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Supporting information 1

Long-chained 4-Aminoquinolines as Quorum Sensing Inhibitors in *Serratia marcescens* and *Pseudomonas aeruginosa*

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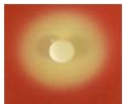
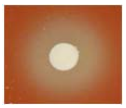
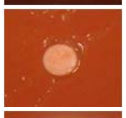
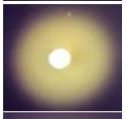
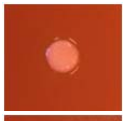
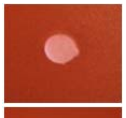
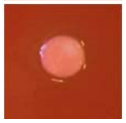
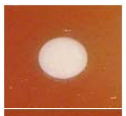
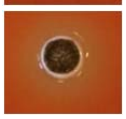
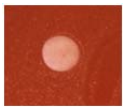
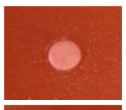
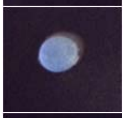
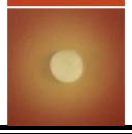
Table 1S. Inhibition of prodigiosin and violacein production in the presence of tested compounds

Compound*	Zones of inhibition (mm)			
	Prodigiosin		Violacein	
1	20±2		20±2	
2	14±2		20±2	
3	14±1		20±2	
4	14±1		26±2	
5	n.a.		24±2	
6	10±1		9±1	
7	n.a.		n.a.	
8	n.a.		20±2	
9	12±1		24±2	
10	n.a.		12±1	
11	16±2		20±1	
12	22±2		30±2	
13	n.a.		9±1	
14	n.a.		30±3	
15	n.a.		14±1	

16	n.a.		16±1	
17	n.a.		n.a.	
18	n.a.		10±1	
19	28±2		36±3	
20	28±2		32±3	
21	n.a.		n.a.	
22	8±1		20±1	
23	n.a.		n.a.	
24	n.a.		n.a.	
25	n.a.		n.a.	
26	n.a.		n.a.	
27	14±1		n.a.	

* Inhibition of pigment production was determined in the presence of 250 µg of tested compound per disk; n.a. – not active;

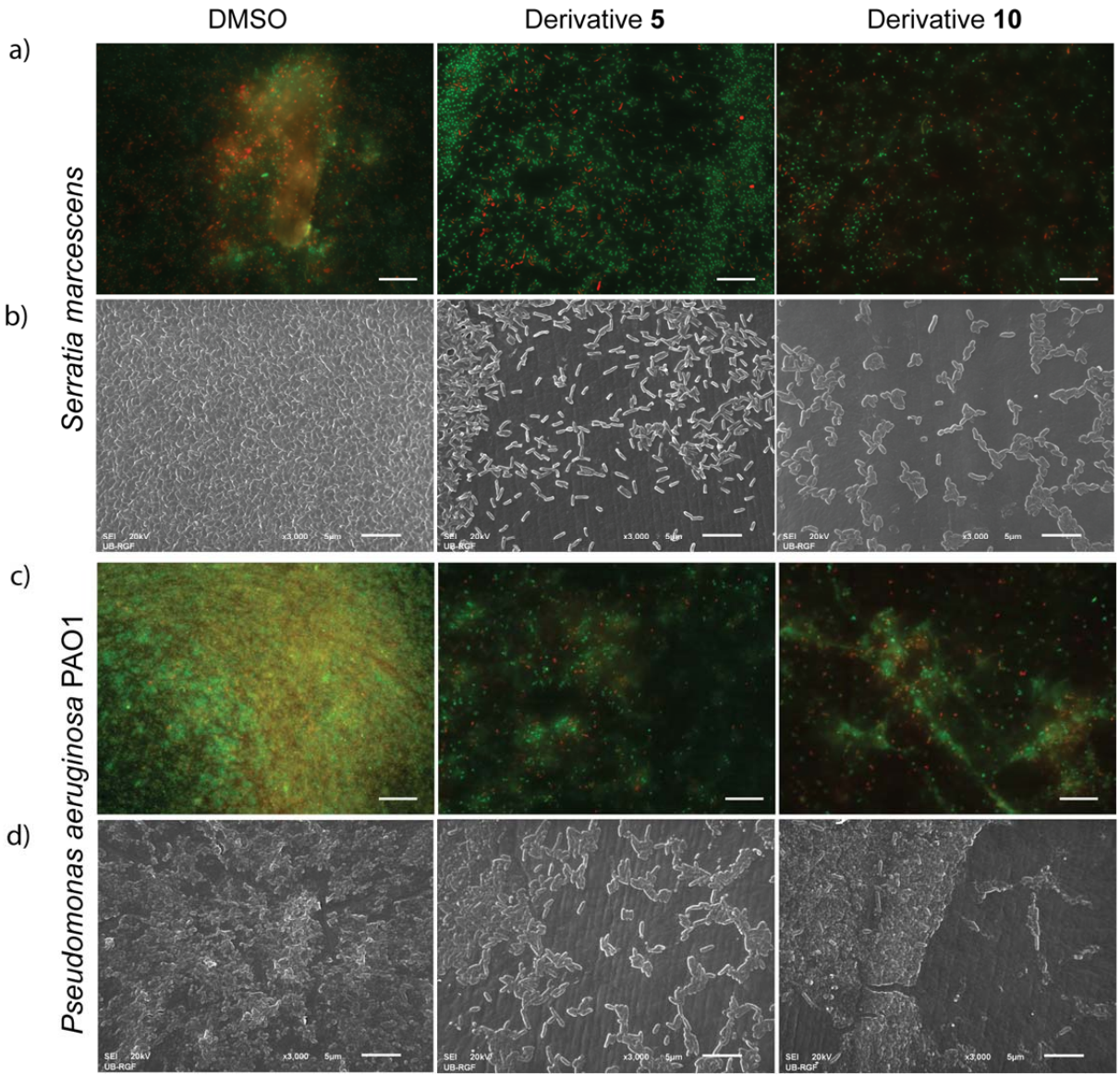


Figure 1S. Inhibition of biofilm formation with 4-AQ derivatives **5** and **10**. Biofilms of *S. marcescens* and *P. aeruginosa* were formed for 24 h in the presence of DMSO (0.1 %), **5** or **10** ($BFIC_{50}$). Biofilms were analysed by fluorescent microscopy (a and c) or scanning electron microscopy (b and d). In a) and c) living bacteria are labeled with Syto9 (green) and dead bacteria were stained with membrane impermeabile dye propidium iodide (red), scale bars represent 10 μm.

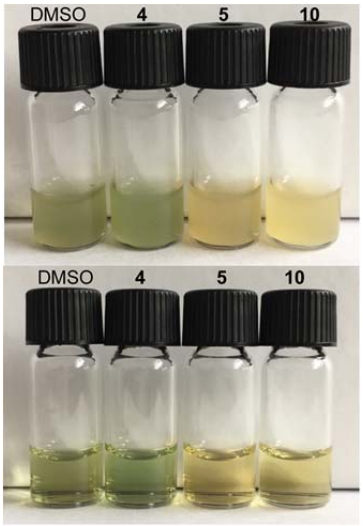
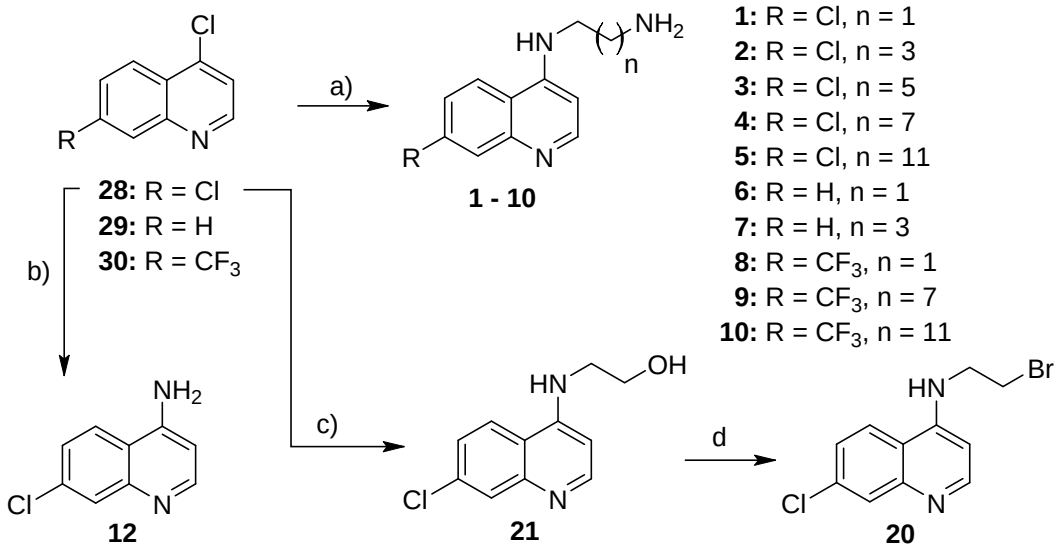


Figure 2S. Inhibition of pyocyanin production in *P. aeruginosa* PA14 incubated for 24h with 50 μg/ml derivatives **4**, **5** or **10** or, 0.1% DMSO. Upper panel demonstrates bacterial cultures and the lower panel shows respective supernatants.

Table 2S. Experimentally determined RM values for standard and examined compounds

Compounds	**logP**[1]	**R_M**	**Compound**	**R_M**
4-Aminophenol	0.04	-1.06	**1**	-0.50
p-Anisidine	0.95	-0.60	**2**	-0.41
Diphenylamine	3.50	0.50	**3**	-0.31
Phenol	1.46	-0.10	**4**	-0.12
4-Nitrophenol	1.91	0.03	**5**	0.37
3-Nitrophenol	2.00	0.10	**6**	-0.79
Benzyl Alcohol	1.10	-0.07	**7**	-0.66
2-Naphtol	2.70	0.35	**8**	-0.43
Naphtylamine	2.25	-0.31	**9**	-0.07
2,4-Dichlorophenol	3.06	0.43	**10**	0.43
Antracene	4.45	1.28	**11**	-0.16
4-Chlorophenol	2.39	0.23	**12**	-0.21
Acetophenone	1.58	0.18	**13**	-0.43
Pyrene	4.88	1.69	**14**	-0.27
Fluorene	4.18	1.19	**15**	-0.31
Acenaphtene	3.92	1.06	**16**	-0.07
Phenantrene	4.46	1.19	**17**	0.25
Simazine	2.18	-0.03	**18**	-0.14
4-Bromoaniline	2.26	-0.37	**19**	-0.45
Benyophenone	3.18	0.69	**20**	-0.12
2-Aminophenol	0.62	-0.69	**21**	-0.31
Bromazepam	2.05	-0.33		
Diazepam	2.82	-0.14		
4-Methoxyphenol	1.58	-0.12		
Benzo(a)anthracene	5.76	1.69		



a) diamine, 120 ^{o}C, 6h; b) $(NH_4)_2CO_3$ / PhOH, 165 ^{o}C, 2h;
c) ethanolamine, 130 ^{o}C, 5h; d) HBr / H_2SO_4, 165 ^{o}C, 3.5h;

Scheme 1S. Reaction schemes for synthesis of tested derivatives.

***Chromobacterium violaceum* disk assay** was performed as previously described[2]. N-(hexanoyl)-L-homoserine lactone (HHL) (5 µM) was used as inducer of violacein production in molten semi-solid LB agar (0.3 % w/v). Cellulose disks containing compounds (250 µg/disk) were placed on solidified agar and incubated for 24 h at 30 °C. Inhibition of violacein synthesis was detected as appearance of colourless halo around a disk.

Fluorescent microscopy

Overnight cultures of bacteria were diluted to 5 x 10^7 cfu mL^{-1} in LB and 2 ml was added per well of 6 well microtiter plate containing plastic cover slips in the presence of DMSO (0.1%) or $BFIC_{50}$ of active compounds. After 24 h, biofilms were washed with 0.9% NaCl and stained with 2.5 µM SYTO9 green fluorescent dye and 2.5 µM propidium iodide (PI) red fluorescent dye of Live/Dead staining kit (LIVE/DEAD® BacLight™ Bacterial Viability Kit, Thermo Fisher Scientific, Waltham, MA, USA). Cells were observed under a fluorescence microscope (Olympus BX51, Applied Imaging Corp., San Jose, USA) under 100× magnification.

Scanning electron microscopy (SEM)

Overnight bacterial cultures were diluted to 5 x 10^7 cfu mL^{-1} in LB and 2 ml was added per

well in 6 well microtiter plate containing 1 cm silicone catheter pieces (Romed, Holland) in the presence of DMSO (0.1%) or $BFIC_{50}$ of active compounds. After 24 h, the catheters were thoroughly washed with phosphate buffered saline (PBS), biofilms were fixed with cold methanol and dried before examination.

Catheters were glued to double-sided conductive carbon tab stuck on standard vacuum-clean stub, and were coated with gold (thickness of 15-20 nm) by sputtering process (Leica EM SCD005 sputtering machine). Sputtering was performed in the vacuum chamber under pressure <0.05 mbar using sputter current of 40 mA, working distance of 50 mm and sputter time of 100 s. Such prepared samples were examined by JEOL JSM-6610LV microscope. An acceleration voltage of 20 kV was used.

7-chloroquinolin-4-amine (12)[3]:

4,7-Dichloroquinoline (2.0 g, 10.0 mmol) was dissolved in phenol (23.7g, 0.1 mol.) with stirring and heating at 110 °C. Ammonium carbonate (4.84g, 0.05 mol) was added in portions as rapidly as the frothing was permitting. After 2 h at 165 °C, the mixture was cooled and diluted with diethyl ether (100 mL), transferred into separatory funnel, washed with 10 % NaOH water solution until all phenol was removed, then with brine, and dried under anh.Na_2SO_4. Solvent was removed under reduce pressure and product was isolated upon column chromatography purification (dry flash, SiO_2, eluent DCM, DCM/MeOH = 9/1, MeOH). Yield 1.44 g (80%). IR (ATR): 3443m, 3321m, 3098s, 2788m, 2707w, 1683w, 1656m, 1634m, 1612m, 1577s, 1505s, 1444s, 1371m, 1329m, 1285m, 1204m, 1165w, 1125m, 1107m, 1075m, 907m, 940w, 877m, 853m, 810m cm^{-1}. ^1H NMR (200 MHz, CD_3OD, δ): 8.22 (*d,* 1H, *J* = 5.35, H-2), 8.0 (*d,* 1H, *J* = 9.0, H-5), 7.72 (*d,* 1H, *J* = 2.2, H-8), 7.31 (*dd,* 1H, J_1 = 9.0, J_2 = 2.2, H-6), 6.57 (*d,* 1H, *J* = 5.35, H-3). ^{13}C NMR (50 MHz, CD_3OD, δ): 154.45 (C4), 151.81 (C2), 149.86 (C8a), 136.57 (C7), 127.29 (C8), 125.81 (C6), 124.97 (C5), 118.27 (C4a), 103.89 (C3). (+)ESI-HRMS (*m*/*z*): calculated for $[C_9H_8ClN_2 + H]^+$ 179.03705, observed 179.03644.

General procedure for 4-diaminoquinoline synthesis:

A mixture of 4,7-dichloroquinoline (5 g, 25 mmol) and 1,2-diaminoethane (15 mL, 224 mmol) was heated slowly to 80 ^oC over 1 h with stirring. Subsequently the temperature was raised to 120 ^oC and stirred for 6 h until the reaction was completed. The reaction mixture was poured into ice/water mixture and left overnight. Precipitate was filtered, washed with

H_2O and dried under reduce pressure. Yield was 5.46 g (97%). If not specified differently, samples were not additionally purified.

***N*-(7-chloroquinolin-4-yl)ethane-1,2-diamine (1)[4]:**

IR (ATR): 3247s, 2923m, 2190w, 1586s, 1542s, 1482m, 1456s, 1427m, 1389m, 1348s, 1323m, 1291m, 1254w, 1211w, 1166w, 1140m, 1112w, 1082w, 1046w, 1023w, 949w, 910w, 867w, 825m,802w, 769w cm^{-1}. ^1H NMR (500 MHz, CD_3OD, δ): 8.36 (d, 1H, J = 5.6, H-2), 8.12 (d, 1H, J = 9.0, H-5), 7.78 (*d,* 1H, *J* = 2.25, H-8), 7.41 (*dd,* 1H, J_1 = 9.0, J_2 = 2.28, H-6), 6.58 (*d,* 1H, *J* = 5.6, H-3), 3.46 (*t,* 2H, *J* = 6.35, H-9), 2.99 (*t,* 2H, *J* = 6.35, H-10). ^{13}C NMR (125 MHz, CD_3OD, δ): 153.0 (C4), 152.62 (C2), 149.84 (C8a), 136.53 (C7), 127.76 (C8), 126.22 (C6), 124.48 (C5), 118.99 (C4a), 99.87 (C3), 46.28 (C9), 40.93 (C10). (+)ESI-HRMS (*m*/*z*): calculated for $[C_{11}H_{13}ClN_3 + H]^+$ 222.07925, observed 222.07881.

***N*-(7-chloroquinolin-4-yl)butane-1,4-diamine (2)[4]:**

IR (ATR): 3285s, 2943s, 1609w, 1580s, 1540m, 1473w, 1452m, 1431w, 1367m, 1329m, 1282w, 1248w, 1203w, 1165w, 1135w, 1078w, 904w, 874w, 853w, 806w, 764w cm^{-1}. ^1H NMR (500 MHz, CD_3OD, δ): 8.34 (*d,* 1H, *J* = 5.7, H-2), 8.09 (*d,* 1H, *J* = 8.9, H-5), 7.77 (*d,* 1H, *J* = 2.2, H-8), 7.38 (*dd,* 1H, J_1 = 8.9, J_2 = 2.2, H-6), 6.51 (*d,* 1H, *J* = 5.7, H-3), 3.38 (*t,* 2H, *J* = 7.1, H-9), 2.76 (*m,* 2H, H-12), 2.78-2.74 (*m,* 2H, H-10), 1.65 (*m,* 2H, H-11). ^{13}C NMR (125 MHz, CD_3OD, δ): 152.87 (C4), 152.58 (C2), 149.85 (C8a), 136.47 (C7), 127.74 (C8), 126.08 (C6), 124.45 (C5), 118.92 (C4a), 99.77 (C3), 43.85 (C9), 42.05 (C12), 30.41 (C10), 26.89 (C11). (+)ESI-HRMS (*m*/*z*): calculated for $[C_{13}H_{17}ClN_3 + H]^+$ 250.11055, observed 250.10956.

***N*-(7-chloroquinolin-4-yl)hexane-1,6-diamine (3)[4]:**

IR (ATR): 3362w, 3274m, 3035m, 2933s, 2857m, 1610w, 1579s, 1541m, 1472m, 1451m, 1429m, 1370m, 1333m, 1256w, 1198w, 1133w, 1081w, 1005w, 937w, 899m, 851m, 799m, 772w, 735w cm^{-1}. ^1H NMR (500 MHz, CD_3OD, δ): 8.34 (*d,* 1H, *J* = 5.7, H-2), 8.09 (*d,* 1H, *J* = 9.1, H-5), 7.77 (*d,* 1H, *J* = 2.15, H-8), 7.38 (*dd,* 1H, J_1 = 9.1, J_2 = 2.15, H-6), 6.5 (*d,* 1H, *J* = 5.5, H-3), 3.36 (*t,* 2H, *J* = 7.2, H-9), 2.72-2.68 (*m,* 2H, H-14), 1.76 (*q,* 2H, *J* = 7.3, H-10), 1.58-1.40 (*m,* 6H, H-11-13). ^{13}C NMR (125 MHz, CD_3OD, δ): 152.91 (C4), 152.56 (C2), 149.88 (C8a), 136.42 (C7), 127.73 (C8), 126.05 (C6), 124.44 (C5), 118.92 (C4a), 99.72 (C3), 44.05 (C9), 42.17 (C14), 32.64 (C10), 29.47 (C13), 28.15 (C11), 27.81 (C12). (+)ESI-HRMS

(*m*/*z*): calculated for $[C_{15}H_{21}ClN_3 + H]^+$ 278.14185, observed 278.14060; calculated for $[C_{15}H_{21}ClN_3 + 2H]^{2+}$ 139.57456, observed 139.5745.

