

$$\text{holo} = ((\text{RNA0} - \text{holo}) * (\text{L0} - \text{holo})) / \text{Kbind}$$

$$\text{Solve}[(\text{RNA0} - \text{holo}) * (\text{L0} - \text{holo}) / \text{Kbind} == \text{holo}, \text{holo}]$$

$$\left\{ \left\{ \text{holo} \rightarrow \frac{1}{2} \left(\text{Kbind} + \text{L0} + \text{RNA0} - \sqrt{(-\text{Kbind} - \text{L0} - \text{RNA0})^2 - 4 \text{L0} \text{RNA0}} \right) \right\}, \right. \\ \left. \left\{ \text{holo} \rightarrow \frac{1}{2} \left(\text{Kbind} + \text{L0} + \text{RNA0} + \sqrt{(-\text{Kbind} - \text{L0} - \text{RNA0})^2 - 4 \text{L0} \text{RNA0}} \right) \right\} \right\}$$

$$\text{holo1}[\text{L0_}, \text{RNA0_}, \text{Kbind_}] :=$$

$$\left(\left(\frac{1}{2} \left(\text{Kbind} + \text{L0} + \text{RNA0} - \sqrt{(-\text{Kbind} - \text{L0} - \text{RNA0})^2 - 4 \text{L0} \text{RNA0}} \right) \right) \right) / \text{RNA0} * 100$$

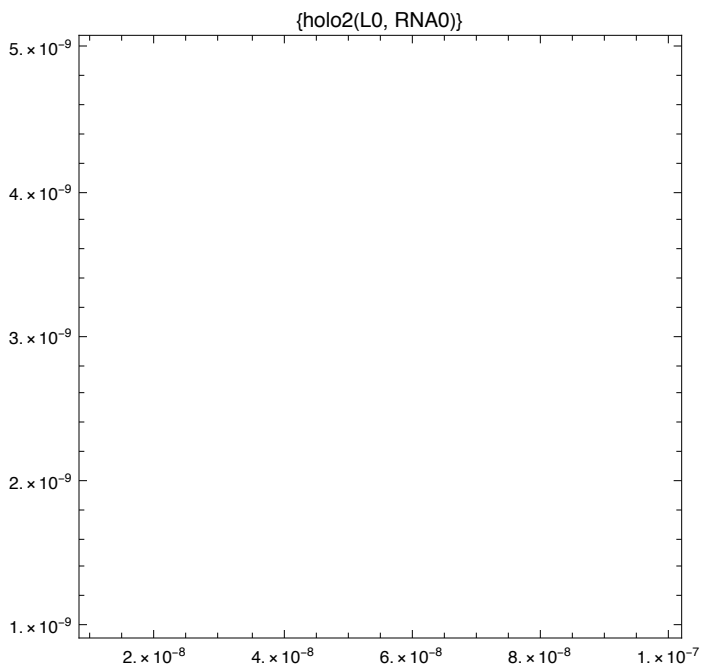
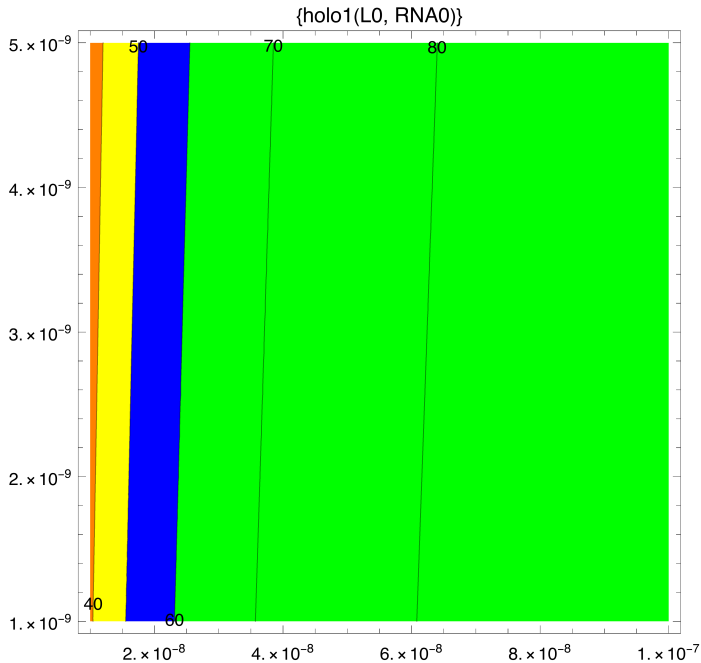
$$\text{holo2}[\text{L0_}, \text{RNA0_}, \text{Kbind_}] :=$$

