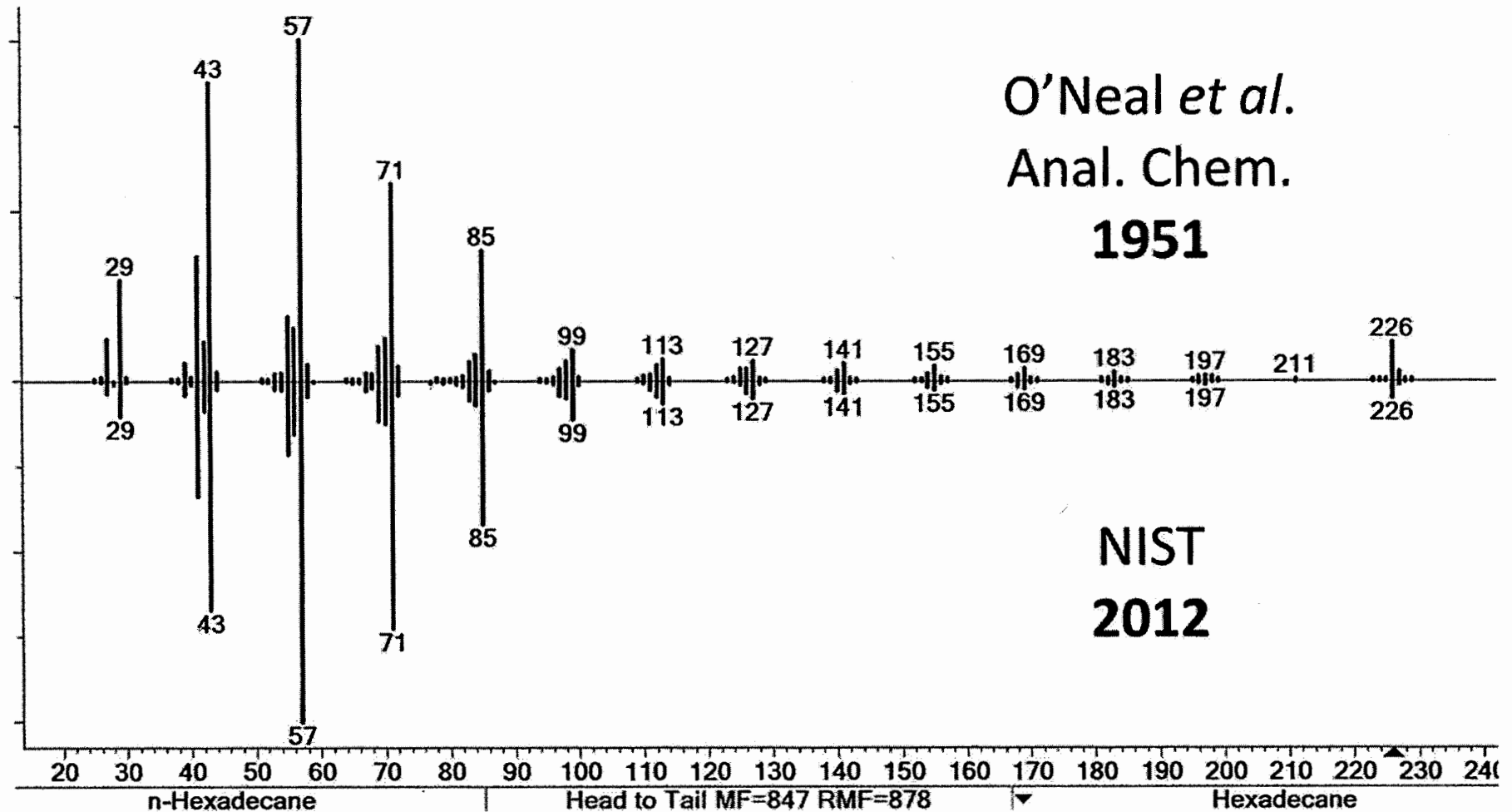
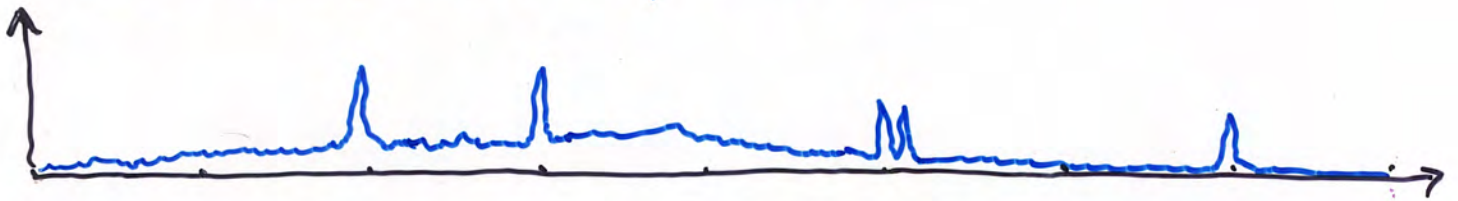