***N*-(7-chloroquinolin-4-yl)octane-1,8-diamine (4):**

A mixture of 4,7-dichloroquinoline (200 mg, 1.02 mmol) and 1,8-diaminooctane (1.03 g, 7.12 mmol) was heated 15 minutes at 55 ^oC, then for 24 hour at 130 ^oC and poured into ice/water mixture and left overnight. Precipitate was filtered, washed thoroughly with H_2O, dried under reduce pressure and purified by column chromatography (dry-flash, SiO_2 column, eluent DCM/MeOH = 95:5 → MeOH → DCM/MeOH/NH_3(aq) = 9:1:1). Yield 240 mg (77 %). IR (ATR): 3248m, 3100m, 2852s, 1612m, 1581s, 1543m, 1477m, 1452m, 1432m, 1371m, 1332m, 1254w, 1136w, 1082w, 1027w, 963m, 908w, 878w, 852w, 802w, 769w, 730w cm^{-1}. ^1H NMR (500 MHz, CD_3OD, δ): 8.32 (*d*, 1H, *J* = 5.7, H-2), 8.07 (*d*, 1H, *J* = 9.1, H-5), 7.76 (*d*, 1H, *J* = 2.15, H-8), 7.36 (*dd*, 1H, J_1 = 9.1, J_2 = 2.15, H-6), 6.44 (*d*, 1H, *J* = 5.7, H-3), 3.30 (*t*, 2H, *J* = 7.15, H-9), 2.62 (*t*, 2H, *J* = 7.15, H-16), 1.77-1.67 (*m*, 2H, H-10), 1.50-1.27 [*m*, 10H, H-(11-15)]. ^{13}C NMR (125 MHz, CD_3OD, δ): 152.83 (C4), 152.51 (C2), 149.83 (C8a), 136.36 (C7), 127.73 (C8), 125.99 (C6), 124.45 (C5), 118.90 (C4a), 99.68 (C3), 44.17 (C9), 42.56 (C16), 33.59 (C10), 30.67 (15), 30.60 (11), 29.52 (C12), 28.33 (C14), 28.07 (C13). (+)ESI-HRMS (*m*/*z*): calculated for $[C_{17}H_{25}ClN_3 + H]^+$ 306.17315, observed 306.17263; calculated for $[C_{17}H_{25}ClN_3 + 2H]^{2+}$ 153.59021, observed 153.59029.

***N*-(7-chloroquinolin-4-yl)dodecane-1,12-diamine (5):**

Compound **5** was obtained according to procedure described for **4**, using 4,7-dichloroquinoline (200 mg, 1.02 mmol) and 1,12-diaminododecane (1.42 g, 7.0 mmol). Solid was triturated with CH_3OH, methanol extract was evaporated to dryness and purified by column chromatography (dry-flash, SiO_2 column, eluent DCM/MeOH = 95:5 → MeOH → DCM/MeOH/NH_3(aq) = 9:1:1). Yield 248 mg (81 %). IR (ATR): 3377m, 3258m, 2938m, 2865m, 1592s, 1548s, 1470m, 1433w, 1380m, 1328s, 1283m, 1206m, 1158m, 1136s, 1118s, 1070m, 962w, 911w, 868w, 810w, 778w, 739w cm^{-1}. ^1H NMR (500 MHz, CD_3OD, δ): 8.32 (*d*, 1H, *J* = 5.7, H-2), 8.08 (*d*, 1H, *J* = 8.85, H-5), 7.76 (*d*, 1H, *J* = 2.0, H-8), 7.36 (*dd*, 1H, J_1 = 8.85, J_2 = 2.0, H-6), 6.46 (*d*, 1H, *J* = 5.7, H-3), 3.34-3.29 (*m*, 2H, overlapped with solvent signal, H-9), 2.64-2.58 (*m*, 2H, H-20), 1.72 (*q*, 2H, H-10), 1.49-1.22 [*m*, 18H, H-(11-19)]. ^{13}C NMR (125 MHz, CD_3OD, δ): 152.86 (C4), 152.53 (C2), 149.86 (C8a), 136.37 (C7), 127.75 (C8), 126.0 (C6), 124.47 (C5), 118.93 (C4a), 99.70 (C3), 44.19 (C9), 42.69 (C20), 33.89 (C10), 30.67 (19), 30.60 (11), 30.85, 30.82, 30.77, 30.65, 29.52, 28.36, 28.19. (+)ESI-HRMS

(*m*/*z*): calculated for $[C_{17}H_{25}ClN_3 + H]^+$ 362.23575, observed 362.23549; calculated for $[C_{17}H_{25}ClN_3 + 2H]^{2+}$ 181.62151, observed 181.62179.

_N_-(quinolin-4-yl)ethane-1,2-diamine (6)[5]:

IR (ATR): 3268s, 3058m, 1668m, 1621m, 1581s, 1542s, 1458m, 1389m, 1342m, 1224m, 1132m, 1136s, 893w, 810w, 763m, 739w cm^{-1}. ^1H NMR (500 MHz, CD_3OD, δ): 8.36 (d, 1H, J = 5.6, H-2), 8.12 (*dd,* 1H, J_1 = 8.5, J_2 = 0.7, H-8), 7.81 (*dd,* 1H, J_1 = 8.5, J_2 = 0.7, H-5), 7.64 (*ddd,* 1H, J_1 = 8.4, J_2 = 6.9, J_3 = 1.4, H-7), 7.45 (*ddd,* 1H, J_1 = 8.4, J_2 = 6.9, J_3 = 1.4, H-6), 6.57 (*d,* 1H, *J* = 5.6, H-3), 3.48 (*t,* 2H, *J* = 6.35, H-9), 3.01 (*t,* 2H, *J* = 6.35, H-10). ^{13}C NMR (125 MHz, CD_3OD, δ): 153.06 (C4), 151.09 (C2), 148.68 (C8a), 130.83 (C8), 128.68 (C7), 125.94 (C6), 122.42 (C5), 120.42 (C4a), 103.89 (C3), 44.19 (C9), 42.69 (C10). (+)ESI-HRMS (*m*/*z*): calculated for $[C_{11}H_{14}CN_3 + H]^+$ 188.11822, observed 188.11795.

_N_-(quinolin-4-yl)butane-1,4-diamine (7)[6]:

IR (ATR): 3311s, 2943s, 2860m, 1582s, 1545m, 1503w, 1478w, 1442w, 1407w, 1379m, 1346m, 1294w, 1262w, 1225w, 1160w, 1128w, 1095w, 1047w, 985w, 958w, 930w, 895w, 864w, 809w, 771m, cm^{-1}. ^1H NMR (200 MHz, CD_3OD, δ): 8.31 (d, 1H, J = 5.6, H-2), 8.07 (d, 1H, J = 8.4, H-8), 7.79 (*d,* 1H, *J* = 8.4, H-5), 7.59 (*td,* 1H, J_1 = 7.6, J_2 = 1.1, H-7), 7.45-7.32 (*m,* 1H, H-7), 6.42 (*d,* 1H, *J* = 5.6, H-3), 3.30 (*t,* 2H, *J* = 6.7, H-9), 2.65 (*t,* 2H, *J* = 6.7, H-12), 1.89-1.40 (*m*, H-10 and H-11). ^{13}C NMR (50 MHz, CD_3OD, δ): 152.65 (C4), 151.30 (C2), 148.97 (C8a), 130.45 (C8), 128.87 (C7), 125.56 (C6), 122.26 (C5), 120.33 (C4a), 99.16 (C3), 43.81 (C9), 42.32 (C12), 31.39 (C10), 26.88 (C11). (+)ESI-HRMS (*m*/*z*): calculated for $[C_{13}H_{17}N_3 + H]^+$ 216.14952, observed 216.14980.

_N_-[7-(trifluoromethyl)quinolin-4-yl]ethane-1,2-diamine (8)[5]:

IR (ATR): 3377m, 3258m, 2938m, 2865m, 1592s, 1549s, 1470m, 1433w, 1380m, 1327s, 1283m, 1206m, 1159s, 1136s, 1118s, 1070m, 962w, 911w, 868w, 810w, 778w, 739w cm^{-1}. ^1H NMR (500 MHz, CD_3OD, δ): 8.46 (*d,* 1H, *J* = 5.6, H-2), 8.32 (*d,* 1H, *J* = 8.75, H-5), 8.09 (*s,* 1H, H-8), 7.62 (*dd,* 1H, J_1 = 8.75, J_2 = 1.7, H-6), 6.66 (*d,* 1H, *J* = 5.6, H-3), 3.49 (*t,* 2H, *J* = 6.2, H-9), 3.03 (*t,* 2H, *J* = 6.2, H-10). ^{13}C NMR (125 MHz, CD_3OD, δ): 153.03 (C2), 152.76 (C4), 148.37 (C8a), 132.28. (d, *J* = 32.5, C7), 126.5 (*d*, *J* = 3.6, C8), 124.47 (C5), 123.44 (*q*, *J* = 269.7, CF_3), 122.35 (C4a), 120.89 (*d*, *J* = 1.8, C6), 100.89 (C3), 46.25 (C9), 40.80 (C10). (+)ESI-HRMS (*m*/*z*): calculated for $[C_{12}H_{12}F_3N_3 + H]^+$ 256.10561, observed 256.10546.

***N*-[7-(trifluoromethyl)quinolin-4-yl]octane-1,8-diamine (9):**

Compound **9** was obtained according to procedure described for **4**, using 4-chloro-7-trifluoromethylquinoline (300 mg, 1.29 mmol) and 1,8-diaminooctane (1.31 g, 9.07 mmol). Product was purified by column chromatography (dry-flash, SiO_2 column, eluent DCM/MeOH = 95:5 → MeOH → DCM/MeOH/NH_3(aq) = 8:12:1). Yield was 419 mg (95%). IR (ATR): 3371w, 3263m, 3161w, 3112w, 3074w, 3028w, 2932s, 2857m, 1584s, 1546m, 1469m, 1435w, 1373s, 1329s, 1281m, 1194w, 1154m, 1137m, 1112s, 1074m, 1027w, 966w, 934w, 912m, 878w, 858w, 809w, 764w, 735w cm^{-1}. ^1H NMR (500 MHz, CD_3OD, δ): 8.42 (*d*, 1H, *J* = 5.6, H-2), 8.29 (*d*, 1H, *J* = 8.85, H-5), 8.07 (*s*, 1H, H-8), 7.60 (*dd*, 1H, J_1 = 8.85, J_2 = 1.8, H-6), 6.56 (*d*, 1H, *J* = 5.6, H-3), 3.37-3.32 (*m*, 2H, H-9), 2.64-2.58 (*m*, 2H, H-16), 1.79-1.70 (*m*, 2H, H-10), 1.50-1.27 [*m*, 10H, H-(11-15)]. ^{13}C NMR (125 MHz, CD_3OD, δ): 152.99 (C2), 152.71 (C4), 148.42 (C8a), 132.24 (*d*, *J* = 32.5, C7), 126.49(C8), 124.41 (C5), 123.44 (*q*, *J* = 269.8, CF_3), 122.32 (C4a), 120.75 (C6), 100.74 (C3), 44.26 (C9), 42.62 (C16), 33.73 (C10), 30.69 (15), 30.60 (11), 29.44 (C12), 28.34 (C14), 28.09 (C13). (+)ESI-HRMS (*m*/*z*): calculated for $[C_{18}H_{24}F_3N_3 + H]^+$ 340.19951, observed 340.19890; calculated for $[C_{18}H_{24}F_3N_3 + 2H]^{2+}$ 170.60339, observed 170.60341.

***N*-[7-(trifluoromethyl)quinolin-4-yl]dodecane-1,12-diamine (10):**

Compound **10** was obtained according to procedure described for **4**, using 4-chloro-7-trifluoromethylquinoline (300 mg, 1.29 mmol) and 1,12-diaminododecane (1.84 g, 9.07 mmol). Product was purified by column chromatography (dry-flash, SiO_2 column, eluent DCM/MeOH = 95:5 → MeOH → DCM/MeOH/NH_3(aq) = 8:2:1). Yield was 418 mg (81%). IR (ATR): 3221m, 3119w, 30375w, 3042w, 2924s, 2851s, 1590s, 1466m, 1433w, 1374m, 1329s, 1279m, 1206w, 1161s, 1117s, 1072w, 911w, 891w, 853w, 815w, 737w cm^{-1}. ^1H NMR (500 MHz, CD_3OD, δ): 8.43 (*d*, 1H, *J* = 5.6, H-2), 8.30 (*d*, 1H, *J* = 8.85, H-5), 8.07 (*s*, 1H, H-8), 7.60 (*dd*, 1H, J_1 = 8.85, J_2 = 1.7, H-6), 6.57 (*d*, 1H, *J* = 5.6, H-3), 3.35 (*t*, *J* = 7.2, 2H, H-9), 2.68-2.61 (*m*, 2H, H-20), 1.75 (*q*, J = 7.4, 2H, H-10), 1.52-1.23 [*m*, 18H, H-(11-19)]. ^{13}C NMR (125 MHz, CD_3OD, δ): 152.99 (C2), 152.74 (C4), 148.43 (C8a), 132.25 (*J* = 32.37, C7), 126.49 (*d*, *J* = 4.5, C8), 124.42 (C5), 123.45 (*q*, *J* = 269.9, CF_3), 122.34 (C4a), 120.76 (*d*, *J* = 2.8, C6), 100.75 (C3), 44.26 (C9), 42.44 (C20), 33.19 (C10), 30.82, 30.71, 30.64, 29.42, 28.36, 28.10. (+)ESI-HRMS (*m*/*z*): calculated for $[C_{22}H_{33}F_3N_3 + H]^+$ 396.26211, observed 396.25993; calculated for $[C_{22}H_{33}F_3N_3 + 2H]^{2+}$ 198.63469, observed 198.63451.

2-[(7-chloroquinolin-4-yl)amino]ethanol (21)[7]:

4,7-Dichloroquinoline (19.8 g, 0.1 mol) was heated in pure ethanolamine (18 mL, 0.3 mol) at 130 °C for 5h. After cooling to room temperature, 10% NaOH solution (100 mL) was added, solid was filtered off, rinsed with water, dried and recrystallized from methanol. Yield was 16.75 g (75%). IR (ATR): 3310s, 3112m, 2964m, 2834m, 1613m, 1582s, 1541m, 1492w, 1450m, 1391w, 1368w, 1340m, 1289w, 1250w, 1223m, 1171m, 1140m, 1140m, 1065m, 925w, 884w, 850w, 801w, 765w cm^{-1}. ^1H NMR (500 MHz, DMSO-d6, δ): 9.19 (*d*, 1H, *J* = 5.5, H-2), 9.08 (*d*, 1H, *J* = 9.15, H-5), 8.59 (*d*, *J* = 2.3, 1H, H-8), 8.24 (*dd*, 1H, J_1 = 9.15, J_2 = 2.2, H-6), 8.08 (*t*, 1H, *J* = 5.3, H-N), 7.30 (*d*, 1H, *J* = 5.5, H-3), 5.70 (*bs*, 1H, H-O), 4.48 (*t*, 2H, *J* = 5.9, H-10), 4.16 (*t*, 2H, *J* = 5.9, H-9). ^{13}C NMR (125 MHz, DMSO-d6, δ): 154.72 (C2), 153.09 (C4), 151.93 (C8a), 136.20 (C7), 130.30 (C8), 126.93 (C5), 126.83 (C6), 120.31 (C4a), 100.52 (C3), 6159 (C10), 47.98 (C9). (+)ESI-HRMS (*m*/*z*): calculated for $[C_{11}H_{11}Cl_3N_2O + H]^+$ 223.06327, observed 223.06335.

***N*-(2-bromoethyl)-7-chloroquinolin-4-amine (20)[8]:**

Alcohol **21** (5.0 g, 22.4 mmol) was heated in 48% HBr (15.84 mL) and 98% H_2SO_4 (2.63 mL) mixture at 165 °C for 3.5 h. After cooling to 50-60 °C, mixture was poured into water/ice mixture, and solid $NaHCO_3$ was added in small portions until pH value of mixture was adjusted to 9. Toluene was added (100 mL), mixture was boiled for 15 minutes, then cooled (50 °C) and layers were separated. Water layer was extracted with toluene (3x15 mL). Combined organic layers were washed with brine and dried with anh. Na_2SO_4. Solution was filtered off and cooled. Separated crystals were filtered and dried under reduce pressure. Yield was 3.8 g (59%). IR (ATR): 3216m, 3062m, 2965m, 1612s, 1577s, 1543s, 1489w, 1454m, 1430m, 1369m, 1327m, 1282w, 1252w, 1228m, 1138m, 1081w, 901w, 874w, 851w, 808w, 769w cm^{-1}. ^1H-NMR (500 MHz, DMSO-d6, δ): 8.42 (*d*, 1H, *J* = 5.5, H-2), 8.25 (*d*, 1H, *J* = 8.95, H-8), 7.81 (*d*, 1H, *J* = 2.25, H-5), 7.65-7.58 (*m*, 1H, H-N), 7.49 (*dd*, 1H, J_1 = 8.95, J_2 = 2.25, H-6), 6.58 (*d*, 1H, *J* = 5.5, H-3), 3.78 – 3.68 (m, 4H, H-9 and H-10). ^{13}C-NMR (125 MHz, DMSO-d6, δ): 153.71 (C2), 151.71 (C4), 150.76 (C8a), 135.72 (C7), 129.33 (C8), 126.48 (C5), 126.0 (C6), 119.33 (C4a), 100.93 (C3), 46.09 (C9), 33.27 (C10). +ESI-MS (*m*/*z* (%)): calculated for $[C_{11}H_{10}BrClN_2 + H]^+$ 284.97886, observed 284.97886.

Chromatographic determination of lipophilicity of AQ derivatives

As a measure of lipophilicity, the distribution coefficient $\log D(o/w)_{exp}$ of the investigated compounds were determined using reversed-phase thin-layer chromatography under acidic

conditions (pH ≈ 1). An HPTLC vertical developing chamber (Camag, Muttenz, Switzerland) in the tank configuration was used for this purpose. A set of standard compounds (Table 2S) and tested substances were simultaneously chromatographed using commercially available sorbent RP-18 W F254s (Art. 13124, Merck, Darmstadt, Germany) and mobile phase containing methanol / HCl / H_2O (60/5/35), pH ≈ 1.

The investigated AQ derivatives and substances used as standards were dissolved in methanol, and the plates were spotted with 0.5 mL aliquots of freshly prepared solutions (C ≈ 1 mg/mL). Before chromatogram development, the chromatographic chamber was equilibrated for 15 min in vapours of the mobile phase. Detection of individual zones was performed using UV lamp (254 nm). All used solvents were of analytical-grade purity. Water was purified using a water purification system Millipore Simplicity 185 S.A., 67120 (Molshem, France). All experiments were performed at room temperature (22 ± 2°C).

