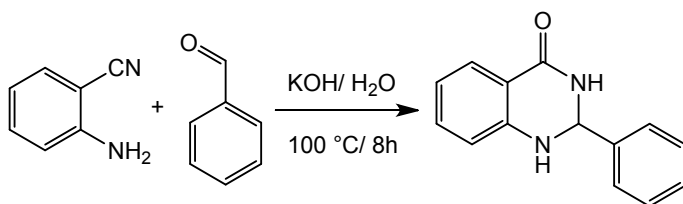


Supporting Information

General remarks:

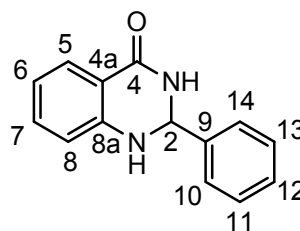
All Chemicals were commercial available and were used without further purification. NMR-data was recorded by a Bruker ARX 300 and Bruker ARX 400 spectrometers. ^{13}C - and ^1H -spectra were referenced to deuterated solvent signals. Peaks were characterized as singlet (*s*), doublet (*d*), doublet of doublet (*dd*), triplet (*t*), doublet of triplets (*dt*), quartet (*q*) and multiplet (*m*). Gas-chromatographie-mass-analysis was measured by an Agilent HP-5890 with Agilent HP-5973 Mass Selective Detector (EI) and HP-5-capillary column using helium as carrier gas. Column-chromatographie was carried out using Merck 60 Silica-Gel (0.043 - 0.06 mm) and distilled solvents were used.

General experimental procedure:



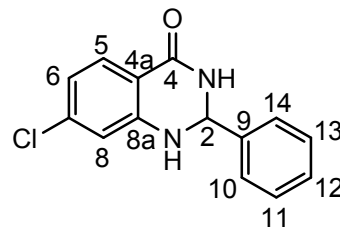
2-Phenyl-2,3-dihydroquinazolin-4(1H)-one

$^1\text{H-NMR}$ (250 MHz, DMSO-*d*₆): δ = 8.28 (*s*, 1H, NH(3)), 7.61 (*dd*, 1H, 3J = 7.8 Hz, 4J = 1.6 Hz, CH(5)), 7.49 (*dd*, 2H, 3J = 7.9 Hz, 4J = 1.9 Hz, CH(10 + 14)), 7.45 - 7.29 (*m*, 3H, CH(11 + 12 + 13)), 7.24 (*ddd*, 1H, 3J = 8.1 Hz, 3J = 7.2 Hz, 3J = 1.6 Hz, CH(7)), 7.11 (*s*, 1H, NH(1)), 6.78 - 6.72 (*m*, 1H, CH(8)), 6.71 - 6.63 (*m*, 1H, CH(6)), 5.75 (*t*, 1H, 3J = 1.9 Hz, CH(2)); $^{13}\text{C-NMR}$ (63 MHz, DMSO-*d*₆): δ = 163.6 (C=O(4)), 147.8 (C_{quart}(8a)), 141.6 (C_{quart}(9)), 133.3 (CH(7)), 128.4 (CH(12)), 128.3 (CH(11 + 13)), 127.3 (CH(5)), 126.8 (CH(10 + 14)), 117.1 (CH(6)), 114.9 (C_{quart}(4a)), 114.4 (CH(8)), 66.5 (CH(2)) ppm; MS: (EI, 70 eV) *m/z* (%) = 224 ([M]⁺, 19), 223 (27), 147 (100), 120 (42), 119 (15), 104 (10), 92 (29), 77 (20), 65 (14), 64 (10), 51 (15).



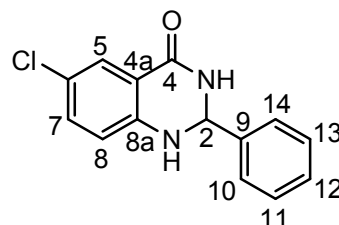
2-Phenyl-7-chloro-2,3-dihydroquinazolin-4(1H)-one

$^1\text{H-NMR}$ (300 MHz, DMSO-*d*₆): δ = 8.47 (*s*, 1H, NH(3)), 7.54 (*d*, 1H, 4J = 2.6 Hz, CH(8)), 7.50 - 7.45 (*m*, 2H, CH(10 + 14)), 7.44 - 7.34 (*m*, 3H, CH(11 + 12 + 13)), 7.34 - 7.32 (*m*, 1H, NH(1)), 7.28 (*dd*, 1H, 3J = 8.7 Hz, 4J = 2.7 Hz, CH(6)), 6.78 (*d*, 1H, 3J = 8.7 Hz, CH(8)), 5.78 (*dd*, 1H, 3J = 1.9 Hz, 3J = 1.9 Hz, CH(2)) ppm; $^{13}\text{C-NMR}$ (75 MHz, DMSO-*d*₆): δ = 162.4 (C=O(4)), 146.6 (C_{quart}(8a)), 141.2 (C_{quart}(9)), 133.1 (C_{quart}(7)), 128.6 (CH(12)), 128.4 (CH(11 + 13)), 126.8 (CH(10 + 14)), 126.4 (CH(5)), 120.7 (CH(6)), 116.4 (CH(8)), 116.0 (C_{quart}(4a)), 66.4 (CH(2)) ppm; MS: (EI, 70 eV) *m/z* (%) = 259 ([M]⁺, 10), 258 (20), 257 (27), 183 (37), 182 (14), 181 (100), 156 (18), 155 (11), 154 (46), 153 (15), 126 (26), 104 (17), 90 (10), 77 (27), 63 (18), 51 (19).



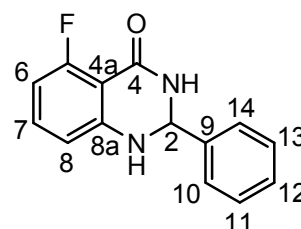
2-Phenyl-6-chloro-2,3-dihydroquinazolin-4(1H)-one

$^1\text{H-NMR}$ (300 MHz, DMSO-*d*₆): δ = 8.49 (*s*, 1H, NH(3)), 7.54 (*d*, 1H, 4J = 2.6 Hz, CH(5)), 7.50 - 7.45 (*m*, 2H, CH(10 + 14)), 7.44 - 7.35 (*m*, 3H, CH(11 + 12 + 13)), 7.34 (*s*, 1H, NH(1)), 7.28 (*dd*, 1H, 3J = 8.7 Hz, 4J = 2.6 Hz, CH(7)), 6.78 (*d*, 1H, 3J = 8.7 Hz, CH(8)), 5.78 (*dd*, 1H, 3J = 1.8 Hz, 3J = 1.8 Hz, CH(2)) ppm; $^{13}\text{C-NMR}$ (75 MHz, DMSO-*d*₆): δ = 162.4 (C=O), 146.6 (C_{quart}(8a)), 141.2 (C_{quart}(9)), 133.1 (C_{quart}(6)), 128.6 (CH(12)), 128.4 (CH(11 + 13)), 126.8 (CH(10 + 14)), 126.4 (CH(5)), 120.7 (CH(7)), 116.4 (CH(8)), 116.0 (C_{quart}(4a)), 66.4 (CH(2)) ppm; MS: (EI, 70 eV) *m/z* (%) = 259 ([M]⁺, 10), 258 (23), 257 (27), 183 (30), 182 (11), 181 (100), 156 (12), 155 (10), 154 (34), 153 (18), 126 (22), 125 (10), 104 (12), 99 (10), 90 (11), 77 (24), 75 (10), 63 (16), 51 (15).



