A new structure-activity relationship for cyanine dyes to improve photostability and fluorescence properties for live cell imaging

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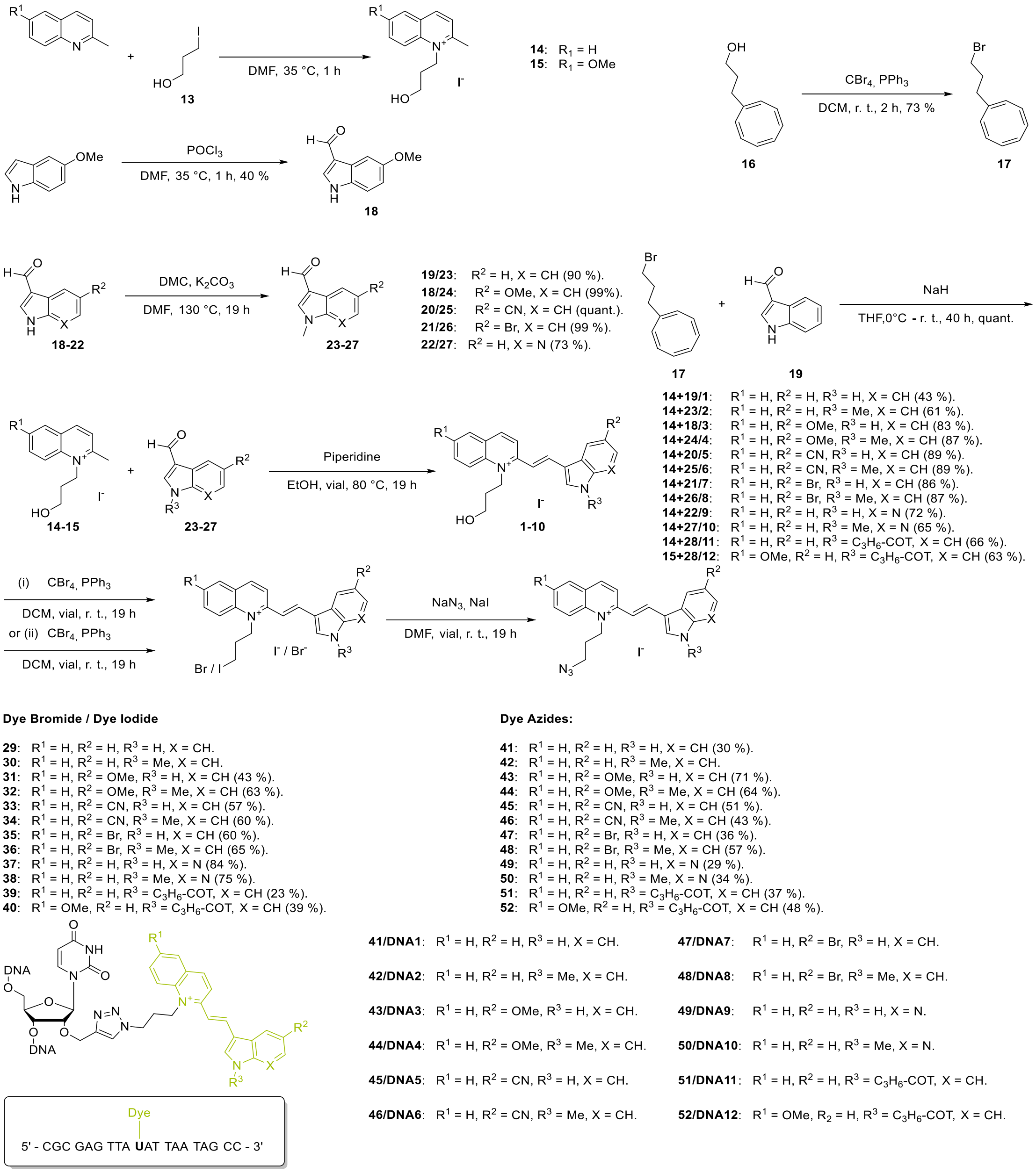
1. Syntheses

Cyanine-styryl dyes (**1**-**10**) are accessible by a Knoevenagel condensation of an aldehyde and a CH-acidic compound. Therefore, differently substituted indoles (**18**-**28**) were synthesized and coupled to the respective quinolinium salt **14** or **15**. Then the cyanine styryl dyes **1**-**10** were converted to their halide derivative **29**-**40** via an Appel reaction and afterwards the corresponding azides (**41**-**52**) were synthesized and used for the copper(I)- catalyzed azide-alkyne cycloaddition (CuAAC) to an alkyne-modified oligonucleotide:



Scheme S1. Synthetic overview.

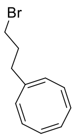
a. Syntheses of 13 and the Quinolinium Salts 14 and 15

The syntheses of the compounds **13**-**15** is described in earlier publications of our working group.[1-2]

b. Syntheses of 17 and the Indoles 18-28

Compound **16** was synthesized by a procedure published by *Altman* et al.[3] and synthesis of **23** is described in earlier publications of our working group.[2]

(1*Z*,3*Z*,5*Z*,7*Z*)-1-(3-bromopropyl)cycloocta-1,3,5,7-tetraene (17):



17

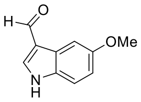
$C_{11}H_{13}Br$

225.1290 g/mol

Under argon atmosphere 5.72 g (3.00 eq, 21.8 mmol) triphenylphosphine and 1.18 g (1.00 eq, 7.27 mmol) **4** were dissolved in 50 mL dry dichloromethane. After addition of 7.95 g (3.30 eq, 7.28 mmol) tetrabromomethane, the solution was stirred 2 h at room temperature. Then, the solvent was removed under reduced pressure and the residue was dissolved in 120 mL methanol. The crude product was extracted 4 x with 150 mL *n*-hexane. The combined hexane layers were dried over sodium sulfate, filtered and the solvent was removed under reduced pressure. After column chromatography (EE / hex v : v = 0 : 1 to v : v = 1 : 0), 1.18 g (5.27 mmol) of the pure compound **5** could be obtained as yellow oil (73 %).

TLC (EE / hex, v : v = 1 : 10): R_f = 0.56. **^{1}H NMR** (300 MHz, $CDCl_3$): δ = 5.92 – 5.57 (m, 3H), 3.49 (t, *J*=6.7, 1H), 2.24 – 2.16 (m, 1H), 1.94 (p, *J*=6.9, 1H). **^{13}C NMR** (75 MHz, $CDCl_3$): δ = 31.4, 33.4, 35.9, 100.1, 127.9, 131.3, 131.7, 132.0, 132.4, 133.9, 142.4. **MS** (EI): m/z (%) = 117.1 (100), 224.1 (10). **HR-MS** (EI): calcd for $C_{11}H_{13}{}^{79}Br_1{}^+$ = 224.0195, found = 224.0196. **IR** (ATR): ṽ (cm^{-1}) = 2997 (m), 1639 (w).

5-methoxy-1*H*-indole-3-carbaldehyde (18):



18

$C_{10}H_9NO_2$

175.1870 g/mol

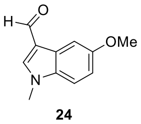
In an oven-dried flask and under argon atmosphere 1.00 g (1.00 eq, 6.79 mmol) 5-methoxy-1*H*-indole were dissolved in 10.5 mL dry *N*,*N*-dimethylformamide. The mixture was stirred and cooled to 0 °C. Afterwards a solution of 1.27 mL (2.08 g, 2.00 eq, 13.6 mmol) phosphorous oxychloride in 10.5 mL 10.5 mL dry *N*,*N*-Dimethylformamide was added dropwise and the solution was heated to 35 °C for 1 h. The reaction was quenched with 80 mL distilled water, basified to pH 6 with 5 M $NaOH_{aq}$ and refluxed for 5 min. After cooling, the crude compound was extracted 3 x with 100 mL ethyl acetate. The combined organic layers were dried over sodium sulfate, filtered and the solvent was removed under reduced pressure. The pure title compound was isolated by column chromatography (EE / hex v : v = 1 : 1) to give 480 mg (2.74 mmol) of a colorless solid (40 %).

TLC (EE / hex, v : v = 1 : 1): R_f = 0.24. **^{1}H NMR** (400 MHz, DMSO): δ = 12.02 (s, 1H), 9.90 (s, 1H), 8.21 (d, *J*=2.4, 1H), 7.59 (d, *J*=2.6, 1H), 7.40 (d, *J*=8.8, 1H), 6.88 (dd, *J*=8.8, 2.6, 1H), 3.78 (s, 3H). **^{13}C NMR** (100 MHz, DMSO): δ=55.3, 102.5, 113.2, 113.3, 118.0, 124.9, 131.8, 138.4, 155.6, 184.8. **MS** (FAB): m/z (%) = 175.1 (62), 176.1 (100), 177.1 (14). **HR-MS** (FAB): calcd for $C_{10}H_{10}O_2N_1{}^+$ = 176.0706, found = 176.0707. **IR** (ATR): ṽ (cm^{-1}) = 3104 (m), 1621 (m), 1208 (s).

General *N*-methylation procedure (23-27):

1 mmol (1.00 eq) of the respective indole, 158 mg (1.00 eq, 1 mmol) potassium carbonate and 4.00 mmol (411 mg, 4.00 eq.) dimethyl carbonate were dissolved in 1 mL dry *N*,*N*-dimethylformamide. The suspension was heated to 130 °C for 19 h. After cooling, the mixture was poured onto 50 mL ice water and the crude product was extracted 3x with 50 mL ethyl acetate. The combined organic layers were washed with 50 mL distilled water. Further the organic phase was dried over sodium sulfate, filtered and the solvent was removed under reduced pressure.

5-methoxy-1-methyl-1*H*-indole-3-carbaldehyde (24):



24

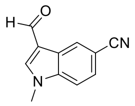
$C_{11}H_{11}NO_2$

189.2140 g/mol

Yield: 99 %.

^{1}H NMR (400 MHz, DMSO): δ = 9.85 (s, 1H), 8.19 (s, 1H), 7.60 (d, *J*=2.5, 1H), 7.48 (d, *J*=8.9, 1H), 6.94 (dd, *J*=8.9, 2.6, 1H), 3.86 (s, 3H), 3.79 (s, 3H). **^{13}C NMR** (100 MHz, DMSO): δ = 33.5, 55.3, 102.6, 111.8, 113.2, 116.7, 125.4, 132.6, 141.4, 156.0, 184.2. **MS** (EI): m/z (%) = 188.1 (40), 189.1 (100), 190.1 (12). **HR-MS** (EI): calcd for $C_{11}H_{11}O_2N_1{}^+$ = 189.0784, found = 189.0783. **IR** (ATR): ṽ (cm^{-1}) = 3104 (w), 2802 (w), 1643 (s), 1220 (m).

3-formyl-1-methyl-1*H*-indole-5-carbonitrile (25):



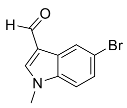
25

$C_{11}H_8N_2O$
184.1980 g/mol

Yield: quant.

^{1}H NMR (400 MHz, DMSO): δ = 9.95 (s, 1H), 8.48 (s, 1H), 8.45 (d, *J*=0.9, 1H), 7.80 (d, *J*=8.5, 1H), 7.71 (dd, *J*=8.5, 1.6, 1H), 3.94 (s, 3H). **^{13}C NMR** (100 MHz, DMSO): δ = 33.7, 39.5, 104.7, 112.6, 116.8, 119.8, 124.3, 125.7, 126.4, 139.3, 143.3, 184.8. **MS** (FAB): m/z (%) = 184.1 (20), 185.1 (100), 186.1 (17). **HR-MS** (FAB): calcd for $C_{11}H_9O_1N_2^+$ = 185.0709, found = 185.0709. **IR** (ATR): ṽ (cm^{-1}) = 2835 (w), 2219 (m), 1654 (s).

5-bromo-1-methyl-1*H*-indole-3-carbaldehyde (26):



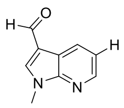
26

$C_{10}H_8BrNO$
238.0840 g/mol

Yield: 99 %.

^{1}H NMR (400 MHz, DMSO): δ = 9.88 (s, 1H), 8.30 (s, 1H), 8.21 (d, *J*=2.0, 1H), 7.55 (d, *J*=8.7, 1H), 7.44 (dd, *J*=8.7, 2.0, 1H), 3.87 (s, 3H). **^{13}C NMR** (100 MHz, DMSO): δ = 33.5, 113.1, 115.3, 116.2, 123.0, 126.0, 126.2, 136.4, 142.4, 184.5. **MS** (EI): m/z (%) = 236.1 (31), 237.1 (34), 238.1 (33), 239.1 (34). **HR-MS** (EI): calcd for $C_{10}H_8O_1N_1{}^{79}Br_1^+$ = 236.9789, found = 236.9788. **IR** (ATR): ṽ (cm^{-1}) = 3104 (w), 2813 (w), 1649 (s), 1240 (w).

1-methyl-1*H*-pyrrolo[2,3-*b*]pyridine-3-carbaldehyde (27):



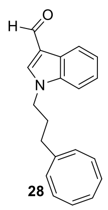
27

$C_9H_8N_2O$
160.1760 g/mol

Yield: 73 %

^{1}H NMR (400 MHz, DMSO) δ = 9.90 (s, 1H), 8.48 (s, 1H), 8.41 (s, 1H), 8.41 – 8.38 (m, 1H), 7.36 – 7.22 (m, 1H), 3.90 (s, 3H). **^{13}C NMR** (100 MHz, DMSO) δ = 31.7, 115.1, 116.8, 118.6, 129.4, 141.5, 144.6, 148.4, 184.9. **MS** (EI): m/z (%) = 159.1 (97), 160.1 (85). **HR-MS** (EI): calcd for $C_9H_8O_1N_2^+$ = 160.0637, found = 160.0638. **IR** (ATR): ṽ (cm^{-1}) = 3089 (w), 2779 (w), 1646 (s), 1205 (w).

1-(3-((1*Z*,3*Z*,5*Z*,7*Z*)-cycloocta-1,3,5,7-tetraen-1-yl)propyl)-1*H*-indole-3-carbaldehyde (28):



28

$C_{20}H_{19}NO$
289.3780 g/mol

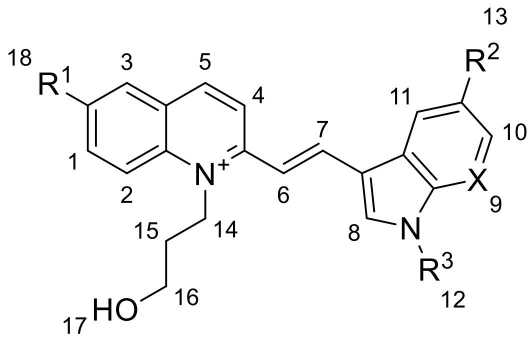
Under argon atmosphere 218 mg (1.00 eq, 1.50 mmol) **7** were dissolved in 5 mL dry tetrahydrofurane and cooled to 0 °C. Then 72.0 mg (1.20 eq, 1.80 mmol) sodium hydride (60 %) were added and the mixture was stirred 15 min at 0 °C. After addition of 405 mg (1.20 eq, 1.80 mmol) **5**, the mixture was slowly heated to room temperature and was stirred 40 h. After the reaction, the mixture was diluted with 50 mL ethyl acetate and 30 mL distilled water. The organic layer was separated and washed with 30 mL Brine. The brine washing solution was back extracted with 25 mL ethyl acetate and the combined organic layers were dried over sodium sulfate, filtered and the solvent was removed under reduced pressure. After high vacuum drying, 434 mg (1.50 mmol) of the pure title compound **28** could be obtained (quant.).

^{1}H NMR (300 MHz, $CDCl_3$): δ = 10.01 (s, 1H), 8.36 – 8.26 (m, 1H), 7.75 (s, 1H), 7.46 – 7.28 (m, 3H), 5.98 – 5.54 (m, 7H), 4.27 (t, *J*=6.9, 2H), 2.12 (t, *J*=6.7, 2H), 2.07 – 1.92 (m, 2H). **^{13}C NMR** (75 MHz, $CDCl_3$): δ = 28.0, 34.6, 46.4, 110.3, 118.2, 122.3, 123.0, 124.0, 125.7, 128.4, 131.5, 131.8, 132.2, 132.4, 132.7, 133.8, 137.4, 138.4, 142.2, 184.6. **MS** (EI): m/z (%) = 289.5 (100), 290.5 (22). **HR-MS** (EI): calcd for $C_{20}H_{19}O_1N_1^+$ = 289.1461, found = 289.1463. **IR** (ATR): ṽ (cm^{-1}) = 2996 (w), 2940 (w), 1654 (s).

c. Syntheses of the Dyes 1-12

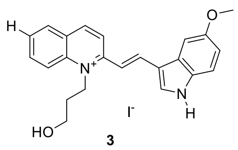
The syntheses of the compounds **1**-**2** is described in earlier publications of our working group.[1-2]

General dye synthesis:



In a headspace vial1 mmol (1.00 eq) of the quinolinium salt **2** or **3** and 2.00 mmol (2.00 eq) of the corresponding indole (**6**-**16**) were dissolved in 10 mL ethanol (100 %). Then, 2.20 mmol (187 mg, 2.20 eq) piperidine were added and the closed headspace vial was heated to 80 °C for 19 h. After cooling to room temperature, 10 mL diethyl ether was added and the formed precipitate was collected and washed 3x with 5 mL diethyl ether.

(*E*)-1-(3-hydroxypropyl)-2-(2-(5-methoxy-1*H*-indol-3-yl)vinyl)quinolin-1-ium iodide (3):



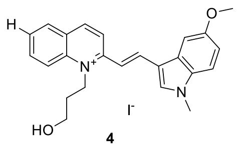
3

$C_{23}H_{23}IN_2O_2$
486.3535 g/mol

Yield: 86 %.

^{1}H NMR (400 MHz, DMSO): δ = 12.26 (s, 1H, H-12), 8.80 (d, *J*=9.2, 1H, H-4/H-5), 8.71 (d, *J*=15.2, 1H, H-6/H-7), 8.63 (d, *J*=9.2, 1H, H-4/H-5), 8.44 (d, *J*=9.0, 1H, H-2/H-3), 8.30 (s, 1H, H-8), 8.25 (d, *J*=7.7, 1H, H-2/H-3), 8.08 (m, 1H, H-1/H-18), 7.83 (m, 1H, H-1/H-18), 7.67 (d, *J*=2.5, 1H, H-11), 7.54 (d, *J*=15.3, 1H, H-6/H-7), 7.45 (d, *J*=8.8, 1H, H-9), 6.93 (dd, *J*=8.9, 2.4, 1H, H-10), 5.15 (t, *J*=4.7, 1H, H-17), 5.01 (t, *J*=8.0, 2H, H-14), 3.89 (s, 3H, H-13), 3.72 (q, *J*=5.3, 2H, H-16), 2.16 (p, *J*=5.7, 2H, H-15). **^{13}C NMR** (100 MHz, DMSO): δ = 31.2 (C-14/C15/C-16), 47.5 (C-14/C15/C-16), 55.5 (Indole-OMe), 57.5 (C-14/C15/C-16), 102.4 (Arom.), 110.0 (Arom.), 113.2 (Arom.), 113.6 (Arom.), 114.7 (Arom.), 118.3 (Arom.), 119.9 (Arom.), 126.2 (Arom.), 126.8 (Arom.), 127.8 (Arom.), 130.0 (Arom.), 132.3 (Arom.), 134.2 (Arom.), 134.4 (Arom.), 138.4 (Arom.), 141.6 (Arom.), 143.6 (Arom.), 155.6 (Arom.), 156.1 (Arom.). **MS** (FAB): m/z (%) = 359.2 (100), 360.2 (28). **HR-MS** (FAB): calcd for $C_{23}H_{23}O_2N_2^+$ = 359.1754, found = 359.1755. **IR** (ATR): ṽ (cm^{-1}) = 3138 (w), 1569 (s), 1208 (s). **EA** calcd for $C_{23}H_{23}O_2N_2I_1$: C, 56.80; H, 4.77; N, 5.76. Found: C, 56.62; H, 4.71; N, 5.74.

(*E*)-1-(3-hydroxypropyl)-2-(2-(5-methoxy-1-methyl-1*H*-indol-3-yl)vinyl)quinolin-1-ium iodide (4):



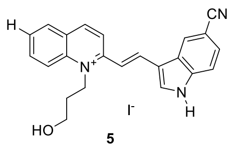
4

$C_{24}H_{25}IN_2O_2$
500.3805 g/mol

Yield: 87 %.

^{1}H NMR (400 MHz, DMSO): δ = 8.78 (d, *J*=9.2, 1H, H-4/H-5), 8.68 (d, *J*=15.2, 1H, H-6/H-7), 8.63 (d, *J*=9.1, 1H, H-4/H-5), 8.42 (d, *J*=9.0, 1H, H-2/H-3), 8.28 (s, 1H, H-8), 8.24 (d, *J*=7.9, 1H, H-2/H-3), 8.02-8.12 (m, 1H, H-1/H-18), 7.82 (m, 1H, H-1/H-18), 7.69 (m, 1H, H-11), 7.53 (d, *J*=9.3, 1H, H-9), 7.50 (d, *J*=15.8, 1H, H-6/H-7), 6.98 (m, 1H, H-10), 5.15 (t, *J*=4.6, 1H, H-17), 4.99 (t, *J*=7.6, 2H,H-14), 3.92 (s, 3H, H-12/H-13), 3.90 (s, 3H, H-12/H-13), 3.72 (q, *J*=5.3, 2H, H-16), 2.16 (p, *J*=6.1, 2H, H-15). **^{13}C NMR** (100 MHz, DMSO): δ = 31.1 (C-14/C15/C-16), 33.8 (Indole-NMe), 47.4 (C-14/C15/C-16), 55.6 (Indole-OMe), 57.5 (C-14/C15/C-16), 102.6 (Arom.), 109.8 (Arom.), 112.3 (Arom.), 113.0 (Arom.), 113.6 (Arom.), 118.3 (Arom.), 119.9 (Arom.), 126.7 (Arom.), 126.8 (Arom.), 127.8 (Arom.), 130.0 (Arom.), 133.0 (Arom.), 134.2 (Arom.), 137.4 (Arom.), 138.4 (Arom.), 141.5 (Arom.), 142.9 (Arom.), 155.9 (Arom.), 156.0 (Arom.). **MS** (FAB): m/z (%) = 373.2 (100), 374.2 (30). **HR-MS** (FAB): calcd for $C_{24}H_{25}O_2N_2^+$ = 373.1911, found = 373.1909. **IR** (ATR): ṽ (cm^{-1}) = 3324 (m), 1589 (s), 1221 (m). **EA** calcd for $C_{24}H_{25}O_2N_2I_1$: C, 57.61; H, 5.04; N, 5.60. Found: C, 57.52; H, 4.99; N, 5.58.