The retardation factor (R_F) of each compound was determined as a ratio of individual zone distance and the solvent front. The corresponding retention mobility (R_M) was calculated from R_F as follows: $\log(1/R_F\text{-}1)$.

In order to determine $\log D(\text{o/w})_{exp}$ values of the investigated compounds, the following linear calibration dependence was obtained between R_M values of standard compounds and their $\log P(\text{o/w})$ values obtained from the literature (Table 2S):

$R_M = 0.489 \log P(\text{o/w}) - 1.007$; $R^2 = 0.891$, $N = 25$, $S.D. = 0.247$, $P < 0.0001$ (**1**)

The $\log D(\text{o/w})_{exp}$ values of the investigated AQs were further calculated simply by substituting their R_M values (Table 2S) into equation 1.

QSAR computations

Before building QSAR models all variables were standardized, *i.e.*, in a column wise fashion from each value the arithmetic mean was subtracted and the difference was divided by the standard deviation. In that way data were mean-centred and expressed in the unit standard deviation.

Furthermore, only the AQ derivatives, i.e., compounds containing quinolone core (**6-27**), were taken into account. Optimal model complexity, in this case the ideal number of PLS components, was determined using cross-validation procedure based on venetian blinds (VB) resampling strategy with 5 splits. The number of PLS components resulting in the model with the lowest cross-validation error (RMSECV) was selected as the optimal one.

In order to increase model performance, variable selection was carried out employing a stepwise PLS regression procedure. In each step variables that contribute to the overall model

better than the average (variable importance to the projection scores - VIP > 1) were retained, and the new PLS model was built. In all instances no further improvements in statistical model performance was noted after the second iteration step. Actually, model deterioration following third and fourth iteration was observed.

The quality of the regression fits was evaluated by the values of determination coefficients for calibration, cross-validation and prediction (R^2_{cal}, R^2_{CV}, R^2_{Pred}) and the corresponding root mean-square errors (*RMSEC*, *RMSECV*, and *RMSEPred*, respectively). Low value of *RMSEC* is desirable but if the high values of *RMSECV* and *RMSEPred* are present at the same time, it indicates the poor predictability of the calibration model. It is considered that model is predictive, if the following conditions are satisfied: $R^2_{cal} > 0.6$, $R^2_{CV} > 0.5$. Predictive performance of a model was assessed in a double cross-validation procedure. The entire data set has been split four times into independent training and test sets using VB algorithm as a part of the outer cross-validation loop. Then, each training set has been further divided into calibration and validation set as a part of the inner cross-validation loop, using five splits in combination with the VB algorithm. In that way each compound has been used as a part of the calibration, validation, and test set but never at the same time. The optimal model complexity was determined based on the model performance criteria obtained from the inner loop, while the performance parameters from the outer loop were used as the model prediction estimates (*RMSEPred* and R^2_{Pred}, respectively).

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Compound 12: ^{1}H NMR spectrum (200 MHz, CD_3OD):

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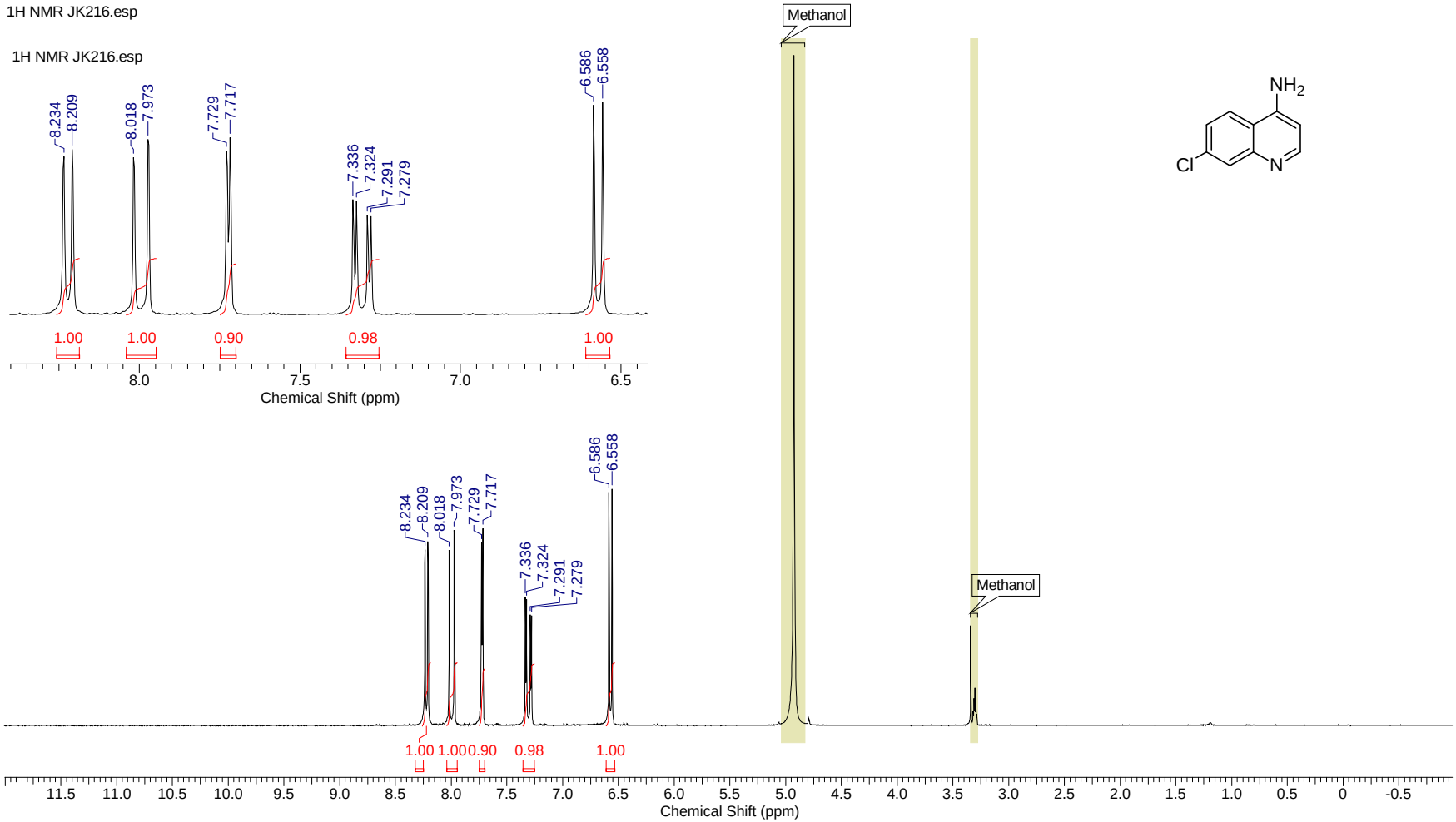

Compound 12: ^{13}C NMR spectrum (50 MHz, CD_3OD):

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Pulse Sequence	s2pul	***Receiver Gain***	25.00	***Solvent***	METHANOL-d4	***Spectrum Offset (Hz)***	4918.2021
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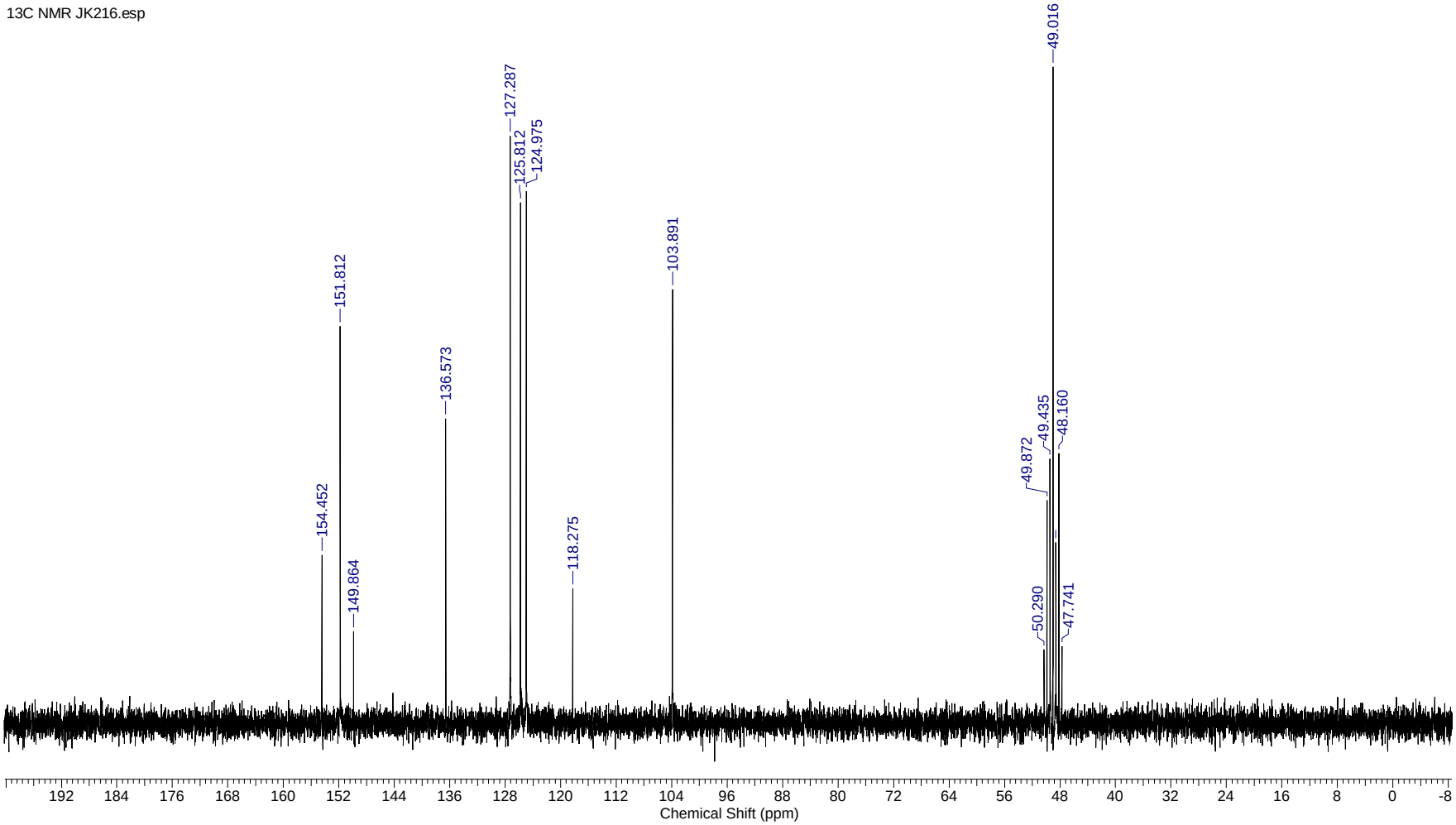

Compound 1: ^{1}H NMR spectrum (500 MHz, CD_3OD)

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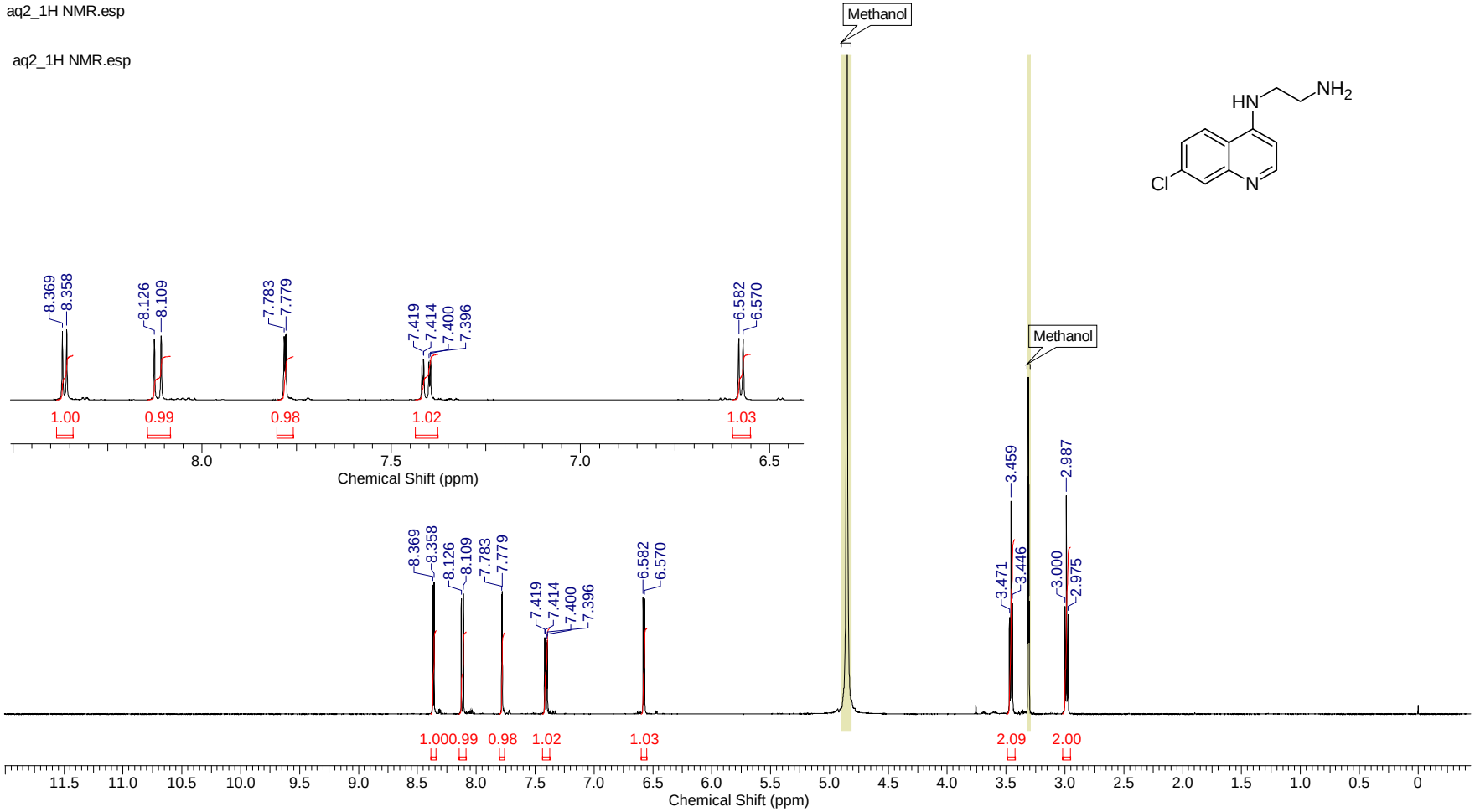

Compound 1: ^{13}C NMR spectrum (500 MHz, CD_3OD)

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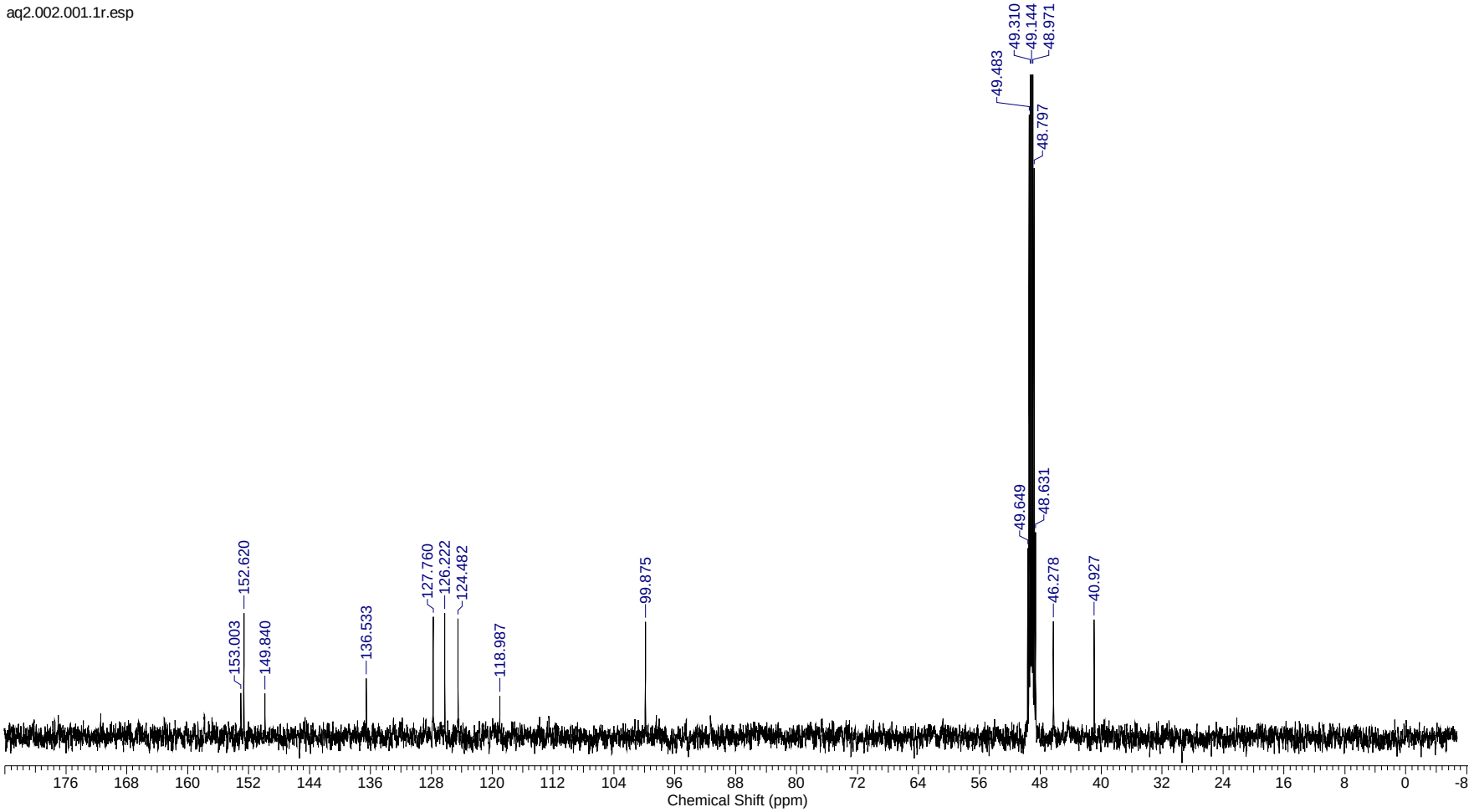

Compound 2: ^{1}H NMR spectrum (500 MHz, CD_3OD)