2-Phenyl-5-fluoro-2,3-dihydroquinazolin-4(1H)-one

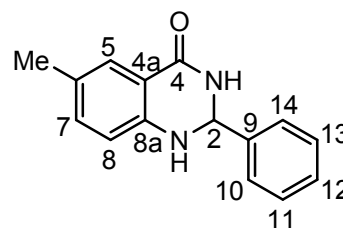
$^1\text{H-NMR}$ (300 MHz, DMSO-*d*₆): δ = 8.33 (*s*, 1H, NH(3)), 7.51 - 7.45 (*m*, 3H, CH(10 + 14) + NH(1)), 7.44 - 7.34 (*m*, 3H, CH(11 + 12 + 13)), 7.21 (*ddd*, 1H, 3J = 8.2 Hz, 3J = 8.2 Hz, 4J = 5.8 Hz, CH(7)), 6.59 (*ddd*, 1H, 3J = 8.2 Hz, 4J = 0.7 Hz, 5J = 0.7 Hz, CH(8)), 6.39 (*ddd*, 1H,



$^3J = 11.5$ Hz, $^3J = 8.1$ Hz, $^4J = 1.0$ Hz, CH(6)), 5.70 (*dd*, 1H, $^3J = 1.9$ Hz, $^3J = 1.9$ Hz, CH(2))) ppm; $^{13}\text{C-NMR}$ (75 MHz, DMSO- d_6): $\delta = 162.3$ (*d*, $^1J = 256.7$ Hz, CF(5)), 160.9 (*d*, $^3J = 2.7$ Hz, C=O(4)), 150.2 (*d*, $^3J = 4.0$ Hz, $\text{C}_{\text{quart}}(8a)$), 141.0 ($\text{C}_{\text{quart}}(9)$), 134.1 (*d*, $^3J = 11.5$ Hz, CH(7)), 128.6 (CH(12)), 128.4 (CH(11 + 13)), 126.9 (CH(10 + 14)), 110.5 (*d*, $^4J = 3.4$ Hz, CH(8)), 104.5 (*d*, $^2J = 21.3$ Hz, CH(6)), 103.83 (*d*, $^2J = 9.3$ Hz, $\text{C}_{\text{quart}}(4a)$), 66.0 (CH(2)) ppm; MS: (EI, 70 eV) m/z (%) = 242 ([M] $^+$, 20), 241 (29), 166 (11), 165 (100), 138 (59), 137 (16), 110 (31), 82 (10), 77 (21), 51 (14).

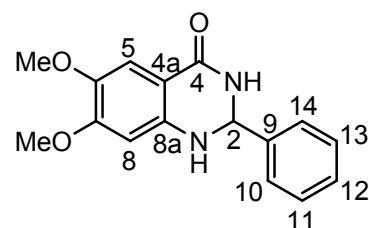
2-Phenyl-6-methyl-2,3-dihydroquinazolin-4(1H)-one

$^1\text{H-NMR}$ (300 MHz, DMSO- d_6): $\delta = 8.24$ (*s*, 1H, NH(3)), 7.51 – 7.46 (*m*, 2H, CH(10 + 14)), 7.44 – 7.26 (*m*, 4H, CH(5 + 11 + 12 + 13)), 7.07 (*dd*, 1H, $^3J = 8.2$ Hz, $^4J = 1.9$ Hz, CH(7)), 6.92 (*s*, 1H, NH(1)), 6.66 (*d*, 1H, $^3J = 8.2$ Hz, CH(8)), 5.70 (*dd*, 1H, $^3J = 1.9$ Hz, CH(2)), 2.18 (*s*, 3H, CH₃) ppm; $^{13}\text{C-NMR}$ (75 MHz, DMSO- d_6): $\delta = 163.7$ (C=O(4)), 145.7 ($\text{C}_{\text{quart}}(8a)$), 141.7 ($\text{C}_{\text{quart}}(9)$), 134.1 ($\text{C}_{\text{quart}}(6)$), 128.4 (CH(12)), 128.3 (CH(11 + 13)), 127.2 (CH(5)), 126.9 (CH(10 + 14)), 125.8 (CH(7)), 115.0 ($\text{C}_{\text{quart}}(4a)$), 114.6 (CH(8)), 66.7 (CH(2)), 20.1 (CH₃) ppm; MS: (EI, 70 eV) m/z (%) = 238 ([M] $^+$, 25), 237 (30), 236 (11), 162 (10), 161 (100), 134 (35), 133 (26), 106 (17), 79 (10), 78 (14), 77 (36), 51 (18).



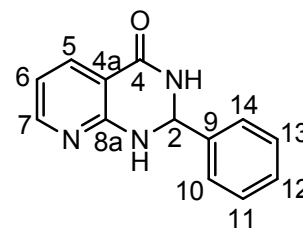
2-Phenyl-6,7-dimethoxy-2,3-dihydroquinazolin-4(1H)-one

$^1\text{H-NMR}$ (400 MHz, DMSO- d_6): $\delta = 8.05$ (*s*, 1H, NH(3)), 7.53 – 7.45 (*m*, 2H, CH(10 + 14)), 7.43 – 7.29 (*m*, 3H, CH(11 + 12 + 13)), 7.11 (*s*, 1H, CH(5)), 6.79 (*s*, 1H, NH(1)), 6.37 (*s*, 1H, CH(8)), 5.68 (*dd*, $^3J = 1.9$ Hz, $^3J = 1.9$ Hz, CH(2)), 3.72 (*s*, 3H, OMe), 3.67 (*s*, 3H, OMe) ppm; $^{13}\text{C-NMR}$ (101 MHz, DMSO- d_6): $\delta = 163.8$ (C=O(4)), 153.9 ($\text{C}_{\text{quart}}(7)$), 143.6 ($\text{C}_{\text{quart}}(8a)$), 141.7 ($\text{C}_{\text{quart}}(9)$), 141.5 ($\text{C}_{\text{quart}}(6)$), 128.4 (CH(12)), 128.2 (CH(11 + 13)), 126.8 (CH(10 + 14)), 109.8 ($\text{C}_{\text{quart}}(4a)$), 106.6 (CH(5)), 97.9 (CH(8)), 66.9 (CH(2)), 55.8 (C(OMe)), 55.4 (C(OMe)) ppm; MS: (EI, 70 eV) m/z (%) = 285 (13), 284 ([M] $^+$, 61), 283 (35), 282 (31), 267 (29), 208 (16), 207 (100), 191 (12), 180 (39), 179 (23), 164 (21), 152 (10), 136 (24), 106 (14), 104 (27), 77 (26), 51 (13).



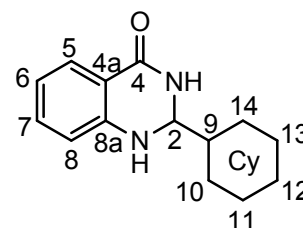
2-Phenyl-2,3-dihydropyrido[2,3-d]pyrimidin-4(1H)-one

$^1\text{H-NMR}$ (300 MHz, DMSO- d_6): $\delta = 8.60$ (*s*, 1H, NH(3)), 8.14 (*dd*, 1H, $^3J = 4.9$ Hz, $^4J = 2.0$ Hz, CH(7)), 8.01 (*s*, 1H, NH(1)), 7.90 (*dd*, 1H, $^3J = 7.5$, $^4J = 2.0$ Hz, CH(5)), 7.62 – 7.14 (*m*, 5H, CH(10 + 11 + 12 + 13 + 14)), 6.70 (*dd*, 1H, $^3J = 7.5$ Hz, $^3J = 4.9$ Hz, CH(6)), 5.83 (*dd*, 1H, $^3J = 2.5$ Hz, $^3J = 2.5$ Hz, CH(2)) ppm; $^{13}\text{C-NMR}$ (75 MHz, DMSO- d_6): $\delta = 162.8$ (C=O(4)), 157.5 ($\text{C}_{\text{quart}}(8a)$), 152.9 (CH(7)), 142.3 ($\text{C}_{\text{quart}}(9)$), 135.7 (CH(5)), 128.4 (CH(12)), 128.3 (CH(11 + 13)), 126.3 (CH(10 + 14)), 113.8 (CH(6)), 109.5 ($\text{C}_{\text{quart}}(4a)$), 65.1 (CH(2)) ppm; MS: (EI, 70 eV) m/z (%) = 225 ([M] $^+$, 14), 224 (26), 148 (100), 121 (27), 93 (28), 77 (17), 51 (14).