$$\left(\left(\frac{1}{2} \left(\text{Kbind} + \text{L0} + \text{RNA0} + \sqrt{(-\text{Kbind} - \text{L0} - \text{RNA0})^2 - 4 \text{L0} \text{RNA0}} \right) \right) \right) / \text{RNA0} * 100$$

```

ContourPlot[holo1[L0, RNA0,  $1.5 \times 10^{-8}$ ], {L0,  $0.01 \times 10^{-6}$ ,  $0.1 \times 10^{-6}$ },
  {RNA0,  $1 \times 10^{-9}$ ,  $5 \times 10^{-9}$ }, Contours → {10, 20, 30, 40, 50, 60, 70, 80, 90, 100},
  ContourShading → {Red, Red, Red, Orange, Yellow, Blue, Green, Green, Green, Green},
  ContourLabels → True, PlotLabel → {"holo1(L0, RNA0)"}, PlotRange → {0, 100}]
ContourPlot[holo2[L0, RNA0,  $1.5 \times 10^{-8}$ ], {L0,  $0.01 \times 10^{-6}$ ,  $0.1 \times 10^{-6}$ },
  {RNA0,  $1 \times 10^{-9}$ ,  $5 \times 10^{-9}$ }, Contours → {10, 20, 30, 40, 50, 60, 70, 80, 90, 100},
  ContourShading → {Red, Red, Red, Orange, Yellow, Blue, Green, Green, Green, Green},
  ContourLabels → True, PlotLabel → {"holo2(L0, RNA0)"}, PlotRange → {0, 100}]

```



```
R = 8.3144621 (*J/mol*K*)
```

```
DeltaHbind = 110470.2357608338`
```

```
DeltaSbind = 238.303284932985`
```

```
holo[L0_, RNA0_, T_] :=
```

$$\left(\left(\frac{1}{2} \left(e^{-\frac{(\text{DeltaHbind} - T \cdot \text{DeltaSbind})}{R \cdot T}} + L0 + \text{RNA0} - \sqrt{\left(-e^{-\frac{(\text{DeltaHbind} - T \cdot \text{DeltaSbind})}{R \cdot T}} - L0 - \text{RNA0} \right)^2 - 4 L0 \text{RNA0}} \right) \right) / \text{RNA0} \right) * 100$$

```
8.31446
```

```
110470.
```

```
238.303
```

```
ContourPlot[holo[L0, 1.5 * 10-9, T], {T, 273, 303},
```

```
{L0, 0.01 * 10-6, 1 * 10-6}, Contours → {10, 20, 30, 40, 50, 60, 70, 80, 90, 100},
```

```
ContourShading → {Red, Red, Red, Orange, Yellow, Blue, Green, Green, Green, Green},
```

```
ContourLabels → True, PlotLabel → {"holo(L0, T)"}, PlotRange → {0, 100}]
```

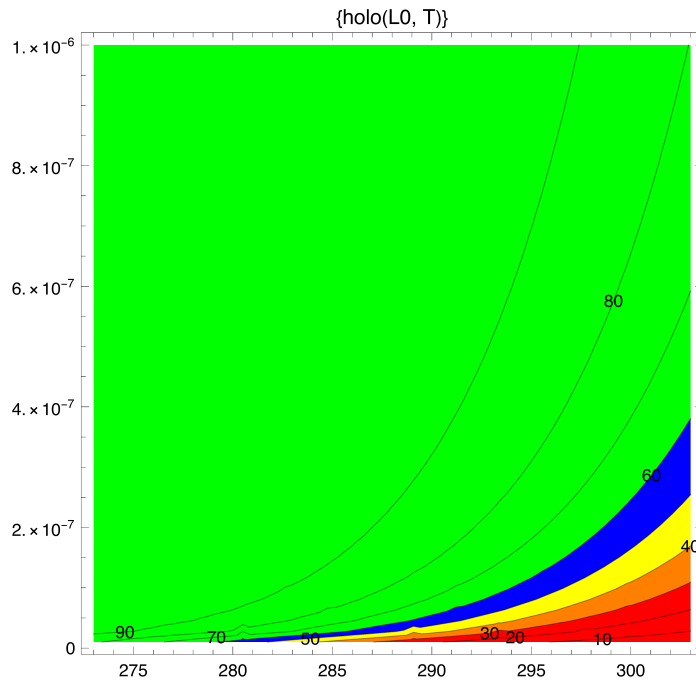
```
p1 = Plot[holo[1 * 10-6, 1.5 * 10-9, T], {T, 273, 303},
```

```
PlotLabel → {"holo(T)"}, PlotRange → {0, 100}, PlotStyle → Red];
```

