```
(*  Paper: Quapp / Bofill, J. Phys Chem B ... 2024 ... *)
(* Publication Date: April 18, 2024
                  Datum
   https://doi.org/10.1021/acs.jpcb.4c00468 *)
(* First we calculate the PES and Newton trajectories (NT) on it *)
  erstes Element
(* main direction (L+d) for dashed NT, comparison with (-1,1) for black NT  *)
(* blue is the corresponding singular NT, red the NT to direction (1,0) *)


(* first molecule LSelA108A + 2GSP6 : no.4 in Table of BB *)
                                                    Tabelle
```

(Debug) In[79]:=

```
ph0 = 0.58 * Pi ;
            Kreis
d0 = 0.33;
k0 = 266.0;
D0 = 201.0;
cc = 0.0;
ph1 = 0.97 * Pi ;
            Kreis
sig = 0.17 * Pi ;
            Kreis
```

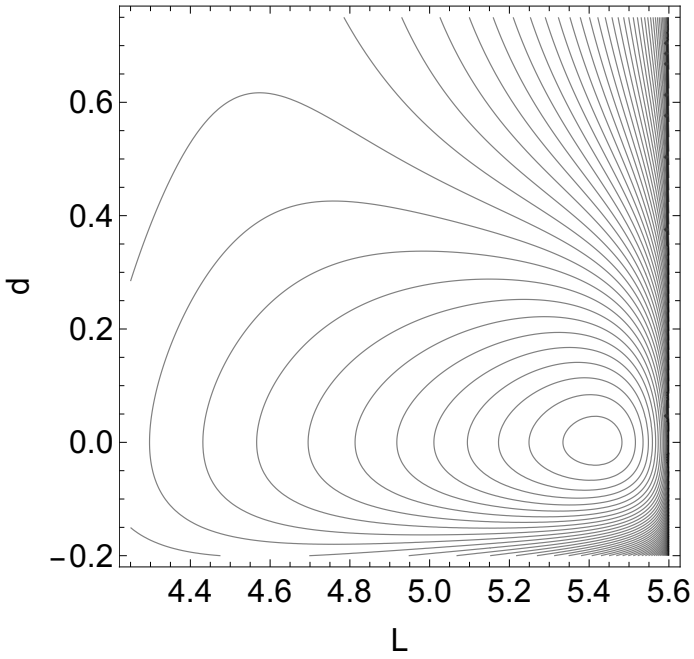
(Debug) In[98]:=

```
PHI[L_] = 2.0 * ArcSin[L / 5.6]
                Arkussinus
De[ph_] = D0 * Exp[-(ph - ph1)^2 / (2. * sig^2)] + cc
              Exponentialfunktion
Vphi[L_] = 0.5 * k0 * (PHI[L] - ph0)^2
Be[d_, ph_] = De[ph] * ((1.0 - Exp[-d / d0])^2 - 1.)
                                Exponentialfunktion
pes[L_, d_, F_] = Vphi[L] + Be[d, PHI[L]] - (L + d) * F
```

(Debug) In[91]:=

```
conBarLSelA = ContourPlot[pes[L, d, 0], {L, 4.25, 5.6},
                Konturgraphik
  {d, -0.2, 0.75}, ContourShading → False, Contours → 50, PlotRange → All,
                   Kontur-Schattierung  falsch  Konturen  Koordinatenb···  alle
  PlotPoints → 53, ContourStyle → Thickness[0.00215], FrameLabel → {"L", "d"},
  Anzahl der Punkte in d···  Konturenstil  Dicke  Rahmenbeschriftung
  AspectRatio → 1, FormatType → TraditionalForm, FrameStyle → FontSize → 16]
  Seitenverhältnis  Formattyp  traditionelle Form  Rahmenstil  Schriftgröße
```

(Debug) Out[91]=




(Debug) In[103]:=

```
(* derivations, here for traditional reasons, the second variable has no.3 *)
p3[L_, d_] = D[pes[L, d, 0], d];
             leite ab
p1[L_, d_] = D[pes[L, d, 0], L];
             leite ab
p11[L_, d_] = D[p1[L, d], L];
              leite ab
p33[L_, d_] = D[p3[L, d], d];
              leite ab
p31[L_, d_] = D[p3[L, d], L];
              leite ab


(* For NTs the gradient has to be parallel to the search direction.
  For-Schleife
  In 2D we can plot the NT by the zero line of the interchanged coefficients
  ei···  leite ab
 of the gradient componenets NT1 is to (1,0),   NT2 is to direction (-1,1) *)
```

```
NewT1 = ContourPlot[p3[L, d], {L, 4.25, 5.6}, {d, -0.2, 0.15},
```
Konturgraphik

```
  ContourShading → False, PlotPoints → 77, Contours → {0.0},
```
Kontur-Schattierung | falsch | Anzahl der Punkte in··· | Konturen

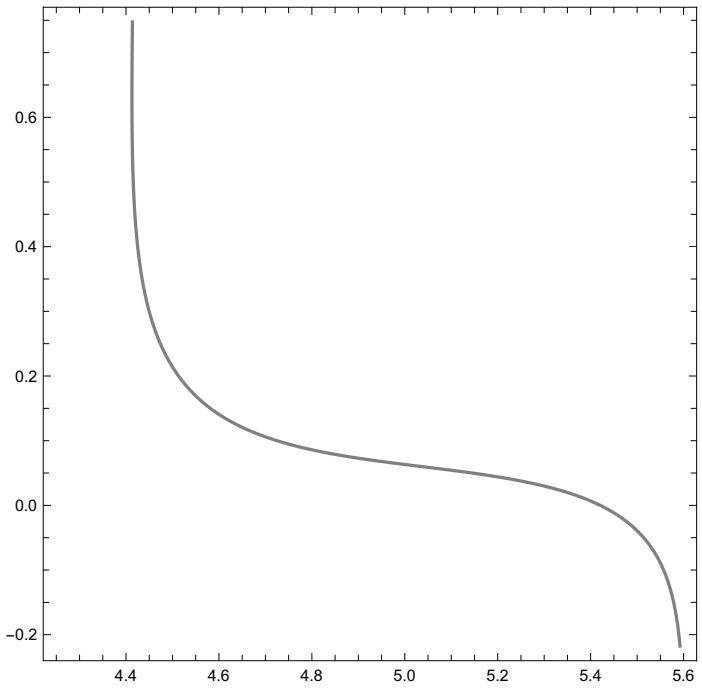
```
  ContourStyle → {Thickness[0.005], Red}]
```
Konturenstil | Dicke | rot

```
NewT2 = ContourPlot[p1[L, d] + p3[L, d], {L, 4.25, 5.6}, {d, -0.22, 0.75},
```
Konturgraphik

```
  ContourShading → False, PlotPoints → 77, Contours → {0.0},
```
Kontur-Schattierung | falsch | Anzahl der Punkte in··· | Konturen

```
  ContourStyle → {Thickness[0.005], Black}]
```
Konturenstil | Dicke | schwarz

*(Debug) Out[∘]=*




```
(* In 2D also the determinant of the Hessian matrix is simple *)
```
ei··· | leite ab

```
DetH[L_, d_] = Simplify[p11[L, d] * p33[L, d] - p31[L, d] * p31[L, d]];
```
vereinfache

```
 (* We search for the line Det(H)=0 on the PES  *)
```
Determinante

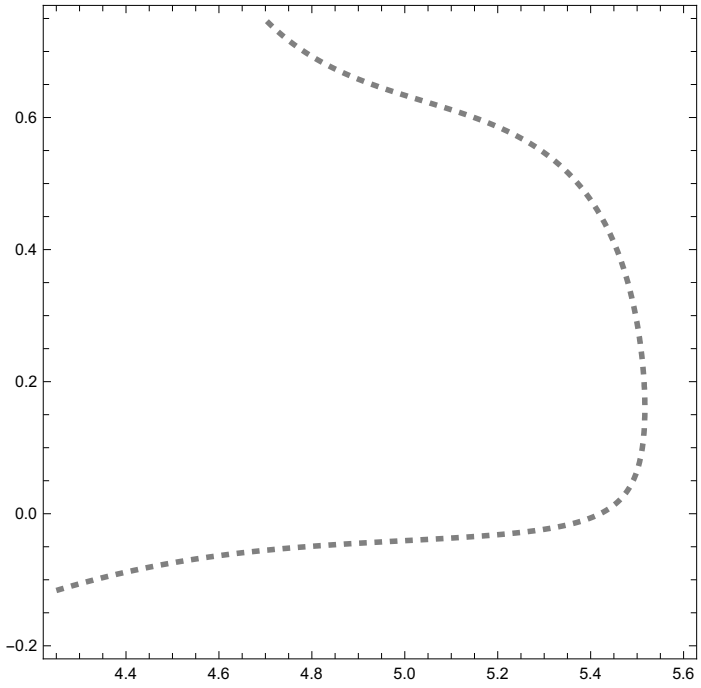
```
 deter1 =
  ContourPlot[Evaluate[DetH[L, d], {L, 4.25, 5.6}, {d, -0.2, 0.75}, ContourShading → False,
```
Konturgraphik | werte aus | Kontur-Schattierung | falsch

```
    PlotPoints → 40, Contours → {0.0}, ContourStyle → {Thickness[0.0046], Green}]]
```
Anzahl der Punkte in··· | Konturen | Konturenstil | Dicke | grün

```
(* NT11 to direction (1,1), that one of main interest *)
```

```
NewT11 = ContourPlot[p3[L, d] - 1.0 * p1[L, d], {L, 4.25, 5.6}, {d, -0.2, 0.75},
          Konturgraphik
  ContourShading → False, PlotPoints → 77, Contours → {0.0},
  Kontur-Schattierung  falsch  Anzahl der Punkte in···  Konturen
  ContourStyle → {Dashed, Thickness[0.0085]}]
  Konturenstil  gestrichelt  Dicke
```