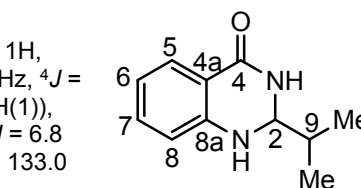
2-Cyclohexyl-2,3-dihydroquinazolin-4(1H)-one

$^1\text{H-NMR}$ (400 MHz, DMSO- d_6): $\delta = 7.87$ (*s*, 1H, NH(3)), 7.55 (*dd*, 1H, $^3J = 7.7$ Hz, $^4J = 1.6$ Hz, CH(5)), 7.23 – 7.16 (*m*, 1H, CH(7)), 6.74 (*dd*, 1H, $^3J = 8.2$ Hz, $^4J = 1.1$ Hz, CH(8)), 6.60 (*ddd*, 1H, $^3J = 7.4$ Hz, $^3J = 7.3$ Hz, $^4J = 1.1$ Hz, CH(6)), 6.55 (*s*, 1H, NH(1)), 4.44 (*ddd*, 1H, $^3J = 4.2$ Hz, $^3J = 1.9$ Hz, $^3J = 1.9$ Hz, CH(2)), 1.77– 1.04 (*m*, 11H, CH₂(Cy)) ppm; $^{13}\text{C-NMR}$ (101 MHz, DMSO- d_6): $\delta = 163.7$ (C=O(4)), 148.3 ($\text{C}_{\text{quart}}(8a)$), 133.0 (CH(7)), 127.2 (CH(5)), 116.4 (CH(6)), 114.8 ($\text{C}_{\text{quart}}(4a)$), 114.1 (CH(8)), 68.6 (CH(2)), 42.9 (CH₂(Cy)), 27.0 (CH₂(Cy)), 26.7 (CH₂(Cy)), 25.9 (CH₂(Cy)), 25.6 (CH₂(Cy)), 25.6 (CH₂(Cy)) ppm; MS: (EI, 70 eV) m/z (%) = 148 (10), 147 (100), 92 (10).

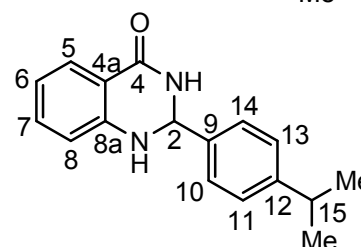


2-Isopropyl-2,3-dihydroquinazolin-4(1H)-one

$^1\text{H-NMR}$ (400 MHz, DMSO- d_6): $\delta = 7.86$ (*s*, 1H, NH(3)), 7.57 (*dd*, $^3J = 7.8$ Hz, $^4J = 1.6$ Hz, 1H, CH(5)), 7.20 (*ddd*, 1H, $^3J = 8.5$ Hz, $^3J = 7.2$ Hz, $^4J = 1.7$ Hz, CH(7)), 6.75 (*dd*, 1H, $^3J = 8.2$ Hz, $^4J = 1.0$ Hz, CH(8)), 6.62 (*ddd*, 1H, $^3J = 7.5$ Hz, $^3J = 7.4$ Hz, $^4J = 1.1$ Hz, CH(6)), 6.51 (*s*, 1H, NH(1)), 4.54 – 4.49 (*m*, 1H, CH(2)), 1.86 (*m*, 1H, CH(9)), 0.94 (*d*, $^3J = 6.9$ Hz, 3H, CH₃), 0.92 (*d*, $^3J = 6.8$ Hz, 3H, CH₃) ppm; $^{13}\text{C-NMR}$ (101 MHz, DMSO- d_6): $\delta = 163.9$ (C=O(4)), 148.5 ($\text{C}_{\text{quart}}(8a)$), 133.0 (CH(7)), 127.2 (CH(5)), 116.5 (CH(6)), 114.7 ($\text{C}_{\text{quart}}(4a)$), 114.1 (CH(8)), 69.2 (CH(2)), 32.7 (CH(9)), 16.9 (CH₃), 16.6 (CH₃) ppm; MS: (EI, 70 eV) m/z (%) = 147 (100), 92 (11), 65 (8).



2-(4-Isopropylphenyl)-2,3-dihydroquinazolin-4(1H)-one



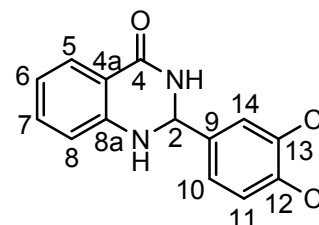
¹H-NMR (400 MHz, DMSO-*d*₆): δ = 8.21 (s, 1H, NH(3)), 7.61 (*dd*, 1H, ³*J* = 7.8 Hz, ⁴*J* = 1.6 Hz, 1H, CH(5)), 7.46 – 7.37 (*m*, 2H, CH(10 + 14)), 7.32 – 7.18 (*m*, 3H, CH(11 + 13 + 7)), 7.05 (s, 1H, NH(1)), 6.79 – 6.70 (*m*, 1H, CH(8)), 6.71 – 6.63 (*m*, 1H, CH(6)), 5.76 – 5.67 (*m*, 1H, CH(2)), 2.88 (*h*, 1H, ³*J* = 6.9 Hz, CH(15)), 1.19 (*d*, 6H, ³*J* = 6.9 Hz, CH₃) ppm; ¹³C-NMR (75 MHz, DMSO-*d*₆): δ = 163.7 (C=O(7)), 148.8 (C_{quart}(12)), 148.0 (C_{quart}(9)), 139.0 (C_{quart}(8a)), 133.3 (CH(7)), 127.4 (CH(5)), 127.0 (CH(11 + 13)), 126.3 (CH(10 + 14)), 117.1 (CH(6)), 115.0 (C_{quart}(4a)), 114.4 (CH(8)), 66.6 (CH(2)), 33.26 (CH(15)), 23.9 (CH₃) ppm; MS: (EI, 70 eV) *m/z* (%) = 266 ([M]⁺, 28), 265 (53), 249 (13), 148 (12), 147 (100), 120 (46), 119 (13), 92 (27), 91 (10), 77 (12), 65 (12).

Crystal data and structure refinement for 2-(4-isopropylphenyl)-2,3-dihydroquinazolin-4(1*H*)-one

Empirical formula	C ₁₇ H ₁₈ N ₂ O
Formula weight	266.33
Temperature	150(2) K
Wavelength	1.54178 Å
Crystal system	monoclinic
Space group (H.M.)	<i>P</i> 2 ₁ / <i>c</i>
Unit cell dimensions	<i>a</i> = 13.7868(3) Å α = 90.00° <i>b</i> = 9.5016(2) Å β = 104.522(1)° <i>c</i> = 10.9971(3) Å γ = 90.00°
Volume	1394.56(6) Å ³
Z	4
Density (calculated)	1.269 Mg/m ³
Absorption coefficient	0.628 mm ⁻¹
F(000)	568
Crystal size	0.44 x 0.42 x 0.08 mm ³
θ range for data collection	3.31 to 63.68°
Index ranges	-16 ≤ <i>h</i> ≤ 14, -6 ≤ <i>k</i> ≤ 11, -12 ≤ <i>l</i> ≤ 12
Reflections collected	9161
Independent reflections	2282 [R(int) = 0.0225]
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.000 and 0.903
Refinement method	Full-matrix least squares on F ²
Data / restraints / parameters	2282 / 0 / 191
Goodness-of-fit on F ²	1.042
Final R indices [I > 2σ(I)]	R1 = 0.0329, wR2 = 0.0857
R indices (all data)	R1 = 0.0349, wR2 = 0.0878

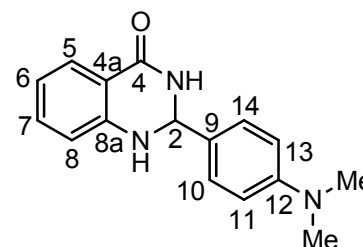
2-(3,4-Dichlorophenyl)-2,3-dihydroquinazolin-4(1*H*)-one

¹H-NMR (400 MHz, DMSO-*d*₆): δ = 8.42 (s, 1H, NH(3)), 7.72 (*d*, 1H, ⁴*J* = 2.0 Hz, CH(14)), 7.66 (*d*, 1H, ³*J* = 8.3 Hz, CH(11)), 7.61 (*dd*, 1H, ³*J* = 7.7 Hz, ⁴*J* = 1.6 Hz, CH(5)), 7.47 (*dd*, 1H, ³*J* = 8.3 Hz, ⁴*J* = 2.1 Hz, CH(7)), 7.29 – 7.22 (*m*, 2H, NH(1) + CH(10)), 6.79 – 6.74 (*m*, 1H, CH(8)), 6.72 – 6.65 (*m*, 1H, CH(6)), 5.80 (*dd*, 1H, ³*J* = 2.3 Hz, ³*J* = 2.3 Hz, CH(2)) ppm; ¹³C-NMR (101 MHz, DMSO-*d*₆): δ = 163.4 (C=O(4)), 147.3 C_{quart}(8a), 143.0 (C_{quart}(9)), 133.5 (CH(7)), 130.9 (C_{quart}(13)), 130.8 (C_{quart}(12)), 130.6 (CH(11)), 128.9 (CH(5)), 127.4 (CH(14)), 127.0 (CH(10)), 117.5 (CH(6)), 114.9 (C_{quart}(4a)), 114.5 (CH(8)), 65.0 (CH(2)) ppm; MS: (EI, 70 eV) *m/z* (%) = 294 (10), 293 (12), 292 ([M]⁺, 15), 291 (16), 148 (10), 147 (100), 120 (44), 119 (21), 92 (30), 65 (12).