(*E*)-2-(2-(5-cyano-1*H*-indol-3-yl)vinyl)-1-(3-hydroxypropyl)quinolin-1-ium iodide (5):



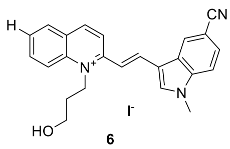
5

$C_{23}H_{20}IN_3O$
481.3375 g/mol

Yield: 89 %.

^{1}H NMR (400 MHz, DMSO): δ = 12.68 (s, 1H, H-12), 8.93 (d, *J*=9.1, 1H, H-4/H-5), 8.77 (s, 1H, H-8), 8.70 (d, *J*=15.7, 1H, H-6/H-7), 8.66 (d, *J*=9.3, 1H, H-4/H-5), 8.52 (d, *J*=9.1, 1H, H-2/H-3), 8.51 (s, 1H, H-11), 8.34-8.25 (m, 1H, H-2/H-3), 8.18-8.08 (m, 1H, H-1/H-18), 7.93-7,84 (m, 1H, H-1/H-18), 7.72 (d, *J*=8.4, 1H, H-9), 7.72 (d, *J*=15.5, 1H, H-6/H-7), 7.65 (dd, *J*=8.5, 1.5, 1H, H-10), 5.19 (t, *J*=4.8, 1H, H-17), 5.09 (t, *J*=7.9, 2H, H-14), 3.72 (q, *J*=5.1, 2H, H-16), 2.16 (p, *J*=6.4, 6.0, 2H, H-15). **^{13}C NMR** (100 MHz, DMSO): δ = 31.4 (C-14/C15/C-16), 47.8 (C-14/C15/C-16), 57.5 (C-14/C15/C-16), 103.8 (Arom.), 112.9 (Arom.), 114.1 (Arom.), 114.6 (Arom.), 118.6 (Arom.), 120.2 (Arom.), 120.2 (Arom.), 125.4 (Arom.), 125.5 (Arom.), 126.0 (Arom.), 127.3 (Arom.), 128.3 (Arom.), 130.2 (Arom.), 134.5 (Arom.), 135.0 (Arom.), 138.4 (Arom.), 139.2 (Arom.), 141.4 (Arom.), 142.6 (Arom.), 156.0 (Arom.). **MS** (FAB): m/z (%) = 354.2 (100), 355.2 (28). **HR-MS** (FAB): calcd for $C_{23}H_{20}O_1N_3^+$ = 354.1601, found = 354.1599. **IR** (ATR): ṽ (cm^{-1}) = 3104 (w), 2224 (m), 1598 (s), 1231 (m). **EA** calcd for $C_{23}H_{20}O_1N_3I_1$: C, 57.39; H, 4.19; N, 8.73. Found: C, 57.50; H, 4.10; N, 8.72.

(*E*)-2-(2-(5-cyano-1-methyl-1*H*-indol-3-yl)vinyl)-1-(3-hydroxypropyl)quinolin-1-ium iodide (6):



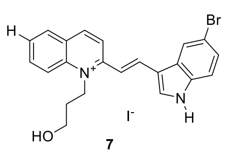
6

$C_{24}H_{22}IN_3O$
495.3645 g/mol

Yield: 89 %.

^{1}H NMR (400 MHz, DMSO): δ = 8.93 (d, *J*=9.0, 1H, H-4/H-5), 8.78 (s, 1H, H-8), 8.72-8.62 (m, 2H, H-6/H-7&H-4/H-5), 8.52 (d, *J*=9.0, 1H, H-2/H-3), 8.49 (s, 1H, H-11), 8.34-8.25 (m, 1H, H-2/H-3), 8.18-8.09 (m, 1H, H-1/H-18), 7.94-7.86 (m, 1H, H-1/H-18), 7.84 (d, *J*=8.5, 1H, H-9), 7.78-7.66 (m, 2H, H-10&H-6/H-7), 5.19 (t, *J*=4.8, 1H, H-17), 5.08 (t, *J*=7.6, 2H, H-14), 4.00 (s, 3H, H-12), 3.72 (q, *J*=5.3, 2H, H-16), 2.16 (p, *J*=6.0, 2H, H-15). **^{13}C NMR** (100 MHz, DMSO): δ = 31.4 (C-14/C15/C-16), 33.8 (Indole-NMe), 47.8 (C-14/C15/C-16), 57.5 (C-14/C15/C-16), 104.0 (Arom.), 112.7 (Arom.), 113.0 (Arom.), 113.6 (Arom.), 118.6 (Arom.), 120.0 (Arom.), 120.2 (Arom.), 125.5 (Arom.), 125.7 (Arom.), 126.0 (Arom.), 127.3 (Arom.), 128.3 (Arom.), 130.2 (Arom.), 134.5 (Arom.), 137.9 (Arom.), 138.4 (Arom.), 139.4 (Arom.), 140.8 (Arom.), 142.7 (Arom.), 155.9 (Arom.). **MS** (FAB): m/z (%) = 368.2 (100), 369.2 (31). **HR-MS** (FAB): calcd for $C_{24}H_{22}O_1N_3^+$ = 368.1757, found = 368.1756. **IR** (ATR): ṽ (cm^{-1}) = 3313 (w), 2221 (m), 1586 (s), 1225 (m). **EA** calcd for $C_{24}H_{22}O_1N_3I_1$: C, 58.19; H, 4.48; N, 8.48. Found: C, 58.04; H, 4.39; N, 8.48.

(*E*)-2-(2-(5-bromo-1*H*-indol-3-yl)vinyl)-1-(3-hydroxypropyl)quinolin-1-ium iodide (7):



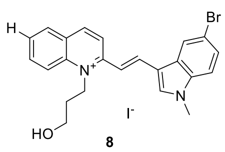
7

$C_{22}H_{20}BrIN_2O$
535.2235 g/mol

Yield: 86 %.

^{1}H NMR (400 MHz, DMSO): δ = 12.44 (s, 1H, H-12), 8.84 (d, *J*=9.1, 1H, H-4/H-5), 8.69 (d, *J*=15.3, 1H, H-6/H-7), 8.66 (d, *J*=9.1, 1H, H-4/H-5), 8.46 (d, *J*=9.0, 1H, H-2/H-3), 8.44-8.37 (m, 2H, H-8&H-11), 8.26 (d, *J*=7.0, 1H, H-2/H-3), 8.14-8.07 (m, 1H, H-1/H-18), 7.90-7.81 (m, 1H, H-1/H-18), 7.61 (d, *J*=15.3, 1H, H-6/H-7), 7.52 (d, *J*=8.6, 1H, H-9), 7.40 (dd, *J*=8.7, 1.8, 1H, H-10), 5.04 (t, *J*=7.8, 2H, H-14), 3.73 (t, *J*=5.5, 2H, H-16), 2.16 (p, *J*=6.9, 2H, H-15). **^{13}C NMR** (100 MHz, DMSO): δ = 31.3 (C-14/C15/C-16), 47.6 (C-14/C15/C-16), 57.6 (C-14/C15/C-16), 111.3 (Arom.), 114.1 (Arom.), 114.6 (Arom.), 114. 9 (Arom.), 118.4 (Arom.), 120.1 (Arom.), 122.3 (Arom.), 125.8 (Arom.), 127.0 (Arom.), 127.5 (Arom.), 128.0 (Arom.), 130.1 (Arom.), 134.3 (Arom.), 134.5 (Arom.), 136.4 (Arom.), 138.4 (Arom.), 142.0 (Arom.), 142.2 (Arom.), 155.9 (Arom.). **MS** (FAB): m/z (%) = 409.1 (100), 410.1 (29). **HR-MS** (FAB): calcd for $C_{22}H_{20}O_1N_2{}^{79}Br_1^+$ = 407.0754, found = 407.0755. **IR** (ATR): ṽ (cm^{-1}) = 3380 (w), 3064 (w), 1591 (s), 1312 (m). **EA** calcd for $C_{22}H_{20}Br_1O_1N_2I_1$: C, 49.37; H, 3.68; N, 5.23. Found: C, 48.90; H, 3.67; N, 5.20.

(*E*)-2-(2-(5-bromo-1-methyl-1*H*-indol-3-yl)vinyl)-1-(3-hydroxypropyl)quinolin-1-ium iodide (8):



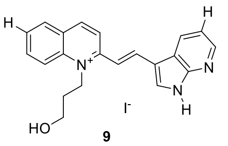
8

$C_{23}H_{22}BrIN_2O$
549.2505 g/mol

Yield: 87 %.

^{1}H NMR (400 MHz, DMSO): δ = 8.86 (d, *J*=9.1, 1H, H-4/H-5), 8.73-8.62 (m, 2H, H-6/H-7&H-4/H-5), 8.51-8.42 (m, 2H, H-2/H-3&H-8), 8.39 (s, 1H, H-11), 8.27 (d, *J*=8.1, 1H, H-2/H-3), 8.15-8.06 (m, 1H, H-1/H-18), 7.91-7.81 (m, 1H, H-1/H-18), 7.61 (d, *J*=8.7, 1H, H-9), 7.60 (d, *J*=15.4, 1H, H-6/H-7), 7.48 (dd, *J*=8.7, 1.8, 1H, H-10), 5.15 (t, *J*=4.7, 1H, H-17), 5.03 (t, *J*=7.5, 2H, H-14), 3.95 (s, 3H, Indole-NMe), 3.73 (q, *J*=5.3, 2H, H-16), 2.15 (p, *J*=7.5, 6.2, 2H, H-15). **^{13}C NMR** (100 MHz, DMSO): δ = 31.3 (C-14/C15/C-16), 33.8 (Indole-NMe), 47.6 (C-14/C15/C-16), 57.5 (C-14/C15/C-16), 111.5 (Arom.), 112.9 (Arom.), 113.4 (Arom.), 115.1 (Arom.), 118.4 (Arom.), 120.1 (Arom.), 122.4 (Arom.), 125.9 (Arom.), 127.1 (Arom.), 127.8 (Arom.), 128.1 (Arom.), 130.1 (Arom.), 134.4 (Arom.), 136.6 (Arom.), 137.1 (Arom.), 138.4 (Arom.), 141.6 (Arom.), 142.1 (Arom.), 155.9 (Arom.). **MS** (FAB): m/z (%) = 421.1 (100), 424.1 (27). **HR-MS** (FAB): calcd for $C_{23}H_{22}O_1N_2{}^{79}Br_1^+$ = 421.0910, found = 421.0911. **IR** (ATR): ṽ (cm^{-1}) = 3315 (m), 1583 (s), 1301 (s), 1224 (m). **EA** calcd for $C_{23}H_{22}Br_1O_1N_2I_1$: C, 50.30; H, 4.04; N, 5.10. Found: C, 50.26; H, 3.99; N, 5.11.

(*E*)-2-(2-(1*H*-pyrrolo[2,3-*b*]pyridin-3-yl)vinyl)-1-(3-hydroxypropyl)quinolin-1-ium iodide (9):



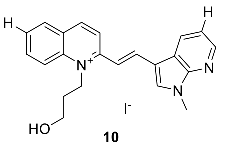
9

$C_{21}H_{20}IN_3O$
457.3155 g/mol

Yield: 72 %.

^{1}H NMR (500 MHz, D_2O/D_2SO_4=10:1) δ = 7.89 (d, *J*=8.0, 1H, H-10/H-11), 7.56 (d, *J*=8.8, 1H, H-4/H-5), 7.40 (d, *J*=6.0, 1H, H-10/H-11), 7.27 (d, *J*=8.9, 1H, H-4/H-5), 7.17 (s, 1H, H-8), 7.15 – 7.04 (m, 2H, H-2/H-3&H-6/H-7), 7.04 – 6.97 (m, 1H, H-1/H-18), 6.89 (d, *J*=8.0, 1H, H-2/H-3), 6.74 (t, *J*=7.5, 1H, H-1/H-18), 6.67 (dd, *J*=8.0, 5.8, 1H, H-13), 6.48 (d, *J*=15.8, 1H, H-6/H-7), 3.95 (t, *J*=7.9, 2H, H-14), 2.90 (t, *J*=5.5, 2H, H-16), 1.33 – 1.16 (m, 2H, H-15). **^{13}C NMR** (100 MHz, DMSO) δ = 31.3 (C-14/C15/C-16), 47.9 (C-14/C15/C-16), 57.4 (C-14/C15/C-16), 111.9 (Arom.), 113.0 (Arom.), 117.9 (Arom.), 118.6 (Arom.), 120.0 (Arom.), 128.3 (Arom.), 129.1 (Arom.), 130.2 (Arom.), 134.5 (Arom.), 134.8 (Arom.), 138.4 (Arom.), 142.6 (Arom.), 142.9 (Arom.), 144.6 (Arom.), 149.9 (Arom.), 156.0 (Arom.). **MS** (FAB): m/z (%) = 330.2 (100), 331.2 (28). **HR-MS** (FAB): calcd for $C_{21}H_{20}O_1N_3^+$ = 330.1601, found = 330.1599. **IR** (ATR): ṽ (cm^{-1}) = 3318 (m), 2864 (w), 1566 (s), 1215 (m). **EA** calcd for $C_{21}H_{20}O_1N_3I_1$: C, 55.15; H, 4.41; N, 9.19. Found: C, 50.28; H, 4.41; N, 9.53.

(*E*)-1-(3-hydroxypropyl)-2-(2-(1-methyl-1*H*-pyrrolo[2,3-*b*]pyridin-3-yl)vinyl)quinolin-1-ium iodide (10):



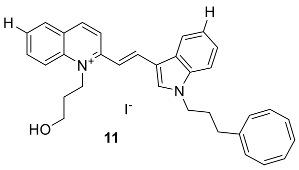
10

$C_{22}H_{22}IN_3O$
471.3425 g/mol

Yield: 65 %.

^{1}H NMR (600 MHz, DMSO) δ = 8.88 (d, *J*=9.0, 1H, H-4/H-5), 8.72 (d, *J*=7.9, 1H, H-10/H-11), 8.64-8.59 (dd, 2H, H-6/H-7&H-4/H-5), 8.51 (d, *J*=8.9, 1H, H-2/H-3), 8.45 (d, *J*=4.5, 1H, H-10/H-11), 8.41 (s, 1H, H-8), 8.27 (d, *J*=8.1, 1H, H-2/H-3), 8.11 (dd, *J*=8.8, 7.1, 1H, H-1/H-8), 7.89 – 7.84 (m, 1H, H-1/H-8), 7.61 (d, *J*=15.3, 1H, H-6/H-7), 7.38-7.34 (m, 1H, H-13), 5.32 (t, *J*=4.4, 1H, H-17), 5.05 (d, *J*=8.0, 2H, H-14), 3.95 (s, 3H, H-12), 3.74 (q, *J*=5.1, 2H, H-16), 2.21 – 2.13 (m, 2H, H-15). **^{13}C NMR** (150 MHz, DMSO) δ = 31.3 (C-14/C15/C-16), 31.7 (Azaindole-NMe, 47.8 (C-14/C15/C-16), 57.4 (C-14/C15/C-16), 111.7 (Arom.), 111.8 (Arom.), 117.6 (Arom.), 118.1 (Arom.), 118.6 (Arom.), 120.0 (Arom.), 127.2 (Arom.), 128.2 (Arom.), 129.4 (Arom.), 130.1 (Arom.), 134.5 (Arom.), 138.4 (Arom.), 142.4 (Arom.), 142.5 (Arom.), 144.4 (Arom.), 148.8 (Arom.), 155.9 (Arom.). **MS** (FAB): m/z (%) = 344.2 (100), 345.2 (28). **HR-MS** (FAB): calcd for $C_{22}H_{22}O_1N_3^+$ = 344.1757, found = 344.1759. **IR** (ATR): ṽ (cm^{-1}) = 3337 (w), 1562 (s), 1315 (m), 1234 (m). **EA** calcd for $C_{22}H_{22}O_1N_3I_1$: C, 56.06; H, 4.70; N, 8.92. Found: C, 54.42; H, 4.56; N, 8.57.

2-((*E*)-2-(1-(3-((1*Z*,3*Z*,5*Z*,7*Z*)-cycloocta-1,3,5,7-tetraen-1-yl)propyl)-1*H*-indol-3-yl)vinyl)-1-(3-hydroxypropyl)quinolin-1-ium iodide (11):



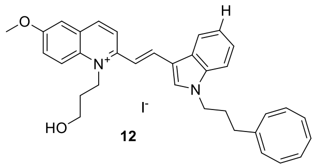
11

$C_{33}H_{33}IN_2O$
600.5445 g/mol

Yield: 66 %.

^{1}H NMR (400 MHz, DMSO) δ = 8.82 (d, *J*=9.1, 1H, H-4/H-5), 8.67 (d, *J*=15.5, 1H, H-6/H-7), 8.62 (d, *J*=9.1, 1H, H-4/H-5), 8.48 (d, *J*=8.9, 1H, H-2/H-3), 8.31 (m, 2H, H-8&H-9/H-11), 8.25 (d, *J*=8.5, 1H, H-2/H-3), 8.15 – 8.03 (m, 1H, H-1/H-18), 7.90 – 7.79 (m, 1H, H-1/H-18), 7.67 (d, *J*=8.0, 1H, H-9/H-11), 7.58 (d, *J*=15.3, 1H, H-6/H-7), 7.44 – 7.27 (m, 2H, H-10/H-13), 5.91 – 5.67 (m, 6H, COT), 5.57 (s, 1H, COT), 5.26 (t, *J*=4.5, 1H, H-17), 5.10 – 4.96 (m, 2H, H-14), 4.35 (t, *J*=7.0, 2H, COT-CH_2), 3.82 – 3.69 (m, 2H, H-16), 2.25-2.12 (m, 2H, H-15), 2.09 (t, *J*=7.3, 2H, Indole-NCH_2), 2.00 – 1.84 (m, 2H, CH_2). **^{13}C NMR** (100 MHz, DMSO) δ = 28.3 (Alkyl), 31.2 (C-14/C15/C-16), 34.0(Alkyl), 45.8 (Alkyl), 47.6 (C-14/C15/C-16), 57.5 (C-14/C15/C-16), 110.5 (Arom.), 111.3 (Arom.), 113.9 (Arom.), 118.4 (Arom.), 119.9 (Arom.), 120.9 (Arom.), 122.4 (Arom.), 123.6 (Arom.), 125.5 (Arom.), 126.9 (Arom.), 127.1 (Arom.), 127.9 (Arom.), 130.0 (Arom.), 131.2 (Arom.), 131.8 (Arom.), 132.2 (Arom.), 134.0 (Arom.), 134.3 (Arom.), 137.2 (Arom.), 137.5 (Arom.), 138.4 (Arom.), 141.9 (Arom.), 142.6 (Arom.), 142.9 (Arom.), 155.9 (Arom.). **MS** (FAB): m/z (%) = 473.1 (100), 474.1 (40). **HR-MS** (FAB): calcd for $C_{33}H_{33}O_1N_2^+$ = 473.2587, found = 473.2587. **IR** (ATR): ṽ (cm^{-1}) = 3306 (w), 1592 (s), 1393 (s), 1244 (m). **EA** calcd for $C_{33}H_{33}O_1N_2I_1$: C, 66.00; H, 5.54; N, 4.66. Found: C, 65.63; H, 5.63; N, 4.75.

2-((*E*)-2-(1-(3-((1*Z*,3*Z*,5*Z*,7*Z*)-cycloocta-1,3,5,7-tetraen-1-yl)propyl)-1*H*-indol-3-yl)vinyl)-1-(3-hydroxypropyl)-6-methoxyquinolin-1-ium iodide (12):



12

$C_{34}H_{35}IN_2O_2$
630.5705 g/mol

Yield: 63 %.

