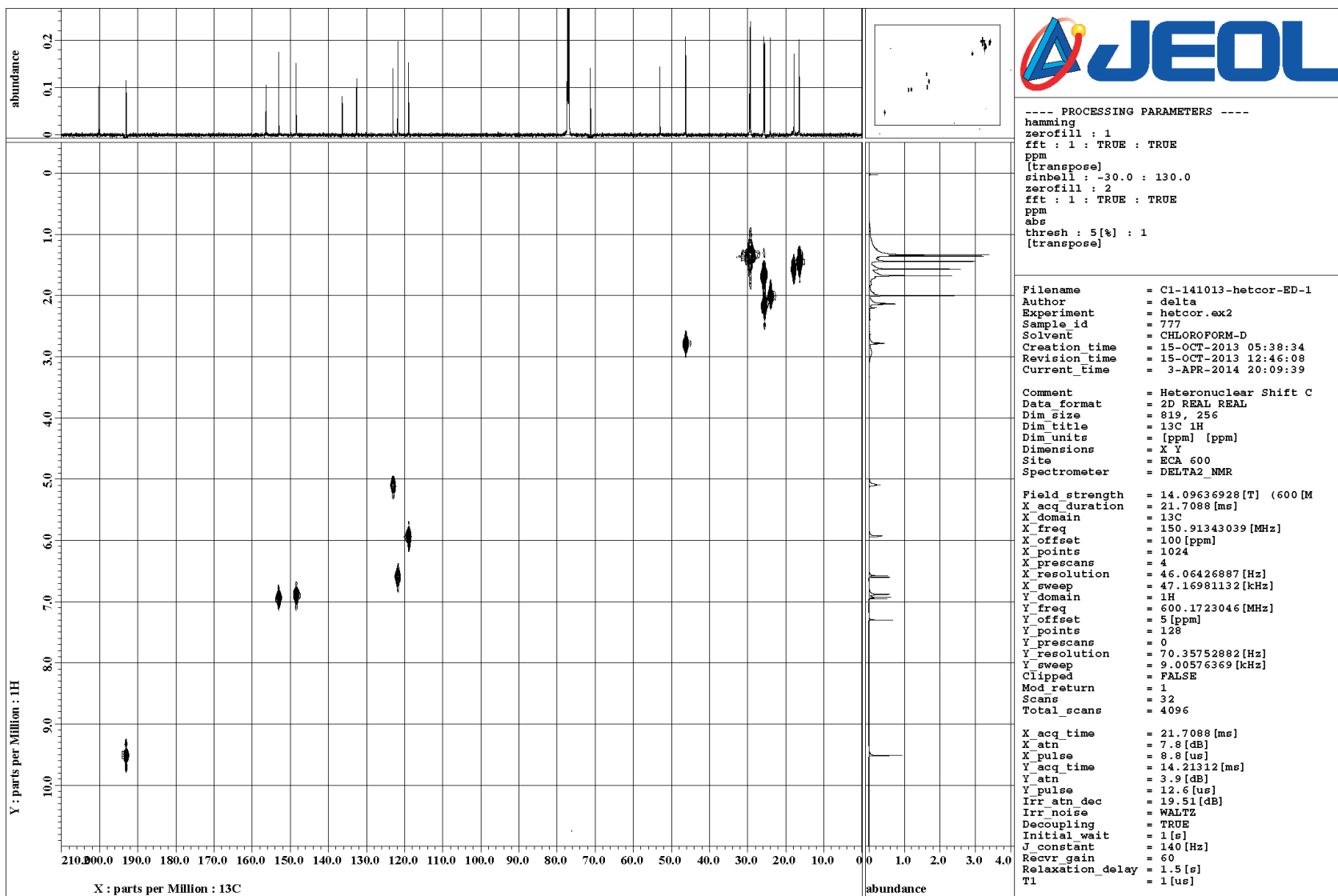


Figure S11. HMBC NMR spectrum of cubelin

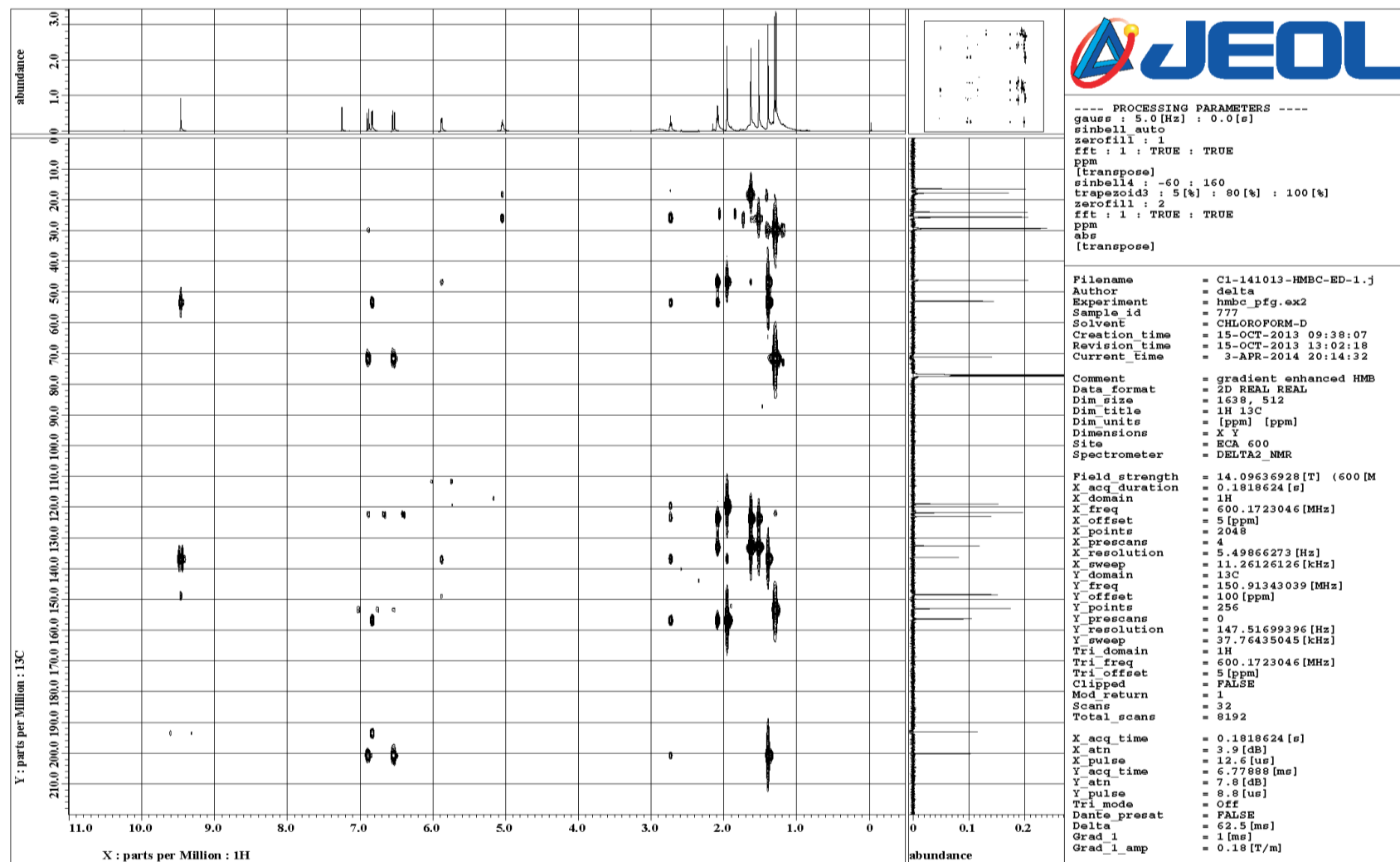


Figure S12. NOESY NMR spectrum of cubelin

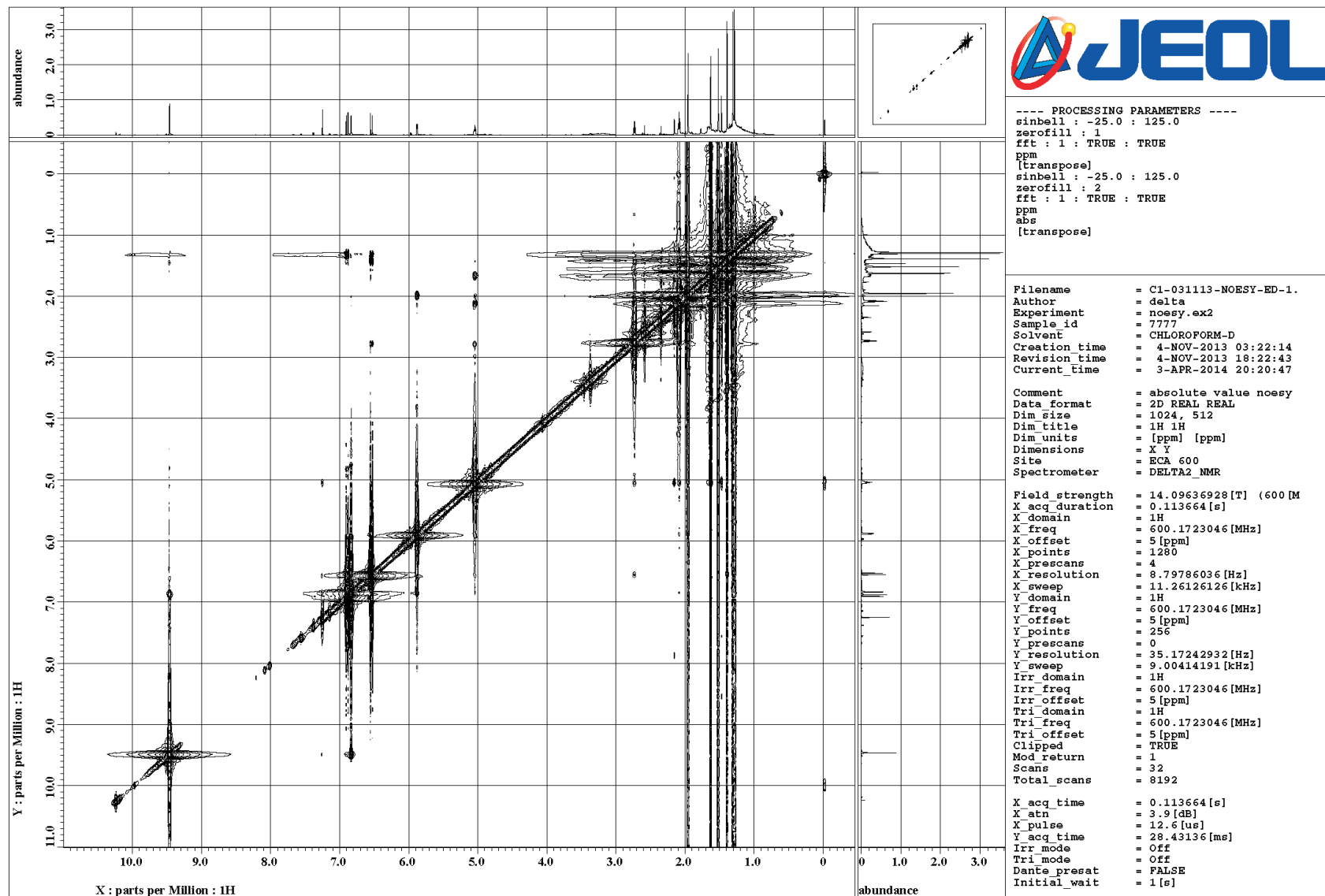


Figure S13. Specific Optical Rotation data of cubelin

P-1000 for windows  
Optical rotation measurement

| Model : P-1030 (A010160639) |           | No. | Sample Mode | Data     | Monitor       | Temp.      | HTV | Date   | Blank | Cell length | Conc.                    | [Alpha] | sugar | coef   | [Alpha]STD | Brix   | Conc.  | Factor | Temp.(STD) | Temp | Coef    | Light | Filter | Cycle  | Time  |
|-----------------------------|-----------|-----|-------------|----------|---------------|------------|-----|--------|-------|-------------|--------------------------|---------|-------|--------|------------|--------|--------|--------|------------|------|---------|-------|--------|--------|-------|
| Comment Sample Name         |           |     |             | Operator |               | Temp Point |     |        |       |             |                          |         |       |        |            |        |        |        |            |      |         |       |        |        |       |
| 1                           | 1 (1/10)  | a   |             | Holder   | Specific O.R. | 272.650    |     | 0.5453 | 20.2  | 406         | Sat Dec 07 13:36:34 2013 | 0.0000  | 10.00 | 2.0000 | 0.000      | 17.313 | 66.450 | 1.00   | 1.0000     | 20.0 | 0.00000 | Na    | 589nm  | 20 sec | 5 sec |