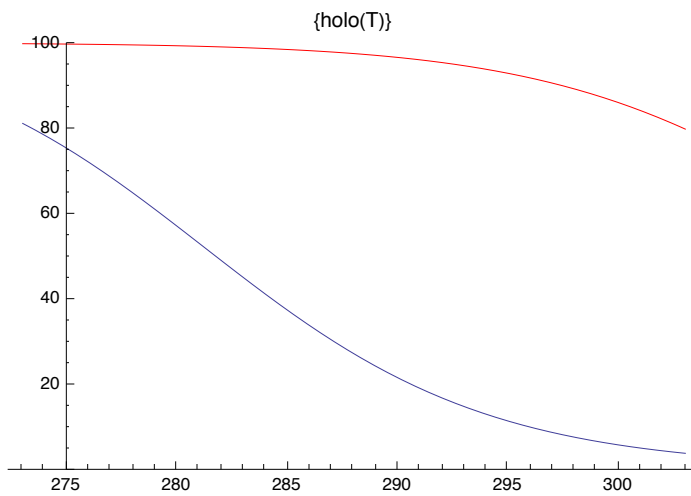
```
p2 = Plot[holo[0.01 * 10-6, 1.5 * 10-9, T], {T, 273, 303},
```

```
PlotLabel → {"holo(T)"}, PlotRange → {0, 100}.PlotStyle → Blue];
```

```
Show[p1, p2]
```



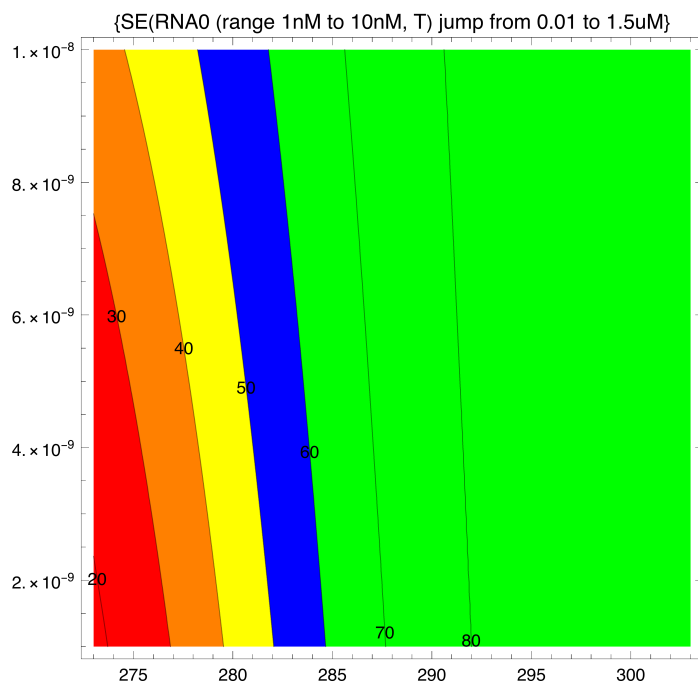
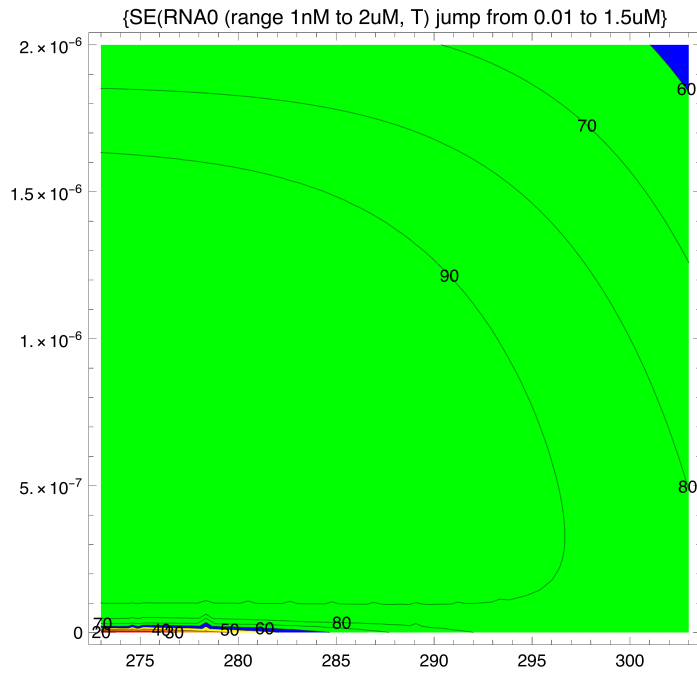
Plot::prng : Value of option PlotRange -> {0, 100}. PlotStyle -> RGBColor[0, 0, 1] is not All, Full, Automatic, a positive machine number, or an appropriate list of range specifications. >>