^{1}H NMR (400 MHz, DMSO) δ = 8.72 (d, *J*=9.1, 1H, H-4/H-5), 8.62 – 8.49 (m, 3H, H-4/H-5&H-6/H-7), 8.42 (d, *J*=9.7, 1H, H-1/H-2), 8.27 (d, J=7.7, 1H, H-9/H-11), 8.23 (s, 1H, H-8) 7.77-7.63 (m, 3H, H-1/H-2&H-3&H-9/H-11), 7.55 (d, *J*=15.4, 1H, H-6/H-7), 7.42 – 7.25 (m, 2H, H-10/H-13), 5.90 – 5.66 (m, 6H, COT), 5.56 (s, 1H, COT), 5.26-5.20 (m, 1H, H-17), 5.08 – 4.94 (m, 2H, H-14), 4.33 (t, *J*=7.1, 2H, COT-CH_2), 3.97 (s, 3H, Quinoline-6-OMe), 3.78 – 3.66 (m, 2H, H-16), 2.21 – 2.10 (m, 2H, H-15), 2.08 (t, *J*=7.3, 2H, Indole-NCH_2), 1.98 – 1.83 (m, 2H, CH_2). **^{13}C NMR** (100 MHz, DMSO) δ = 28.3 (Alkyl), 31.4 (C-14/C15/C-16), 34.0 (Alkyl), 45.7 (Alkyl), 47.8 (C-14/C15/C-16), 56.1 (Quinoline-6-OMe, 57.4 (C-14/C15/C-16), 109.1 (Arom.), 110.7 (Arom.), 111.2 (Arom.), 113.6 (Arom.), 120.3 (Arom.), 120.4 (Arom.), 120.8 (Arom.), 122.1 (Arom.), 123.4 (Arom.), 125.0 (Arom.), 125.5 (Arom.), 127.1 (Arom.), 128.8 (Arom.), 131.2 (Arom.), 131.7 (Arom.), 132.2 (Arom.), 133.5 (Arom.), 134.0 (Arom.), 136.3 (Arom.), 137.4 (Arom.), 141.0 (Arom.), 141.3 (Arom.), 142.6 (Arom.), 153.6 (Arom.), 158.1 (Arom.). **MS** (FAB): m/z (%) = 503.1 (100), 504.2 (40). **HR-MS** (FAB): calcd for $C_{34}H_{35}O_2N_2^+$ = 503.2693, found = 503.2693. **IR** (ATR): ṽ (cm^{-1}) = 3373 (w), 1512 (s), 1392 (m), 1240 (m). **EA** calcd for $C_{34}H_{35}O_2N_2I_1$: C, 64.76; H, 5.59; N, 4.44. Found: C, 63.67; H, 5.51; N, 4.34.

d. Syntheses of the Dye-Bromides/-Iodides 29-40

General dye bromide synthesis (31-36, 39-40):

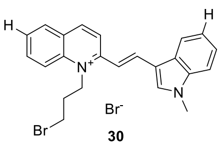
In a headspace vial 200 µmol (1.00 eq) dye, 660 µmol (3.30 eq) tetrabromomethane and 600 µmol (3.00 eq) triphenylphosphine were dissolved in 2 mL dry dichloromethane and stirred at room temperature for 19 h. Then the solvent was removed and 2 mL methanol was added. The suspension was exposed to ultrasound for 10 min, filtered and the solid was washed 3x with 5 mL diethyl ether. The solid was then mixed with 2 g sodium bromide and the mixture was distributed between 150 mL dichloromethane and 50 mL distilled water. The aqueous phase was 3x back extracted with 100 mL dichloromethane. Under reduced pressure, the combined organic layers were evaporated to dryness. The formed solid was again suspended in 2 mL methanol, exposed to ultrasound for 10 min, filtered and washed 3x with 5 mL diethyl ether.

General dye iodide synthesis (37-38):

The synthesis of **29** is described in earlier publications of our group.[1]

In a headspace vial 500 µmol (1.00 eq) dye, 550 µmol (1.10 eq) triphenylphosphine, 2.00 mmol (4.00 eq) imidazole and 550 µmol (1.10 eq) iodine were dissolved in 5 mL dry dichloromethane and stirred at room temperature for 19 h. Then, the solvent was removed and 5 mL methanol was added. The suspension was exposed to ultrasound for 30 min and the solid collected and washed 3x with 5 mL diethyl ether.

(*E*)-1-(3-iodopropyl)-2-(2-(1-methyl-1*H*-indol-3-yl)vinyl)quinolin-1-ium iodide (30):



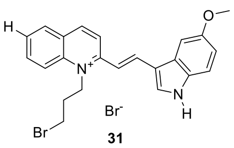
30

$C_{23}H_{22}Br_2N_2$
486.2510 g/mol

Yield: 56 %.

^{1}H NMR (400 MHz, DMSO) δ = 8.81 (d, *J*=9.1, 1H), 8.75 – 8.58 (m, 2H), 8.44 (d, *J*=8.9, 1H), 8.36 (s, 1H), 8.24 (t, *J*=7.1, 2H), 8.09 (dd, *J*=8.8, 6.9, 1H), 7.84 (t, *J*=7.5, 1H), 7.63 (d, *J*=7.8, 1H), 7.49 – 7.28 (m, 3H), 5.07 (t, *J*=7.9, 2H), 3.95 (s, 3H), 3.58 – 3.36 (m, 2H). **^{13}C NMR** (100 MHz, DMSO) δ = 30.6, 31.3, 33.6, 48.6, 110.2, 111.5, 113.6, 118.2, 120.0, 120.5, 122.3, 123.6, 125.5, 126.9, 128.0, 130.2, 134.4, 138.1, 138.2, 138.4, 142.0, 143.2, 156.1. **MS** (FAB): m/z (%) = 405.3 (97), 406.3 (33), 407.3 (100), 408.3 (28). **HR-MS** (FAB): calcd for $C_{23}H_{22}N_2{}^{79}Br_1{}^+$ = 405.0961, found = 405.0961. **IR** (ATR): ṽ (cm^{-1}) = 3001 (w), 1585 (s), 1333 (w), 1243 (m).

(*E*)-1-(3-bromopropyl)-2-(2-(5-methoxy-1*H*-indol-3-yl)vinyl)quinolin-1-ium bromide (31):



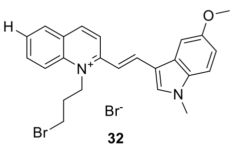
31

$C_{23}H_{22}Br_2N_2O$
502.2500 g/mol

Yield: 43 %.

^{1}H NMR (400 MHz, DMSO) δ = 12.31 (s, 1H), 8.81 (d, *J*=9.2, 1H), 8.74 (d, *J*=15.1, 1H), 8.65 (d, *J*=9.3, 1H), 8.42 (d, *J*=8.9, 1H), 8.39 (d, *J*=3.2, 1H), 8.28 – 8.23 (m, 1H), 8.13-8.06 (m, 1H), 7.84 (t, *J*=7.5, 1H), 7.69 (d, *J*=2.4, 1H), 7.49 – 7.37 (m, 2H), 6.93 (dd, *J*=8.8, 2.4, 1H), 5.14 – 5.01 (m, 2H), 3.96 – 3.84 (m, 6H), 2.50 (under DMSO signal, 2H). **^{13}C NMR** (100 MHz, DMSO) δ = 30.8, 31.0, 48.5, 55.7, 102.6, 109.8, 113.0, 113.7, 114.6, 118.1, 120.1, 126.4, 126.9, 127.9, 130.2, 132.2, 134.3, 138.4, 141.8, 143.8, 155.6, 156.3. **MS** (FAB): m/z (%) = 421.1 (100), 424.1 (28). **HR-MS** (FAB): calcd for $C_{23}H_{22}O_1N_2{}^{79}Br_1{}^+$ = 421.0915, found = 421.0914. **IR** (ATR): ṽ (cm^{-1}) = 3044 (w), 1583 (m), 1331 (w), 1254 (m).

(*E*)-1-(3-bromopropyl)-2-(2-(5-methoxy-1-methyl-1*H*-indol-3-yl)vinyl)quinolin-1-ium bromide (32):



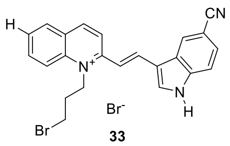
32

$C_{24}H_{24}Br_2N_2O$
516.2770 g/mol

Yield: 63 %.

^{1}H NMR (400 MHz, DMSO) δ = 8.79 (dd, *J*=9.2, 3.6, 1H), 8.69 (dd, *J*=15.1, 8.1, 1H), 8.64 (dd, *J*=9.3, 6.1, 1H), 8.41 (t, *J*=8.8, 1H), 8.32 (d, *J*=27.3, 1H), 8.27 – 8.20 (m, 1H), 8.12 – 8.03 (m, 1H), 7.88 – 7.78 (m, 1H), 7.70 (dd, *J*=6.3, 2.4, 1H), 7.54 (dd, *J*=8.9, 2.9, 1H), 7.02 – 6.95 (m, 1H), 5.09 – 4.93 (m, 2H), 3.92 (d, *J*=4.2, 3H), 3.90 (s, 3H), 3.76 – 3.68 (m, 1H), 2.50 (under DMSO signal, 2H), 2.20 – 2.11 (m, 1H). **^{13}C NMR** (100 MHz, DMSO) δ = 30.7, 31.1, 33.8, 47.4, 55.6, 102.6, 109.8, 113.1, 113.5, 113.6, 118.3, 120.1, 126.8, 126.8, 127.8, 130.2, 134.2, 138.4, 141.5, 143.1, 156.0. **MS** (FAB): m/z (%) = 435.1 (38), 438.1 (11). **HR-MS** (FAB): calcd for $C_{24}H_{24}O_1N_2{}^{79}Br_1{}^+$ = 435.0172, found = 435.1070. **IR** (ATR): ṽ (cm^{-1}) = 3349 (w), 1589 (s), 1306 (m), 1217 (s).

(*E*)-1-(3-bromopropyl)-2-(2-(5-cyano-1*H*-indol-3-yl)vinyl)quinolin-1-ium bromide (33):



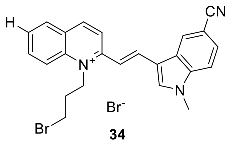
33

$C_{23}H_{19}Br_2N_3$
497.2340 g/mol

Yield: 57 %.

^{1}H NMR (400 MHz, DMSO) δ = 12.73 (s, 1H), 8.95 (d, *J*=9.1, 1H), 8.80 – 8.58 (m, 4H), 8.51 (d, *J*=9.0, 1H), 8.35 – 8.26 (m, 1H), 8.20 – 8.09 (m, 1H), 7.89 (t, *J*=7.5, 1H), 7.73 (d, *J*=8.5, 1H), 7.68 – 7.56 (m, 2H), 5.17 (t, *J*=8.1, 2H), 3.92 (t, *J*=6.2, 2H), 2.50 (under DMSO signal, 2H). **^{13}C NMR** (100 MHz, DMSO) δ = 30.9, 31.2, 48.9, 103.7, 112.7, 114.1, 114.4, 118.4, 120.1, 120.4, 125.3, 125.5, 126.0, 127.4, 128.4, 130.3, 134.7, 135.1, 138.3, 139.0, 141.9, 142.9, 156.2. **MS** (FAB): m/z (%) = 418.1 (100), 419.1 (28). **HR-MS** (FAB): calcd for $C_{23}H_{19}N_3{}^{79}Br_1{}^+$ = 416.0762, found = 416.0761. **IR** (ATR): ṽ (cm^{-1}) = 3013 (m), 2220 (w), 1589 (s), 1312 (w), 1252 (m).

(*E*)-1-(3-bromopropyl)-2-(2-(5-cyano-1-methyl-1*H*-indol-3-yl)vinyl)quinolin-1-ium bromide (34):



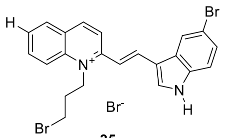
34

$C_{24}H_{21}Br_2N_3$
511.2610 g/mol

Yield: 60 %.

^{1}H NMR (400 MHz, DMSO) δ = 8.95 (d, *J*=9.0, 1H), 8.78 (d, *J*=1.5, 1H), 8.69 (dd, *J*=12.4, 3.3, 2H), 8.59 – 8.46 (m, 2H), 8.35 – 8.28 (m, 1H), 8.20-8.11 (m, 1H), 8.06 – 7.95 (m, 1H), 7.95 – 7.81 (m, 3H), 7.78 – 7.71 (m, 1H), 7.59 (d, *J*=15.5, 1H), 5.17 (d, *J*=16.4, 2H), 4.01 (s, 3H), 3.91 (t, *J*=6.3, 2H), 2.50 (under DMSO signal, 2H). **^{13}C NMR** (100 MHz, DMSO) δ = 30.9, 31.0, 33.8, 48.9, 104.0, 112.8, 113.5, 118.4, 120.0, 120.4, 125.5, 125.7, 126.0, 127.4, 128.4, 130.3, 134.7, 138.4, 139.5, 141.2, 143.0, 156.1. **MS** (FAB): m/z (%) = 432.1 (100), 433.1 (30). **HR-MS** (FAB): calcd for $C_{24}H_{21}N_3{}^{79}Br_1{}^+$ = 430.0919, found = 430.0920. **IR** (ATR): ṽ (cm^{-1}) = 2219 (m), 1585 (s), 1350 (s), 1257 (s).

(*E*)-2-(2-(5-bromo-1*H*-indol-3-yl)vinyl)-1-(3-bromopropyl)quinolin-1-ium bromide (35):



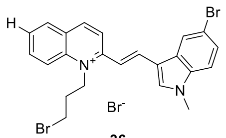
35

$C_{22}H_{19}Br_3N_2$
551.1200 g/mol

Yield: 60 %.

^{1}H NMR (400 MHz, DMSO) δ = 12.52 (s, 1H), 8.87 (d, *J*=9.2, 1H), 8.73 (d, *J*=15.3, 1H), 8.68 (d, *J*=9.2, 1H), 8.51 (d, *J*=3.0, 1H), 8.47 (d, *J*=9.0, 1H), 8.40 (d, *J*=1.9, 1H), 8.32 – 8.23 (m, 1H), 8.16-8.06 (m, 1H), 7.86 (t, *J*=7.5, 1H), 7.56 – 7.43 (m, 2H), 7.40 (dd, *J*=8.8, 1.8, 1H), 5.17 – 5.04 (m, 2H), 3.93 (t, *J*=6.2, 2H), 2.50 (under DMSO signal, 2H). **^{13}C NMR** (100 MHz, DMSO) δ = 30.8, 31.2, 48.7, 111.2, 113.9, 114.6, 114.8, 118.3, 120.2, 122.3, 125.9, 127.1, 127.3, 128.1, 130.2, 134.5, 134.7, 136.1, 138.3, 142.4, 142.8, 156.2. **MS** (FAB): m/z (%) = 469.0 (51), 470.0 (20), 471.0 (100), 472.0 (30), 473.0 (50), 474.0 (13), 475.0 (2). **HR-MS** (FAB): calcd for $C_{22}H_{19}N_2{}^{79}Br_2{}^+$ = 468.9915, found = 468.9918; calcd for $C_{22}H_{19}N_2{}^{79}Br_1{}^{81}Br_1{}^+$ = 470.9894, found = 470.9893. **IR** (ATR): ṽ (cm^{-1}) = 3088 (w), 1597 (s), 1320 (s), 1251 (s).

(*E*)-2-(2-(5-bromo-1-methyl-1*H*-indol-3-yl)vinyl)-1-(3-bromopropyl)quinolin-1-ium bromide (36):



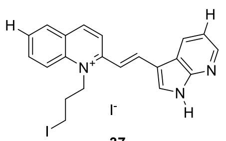
36

$C_{23}H_{21}Br_3N_2$
565.1470 g/mol

Yield: 65 %.

^{1}H NMR (400 MHz, DMSO) δ = 8.86 (d, *J*=9.1, 1H), 8.69 (d, *J*=6.9, 1H), 8.66 (s, 1H), 8.45 (d, *J*=9.2, 1H), 8.42 (s, 1H), 8.27 (dd, *J*=8.2, 1.6, 1H), 8.16-8.07 (m, 1H), 7.87 (t, *J*=7.5, 1H), 7.62 (d, *J*=8.7, 1H), 7.53 – 7.40 (m, 2H), 5.15 – 5.04 (m, 1H), 3.95 (s, 3H), 3.91 (t, *J*=6.2, 2H), 2.50 (under DMSO signal, 2H). **^{13}C NMR** (100 MHz, DMSO) δ = 30.8, 31.0, 33.8, 48.7, 111.2, 112.8, 113.5, 115.1, 118.3, 120.2, 122.4, 126.0, 127.1, 127.6, 128.2, 130.2, 134.5, 136.7, 137.7, 138.3, 142.1, 142.3, 156.1. **MS** (FAB): m/z (%) = 483.0 (53), 484.0 (18), 485.0 (100), 486.0 (30), 487.0 (52), 488.0 (14), 489.0 (3). **HR-MS** (FAB): calcd for $C_{23}H_{21}N_2{}^{79}Br_2{}^+$ = 483.0071, found = 483.0074; calcd for $C_{23}H_{21}N_2{}^{79}Br_1{}^{81}Br_1{}^+$ = 485.0051, found = 485.0053. **IR** (ATR): ṽ (cm^{-1}) = 3007 (w), 1590 (s), 1309 (s), 1231 (m).

(*E*)-2-(2-(1*H*-pyrrolo[2,3-*b*]pyridin-3-yl)vinyl)-1-(3-iodopropyl)quinolin-1-ium iodide (37):



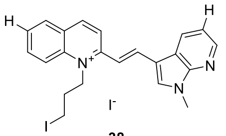
37

$C_{21}H_{19}I_2N_3$
567.2129 g/mol

The conversion to the iodide yielded not in pure products. Corresponding bromide synthesis is recommended.

(**^{1}H NMR** (400 MHz, DMSO) δ = 12.89 – 12.76 (m, 1H), 8.91 (dd, *J*=9.2, 5.6, 1H), 8.75 – 8.55 (m, 4H), 8.55 – 8.45 (m, 2H), 8.45 – 8.35 (m, 1H), 8.35 – 8.24 (m, 1H), 8.19 – 8.07 (m, 1H), 7.95 – 7.82 (m, 1H), 7.42 – 7.27 (m, 1H), 5.13 – 5.00 (m, 2H), 3.74 (t, *J*=5.3, 1H), 3.62 (t, *J*=6.7, 1H), 2.50 (under DMSO signal, 1H), 2.23 – 2.05 (m, 1H).. **^{13}C NMR** (100 MHz, DMSO) δ = 31.4, 50.8, 57.4, 111.9, 111.9, 113.0, 117.3, 118.6, 120.3, 127.4, 128.3, 129.1, 134.2, 134.5, 134.6, 138.4, 142.6, 142.8, 144.6, 149.8, 156.2.**)** **MS** (FAB): m/z (%) = 440.1 (100), 441.1 (30). **HR-MS** (FAB): calcd for $C_{21}H_{19}N_3{}^{127}I_1{}^+$ = 440.0624, found = 440.0626. **IR** (ATR): ṽ (cm^{-1}) = 3320 (w), 2717 (w), 1566 (s), 1316 (m), 1273 (m).

(*E*)-1-(3-iodopropyl)-2-(2-(1-methyl-1*H*-pyrrolo[2,3-*b*]pyridin-3-yl)vinyl)quinolin-1-ium iodide (38):



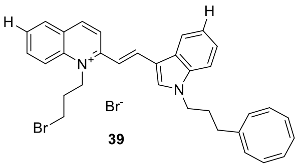
38

$C_{22}H_{21}I_2N_3$
581.2399 g/mol

The conversion to the iodide yielded not in pure products. Corresponding bromide synthesis is recommended.

(^{1}H NMR (400 MHz, DMSO) δ = 2.50, 3.97, 4.04, 5.16, 7.40, 7.52, 7.88, 8.14, 8.30, 8.47, 8.49, 8.49, 8.63, 8.64, 8.64, 8.91. **^{13}C NMR** (100 MHz, DMSO) δ = 30.6, 31.5, 42.2, 47.6, 117.7, 111.5, 128.0, 134.3, 129.9, 143.9, 118.1, 137.2, 142.2, 128.9, 119.9, 142.5.**) MS** (FAB): m/z (%) = 454.1 (72), 455.1 (21). **HR-MS** (FAB): calcd for $C_{22}H_{21}N_3{}^{127}I_1{}^+$ = 454.0780, found = 454.0783. **IR** (ATR): ṽ (cm^{-1}) = 3041 (w), 1588 (s), 1306 (s), 1280 (w).

1-(3-bromopropyl)-2-((*E*)-2-(1-(3-((1*Z*,3*Z*,5*Z*,7*Z*)-cycloocta-1,3,5,7-tetraen-1-yl)propyl)-1*H*-indol-3-yl)vinyl)quinolin-1-ium bromide (39):



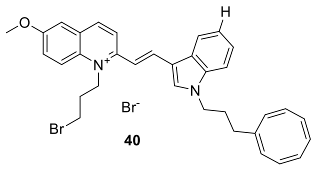
39

$C_{33}H_{32}Br_2N_2$
616.4410 g/mol

Yield: 23 %.

^{1}H NMR (500 MHz, DMSO) δ = 8.85 (d, *J*=9.1, 1H), 8.70 (d, *J*=15.2, 1H), 8.64 (d, *J*=9.3, 1H), 8.46 (d, *J*=9.0, 1H), 8.37 (s, 1H), 8.26 (t, *J*=8.3, 2H), 8.16 (m, 1H), 7.85 – 7.83 (m, 1H), 7.70 (d, *J*=8.2, 1H), 7.48 (d, *J*=15.2, 1H), 7.39 (t, *J*=7.8, 1H), 7.34 (t, *J*=7.7, 1H), 5.88 – 5.70 (m, 6H), 5.57 (s, 1H), 5.10 (t, *J*=8.1, 2H), 4.37 (t, *J*=7.0, 2H), 3.94 (t, *J*=6.2, 2H), 2.09 (t, *J*=7.2, 2H), 1.99 – 1.89 (m, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ = 28.3, 30.6, 31.4, 34.0, 45.9, 48.7, 110.6, 111.5, 113.9, 118.2, 120.1, 120.7, 122.3, 123.7, 125.7, 127.0, 128.0, 130.2, 131.2, 131.8, 132.3, 134.1, 134.4, 136.9, 137.5, 138.4, 142.2, 142.6, 143.1, 156.2. **MS** (FAB): m/z (%) = 535.2 (100), 538.2 (37). **HR-MS** (FAB): calcd for $C_{33}H_{32}N_2{}^{79}Br_1{}^+$ = 535.1743, found = 535.1745. **IR** (ATR): ṽ (cm^{-1}) = 3369 (w), 2919 (m), 2850 (w), 1730 (w), 1586 (s), 1311 (w), 1251 (w).