| 2                           | 1 (2/10)  | a   |             | Holder   | Specific O.R. | 274.550    |     | 0.5491 | 20.1  | 386         | Sat Dec 07 13:36:55 2013 | 0.0000  | 10.00 | 2.0000 | 0.000      | 17.313 | 66.450 | 1.00   | 1.0000     | 20.0 | 0.00000 | Na    | 589nm  | 20 sec | 5 sec |
| 3                           | 1 (3/10)  | a   |             | Holder   | Specific O.R. | 275.200    |     | 0.5504 | 20.1  | 410         | Sat Dec 07 13:37:15 2013 | 0.0000  | 10.00 | 2.0000 | 0.000      | 17.313 | 66.450 | 1.00   | 1.0000     | 20.0 | 0.00000 | Na    | 589nm  | 20 sec | 5 sec |
| 4                           | 1 (4/10)  | a   |             | Holder   | Specific O.R. | 275.050    |     | 0.5501 | 20.1  | 390         | Sat Dec 07 13:37:35 2013 | 0.0000  | 10.00 | 2.0000 | 0.000      | 17.313 | 66.450 | 1.00   | 1.0000     | 20.0 | 0.00000 | Na    | 589nm  | 20 sec | 5 sec |
| 5                           | 1 (5/10)  | a   |             | Holder   | Specific O.R. | 273.350    |     | 0.5467 | 20.1  | 390         | Sat Dec 07 13:37:56 2013 | 0.0000  | 10.00 | 2.0000 | 0.000      | 17.313 | 66.450 | 1.00   | 1.0000     | 20.0 | 0.00000 | Na    | 589nm  | 20 sec | 5 sec |
| 6                           | 1 (6/10)  | a   |             | Holder   | Specific O.R. | 273.950    |     | 0.5479 | 20.1  | 401         | Sat Dec 07 13:38:16 2013 | 0.0000  | 10.00 | 2.0000 | 0.000      | 17.313 | 66.450 | 1.00   | 1.0000     | 20.0 | 0.00000 | Na    | 589nm  | 20 sec | 5 sec |