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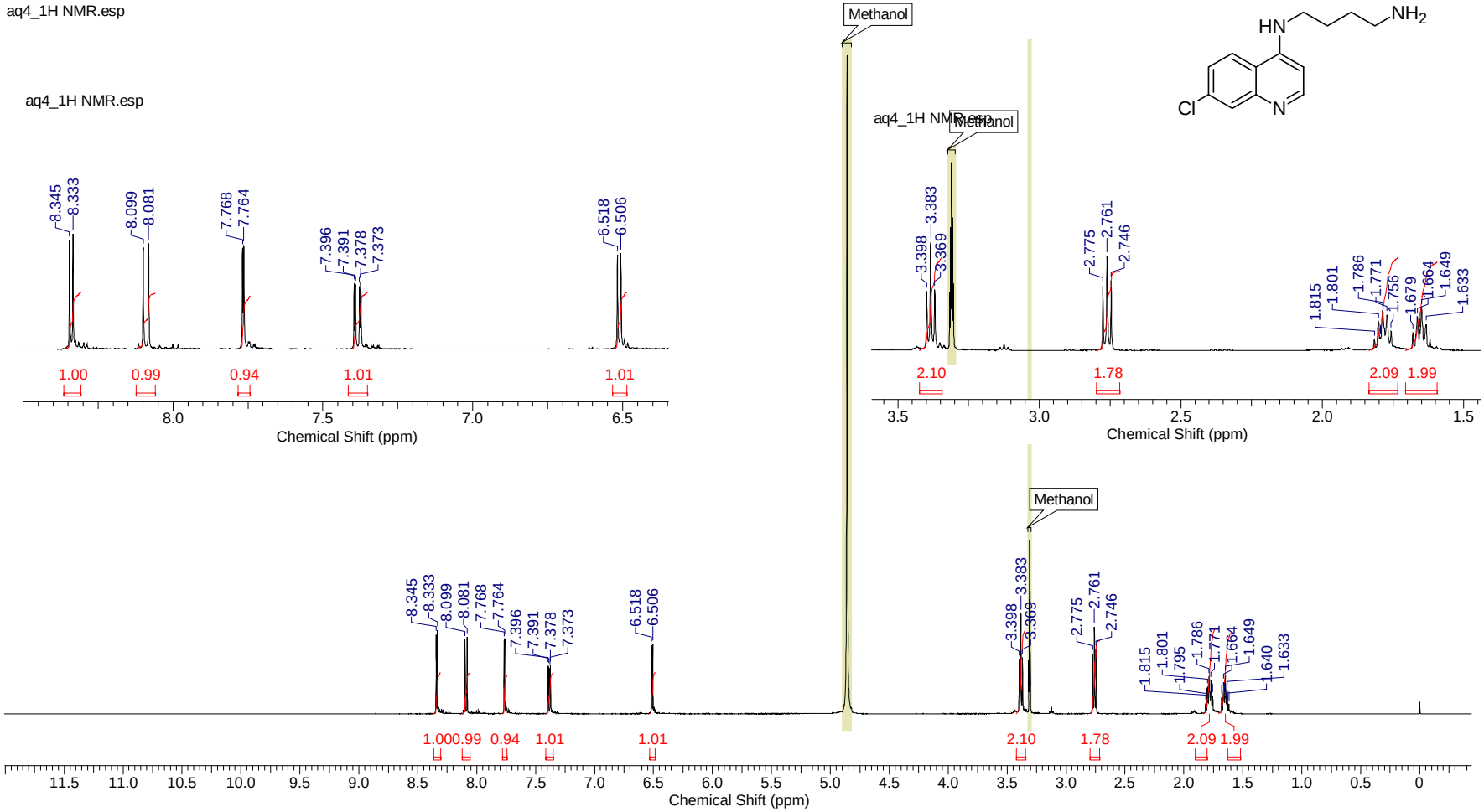

Compound 2: ^{13}C NMR spectrum (500 MHz, CD_3OD)

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Frequency (MHz)	125.79	***Nucleus***	13C	***Number of Transients***	2103	***Origin***	spect
Original Points Count	16384	***Owner***	nmrsu	***Points Count***	32768	***Pulse Sequence***	zgpg30
Receiver Gain	2050.00	***SW(cyclical) (Hz)***	29761.90	***Solvent***	METHANOL-d4	***Spectrum Offset (Hz)***	14031.4922
Spectrum Type	STANDARD	***Sweep Width (Hz)***	29761.00	***Temperature (degree C)***	25.000		

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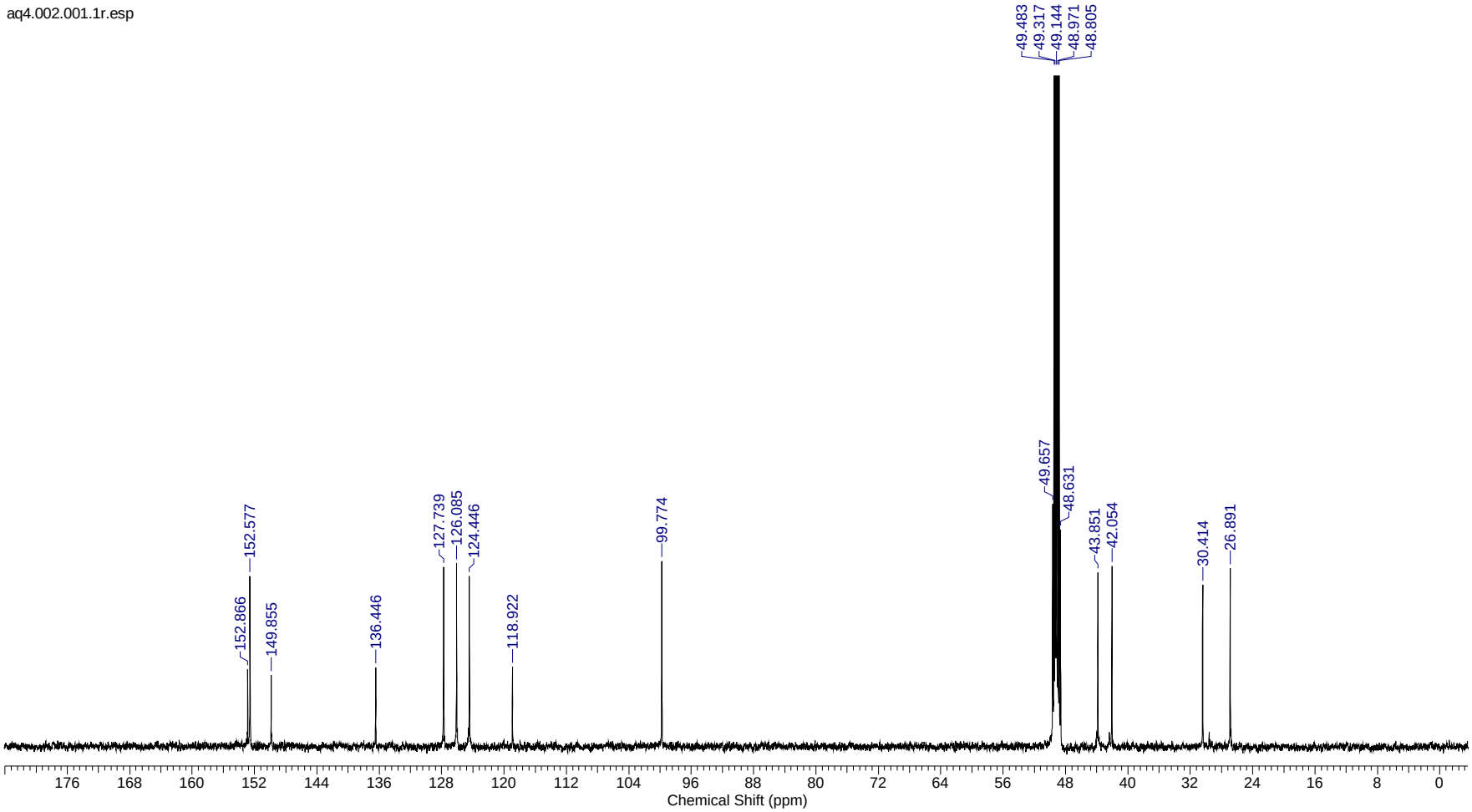
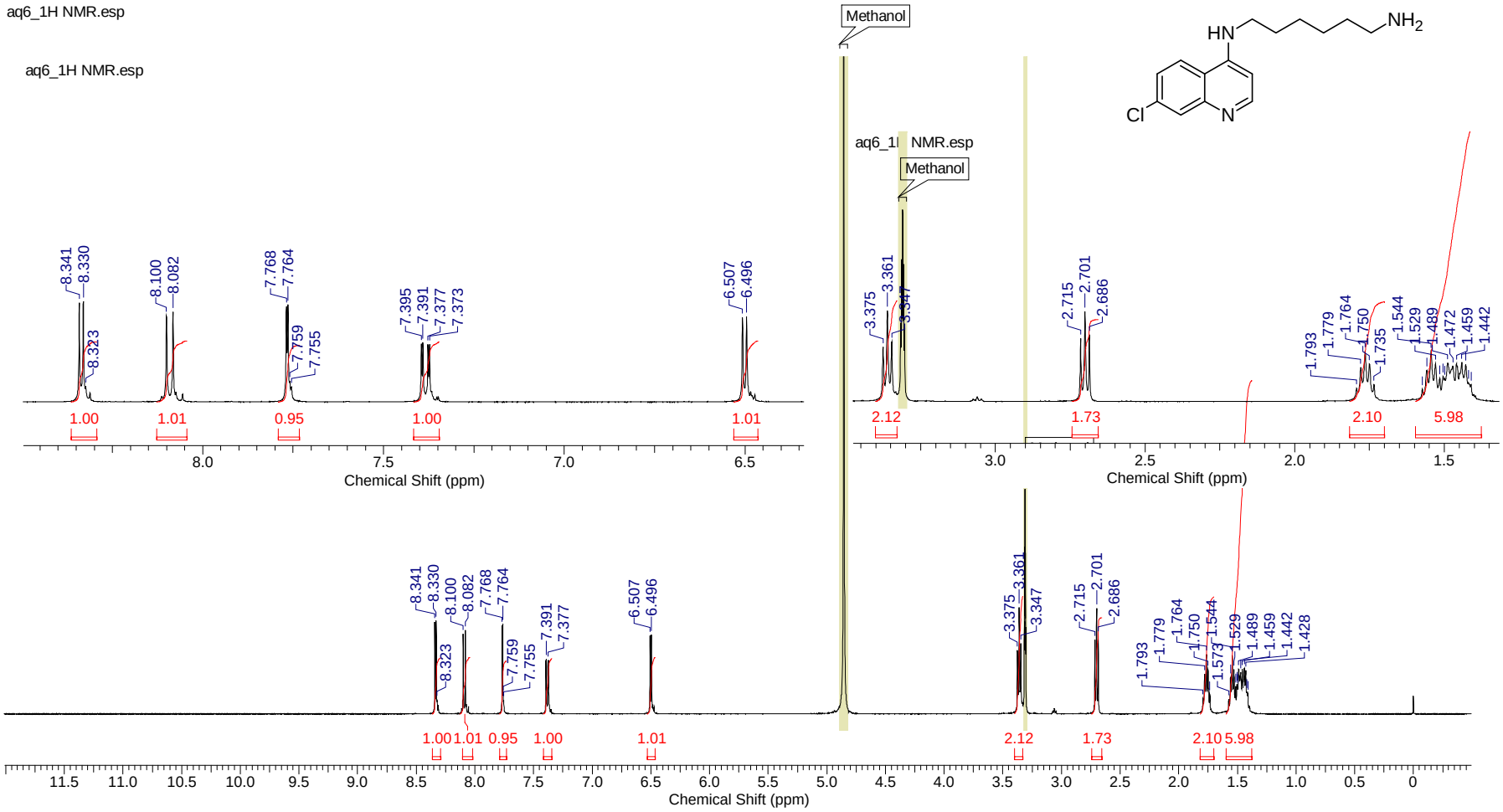


Compound 3: ^{1}H NMR spectrum (500 MHz, CD_3OD)

Acquisition Time (sec)	2.1823	***Comment***	5 mm BBO BB-1H/D Z-GRD Z8007/0118			***Date***	28 Oct 2015 10:42:24
Date Stamp	28 Oct 2015 10:42:24			***File Name***	C:\Users\Dejan Opsenica\Documents\Radni dnevnik\AQ 6\aq6\1\pdata\1\1r		
Frequency (MHz)	500.26	***Nucleus***	1H	***Number of Transients***	10	***Origin***	spect
Original Points Count	16384	***Owner***	nmrsu	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	406.00	***SW(cyclical) (Hz)***	7507.51	***Solvent***	METHANOL-d4	***Spectrum Offset (Hz)***	3492.6926
Spectrum Type	STANDARD	***Sweep Width (Hz)***	7507.28	***Temperature (degree C)***	25.000		



Compound 3: ^{13}C NMR spectrum (500 MHz, CD_3OD)

Acquisition Time (sec)	0.5505	***Comment***	5 mm BBO BB-1H/D Z-GRD Z8007/0118			***Date***	28 Oct 2015 10:42:24
Date Stamp	28 Oct 2015 10:42:24			***File Name***	C:\Users\Dejan Opsenica\Documents\Radni dnevnik\AQ 6\aq6\2\pdata\1\1r		
Frequency (MHz)	125.79	***Nucleus***	13C	***Number of Transients***	134	***Origin***	spect
Original Points Count	16384	***Owner***	nmrsu	***Points Count***	32768	***Pulse Sequence***	zgpg30
Receiver Gain	2050.00	***SW(cyclical) (Hz)***	29761.90	***Solvent***	METHANOL-d4	***Spectrum Offset (Hz)***	14031.4922
Spectrum Type	STANDARD	***Sweep Width (Hz)***	29761.00	***Temperature (degree C)***	25.200		

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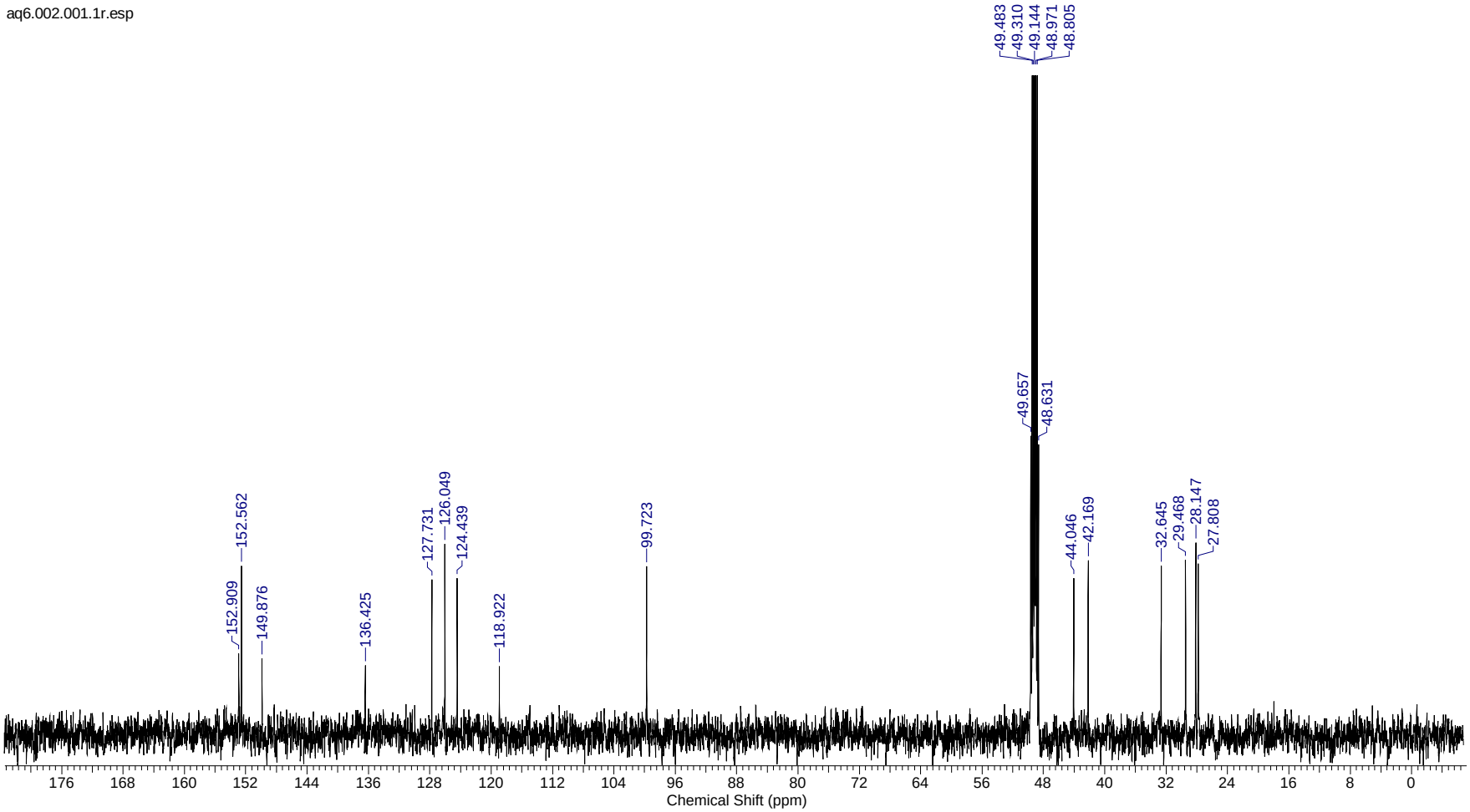
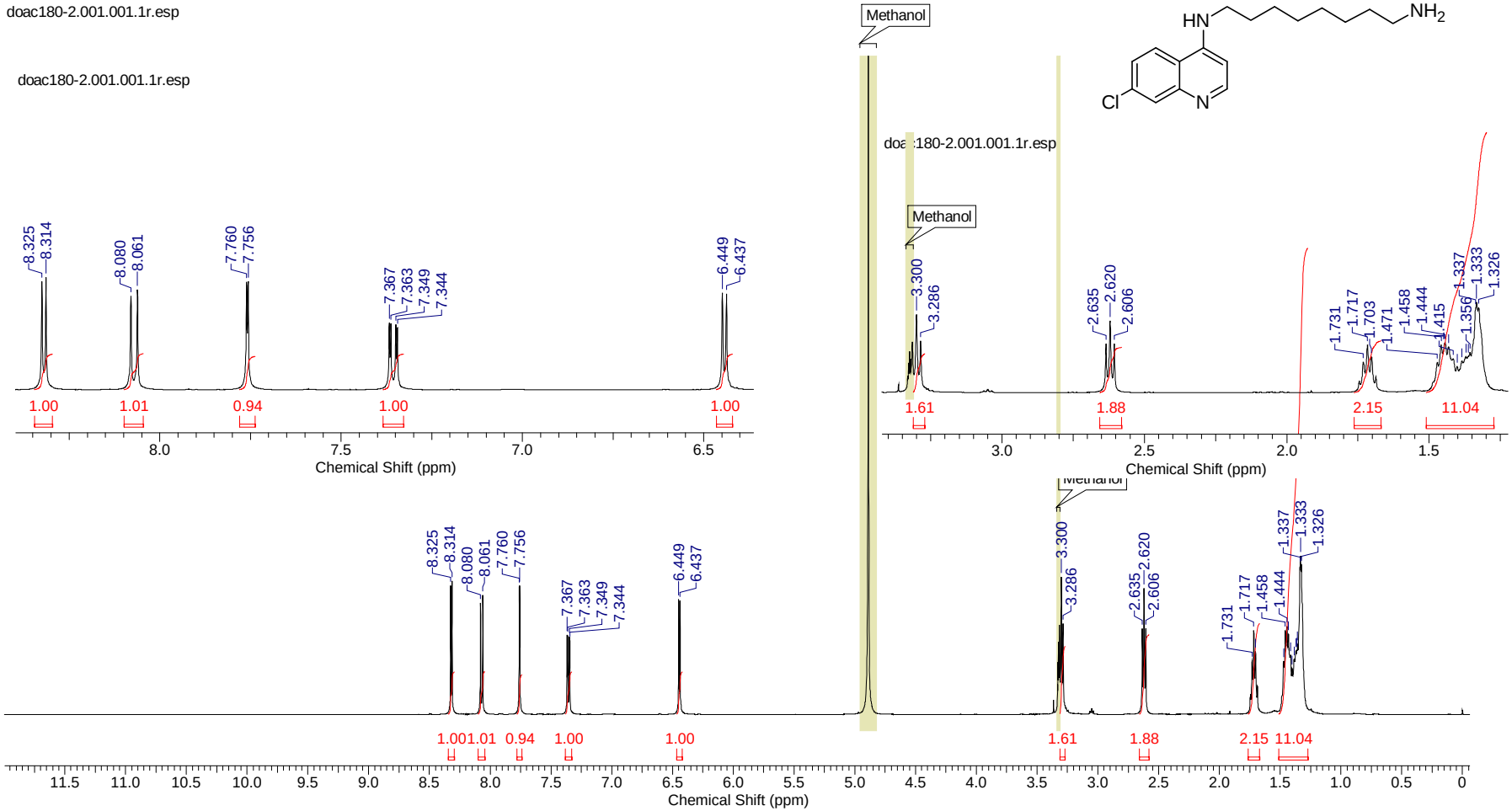