1-(3-bromopropyl)-2-((*E*)-2-(1-(3-((1*Z*,3*Z*,5*Z*,7*Z*)-cycloocta-1,3,5,7-tetraen-1-yl)propyl)-1*H*-indol-3-yl)vinyl)-6-methoxyquinolin-1-ium bromide (40):



40

$C_{34}H_{34}Br_2N_2O$
646.4670 g/mol

Yield: 39 %:

^{1}H NMR (400 MHz, DMSO) δ = 8.75 (d, *J*=9.1, 1H), 8.65 – 8.52 (m, 2H), 8.41 (d, *J*=9.7, 1H), 8.30 (s, 1H), 8.23 (d, *J*=7.9, 1H), 7.80 – 7.64 (m, 3H), 7.45 (d, *J*=15.3, 1H), 7.41 – 7.27 (m, 2H), 5.88 – 5.68 (m, 6H), 5.56 (s, 1H), 5.09 (t, *J*=7.7, 2H), 4.40 – 4.30 (m, 2H), 3.98 (s, 3H), 3.92 (t, *J*=6.4, 2H), 2.08 (t, *J*=7.4, 2H), 1.98 – 1.87 (m, 2H), 2.50 (under DMSO signal, 2H). **^{13}C NMR** (100 MHz, DMSO) δ = 28.3, 30.8, 31.3, 34.0, 45.8, 48.9, 56.1, 109.2, 110.7, 111.4, 113.6, 120.1, 120.6, 122.0, 123.5, 125.1, 125.7, 127.1, 128.9, 131.7, 132.3, 133.5, 136.0, 137.4, 141.3, 141.5, 142.6, 153.9, 158.1. **MS** (FAB): m/z (%) = 565.2 (94), 566.2 (42), 567.2(100), 568.2 (38). **HR-MS** (FAB): calcd for $C_{34}H_{34}O_1N_2{}^{79}Br_1{}^+$ = 565.1855, found = 565.1855. **IR** (ATR): ṽ (cm^{-1}) = 2991 (w), 1569 (s), 1374 (m), 1252 (m).

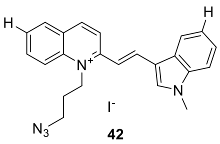
e. Syntheses of the Dye-Azides 41-52

The synthesis of compound **41** is described in earlier publications of our group.[1]

General dye-azide synthesis (41-52):

In a headspace vial 60 µmol (1.00 eq) dye-bromide/-iodide, 200 µmol (3.33 eq) sodium iodide and 600 µmol (3.00 eq) sodium azide were dissolved in 1.6 mL dry dimethylformamide and stirred at room temperature for 19 h. Then the mixture is poured into 150 mL diethyl ether and 50 mL *n*-hexane and let stand until the precipitate settled. The supernatant fluid was decanted and the remaining solid was then mixed with 2 g sodium iodide. The mixture was distributed between 150 mL dichloromethane and 50 mL distilled water. The aqueous phase was 3x back extracted with 100 mL dichloromethane. Under reduced pressure the combined organic layers were evaporated to dryness. The formed solid was suspended in 2 mL methanol, exposed to ultrasound for 10 min, filtered and washed 3x with 5 mL diethyl ether.

(*E*)-1-(3-azidopropyl)-2-(2-(1-methyl-1*H*-indol-3-yl)vinyl)quinolin-1-ium iodide (42):



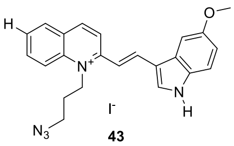
42

$C_{23}H_{22}IN_5$
495.3685 g/mol

Yield: 77 %.

^{1}H NMR (400 MHz, DMSO) δ = 8.80 (d, *J*=9.1, 1H), 8.73 – 8.57 (m, 2H), 8.44 (d, *J*=8.9, 1H), 8.32 (s, 1H), 8.25 (ddd, *J*=7.4, 5.3, 1.6, 2H), 8.14-8.03 (m, 1H), 7.84 (t, *J*=7.5, 1H), 7.62 (dd, *J*=7.8, 1.4, 1H), 7.48 – 7.28 (m, 3H), 4.99 (t, *J*=8.2, 2H), 3.94 (s, 3H), 3.82 (t, *J*=6.2, 2H), 2.17 (q, *J*=7.3, 6.0, 2H). **^{13}C NMR** (100 MHz, DMSO) δ = 27.3, 33.5, 47.3, 48.1, 110.1, 111.5, 113.6, 118.2, 119.9, 120.4, 122.3, 123.6, 125.4, 126.8, 127.9, 130.1, 134.3, 138.3, 138.5, 139.2, 141.9, 143.2, 155.9. **MS** (FAB): m/z (%) = 368.2 (100), 369.2 (28) 370.2 (3). **HR-MS** (FAB): calcd for $C_{23}H_{22}N_5^+$ = 368.1870, found = 384.1867. **IR** (ATR): ṽ (cm^{-1}) = 2086 (m), 1514 (m), 1224 (m).

(*E*)-1-(3-azidopropyl)-2-(2-(5-methoxy-1*H*-indol-3-yl)vinyl)quinolin-1-ium iodide (43):



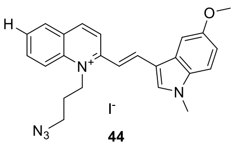
43

$C_{23}H_{22}IN_5O$
511.3675 g/mol

Yield: 71 %.

^{1}H NMR (600 MHz, DMSO): δ = 12.29 (s, 1H), 8.80 (d, *J*=9.1, 1H), 8.73 (d, *J*=15.1, 1H), 8.63 (d, *J*=9.2, 1H), 8.42 (d, *J*=8.9, 1H), 8.36 (s, 1H), 8.25 (d, *J*=7.3, 1H), 8.12-8.06 (m, 1H), 7.84 (t, *J*=7.4, 1H), 7.71 (d, *J*=2.6, 1H), 7.47 (d, *J*=8.7, 1H), 7.41 (d, *J*=15.2, 1H), 6.95 (dd, *J*=8.9, 2.3, 1H), 5.01 (t, *J*=7.7, 2H), 3.89 (s, 3H), 3.79 (t, *J*=6.3, 2H), 2.20 (p, *J*=6.7, 2H). **^{13}C NMR** (100 MHz, DMSO): δ = 27.3, 39.5, 47.2, 48.0, 55.6, 103.1, 109.7, 112.5, 113.6, 114.6, 118.2, 119.9, 126.2, 126.8, 127.8, 130.1, 132.4, 134.3, 134.9, 138.3, 141.7, 143.8, 155.6, 156.1. **MS** (FAB): m/z (%) = 384.2 (100), 385.2 (31). **HR-MS** (FAB): calcd for $C_{23}H_{22}O_1N_5^+$ = 384.1819, found = 384.1817. **IR** (ATR): ṽ (cm^{-1}) = 3148 (w), 2103 (m), 1507 (m), 1223 (w).

(*E*)-1-(3-azidopropyl)-2-(2-(5-methoxy-1-methyl-1*H*-indol-3-yl)vinyl)quinolin-1-ium iodide (44):



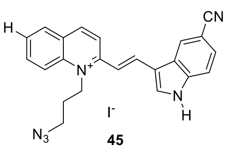
44

$C_{24}H_{24}IN_5O$
525.3945 g/mol

Yield: 64 %.

^{1}H NMR (600 MHz, DMSO): δ = 8.79 (d, *J*=9.1, 1H), 8.70 (d, *J*=15.2, 1H), 8.63 (d, *J*=9.2, 1H), 8.41 (d, *J*=9.5, 1H), 8.32 (s, 1H), 8.24 (d, *J*=8.0, 1H), 8.12-8.07 (m, 1H), 7.83 (t, *J*=7.5, 1H), 7.73 (d, *J*=2.4, 1H), 7.56 (d, *J*=9.0, 1H), 7.38 (d, *J*=15.2, 1H), 7.03 (dd, *J*=8.9, 2.4, 1H), 5.00 (t, *J*=7.9, 2H), 3.93 (s, 3H), 3.90 (s, 3H), 3.78 (t, *J*=6.3, 2H), 2.20 (p, *J*=7.3, 2H). **^{13}C NMR** (100 MHz, DMSO): δ = 27.3, 33.8, 47.2, 48.0, 55.6, 103.3, 109.6, 112.3, 112.4, 113.5, 118.2, 119.9, 126.7, 126.8, 127.8, 130.1, 133.2, 134.3, 137.9, 138.3, 141.7, 143.2, 156.0, 156.0. **MS** (FAB): m/z (%) = 398.2 (100), 399.2 (32). **HR-MS** (FAB): calcd for $C_{24}H_{24}O_1N_5^+$ = 398.1975, found = 398.1976. **IR** (ATR): ṽ (cm^{-1}) = 3008 (w), 2096 (m), 1589 (s), 1217 (s).

(*E*)-1-(3-azidopropyl)-2-(2-(5-cyano-1*H*-indol-3-yl)vinyl)quinolin-1-ium iodide (45):



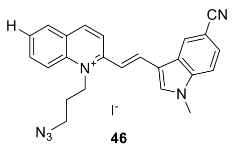
45

$C_{23}H_{19}IN_6$
506.3515 g/mol

Yield: 51 %.

^{1}H NMR (600 MHz, DMSO): δ = 12.71 (s, 1H), 8.95 (d, *J*=9.0, 1H), 8.80-8.76 (m, 1H), 8.71 (d, *J*=15.5, 1H), 8.67 (d, *J*=9.1, 1H), 8.57 (s, 1H), 8.51 (d, *J*=9.0, 1H), 8.34-8.28 (m, 1H), 8.20-8.11 (m, 1H), 7.90 (t, *J*=7.5, 1H), 7.74 (d, *J*=8.5, 1H), 7.67 (dd, *J*=8.5, 1.5, 1H), 7.63 (d, *J*=15.6, 1H), 5.13 (t, *J*=8.1, 2H), 3.76 (t, *J*=6.3, 2H), 2.21 (p, *J*=6.5, 2H). **^{13}C NMR** (150 MHz, DMSO): δ = 27.5, 47.7, 48.0, 103.8, 112.9, 114.2, 114.5, 118.6, 120.1, 120.3, 125.3, 125.4, 126.0, 127.4, 128.4, 130.3, 134.7, 135.2, 138.3, 139.1, 141.7, 142.9, 156.1. **MS** (FAB): m/z (%) = 379.2 (100), 380.2 (31). **HR-MS** (FAB): calcd for $C_{23}H_{19}N_6^+$ = 379.1666, found = 379.1666. **IR** (ATR): ṽ (cm^{-1}) = 2997 (w), 2217 (w), 2104 (m), 1592 (s), 1229 (m).

(*E*)-1-(3-azidopropyl)-2-(2-(5-cyano-1-methyl-1*H*-indol-3-yl)vinyl)quinolin-1-ium iodide (46):



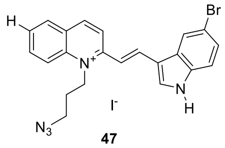
46

$C_{24}H_{21}IN_6$
520.3785 g/mol

Yield: 43 %.

^{1}H NMR (400 MHz, DMSO) δ = 8.68 (d, *J*=15.3, 1H), 8.66 – 8.62 (m, 1H), 8.95 (d, *J*=9.0, 1H), 8.79 (s, 1H), 8.67 (d, *J*=9.5, 2H), 8.53 (s, 1H), 8.51 (d, *J*=8.7, 1H), 8.34-8.23 (m, 1H), 8.20-8.12 (m, 1H), 7.90 (t, *J*=7.6, 1H), 7.86 (d, *J*=8.6, 1H), 7.79-7.73 (m, 1H), 7.60 (d, *J*=15.6, 1H), 5.12 (t, *J*=7.7, 2H), 4.01 (s, 3H), 3.76 (t, *J*=6.4, 2H), 2.21 (p, *J*=6.8, 2H). **^{13}C NMR** (100 MHz, DMSO): δ = 27.5, 33.8, 47.6, 48.0, 104.1, 112.8, 112.9, 113.6, 118.5, 112.0, 120.3, 125.5, 125.6, 126.0, 127.4, 128.4, 130.3, 134.7, 138.3, 138.4, 139.5, 141.1, 142.9, 156.0. **MS** (FAB): m/z (%) = 393.2 (100), 394.2 (32). **HR-MS** (FAB): calcd for $C_{24}H_{21}N_6^+$ = 393.1822, found = 393.1820. **IR** (ATR): ṽ (cm^{-1}) = 3009 (w), 2224 (w), 2094 (m), 1592 (s), 1229 (m).

(*E*)-1-(3-azidopropyl)-2-(2-(5-bromo-1*H*-indol-3-yl)vinyl)quinolin-1-ium iodide (47):



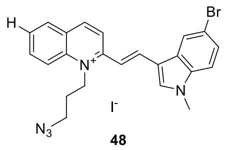
47

$C_{22}H_{19}BrIN_5$
560.2375 g/mol

Yield: 36 %.

^{1}H NMR (600 MHz, DMSO): δ = 12.48 (s, 1H), 8.87 (d, *J*=9.1, 1H), 8.71 (d, *J*=15.3, 1H), 8.66 (d, *J*=9.1, 1H), 8.46 (d, *J*=8.9, 1H), 8.45 (s, 1H), 8.44-8.41 (m, 1H), 8.30-8.25 (m, 1H), 8.15-8.09 (m, 1H), 7.87 (t, *J*=7.5, 1H), 7.54 (d, *J*=8.5, 1H), 7.49 (d, *J*=15.3, 1H), 7.43 (dd, *J*=8.6, 1.8, 1H), 5.06 (t, *J*=7.8, 2H), 3.79 (t, *J*=6.3, 2H), 2.20 (p, *J*=6.5, 2H). **^{13}C NMR** (100 MHz, DMSO): δ = 27.4, 47.5, 48.0, 111.4, 113.9, 114.6, 114.9, 118.4, 120.1, 122.3, 125.9, 127.1, 127.3, 128.2, 130.2, 134.5, 134.8, 136.2, 138.3, 142.4, 142.7, 156.1. **MS** (FAB): m/z (%) = 432.1 (25), 435.1 (7). **HR-MS** (FAB): calcd for $C_{22}H_{19}N_5{}^{79}Br_1^+$ = 432.0818, found = 432.0820. **IR** (ATR): ṽ (cm^{-1}) = 3163 (w), 2101 (m), 1594 (s), 1315 (s), 1241 (m).

(*E*)-1-(3-azidopropyl)-2-(2-(5-bromo-1-methyl-1*H*-indol-3-yl)vinyl)quinolin-1-ium iodide (48):



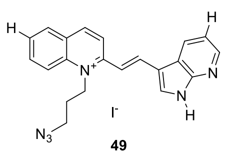
48

$C_{23}H_{21}BrIN_5$
574.2645 g/mol

Yield: 57 %.

^{1}H NMR (600 MHz, DMSO): δ = 8.86 (d, *J*=9.1, 1H), 8.68 (d, *J*=15.4, 1H), 8.66 (d, *J*=9.1, 1H), 8.45 (d, *J*=9.1, 1H), 8.43 (s, 1H), 8.42 (s, 1H), 8.27 (d, *J*=7.3, 1H), 8.15-8.08 (m, 1H), 7.86 (t, *J*=7.5, 1H), 7.62 (d, *J*=8.7, 1H), 7.50 (dd, *J*=8.9, 1.8, 1H), 7.45 (d, *J*=15.4, 1H), 5.04 (t, *J*=8.0, 2H), 3.95 (s, 3H), 3.79 (t, *J*=6.4, 2H), 2.19 (p, *J*=6.8, 2H). **^{13}C NMR** (150 MHz, DMSO): δ = 27.4, 33.8, 47.4, 48.0, 111.3, 112.9, 113.5, 115.1, 118.4, 120.1, 122.4, 125.9, 127.1, 127.6, 128.1, 130.2, 134.5, 136.8, 137.8, 138.3, 142.0, 142.3, 156.0. **MS** (FAB): m/z (%) = 446.1 (36), 449.1 (10). **HR-MS** (FAB): calcd for $C_{23}H_{21}N_5{}^{79}Br_1^+$ = 446.0975, found = 446.0973. **IR** (ATR): ṽ (cm^{-1}) = 3007 (w), 2091 (m), 1592 (s), 1311 (s), 1230 (m).

(*E*)-2-(2-(1*H*-pyrrolo[2,3-*b*]pyridin-3-yl)vinyl)-1-(3-azidopropyl)quinolin-1-ium iodide (49):



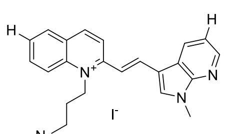
49

$C_{21}H_{19}IN_6$
482.3295 g/mol

Yield: 29 %.

^{1}H NMR (500 MHz, DMSO) δ = 12.82 (s, 1H), 8.91 (d, *J*=9.1, 1H), 8.75-8.68 (m, 1H), 8.66 – 8.57 (m, 2H), 8.52 (d, *J*=9.0, 1H), 8.45-8.40 (m, 1H), 8.39 (s, 1H), 8.33-8.25 (m, 1H), 8.16-8.08 (m, 1H), 7.88 (t, *J*=7.5, 1H), 7.65 (d, *J*=15.6, 1H), 7.33 (dd, *J*=7.9, 4.7, 1H), 5.07 (t, *J*=8.1, 2H), 3.74 (q, *J*=5.1, 2H), 2.24 – 2.12 (m, 2H). **^{13}C NMR** (125 MHz, DMSO) δ = 31.3, 47.9, 57.4, 111.9, 113.0, 117.4, 117.9, 118.7, 120.0, 127.2, 128.3, 129.1, 130.2, 134.5, 135.0, 138.4, 142.6, 142.9, 144.7, 150.0, 156.1. **MS** (FAB): m/z (%) = 355.1 (72), 356.1 (28). **HR-MS** (FAB): calcd for $C_{21}H_{19}N_6^+$ = 355.1671, found = 355.1670. **IR** (ATR): ṽ (cm^{-1}) = 3321 (w), 2099 (m), 1568 (s), 1317 (m), 1275 (m).

(*E*)-1-(3-azidopropyl)-2-(2-(1-methyl-1*H*-pyrrolo[2,3-*b*]pyridin-3-yl)vinyl)quinolin-1-ium iodide (50):



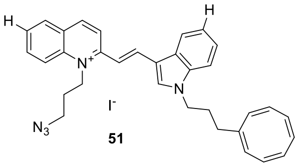
50

$C_{22}H_{21}IN_6$
496.3565 g/mol

Yield: 34 %.

^{1}H NMR (400 MHz, DMSO) δ = 8.91 (d, *J*=9.3, 1H), 8.73 – 8.58 (m, 3H), 8.53 – 8.43 (m, 3H), 8.30 (d, *J*=8.4, 1H), 8.14 (t, *J*=7.8, 1H), 7.89 (t, *J*=7.5, 1H), 7.52 (d, *J*=15.4, 1H), 7.39 (dd, *J*=7.3, 4.3, 1H), 5.08 (t, *J*=8.0, 2H), 3.97 (s, 3H), 3.78 (t, *J*=6.2, 2H), 2.27 – 2.17 (m, 2H). **^{13}C NMR** (100 MHz, DMSO) δ = 27.5, 31.7, 47.6, 48.0, 111.6, 111.9, 117.7, 118.0, 118.5, 120.2, 127.2, 128.3, 129.0, 130.2, 134.6, 137.8, 138.3, 142.5, 142.7, 144.5, 148.8, 156.0. **MS** (FAB): m/z (%) = 369.1 (100), 370.1 (30). **HR-MS** (FAB): calcd for $C_{22}H_{21}N_6^+$ = 369.1828, found = 369.1827. **IR** (ATR): ṽ (cm^{-1}) = 2099 (s), 1563 (s), 1349 (m), 1282 (m).

1-(3-azidopropyl)-2-((*E*)-2-(1-(3-((1*Z*,3*Z*,5*Z*,7*Z*)-cycloocta-1,3,5,7-tetraen-1-yl)propyl)-1*H*-indol-3-yl)vinyl)quinolin-1-ium iodide (51):



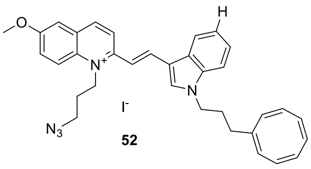
51

$C_{33}H_{32}IN_5$
625.5585 g/mol

Yield: 37 %.

^{1}H NMR (600 MHz, DMSO) δ = 8.84 (d, *J*=9.1, 1H), 8.68 (d, *J*=15.3, 1H), 8.63 (d, *J*=9.2, 1H), 8.46 (d, *J*=9.0, 1H), 8.33 (s, 1H), 8.28 (d, *J*=8.0, 1H), 8.26 (d, *J*=8.1, 1H), 8.16 – 8.06 (m, 1H), 7.86 (t, *J*=7.5, 1H), 7.71 (d, *J*=8.2, 1H), 7.48 (d, *J*=15.2, 1H), 7.40 (t, *J*=7.5, 1H), 7.35 (t, *J*=7.4, 1H), 5.90 – 5.68 (m, 6H), 5.56 (s, 1H), 5.03 (t, *J*=8.3, 2H), 4.37 (t, *J*=7.2, 2H), 3.80 (t, *J*=6.0, 2H), 2.28 – 2.14 (m, 2H), 2.08 (t, *J*=7.4, 2H), 2.03 – 1.86 (m, 2H). **^{13}C NMR** (150 MHz, DMSO) δ = 27.4, 28.3, 34.0, 45.9, 47.4, 48.1, 110.6, 111.6, 113.9, 118.4, 120.0, 120.6, 122.3, 123.7, 125.6, 127.0, 127.1, 128.0, 130.2, 131.2, 131.8, 132.3, 134.1, 134.4, 137.3, 137.6, 138.3, 142.1, 142.6, 143.1, 156.1. **MS** (FAB): m/z (%) = 498.3 (100), 499.3 (41). **HR-MS** (FAB): calcd for $C_{33}H_{32}N_5^+$ = 498.2652, found = 498.2651. **IR** (ATR): ṽ (cm^{-1}) = 2095 (m), 1566 (m), 1350 (w), 1238 (m).

