SUPPORTING INFORMATION

Novel triterpenoid derivatives from *Eucomis bicolor* Bak. (Hyacinthaceae: Hyacinthoideae)

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<td>76-81</td>
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</tbody>
</table>
S.1 Structures of all compounds isolated from *Eucomis bicolor*.

**Figure S1.1** Known compounds isolated from the dichloromethane extract (EB 1-7) and methanol extract (EB 8) of *Eucomis bicolor*

EB 1 = (R)-5,7-dihydroxy-8-methoxy-3-(4’-methoxybenzyl)-4-chromanone; EB 2 = 3,5,7-trihydroxy-3-(4’-methoxybenzyl)-4-chromanone; EB 3 = (R)-5,7-dihydroxy-3-(4’-methoxybenzyl)-4-chromanone; EB 4 = eucosterol; EB 5 = (17S,23S)-23,17-epoxy-3β,28,29-trihydroxy-27-norlanost-8-en-24-one; EB 6 = 15-deoxoeucosterol; EB 7 = 3-dehydro-15-deoxoeucosterol; EB 8 = (R)-5,7-dihydroxy-3-(4’-hydroxybenzyl)-4-chromanone.
Figure S 1.2: New compounds isolated from the dichloromethane extract of *Eucomis bicolor*.

Figure S 1.3: Monosaccharide triterpenoid derivatives isolated from the methanol extract of *Eucomis bicolor* (after acetylation of a complex mixture)

Figure S 1.3: Disaccharide triterpenoid derivatives isolated from the methanol extract of *Eucomis bicolor* (after acetylation of a complex mixture).


Figure S 1.4: Trisaccharide triterpenoid derivative isolated from the methanol extract of *Eucomis bicolor* after acetylation.

14Ac = (17S,23S)-29-acetoxy-23,17-epoxy-3β-[2′,3′,4′-tri-O-acetyl-β-D-glucopyranoside-(6′→1′′)-2″,3″,4″′-tri-O-acetyl-β-D-arabinopyranosyl-(3′→1′′′)-2″″,3″″,4″″′-tri-O-acetyl-β-D-xylopyranosyl]-27-norlanost-8-ene-15,24-dione.
S.2.1: Flow chart of the compounds isolated from the dichloromethane extract of *Eucomis bicolor* Bak.

![Flow chart diagram]

- **SC** - small column-silica, 1 cm diameter, 2 ml fractions collected
- **SC-Sephadex** - small column-sephadex, 1cm diameter, 2 ml fractions collected
- **LC** - large column-silica, 5 cm diameter, 75 ml fractions collected
- **PTLC** - Preparative TLC
- **D** - DCM
- **M** - MeOH
- **Et** - Ethyl acetate
- **E** - Diethyl ether
S. 2.2 Flow chart of the compounds isolated from the methanol extract of *Eucomis bicolor* Bak.

**Eucomis bicolor** (104.87g)

- **LC/3% M**: 97% D
  - Fr 13-17
  - **LC/8% Et**: 92% D
    - Fr 4-5
    - **EB 8 (8.2 mg)**

- **Fr 115 (6Ac, 1.9 mg), Fr 58-51 (8Ac, 1.8 mg), Fr 34-35 (10Ac, 2.3 mg), Fr 21-22 (12Ac, 2.1 mg)**

- **LC/15% M**: 85% D
  - Fr 30-33
  - **SC/50% Et**: 50% D
    - Fr 12-16
    - **PTLC x 2/10% M**: 90% D
      - **No separation**
      - **SC-Sep/50% M**: 50% D
        - Fr 9-14
        - **Ac/SC/8%Et**: 92% D

- **Fr 115 (6Ac, 1.9 mg), Fr 58-51 (8Ac, 1.8 mg), Fr 34-35 (10Ac, 2.3 mg), Fr 21-22 (12Ac, 2.1 mg)**

- **LC/20% M**: 80% D
  - Fr 40-45
  - **SC/50% Et**: 50% D
    - Fr 20-24
    - **PTLC x 2/15% M**: 90% D
      - **No separation**
      - **SC-Sep/50% M**: 50% D
        - Fr 7-11
        - **Ac/SC/8%Et**: 92% D

- **Fr 101 (7Ac, 1.2 mg), Fr 43 (9Ac, 1.1 mg), Fr 19-20 (11Ac, 0.8 mg), Fr 10-11 (13Ac, 1.7 mg), Fr 123 (14Ac, 1.4 mg)**

- **Fr 4-5 (8.2 mg)**
S.3 Details for the LSD input file

; The LSD input file starts below the row of stars.
; The lines must be copied in a text editor
; such as textedit (Mac), gedit (Linux) or notepad++ (Windows)
; and saved as simple text.