Vergleich Massenspektren GC/MS



- Fragmentierung durch Electron Ionization (EI) ist hochgradig reproduzierbar
- Massengenauigkeit GC/MS üblicherweise nur ganze Zahlen

Gemessenes Spektrum



$$\mathcal{M}' = \{ 200, 300, 500, 515, 700 \}$$

Referenzspektren



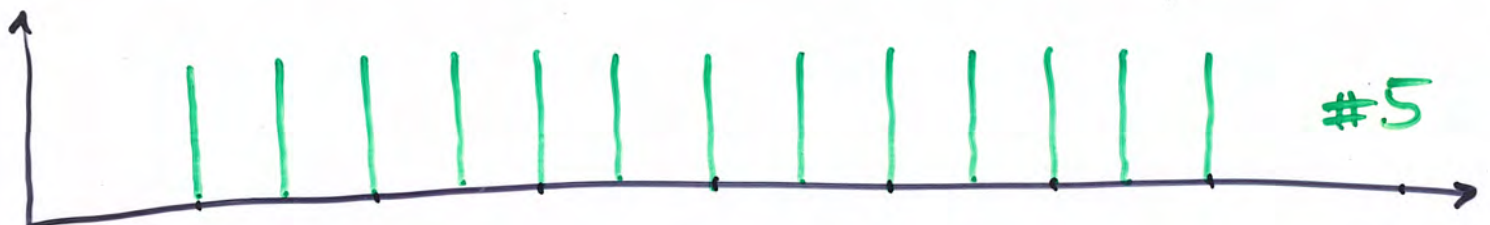
$$\mathcal{M}_1 = \{ 100, 175, 350, 480, 490, 550 \}$$

$$\mathcal{M}_2 = \{ 200, 270, 305, 400, 450 \}$$

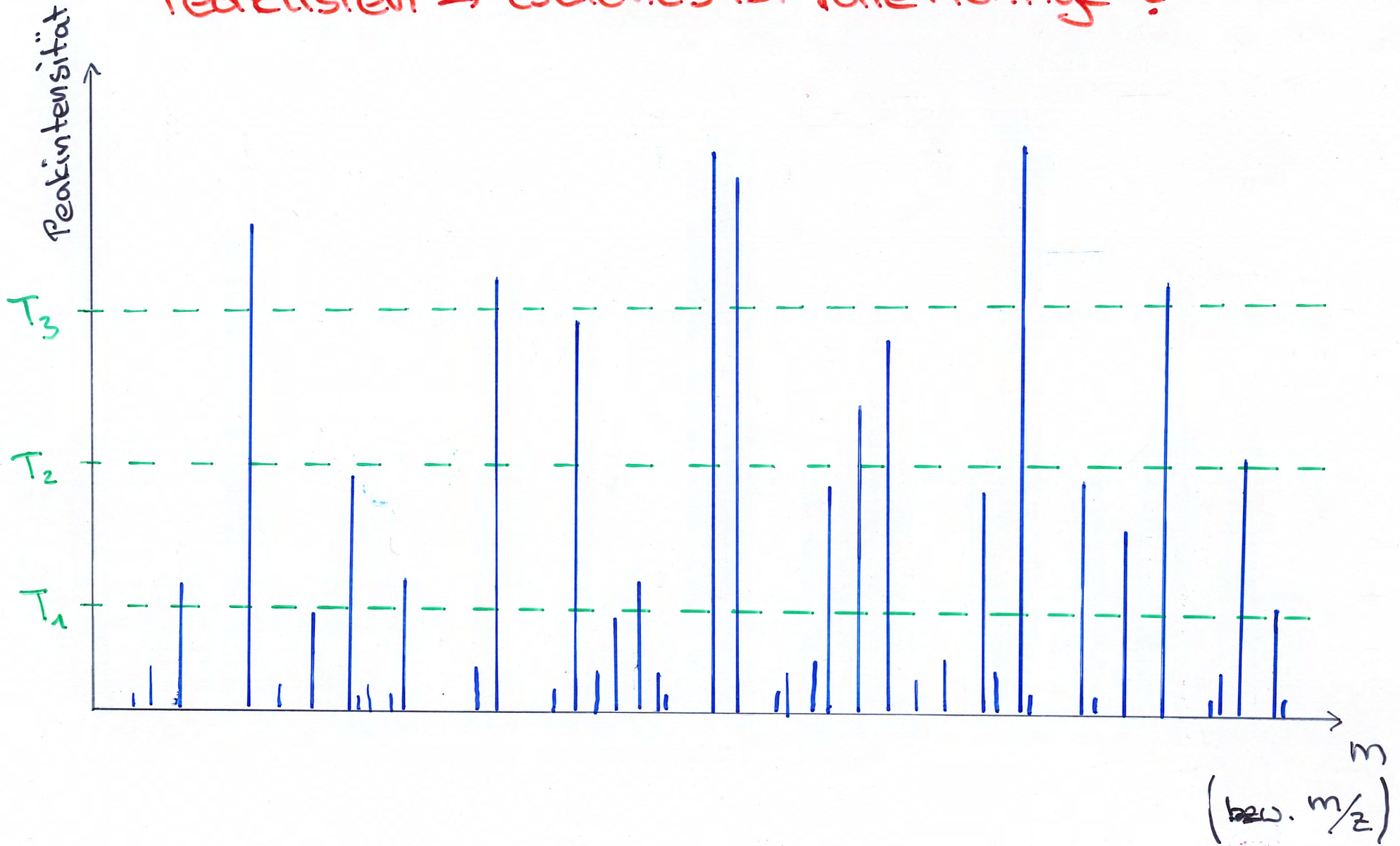
$$\mathcal{M}_3 = \{ 200, 510, 705, 850 \}$$