1-(3-azidopropyl)-2-((*E*)-2-(1-(3-((1*Z*,3*Z*,5*Z*,7*Z*)-cycloocta-1,3,5,7-tetraen-1-yl)propyl)-1*H*-indol-3-yl)vinyl)-6-methoxyquinolin-1-ium iodide (52):



52

$C_{34}H_{34}IN_5O$
655.5845 g/mol

Yield: 48 %.

^{1}H NMR (600 MHz, DMSO) δ = 8.74 (d, *J*=9.1, 1H), 8.65 – 8.50 (m, 2H), 8.41 (d, *J*=9.7, 1H), 8.28 (s, 1H), 8.25 (d, *J*=7.9, 1H), 7.75 (d, *J*=3.0, 1H), 7.71 (dd, *J*=9.7, 2.9, 1H), 7.67 (d, *J*=8.2, 1H), 7.43 (d, *J*=15.3, 1H), 7.37 (t, *J*=7.8, 1H), 7.32 (t, *J*=7.5, 1H), 5.92-5.67 (m, 6H), 5.56 (s, 1H), 5.01 (t, *J*=8.4, 2H), 4.34 (t, *J*=7.2, 2H), 3.97 (s, 3H), 3.78 (t, *J*=6.2, 2H), 2.25 – 2.12 (m, 2H), 2.08 (t, *J*=7.4, 2H), 2.00 – 1.84 (m, 2H).**^{13}C NMR** (150 MHz, $CDCl_3$) δ = 27.6, 28.3, 34.0, 45.7, 47.6, 48.0, 56.1, 109.2, 110.7, 111.4, 113.6, 120.2, 120.5, 120.5, 122.1, 123.5, 125.1, 125.6, 127.1, 128.8, 131.2, 131.8, 132.3, 133.4, 134.1, 136.4, 137.4, 141.2, 141.5, 142.6, 153.7, 158.1. **MS** (FAB): m/z (%) = 528.3 (51), 529.3 (22). **HR-MS** (FAB): calcd for $C_{34}H_{34}O_1N_5^+$ = 528.2758, found = 528.2759. **IR** (ATR): ṽ (cm^{-1}) = 2094 (m), 1570 (w), 1347 (m), 1262 (w).

2. DNA-Synthesis and *Click*-Conjugation

a. DNA-Synthesis

The oligonucleotides were synthesized using an *Expedite 8900 Nucleic Acid Synthesizer* from *Applied Biosystems* (*ABI*). The standard phosphoramidite solid phase synthesis was used. The used reagents were purchased from *ABI* and *Proligo*. The phosphoramidites of the natural bases were used as 0.067 M solutions in acetonitrile (*amidite diluent* from *ABI*). The artificial building block 2-'*O*-propargyluridine (cU) was purchased from *ChemGenes* and used as a 0.083 M solution in acetonitrile. The CPG columns from *Glen Research* were used as a solid phase with a pore size of 500 Å and a coating density of 1 µmol. Unmodified DNA strands were obtained from *Metabion international* in HPLC purified state.
The individual reagents are listed below:

Table S1. Used reagents in the phosphoramidite synthesis.

Reagent	Composition
Deblock (Dblk)	3% dichloroacetic acid in dichloromethane
Wash (wsh)	acetonitrile
Activator (Act)	0.45 M tetrazole in acetonitrile
Cap A	acetic anhydride in tetrahydrofuran / pyridine
Cap B	N-methylimidazole in tetrahydrofuran / pyridine
Oxidizer (Ox)	iodine in water / tetrahydrofuran / pyridine

The following coupling protocol was used for the insertion of standard bases (Table S2). Here, for example, thymidine:

Table S2. Coupling protocol for standard bases.

Coding	Function	Mode	Pulse	Time t_c [s]
		$Deblocking		
144	Index Fract. Coll	NA	1	0
0	Default	WAIT	0	1.5
141	Trityl Mon. On / Off	PULSE	1	1
16	Dblk	PULSE	10	0
16	Dblk	PULSE	50	49
38	Diverted Wsh A	PULSE	40	0
141	Trityl Mon. On / Off	NA	0	1
38	Diverted Wsh A	PULSE	40	0
144	Index Fract. Coll	NA	2	0
		$Coupling		
1	Wsh	PULSE	5	0
2	Act	PULSE	5	0
21	T + Act	PULSE	5	0
21	T + Act	PULSE	2	16
2	Act	PULSE	3	24

1	Wsh	PULSE	7	56
1	Wsh	PULSE	8	0
		$Capping		
12	Wsh A	PULSE	20	0
13	Caps	PULSE	8	0
12	Wsh A	PULSE	6	15
12	Wsh A	PULSE	14	0
		$Oxidizing		
15	Ox	PULSE	15	0
12	Wsh A	PULSE	15	0
		$Capping		
13	Caps	PULSE	7	0
12	Wsh A	PULSE	30	0

To insert the **cU** building block, the coupling protocol was modified in the coupling step:

Table S3. Coupling protocol for 2-'*O*-propargyluridine.

Coding	Function	Mode	Pulse	Time t_c [s]
		$Coupling		
1	Wsh	PULSE	5	0
2	Act	PULSE	6	0
24	6 + Act	PULSE	5	0
24	6 + Act	PULSE	2	84
2	Act	PULSE	4	84
1	Wsh	PULSE	7	56
1	Wsh	PULSE	8	0

Following the solid phase synthesis, the CPG column was dried overnight on a *Christ Alpha 1-2 LD Plus* lyophilization system. After opening the CPG column, the CPG granules were transferred into an *Eppendorf* reaction vessel. Then, 700 µL of ammonium hydroxide solution (>25%, *trace select*, *Fluka*) was added to the cleavage from the solid phase and for the deprotection of the bases, and the mixture was heated at 55 °C overnight. After cooling to room temperature, the ammonia was removed (60 min, heating: 55 min, 34 °C., 100 mbar) on a *Christ Alpha AVC* vacuum concentrator with a *Christ Alpha 1-2 LD Plus* lyophilization system. Finally, the supernatant solution was removed and the remaining CPG granules were washed 3x with 200 µL of *Millipore* water. The solvent of the combined extracts was removed on a vacuum concentrator (14 h, 25 °C, 0.1 mbar).

b. *Click*-Conjugation

The dried DNA strands were dissolved in 50 µl of Millipore water and 114 µl of 10 mM azide solution (in DMSO / *t*-BuOH v: v = 3: 1), 34 µl of 100 mM TBTA solution (in DMSO / *t*-BuOH v: V: 3: 1), 25 µL 400 mM sodium ascorbate solution (in *Millipore* water) and 17 µL 100 mM tetrakis(acetonitrile)copper(I) hexafluorophosphate (in DMSO / t-BuOH v: v = 3: 1). The reaction solution was heated to 60 °C for 2 h. After cooling to room temperature, the solution was mixed with 150 µL of 50 mM disodium EDTA solution (in *Millipore* water), 450 µl of 0.3 M sodium acetate solution (in *Millipore* water) and filled up to 10 ml with ethanol (99.6%). To precipitate the DNA, the mixture was incubated overnight at -32 °C. The precipitate was centrifuged (10 min, 4000 rpm) and the supernatant solution was separated off. The residue was washed 3x with 1 mL of 80 % ethanol solution (in *Millipore* water) and finally dried overnight on a Christ Alpha 1-2 LD Plus lyophilization system.

c. Purification of DNA-Dye Bioconjugates

The high-performance liquid chromatography (HPLC) of DNA was carried out on a modular HPLC system from *Shimadzu* (Autosampler *SIL-10AD*, pump module *LC-10AT*, control unit *SCL-10A*, multidiode array *SPD-M10A*, fluorescence detector *RF-10A XL*). Detection, control and evaluation were carried out with the software *Class VP*. Semi-preparative separations were carried out via a reversed phase *Supelcosil* ™ *LC-318* column (250 × 10 mm, 5 µm). The flow rate for semipreparative separations was 2.5 mL/min. The corresponding column was equilibrated with 50 mM ammonium acetate buffer for DNA (pH 6.5, eluent A) and then eluted with different acetonitrile gradients (eluent B). The detection was carried out via the DNA typical UV/VIS absorption at λ=260 nm. The characteristic UV/VIS absorption of DNA strands with covalently bound dyes was additionally detected. For HPLC purification, high-purity (HPLC grade) *Fischer* solvents and water, which had previously been deionized and freshly ultrafiltered in a *Millipore Q8* lab water system, were used. A gradient from 0 to 20 % B over 30 min was chosen followed by an ongoing isocratic flow for 10 min at 40 °C.

3. Extinction Coefficients

To determine the extinction coefficient, a certain amount of the respective dye was dissolved in 20% ethanol (99.6 %). A total of five samples were carried out per dye. For this purpose, the weighed dye was first dissolved in 10 ml of ethanol (99.6 %) and treated in an ultrasonic bath for 10 minutes. After cooling to room temperature, *Millipore* water was added to 50 ml. These solutions (in 20 % ethanol) were further diluted (1:1) with 10% ethanol to result in ten different dye concentrations. An absorption spectrum was recorded from each of the solutions obtained and the absorbances in the respective maximum (λ_{max}) were plotted against the concentration c of the respective dye solution. For this purpose, a quartz glass cuvette with a layer thickness d=1 cm was used. The absorption spectra were recorded on a *Lambda 750* UV/VIS spectrometer with temperature controller (*PTP 6+6 Peltier Temperature Programmer*) from *PerkinElmer*. According to the *Beer-Lambert* law, the extinction coefficients are obtained as the slope of the regression line. For the determination of the extinction coefficient, only absorbance values less than one were used in order to ensure the linearity of the detector sensitivity. Furthermore, the extinction coefficient at λ=260 nm was determined in order to be able to determine the concentrations of the modified DNA strands.

Table S4. Extinction coefficients ε of the dyes **1**-**12**.

Dye	λ_{max}	ε_{max} [mM^{-1}cm^{-1}]	$\Delta\varepsilon_{max}$ [mM^{-1}cm^{-1}]	ε_{260nm} [mM^{-1}cm^{-1}]
1	465	41.7	0.14	9.2
2[a]	470	42.6	0.25	8.4
3	471	43.7	0.49	10.8
4	481	45.9	0.4	8.4
5	447	33.6	0.44	15
6	456	29.3	0.13	21.0
7	459	39.5	0.37	9.7
8	476	39.5	0.62	10.5
9	435	37.2	1.01	11.1
10	444	33.4	0.48	12.6
11	477	45.1	0.71	9.2
12	475	43.7	1.49	9.9

[a]Extinction coefficient was measured in 10 % ethanol.

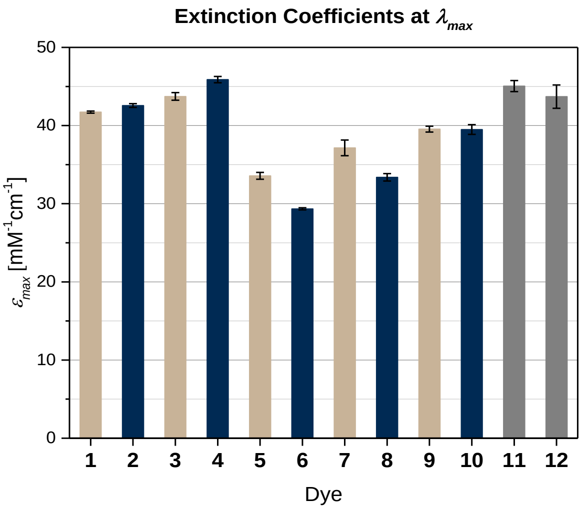


Figure S1. Extinction coefficients ε of the dyes **1**-**12**.

4. Relationship between Nucleophilicity and Extinction Coefficient

The relationship between nucleophilicity and extinction coefficient ε was determined by line fitting of the plot of the nucleophilicity parameter *N* against the extinction coefficient of the absorption maxima of the appropriate dye ε_{max}. Since the dyes differ only in their indole moiety (except dye **12**), the electron density and therefore the nucleophilicity is mainly influenced by the substituent at the indole moiety. Following this, plotting the known nucleophilicity parameters from Mayr *et al.* against the measured extinction coefficients of the respective dye (**1**-**3**, **5**, **7** and **9**) resulted in a line function.[4]

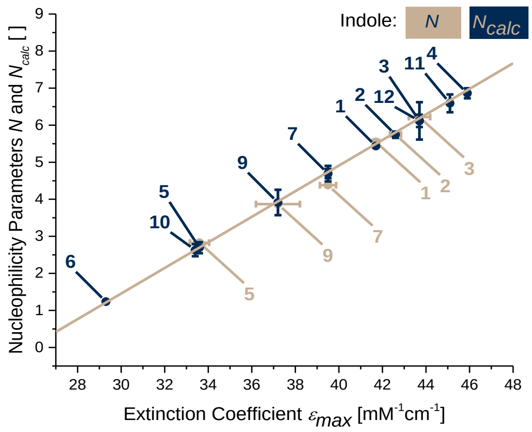


Figure S2. Relationship between nucleophilicity *N* and extinction coefficient ε. Since the dyes **7** and **8** have the same absorption coefficient, both of them possess the same Ncalc value

Table S5. Fit-Parameters for the relationship between nucleophilicity *N* and extinction coefficient ε.

	Value
Intercept	-8.9054
Slope	0.34535
Pearson's r	0.98755
R-Square(COD)	0.97526
Adj. R-Square	0.96907

The remaining nucleophilicity parameters could be calculated via the following linear relationship and the error was estimated as first derivative multiplied with the standard error of the determined extinction coefficient ε_{max}:

$$N_{calc} = 0.35 \cdot \varepsilon_{max} - 8.91 \qquad \Delta N_{calc} = 0.35 \cdot \Delta\varepsilon_{max}$$

Table S6. Calculated nucleophilicity parameter N_{calc}.

Dye	N [ ]	ΔN_{calc} [ ]
1	5.44	0.05
2	5.74	0.08
3	6.12	0.17
4	6.86	0.14
5	2.69	0.15
6	1.24	0.04
7	4.69	0.13
8	4.69	0.21
9	3.91	0.34
10	2.63	0.16
11	6.59	0.24
12	6.12	0.50

5. Concentration of ssDNAs

The concentration determination was carried out analogously to the *Beer-Lambert* law at λ=260 nm:

$$A_{260\,nm} = \varepsilon_{260\,nm} \cdot c \cdot d$$

$A_{260\,nm}$: Absorbance at λ=260 nm, unitless.
$\varepsilon_{260\,nm}$: Extinction coefficient at λ=260 nm, in [$L \cdot cm^{-1} \cdot mmol^{-1}$].
c: Concentration of the substance in the solution, in [mmol/L].
d: Layer thickness of the irradiated solution, in [cm].

For this purpose, the absorbance *A* was determined at λ=260 nm on an *ND-1000* spectrophotometer from *NanoDrop* in the nucleic acid mode, the layer thickness of the irradiated solution is d = 1 cm. For this purpose, 1.00 µL of the stock solution was used in each case. The extinction coefficient of the respective unmodified oligonucleotide was determined by the following equation:

$$\varepsilon_{260\,nm} = (A \cdot \varepsilon_A + C \cdot \varepsilon_C + G \cdot \varepsilon_G + T \cdot \varepsilon_T) \cdot 0.9$$

$\varepsilon_{260\,nm}$: Extinction coefficient of the oligonucleotide at λ=260 nm, [L · cm-1·mol-1].
A, C, G, T: Number of the respective base in the sequence, unitless.
ε_A: Extinction coefficient of A at λ=260 nm, ε_A=15.4 $L \cdot cm^{-1} \cdot mmol^{-1}$.
ε_C: Extinction coefficient of C at λ=260 nm, ε_C=7.3 $L \cdot cm^{-1} \cdot mmol^{-1}$.
ε_G: Extinction coefficient of G at λ=260 nm, ε_G=11.7 $L \cdot cm^{-1} \cdot mmol^{-1}$.
ε_T: Extinction coefficient of T at λ=260 nm, ε_T=8.8 $L \cdot cm^{-1} \cdot mmol^{-1}$.

The factor 0.9 takes the hypochromicity into account. In the calculation of the extinction coefficient of the dye-modified strands, the extinction coefficient of the modified base was added.

Table S7. Extinction coefficients ε, retention time *RT*, calculated (M_{calcd}) and found masses (M_{found}) of the **DNA1**-**12**.

DNA	ε_{260} [$mM^{-1}cm^{-1}$]	RT[a] [min]	M_{calcd}	M_{found} [m/z]
1	209	18.8	6507	6502
2	209	19.4	6521	6518
3	212	19.2	6537	6533
4	210	19.5	6551	6548
5	216	19.3	6532	6534
6	222	19.6	6546	6538
7	211	19.8	6585	6583
8	217	19.7	6599	6600
9	211	18.5	6508	6502
10	213	18.5	6522	6520
11	209	23.7	6651	6637
12	210	24.7	6681	6677

[a]Determined from the UV-vis chromatogram at 260 nm.

6. Optical Characterization of ss and dsDNA1-12

a. Quantum Yields

Absolute quantum yields were determined on *Quantaurus QY C11347* in 5 mL quartz glass cuvettes from *Hamamatsu*. A solution of 10 mM NaP_i buffer (pH 7) and 250 mM NaCl in *Millipore* water was used for the base line correction. Afterwards, the quantum yields of the single and double strands were determined from a solution of 2.5 µM respective DNA, 10 mM NaP_i buffer (pH 7) and 250 mM NaCl in *Millipore* water. In addition, the quantum yields of the pure dyes (2.5 µM) in presence (12.5 µM dsDNA) and absence of double stranded DNA under same salt and buffer conditions in 5 % ethanol in water are given in the following table:

Table S8. Quantum yields Φ_F and brightnesses *B* of single and double stranded **DNA1**-**DNA12** in comparison to non-attached dyes **1-10** in presence (non-covalently bound) and absence of double stranded DNA.

DNA	Φ_F ss	$\Delta\Phi_F$ ss	*B ss* $mM^{-1}cm^{-1}$	ΔB ss $mM^{-1}cm^{-1}$	Φ_F ds	$\Delta\Phi_F$ ds	*B ds* $mM^{-1}cm^{-1}$	ΔB ds $mM^{-1}cm^{-1}$	$\Phi_{F,Dye}$	$\Phi_{F,Dye+dsDNA}$
1	0.21	0.06	8.76	2.53	0.11	0.002	3.75	0.10	0.01	0.04
2	0.35	0.002	15.0	0.16	0.20	0.002	8.55	0.11	0.01	0.07
3	0.03	0.002	1.31	0.10	0.01	0.004	0.44	0.18	0.01	0.02
4	0.05	0.002	2.30	0.11	0.04	0.002	1.84	0.11	0.02	0.03
5	0.26	0.006	8.74	0.32	0.32	0.012	10.8	0.54	0.01	0.02
6	0.28	0.004	8.20	0.15	0.19	0.005	5.57	0.17	0.01	0.04
7	0.22	0.003	8.69	0.20	0.32	0.01	12.6	0.51	0.01	0.06
8	0.30	0.005	11.9	0.38	0.30	0.005	11.9	0.38	0.01	0.11
9	0.49	0.011	18.2	0.90	0.20	0.005	7.44	0.39	0.01	0.01
10	0.51	0.011	17.0	0.61	0.22	0.013	7.35	0.54	0.01	0.02
11	0.46	0.002	20.7	0.42	0.20	0.002	8.57	0.23	-[a]	-[a]
12	0.39	0.073	17.0	3.77	0.17	0.002	7.43	0.34	-[a]	-[a]

[a] No reliable data could be recorded due to their poor solubility in water.

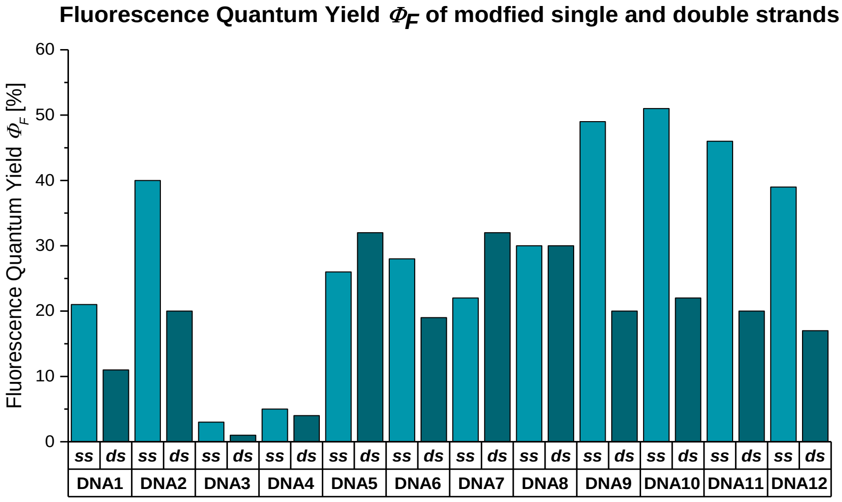


Figure S3. Quantum yields Φ_F for single- and double-stranded **DNA1**-**12**.

b. Absorption and Emission Spectra

Absorption and emission spectroscopy was carried out in quartz glass cuvettes from *Starna* with a layer thickness of $d = 1$ cm. Measurements are taken, unless otherwise stated, at a temperature of 20 °C. The absorption spectra were recorded on a *PerkinElmer Lambda 750* UV / VIS spectrometer with temperature controller (*PTP 6 + 6 Peltier Temperature Programmer*). The spectra were baseline corrected against the absorption of the solvent. All measurements were made in 10 mM NaPi buffer (pH 7) and 250 mM NaCl in Millipore water. The DNA concentration of the modified strands and unmodified strands is 2.5 μM. The following measurement parameters were used: SBW 2.0 nm, Average time 0.1 s, Data interval 1.0 nm, Light source change over 350 nm.