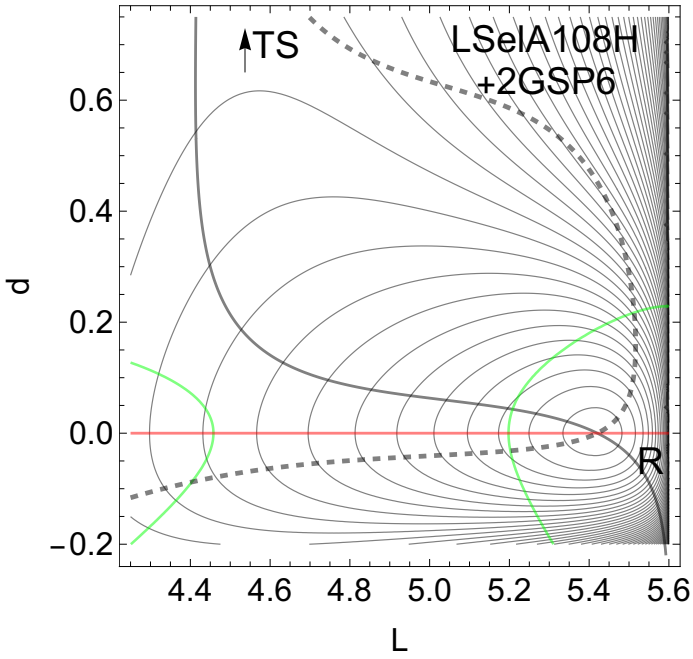
(Debug) Out[•]=




```
(* next are data for the figures *)
```

```
spArr = Graphics[Arrow[{{4.537, 0.65}, {4.537, 0.73}}]]
textLSelA = Show[Graphics[{Text[Style["R"], {5.5540, -0.05}],
      Text[Style["TS"], {4.615, 0.7}],
      Text[Style["LSelA108H"], {5.29, 0.71}],
      Text[Style["+2GSP6"], {5.293, 0.635}]},
    PlotRange → {{L, 1.5, 5.5}, {d, -.25, 0.5}}]];
BiLSelA = Show[conBarLSelA, NewT2, deter1,
  NewT1, NewTNT11, spArr, textLSelA, TextStyle → FontSize → 19]
```

(Debug) Out[∗]=




```
Export["BildLSelA108H.pdf", BiLSelA, ImageResolution → 400, ImageSize → Automatic]
```

```
(*  NEXT EXAMPLE  xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx*)
```

(Debug) In[8]:=

```
(*  LSelN138G + PSGL1   :  no.2 in BB tabelle *)
ph0 = 0.58 * Pi ;
d0 = 0.29;
k0 = 220.0;
D0 = 210.0;
cc = 0.0;
ph1 = Pi ;
sig = 0.12 * Pi;
```

(Debug) In[•]:=

```
PHI[L_] = 2.0 * ArcSin[L / 5.6]
```
Arkussinus

```
De[ph_] = D0 * Exp[-(ph - ph1)^2 / (2. * sig^2)] + cc
```
Exponentialfunktion

```
Vphi[L_] = 0.5 * k0 * (PHI[L] - ph0)^2
Be[d_, ph_] = De[ph] * ((1.0 - Exp[-d / d0])^2 - 1.)
```
Exponentialfunktion

```
pes[L_, d_, F_] = Vphi[L] + Be[d, PHI[L]] - (L + d) * F
```

(Debug) In[•]:=

```
conBarLSelN = ContourPlot[pes[L, d, 0], {L, 4.25, 5.6},
  {d, -0.2, 0.65}, ContourShading → False, Contours → 50, PlotRange → All,
  PlotPoints → 53, ContourStyle → Thickness[0.00215], FrameLabel → {"L", "d"},
  AspectRatio → 1, FormatType → TraditionalForm, FrameStyle → FontSize → 16]
```
Konturgraphik; Kontur-Schattierung: falsch; Konturen; Koordinatenb…: alle; Anzahl der Punkte in d…; Konturenstil; Dicke; Rahmenbeschriftung; Seitenverhältnis; Formattyp; traditionelle Form; Rahmenstil; Schriftgröße

```
p3[L_, d_] = D[pes[L, d, 0], d];
```
leite ab

```
p1[L_, d_] = D[pes[L, d, 0], L];
```
leite ab

```
p11[L_, d_] = D[p1[L, d], L];
```
leite ab

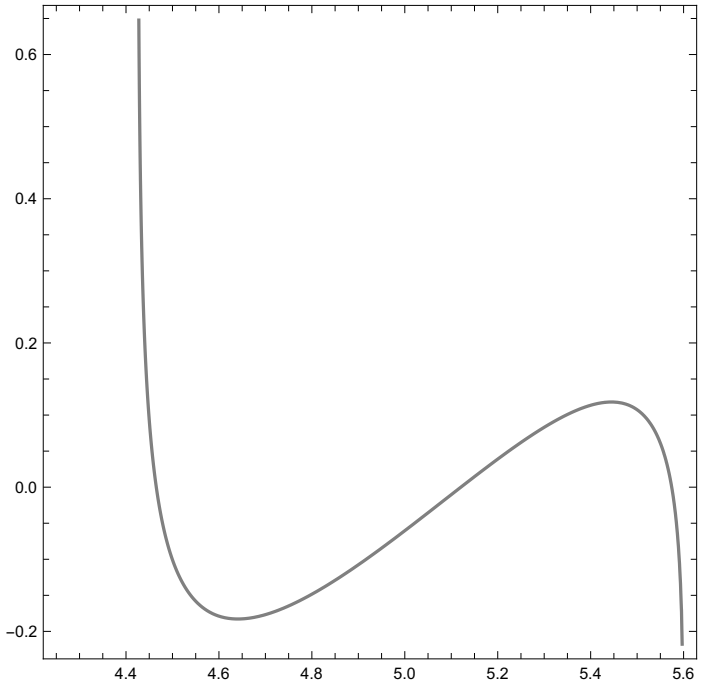
```
p33[L_, d_] = D[p3[L, d], d];
```
leite ab

```
p31[L_, d_] = D[p3[L, d], L];
```
leite ab

```
NewT1 = ContourPlot[p3[L, d], {L, 4.25, 5.6}, {d, -0.2, 0.15},
  ContourShading → False, PlotPoints → 77, Contours → {0.0},
  ContourStyle → {Thickness[0.005], Red}]
```
Konturgraphik; Kontur-Schattierung: falsch; Anzahl der Punkte in…; Konturen; Konturenstil; Dicke; rot

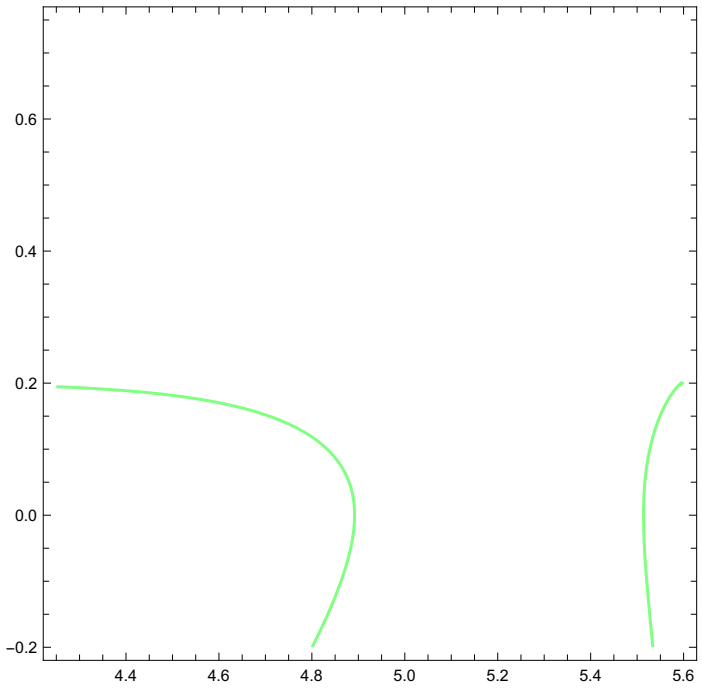
```
NewT2 = ContourPlot[p1[L, d] + p3[L, d], {L, 4.25, 5.6}, {d, -0.22, 0.65},
        Konturgraphik
  ContourShading → False, PlotPoints → 77, Contours → {0.0},
  Kontur-Schattierung  falsch  Anzahl der Punkte in···  Konturen
  ContourStyle → {Thickness[0.005], Black}]
  Konturenstil  Dicke  schwarz
```

