

Supplementary Materials

N-(6-Chloro-3-nitropyridin-2-yl)-5-(1-methyl-1*H*-pyrazol-4-yl)isoquinolin-3-amine

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Figure S1: ¹H-NMR spectrum of **5**

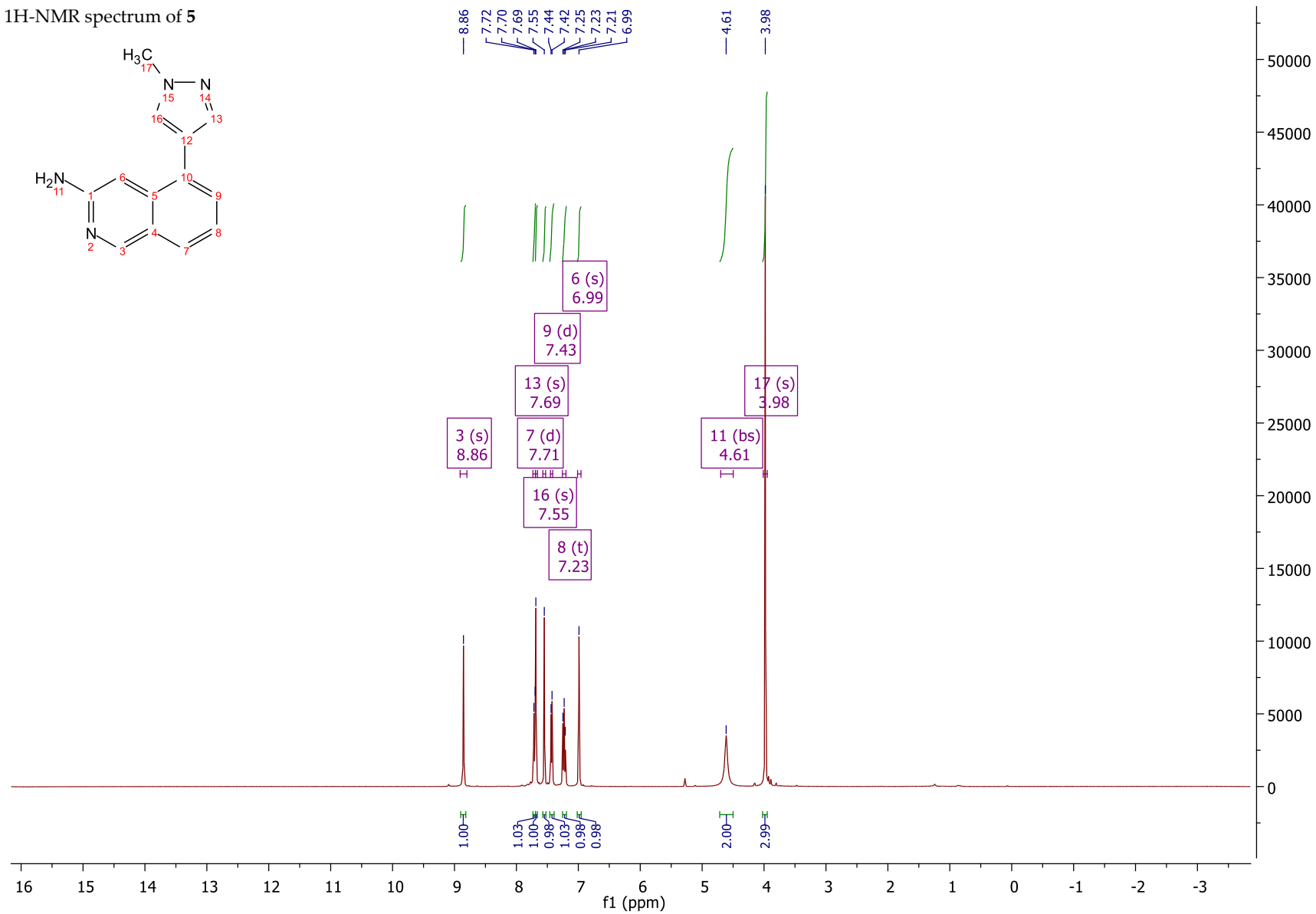


Figure S2: ¹³C-NMR spectrum of **5**

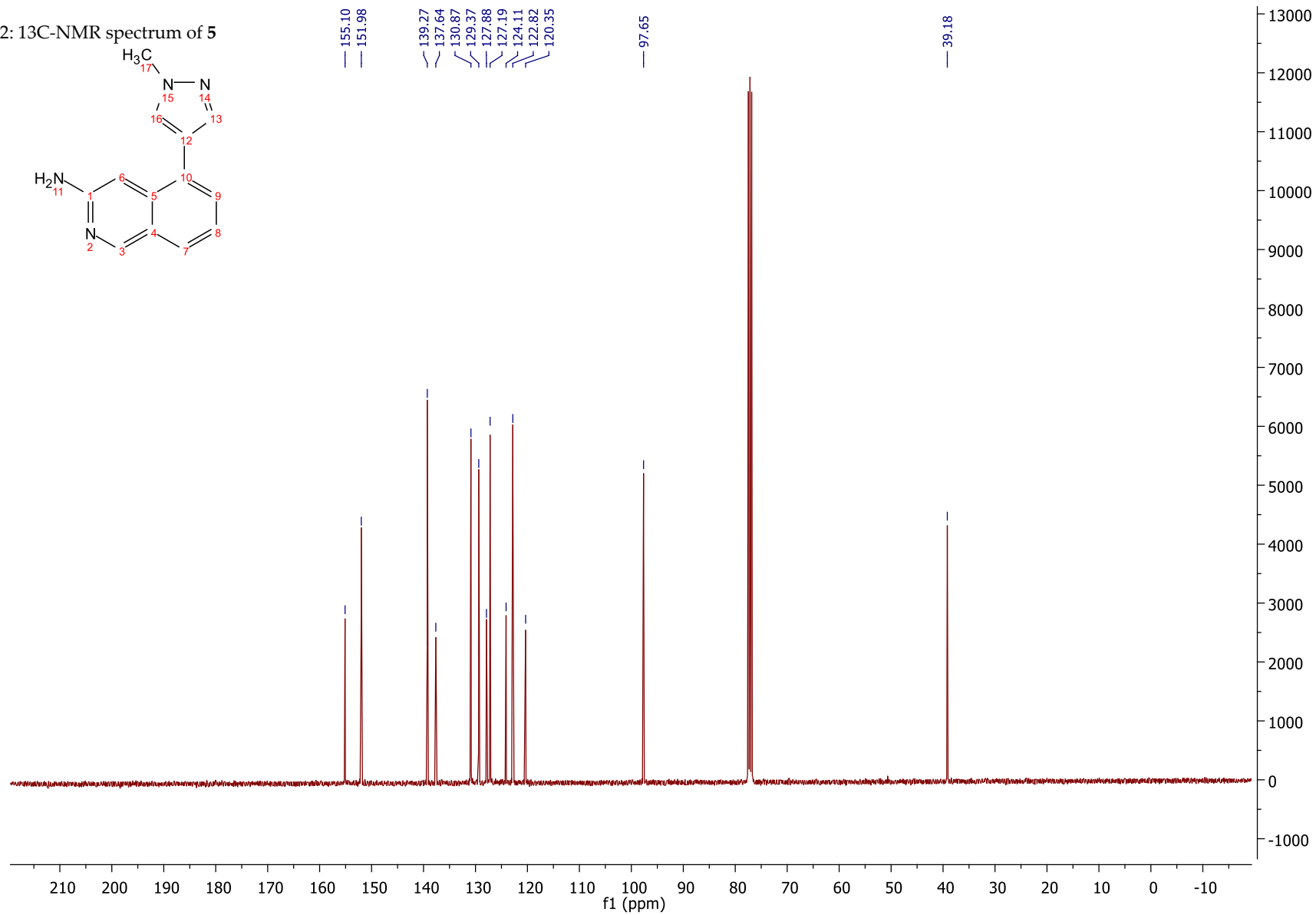


Figure S3: HSQC-2D-NMR spectrum of **5**

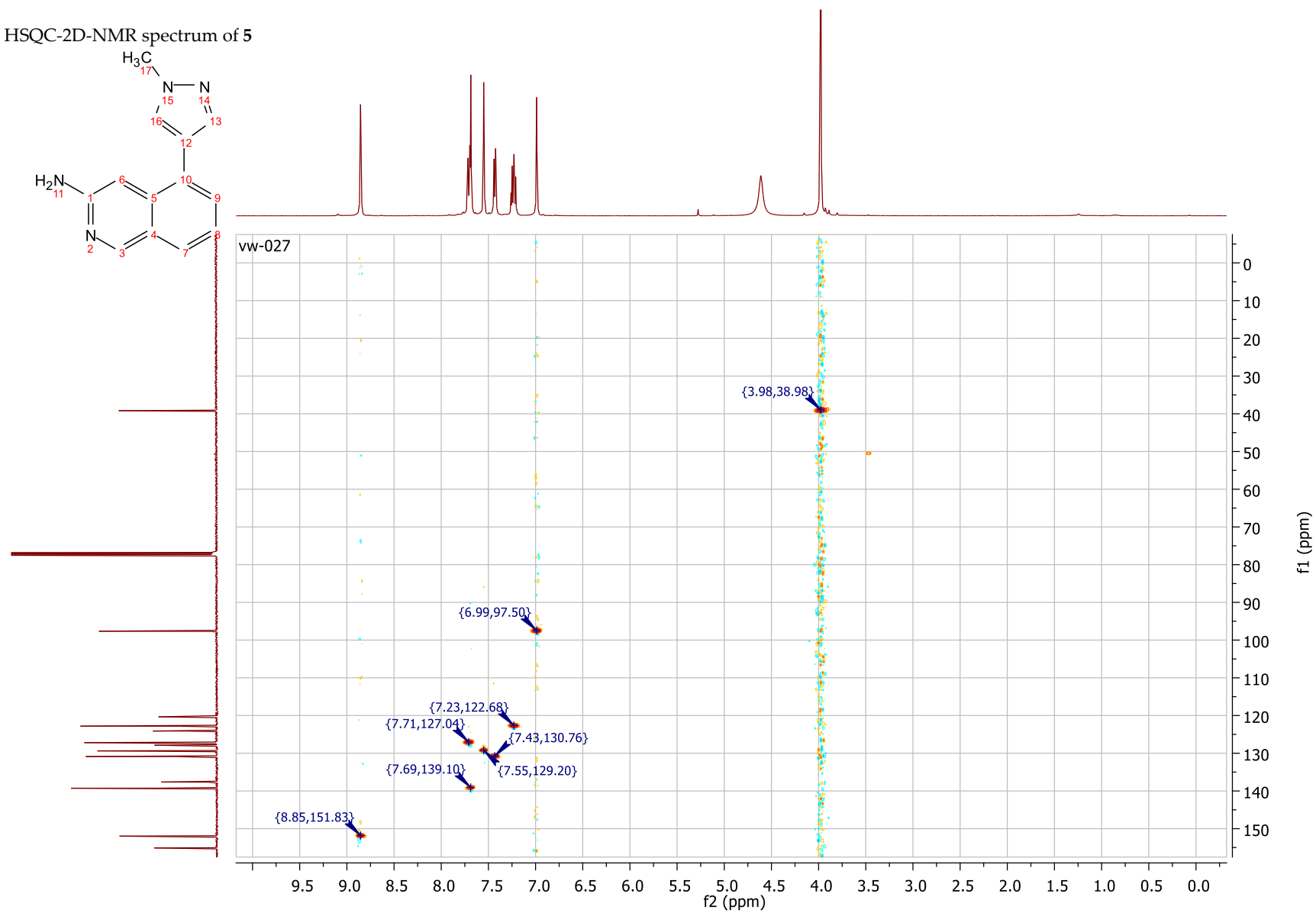


Figure S4: ESI-MS of 5