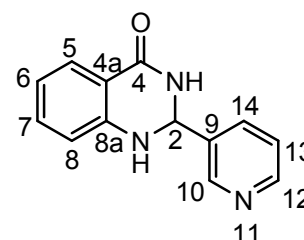
2-(4-(Dimethylamino)phenyl)-2,3-dihydroquinazolin-4(1*H*)-one

¹H-NMR (400 MHz, DMSO-*d*₆): δ = 8.07 (s, 1H, NH(3)), 7.61 (*dd*, ³*J* = 7.7 Hz, ⁴*J* = 1.6 Hz, 1H, CH(5)), 7.33 – 7.27 (*m*, 2H, CH(10 + 14)), 7.22 (*ddd*, 1H, ³*J* = 7.9 Hz, ³*J* = 7.1 Hz, ⁴*J* = 1.6 Hz, CH(7)), 6.91 (s, 1H, NH(1)), 6.75 – 6.69 (*m*, 3H, CH(8 + 11 + 13)), 6.69 – 6.63 (*m*, 1H, CH(6)), 5.65 – 5.62 (*m*, 1H, CH(2)), 3.34 (s, 6H, CH₃) ppm; ¹³C-NMR (101 MHz, DMSO-*d*₆): δ = 163.8 (C=O(4)), 150.7 (C_{quart}(9)), 148.2 (C_{quart}(8a)), 133.1 (CH(7)), 128.7 (CH(5)), 127.7 (C_{quart}(12)), 127.3 (CH(10 + 14)), 116.9 (CH(6)), 115.0 (C_{quart}(4a)), 114.4 (CH(8)), 111.9 (CH(11 + 13)), 66.6 (CH(2)), 40.16 (CH₃) ppm; MS: (EI, 70 eV) *m/z* (%) = 266 ([M-H]⁺, 18), 265 (100), 264 (45), 146 (21), 145 (18), 119 (18).



2-(Pyridin-3-yl)-2,3-dihydroquinazolin-4(1*H*)-one

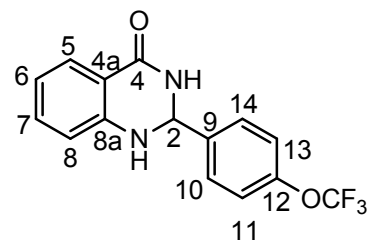
¹H-NMR (300 MHz, DMSO-*d*₆): δ = 8.66 (*d*, 1H, ⁴*J* = 2.3 Hz, CH(10)), 8.55 (*dd*, ³*J* = 4.8 Hz, ⁴*J* = 1.7 Hz, CH(12)), 8.40 (s, 1H, NH(3)), 7.89 (*dd*, ³*J* = 8.0 Hz, ⁴*J* = 2.0 Hz, CH(14)), 7.63 (*dd*, 1H, ³*J* = 7.8 Hz, ⁴*J* = 1.6 Hz, CH(5)), 7.43 (*ddd*, 1H, ³*J* = 8.0 Hz, ³*J* = 4.8 Hz, ⁴*J* = 0.9 Hz, CH(13)), 7.27 (*ddd*, 1H, ³*J* = 8.5 Hz, ³*J* = 7.2 Hz, ⁴*J* = 1.6 Hz, CH(7)), 7.18 (s, 1H,



NH(1)), 6.84 – 6.66 (*m*, 2H, CH(8 + 6)), 5.85 (*dd*, 1H, $^3J = 1.8$ Hz, $^3J = 1.8$ Hz, CH(2)) ppm; $^{13}\text{C-NMR}$ (101 MHz, DMSO- d_6): $\delta = 163.6$ (C=O(4)), 149.7 (CH(10), 148.4 (CH(12)), 147.7 (C_{quart} (8a)), 136.8 CH(14)), 134.7 (C_{quart} (9)), 133.6 (CH(7)), 127.4 (CH(5)), 123.6 (CH(13)), 117.6 (CH(6)), 115.0 (C_{quart} (4a)), 114.6 (CH(4)), 64.7 (CH(2)) ppm; MS: (EI, 70 eV) *m/z* (%) = 225 ($[\text{M}]^+$, 15), 242 (12), 148 (11), 147 (100), 120 (35), 119 (19), 92 (31), 65 (14), 64 (11), 63 (11), 51 (18).

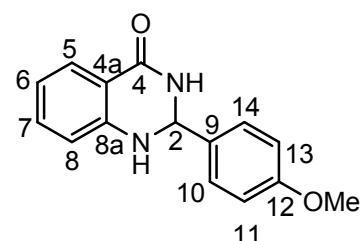
2-(4-(Trifluoromethoxy)phenyl)-2,3-dihydroquinazolin-4(1H)-one

$^1\text{H-NMR}$ (300 MHz, DMSO- d_6): $\delta = 8.37$ (*s*, 1H, NH(3)), 7.68 – 7.60 (*m*, 3H, CH(5 + 10 + 14)), 7.40 (*ddd*, 2H, $^3J = 7.8$ Hz, $^3J = 2.1$ Hz, $^5J = 1.1$ Hz, CH(11 + 13)), 7.26 (*ddd*, 1H, $^3J = 8.1$ Hz, $^3J = 7.2$ Hz, $^4J = 1.6$ Hz, CH(7)), 7.18 (*s*, 1H, NH(1)), 6.77 (*dd*, 1H, $^3J = 8.2$ Hz, $^4J = 1.0$ Hz, CH(8)), 6.74 – 6.66 (*m*, 1H, CH(6)), 5.83 (*dd*, 1H, $^3J = 1.9$ Hz, $^3J = 1.9$ Hz, CH(2)) ppm; $^{13}\text{C-NMR}$ (75 MHz, DMSO- d_6): $\delta = 163.6$ (C=O(4)), 148.4 (*d*, $^3J = 1.7$ Hz, C_{quart} (12)), 147.7 (C_{quart} (8a)), 141.0 (C_{quart} (9)), 133.5 (CH(7)), 129.0 (CH(10 + 14)), 127.4 (CH(5)), 121.02 (CH(11 + 13)), 120.11 (*q*, $^1J = 256.3$ Hz, OCF_3), 117.4 (CH(6)), 114.9 (C_{quart} (4a)), 114.5 (CH(8)), 65.9 (CH(2)) ppm; $^{19}\text{F-NMR}$ (282 MHz, DMSO- d_6): $\delta = -56.47$ (*s*, OCF_3) ppm; MS: (EI, 70 eV) *m/z* (%) = 308 ($[\text{M}]^+$, 32), 307 (45), 188 (10), 148 (10), 147 (100), 120 (63), 119 (27), 95 (10), 92 (44), 91 (10), 69 (24), 65 (20), 64 (16), 63 (15).



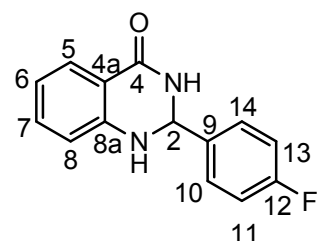
2-(4-Methoxyphenyl)-2,3-dihydroquinazolin-4(1H)-one

$^1\text{H-NMR}$ (300 MHz, DMSO- d_6): $\delta = 8.21$ (*s*, 1H, NH(3)), 7.62 (*dd*, 1H, $^3J = 7.8$ Hz, $^4J = 1.6$ Hz, CH(5)), 7.48 – 7.38 (*m*, 2H, CH(10 + 14)), 7.24 (*ddd*, 1H, $^3J = 8.1$ Hz, $^3J = 7.2$ Hz, $^4J = 1.6$ Hz, CH(7)), 7.05 (*s*, 1H, NH(1)), 6.99 – 6.90 (*m*, 2H, CH(11 + 13)), 6.75 (*ddd*, 1H, $^3J = 8.2$ Hz, $^4J = 1.1$, $^5J = 0.5$ Hz, CH(8)), 6.68 (*ddd*, 1H, $^3J = 7.7$ Hz, $^3J = 7.2$ Hz, $^4J = 1.1$ Hz, CH(6)), 5.72 (*dd*, 1H, $^3J = 1.7$ Hz, $^3J = 1.7$ Hz, CH(2)), 3.74 (*s*, 3H, CH₃) ppm; $^{13}\text{C-NMR}$ (101 MHz, DMSO- d_6): $\delta = 163.7$ (C=O(4)), 159.4 (C_{quart} (12)), 148.0 (C_{quart} (8a)), 133.5 (CH(7)), 133.3 (C_{quart} (9)), 128.2 (CH(10 + 14)), 127.4 (CH(5)), 117.1 (CH(6)), 115.0 (C_{quart} (4a)), 114.4 (CH(8)), 113.6 (CH(11 + 13)), 66.3 (CH(2)), 55.2 (OMe) ppm; MS: (EI, 70 eV) *m/z* (%) = 254 ($[\text{M}]^+$, 50), 253 (100), 252 (16), 147 (70), 134 (13), 120 (75), 119 (31), 92 (49), 91 (17), 77 (16), 65 (21), 64 (20), 63 (17).