(Debug) Out[•]=

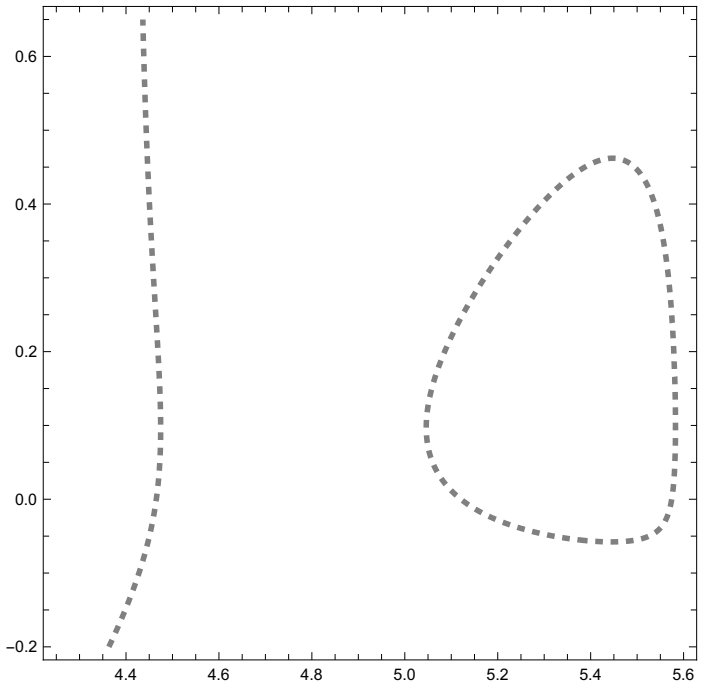


```
DetH[L_, d_] = Simplify[p11[L, d] * p33[L, d] - p31[L, d] * p31[L, d]];
                vereinfache

deter1 =
 ContourPlot[Evaluate[DetH[L, d], {L, 4.25, 5.6}, {d, -0.2, 0.75}, ContourShading → False,
  Konturgraphik  werte aus                                        Kontur-Schattierung  falsch
   PlotPoints → 40, Contours → {0.0}, ContourStyle → {Thickness[0.0046], Green}]]
    Anzahl der Punkte in···  Konturen  Konturenstil  Dicke  grün

NewTNT11 = ContourPlot[p3[L, d] - 1.0 * p1[L, d], {L, 4.25, 5.6}, {d, -0.2, 0.65},
            Konturgraphik

  ContourShading → False, PlotPoints → 77, Contours → {0.0},
   Kontur-Schattierung  falsch  Anzahl der Punkte in···  Konturen

  ContourStyle → {Dashed, Thickness[0.0085]}]
   Konturenstil  gestrichelt  Dicke
```

(Debug) Out[•]=

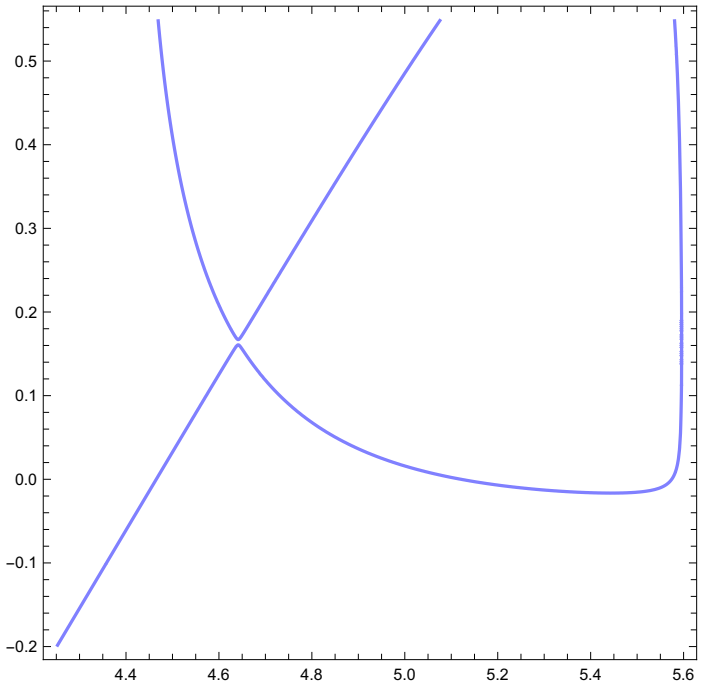



(Debug) Out[•]=



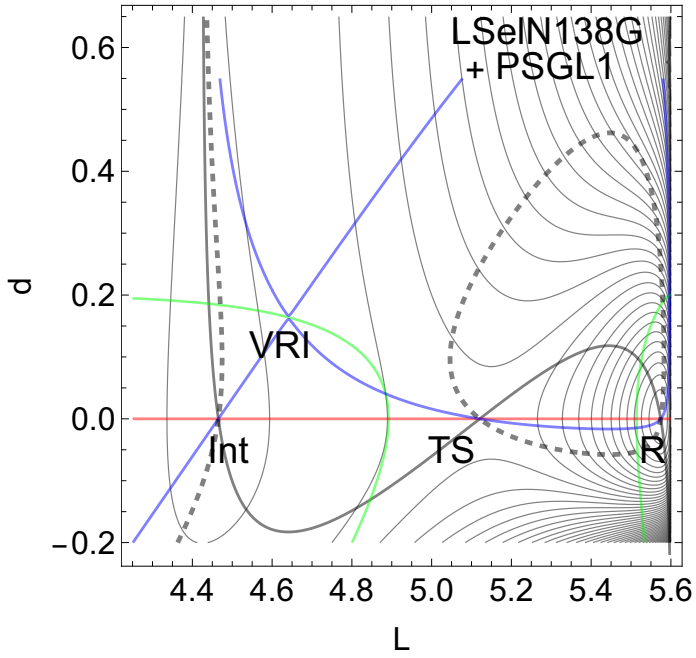
```
(* The singular NT through the VRI point must be determined by hand,
it means one has to probe the coefficients for the searched
 intersection of the two branches of the NT , drawn in blue *)

NewTSi = ContourPlot[-0.296 * p1[L, d] + 1.445 * p3[L, d], {L, 4.25, 5.6},
          Konturgraphik

  {d, -0.2, 0.55}, ContourShading → False, PlotPoints → 77, Contours → {0.0},
                   Kontur-Schattierung   falsch   Anzahl der Punkte in···   Konturen

   ContourStyle → {Thickness[0.005], Blue}]
    Konturenstil          Dicke              blau
```

(Debug) Out[ ]=



```
textLSelN = Show[Graphics[{Text[Style["R"], {5.5540, -0.05}],
                zei··· Graphik Text Stil
      Text[Style["TS"], {5.05, -0.05}],
      Text Stil
      Text[Style["LSelN138G"], {5.29, 0.626}],
      Text Stil
      Text[Style["+ PSGL1"], {5.273, 0.57}],
      Text Stil
      Text[Style["VRI"], {4.62, 0.12}],
      Text Stil
      Text[Style["Int"], {4.49, -0.05}]},
      Text Stil
    PlotRange → {{L, 1.5, 5.5}, {d, -.25, 0.5}}]];
    Koordinatenbereich der Graphik
BiLSelN = Show[conBarLSelN, NewT2, deter1,
          zeige an
  NewT1, NewTSi, NewTNT11, textLSelN, TextStyle → FontSize → 19]
                                  Textstil  Schriftgröße
```

(Debug) Out[ ]=




```
Export["BildLSelN138G.pdf", BiLSelN, ImageResolution → 400, ImageSize → Automatic]
exportiere                    Bildauflösung          Bildgröße    automatisch
```

(Debug) In[15]:=

```
(*  L-selectin + 2GSP6  no.3 in BB Table *)
                          Tabelle
ph0 = 0.58 * Pi ;
      Kreiszahl π
d0 = 0.33;
k0 = 266.0;
D0 = 217.0;
cc = 0.0;
ph1 = 0.98 * Pi ;
      Kreiszahl π
sig = 0.09 * Pi;
      Kreiszahl π
```

(Debug) In[•]:=

```
PHI[L_] = 2.0 * ArcSin[L / 5.6]
```
Arkussinus

```
De[ph_] = D0 * Exp[-(ph - ph1)^2 / (2. * sig^2)] + cc
```
Exponentialfunktion

```
Vphi[L_] = 0.5 * k0 * (PHI[L] - ph0)^2
Be[d_, ph_] = De[ph] * ((1.0 - Exp[-d / d0])^2 - 1.)
```
Exponentialfunktion

```
pes[L_, d_, F_] = Vphi[L] + Be[d, PHI[L]] - (L + d) * F
```