; *****************************************************

; Compound 1
ELIM 1 4 ; 1 HMBC correlation can be 4J

; LSD atom numbering (Hs excepted)
MULT 1 C 2 0 ; Atom 1 is a C, is hybridized sp2, and has 0 H atom attached
MULT 2 C 2 0
MULT 3 C 2 0
MULT 4 C 2 0
MULT 5 C 3 0
MULT 6 C 3 0
MULT 7 C 3 1
MULT 8 C 3 0
MULT 9 C 3 1
MULT 10 C 3 1
MULT 11 C 3 2
MULT 12 C 3 2
MULT 13 C 3 2
MULT 14 C 3 2
MULT 15 C 3 0
MULT 16 C 3 2
MULT 17 C 3 3
MULT 18 C 3 2
MULT 19 C 3 2
MULT 20 C 3 2
MULT 21 C 3 2
MULT 22 C 3 3
MULT 23 C 3 3
MULT 24 C 3 3
MULT 25 C 3 3
MULT 26 O 2 0
MULT 27 O 2 0
MULT 28 O 3 0

SHIX 1 213.1 ; The chemical shift of C-1 is 213.1 ppm
SHIX 2 177.1
SHIX 3 135.8
SHIX 4 133.1
SHIX 5 98.4

; the SHIX commands are ignored by LSD
HSQC 1 1 ; see below about HMBC (11 18 21)
HSQC 2 2 ; idem
HSQC 3 3 ; idem
HSQC 4 4 ; idem
HSQC 5 5 ; idem
HSQC 6 6 ; idem
HSQC 7 7

; HMBC (11 18 21) 5
HSQC 14 14
HSQC 15 15 ; idem
HSQC 16 16
HSQC 17 17
HSQC 18 18 ; C-18 is bound to H-18 (even though there are two of them)
HSQC 19 19
HSQC 20 20
HSQC 21 21
HSQC 22 22
HSQC 23 23
HSQC 24 24
HSQC 25 25

COSY 7 9 ; H-7 and H-9 correlate in the COSY spectrum (strong intensity, 3J)
COSY 7 20
COSY 10 12
COSY 13 14
COSY 23 10
COSY 25 9

BOND 1 26 ; C=O ketone
BOND 2 27 ; C=O lactone
BOND 2 28 ; C-O lactone
BOND 5 28 ; O-C lactone
BOND 3 4 ; C=C

HMBC 1 13 ; C-1 correlates with H-13 in the HMBC spectrum
HMBC 1 9
HMBC 1 14
HMBC 1 25

HMBC 2 12
HMBC 2 10
HMBC 2 12

HMBC 3 20 ; low intensity
HMBC 3 16 ; idem
HMBC 3 17

HMBC 4 14 ; idem
HMBC 4 19 ; idem
HMBC 4 24

; C-5 correlates with H-11 or H-18 or H-21
; This should be written HMBC 5 (11 18 21).

; The LSD syntax does not allow it, sorry.
; This is equivalent to HMBC (11 18 21) 5
; because of the numbering of Hs according to Cs using HSQC data.
; this forces to "invent" an H-5 that does not exist
; and explains why a few quaternary Cs (among which C-5)
; are declared in the HSQC section.
Therefore:
HMBC (11 18 21) 5
HMBC 5 12
HMBC 5 16
HMBC 5 23
HMBC 5 22

