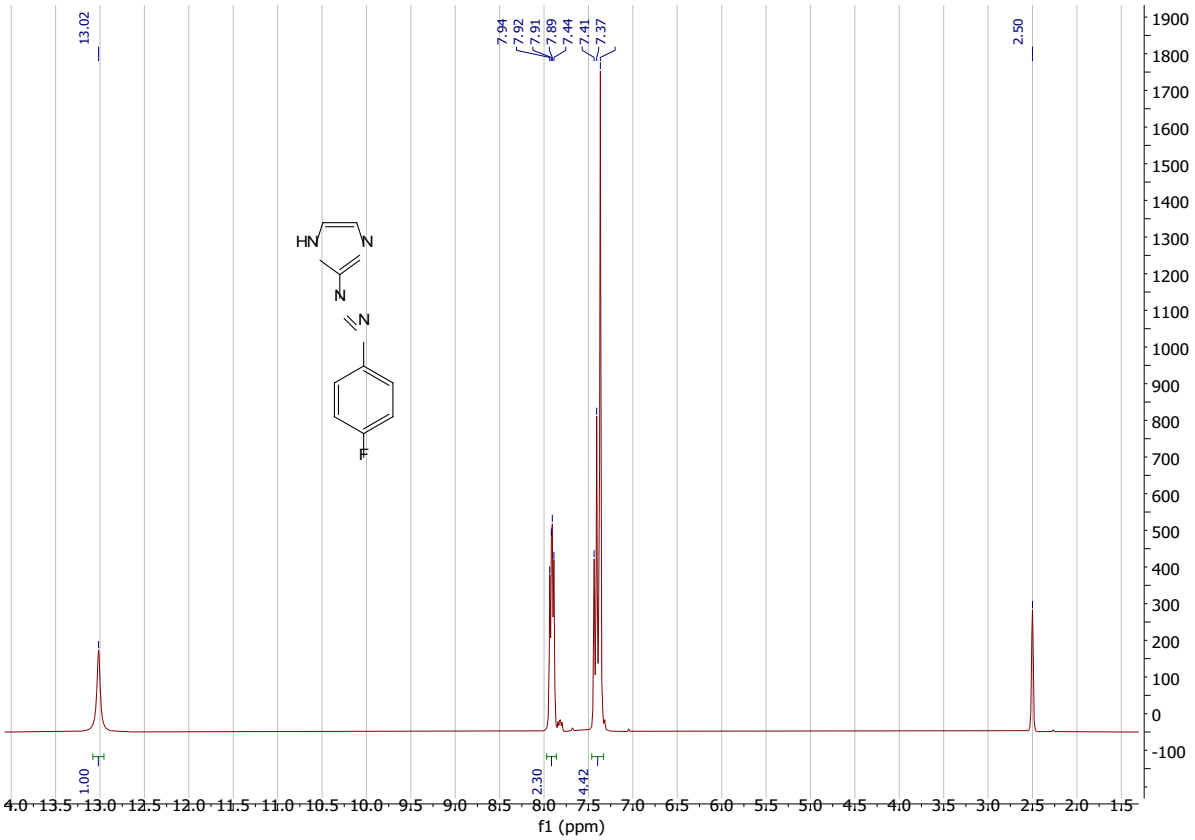
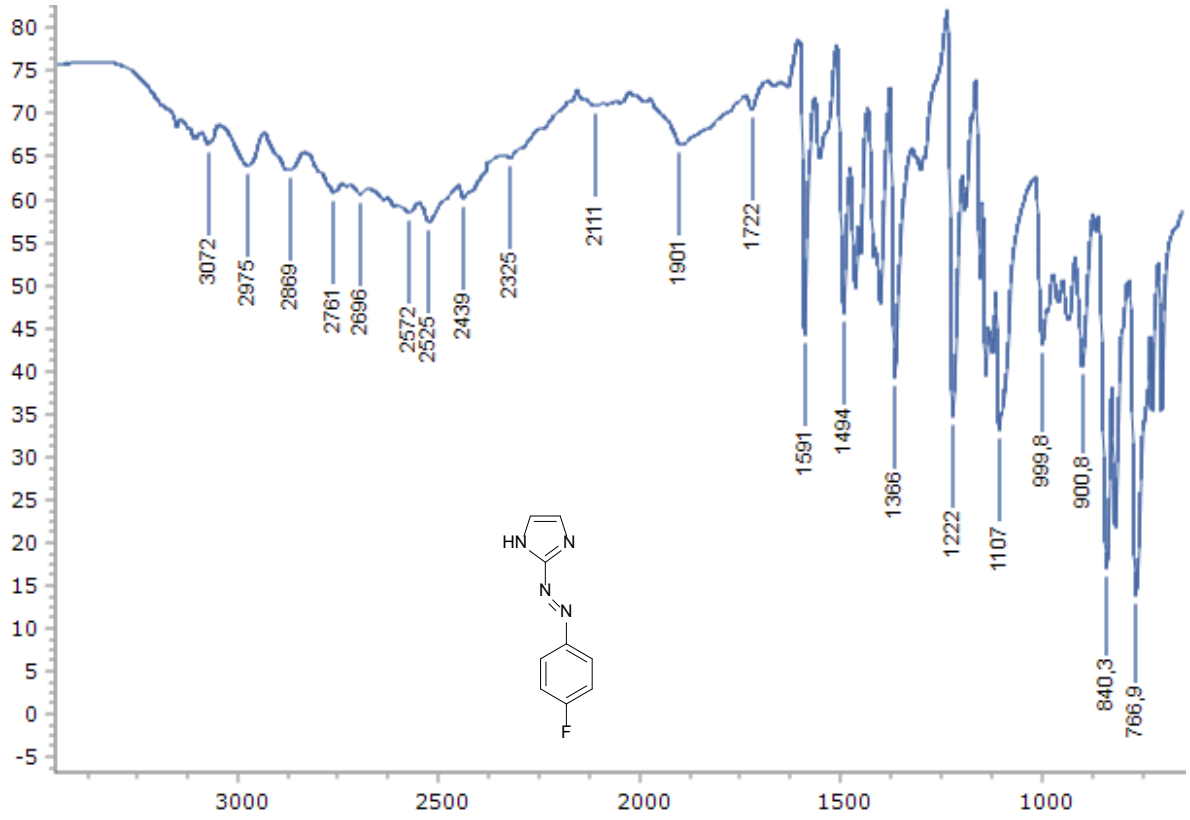
2 Anhang