The emission spectra were recorded on a *Fluoromax-4 Spectrofluorometer* from *HORIBA Scientific* with a Peltier element. The measurements were carried out at a temperature of 20 ± 0.001 °C. The background correction of the spectra was against Raman scattering of the pure solvent. The following settings were used: increment: 1.0 nm, increment time: 0.2 s, slit: 3 nm.

Table S9. Optical properties of **DNA1**-**DNA12**.

DNA	$\lambda_{exc\ ss}$ nm	$\lambda_{em\ ss}$ nm	$\lambda_{Stokes\ ss}$ nm	$\lambda_{exc\ ds}$ nm	$\lambda_{em\ ds}$ nm	$\lambda_{Stokes\ ds}$ nm
1	500	572	72	499	571	72
2	507	564	56	502	556	54
3	499	565	66	499	583	84
4	512	574	62	509	581	72
5	479	558	79	461	532	71
6	484	556	72	467	541	74
7	490	559	69	475	543	68
8	498	565	67	483	540	57
9	477	546	69	459	541	82
10	479	545	66	466	551	85
11	522	565	43	515	587	72
12	509	567	58	509	580	71

ssDNA1-12:

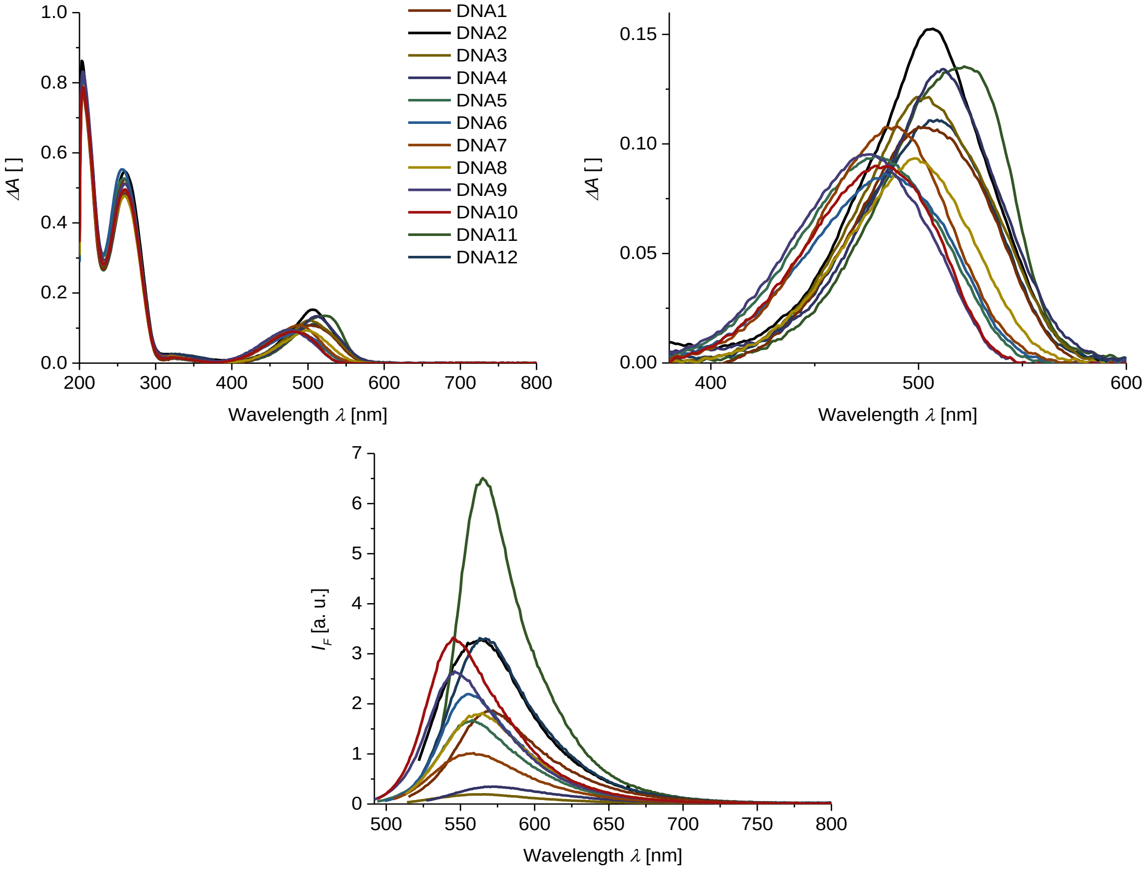


Figure S4. Absorption (top left and right) and emission spectra (bottom) of ss**DNA1**-**12**.

dsDNA1-12:

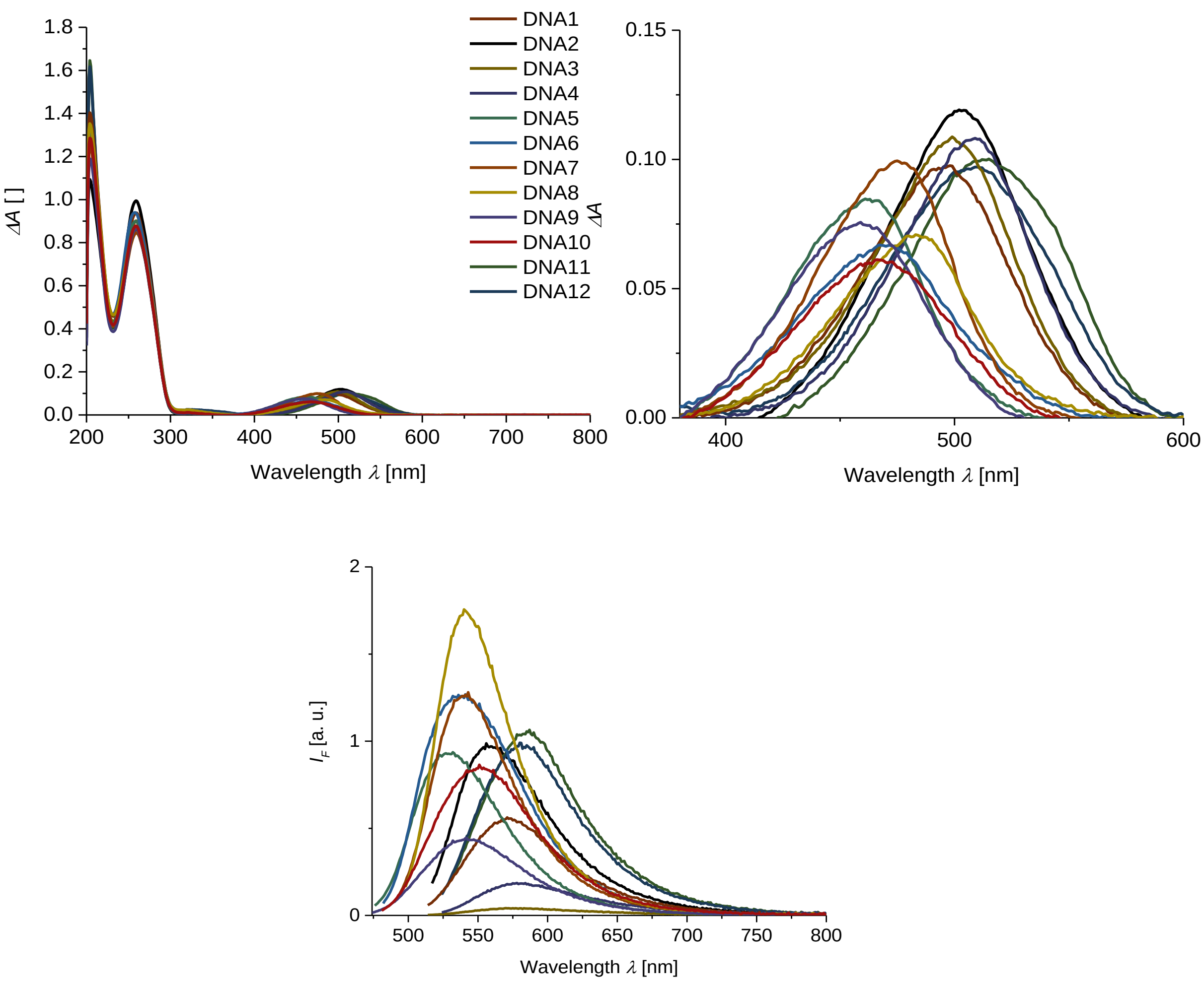


Figure S5. Absorption (top left and right) and emission spectra (bottom) of ds**DNA1**-**12**.

DNA1:

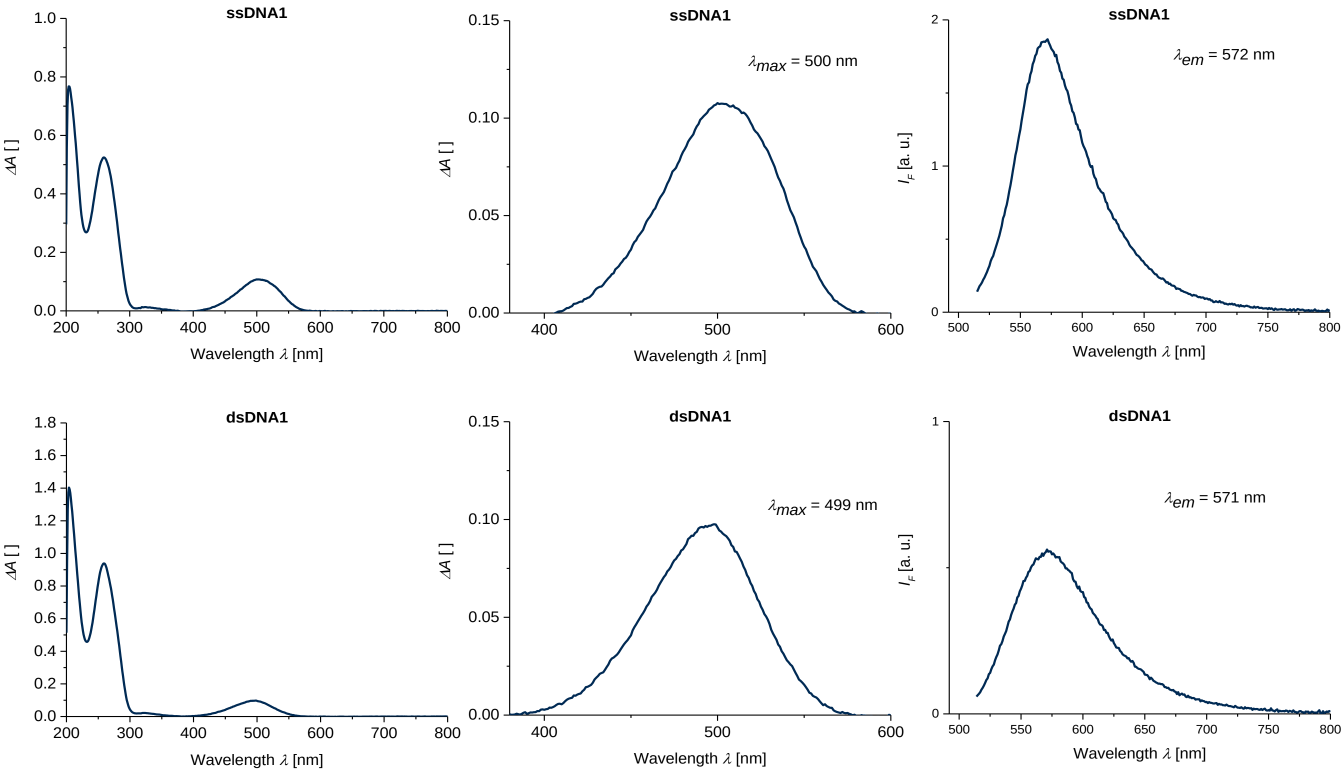


Figure S6. Absorption (left and middle) and emission spectra (right) of single-stranded (top) and double-stranded **DNA1**.

DNA2:

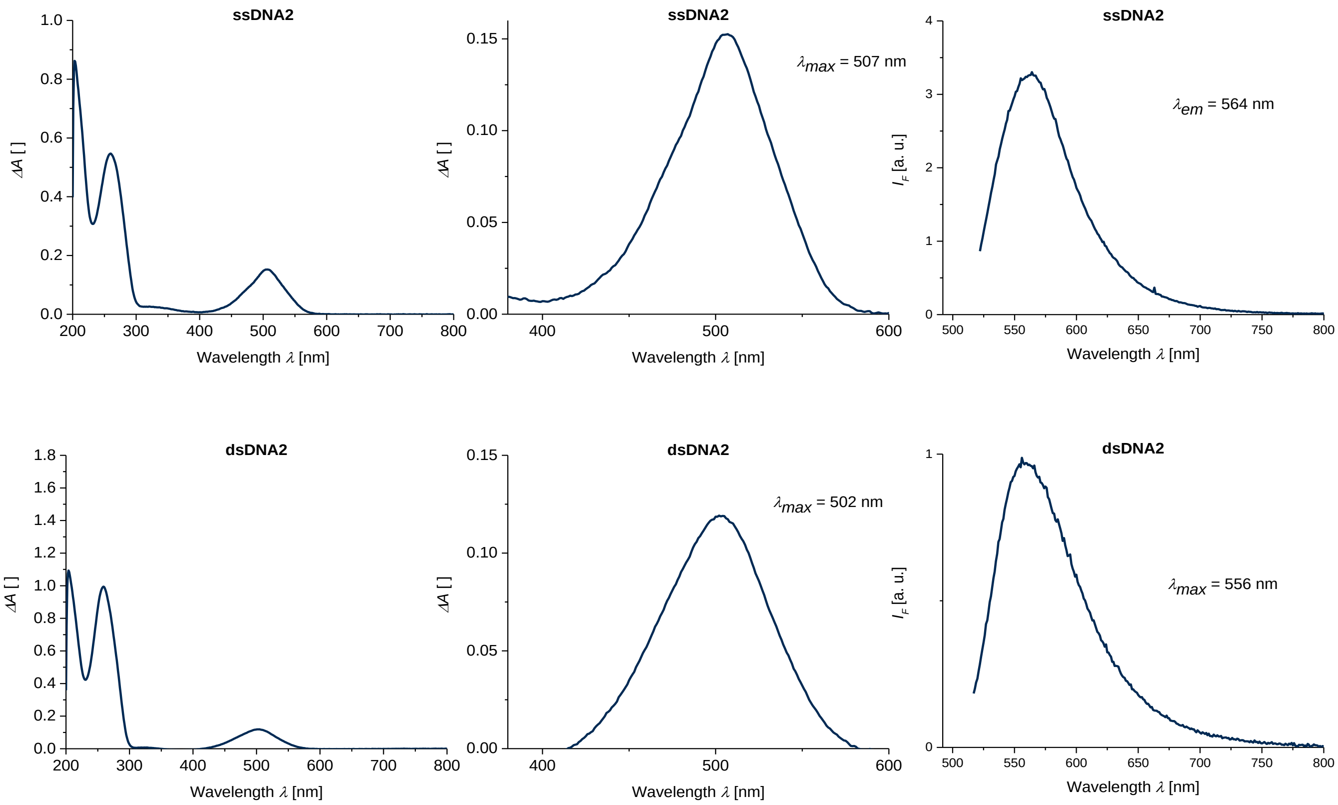


Figure S7. Absorption (left and middle) and emission spectra (right) of single-stranded (top) and double-stranded **DNA2**.

DNA3:

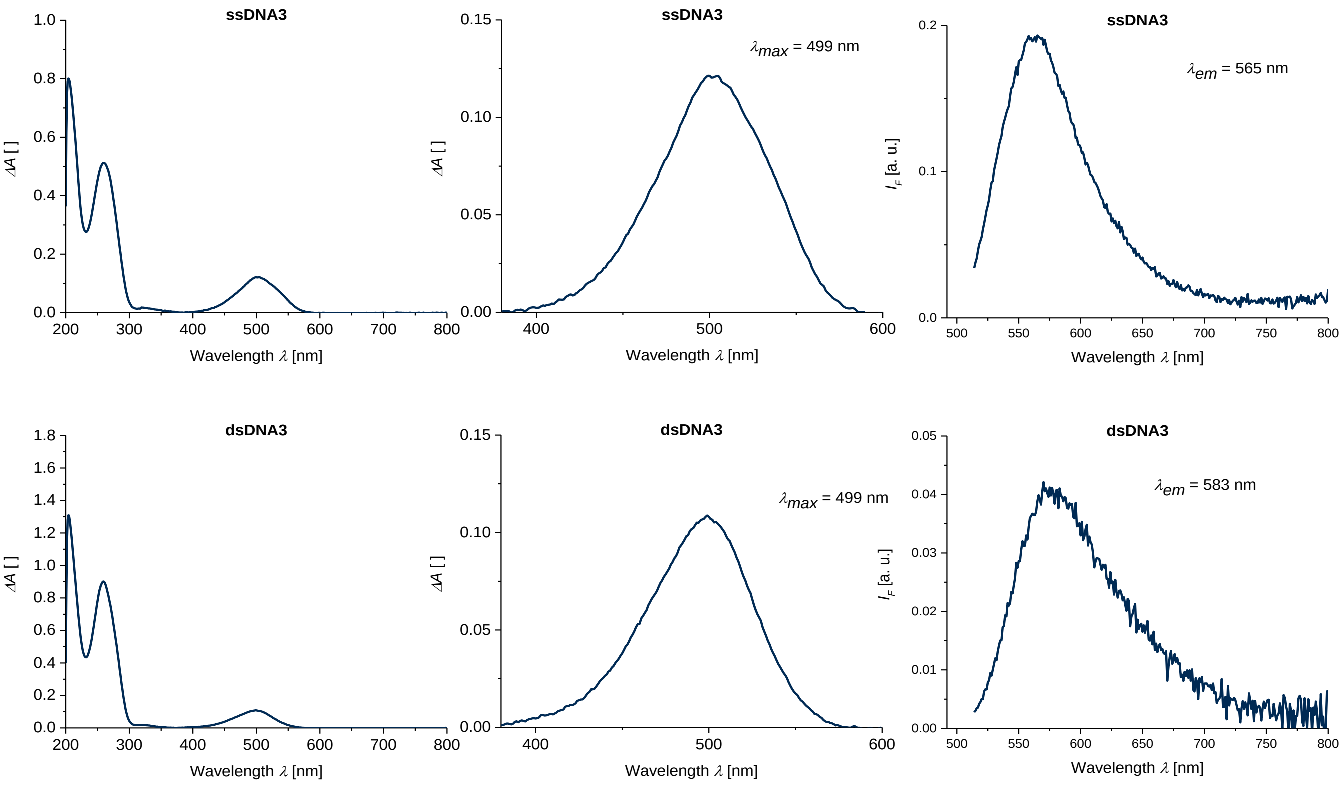


Figure S8. Absorption (left and middle) and emission spectra (right) of single-stranded (top) and double-stranded **DNA3**.

DNA4:

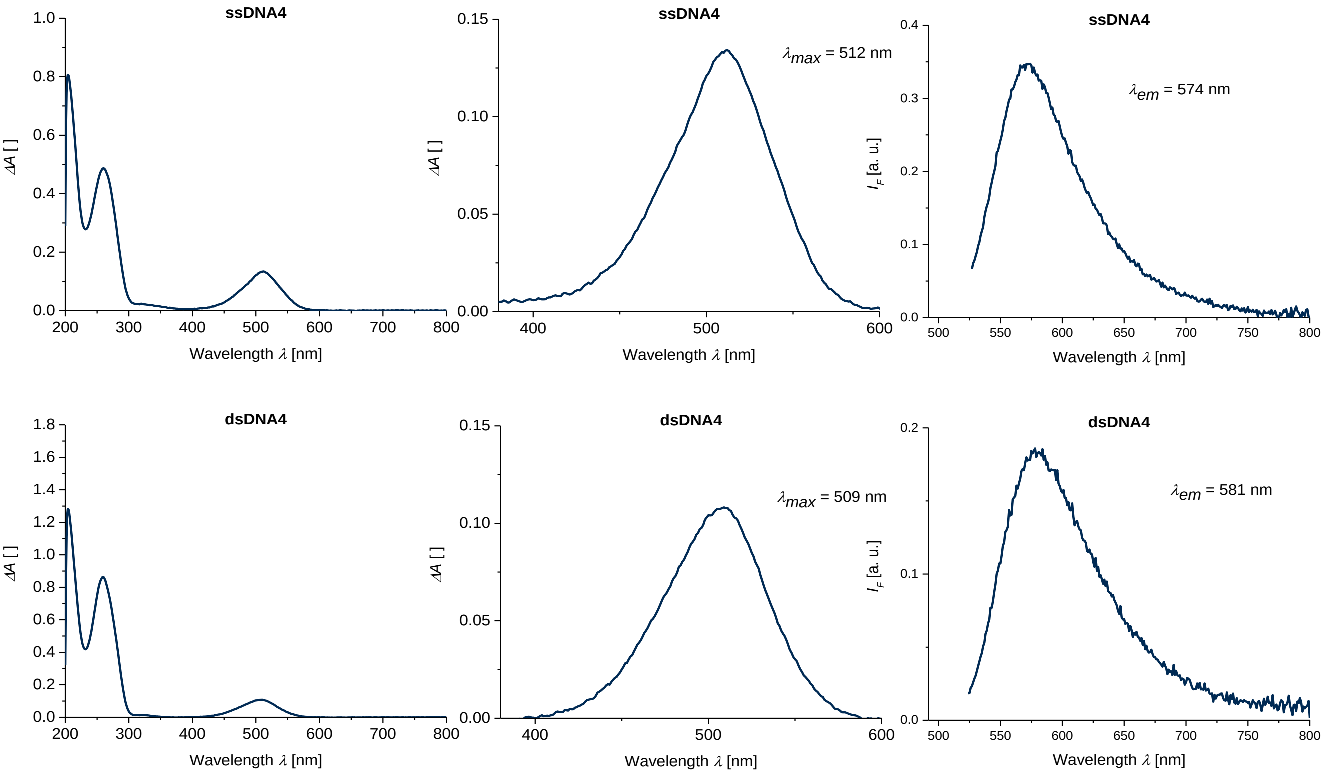


Figure S9. Absorption (left and middle) and emission spectra (right) of single-stranded (top) and double-stranded **DNA4**.