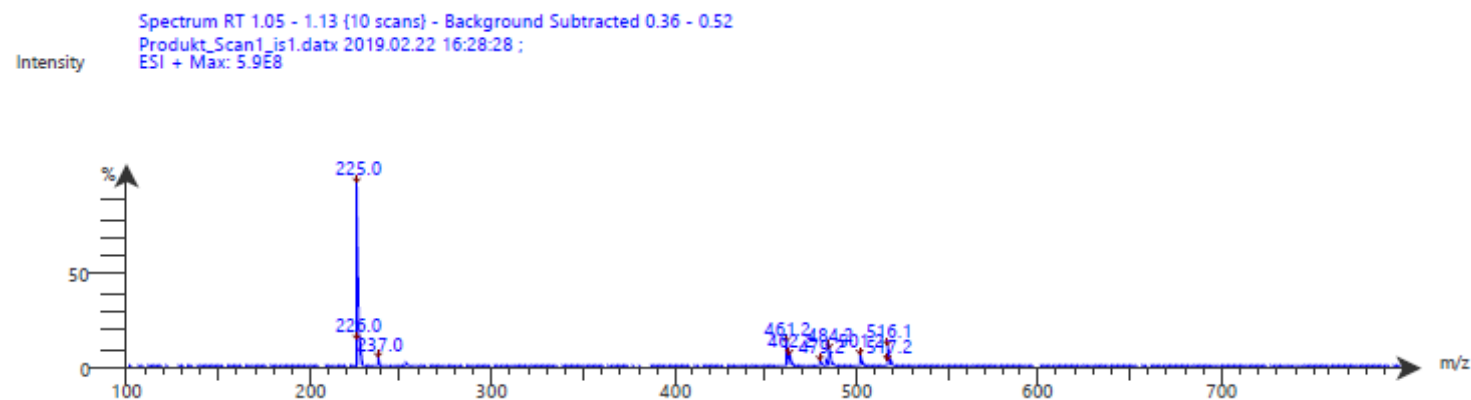
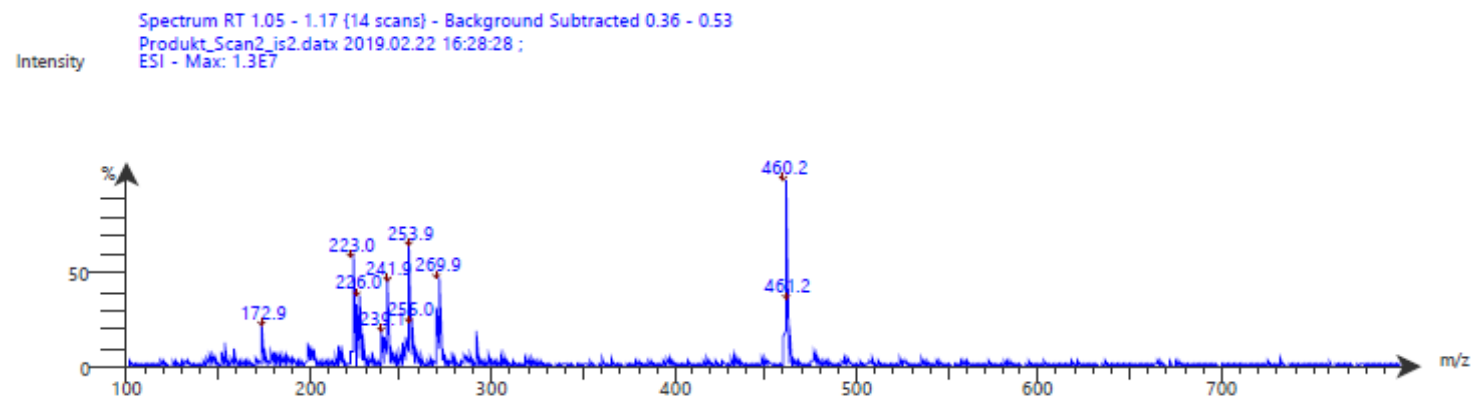
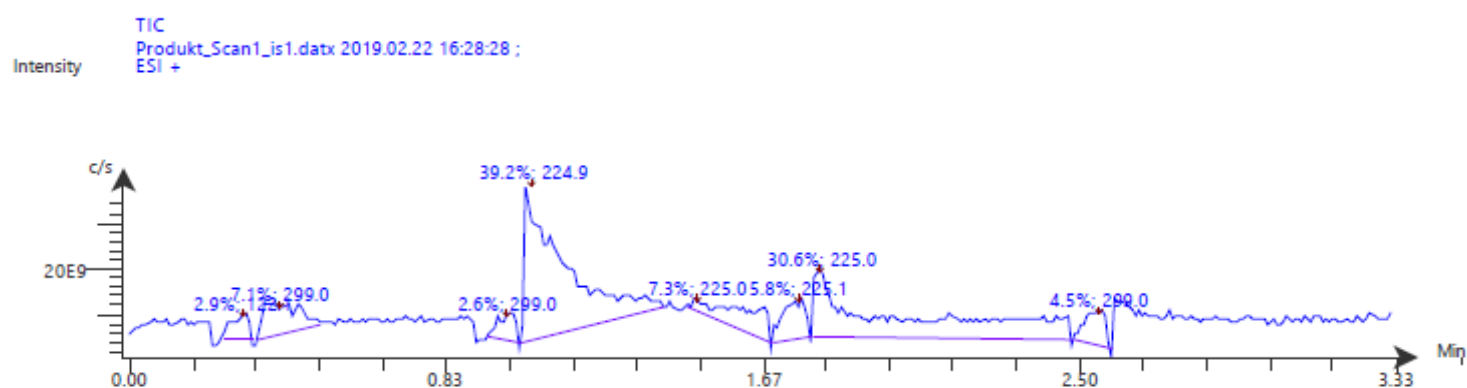
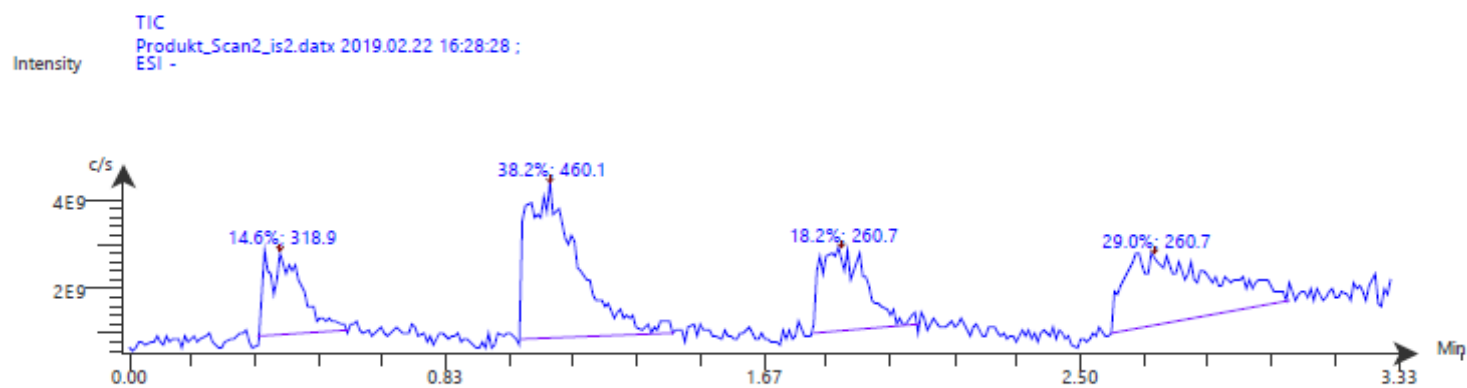
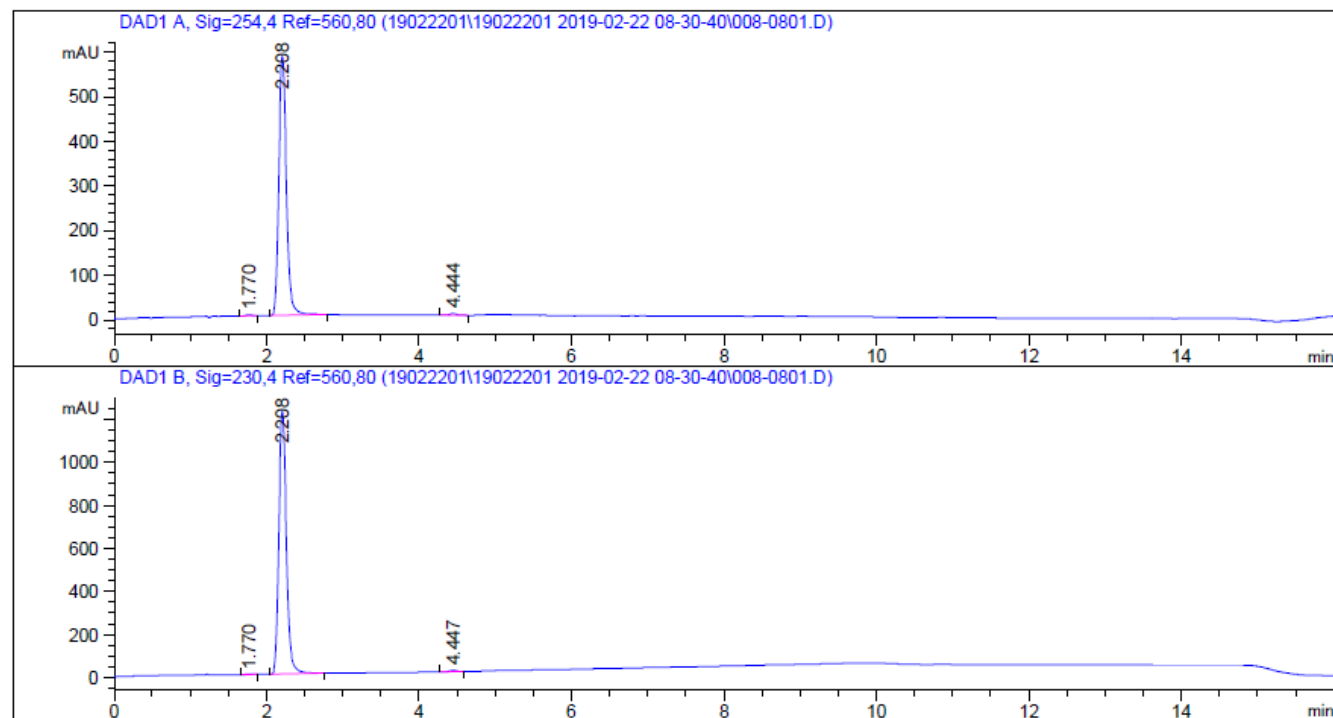