$$\mathcal{M}_4 = \{ 190, 310, 490, 710 \}$$

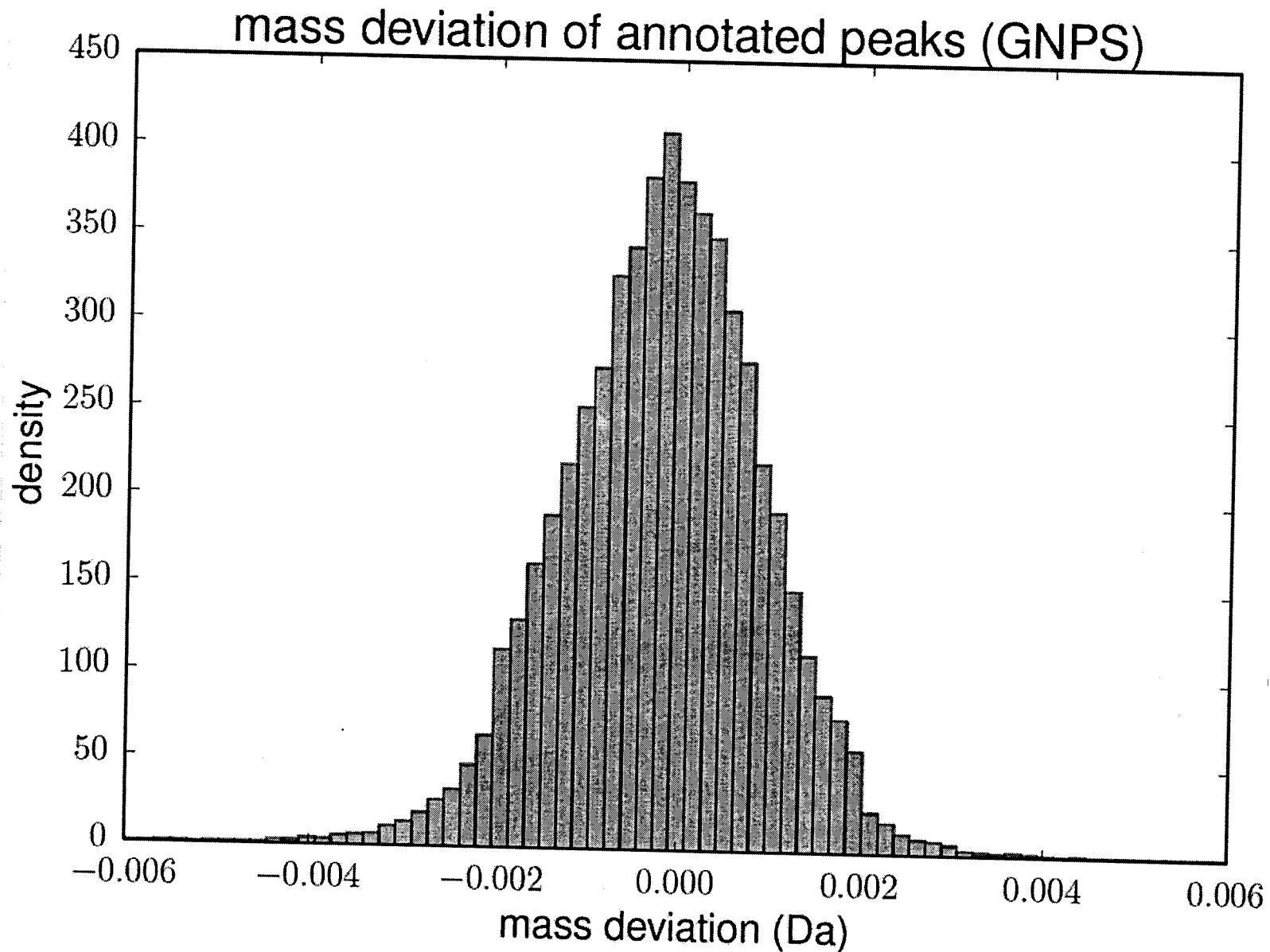
$$\mathcal{M}_5 = \{ 100, 150, 200, 250, \dots, 600, 650, 700 \}$$