(Debug) In[•]:=

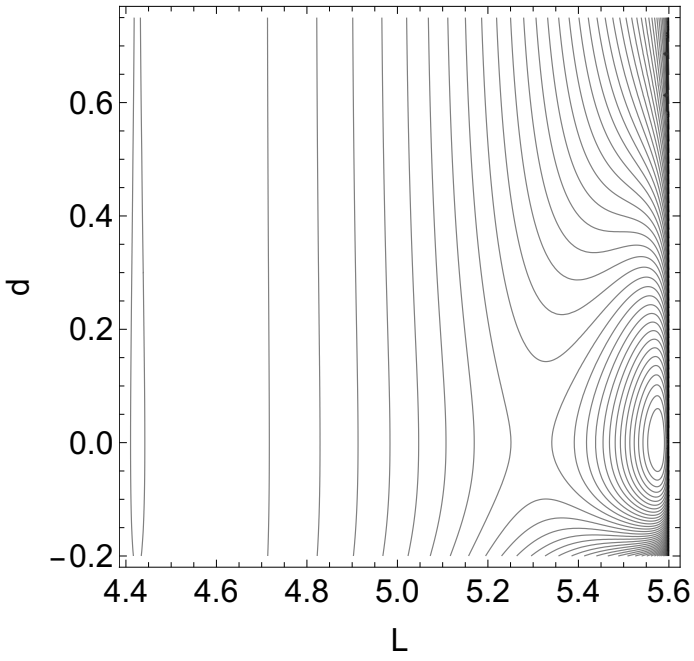
```
conBarL2G = ContourPlot[pes[L, d, 0], {L, 4.25, 5.6},
```
Konturgraphik

```
  {d, -0.2, 0.75}, ContourShading → False, Contours → 50, PlotRange → All,
```
Kontur–Schattierung | falsch | Konturen | Koordinatenb··· | alle

```
  PlotPoints → 53, ContourStyle → Thickness[0.00215], FrameLabel → {"L", "d"},
```
Anzahl der Punkte in d··· | Konturenstil | Dicke | Rahmenbeschriftung

```
  AspectRatio → 1, FormatType → TraditionalForm, FrameStyle → FontSize → 16]
```
Seitenverhältnis | Formattyp | traditionelle Form | Rahmenstil | Schriftgröße

(Debug) Out[•]=




(Debug) In[•]:=

```
p3[L_, d_] = D[pes[L, d, 0], d];
```
leite ab

```
p1[L_, d_] = D[pes[L, d, 0], L];
```
leite ab

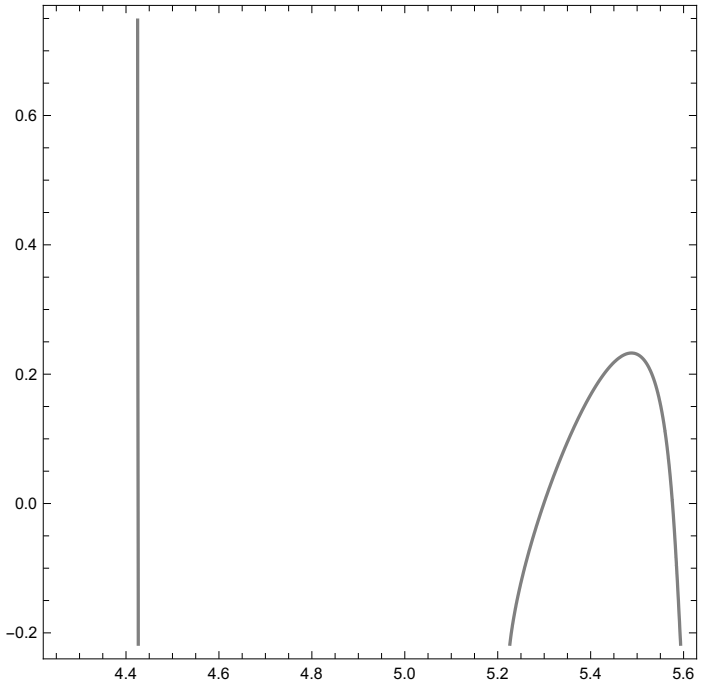
```
p11[L_, d_] = D[p1[L, d], L];
```
leite ab

```
p33[L_, d_] = D[p3[L, d], d];
```
leite ab

```
p31[L_, d_] = D[p3[L, d], L];
```
leite ab

```
NewT2 = ContourPlot[p1[L, d] + p3[L, d], {L, 4.25, 5.6}, {d, -0.22, 0.75},
        Konturgraphik
  ContourShading → False, PlotPoints → 77, Contours → {0.0},
  Kontur-Schattierung  falsch  Anzahl der Punkte in···  Konturen
  ContourStyle → {Thickness[0.005], Black}]
  Konturenstil  Dicke  schwarz
```

(Debug) Out[•]=

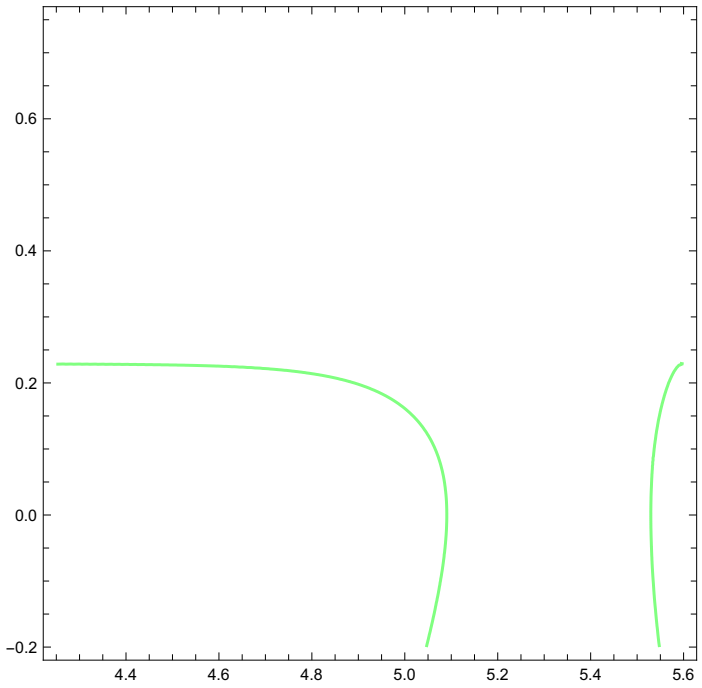



```
NewT1 = ContourPlot[p3[L, d], {L, 4.25, 5.6}, {d, -0.2, 0.15},
        Konturgraphik
  ContourShading → False, PlotPoints → 77, Contours → {0.0},
  Kontur-Schattierung  falsch  Anzahl der Punkte in···  Konturen
  ContourStyle → {Thickness[0.005], Red}]
  Konturenstil  Dicke  rot
```

(Debug) In[•]:=

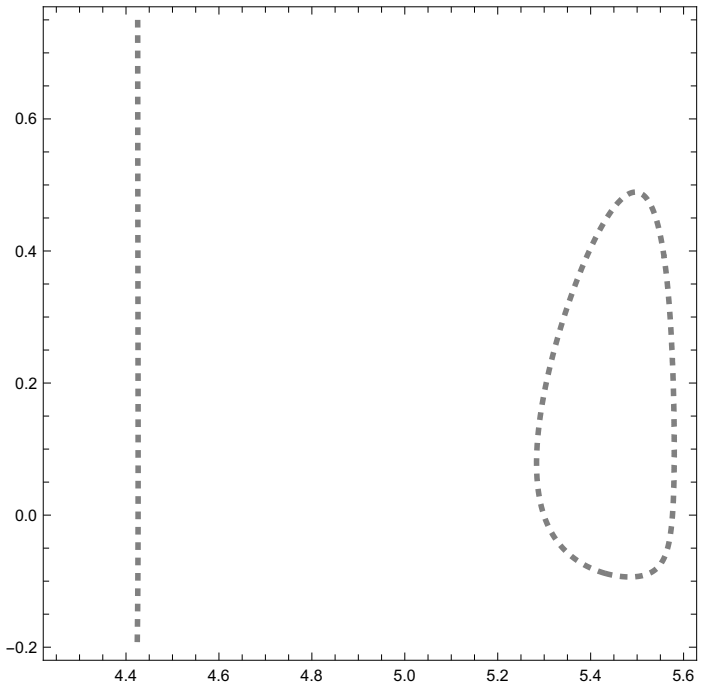
```
DetH[L_, d_] = Simplify[p11[L, d] * p33[L, d] - p31[L, d] * p31[L, d]];
               vereinfache

deter1 =
 ContourPlot[Evaluate[DetH[L, d], {L, 4.25, 5.6}, {d, -0.2, 0.75}, ContourShading → False,
  Konturgraphik  werte aus                                          Kontur-Schattierung  falsch
   PlotPoints → 40, Contours → {0.0}, ContourStyle → {Thickness[0.0046], Green}]]
    Anzahl der Punkte in···  Konturen  Konturenstil  Dicke  grün
```