HMBC 7 9
HMBC (14 18) 7
HMBC 7 20
HMBC 7 24
HMBC 7 25

HMBC 8 19
HMBC (11 18 21) 8
HMBC 8 19
HMBC (16 20) 8
HMBC 8 17
HMBC 8 22

HMBC 9 13
HMBC (11 18 21) 9
HMBC 9 7
HMBC 9 25

HMBC 10 12
HMBC (11 18 21) 10
HMBC 10 12
HMBC 10 23

HMBC 11 16

HMBC 12 10
HMBC 12 23
| HMBC 13 14 | HMBC 19 22 |
| HMBC 14 13 | HMBC 20 9 |
| HMBC 14 24 | HMBC (14 18) 20 |
| HMBC 15 13 | HMBC 20 7 |
| HMBC 15 14 | HMBC 21 19 |
| HMBC 15 20 |
| HMBC 15 7 |
| HMBC 15 24 | HMBC 22 19 |
| HMBC (11 18 21) 16 | HMBC 23 12 |
| HMBC 16 17 | HMBC 23 10 |
| HMBC 17 16 | HMBC 24 14 |
| HMBC 18 20 | HMBC 24 7 |
| HMBC 20 7 |
| HMBC 21 19 |
| HMBC 22 19 |
| HMBC 23 12 |
| HMBC 23 10 |
| HMBC 24 14 |
| HMBC 24 7 |

**QUAT L1 ; L1 is the list of quaternary carbons**
**LIST L2 17 22 24 ; L2 is the list of the indexes of methyl singlets**
**PROP L2 1 L1 ; each singlet methyl has exactly one quaternary carbon as neighbor**

**CH L3 ; L3 is the list of methine carbons**
**LIST L4 23 25 ; L4 is the list of the indexes of methyl doublets**
**PROP L4 1 L3 ; each doublet methyl has exactly one methine carbon as neighbor**
NMR spectra for compounds 1-5 and 6Ac-14Ac. (See Figures S1.1, S 1.2, S 1.3 and S 1.4 for names and structures).
Spectrum S.3.1.2: FTIR spectrum for compound 1

Spectrum S.3.1.3: $^1$H NMR spectrum for compound 1 in CDCl$_3$
Spectrum S.3.1.4: $^{13}$C NMR spectrum for compound 1 in CDCl$_3$

Spectrum S.3.1.5: DEPT spectrum for compound 1 in CDCl$_3$
Spectrum S.3.1.6: HSQCDEPT spectrum for compound 1 in CDCl₃

Spectrum S.3.1.7: HMBC spectrum for compound 1 in CDCl₃
Spectrum S.3.2.1: Mass spectrum for compound 2Ac

Spectrum S.3.2.2: FTIR spectrum for compound 2Ac
Spectrum S.3.2.3: $^1$H NMR spectrum for compound 2Ac in CDCl$_3$

Spectrum S.3.2.4: $^{13}$C NMR spectrum for compound 2Ac in CDCl$_3$
Spectrum S.3.2.5: DEPT spectrum for compound 2Ac in CDCl$_3$

Spectrum S.3.2.6: HSQCDEPT spectrum for compound 2Ac in CDCl$_3$
Spectrum S.3.2.7: HMBC spectrum for compound 2Ac in CDCl₃

Spectrum S.3.2.8: COSY spectrum for compound 2Ac in CDCl₃
Spectrum S.3.2.9: NOESY spectrum for compound 2Ac in CDCl₃

Spectrum S.3.3.1: Mass spectrum for compound 3
Spectrum S.3.3.2: FTIR spectrum for compound 3

Spectrum S.3.3.3: $^1$H NMR spectrum for compound 3 in CDCl$_3$
Spectrum S.3.3.4: $^{13}$C NMR spectrum for compound 3 in CDCl$_3$.