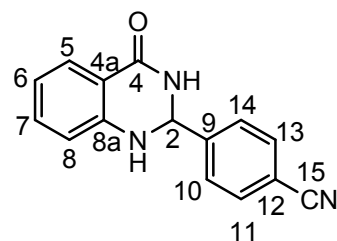
2-(4-Fluorophenyl)-2,3-dihydroquinazolin-4(1H)-one

$^1\text{H-NMR}$ (400 MHz, DMSO- d_6): $\delta = 8.31$ (*s*, 1H, NH(3)), 7.63 (*dd*, 1H, $^3J = 7.8$ Hz, $^4J = 1.6$ Hz, CH(5)), 7.59 – 7.52 (*m*, 2H, CH(10 + 14)), 7.30 – 7.18 (*m*, 3H, CH(7 + 11 + 13)), 7.12 (*s*, 1H, NH(1)), 6.77 (*dd*, 1H, $^3J = 8.2$ Hz, $^4J = 1.0$ Hz, CH(8)), 6.69 (*ddd*, 1H, $^3J = 7.5$ Hz, $^3J = 7.4$ Hz, $^4J = 1.0$ Hz, CH(6)), 5.79 (*dd*, 1H, $^3J = 1.7$ Hz, $^3J = 1.7$ Hz, CH(2)) ppm; $^{13}\text{C-NMR}$ (101 MHz, DMSO- d_6): $\delta = 163.6$ (C=O(4)), 162.1 (*d*, $^1J = 244.1$ Hz, C_{quart} (12)), 147.8 (C_{quart} (8a)), 137.8 (*d*, $^4J = 2.9$ Hz, C_{quart} (9)), 133.4 (CH(7)), 129.1 (*d*, $^3J = 8.3$ Hz, CH(10 + 14)), 127.4 (CH(5)), 117.3 (CH(6)), 115.1 (*d*, $^2J = 21.5$ Hz, CH(11 + 13)), 115.0 (C_{quart} (4a)), 114.5 (CH(8)), 66.0 (CH(2)) ppm; $^{19}\text{F-NMR}$ (282 MHz, DMSO- d_6): $\delta = -112.44$ – -114.78 (*m*, CF) ppm; MS: (EI, 70 eV) *m/z* (%) = 242 ($[\text{M}]^+$, 32), 241 (45), 148 (10), 147 (100), 122 (11), 120 (76), 119 (23), 95 (12), 92 (40), 65 (17), 64 (11).



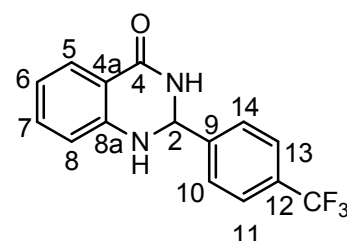
2-(4-cyanophenyl)-2,3-dihydroquinazolin-4(1H)-one

$^1\text{H-NMR}$ (300 MHz, DMSO- d_6): $\delta = 8.49$ – 8.44 (*m*, 1H, NH(3)), 7.90 – 7.82 (*m*, 2H,), 7.68 – 7.63 (*m*, 2H), 7.60 (*dd*, 1H, $^3J = 7.7$ Hz, $^4J = 1.6$ Hz, CH(5)), 7.33 – 7.20 (*m*, 2H, CH(7) + NH(1)), 6.75 (*dd*, 1H, $^3J = 8.1$ Hz, $^4J = 1.1$ Hz, CH(8)), 6.68 (*ddd*, 1H, $^3J = 7.5$ Hz, $^3J = 7.5$ Hz, $^4J = 1.1$ Hz, CH(6)), 5.84 (*dd*, 1H, $^3J = 2.4$ Hz, $^3J = 2.4$ Hz, CH(2)); $^{13}\text{C-NMR}$ (75 MHz, DMSO): $\delta = 163.3$ (C=O(4)), 147.4 (C_{quart} (9)), 147.3 (C_{quart} (8a)), 133.6 (CH(7)), 132.4 (CH(10 + 14)), 127.7 (11 + 13), 127.4 (CH(5)), 118.7 (CN(15)), 117.4 (CH(6)), 114.9 (C_{quart} (4a)), 114.5 (CH(8)), 111.1 (C_{quart} (12)), 65.5 (CH(2)); MS: (EI, 70 eV) *m/z* (%) = 249 ($[\text{M}]^+$, 18), 248 (18), 148 (10), 147 (100), 120 (40), 119 (20), 102 (10), 92 (25), 65 (10).



2-(4-(Trifluoromethyl)phenyl)-2,3-dihydroquinazolin-4(1H)-one

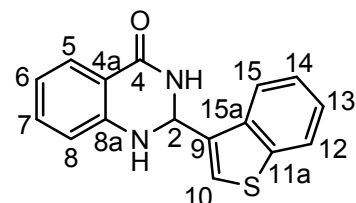
$^1\text{H-NMR}$ (400 MHz, DMSO- d_6): $\delta = 8.44$ (*m*, 1H, NH(3)), 7.77 (*d*, 2H, $^3J = 8.3$ Hz, CH(11 + 13)), 7.71 (*d*, 1H, $^3J = 8.2$ Hz, CH(10 + 14)), 7.62 (*dd*, 1H, $^3J = 7.8$ Hz, $^4J = 1.6$ Hz, CH(5)), 7.31 – 7.20 (*m*, 2H, CH(7) + NH(1)), 6.76 (*dd*, 1H, $^3J = 8.2$ Hz, $^4J = 1.0$ Hz, CH(8)), 6.69 (*ddd*, 1H, $^3J = 8.1$ Hz, $^3J = 7.3$ Hz, $^4J = 1.1$ Hz, CH(6)), 5.87 (*dd*, 1H, $^3J = 2.2$ Hz, $^3J = 2.2$ Hz, CH(2)) ppm; $^{13}\text{C-NMR}$ (101 MHz, DMSO- d_6): $\delta = 163.4$ (C=O(4)), 147.5 (C_{quart} (8a)), 146.4 (C_{quart} (9)), 133.5 (CH(7)), 128.9 (*q*, $^2J = 31.6$ Hz, CH(12)), 127.7 (CH(10 + 14)), 127.4 (CH(5)), 125.31 (*q*, $^3J = 3.7$ Hz, CH(11 + 13)), 124.16 (*q*, $^1J = 272.2$



Hz, CF₃), 117.4 (CH(6)), 114.9 (CH(4a)), 114.5 (CH(8)), 65.7 (CH(2)) ppm; ¹⁹F-NMR (282 MHz, DMSO-*d*₆): δ = -60.59 (CF₃) ppm; MS: (EI, 70 eV) *m/z* (%) = 292 ([M]⁺, 23), 291 (24), 148 (10), 147 (100), 120 (43), 119 (20), 92 (27), 65 (10).