DNA5:

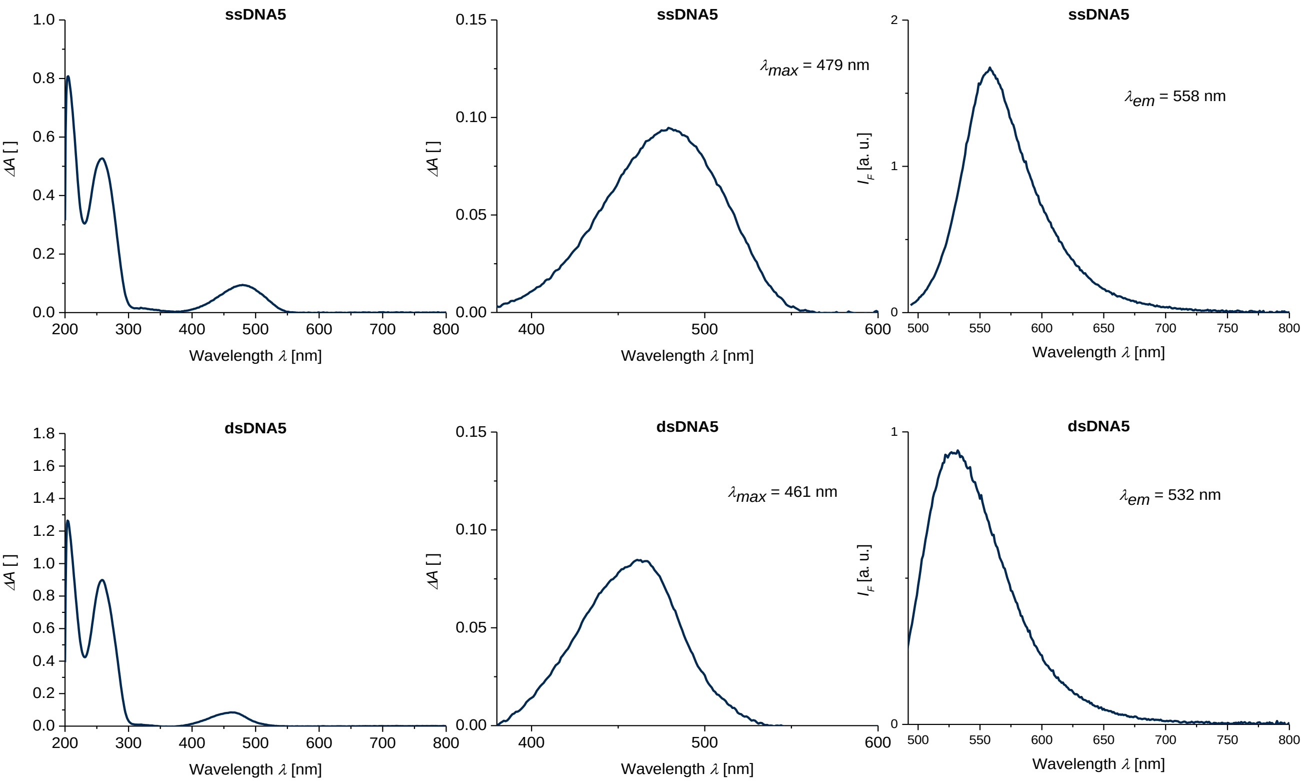


Figure S10. Absorption (left and middle) and emission spectra (right) of single-stranded (top) and double-stranded **DNA5**.

DNA6:

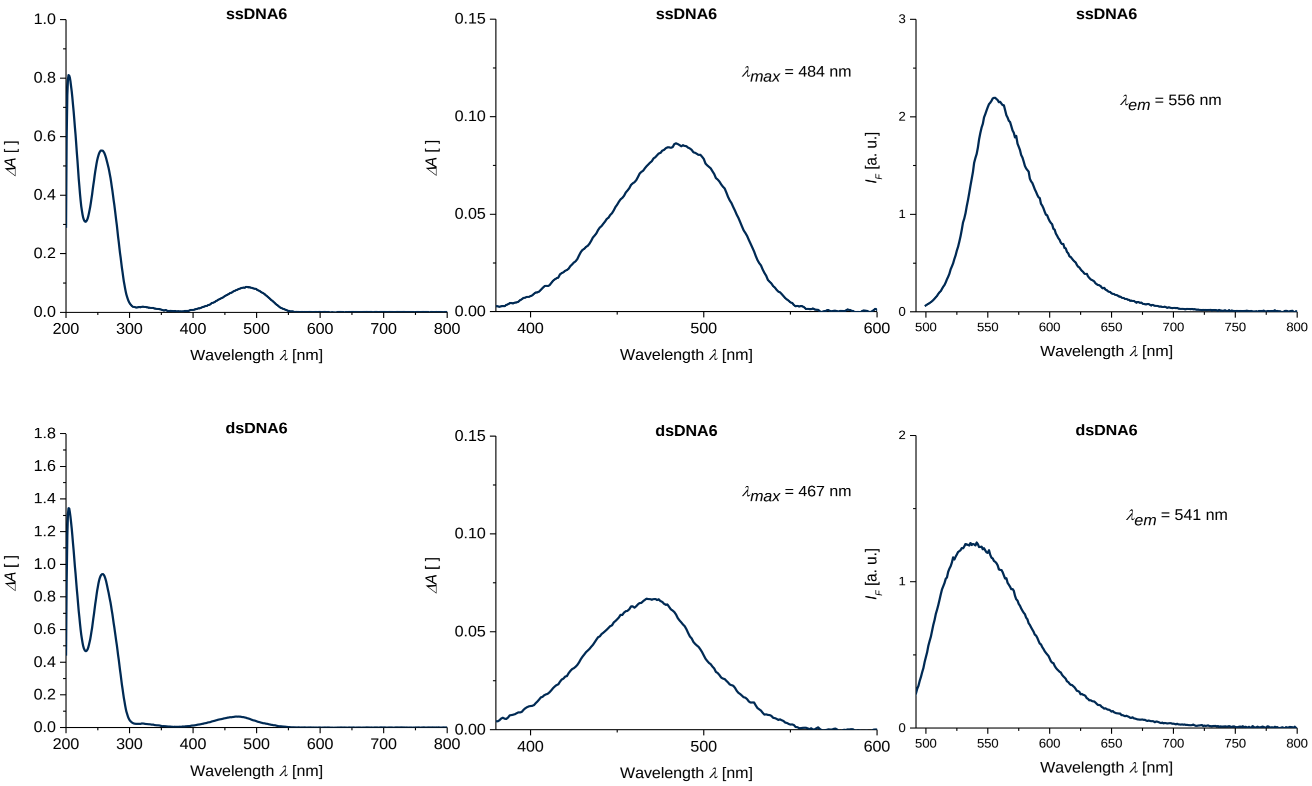


Figure S11. Absorption (left and middle) and emission spectra (right) of single-stranded (top) and double-stranded **DNA6**.

DNA7:

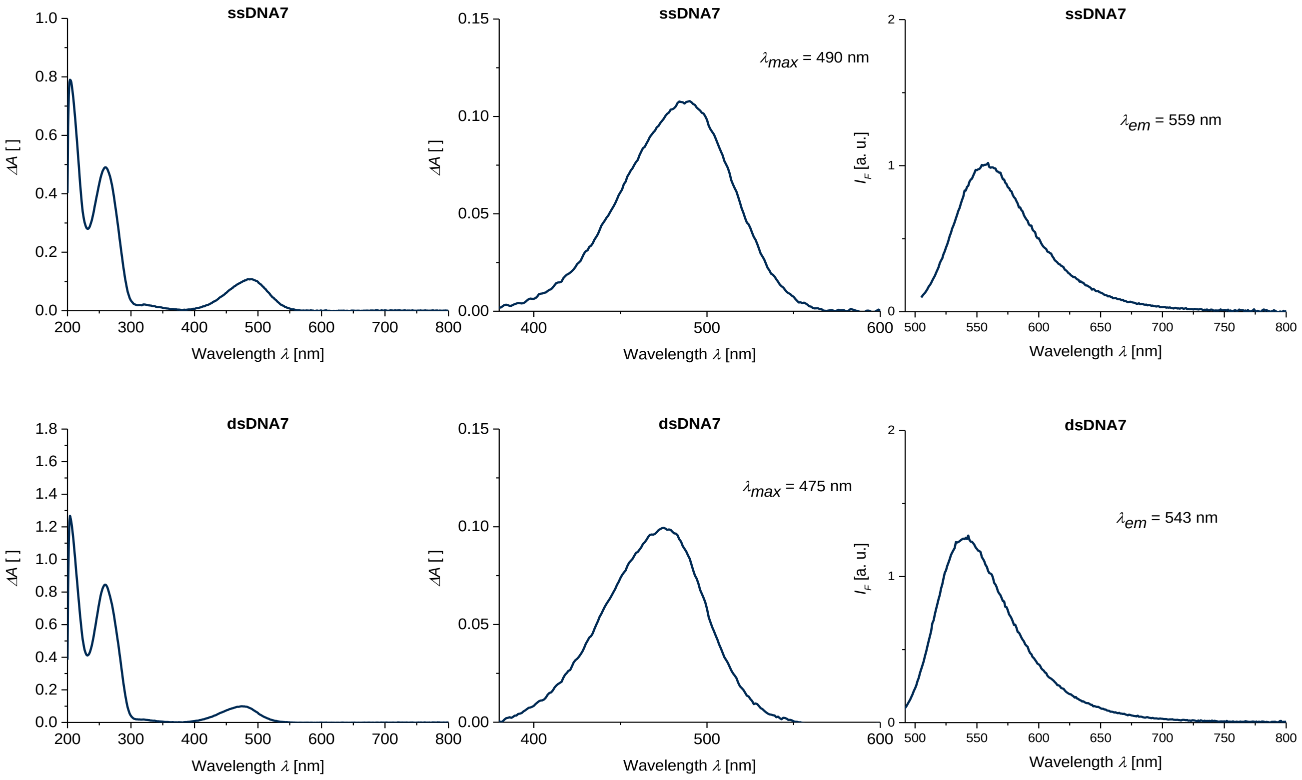


Figure S12. Absorption (left and middle) and emission spectra (right) of single-stranded (top) and double-stranded **DNA7**.

DNA8:

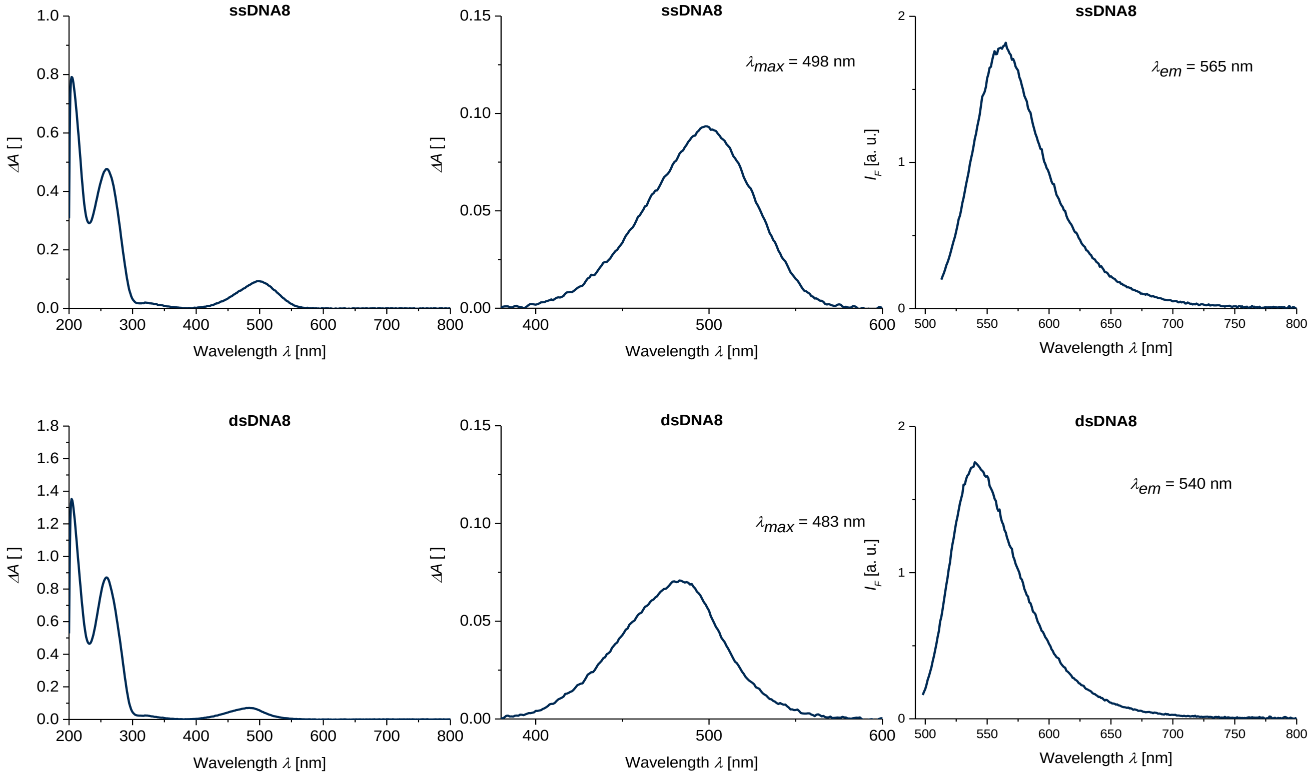


Figure S13. Absorption (left and middle) and emission spectra (right) of single-stranded (top) and double-stranded **DNA8**.

DNA9:

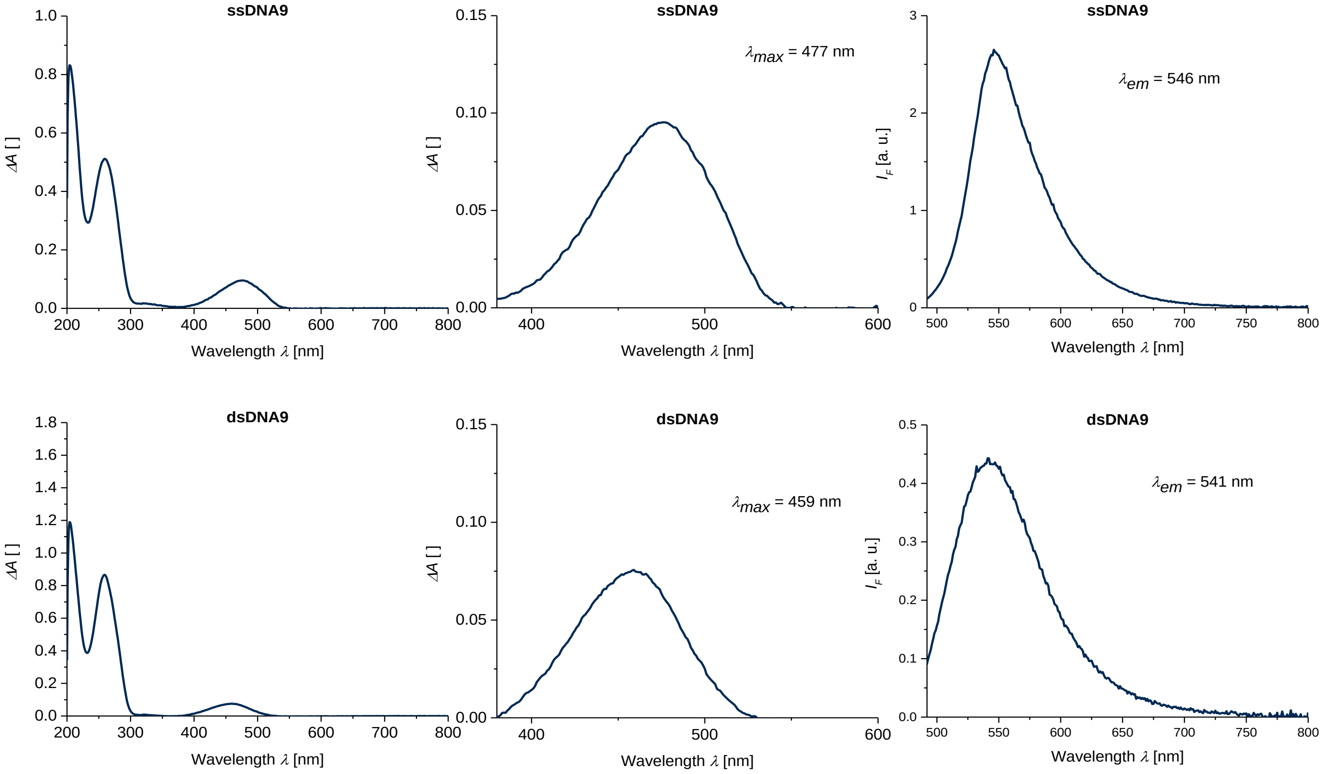


Figure S14. Absorption (left and middle) and emission spectra (right) of single-stranded (top) and double-stranded **DNA9**.

DNA10:

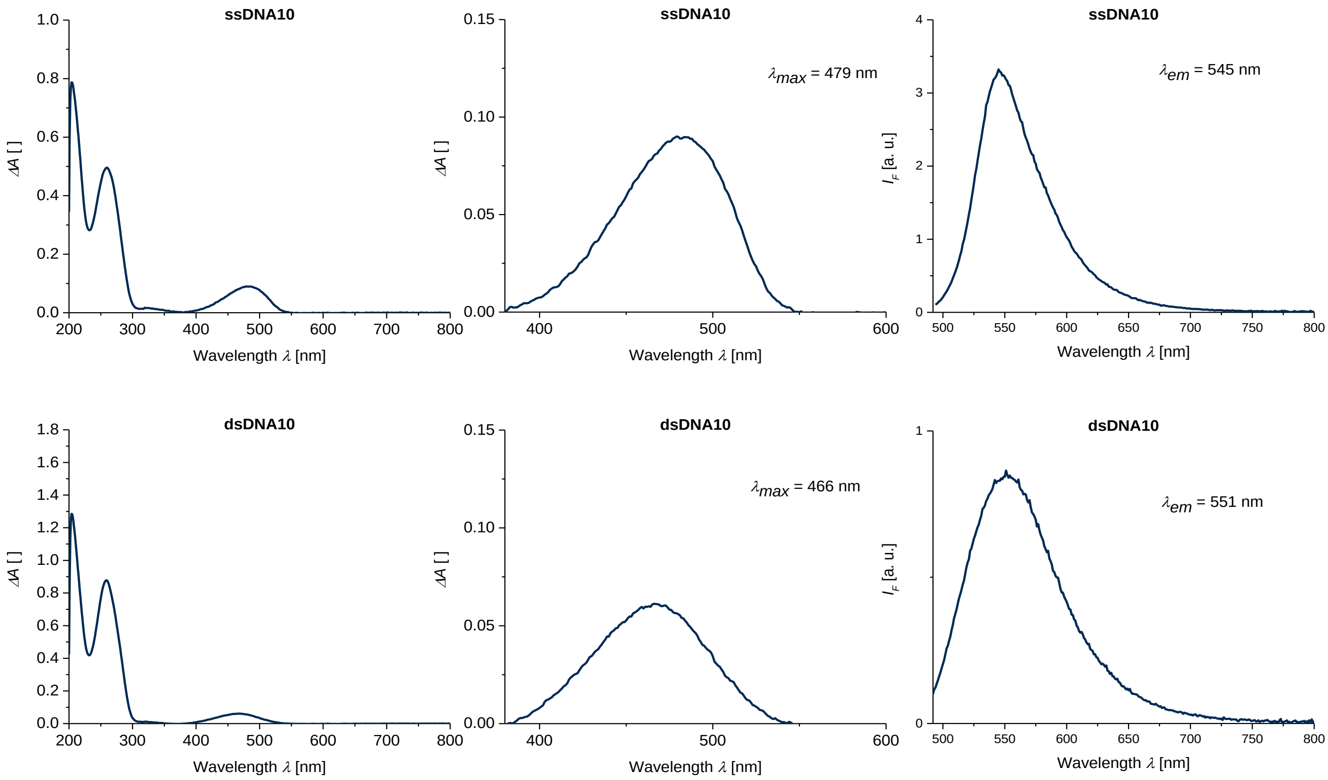


Figure S15. Absorption (left and middle) and emission spectra (right) of single-stranded (top) and double-stranded **DNA10**.