| 7                           | 1 (7/10)  | a   |             | Holder   | Specific O.R. | 274.250    |     | 0.5485 | 20.2  | 382         | Sat Dec 07 13:38:36 2013 | 0.0000  | 10.00 | 2.0000 | 0.000      | 17.313 | 66.450 | 1.00   | 1.0000     | 20.0 | 0.00000 | Na    | 589nm  | 20 sec | 5 sec |
| 8                           | 1 (8/10)  | a   |             | Holder   | Specific O.R. | 274.000    |     | 0.5480 | 20.2  | 405         | Sat Dec 07 13:38:57 2013 | 0.0000  | 10.00 | 2.0000 | 0.000      | 17.313 | 66.450 | 1.00   | 1.0000     | 20.0 | 0.00000 | Na    | 589nm  | 20 sec | 5 sec |
| 9                           | 1 (9/10)  | a   |             | Holder   | Specific O.R. | 273.250    |     | 0.5465 | 20.1  | 406         | Sat Dec 07 13:39:17 2013 | 0.0000  | 10.00 | 2.0000 | 0.000      | 17.313 | 66.450 | 1.00   | 1.0000     | 20.0 | 0.00000 | Na    | 589nm  | 20 sec | 5 sec |
| 10                          | 1 (10/10) | a   |             | Holder   | Specific O.R. | 274.000    |     | 0.5480 | 20.1  | 398         | Sat Dec 07 13:39:37 2013 | 0.0000  | 10.00 | 2.0000 | 0.000      | 17.313 | 66.450 | 1.00   | 1.0000     | 20.0 | 0.00000 | Na    | 589nm  | 20 sec | 5 sec |