Figure S5: HPLC chromatogram of 5



Signal 1: DAD1 A, Sig=254,4 Ref=560,80

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	1.770	BB	0.0793	12.26213	2.33235	0.3040
2	2.208	BB	0.1062	3995.54053	581.15881	99.0618
3	4.444	BB	0.1014	25.58060	3.85645	0.6342

Totals : 4033.38326 587.34761

Signal 2: DAD1 B, Sig=230,4 Ref=560,80

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	1.770	BB	0.0811	11.58911	2.21464	0.1375
2	2.208	BB	0.1061	8379.92969	1220.38330	99.3913
3	4.447	BB	0.0966	39.73557	6.38465	0.4713

Totals : 8431.25437 1228.98259

Figure S6: ¹H-NMR spectrum of **1**

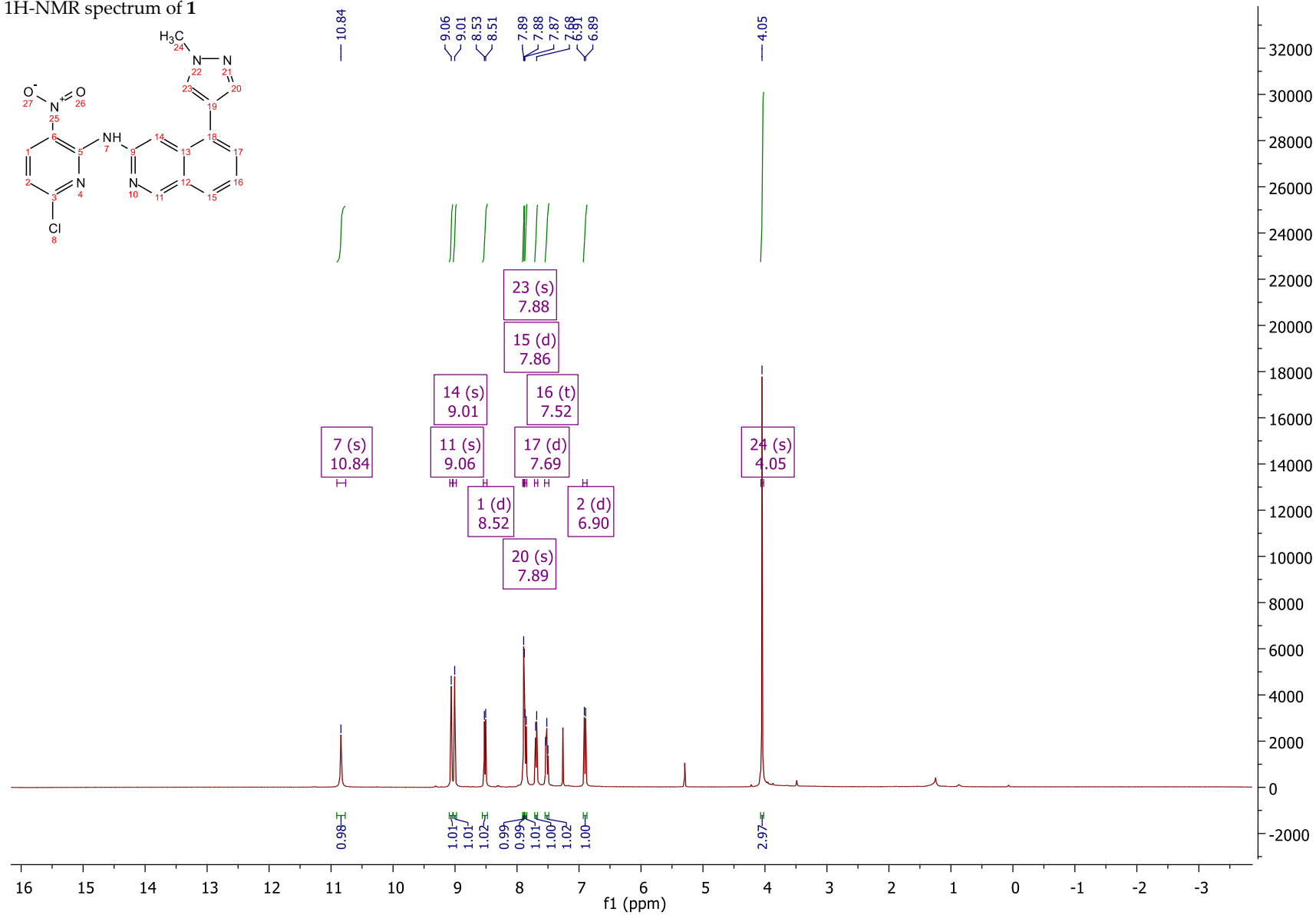


Figure
S7: ^{13}C -
NMR
spectrum
of **1**

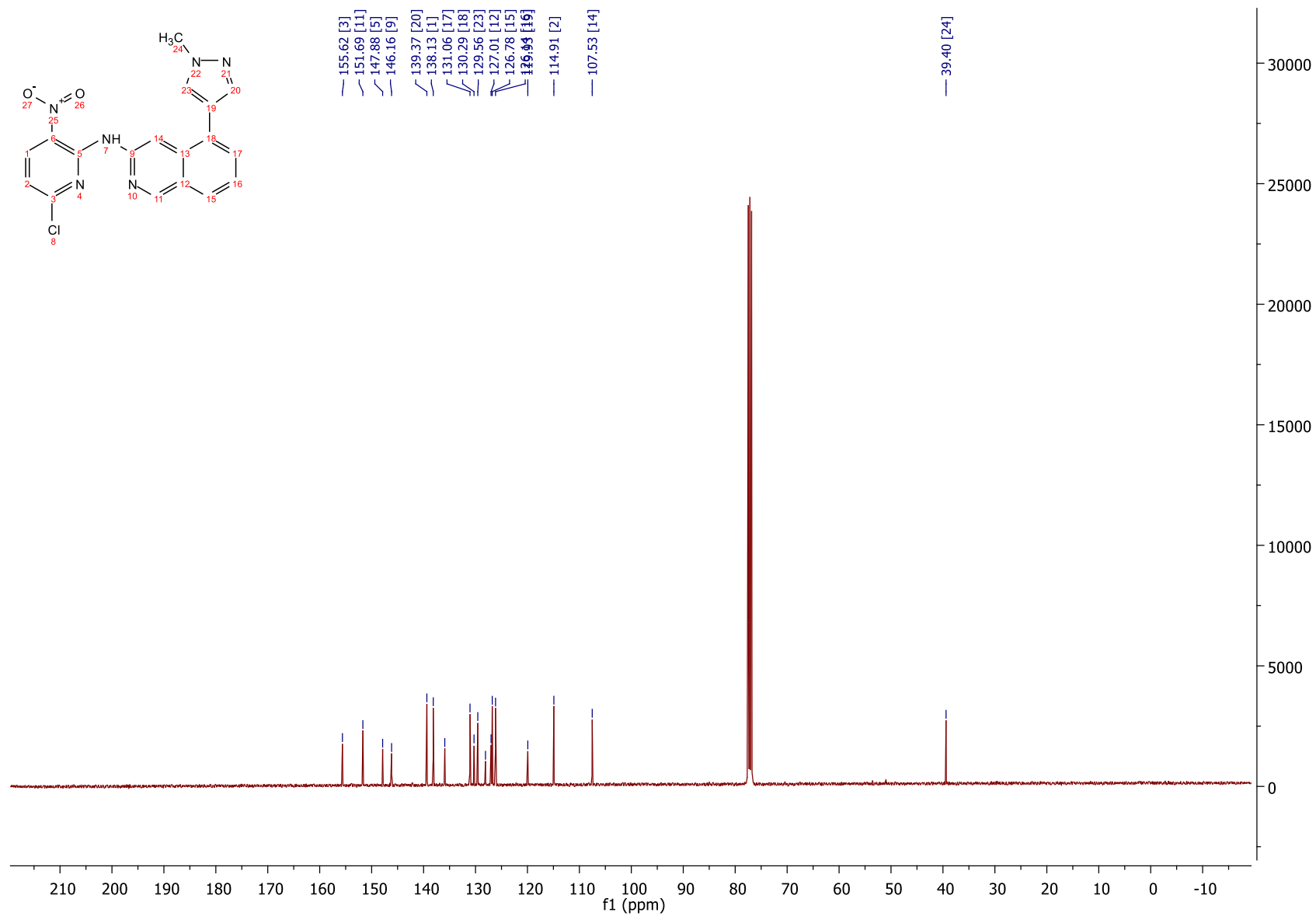