Spectrum S.3.3.5: DEPT spectrum for compound 3 in CDCl$_3$.
Spectrum S.3.3.6: HSQCDEPT spectrum for compound 3 in CDCl₃

Spectrum S.3.3.7: HMBC spectrum for compound 3 in CDCl₃
Spectrum S.3.3.9: COSY spectrum for compound 3 in CDCl₃

Spectrum S.3.3.9: NOESY spectrum for compound 3 in CDCl₃
Spectrum S.3.4.1: Mass spectrum for compound 4

Spectrum S.3.4.2: FTIR spectrum for compound 4
Spectrum S.3.4.3: $^1$H NMR spectrum for compound 4 in CDCl$_3$
Spectrum S.3.4.4: DEPT spectrum for compound 4 in CDCl₃

Spectrum S.3.4.6: HSQCDEPT spectrum for compound 4 in CDCl₃
Spectrum S.3.4.7: HMBC spectrum for compound 4 in CDCl₃
Spectrum S.3.5.1: Mass spectrum for compound 5

Spectrum S.3.5.2: FTIR spectrum for compound 5
Spectrum S.3.5.4: $^{13}$C NMR spectrum for compound 5 in CDCl$_3$

Spectrum S.3.5.5: DEPT spectrum for compound 5 in CDCl$_3$
Spectrum S.3.5.6: HSQCDEPT spectrum for compound 5 in CDCl₃

Spectrum S.3.5.7: HMBC spectrum for compound 5 in CDCl₃
Spectrum S3.5.8: COSY spectrum for compound 5 in CDCl₃

Spectrum S3.5.9: NOESY spectrum for compound 5 in CDCl₃
Spectrum S3.6.2: FTIR spectrum for compound 6Ac

Spectrum S3.6.1: Mass spectrum for compound 6Ac
Spectrum S3.6.5: DEPT spectrum for compound 6Ac in CDCl₃

Spectrum S3.6.6: HSQCDEPT spectrum for compound 6Ac in CDCl₃
Spectrum S3.6.7: HMBC spectrum for compound 6Ac in CDCl3.

Spectrum S3.6.8: COSY spectrum for compound 6Ac in CDCl3.
Spectrum S3.6.9: NOESY spectrum for compound 6Ac in CDCl₃

Spectrum S3.7.1: Mass spectrum for compound 7Ac
Spectrum S.3.7.2: FTIR spectrum for compound 7Ac

Spectrum S.3.7.3: $^1$H NMR spectrum for compound 7Ac in CDCl$_3$
Spectrum S.3.7.4: $^1$C NMR spectrum for compound 7Ac in CDCl$_3$

Spectrum S.3.7.5: DEPT spectrum for compound 7Ac in CDCl$_3$
Spectrum S.3.7.8: COSY spectrum for compound 7Ac in CDCl₃

Spectrum S.3.7.9: NOESY spectrum for compound 7Ac in CDCl₃
Mass Spectrum SmartFormula Report

Analysis Info
Analysis Name: 1406_data_pulver_12/MSS 10984b_55_01_44084.d
Method: 2.5min_cat_sample_eros_Naf_11-10-10.m
Sample Name: MSS 10984b
Comment: 

Acquisition Date: 25/06/2012 17:15:42
Operator: Mass Spec
Instrument / Ser#: microTOF 512

Acquisition Parameter
Source Type: ESI
Focus: Not active
Scan Begin: 100 m/z
Scan End: 1000 m/z
Ion Polarity: Positive
Set Nebulizer: 2.0 Bar
Set Capillary: 4500 V
Set Dry Heater: 181 °C
Set Dry Gas: 10.0 l/min
Set Divert Valve: Source
Set End Plate Offset: -500 V

This is the measured mass spectrum of your compound.

Spectrum S3.8.1: Mass spectrum for compound 8Ac

Spectrum S3.8.2: FTIR spectrum for compound 8A
Spectrum S3.8.3: $^1$H NMR spectrum for compound 8Ac in CDCl₃

Spectrum S3.8.4: $^{13}$C NMR spectrum for compound 8Ac in CDCl₃
Spectrum S3.8.5: DEPT spectrum for compound 8Ac in CDCl₃

Spectrum S3.8.6: HSQCDEPT spectrum for compound 8Ac in CDCl₃
Mass Spectrum SmartFormula Report

Analysis Info
Analysis Name: 5000-Data-12/MSS 10983b_15_01_445683.d
Method: 2.5min_cal_sample_pos_Naf_Mid_mass.m
Sample Name: MSS 10983b
Comment:

Acquisition Info
Acquisition Date: 25/06/2012 17:12:12
Operator: Mass Spec
Instrument: Sent microTOF 92

Acquisition Parameter
Source Type: ESI
Flow: Not active
Scan Begin: 100 m/z
Scan End: 1500 m/z
Ion Polarity: Positive
Set Nebulizer: 2.0 Bar
Set Capillary: 4500 V
Set End Plate Offset: -500 V
Set Dry Heater: 180 °C
Set Dry Gas: 10.0 l/min
Set Divert Valve: Source

Spectrum S3.9.1: Mass spectrum for compound 9Ac

Spectrum S3.9.3: 1H NMR spectrum for compound 9Ac in CDCl₃
Spectrum S3.9.4: $^{13}$C NMR spectrum for compound 9Ac in CDCl$_3$

Spectrum S3.9.5: DEPT spectrum for compound 9Ac in CDCl$_3$
Spectrum S3.9.6: HSQCDEPT spectrum for compound 9Ac in CDCl₃

Spectrum S3.9.7: HMBC spectrum for compound 9Ac in CDCl₃
Spectrum S3.9.8: COSY spectrum for compound 9Ac in CDCl₃

Spectrum S3.9.9: NOESY spectrum for compound 9Ac in CDCl₃
Spectrum S3.10.1: Mass spectrum for compound 10Ac

Spectrum S3.10.2: FTIR spectrum for compound 10Ac
Spectrum S3.10.3: $^1$H NMR spectrum for compound 10Ac in CDCl$_3$.

Spectrum S3.10.4: $^{13}$C NMR spectrum for compound 10Ac in CDCl$_3$. 
Spectrum S3.10.5: DEPT spectrum for compound 10Ac in CDCl₃

Spectrum S3.10.6: HSQCDEPT spectrum for compound 10Ac in CDCl₃
Spectrum S3.10.9: NOESY spectrum for compound 10Ac in CDCl₃

### Mass Spectrum SmartFormula Report

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This is the measured mass spectrum of your compound.

**Spectrum S3.11.1**: Mass spectrum for compound 11Ac
Spectrum S3.11.2: FTIR spectrum for compound 11Ac

Spectrum S3.11.3: $^1$H NMR spectrum for compound 11Ac in CDCl$_3$
Spectrum S.3.11.4: $^{13}$C NMR spectrum for compound 11Ac in CDCl$_3$

Spectrum S.3.11.5: DEPT spectrum for compound 11Ac in CDCl$_3$
Spectrum S.3.11.6: HSQCDEPT spectrum for compound 11Ac in CDCl₃

Spectrum S.3.11.7: HMBC spectrum for compound 11Ac in CDCl₃
Spectrum S.3.11.6: COSY spectrum for compound II Ac in CDCl₃

Spectrum S.3.11.9: NOESY spectrum for compound II Ac in CDCl₃
Mass Spectrum SmartFormula Report

Analysis Info
Analysis Name: Z:\Sep 11MSS09703_19_01_32461.d
Method: 2.5min_old_sample_pos_Hif_11-10-10.m
Sample Name: MSS09703
Comment: 

Acquisition Date: 16/09/2011 10:58 am
Operator: Mass Spec
Instrument/Seq: hiTOF 92

Acquisition Parameter
Source Type: ESI
Focus: Not active
Scan Begin: 100 m/z
Scan End: 1600 m/z
Ion polarity: Positive
Set Nebulizer: 2.0 Bar
Set Dry Heater: 190 °C
Set Dry Gas: 13.0 l/min
Set End Plate Offset: -500 V
Set Ejector Valve: Source

This is the measured mass spectrum of your compound.