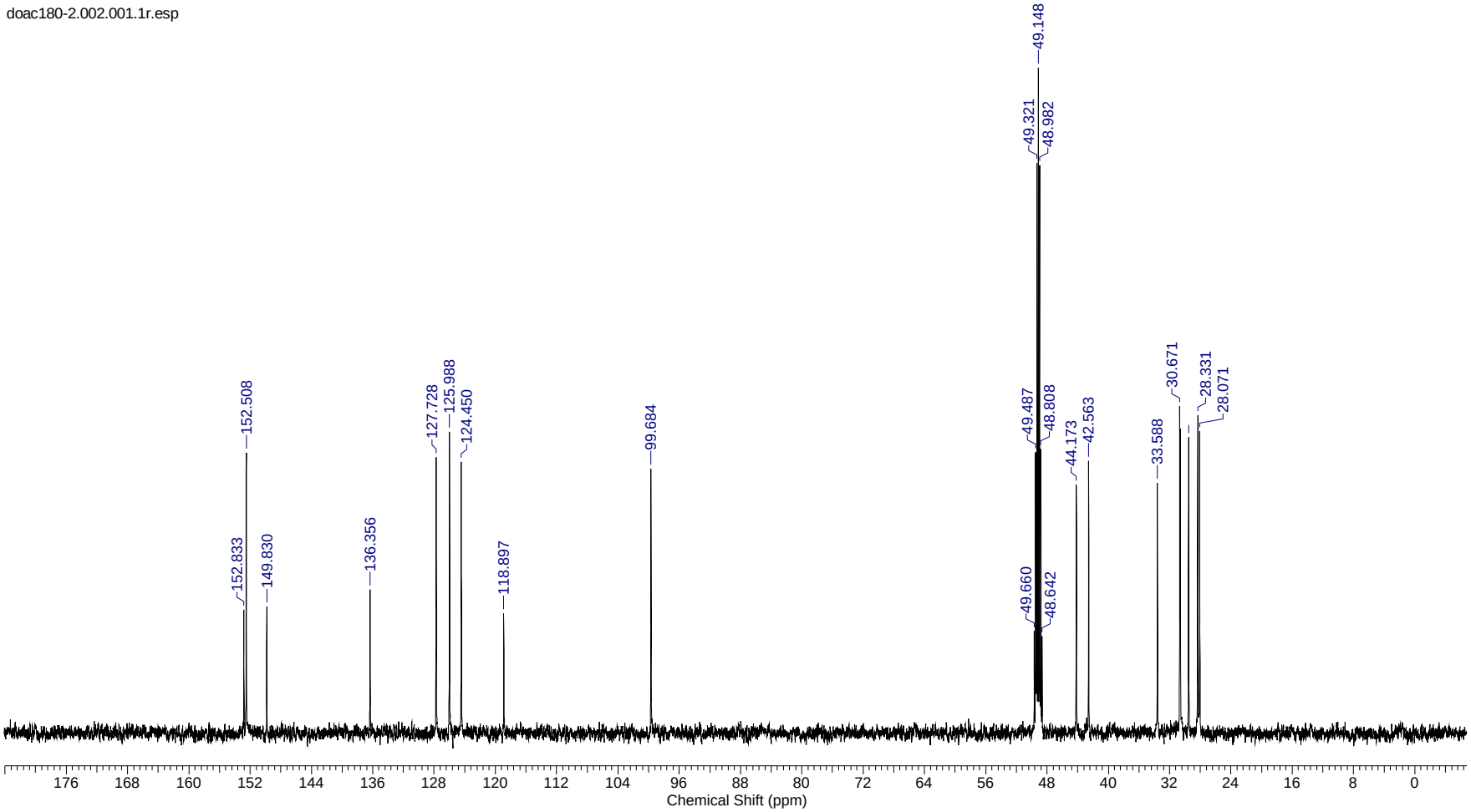
Compound 4: ^{1}H NMR spectrum (500 MHz, CD_3OD)

Acquisition Time (sec)	2.1823	***Comment***	5 mm BBO BB-1H/D Z-GRD Z8007/0118			***Date***	07 Sep 2015 10:00:00
Date Stamp	07 Sep 2015 10:00:00			***File Name***	C:\Users\Dejan Opsenica\Documents\Radni dnevnik\DOAC\DOAC180\doac180-2\1\pdata\1\1r		
Frequency (MHz)	500.26	***Nucleus***	1H	***Number of Transients***	64	***Origin***	spect
Original Points Count	16384	***Owner***	nmrsu	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	71.80	***SW(cyclical) (Hz)***	7507.51	***Solvent***	METHANOL-d4	***Spectrum Offset (Hz)***	3499.8916
Spectrum Type	STANDARD	***Sweep Width (Hz)***	7507.28	***Temperature (degree C)***	25.000		



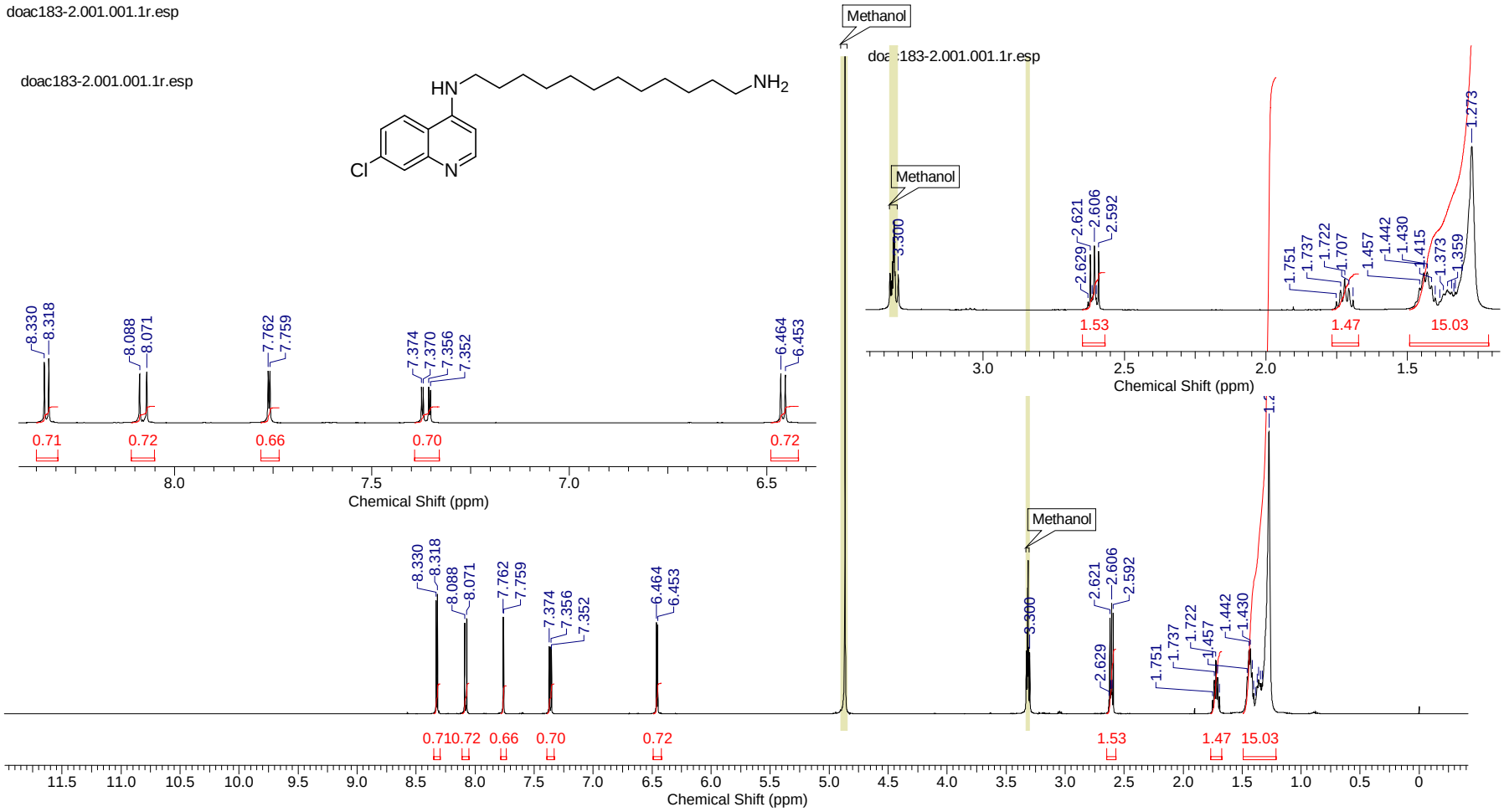
Compound 4: ^{13}C NMR spectrum (500 MHz, CD_3OD)

Acquisition Time (sec)	0.5505	***Comment***	5 mm BBO BB-1H/D Z-GRD Z8007/0118			***Date***	07 Sep 2015 10:04:16
Date Stamp	07 Sep 2015 10:04:16			***File Name***	C:\Users\Dejan Opsenica\Documents\Radni dnevnik\DOAC\DOAC180\doac180-2\2\pdata\1\1r		
Frequency (MHz)	125.79	***Nucleus***	13C	***Number of Transients***	116	***Origin***	spect
Original Points Count	16384	***Owner***	nmrsu	***Points Count***	32768	***Pulse Sequence***	zgpg30
Receiver Gain	2050.00	***SW(cyclical) (Hz)***	29761.90	***Solvent***	METHANOL-d4	***Spectrum Offset (Hz)***	14029.2275
Spectrum Type	STANDARD	***Sweep Width (Hz)***	29761.00	***Temperature (degree C)***	25.000		



Compound 5: ^{1}H NMR spectrum (500 MHz, CD_3OD)

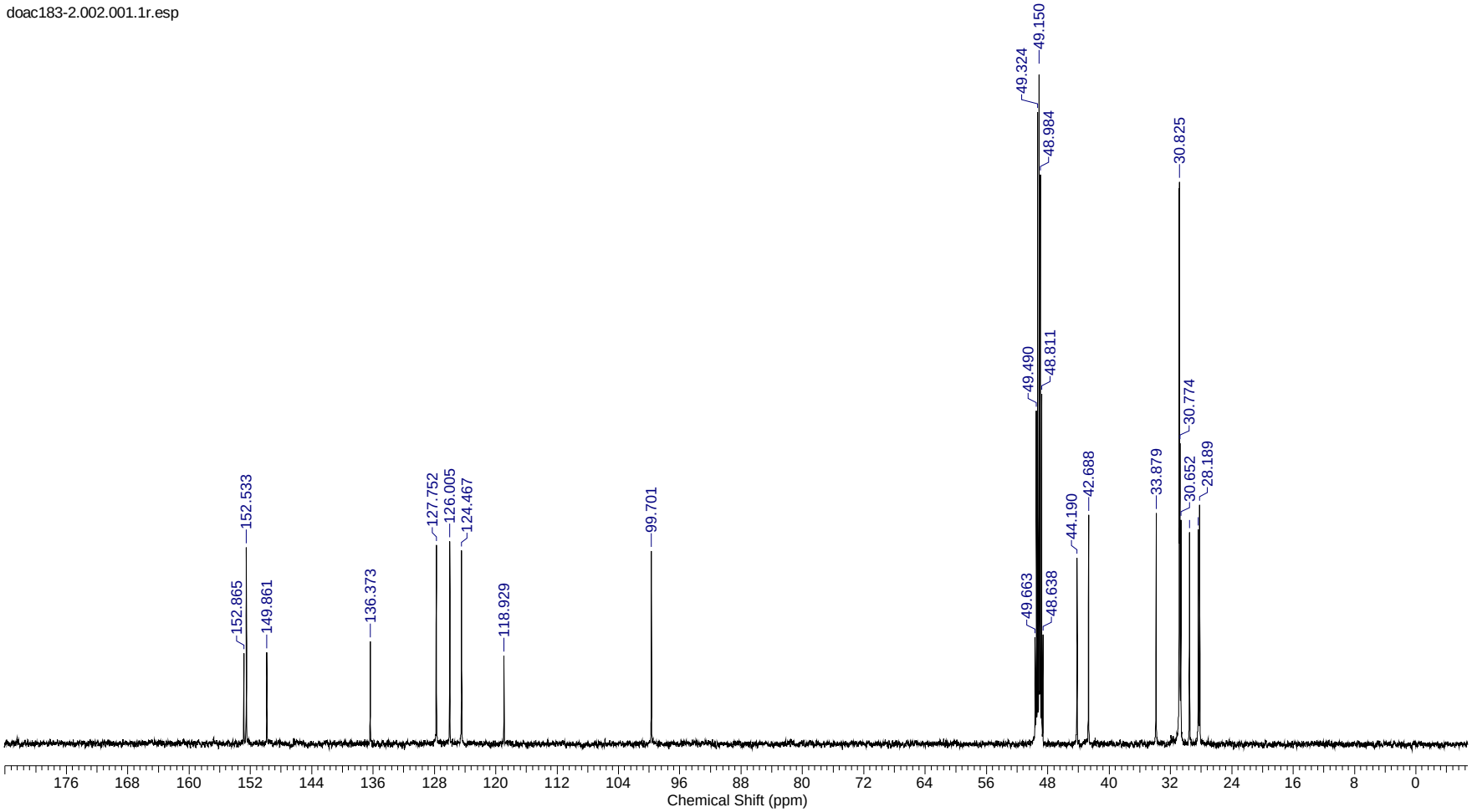
Acquisition Time (sec)	2.1823	***Comment***	5 mm BBO BB-1H/D Z-GRD Z8007/0118			***Date***	07 Sep 2015 10:10:40
Date Stamp	07 Sep 2015 10:10:40			***File Name***	C:\Users\Dejan Opsenica\Documents\Radni dnevnik\DOAC\DOAC183\doac183-2\1\pdata\1\1r		
Frequency (MHz)	500.26	***Nucleus***	1H	***Number of Transients***	14	***Origin***	spect
Original Points Count	16384	***Owner***	nmrsu	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	71.80	***SW(cyclical) (Hz)***	7507.51	***Solvent***	METHANOL-d4	***Spectrum Offset (Hz)***	3496.1145
Spectrum Type	STANDARD	***Sweep Width (Hz)***	7507.28	***Temperature (degree C)***	25.000		



Compound 5: ^{13}C NMR spectrum (500 MHz, CD_3OD)

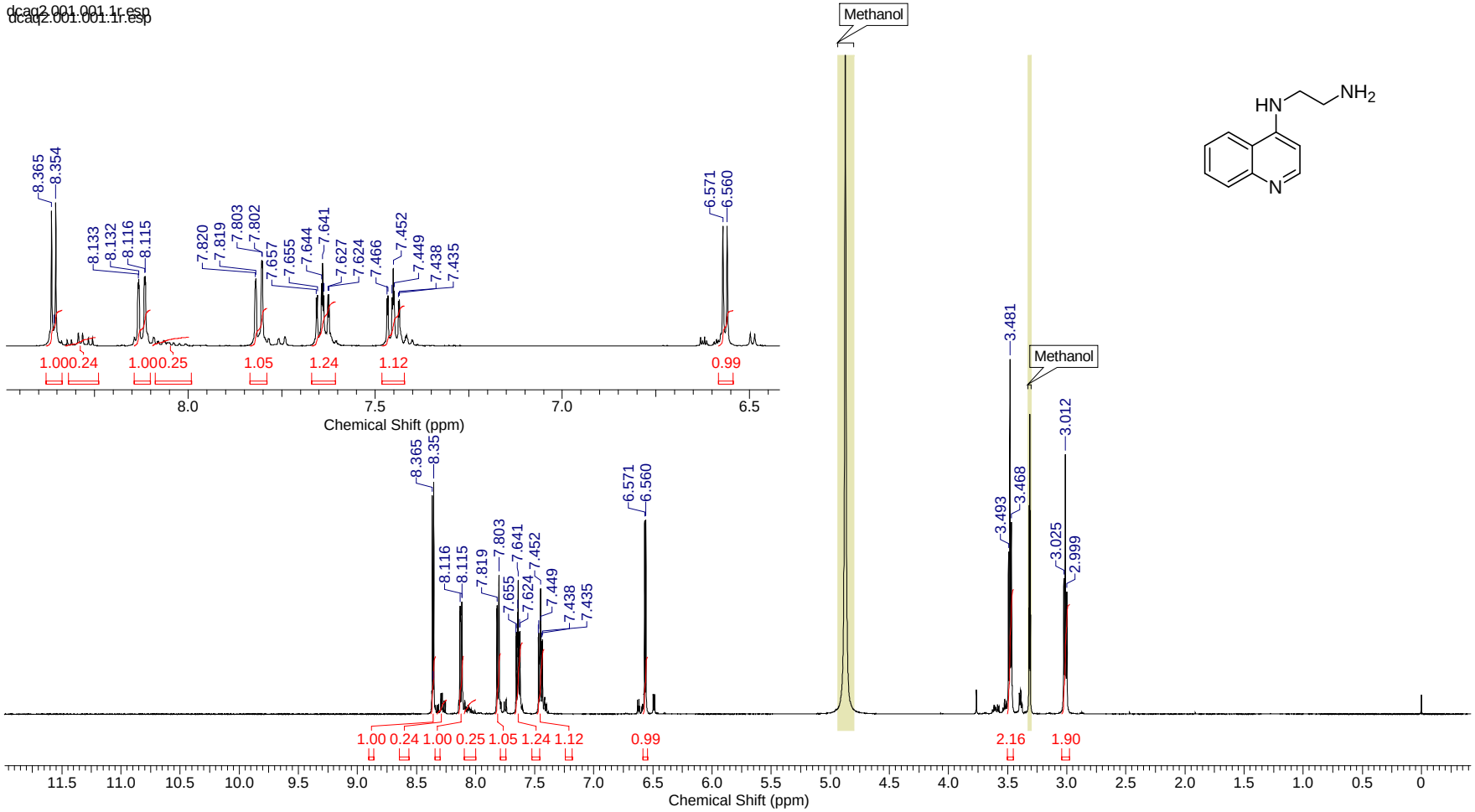
Acquisition Time (sec)	0.5505	*Comment*	5 mm BBO BB-1H/D Z-GRD Z8007/0118			*Date*	07 Sep 2015 10:12:48
Date Stamp	07 Sep 2015 10:12:48			*File Name*	C:\Users\Dejan Opsenica\Documents\Radni dnevnik\DOAC\DOAC183\doac183-2\2\pdata\1\1r		
Frequency (MHz)	125.79	*Nucleus*	13C	*Number of Transients*	973	*Origin*	spect
Original Points Count	16384	*Owner*	nmrsu	*Points Count*	32768	*Pulse Sequence*	zgpg30
Receiver Gain	2050.00	*SW(cyclical) (Hz)*	29761.90	*Solvent*	METHANOL-d4	*Spectrum Offset (Hz)*	14030.4727
Spectrum Type	STANDARD	*Sweep Width (Hz)*	29761.00	*Temperature (degree C)*	25.100		

doac183-2.002.001.1r.esp



Compound 6: ^{1}H NMR spectrum (500 MHz, CD_3OD)