Figure S8:
90DEPT-NMR
spectrum of **1**

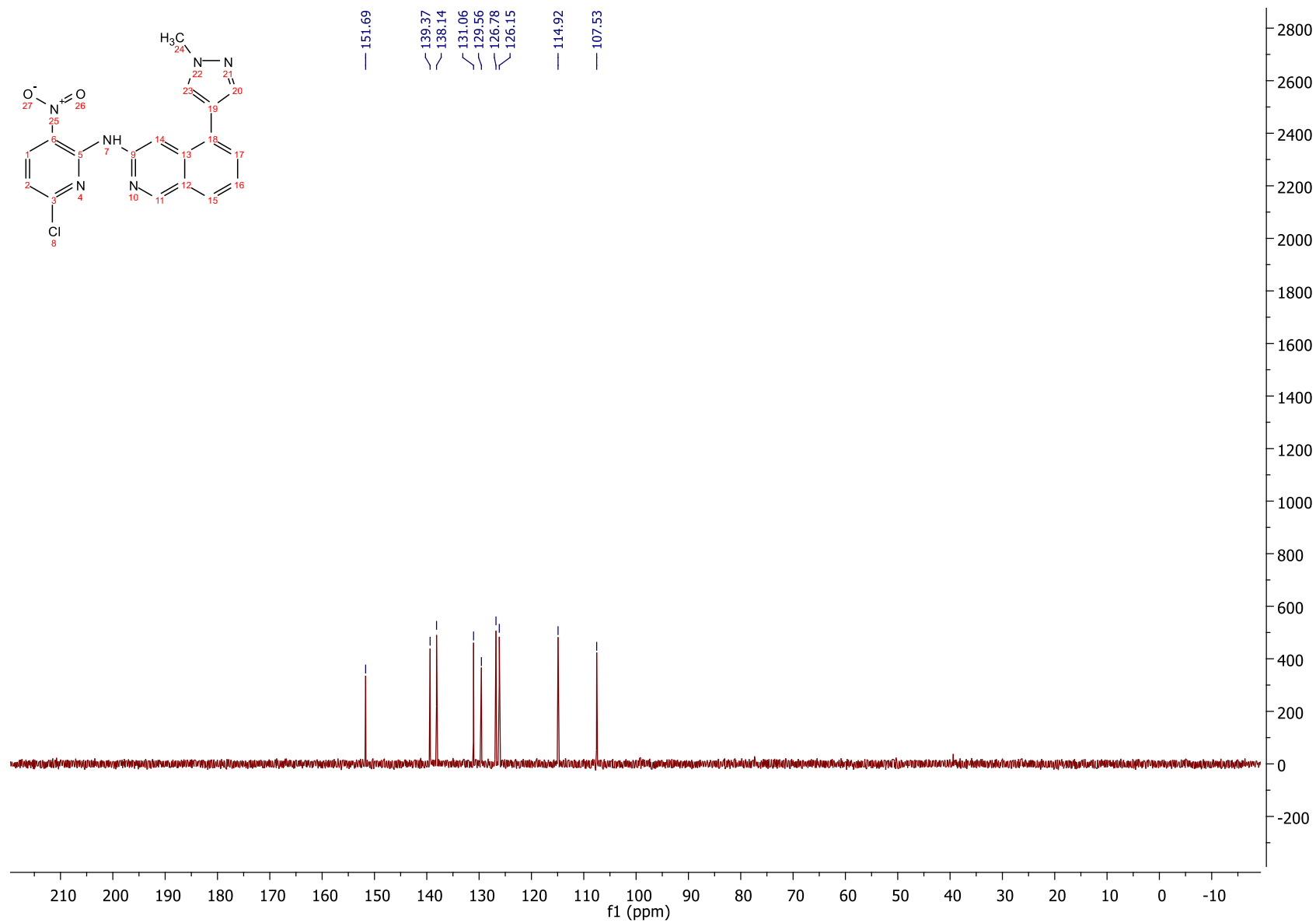


Figure S9: HSQC-
2D-NMR
spectrum of **1**

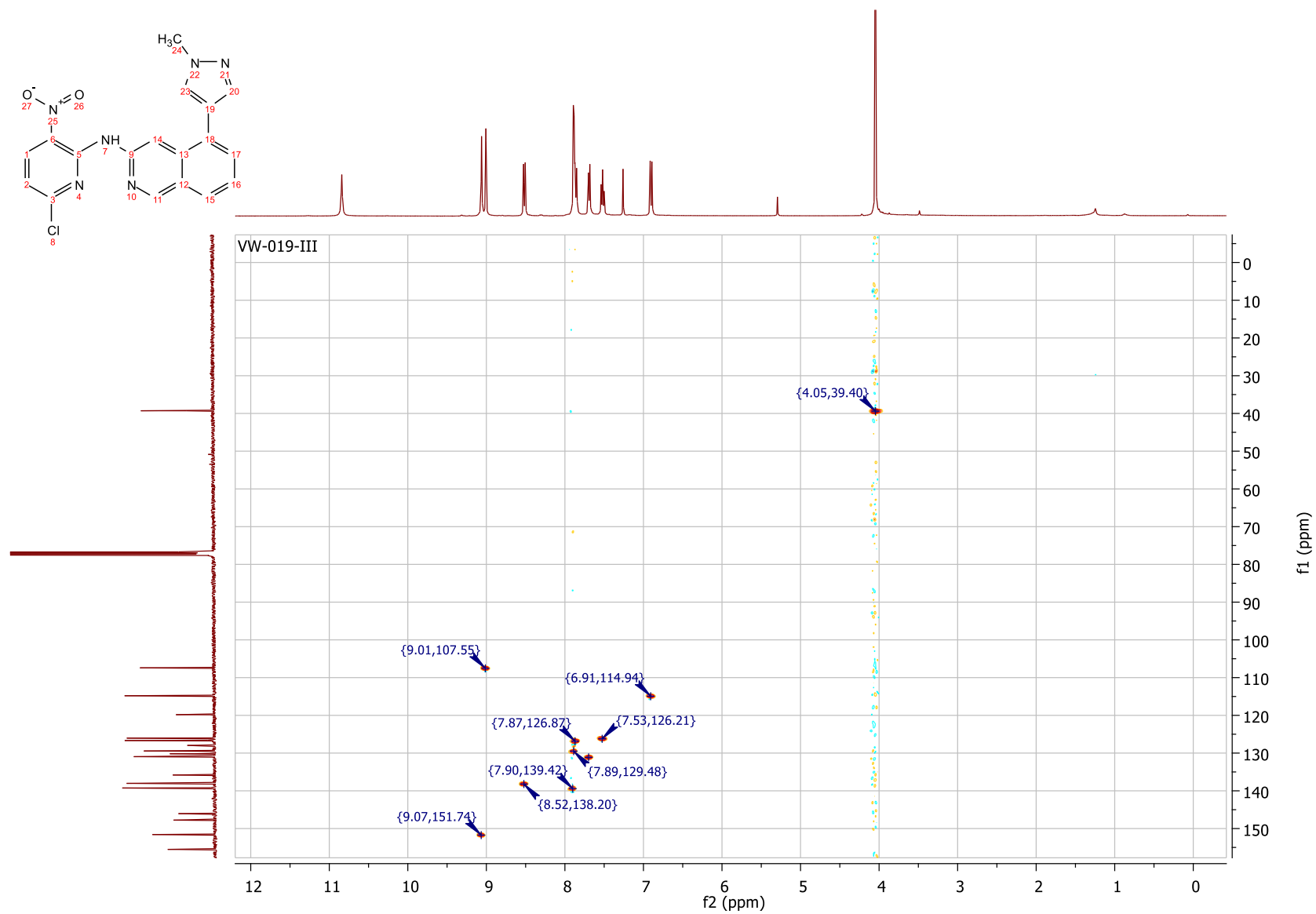


Figure S10: COSY-
2D-NMR spectrum
of **1**

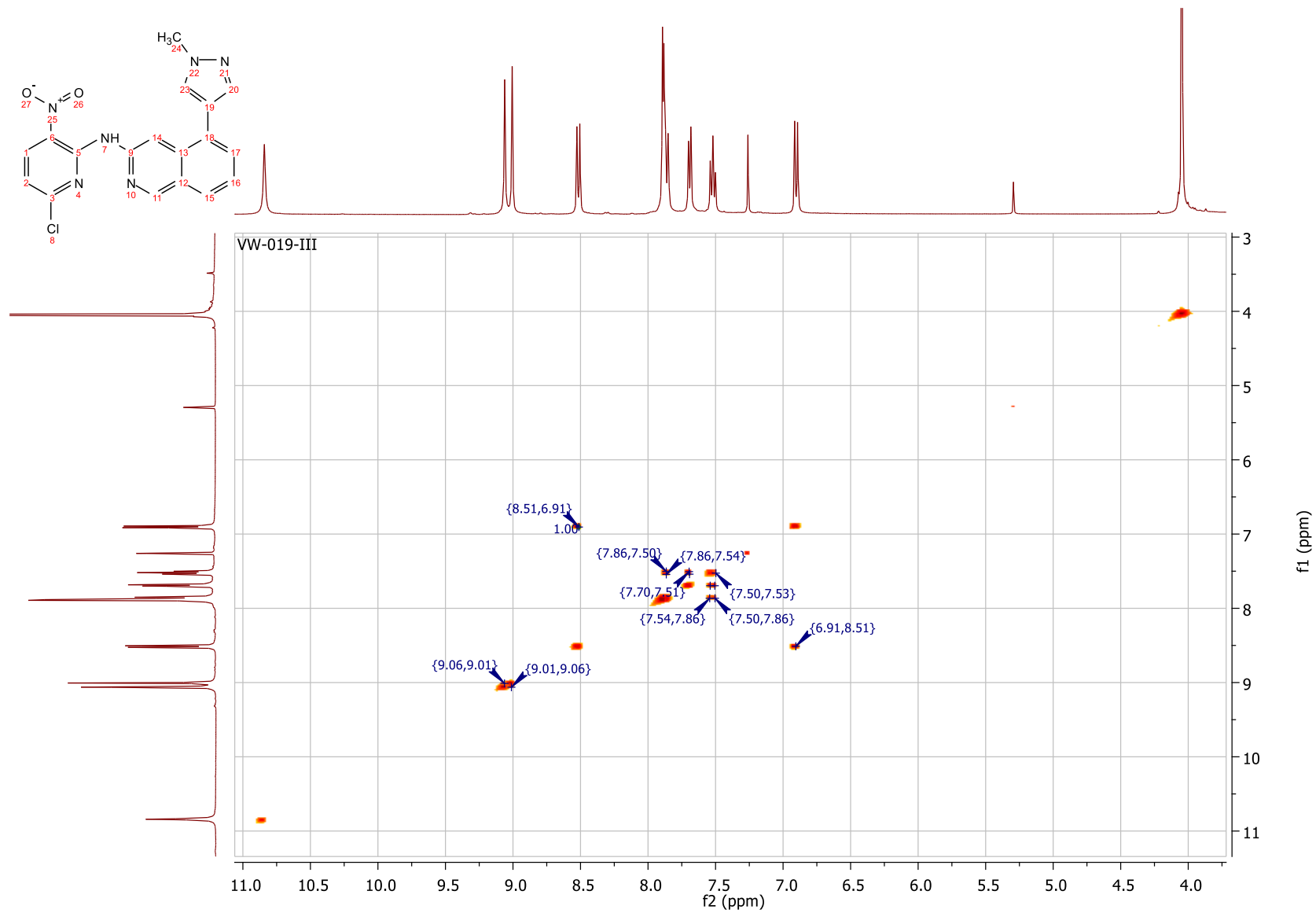


Figure S11:
HMBC-2D-NMR
spectrum of **1**

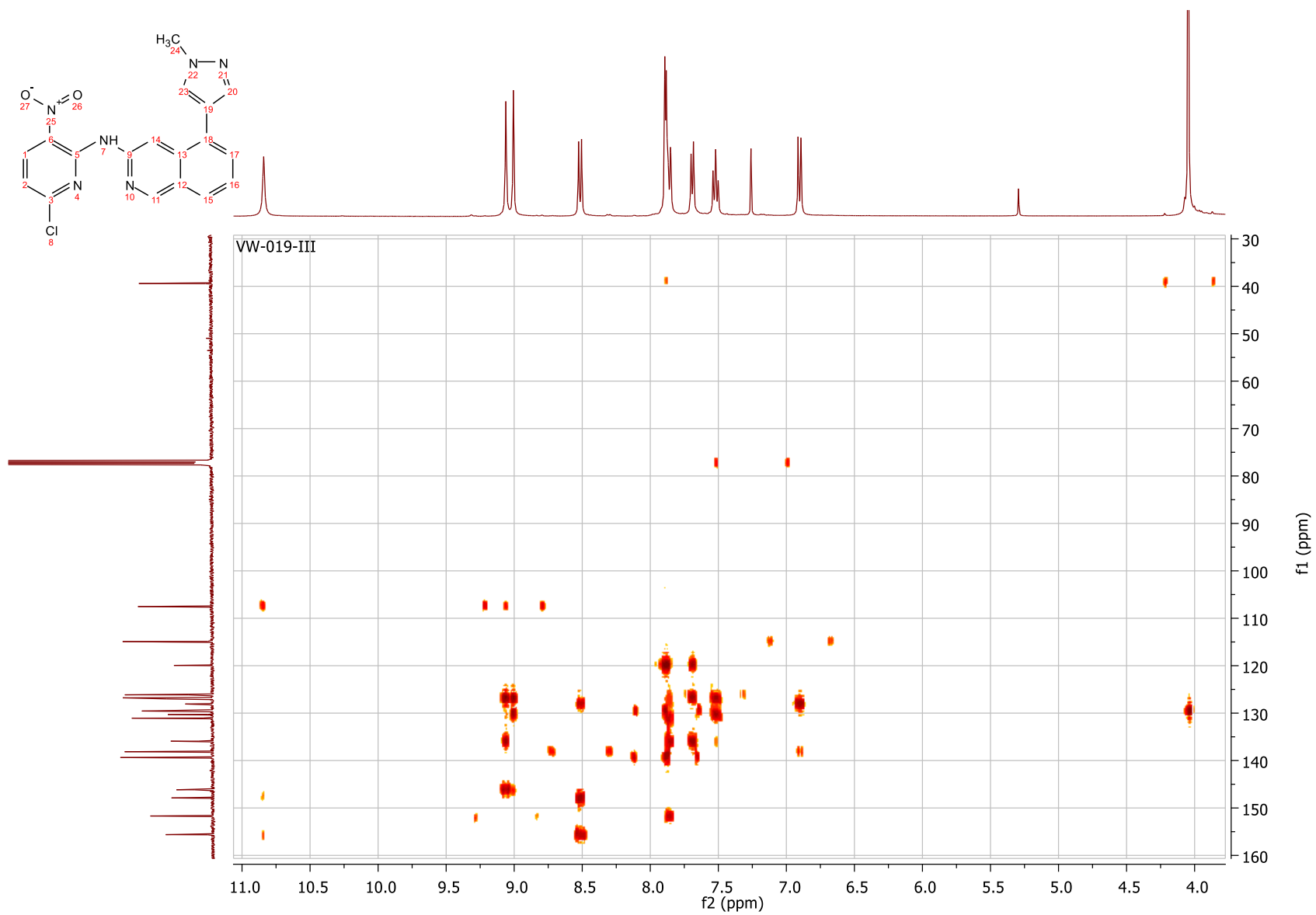