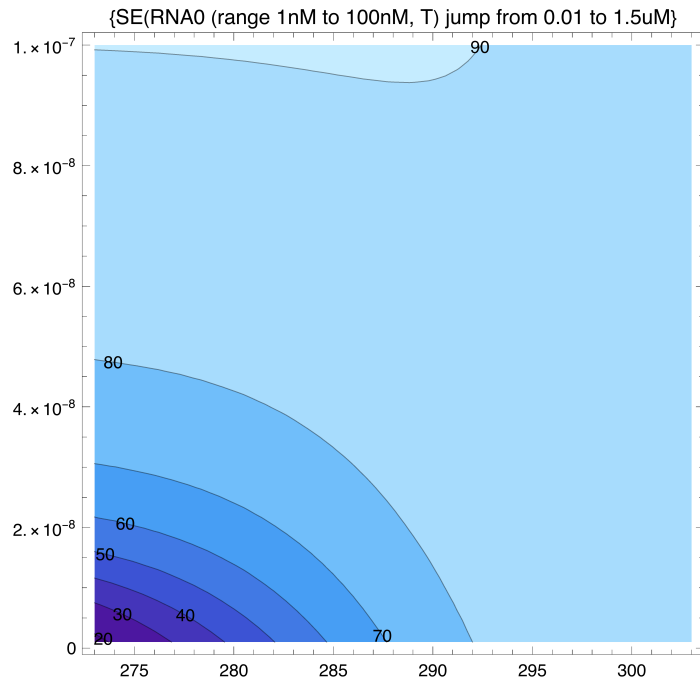


```

ContourPlot[holo[ $1.5 \times 10^{-6}$ , RNA0, T] - holo[ $0.01 \times 10^{-6}$ , RNA0, T], {T, 273, 303},
  {RNA0,  $1 \times 10^{-9}$ ,  $2 \times 10^{-6}$ }, Contours → {10, 20, 30, 40, 50, 60, 70, 80, 90, 100},
  ContourShading → {Red, Red, Red, Orange, Yellow, Blue, Green, Green, Green, Green},
  ContourLabels → True, PlotLabel →
    {"SE(RNA0 (range 1nM to 2uM, T) jump from 0.01 to 1.5uM"}, PlotRange → {0, 100}]
ContourPlot[holo[ $1.5 \times 10^{-6}$ , RNA0, T] - holo[ $0.01 \times 10^{-6}$ , RNA0, T], {T, 273, 303},
  {RNA0,  $1 \times 10^{-9}$ ,  $1 \times 10^{-8}$ }, Contours → {10, 20, 30, 40, 50, 60, 70, 80, 90, 100},
  ContourShading → {Red, Red, Red, Orange, Yellow, Blue, Green, Green, Green, Green},
  ContourLabels → True, PlotLabel →
    {"SE(RNA0 (range 1nM to 10nM, T) jump from 0.01 to 1.5uM"}, PlotRange → {0, 100}]
ContourPlot[holo[ $1.5 \times 10^{-6}$ , RNA0, T] - holo[ $0.01 \times 10^{-6}$ , RNA0, T],
  {T, 273, 303}, {RNA0,  $1 \times 10^{-9}$ ,  $1 \times 10^{-7}$ },
  Contours → {10, 20, 30, 40, 50, 60, 70, 80, 90, 100},
  ColorFunction → ColorData["DeepSeaColors"], ContourLabels → True,
  PlotLabel → {"SE(RNA0 (range 1nM to 100nM, T) jump from 0.01 to 1.5uM"},
  PlotRange → {0, 100}]