(Debug) Out[•]=




```
NewTNT11 = ContourPlot[p3[L, d] - 1.0 * p1[L, d], {L, 4.25, 5.6}, {d, -0.2, 0.75},
            Konturgraphik

   ContourShading → False, PlotPoints → 77, Contours → {0.0},
    Kontur-Schattierung  falsch  Anzahl der Punkte in···  Konturen

   ContourStyle → {Dashed, Thickness[0.0085]}]
    Konturenstil  gestrichelt  Dicke
```

(Debug) Out[•]=



(Debug) In[•]:=

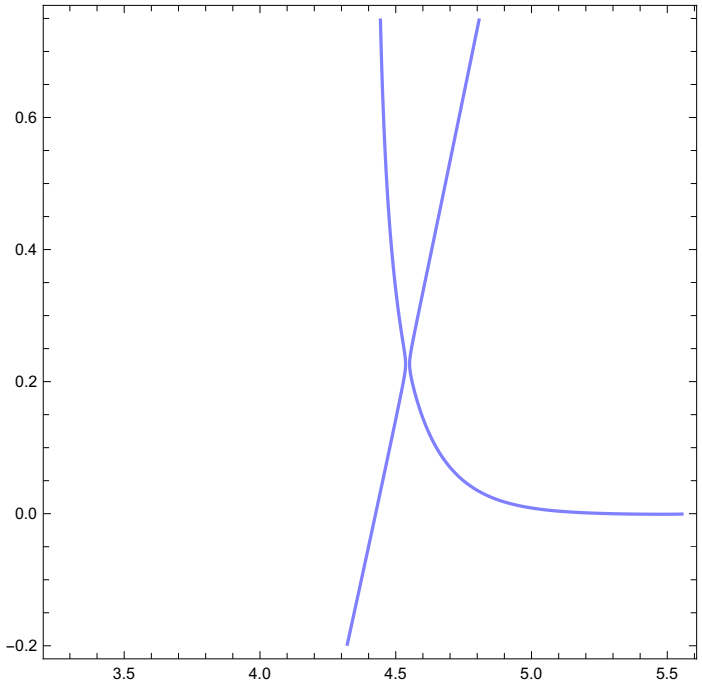
```
p3[4.25, 0.1273]
```

(Debug) Out[•]=

```
12.2701
```

```
NewTSi = ContourPlot[-0.04040 * p1[L, d] + 9.133 * p3[L, d], {L, 3.25, 5.56},
                     Konturgraphik
  {d, -0.2, 0.75}, ContourShading → False, PlotPoints → 77, Contours → {0.0},
                   Kontur-Schattierung  falsch  Anzahl der Punkte in···  Konturen
  ContourStyle → {Thickness[0.005], Blue}]
                 Konturenstil          Dicke          blau
```

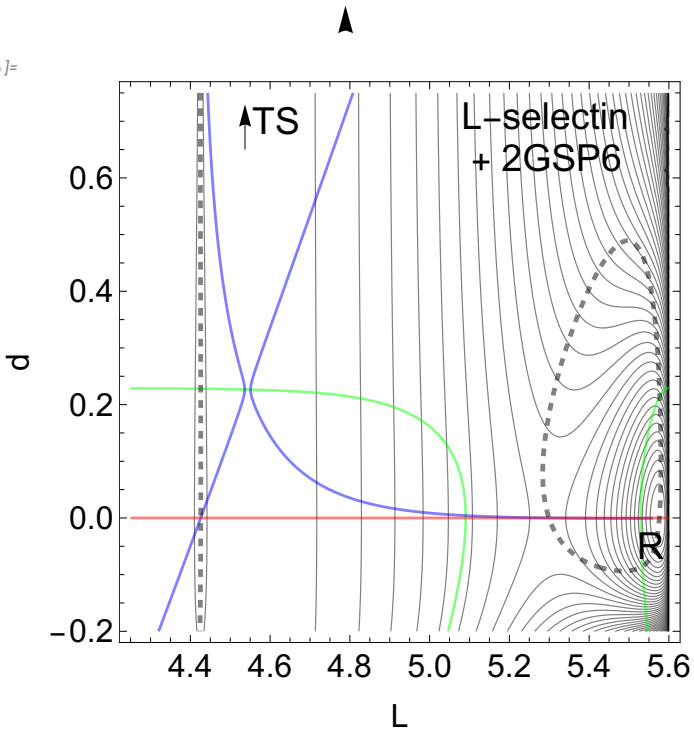
(Debug) Out[•]=



```
spArr = Graphics[Arrow[{{4.537, 0.65}, {4.537, 0.73}}]]
        Graphik  Pfeil
textLG2 = Show[Graphics[{Text[Style["R"], {5.5540, -0.05}],
          zei…  Graphik  Text  Stil
      Text[Style["TS"], {4.615, 0.7}],
      Text  Stil
      Text[Style["L-selectin"], {5.29, 0.71}],
      Text  Stil
      Text[Style["+ 2GSP6"], {5.293, 0.635}]},
      Text  Stil
    PlotRange → {{L, 1.5, 5.5}, {d, -.25, 0.5}}]];
    Koordinatenbereich der Graphik
BiL2G = Show[conBarL2G, deter1, NewTSi,
        zeige an
  NewT1, NewTNT11, spArr, textLG2, TextStyle → FontSize → 19]
                                   Textstil  Schriftgröße
```

(Debug) Out[ ]=

(Debug) Out[ ]=




```
Export["BildLselec2GSP6.pdf", BiL2G, ImageResolution → 400, ImageSize → Automatic]
exportiere                    Bildauflösung  Bildgröße  automatisch
```

(Debug) In[22]:=

```
(*  L-selectin + PSGL1  vorher falsch k0=299.0  XXXXXXXXXXXXXXXXX Haupteil !!!  *)
(*  No 1 in Tabelle in PNAS ist auch gleich !!!!! D.h. L-selectin alles wie vorher *)
                                                  leite ab
ph0 = 0.58 * Pi ;
            Kreiszahl π
d0 = 0.29;
k0 = 266.0;
D0 = 237.0;
cc = 0.0;
ph1 = Pi ;
      Kreiszahl π
sig = 0.12 * Pi;
            Kreiszahl π
```

(Debug) In[29]:=

```
(* phi(L) indirekt gegeben !! W=2.8  *)
PHI[L_] = 2.0 * ArcSin[L / 5.6]
```

Arkussinus

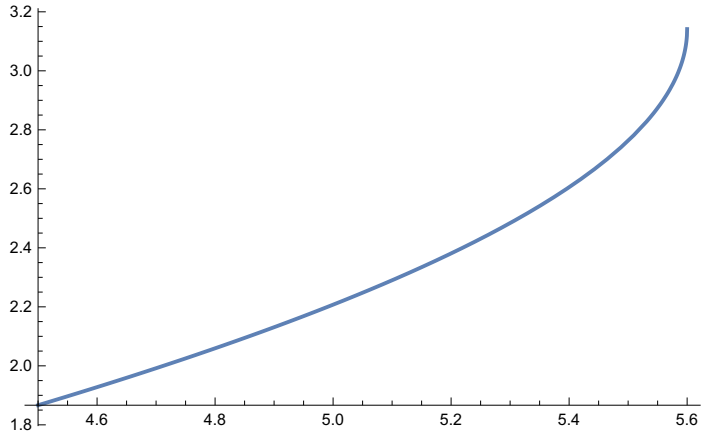
```
Plot[PHI[L], {L, 4.5, 5.6}]
```

stelle Funktion graphisch dar

(Debug) Out[29]=

$$2.\ \text{ArcSin}\left[0.178571\ L\right]$$

(Debug) Out[30]=




(Debug) In[31]:=

```
theta0 = 0.58 * Pi
```

Kreiszahl $\pi$

```
L0 = 5.6 * Sin[theta0 / 2.]
```

Sinus

(Debug) Out[31]=

1.82212

(Debug) Out[32]=

4.42487

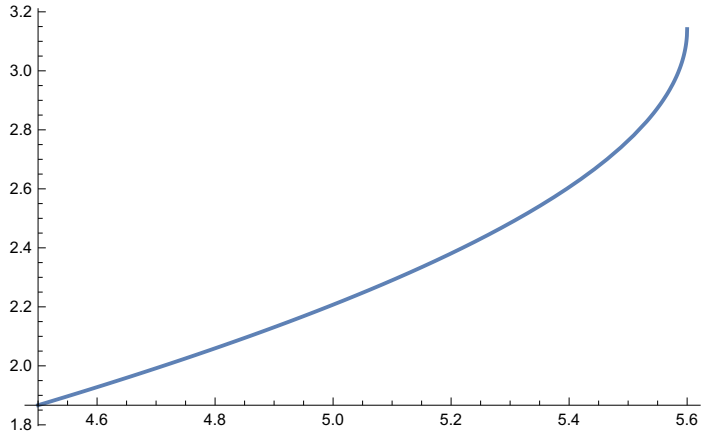
(Debug) In[33]:=

```
(* phi(L) indirekt gegeben !! W=2.8  *)
PHI[L_] = 2.0 * ArcSin[L / 5.6]
          | Arkussinus
Plot[PHI[L], {L, 4.5, 5.6}]
| stelle Funktion graphisch dar
De[ph_] = D0 * Exp[-(ph - ph1) ^ 2 / (2. * sig ^ 2)] + cc
          | Exponentialfunktion
Vphi[L_] = 0.5 * k0 * (PHI[L] - ph0) ^ 2
Be[d_, ph_] = De[ph] * ((1.0 - Exp[-d / d0]) ^ 2 - 1.)
                       | Exponentialfunktion
pes[L_, d_, F_] = Vphi[L] + Be[d, PHI[L]] - (L + d) * F
```