Unterschiedliche Thresholds ergeben unterschiedliche Peaklisten → welches ist „die richtige“?

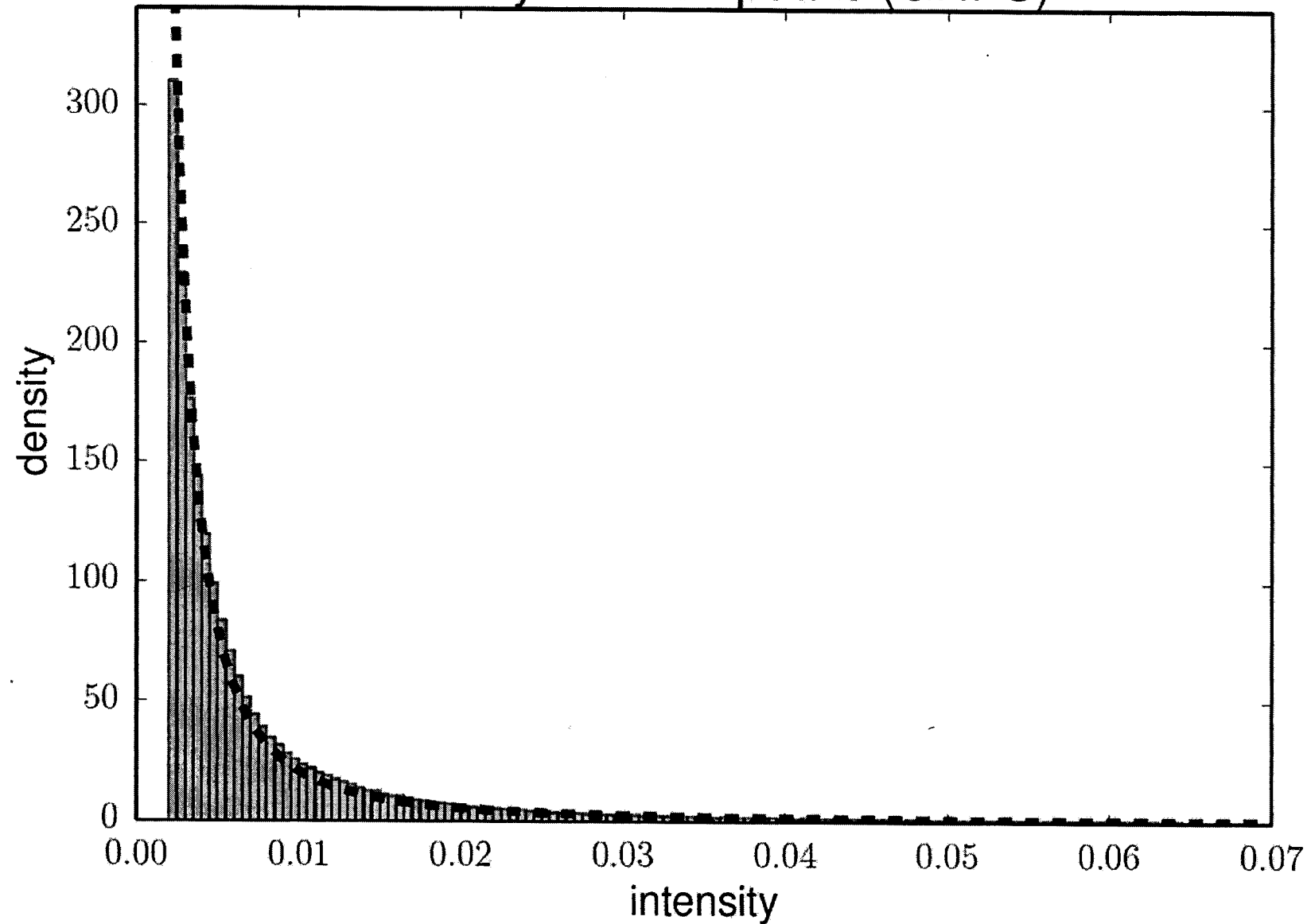