| 11                          | 2 (1/10)  | a   |             | Holder   | Specific O.R. | 277.600    |     | 0.2776 | 20.1  | 390         | Sat Dec 07 13:44:29 2013 | 0.0000  | 10.00 | 1.0000 | 0.000      | 17.313 | 66.450 | 1.00   | 1.0000     | 20.0 | 0.00000 | Na    | 589nm  | 20 sec | 5 sec |
| 12                          | 2 (2/10)  | a   |             | Holder   | Specific O.R. | 279.200    |     | 0.2792 | 20.2  | 375         | Sat Dec 07 13:44:49 2013 | 0.0000  | 10.00 | 1.0000 | 0.000      | 17.313 | 66.450 | 1.00   | 1.0000     | 20.0 | 0.00000 | Na    | 589nm  | 20 sec | 5 sec |
| 13                          | 2 (3/10)  | a   |             | Holder   | Specific O.R. | 276.300    |     | 0.2763 | 20.2  | 382         | Sat Dec 07 13:45:10 2013 | 0.0000  | 10.00 | 1.0000 | 0.000      | 17.313 | 66.450 | 1.00   | 1.0000     | 20.0 | 0.00000 | Na    | 589nm  | 20 sec | 5 sec |
| 14                          | 2 (4/10)  | a   |             | Holder   | Specific O.R. | 272.400    |     | 0.2724 | 20.1  | 398         | Sat Dec 07 13:45:30 2013 | 0.0000  | 10.00 | 1.0000 | 0.000      | 17.313 | 66.450 | 1.00   | 1.0000     | 20.0 | 0.00000 | Na    | 589nm  | 20 sec | 5 sec |
| 15                          | 2 (5/10)  | a   |             | Holder   | Specific O.R. | 274.500    |     | 0.2745 | 20.1  | 382         | Sat Dec 07 13:45:50 2013 | 0.0000  | 10.00 | 1.0000 | 0.000      | 17.313 | 66.450 | 1.00   | 1.0000     | 20.0 | 0.00000 | Na    | 589nm  | 20 sec | 5 sec |