2.1 Spektrenkatalog



Spektrum 1: H-NMR, 2-((4-Fluorphenyl) diazenyl)-1H-imidazol (9)


80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
0
-5
3000
2500
2000
1500
1000
3072
2975
2869
2761
2696
2572
2525
2439
2325
2111
1901
1722
1591
1494
1366
1222
1107
999,8
900,8
840,3
766,9
HN
N
N
N
F

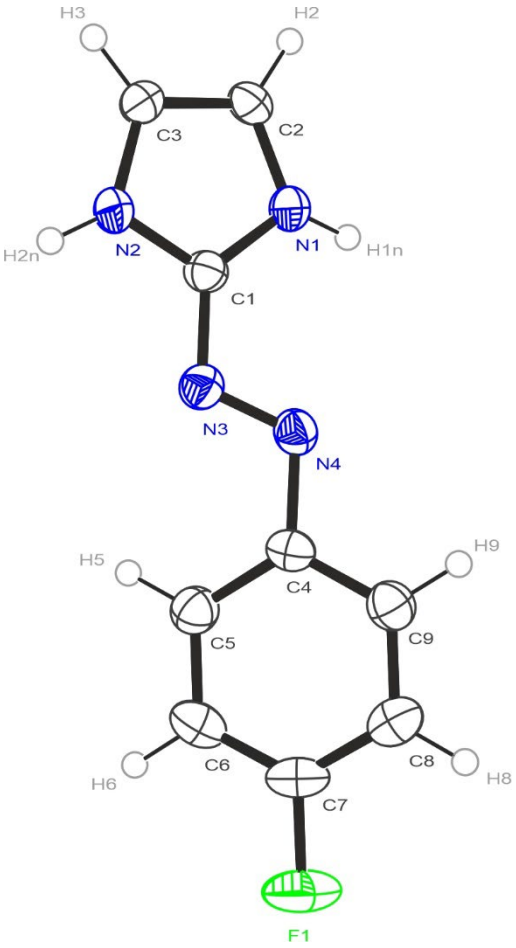

H3
H2
C3
C2
N2
N1
H2n
H1n
C1
N3
N4
H5
H9
C4
C5
C9
C6
C8
H6
H8
C7
F1

Abbildung 9: Kristallstruktur 2-((4-Fluorphenyl) diazenyl)-1H-imidazol (9)

Tabelle 3: Kristalldaten 2-((4-Fluorphenyl) diazenyl)-1H-imidazol (9)

Crystal data	
Chemical formula	$C_9H_7FN_4$
M_r	190.19
Crystal system, space group	Triclinic, *P*
Temperature (K)	183
a, *b*, *c* (Å)	7.0756 (4), 7.7929 (5), 8.8199 (6)
α, β, γ (°)	70.801 (2), 74.9153 (19), 83.689 (2)
V (Å^3)	443.29 (5)
Z	2
Radiation type	Mo *K*α
μ (mm^{-1})	0.11
Crystal size (mm)	0.16 × 0.11 × 0.08
Data collection	
Diffractometer	Bruker D8 QUEST PHOTON 100
Absorption correction	Multi-scan Bruker *SADABS2014*/5)
T_{min}, T_{max}	0.925, 0.971
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	10043, 1560, 1312
R_{int}	0.039
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.594
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.039, 0.100, 1.09
No. of reflections	1560
No. of parameters	136
No. of restraints	2

H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.19, −0.28