```





(*Werte für die NMR Magnesium Bedingungen*)

R = 8.3144621 (*J/mol*K*)

DeltaHbind = 132703.18846113922`

DeltaSbind = 370.02936714423925`

holo[L0_, RNA0_, T_] :=

$$\left(\left(\frac{1}{2} \left(e^{-\frac{(\text{DeltaHbind} - T \cdot \text{DeltaSbind})}{R \cdot T}} + L0 + \text{RNA0} - \sqrt{\left(-e^{-\frac{(\text{DeltaHbind} - T \cdot \text{DeltaSbind})}{R \cdot T}} - L0 - \text{RNA0} \right)^2 - 4 L0 \text{RNA0}} \right) \right) / \text{RNA0} \right) * 100$$

ContourPlot[holo1[L0, 1.5 * 10⁻⁹, T], {T, 273, 303}, {L0, 0.01 * 10⁻⁶, 1 * 10⁻⁶},
Contours → {10, 20, 30, 40, 50, 60, 70, 80, 90, 100},
ContourShading → {Red, Red, Red, Orange, Yellow, Blue, Green, Green, Green, Green},
ContourLabels → True, PlotLabel → {"holo1(L0, T)"}, PlotRange → {0, 100}]

p1 = Plot[holo1[1 * 10⁻⁶, 1.5 * 10⁻⁹, T], {T, 273, 303},
PlotLabel → {"holo1(T)"}, PlotRange → {0, 100}, PlotStyle → Red];

p2 = Plot[holo1[0.01 * 10⁻⁶, 1.5 * 10⁻⁹, T], {T, 273, 303},
PlotLabel → {"holo1(T)"}, PlotRange → {0, 100}.PlotStyle → Blue];

Show[

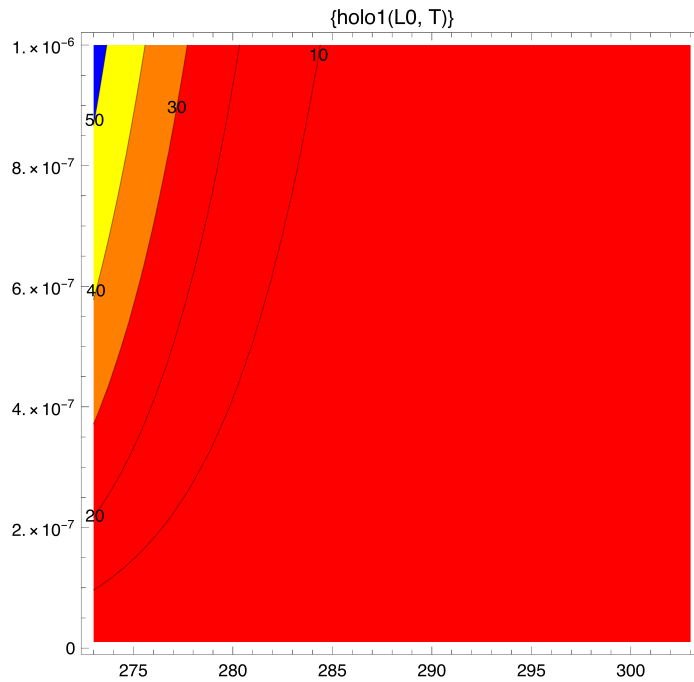
p1,

p2]

8.31446

132 703.

370.029



Plot::prng : Value of option PlotRange $\rightarrow \{0, 100\}$. PlotStyle $\rightarrow \text{RGBColor}[0, 0, 1]$ is not All, Full, Automatic, a positive machine number, or an appropriate list of range specifications. \gg