(Debug) Out[33]=

$$2.\ \text{ArcSin}[0.178571\ L]$$

(Debug) Out[34]=




(Debug) Out[35]=

$$0. + 237.\ e^{-3.5181\ (\text{ph}-\pi)^2}$$

(Debug) Out[36]=

$$133.\ (-1.82212 + 2.\ \text{ArcSin}[0.178571\ L])^2$$

(Debug) Out[37]=

$$\left(0. + 237.\ e^{-3.5181\ (\text{ph}-\pi)^2}\right)\left(-1. + \left(1. - e^{-3.44828\ d}\right)^2\right)$$

(Debug) Out[38]=

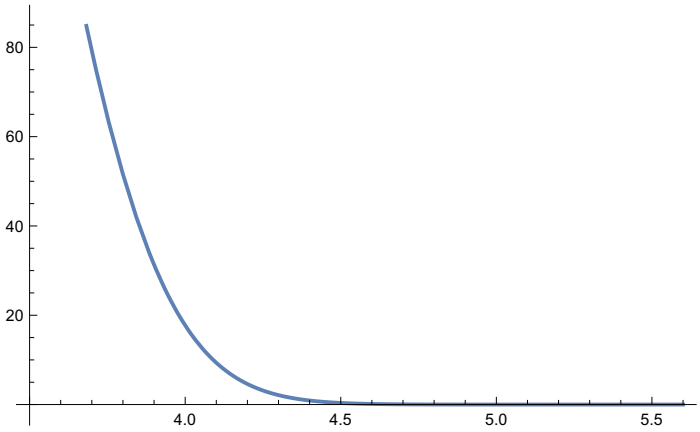
$$\left(0. + 237.\ e^{-3.5181\ \left(-\pi+2.\ \text{ArcSin}[0.178571\ L]\right)^2}\right)\left(-1. + \left(1. - e^{-3.44828\ d}\right)^2\right) - F\ (d + L) + 133.\ (-1.82212 + 2.\ \text{ArcSin}[0.178571\ L])^2$$

(Debug) In[◦]:=

```
Plot[De[ph], {ph, 3.5, 5.6}]
```

stelle Funktion graphisch dar

(Debug) Out[◦]=

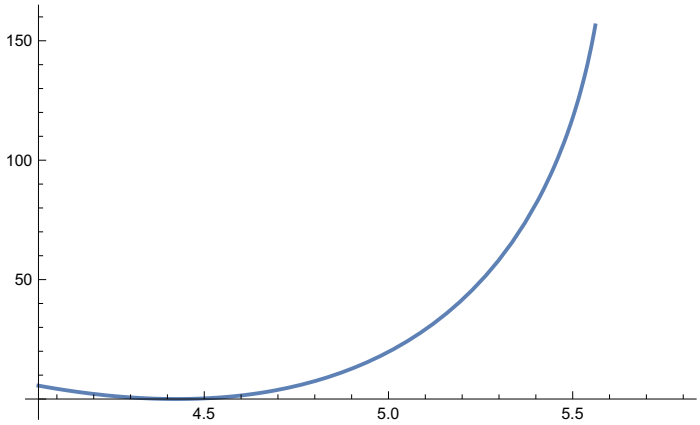



(Debug) In[◦]:=

```
Plot[Vphi[L], {L, 4.05, 5.8}]
```

stelle Funktion graphisch dar

(Debug) Out[◦]=

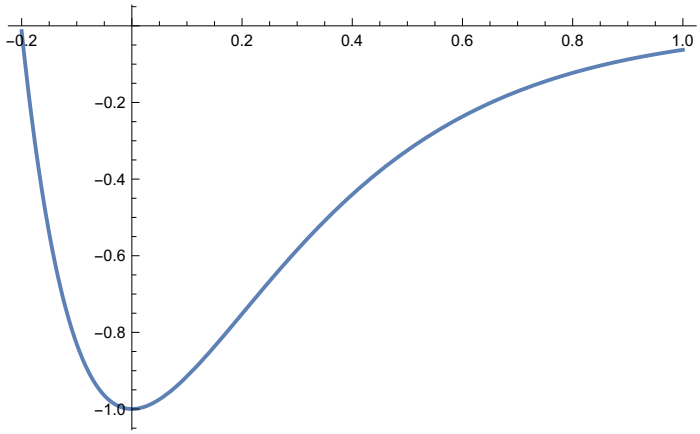



(Debug) In[◦]:=

```
Plot[(1.0 - Exp[-d / d0])^2 - 1., {d, -0.2, 1.0}]
```

stelle Funkt·· Exponentialfunktion

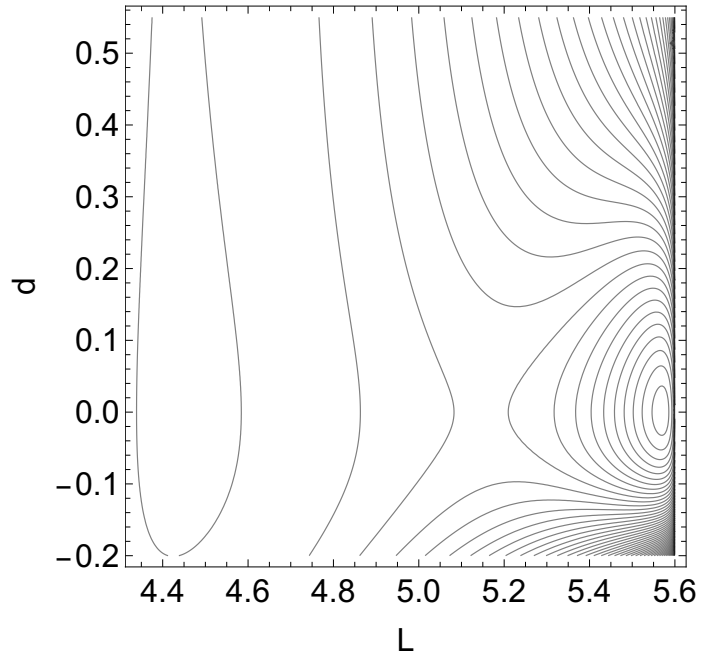
(Debug) Out[◦]=



(Debug) In[39]:=

```
conBarL = ContourPlot[pes[L, d, 0], {L, 4.25, 5.6},
          Konturgraphik
  {d, -0.2, 0.55}, ContourShading → False, Contours → 50, PlotRange → All,
                   Kontur-Schattierung  falsch  Konturen  Koordinatenb···  alle
  PlotPoints → 53, ContourStyle → Thickness[0.00215], FrameLabel → {"L", "d"},
  Anzahl der Punkte in d···  Konturenstil  Dicke  Rahmenbeschriftung
  AspectRatio → 1, FormatType → TraditionalForm, FrameStyle → FontSize → 16]
  Seitenverhältnis  Formattyp  traditionelle Form  Rahmenstil  Schriftgröße
```

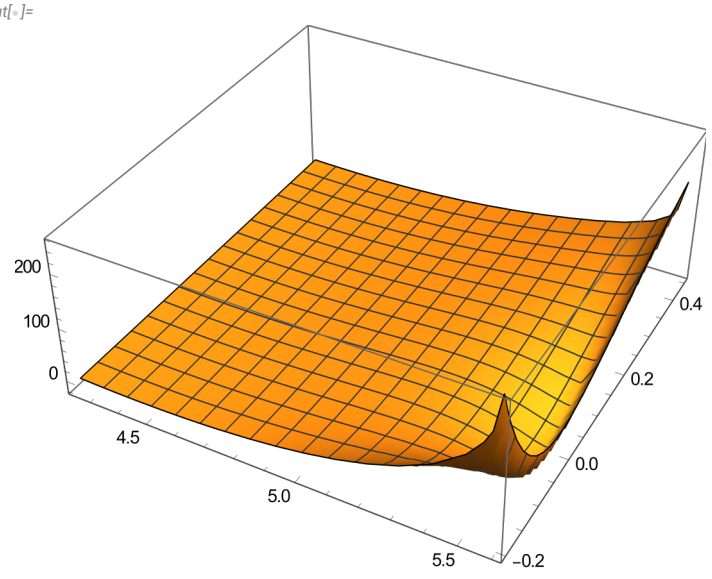
(Debug) Out[39]=




(Debug) In[ ]:=

```
Plot3D[pes[L, d, 0], {L, 4.25, 5.6}, {d, -0.2, 0.45}, PlotRange → All]
  stelle Funktion graphisch in 3D dar  Koordinatenb···  alle
```