Theoretical isotope model: C_6H_6NaO_15: [867.4147]

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<th>Meas. m/z</th>
<th># Formula</th>
<th>m/z err [ppm]</th>
<th>Mean err [ppm]</th>
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<th>e'</th>
<th>Conf</th>
<th>mSigma</th>
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<tr>
<td>867.4147</td>
<td>1 C_65H_64NaO_15</td>
<td>+1.1</td>
<td>+1.9</td>
<td>13.5</td>
<td>even</td>
<td>50.49</td>
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</tr>
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Spectrum S.3.12.1: Mass spectrum for compound 12Ac

Spectrum S.3.12.2: FTIR spectrum for compound 12Ac
Spectrum S3.12.3: $^1$H NMR spectrum for compound 12Ac in CDCl$_3$. 
Spectrum S3.12.4: $^{13}$C NMR spectrum for compound 12Ac in CDCl$_3$

Spectrum S3.12.5: DEPT spectrum for compound 12Ac in CDCl$_3$
Spectrum S3.12.6: HSQCDEPT spectrum for compound 12Ac in CDCl₃

Spectrum S3.12.7: HMBC spectrum for compound 12Ac in CDCl₃
Spectrum S3.12.8: COSY spectrum for compound 12Ac in CDCl₃

Spectrum S3.12.9: NOESY spectrum for compound 12Ac in CDCl₃
Mass Spectrum SmartFormula Report

Analysis Info
Analysis Name: UnofDat Jun 12 MSS 10982_55_01_43046.d
Method: 2.5 min_cal_sample_pos_Nat_Mid_mass.m
Sample Name: MSS 10982
Comment:

Acquisition Info
Acquisition Date: 22/06/2012 14:13:50
Operator: Mass Spec
Instrument / Ser#: microTOF 92

Acquisition Parameter
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Focus: Not active
Scan Begin: 100 m/z
Scan End: 1500 m/z
Scan Rate: 5000 V
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Set End Plate Offset: -500 V
Set Nebulizer: 2.0 Bar
Set Dry Heater: 100 °C
Set Dry Gas: 10.0 L/min
Set Divert valve: Source

This is the measured mass spectrum of your compound.

Theoretical Isotope Model: C 54 H 76 Na D 21 + 1083.48

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<td>102.74</td>
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Spectrum S3.13.3: $^1$H NMR spectrum for compound 13Ac in CDCl$_3$.

Spectrum S3.13.4: $^{13}$C NMR spectrum for compound 13Ac in CDCl$_3$.
Spectrum S3.13.5: DEPT spectrum for compound 13Ac in CDCl₃

Spectrum S3.13.6: HSQCDEPT spectrum for compound 13Ac in CDCl₃
Spectrum S3.13.7: HMBC spectrum for compound 13Ac in CDCl₃

Spectrum S3.13.8: COSY spectrum for compound 13Ac in CDCl₃
Spectrum S3.14.2: FTIR spectrum for compound 14Ac

Spectrum S3.14.3: 1H NMR spectrum for compound 14Ac in CDCl3
Spectrum S3.14.4: $^{13}$C NMR spectrum for compound 14Ac in CDCl$_3$

Spectrum S3.14.5: DEPT spectrum for compound 14Ac in CDCl$_3$
Spectrum S3.14.8: COSY spectrum for compound 14Ac in CDCl₃

Spectrum S3.14.9: NOESY spectrum for compound 14Ac in CDCl₃
S.5 NCI 59 CELL SCREENING DATA FOR COMPOUNDS

The following compounds were submitted to the NCI-59 Panel:

5,7-dihydroxy-8-methoxy-3-(4′-methoxybenzyl)-4-chromanone (EB1), eucosterol (EB4), (23S)-17α,23-epoxy-3β,28,29-trihydroxy-27-norlanost-8-en-24-one (EB5), 2Ac, 3, 4 and 5.

Structures are provided in S.1

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Figure S.4.1: Single dose screen report for compound EB1
**Figure S.4.2: Single dose screen report for compound EB4**
Figure S.4.3: Single dose screen report for compound EB5
### Figure S.4.4: Single dose screen report for compound 2Ac

<table>
<thead>
<tr>
<th>Panel/Cell Line</th>
<th>Growth Percent</th>
<th>Mean Growth Percent - Growth Percent</th>
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<tbody>
<tr>
<td>Leukemia</td>
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</tr>
<tr>
<td>CCRF-CEM</td>
<td>93.48</td>
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The graph shows the growth percent and mean growth percent for various cell lines treated with compound 2Ac.
Figure S.4.5: Single dose screen report for compound 3
Figure S.4.6: Single dose screen report for compound 5