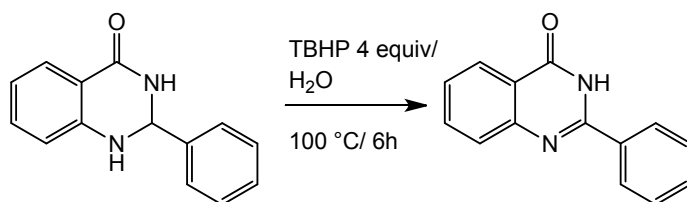
2-(Benzo[*b*]thiophen-3-yl)-2,3-dihydroquinazolin-4(1*H*)-one

¹H-NMR (400 MHz, DMSO-*d*₆): δ = 8.35 (s, 1H, NH(3)), 8.21 – 8.14 (*m*, 1H, CH(12)), 8.05 – 7.96 (*m*, 1H, CH(15)), 7.77 (s, 1H, CH(10)), 7.67 (*dd*, 1H, ³*J* = 7.8 Hz, ⁴*J* = 1.6 Hz, (CH(5))), 7.46 – 7.36 (*m*, 2H, CH(13 + 14)), 7.26 (*ddd*, 1H, ³*J* = 8.3 Hz, ³*J* = 7.2 Hz, ⁴*J* = 1.6 Hz, (CH(7))), 7.14 (s, 1H, NH(1)), 6.77 (*dd*, 1H, ³*J* = 8.2 Hz, ⁴*J* = 1.0 Hz, CH(8)), 6.72 (*ddd*, 1H, ³*J* = 7.5 Hz, ⁴*J* = 1.0 Hz, CH(6)), 6.20 (*dd*, 1H, ³*J* = 1.5 Hz, CH(2)) ppm; ¹³C-NMR (101 MHz, DMSO): δ = 163.9 (C=O), 148.1 (C_{quart}(8a)), 140.3 (C_{quart}(9)), 136.8 (C_{quart}(11a)), 135.4 (C_{quart}(15a)), 133.3 (CH(7)), 127.5 (CH(5)), 126.6 (CH(13)), 124.6 (CH(14)), 124.0 CH(15), 123.5 (CH(10)), 123.0 (CH(12)), 117.3 CH(6), 115.1 (C_{quart}(4a)), 114.5 (CH(8)), 62.6 (CH(2)) ppm; MS: (EI, 70 eV) *m/z* (%) = 281 (16), 280 ([M]⁺, 74), 279 (100), 160 (16), 147 (51), 134 (17), 120 (94), 119 (20), 92 (39), 89 (20), 95 (15), 63 (10).

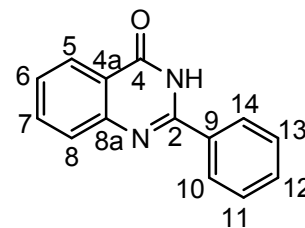


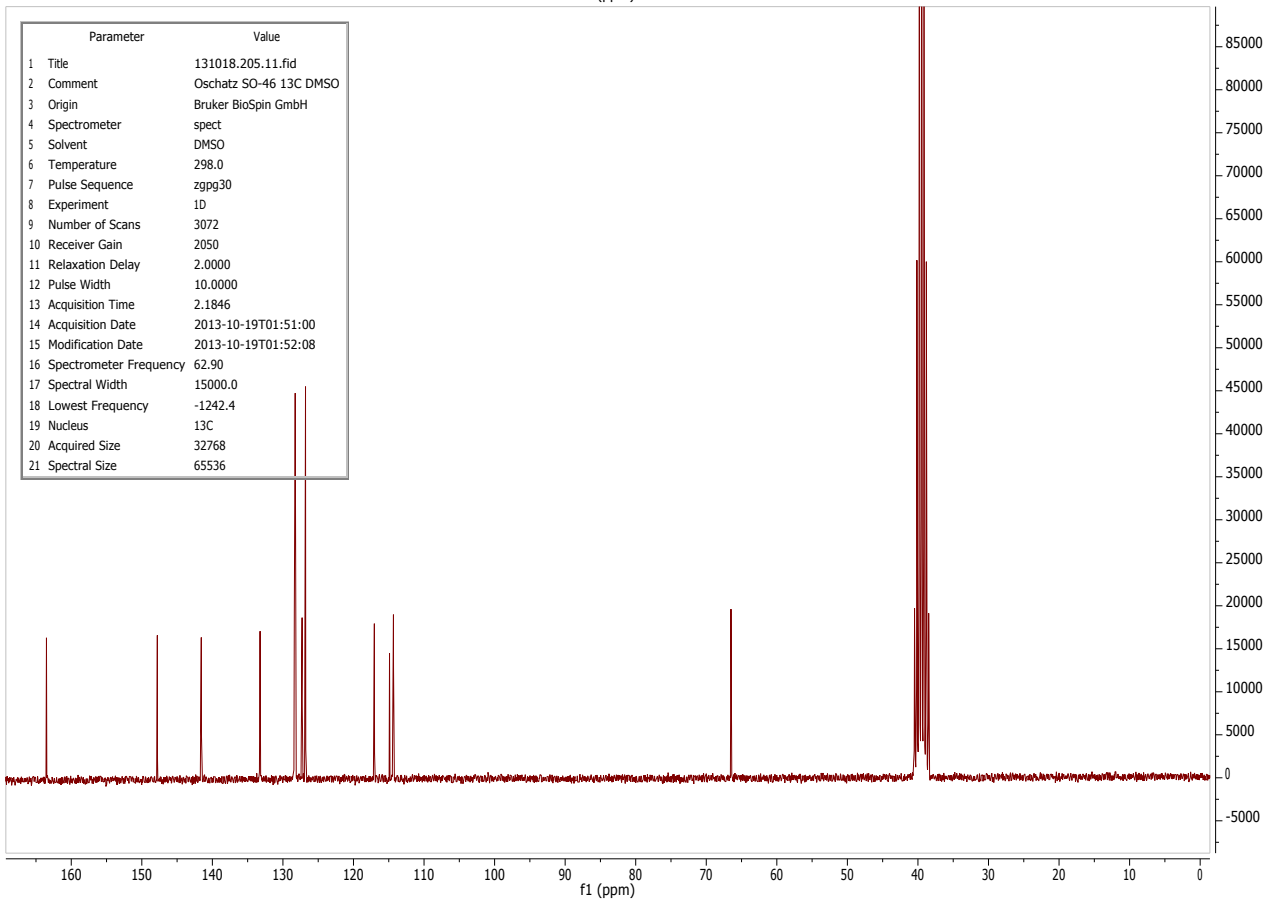
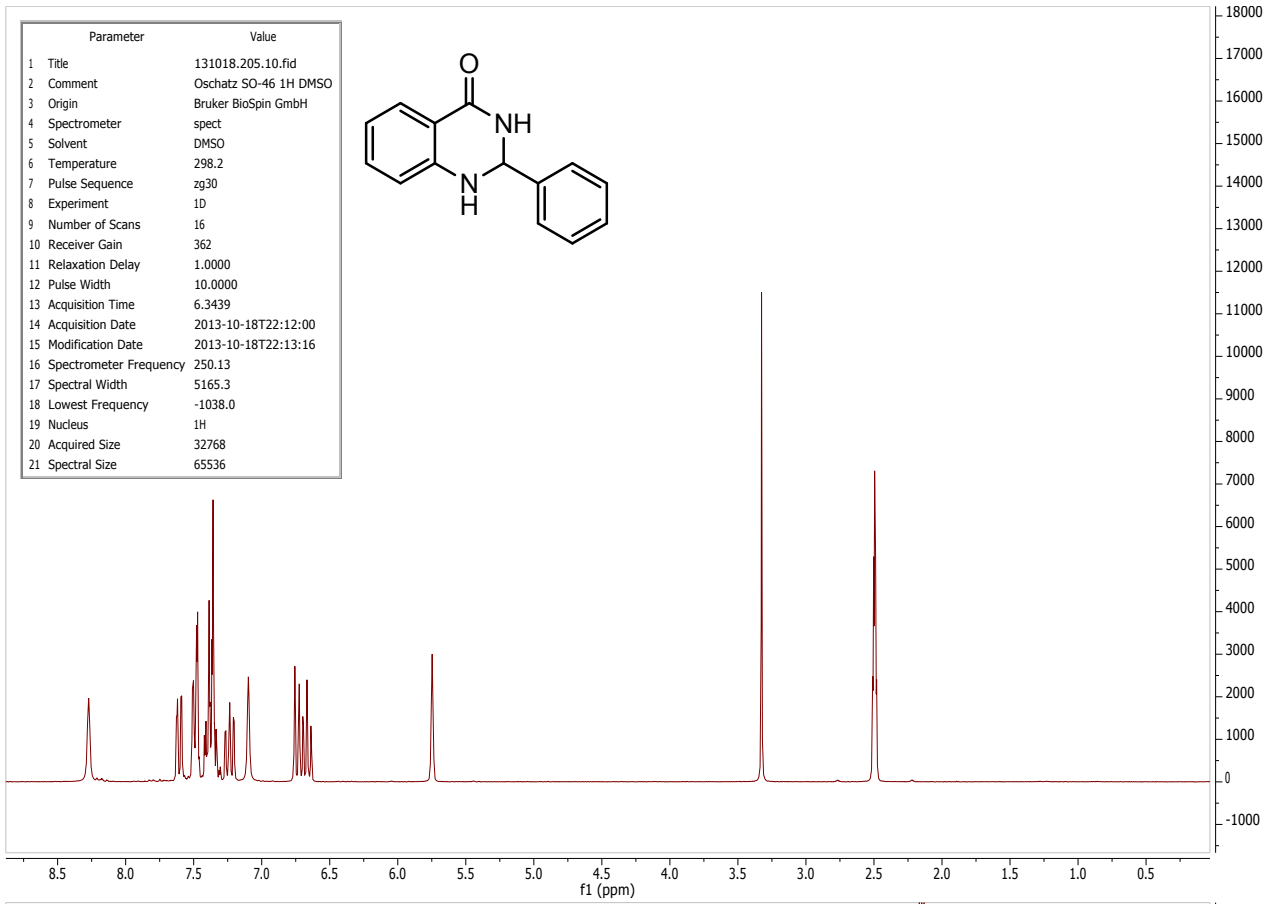
2-phenyl-quinazolinone