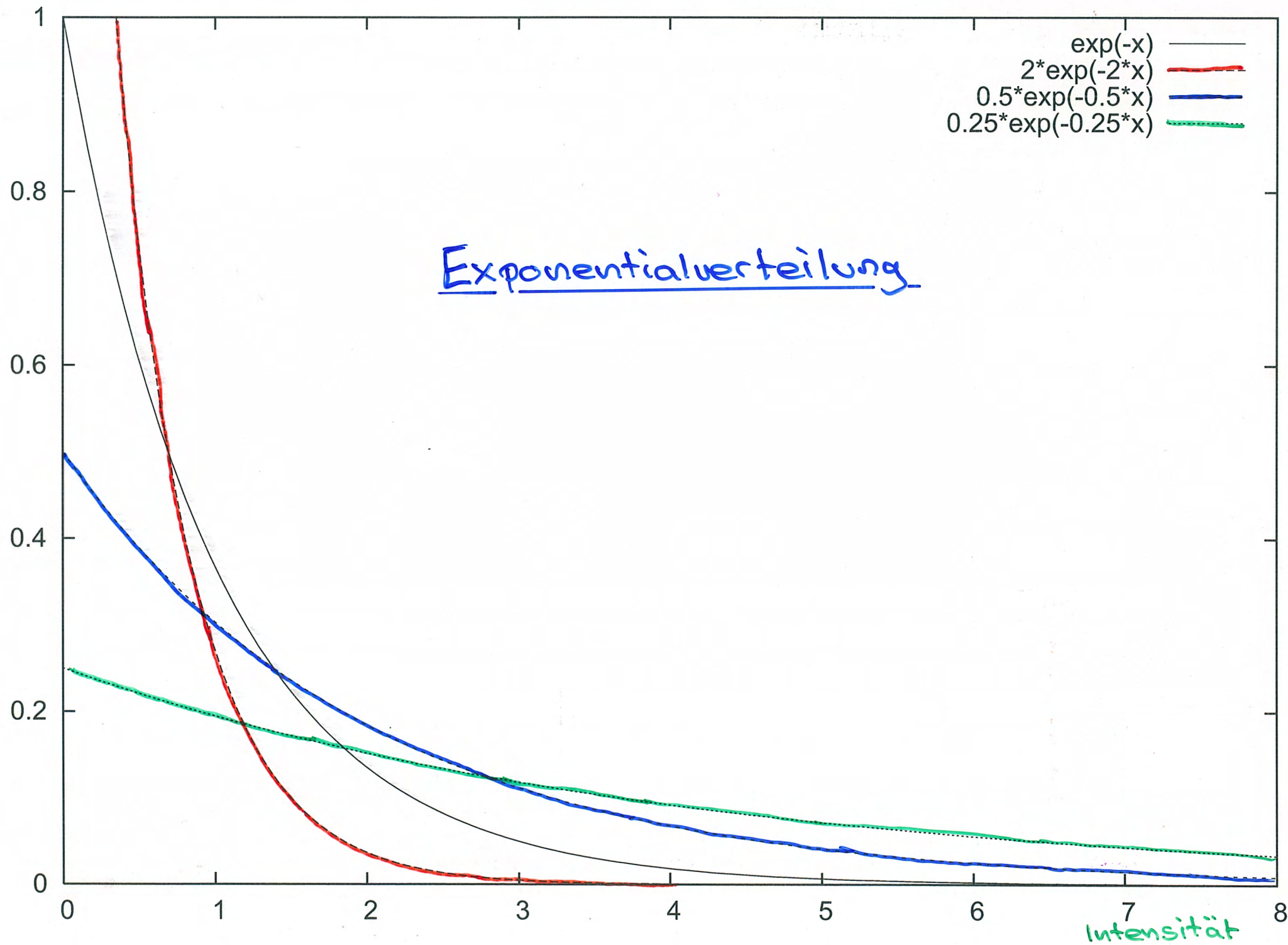
Massenabweichungen Tandem MS



Intensitäten Rauschpeaks Tandem MS

intensity of noise peaks (GNPS)





Exponentialverteilung

Intensität