| 16                          | 2 (6/10)  | a   |             | Holder   | Specific O.R. | 275.700    |     | 0.2757 | 20.1  | 378         | Sat Dec 07 13:46:11 2013 | 0.0000  | 10.00 | 1.0000 | 0.000      | 17.313 | 66.450 | 1.00   | 1.0000     | 20.0 | 0.00000 | Na    | 589nm  | 20 sec | 5 sec |
| 17                          | 2 (7/10)  | a   |             | Holder   | Specific O.R. | 275.800    |     | 0.2758 | 20.1  | 404         | Sat Dec 07 13:46:31 2013 | 0.0000  | 10.00 | 1.0000 | 0.000      | 17.313 | 66.450 | 1.00   | 1.0000     | 20.0 | 0.00000 | Na    | 589nm  | 20 sec | 5 sec |
| 18                          | 2 (8/10)  | a   |             | Holder   | Specific O.R. | 276.500    |     | 0.2765 | 20.2  | 374         | Sat Dec 07 13:46:51 2013 | 0.0000  | 10.00 | 1.0000 | 0.000      | 17.313 | 66.450 | 1.00   | 1.0000     | 20.0 | 0.00000 | Na    | 589nm  | 20 sec | 5 sec |
| 19                          | 2 (9/10)  | a   |             | Holder   | Specific O.R. | 278.800    |     | 0.2788 | 20.2  | 405         | Sat Dec 07 13:47:12 2013 | 0.0000  | 10.00 | 1.0000 | 0.000      | 17.313 | 66.450 | 1.00   | 1.0000     | 20.0 | 0.00000 | Na    | 589nm  | 20 sec | 5 sec |
| 20                          | 2 (10/10) | a   |             | Holder   | Specific O.R. | 277.400    |     | 0.2774 | 20.2  | 378         | Sat Dec 07 13:47:32 2013 | 0.0000  | 10.00 | 1.0000 | 0.000      | 17.313 | 66.450 | 1.00   | 1.0000     | 20.0 | 0.00000 | Na    | 589nm  | 20 sec | 5 sec |