Experimental procedure:

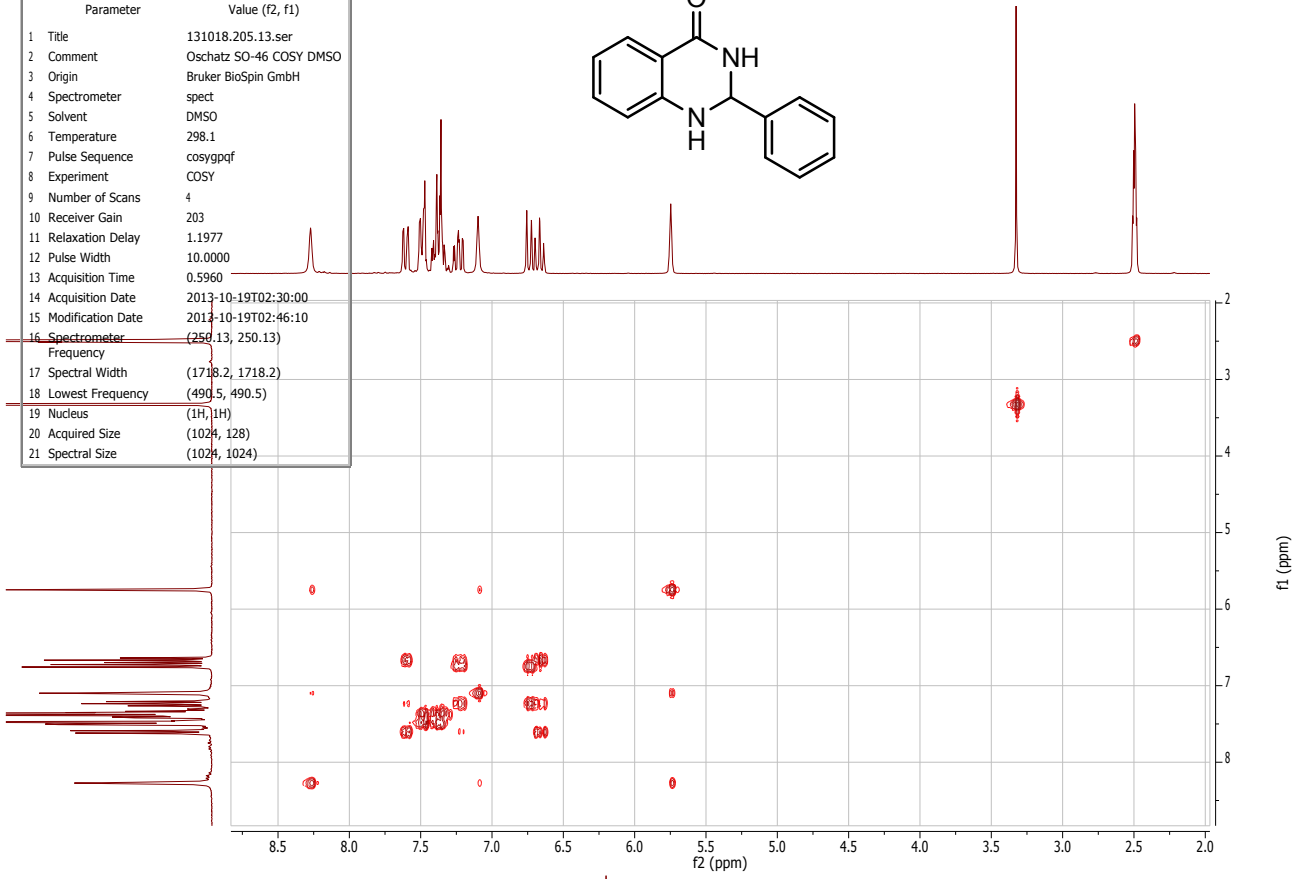
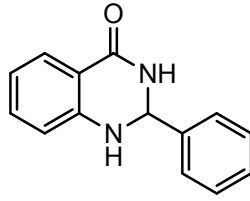


¹H-NMR (300 MHz, DMSO-*d*₆): δ = 12.55 (s, 1H, NH), 8.23 – 8.13 (*m*, 3H, CH(7 + 10 + 14)), 7.85 (*ddd*, ³*J* = 8.5 Hz, ³*J* = 7.0 Hz, ³*J* = 1.6 Hz, CH(5)), 7.77 – 7.71 (*m*, 1H, CH(12)), 7.62 – 7.49 (*m*, 4H, CH(4 + 6 + 11 + 13)) ppm; ¹³C-NMR (75 MHz, DMSO-*d*₆): δ = 162.3 (C=O(4)), 152.4 (C_{quart}(2)), 148.7 (C_{quart}(8a)), 134.6 (CH(7)), 132.8 (C_{quart}(9)), 131.4 (CH(12)), 128.6 (CH(10 + 14)), 127.8 (CH(11 + 13)), 127.4 CH(6), 126.6 (CH(7)), 125.8 (CH(5)), 121.0 (C_{quart}(4a)) ppm; MS (EI, 70 eV): *m/z* (%) = 222 ([M]⁺, 100), 119 (99), 104 (11), 92 (14), 90 (17), 77 (22), 76 (11), 51 (10).