Figure S12: NOESY-
2D-NMR spectrum of
1

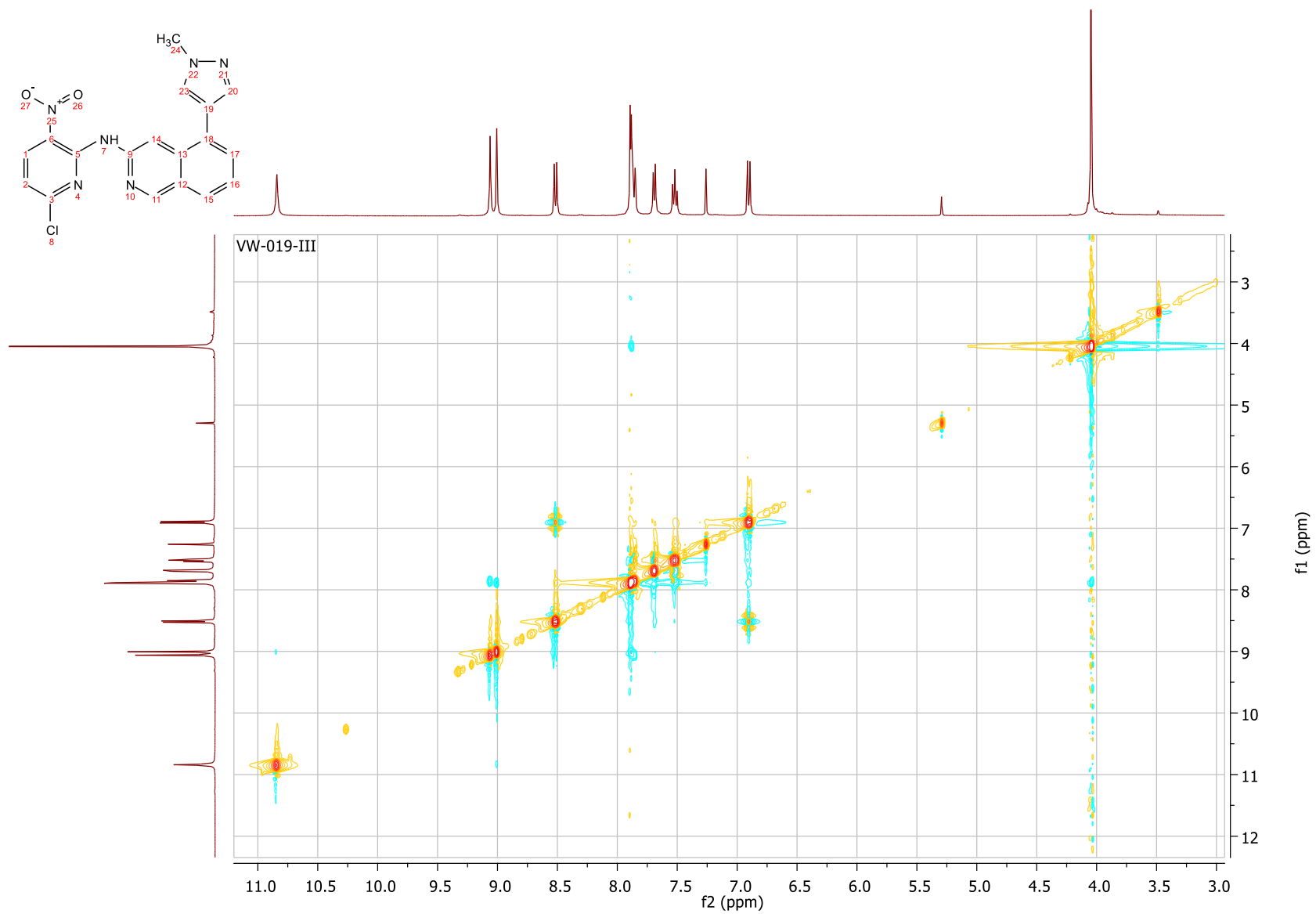


Figure S13: ESI-HRMS of 1

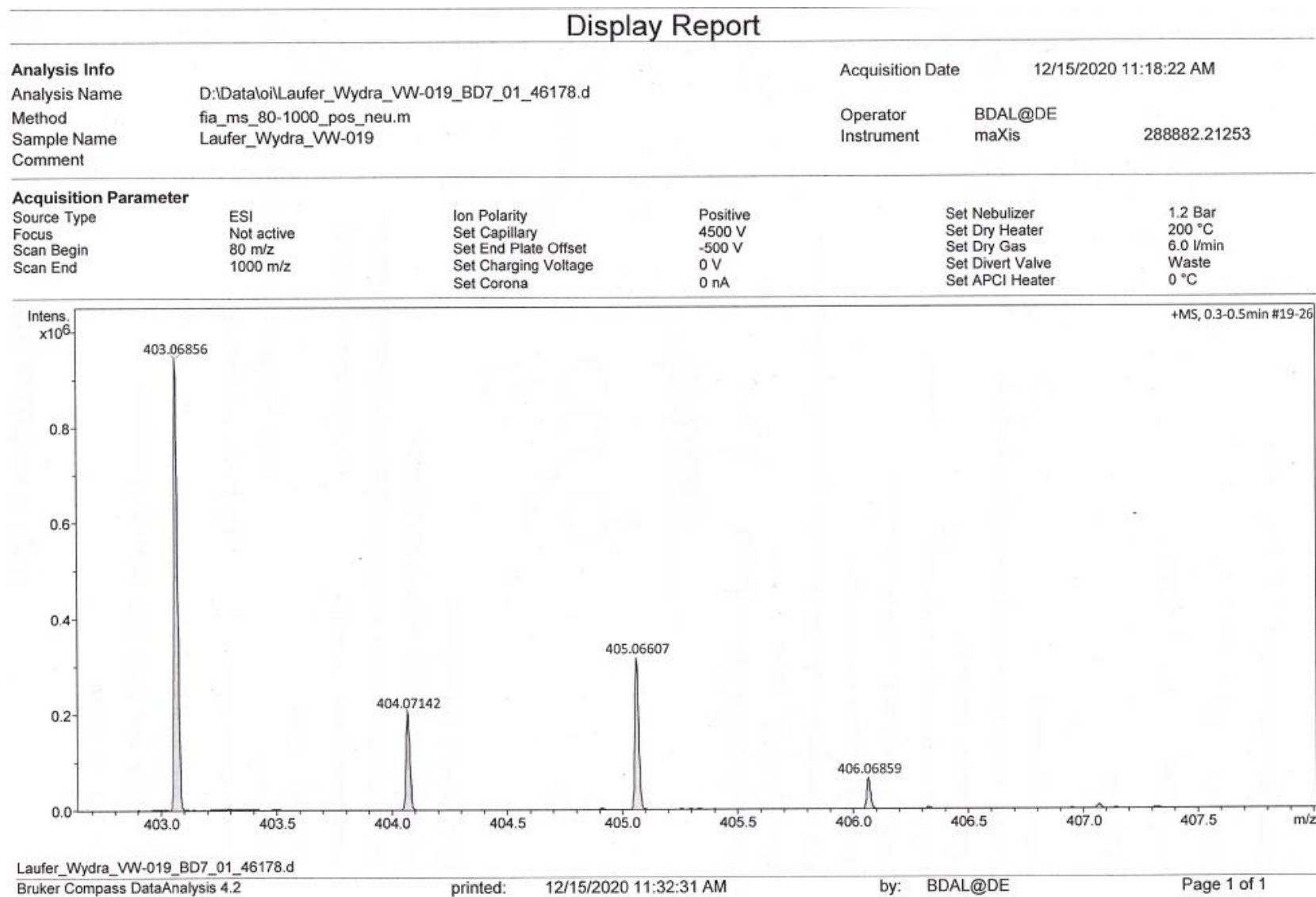
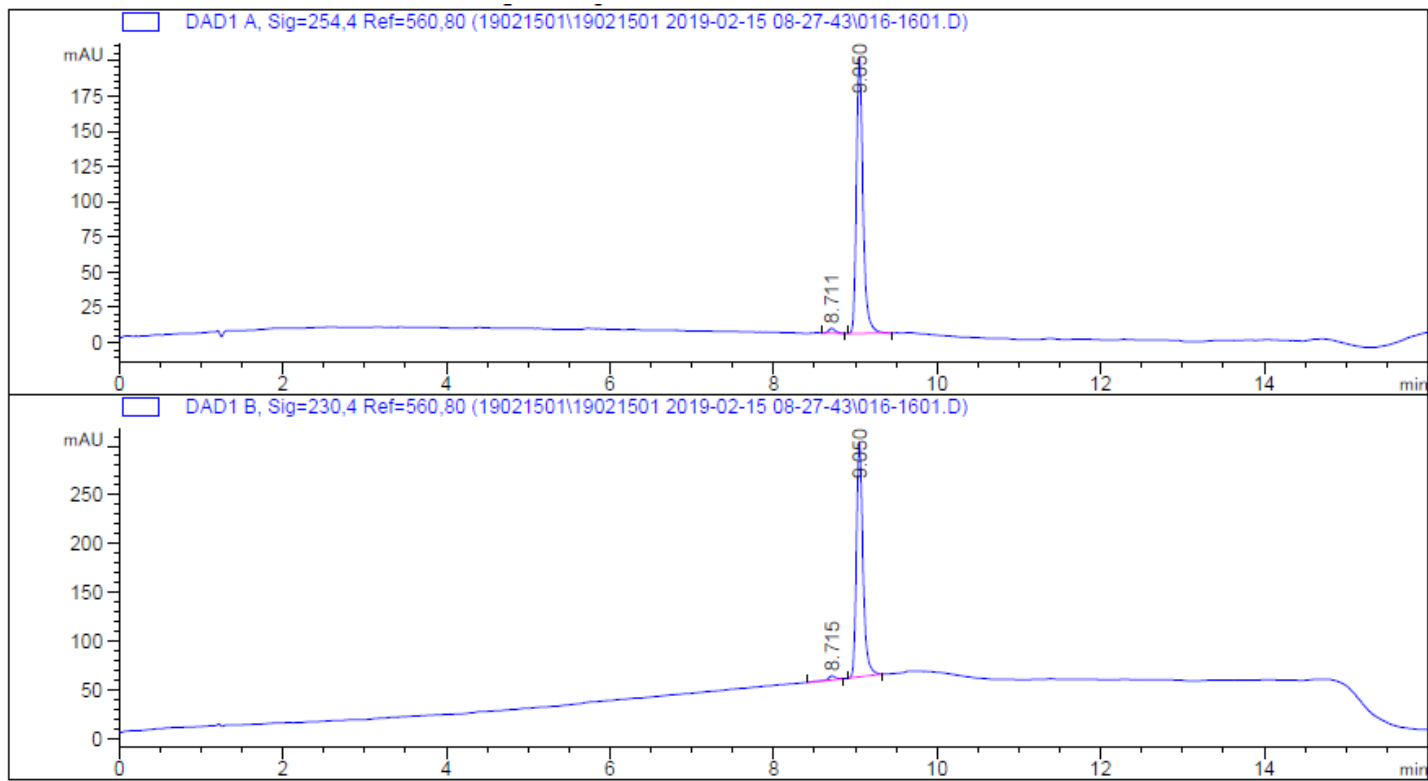


Figure S14: HPLC chromatogram of 1



Signal 1: DAD1 A, Sig=254,4 Ref=560,80

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.711	BB	0.0864	19.71092	3.46197	1.7679
2	9.050	BB	0.0852	1095.20520	195.97061	98.2321

Totals : 1114.91612 199.43258

Signal 2: DAD1 B, Sig=230,4 Ref=560,80

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.715	BB	0.0934	25.21171	4.00476	1.8509
2	9.050	BB	0.0847	1336.89111	240.94110	98.1491

Totals : 1362.10283 244.94586

Figure S15: IR spectrum of 1