(Debug) Out[ ]=



(Debug) In[40]:=

```
p3[L_, d_] = D[pes[L, d, 0], d];
```
leite ab

```
p1[L_, d_] = D[pes[L, d, 0], L];
```
leite ab

```
p11[L_, d_] = D[p1[L, d], L];
```
leite ab

```
p33[L_, d_] = D[p3[L, d], d];
```
leite ab

```
p31[L_, d_] = D[p3[L, d], L];
```
leite ab

(Debug) In[•]:=

```
FindRoot[{p1[L, d], p3[L, d]}, {{L, 4.46}, {d, 0.0}}]
```
ermittle Nullstelle

(Debug) Out[•]=

```
{L → 4.46192, d → 0.}
```

```
{L → 4.461915723575546`, d → 0.`} (*  Intermediate *)
```

(Debug) In[•]:=

```
pes[4.461915723575546, 0.0, 0]
```

(Debug) Out[•]=

```
-0.570468
```

(Debug) In[•]:=

```
FindRoot[{p1[L, d], p3[L, d]}, {{L, 5.15}, {d, 0.0}}]
```
ermittle Nullstelle

(Debug) Out[•]=

```
{L → 5.15091, d → 0.}
```

```
{L → 5.150914868876448`, d → 0.`} (*  SP *)
```

(Debug) In[•]:=

```
pes[5.15091, 0.0, 0]
```

(Debug) Out[•]=

```
10.9567
```

(Debug) In[•]:=

```
FindRoot[{p1[L, d], p3[L, d]}, {{L, 5.59}, {d, 0.0}}]
```
ermittle Nullstelle

(Debug) Out[•]=

```
{L → 5.57025, d → 0.}
```

```
{L → 5.570252566046982`, d → 0.`} (*  Min R *)
```
kleinstes E

(Debug) In[•]:=

```
pes[5.57025256, 0.0, 0]
```

(Debug) Out[•]=

```
-39.2368
```

(Debug) In[•]:=

```
Bar0 = 10.956699577153884 + 39.23677075785412
```

(Debug) Out[•]=

```
50.1935
```

```
(*  Control of kind of stat points *)
```
Bedienelement

(Debug) In[◦]:=

```
H[L_, d_] = {{p11[L, d], p31[L, d]}, {p31[L, d], p33[L, d]}};

Eigensystem[H[4.461915723, 0.0]]
```
Eigensystem

(Debug) Out[◦]=

```
{{76.0267, 15.0614}, {{-1., 0.}, {0., -1.}}}
```

(Debug) In[◦]:=

```
Eigensystem[H[5.15091, 0.0]]
```
Eigensystem

(Debug) Out[◦]=

```
{{571.958, -280.949}, {{0., 1.}, {-1., 0.}}}
```

(Debug) In[◦]:=

```
Eigensystem[H[5.57025256, 0.0]]
```
Eigensystem

(Debug) Out[◦]=

```
{{15 313.4, 4852.83}, {{-1., 0.}, {0., -1.}}}
```

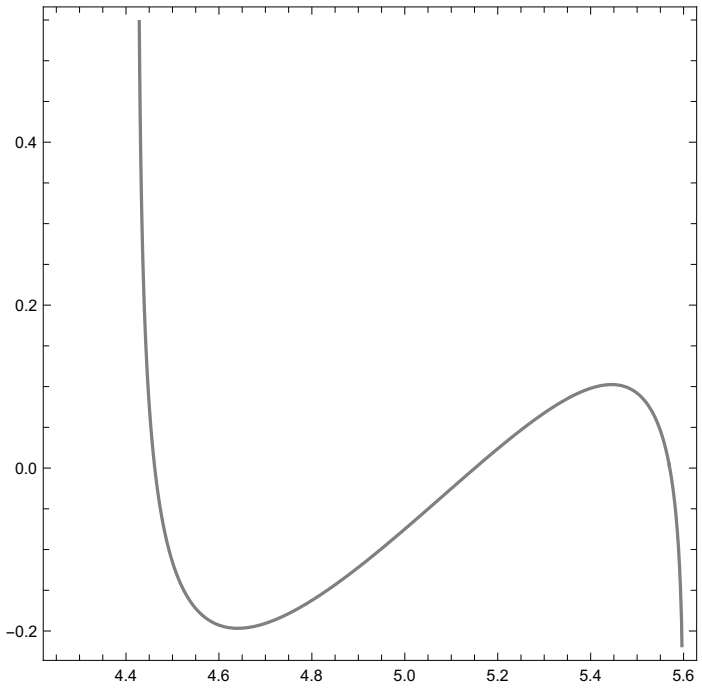
(Debug) In[45]:=

```
NewT2 = ContourPlot[p1[L, d] + p3[L, d], {L, 4.25, 5.6}, {d, -0.22, 0.55},
```
Konturgraphik

```
  ContourShading → False, PlotPoints → 77, Contours → {0.0},
```
Kontur-Schattierung | falsch | Anzahl der Punkte in··· | Konturen

```
  ContourStyle → {Thickness[0.005], Black}]
```
Konturenstil | Dicke | schwarz

(Debug) Out[45]=




```
(*  vorher NewT1 *)

NewTed = ContourPlot[p3[L, d], {L, 4.25, 5.6}, {d, -0.2, 0.15},
```
Konturgraphik

```
  ContourShading → False, PlotPoints → 77, Contours → {0.0},
```
Kontur-Schattierung | falsch | Anzahl der Punkte in··· | Konturen

```
  ContourStyle → {Thickness[0.005], Red}] ;
```
Konturenstil | Dicke | rot

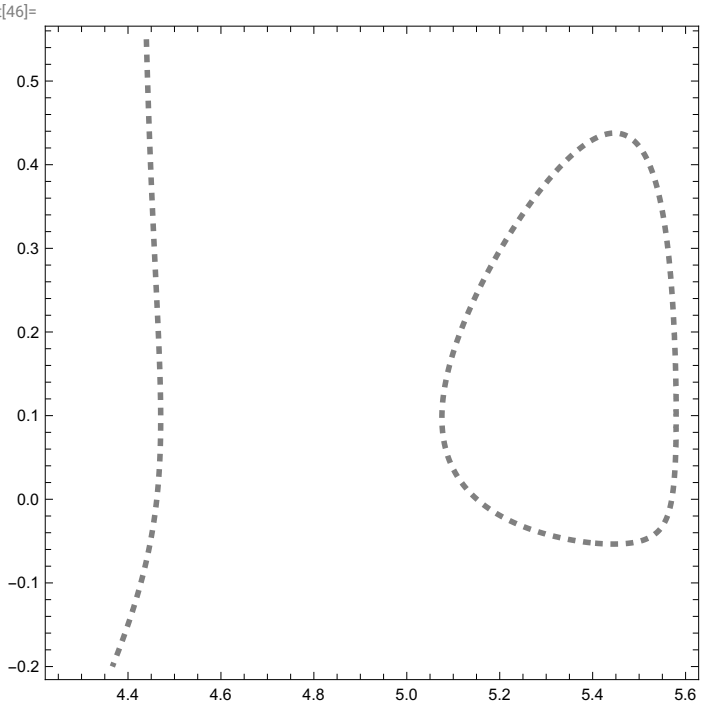
(Debug) In[•]:=

```
DetH[L_, d_] = Simplify[p11[L, d] * p33[L, d] - p31[L, d] * p31[L, d]];
                vereinfache

deter1 =
 ContourPlot[Evaluate[DetH[L, d], {L, 4.25, 5.6}, {d, -0.2, 0.45}, ContourShading → False,
  Konturgraphik  werte aus                                          Kontur-Schattierung  falsch

   PlotPoints → 40, Contours → {0.0}, ContourStyle → {Thickness[0.0046], Green}]]
    Anzahl der Punkte in···  Konturen  Konturenstil  Dicke  grün
```

(Debug) In[46]:=

```
NewT11 = ContourPlot[p3[L, d] - 1.0 * p1[L, d], {L, 4.25, 5.6}, {d, -0.2, 0.55},
          Konturgraphik

  ContourShading → False, PlotPoints → 77, Contours → {0.0},
   Kontur-Schattierung  falsch  Anzahl der Punkte in···  Konturen

  ContourStyle → {Dashed, Thickness[0.0085]}]
   Konturenstil  gestrichelt  Dicke
```