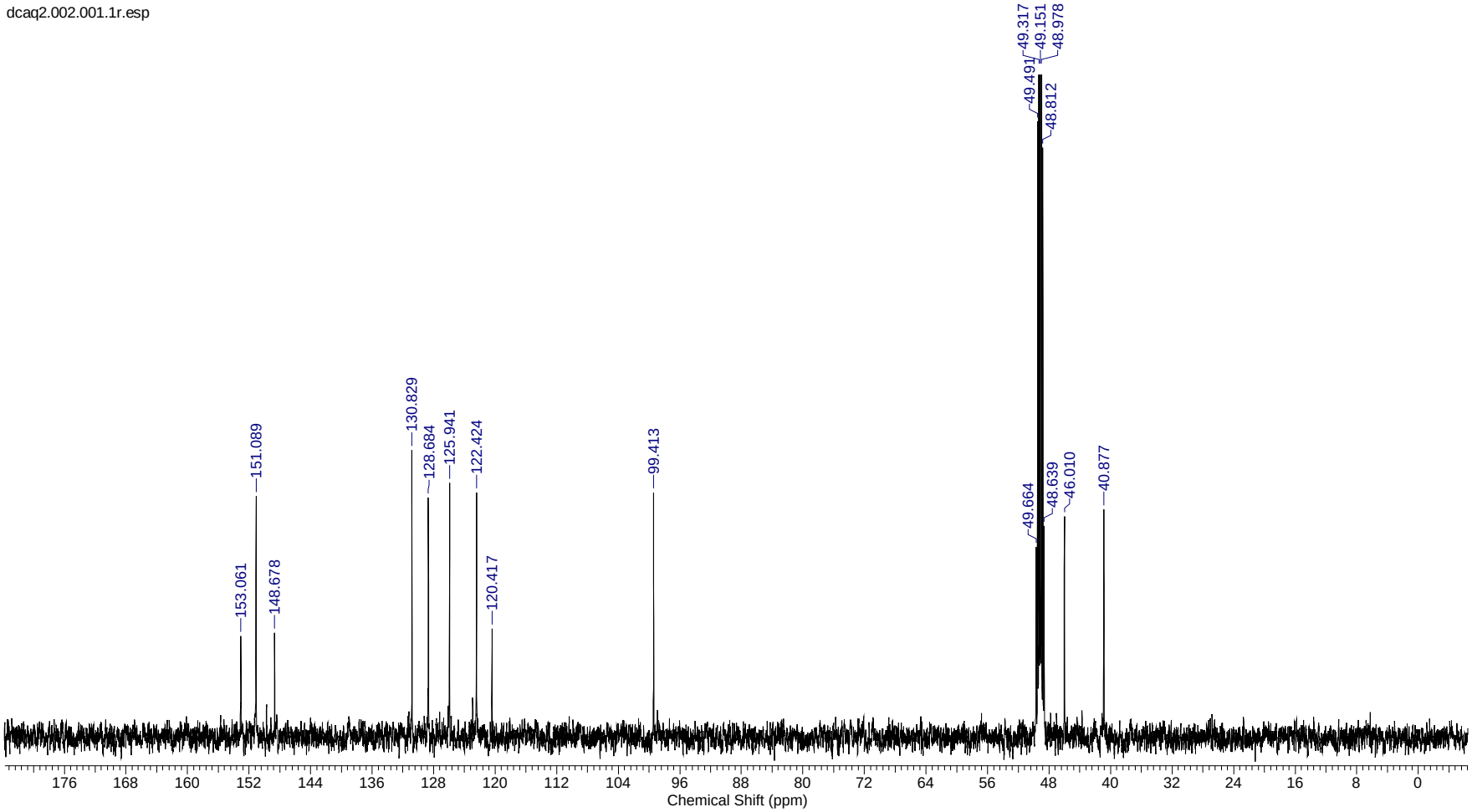
Acquisition Time (sec)	2.1823	***Comment***	5 mm BBO BB-1H/D Z-GRD Z8007/0118			***Date***	28 Oct 2015 10:23:12
Date Stamp	28 Oct 2015 10:23:12			***File Name***	C:\Users\Dejan Opsenica\Documents\Radni dnevnik\DCAQ2\dcaq2\1\pdata\1\1r		
Frequency (MHz)	500.26	***Nucleus***	1H	***Number of Transients***	16	***Origin***	spect
Original Points Count	16384	***Owner***	nmrsu	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	406.00	***SW(cyclical) (Hz)***	7507.51	***Solvent***	METHANOL-d4	***Spectrum Offset (Hz)***	3494.4385
Spectrum Type	STANDARD	***Sweep Width (Hz)***	7507.28	***Temperature (degree C)***	25.000		



Compound 6: ^{13}C NMR spectrum (500 MHz, CD_3OD)

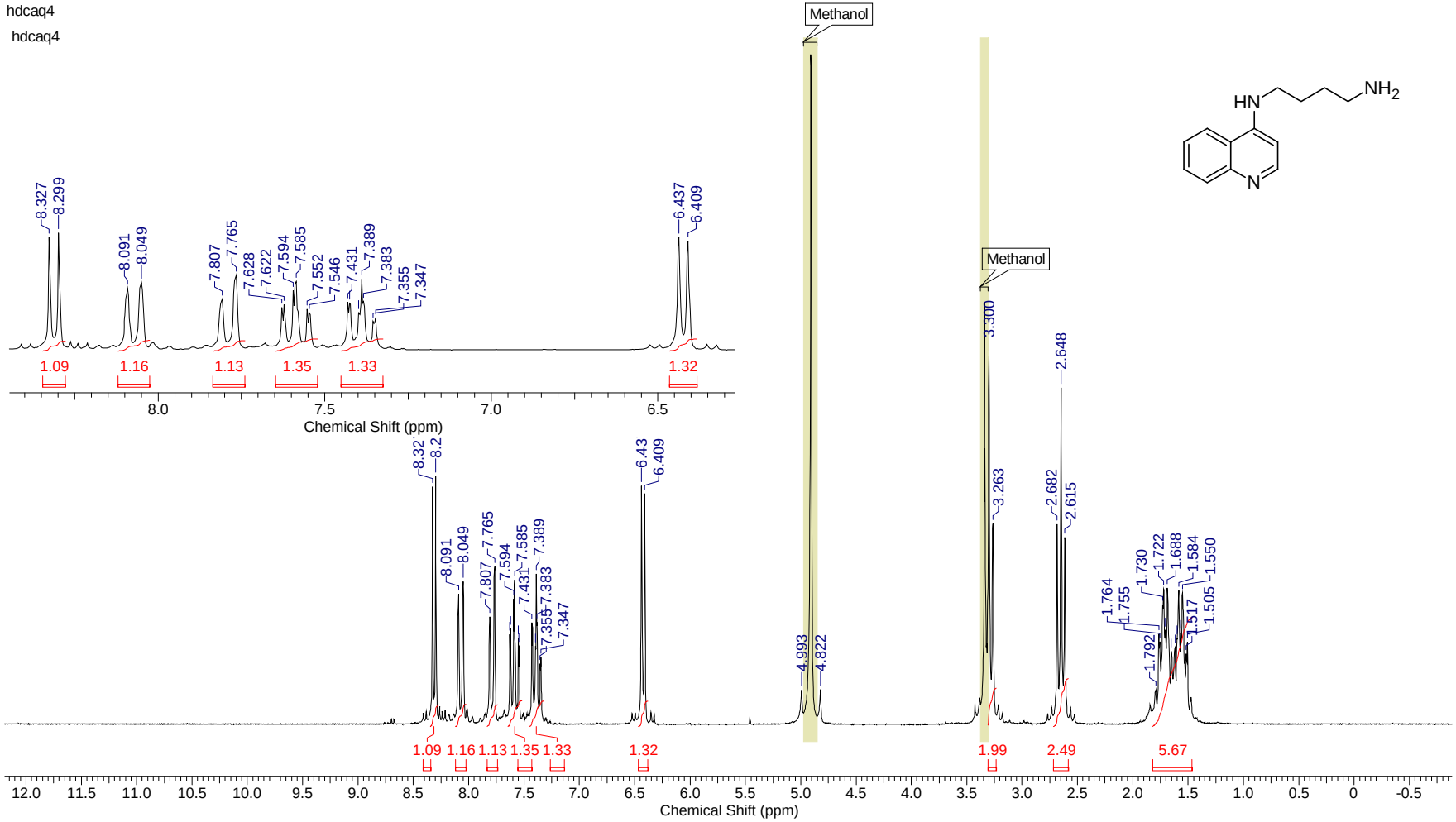
Acquisition Time (sec)	0.5505	***Comment***	5 mm BBO BB-1H/D Z-GRD Z8007/0118			***Date***	28 Oct 2015 10:27:28
Date Stamp	28 Oct 2015 10:27:28			***File Name***	C:\Users\Dejan Opsenica\Documents\Radni dnevnik\DCAQ2\dcaq2\2\pdata\1\1r		
Frequency (MHz)	125.79	***Nucleus***	13C	***Number of Transients***	114	***Origin***	spect
Original Points Count	16384	***Owner***	nmrsu	***Points Count***	32768	***Pulse Sequence***	zgpg30
Receiver Gain	2050.00	***SW(cyclical) (Hz)***	29761.90	***Solvent***	METHANOL-d4	***Spectrum Offset (Hz)***	14031.4922
Spectrum Type	STANDARD	***Sweep Width (Hz)***	29761.00	***Temperature (degree C)***	25.000		

dcaq2.002.001.1r.esp



Compound 7: ^{1}H NMR spectrum (500 MHz, CD_3OD)

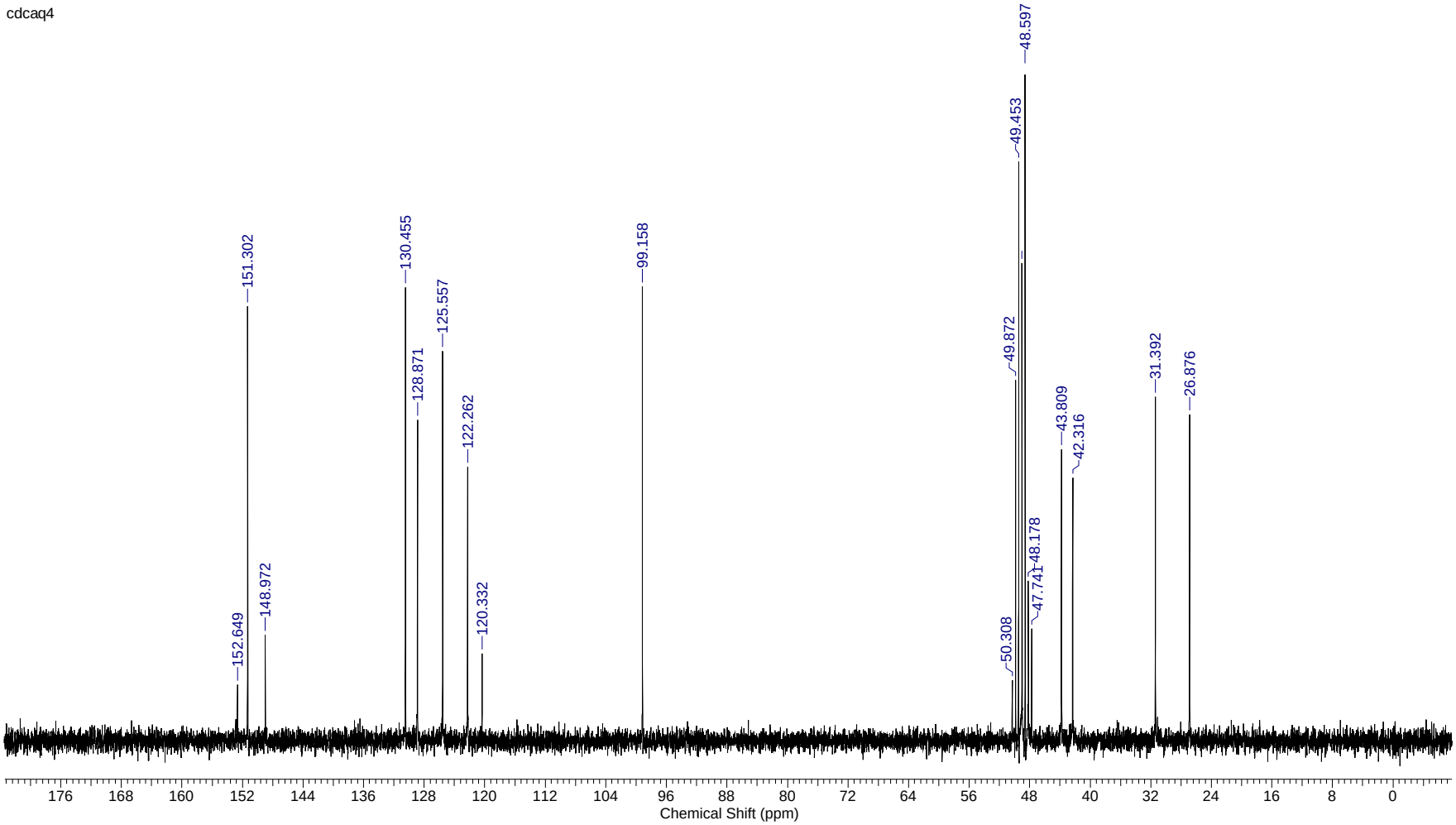
Acquisition Time (sec)	1.4400	***Comment***	DCAQ4	***Date***	Nov 1 13	***Date Stamp***	Nov 1 13
File Name	C:\Users\Dejan Opsenica\Documents\Radni dnevnik\DCAQ4\dcaq4\hdcaq4.fid\fid					***Frequency (MHz)***	199.97
Nucleus	1H	***Number of Transients***	64	***Original Points Count***	6624	***Points Count***	8192
Pulse Sequence	s2pul	***Receiver Gain***	2.00	***Solvent***	METHANOL-d4		
Spectrum Offset (Hz)	1682.8494	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	4600.00	***Temperature (degree C)***	AMBIENT TEMPERATURE



Compound 7: ^{13}C NMR spectrum (500 MHz, CD_3OD)

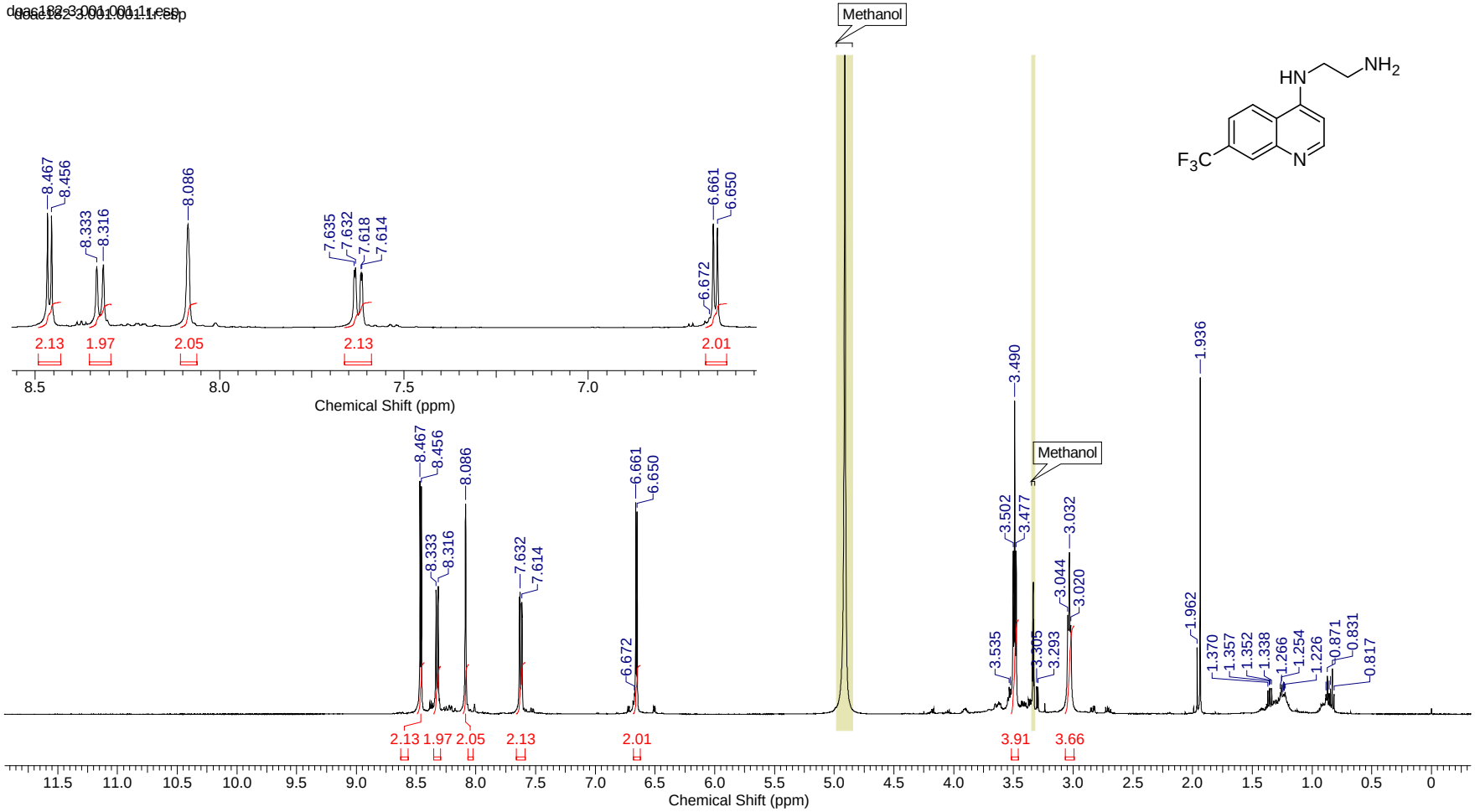
Acquisition Time (sec)	1.0667	***Comment***	DSAQ4	***Date***	Nov 1 13	***Date Stamp***	Nov 1 13
File Name	C:\Users\Dejan Opsenica\Documents\Radni dnevnik\DCAQ4\dcaq4\cdcaq4.fid\fid					***Frequency (MHz)***	50.29
Nucleus	13C	***Number of Transients***	363	***Original Points Count***	16000	***Points Count***	16384
Pulse Sequence	s2pul	***Receiver Gain***	25.00	***Solvent***	METHANOL-d4	***Spectrum Offset (Hz)***	4919.1177
Spectrum Type	STANDARD	***Sweep Width (Hz)***	15000.00	***Temperature (degree C)***	AMBIENT TEMPERATURE		