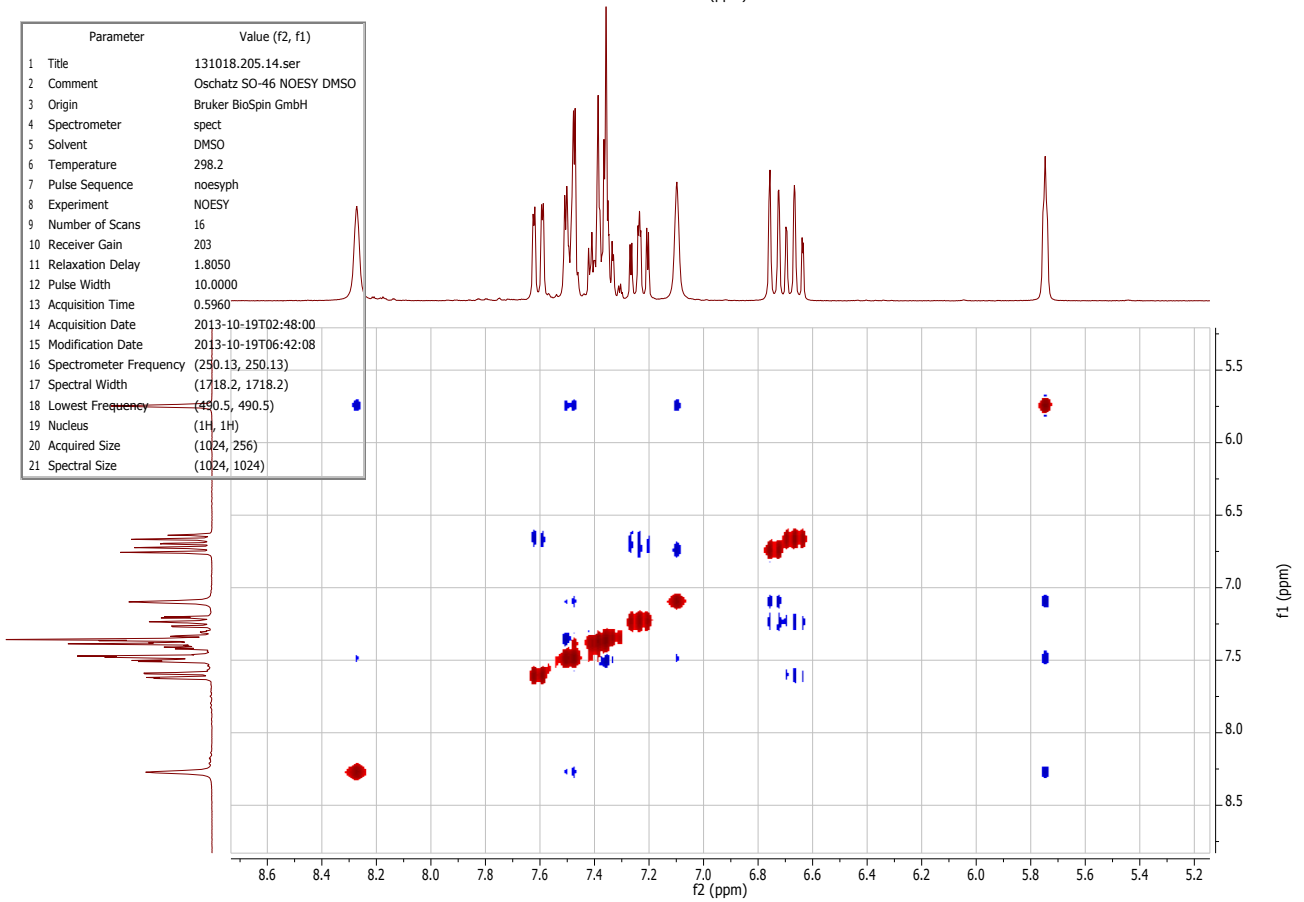




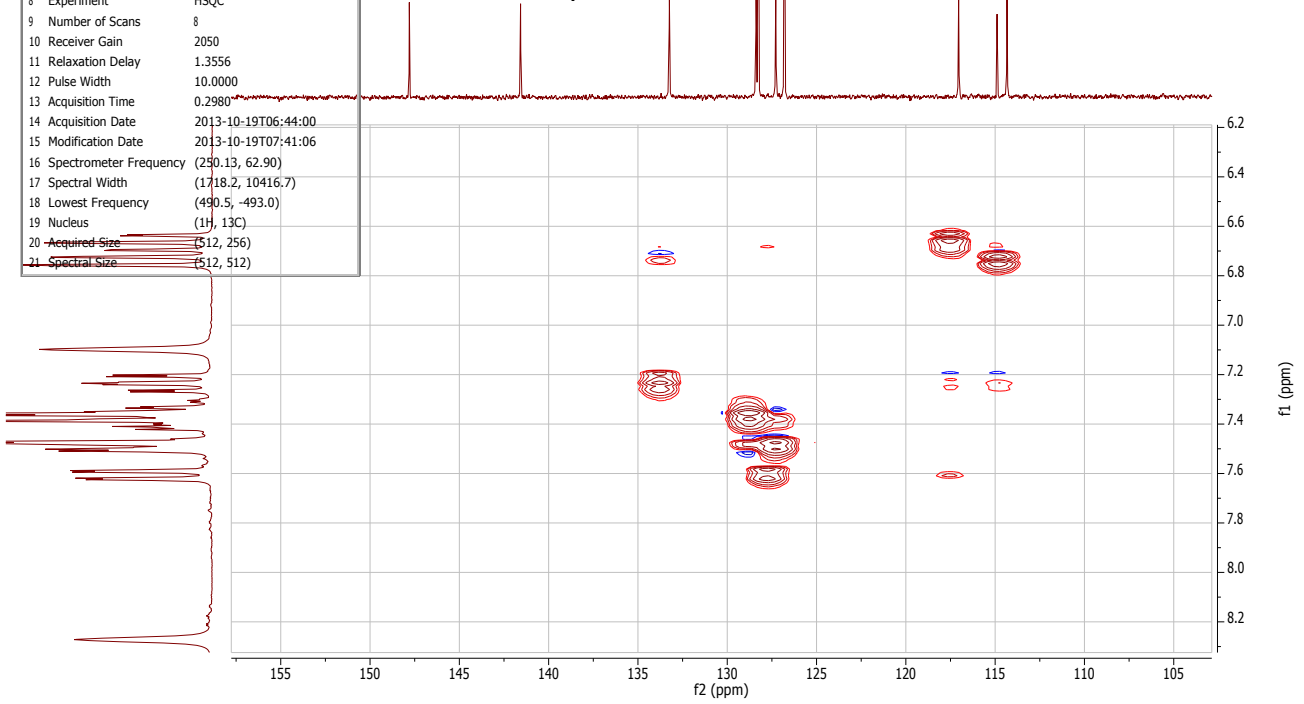
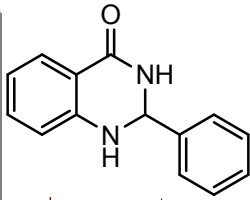
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1 Title	131018.205.13.ser
2 Comment	Oschatz SO-46 COSY DMSO
3 Origin	Bruker BioSpin GmbH
4 Spectrometer	spect
5 Solvent	DMSO
6 Temperature	298.1
7 Pulse Sequence	cosyppqf
8 Experiment	COSY
9 Number of Scans	4
10 Receiver Gain	203
11 Relaxation Delay	1.1977
12 Pulse Width	10.0000
13 Acquisition Time	0.5960
14 Acquisition Date	2013-10-19T02:30:00
15 Modification Date	2013-10-19T02:46:10
16 Spectrometer Frequency	(250.13, 250.13)
17 Spectral Width	(1718.2, 1718.2)
18 Lowest Frequency	(490.5, 490.5)
19 Nucleus	(1H, 1H)
20 Acquired Size	(1024, 128)
21 Spectral Size	(1024, 1024)



Parameter	Value (f2, f1)
1 Title	131018.205.14.ser
2 Comment	Oschatz SO-46 NOESY DMSO
3 Origin	Bruker BioSpin GmbH
4 Spectrometer	spect
5 Solvent	DMSO
6 Temperature	298.2
7 Pulse Sequence	noesyph
8 Experiment	NOESY
9 Number of Scans	16
10 Receiver Gain	203
11 Relaxation Delay	1.8050
12 Pulse Width	10.0000
13 Acquisition Time	0.5960
14 Acquisition Date	2013-10-19T02:48:00
15 Modification Date	2013-10-19T06:42:08
16 Spectrometer Frequency	(250.13, 250.13)
17 Spectral Width	(1718.2, 1718.2)
18 Lowest Frequency	(490.5, 490.5)
19 Nucleus	(1H, 1H)
20 Acquired Size	(1024, 256)
21 Spectral Size	(1024, 1024)



Parameter	Value (f2, f1)
1 Title	131018.205.15.ser
2 Comment	Oschatz SO-46 HSQC DMSO
3 Origin	Bruker BioSpin GmbH
4 Spectrometer	spect
5 Solvent	DMSO
6 Temperature	298.2
7 Pulse Sequence	hsqcetpsi2
8 Experiment	HSQC
9 Number of Scans	8
10 Receiver Gain	2050
11 Relaxation Delay	1.3556
12 Pulse Width	10.0000
13 Acquisition Time	0.2980
14 Acquisition Date	2013-10-19T06:44:00
15 Modification Date	2013-10-19T07:41:06
16 Spectrometer Frequency	(250.13, 62.90)
17 Spectral Width	(1718.2, 10416.7)
18 Lowest Frequency	(490.5, -493.0)
19 Nucleus	(1H, 13C)
20 Acquired Size	(512, 256)
21 Spectral Size	(512, 512)



Parameter	Value (f2, f1)
1 Title	131018.205.16.ser
2 Comment	Oschatz SO-46 HMBC DMSO
3 Origin	Bruker BioSpin GmbH
4 Spectrometer	spect
5 Solvent	DMSO
6 Temperature	298.2
7 Pulse Sequence	hmbcgpndf
8 Experiment	HMBC
9 Number of Scans	64
10 Receiver Gain	2050
11 Relaxation Delay	0.9225
12 Pulse Width	10.0000
13 Acquisition Time	1.1920
14 Acquisition Date	2013-10-19T07:45:00
15 Modification Date	2013-10-19T12:41:40
16 Spectrometer Frequency	(250.13, 62.90)
17 Spectral Width	(1718.2, 13966.5)
18 Lowest Frequency	(490.5, -704.2)
19 Nucleus	(1H, 13C)
20 Acquired Size	(2048, 128)
21 Spectral Size	(2048, 512)