(Debug) Out[46]=




(Debug) In[•]:=

```
(*  VRI point ~ (4.64, 0.1675)  *)
p1[4.64, 0.1675]
```

(Debug) Out[•]=

```
15.1316
```

(Debug) In[•]:=

```
p3[4.64, 0.1675]
```

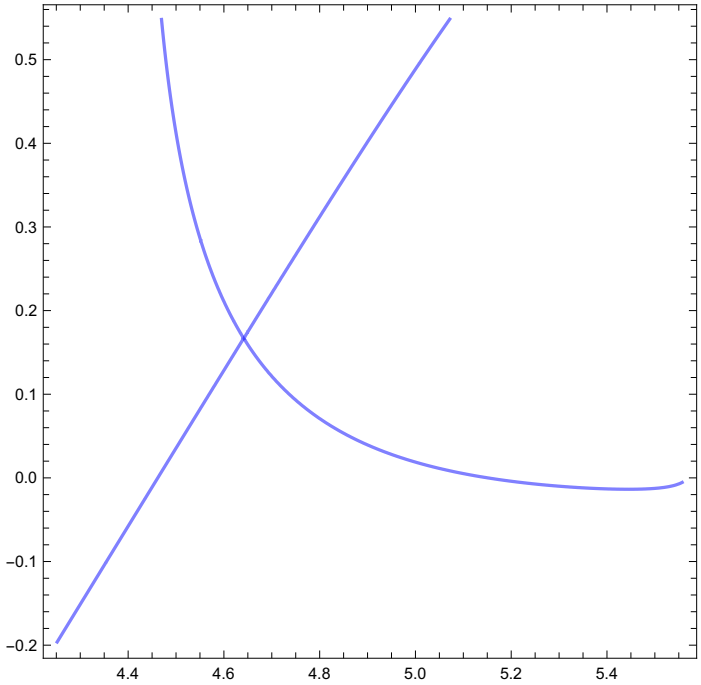
(Debug) Out[•]=

```
2.79638
```

(Debug) In[47]:=

```
NewTSi = ContourPlot[-0.27963771199820813 * p1[L, d] + 1.5131569585841813 * p3[L, d],
          Konturgraphik
  {L, 4.25, 5.56}, {d, -0.2, 0.55}, ContourShading → False, PlotPoints → 77,
                                     Kontur-Schattierung   falsch   Anzahl der Punkte in der Graphil
  Contours → {0.0}, ContourStyle → {Thickness[0.005], Blue}]
   Konturen          Konturenstil        Dicke          blau
```

(Debug) Out[47]=




(Debug) In[•]:=

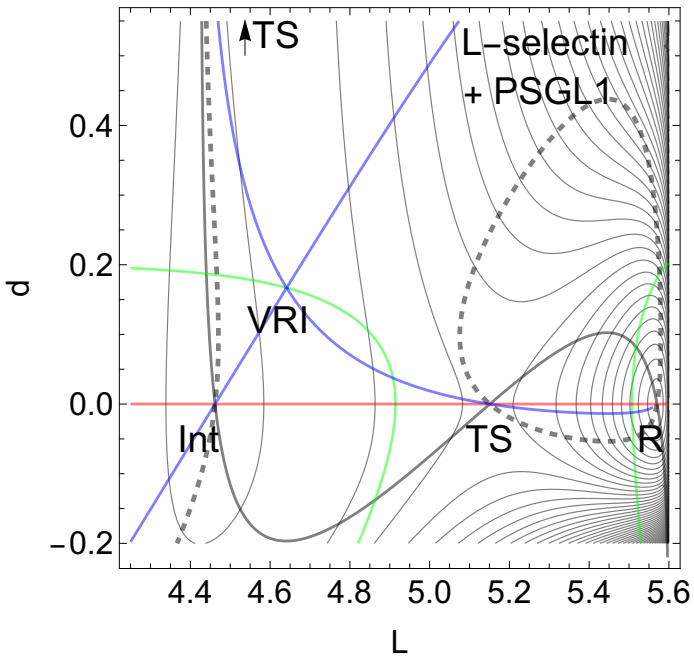
```
spArr = Graphics[Arrow[{{4.537, 0.5}, {4.537, 0.553}}]]
         Graphik   Pfeil
```

(Debug) In[•]:=

```
text = Show[Graphics[{Text[Style["R"], {5.5540, -0.05}],
        zei···  Graphik    Text  Stil

      Text[Style["TS"], {5.15, -0.05}],
      Text  Stil

      Text[Style["TS"], {4.615, 0.53}],
      Text  Stil

      Text[Style["L-selectin"], {5.29, 0.52}],
      Text  Stil

      Text[Style["+ PSGL1"], {5.273, 0.45}],
      Text  Stil

      Text[Style["VRI"], {4.62, 0.12}],
      Text  Stil

      Text[Style["Int"], {4.4, -0.05}]},
      Text  Stil

     PlotRange → {{L, 1.5, 5.5}, {d, -.25, 0.5}}]];
     Koordinatenbereich der Graphik
```

```
BiL = Show[conBarL, NewT1, deter1, NewT1,
      zeige an
  NewTSi, NewTNT11, spArr, text, TextStyle → FontSize → 19]
                                 Textstil      Schriftgröße
```

(Debug) Out[•]=




```
Export["BildLselectin.pdf", BiL, ImageResolution → 400, ImageSize → Automatic]
exportiere                    Bildauflösung              Bildgröße    automatisch
```

```
(*   xxxxxxxxxxxxxxxxx XXXXXXXXXXXXXXXXXXX  xxxxxxxxxxxxxx  *)
(*   !!! Calculation of the catch bond barriers !!! *)
```

(Debug) In[92]:=

```
p1F[L_, d_, F_] = D[pes[L, d, F], L];
                  leite ab
p3F[L_, d_, F_] = D[pes[L, d, F], d];
                  leite ab

Lo = 5.560;
do = 0.0;
Minweg = Table[{mini = FindRoot[p1F[L, d, F] == 0 && p3F[L, d, F] == 0, {L, Lo}, {d, do}];
          Tabelle          ermittle Nullstelle
    {Lo, do} = {L, d} /. mini;
    pes[Lo, do, F]}, {F, 0.0, 100, 5}]
(
```

(Debug) Out[96]=

```
{{-61.3128}, {-88.4327}, {-115.586}, {-142.771}, {-169.986}, {-197.23}, {-224.502},
 {-251.801}, {-279.126}, {-306.477}, {-333.851}, {-361.25}, {-388.672}, {-416.118},
 {-443.585}, {-471.074}, {-498.585}, {-526.117}, {-553.671}, {-581.244}, {-608.839}}
```

```
(*   ++++++++++++++++ SP    *)
```

(Debug) In[63]:=

```
(*  TS  *)
Lo = 5.160;
do = 0.01;
MinSP = Table[{saddle = FindRoot[p1F[L, d, F] == 0 && p3F[L, d, F] == 0, {L, Lo}, {d, do}];
                Tabelle          ermittle Nullstelle
   {Lo, do} = {L, d} /. saddle;
   pes[Lo, do, F]}, {F, 0.0, 100, 5}]
```

(Debug) Out[65]=

```
{{10.9567}, {-14.7762}, {-40.4728}, {-66.1545}, {-91.8726}, {-117.727}, {-143.838},
 {-170.277}, {-197.057}, {-224.159}, {-251.554}, {-279.212}, {-307.106}, {-335.209},
 {-363.498}, {-391.951}, {-420.552}, {-449.283}, {-478.129}, {-507.078}, {-536.118}}
```

(Debug) In[74]:=

```
barrier = Flatten[MinSP - Minweg]
                  ebne ein
```

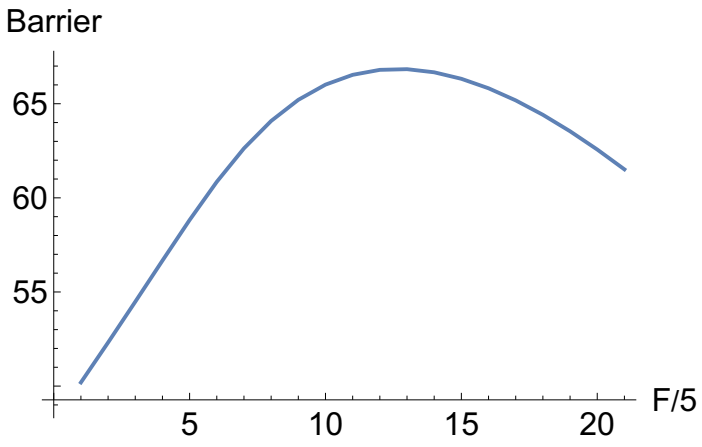
(Debug) Out[74]=

```
{50.1935, 52.3152, 54.4801, 56.6666, 58.8234, 60.8512,
 62.6288, 64.0845, 65.2068, 66.0142, 66.5351, 66.7994, 66.8355,
 66.6692, 66.324, 65.8207, 65.1778, 64.4118, 63.5373, 62.5672, 61.5132}
```

(Debug) In[97]:=

```
BiListe = ListLinePlot[barrier, AxesLabel → {"F/5", "Barrier"}, AxesStyle → FontSize → 16]
                  listenbezogene Liniengraphik  Achsenbeschriftungen          Achsenstile  Schriftgröße
```

(Debug) Out[97]=




```
(* here we obtain a nice catch bond behavior *)
```