cdcaq4



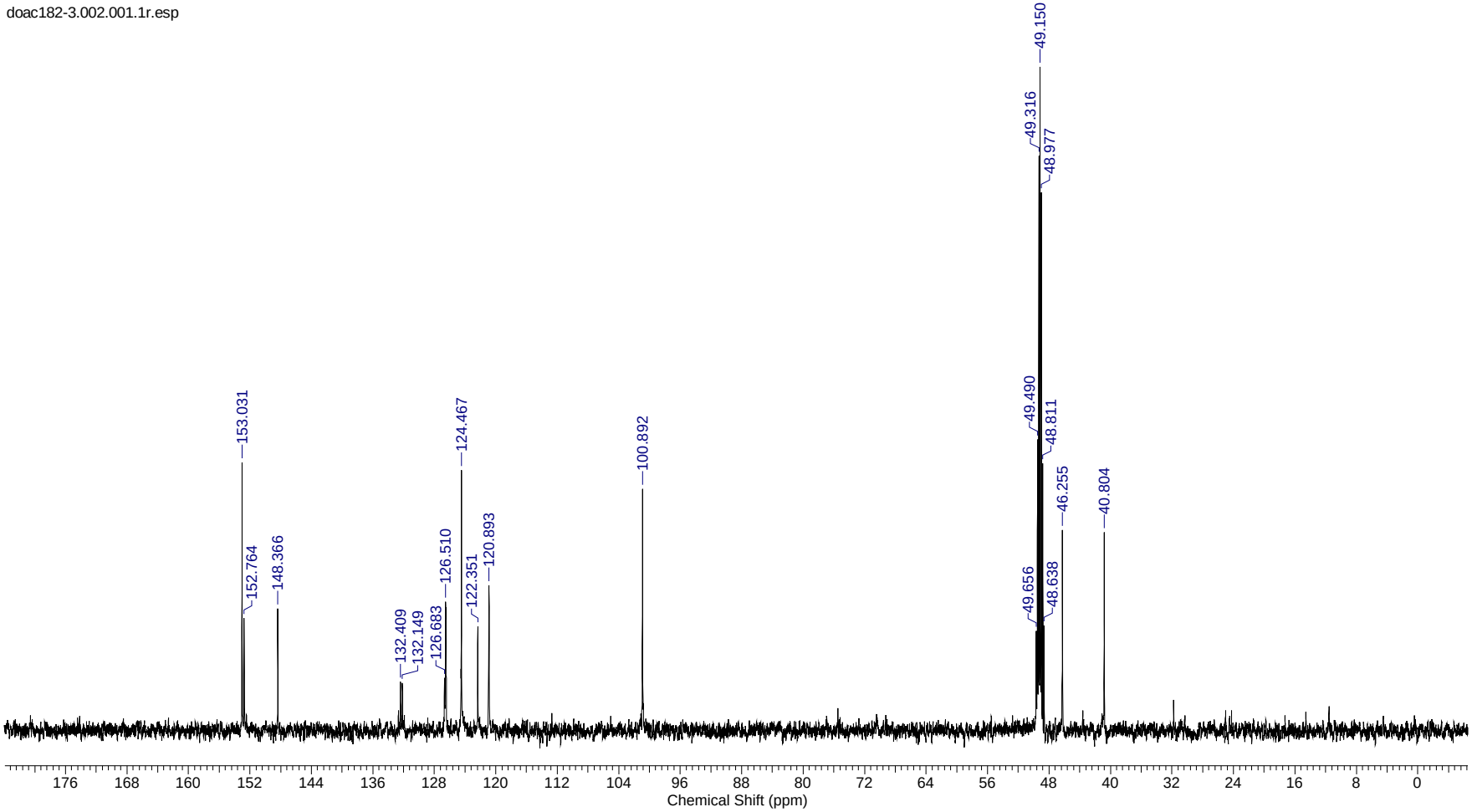
Compound 8: ^{1}H NMR spectrum (500 MHz, CD_3OD)

Acquisition Time (sec)	2.1823	***Comment***	5 mm BBO BB-1H/D Z-GRD Z8007/0118			***Date***	07 Sep 2015 09:47:12
Date Stamp	07 Sep 2015 09:47:12			***File Name***	C:\Users\Dejan Opsenica\Documents\Radni dnevnik\DOAC\DOAC182\doac182-3\1\pdata\1\1r		
Frequency (MHz)	500.26	***Nucleus***	1H	***Number of Transients***	11	***Origin***	spect
Original Points Count	16384	***Owner***	nmrsu	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	71.80	***SW(cyclical) (Hz)***	7507.51	***Solvent***	METHANOL-d4	***Spectrum Offset (Hz)***	3504.8240
Spectrum Type	STANDARD	***Sweep Width (Hz)***	7507.28	***Temperature (degree C)***	25.000		



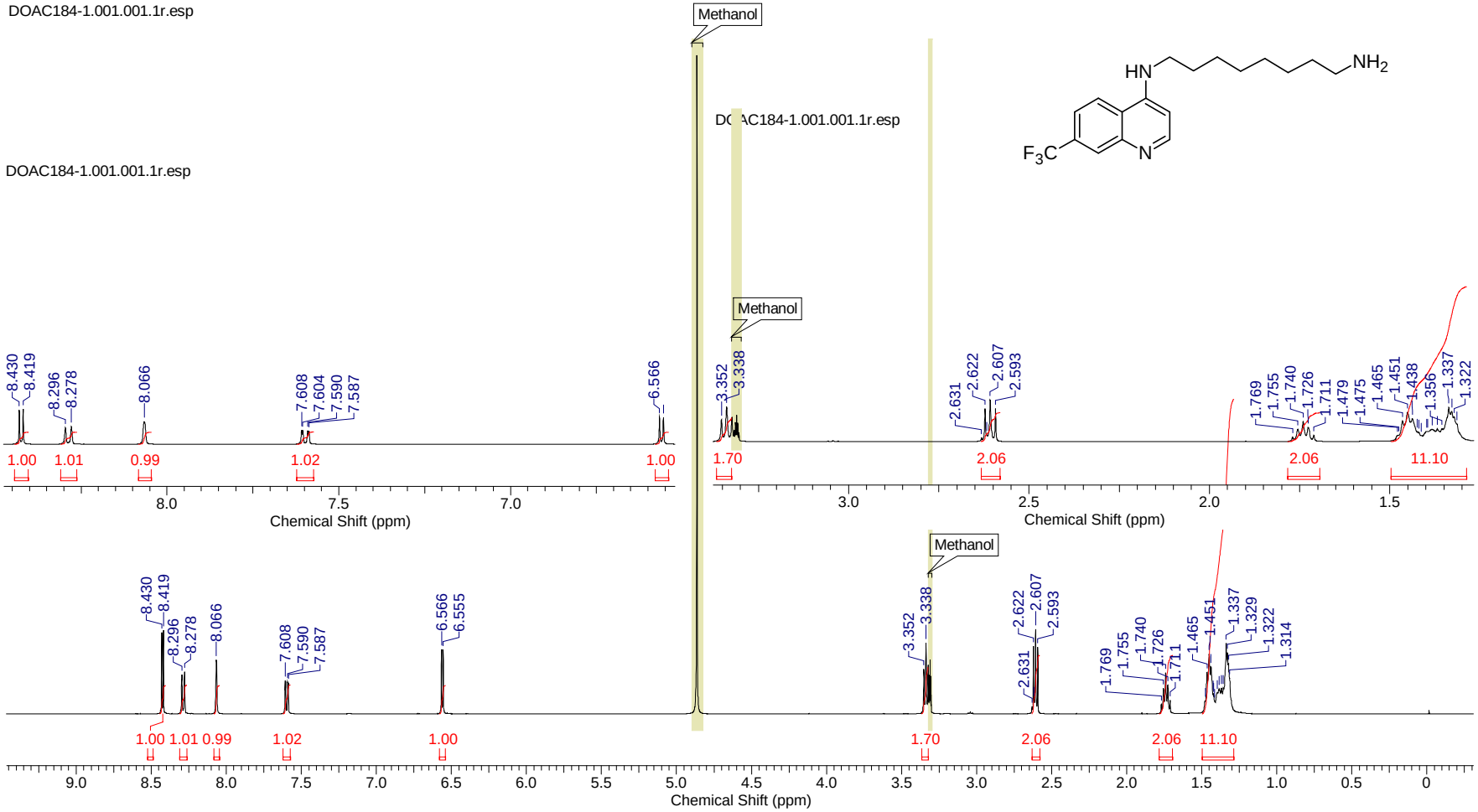
Compound 8: ^{13}C NMR spectrum (500 MHz, CD_3OD)

Acquisition Time (sec)	0.5505	***Comment***	5 mm BBO BB-1H/D Z-GRD Z8007/0118			***Date***	07 Sep 2015 09:49:20
Date Stamp	07 Sep 2015 09:49:20			***File Name***	C:\Users\Dejan Opsenica\Documents\Radni dnevnik\DOAC\DOAC182\doac182-3\2\pdata\1\1r		
Frequency (MHz)	125.79	***Nucleus***	13C	***Number of Transients***	91	***Origin***	spect
Original Points Count	16384	***Owner***	nmrsu	***Points Count***	32768	***Pulse Sequence***	zgpg30
Receiver Gain	2050.00	***SW(cyclical) (Hz)***	29761.90	***Solvent***	METHANOL-d4	***Spectrum Offset (Hz)***	14030.4727
Spectrum Type	STANDARD	***Sweep Width (Hz)***	29761.00	***Temperature (degree C)***	25.100		



Compound 9: ^{1}H NMR spectrum (500 MHz, CD_3OD)

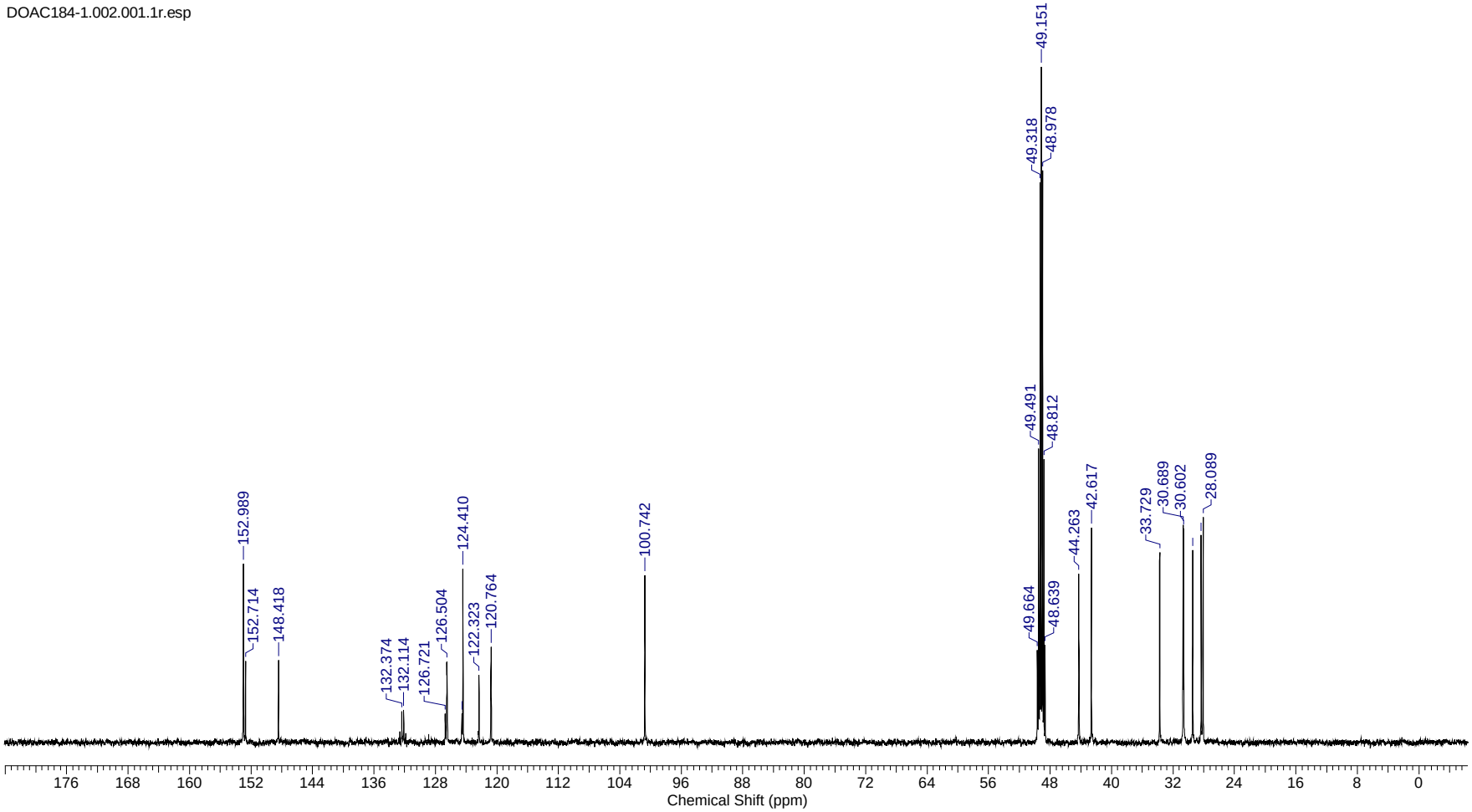
Acquisition Time (sec)	3.2768	***Comment***	5 mm BBO BB-1H/D Z-GRD Z8007/0118			***Date***	13 Oct 2015 12:27:12
Date Stamp	13 Oct 2015 12:27:12			***File Name***	C:\Users\Dejan Opsenica\Documents\Radni dnevnik\DOAC\DOAC184\DOAC184-1\1\pdata\1\1r		
Frequency (MHz)	500.26	***Nucleus***	1H	***Number of Transients***	16	***Origin***	spect
Original Points Count	16384	***Owner***	nmrsu	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	114.00	***SW(cyclical) (Hz)***	5000.00	***Solvent***	METHANOL-d4	***Spectrum Offset (Hz)***	2243.4446
Spectrum Type	STANDARD	***Sweep Width (Hz)***	4999.85	***Temperature (degree C)***	25.000		



Compound 9: ^{13}C NMR spectrum (500 MHz, CD_3OD)

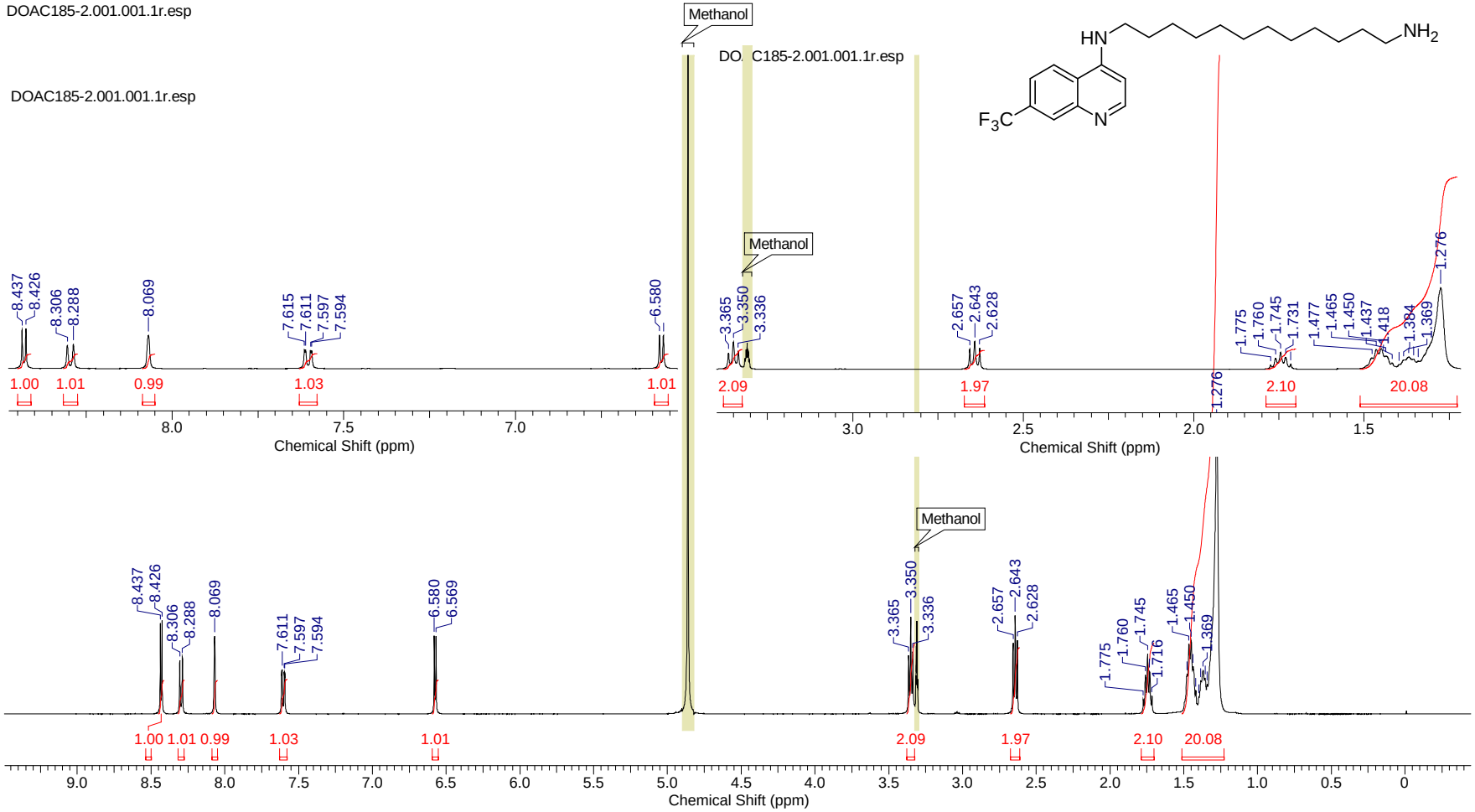
Acquisition Time (sec)	0.5505	***Comment***	5 mm BBO BB-1H/D Z-GRD Z8007/0118			***Date***	13 Oct 2015 12:31:28
Date Stamp	13 Oct 2015 12:31:28			***File Name***	C:\Users\Dejan Opsenica\Documents\Radni dnevnik\DOAC\DOAC184\DOAC184-1\2\pdata\1\1r		
Frequency (MHz)	125.79	***Nucleus***	13C	***Number of Transients***	400	***Origin***	spect
Original Points Count	16384	***Owner***	nmrsu	***Points Count***	32768	***Pulse Sequence***	zgpg30
Receiver Gain	2050.00	***SW(cyclical) (Hz)***	29761.90	***Solvent***	METHANOL-d4	***Spectrum Offset (Hz)***	14031.5176
Spectrum Type	STANDARD	***Sweep Width (Hz)***	29761.00	***Temperature (degree C)***	25.000		

DOAC184-1.002.001.1r.esp



Compound 10: ^{1}H NMR spectrum (500 MHz, CD_3OD)

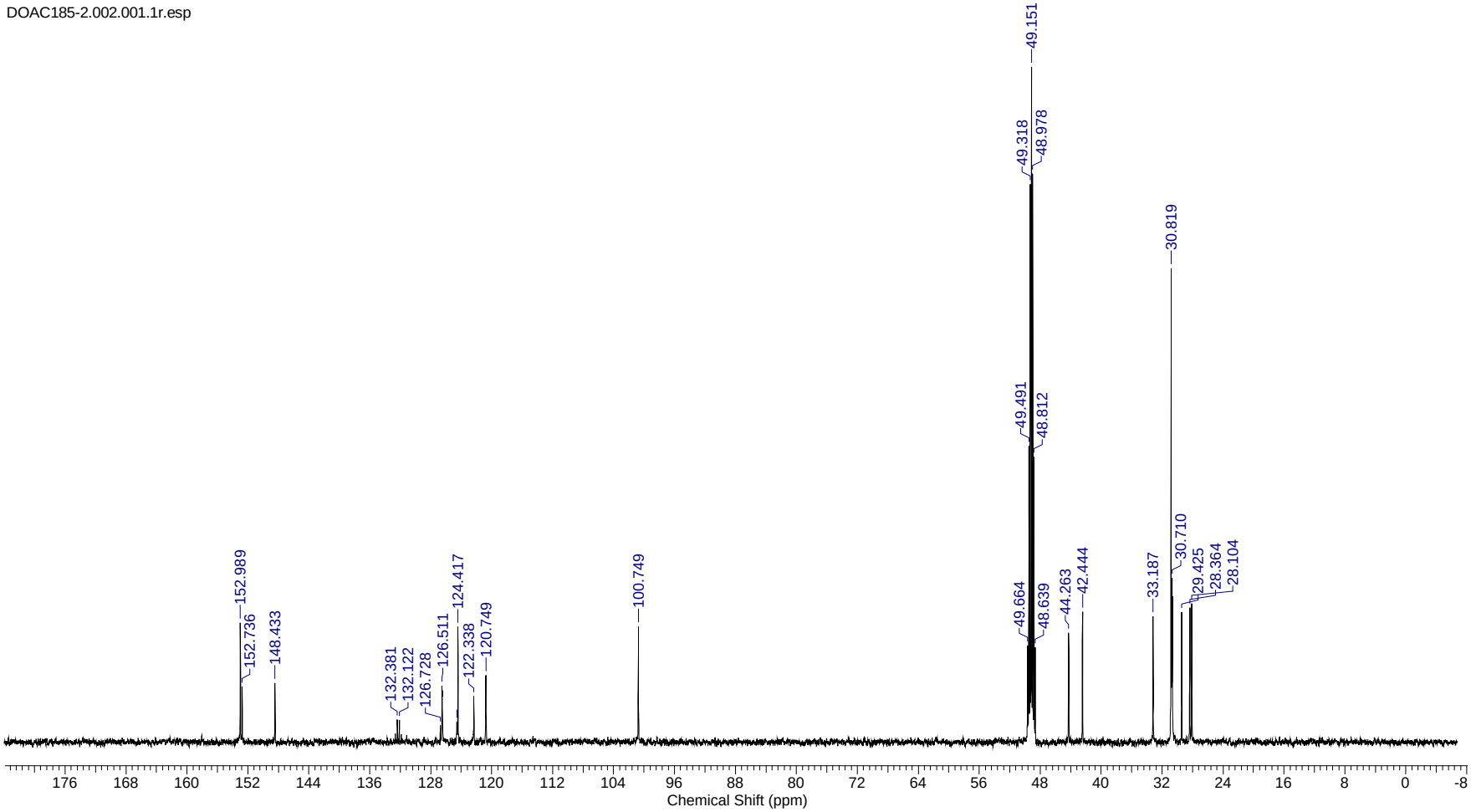
Acquisition Time (sec)	3.2768	***Comment***	5 mm BBO BB-1H/D Z-GRD Z8007/0118			***Date***	14 Oct 2015 12:22:56
Date Stamp	14 Oct 2015 12:22:56			***File Name***	C:\Users\Dejan Opsenica\Documents\Radni dnevnik\DOAC\DOAC185\DOAC185-2\1\pdata\1\1r		
Frequency (MHz)	500.26	***Nucleus***	1H	***Number of Transients***	16	***Origin***	spect
Original Points Count	16384	***Owner***	nmrsu	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	114.00	***SW(cyclical) (Hz)***	5000.00	***Solvent***	METHANOL-d4	***Spectrum Offset (Hz)***	2251.9424
Spectrum Type	STANDARD	***Sweep Width (Hz)***	4999.85	***Temperature (degree C)***	25.000		



Compound 10: ^{13}C NMR spectrum (500 MHz, CD_3OD)

Acquisition Time (sec)	0.5505	***Comment***	5 mm BBO BB-1H/D Z-GRD Z8007/0118			***Date***	14 Oct 2015 12:33:36
Date Stamp	14 Oct 2015 12:33:36			***File Name***	C:\Users\Dejan Opsenica\Documents\Radni dnevnik\DOAC\DOAC185\DOAC185-2\2\pdata\1\1r		
Frequency (MHz)	125.79	***Nucleus***	13C	***Number of Transients***	513	***Origin***	spect
Original Points Count	16384	***Owner***	nmrsu	***Points Count***	32768	***Pulse Sequence***	zgpg30
Receiver Gain	2050.00	***SW(cyclical) (Hz)***	29761.90	***Solvent***	METHANOL-d4	***Spectrum Offset (Hz)***	14031.5176
Spectrum Type	STANDARD	***Sweep Width (Hz)***	29761.00	***Temperature (degree C)***	25.000		

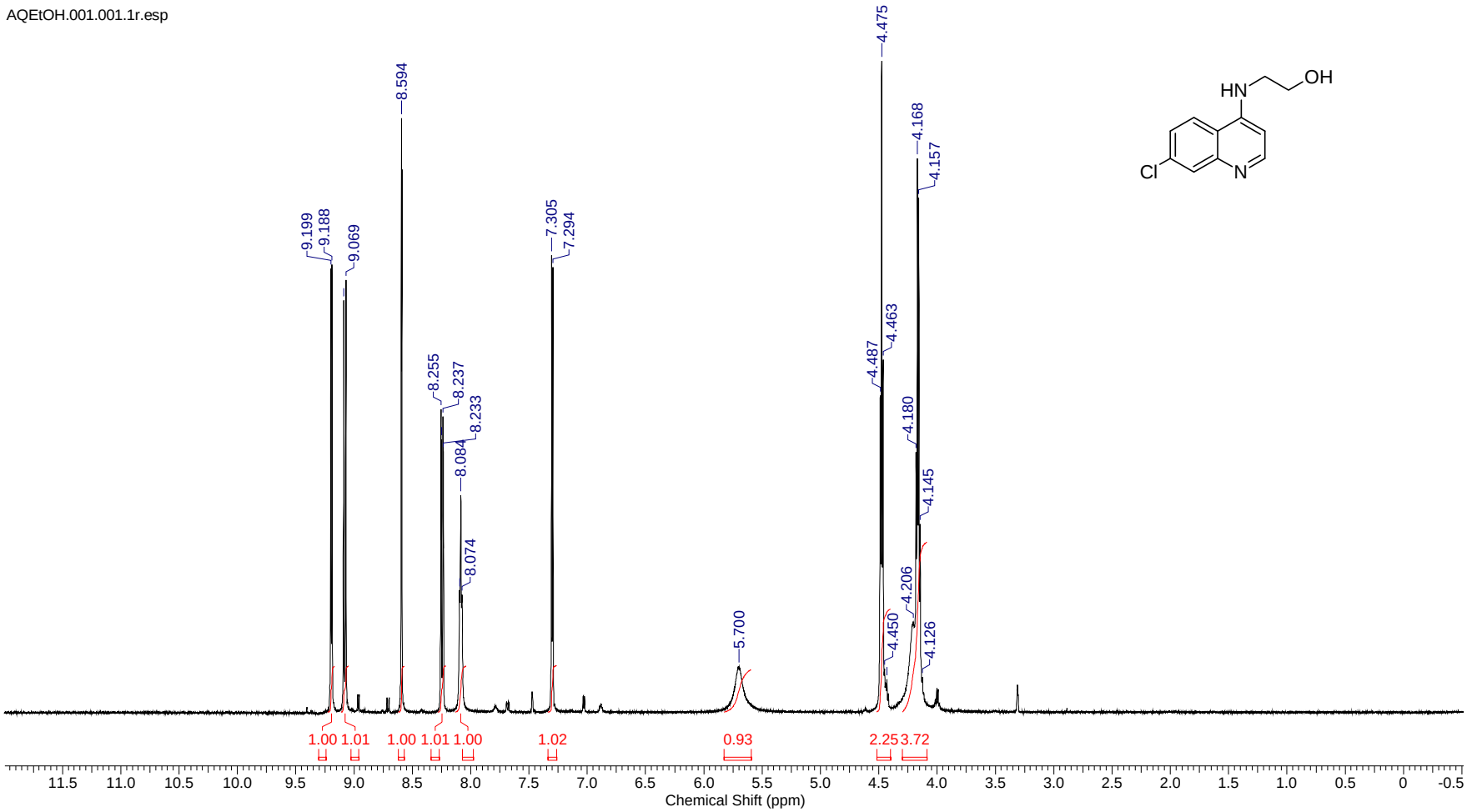
DOAC185-2.002.001.1r.esp



Compound 21: ^{1}H NMR spectrum (500 MHz, DMSO-d6)

Acquisition Time (sec)	2.1823	***Comment***	Z8007_0118 (PH BBO 500S2 BB-H-D-05 Z)			***Date***	06 Apr 2016 13:05:36
Date Stamp	06 Apr 2016 13:05:36			***File Name***	C:\Users\Dejan Opsenica\Documents\Radni dnevnik\AQEtOH\1\pdata\1\1r		
Frequency (MHz)	500.26	***Nucleus***	1H	***Number of Transients***	4	***Origin***	spect
Original Points Count	16384	***Owner***	nmrsu	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	114.00	***SW(cyclical) (Hz)***	7507.51	***Solvent***	METHANOL-d4	***Spectrum Offset (Hz)***	3496.4045
Spectrum Type	STANDARD	***Sweep Width (Hz)***	7507.28	***Temperature (degree C)***	25.000		

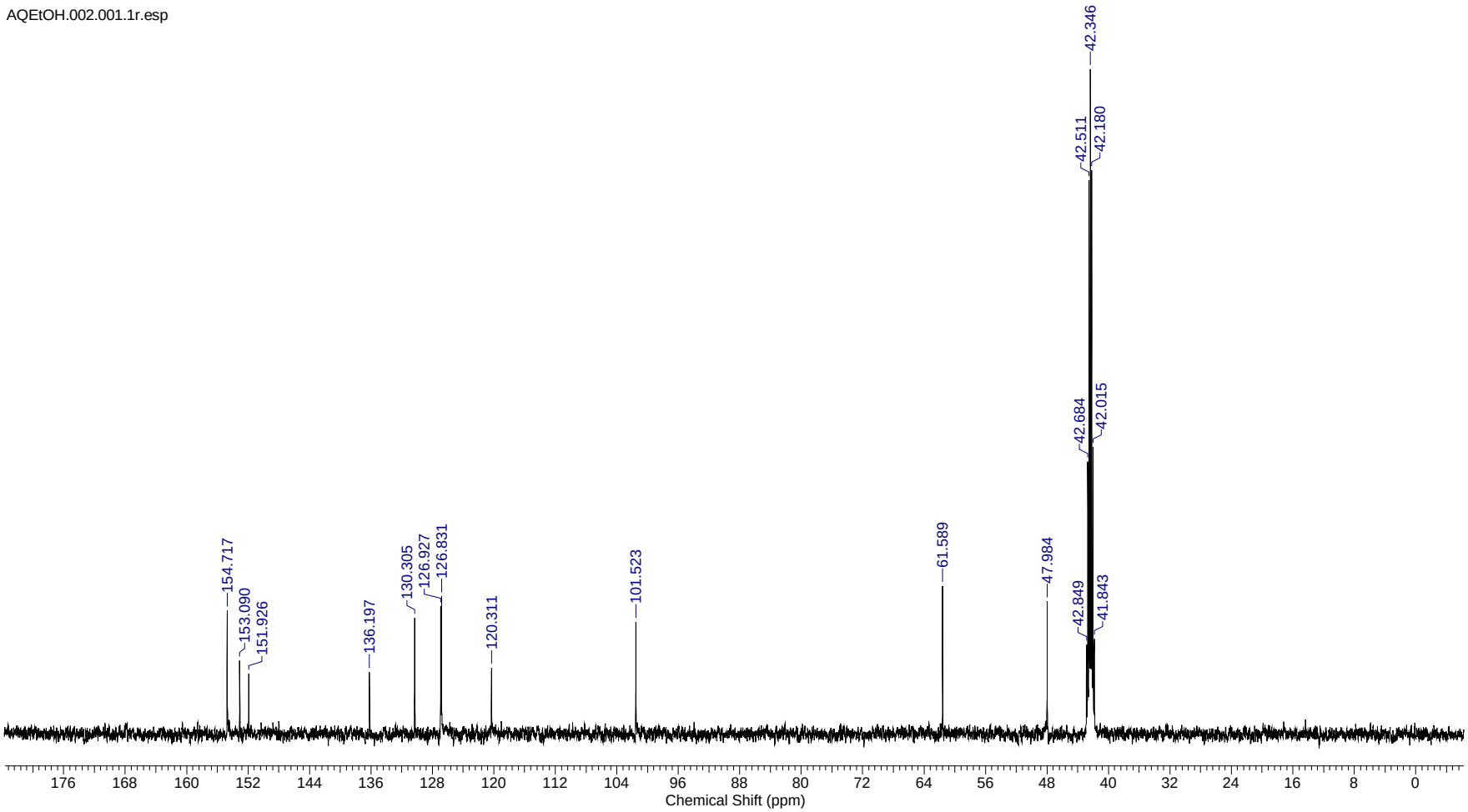
AQEtOH.001.001.1r.esp



Compound 21: ^{13}C NMR spectrum (500 MHz, DMSO-d6)

Acquisition Time (sec)	0.5767	***Comment***	Z8007_0118 (PH BBO 500S2 BB-H-D-05 Z)			***Date***	06 Apr 2016 13:07:44
Date Stamp	06 Apr 2016 13:07:44			***File Name***	C:\Users\Dejan Opsenica\Documents\Radni dnevnik\AQEtOH\2\pdata\1\1r		
Frequency (MHz)	125.79	***Nucleus***	13C	***Number of Transients***	40	***Origin***	spect
Original Points Count	16384	***Owner***	nmrsu	***Points Count***	32768	***Pulse Sequence***	zgpg30
Receiver Gain	2050.00	***SW(cyclical) (Hz)***	28409.09	***Solvent***	METHANOL-d4	***Spectrum Offset (Hz)***	13403.0127
Spectrum Type	STANDARD	***Sweep Width (Hz)***	28408.22	***Temperature (degree C)***	25.000		

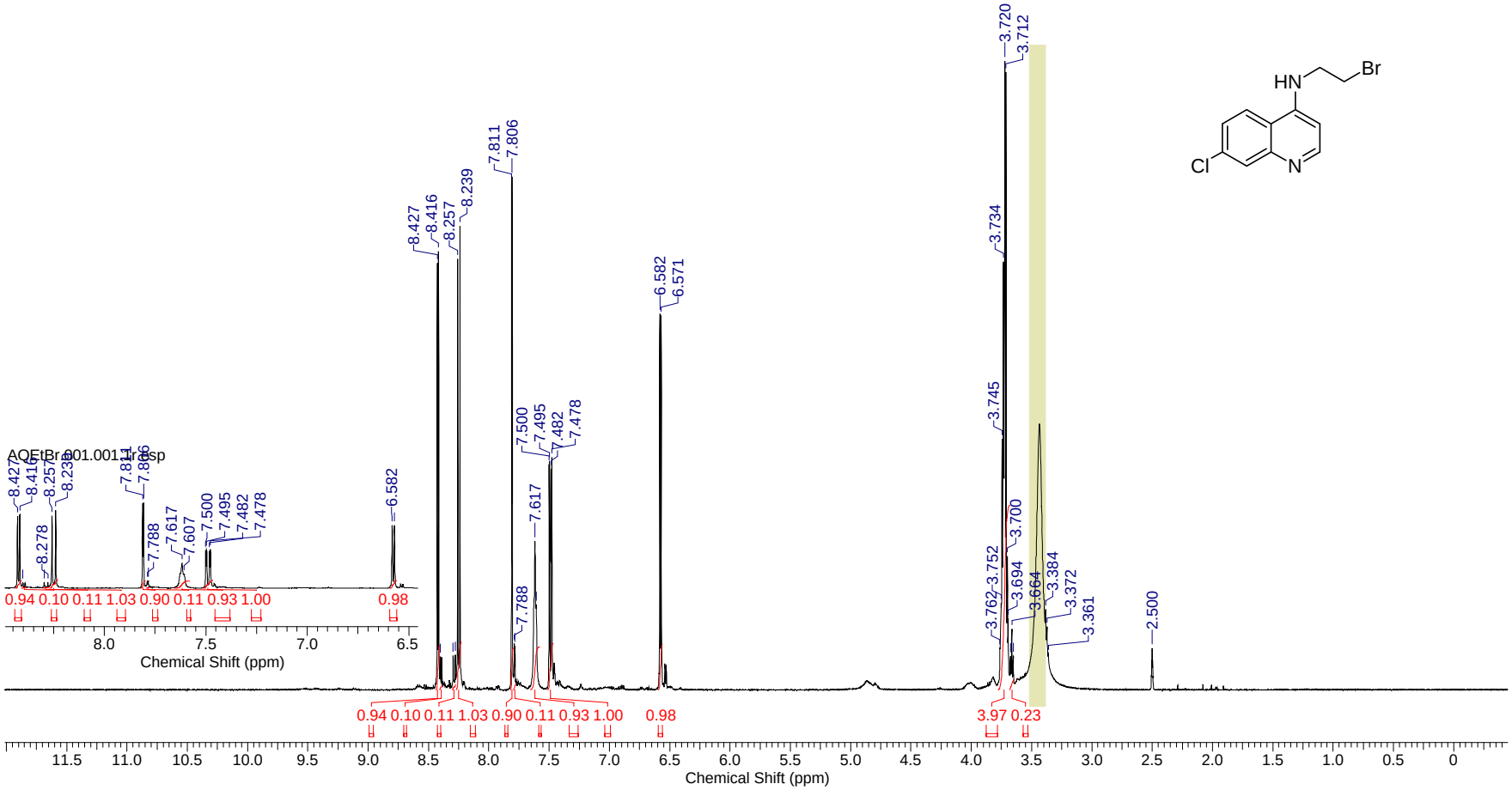
AQEtOH.002.001.1r.esp



Compound 20: ^{1}H NMR spectrum (500 MHz, DMSO-d6)

Acquisition Time (sec)	2.1823	***Comment***	Z8007_0118 (PH BBO 500S2 BB-H-D-05 Z)			***Date***	06 Apr 2016 12:57:04
Date Stamp	06 Apr 2016 12:57:04			***File Name***	C:\Users\Dejan Opsenica\Documents\Radni dnevnik\AQEtBr\1\pdata\1\1r		
Frequency (MHz)	500.26	***Nucleus***	1H	***Number of Transients***	4	***Origin***	spect
Original Points Count	16384	***Owner***	nmrsu	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	114.00	***SW(cyclical) (Hz)***	7507.51	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	3496.4045
Spectrum Type	STANDARD	***Sweep Width (Hz)***	7507.28	***Temperature (degree C)***	25.000		

AQEtBr.001.001.1r.esp



Compound 20: ^{13}C NMR spectrum (500 MHz, DMSO-d6)

Acquisition Time (sec)	0.5767	***Comment***	Z8007_0118 (PH BBO 500S2 BB-H-D-05 Z)			***Date***	06 Apr 2016 12:59:12
Date Stamp	06 Apr 2016 12:59:12			***File Name***	C:\Users\Dejan Opsenica\Documents\Radni dnevnik\AQEtBr\2\pdata\1\1r		
Frequency (MHz)	125.79	***Nucleus***	13C	***Number of Transients***	50	***Origin***	spect
Original Points Count	16384	***Owner***	nmrsu	***Points Count***	32768	***Pulse Sequence***	zgpg30
Receiver Gain	2050.00	***SW(cyclical) (Hz)***	28409.09	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	13403.0127
Spectrum Type	STANDARD	***Sweep Width (Hz)***	28408.22	***Temperature (degree C)***	25.200		

AQEtBr.002.001.1r.esp