DNA11:

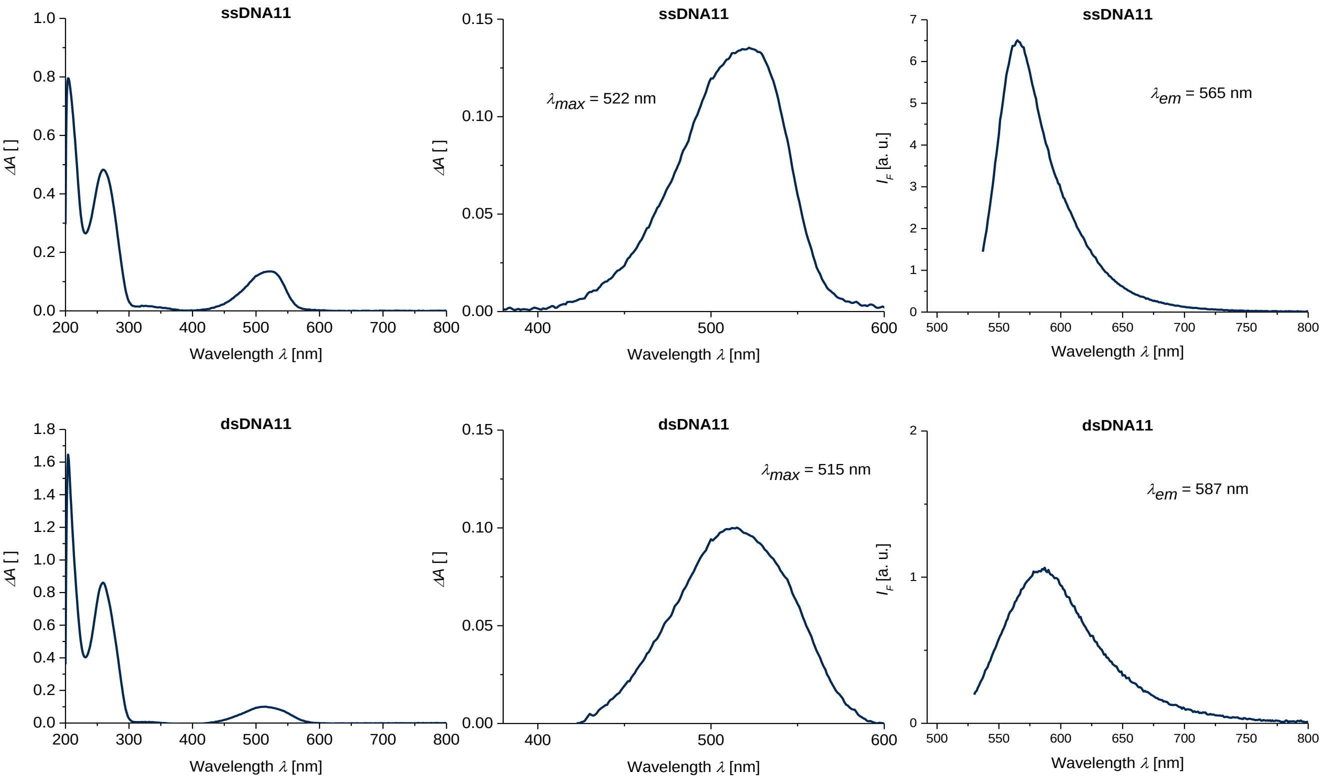


Figure S16. Absorption (left and middle) and emission spectra (right) of single-stranded (top) and double-stranded **DNA11**.

DNA12:

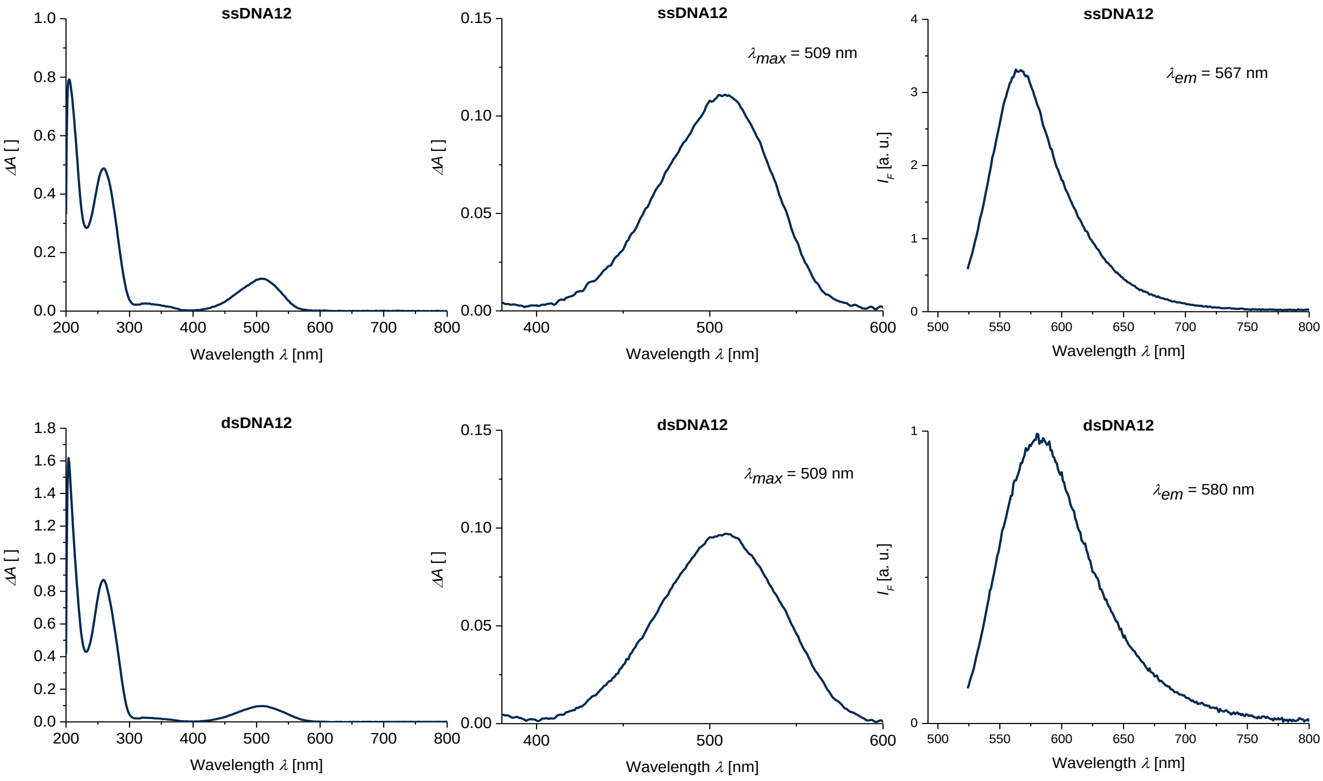


Figure S17. Absorption (left and middle) and emission spectra (right) of single-stranded (top) and double-stranded **DNA12**.

7. Melting Temperature of dsDNAs

For hybridization, the respective single strands and their counter strand were mixed together in 10 mM NaPi buffer (pH 7), 250 mM NaCl in *Millipore* water. Then, these solutions were heated to 90 °C for 10 minutes and cooled slowly to room temperature.
Melting temperature measurements were carried out on a *Varian Cary 100* Bio with temperature controller (*Cary 100 Temperature Controller*) and the *Thermal* program. The absorption change of the DNA was followed at λ=260 nm. The measurements were carried out over a temperature range of 10 °C to 90 °C. The heating and cooling rate was 0.7 °C/min and the data was recorded in 0.5 °C steps.

Table S10. Melting temperatures of **DNA1**-**DNA12**.

DNA	T_m[a] [°C]
1	66
2	67
3	65
4	65
5	66
6	65
7	67
8	67
9	66
10	66
11	66
12	65

[a]unmodified double strand – T_m = 66 °C.

8. Fluorescence Lifetime of ssDNAs and dsDNAs

Fluroescence lifetimes τ were measured via time correlated single photon counting (TCSPC) technique on a *Fluoromax-4 Spectrofluorometer* with equipped *DeltaTime-NL* timing module and *NL-C2* pulsed diode controller from *HORIBA Scientific*. As excitation light source a *NanoLED* (λ = 456 nm) from *HORIBA Scientific* with a repetition rate of 1 MHz was used. The measurements were carried out at a temperature of 20 °C.

For the decay measurement 2.5 µM respective DNA, 10 mM NaP_i buffer (pH 7) and 250 mM NaCl in *Millipore* water was used and for the prompt (intrument respond function) a dilution of *LUDOX*® (colloidal silica in water, 30 wt. %) from *Sigma Aldrich* was used.

The decay and corresponding prompt measurements were evaluated with the software *DAS6 v 6.8* from *HORIBA Scientific*. Therefore, a biexponential curve fitting was used and a χ^2 value of 1.2 was intended.

The average lifetime was calculated using the following equation:[5]

$$\langle \tau_F \rangle = \frac{B1 \cdot T1^2 + B2 \cdot T2^2}{B1 \cdot T1 + B2 \cdot T2}$$

ssDNA1:

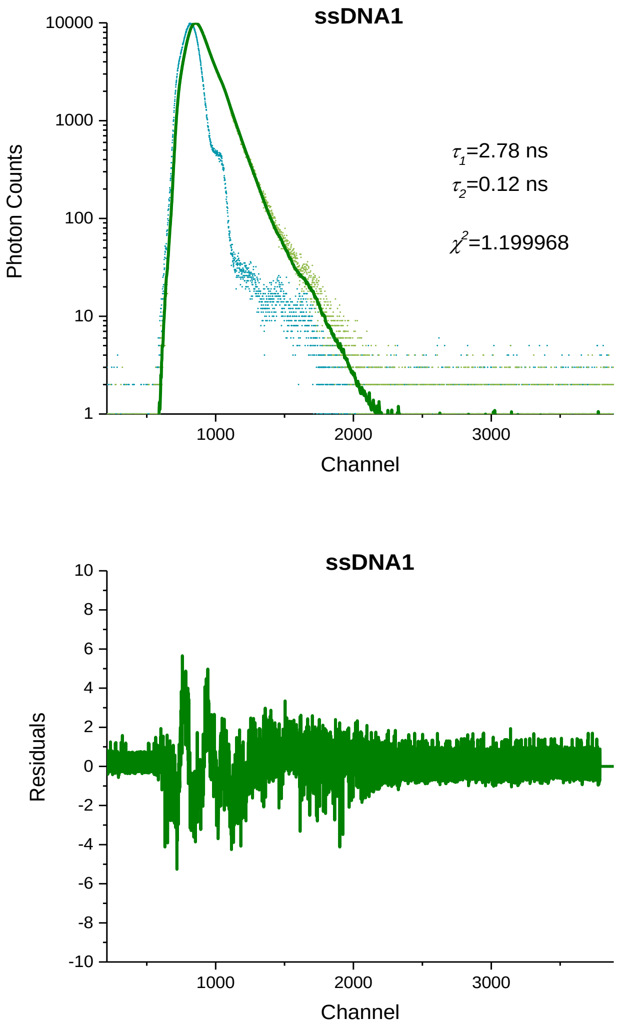


Figure S18. Fluorescence decay (top) and residuals (bottom) of ss**DNA1**.

The initial parameters are:

Shift Value = 0 ch
0 sec
Shift Limit = 100 ch
2.743484E-09 sec

T1 Estimate = 41.03476 ch
1.125782E-09 sec
T2 Estimate = 164.139 ch
4.503129E-09 sec

A Free
B1 Free
B2 Free

Prompt and decay LO = 211 ch
5.788752E-09 sec
Prompt and decay HI = 3889 ch
1.066941E-07 sec

Background on prompt = 0.9598997
Time calibration = 2.743484E-11 sec/ch

The fitted parameters are:

Hi reduced to: 3789 ch

SHIFT = 5.512647 ch
1.512386E-10 sec
S.Dev = 3.707082E-12 sec

T1 = 4.216256 ch
1.156723E-10 sec
S.Dev = 1.274112E-11 sec
T2 = 101.2487 ch
2.777743E-09 sec
S.Dev = 4.82858E-12 sec

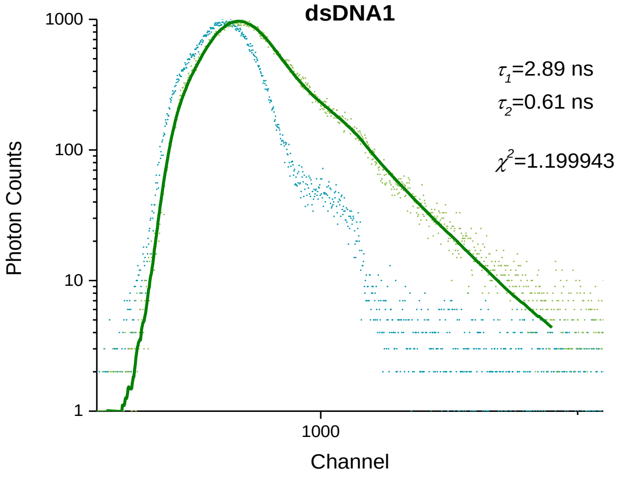
A = 0.1515428
S.Dev = 2.267227E-02

B1 = 9.794793E-02
[26.15 Rel.Ampl]
S.Dev = 3.04294E-04
B2 = 0.0115217
[73.85 Rel.Ampl]
S.Dev = 1.347935E-05

CHISQ = 1.199968
[3573 degrees of freedom]

Chi-squared Probability = 9.0869E-14%
Durbin-Watson Parameter = 1.181519
Negative residuals = 44.53758%
Residuals < 1 s.dev = 73.90333%
Residuals < 2 s.dev = 93.40598%
Residuals < 3 s.dev = 97.90444%
Residuals < 4 s.dev = 99.41325%

dsDNA1:



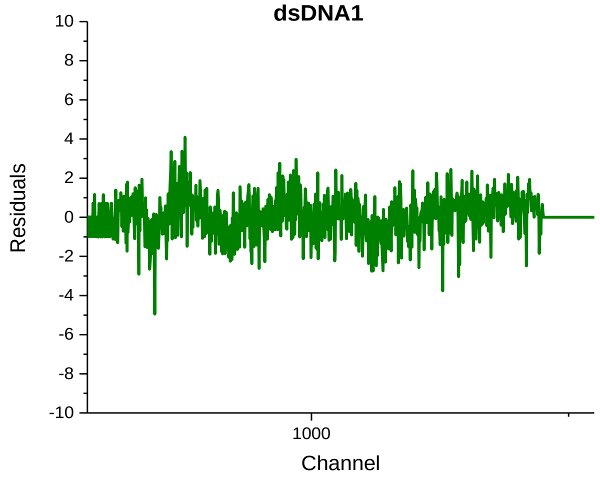


Figure S19. Fluorescence decay (top) and residuals (bottom) of ds**DNA1**.

The initial parameters are:

Shift Value = 0 ch
0 sec
Shift Limit = 100 ch
2.743484E-09 sec

T1 Estimate = 31.42899 ch
8.622493E-10 sec
T2 Estimate = 125.7159 ch
3.448997E-09 sec

A Free
B1 Free
B2 Free

Prompt and decay LO = 564 ch
1.547325E-08 sec
Prompt and decay HI = 1550 ch
4.252401E-08 sec

Background on prompt = 4.2
Time calibration = 2.743484E-11 sec/ch

The fitted parameters are:

Hi reduced to: 1450 ch

SHIFT = -4.070872 ch
-1.116837E-10 sec
S.Dev = 6.344333E-12 sec

T1 = 22.41422 ch
6.149307E-10 sec
S.Dev = 6.032423E-11 sec
T2 = 105.3969 ch
2.891546E-09 sec
S.Dev = 2.565795E-11 sec

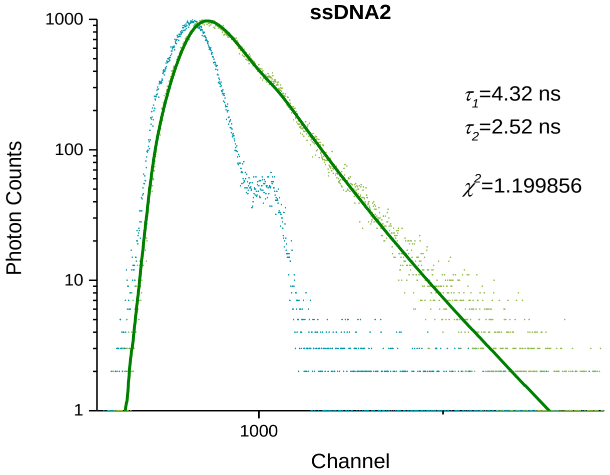
A = 0.983838
S.Dev = 0.1066143

B1 = 2.706392E-02
[42.51 Rel.Ampl]
S.Dev = 1.991261E-04
B2 = 7.784688E-03
[57.49 Rel.Ampl]
S.Dev = 4.448426E-05

CHISQ = 1.199943
[881 degrees of freedom]

Chi-squared Probability = 3.7622E-03%
Durbin-Watson Parameter = 1.575354
Negative residuals = 42.7283%
Residuals < 1 s.dev = 64.48704%
Residuals < 2 s.dev = 93.01015%
Residuals < 3 s.dev = 99.32356%
Residuals < 4 s.dev = 99.77452%

ssDNA2:



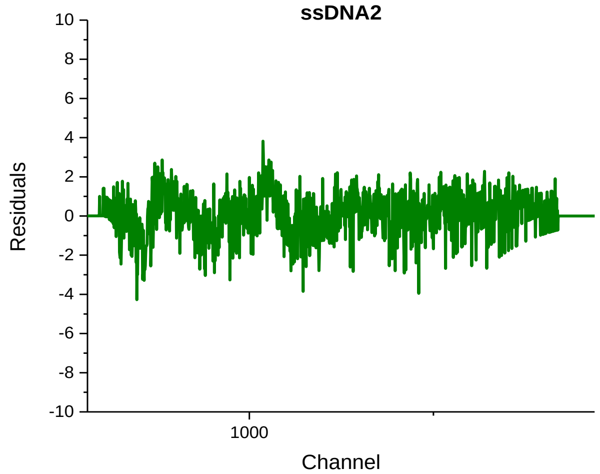


Figure S20. Fluorescence decay (top) and residuals (bottom) of ss**DNA2**.

The initial parameters are:

Shift Value = 0 ch
0 sec
Shift Limit = 100 ch
2.743484E-09 sec

T1 Estimate = 48.02121 ch
1.317454E-09 sec
T2 Estimate = 192.0848 ch
5.269817E-09 sec

A Free
B1 Free
B2 Free

Prompt and decay LO = 560 ch
1.536351E-08 sec
Prompt and decay HI = 1938 ch
5.316873E-08 sec

Background on prompt = 2.244681
Time calibration = 2.743484E-11 sec/ch

The fitted parameters are:

Hi reduced to: 1838 ch

SHIFT = -8.091501 ch
-2.219891E-10 sec
S.Dev = 6.764616E-12 sec

T1 = 91.72512 ch
2.516464E-09 sec
S.Dev = 1.477966E-10 sec
T2 = 157.5165 ch
4.321441E-09 sec
S.Dev = 1.181433E-10 sec

A = -4.212842E-03
S.Dev = 6.803325E-02

B1 = 1.391071E-02
[73.53 Rel.Ampl]
S.Dev = 8.959865E-05
B2 = 2.916736E-03
[26.47 Rel.Ampl]
S.Dev = 5.120749E-05

CHISQ = 1.199856
[1273 degrees of freedom]

Chi-squared Probability = 1.0069E-04%
Durbin-Watson Parameter = 1.444203
Negative residuals = 41.51681%
Residuals < 1 s.dev = 65.67631%
Residuals < 2 s.dev = 93.04144%
Residuals < 3 s.dev = 99.29633%
Residuals < 4 s.dev = 99.92181%

dsDNA2:

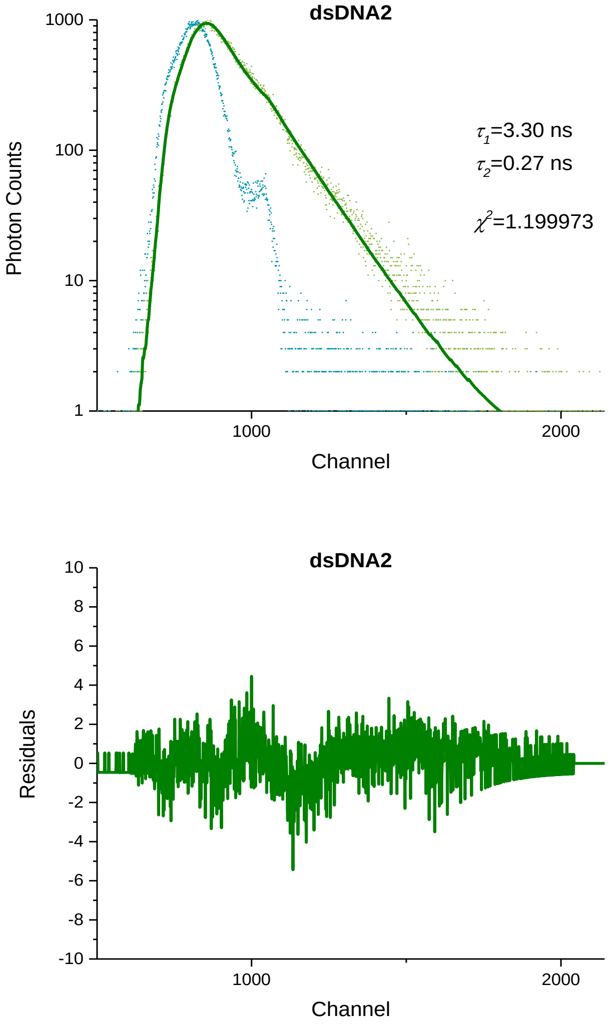


Figure S21. Fluorescence decay (top) and residuals (bottom) of ds**DNA2**.

The initial parameters are:

Shift Value = 0 ch
0 sec
Shift Limit = 100 ch
2.743484E-09 sec

T1 Estimate = 48.92282 ch
1.34219E-09 sec
T2 Estimate = 195.6913 ch
5.36876E-09 sec

A Free
B1 Free
B2 Free

Prompt and decay LO = 501 ch
1.374486E-08 sec
Prompt and decay HI = 2141 ch
5.8738E-08 sec

Background on prompt = 1.842767
Time calibration = 2.743484E-11 sec/ch

The fitted parameters are:

Hi reduced to: 2041 ch

SHIFT = 6.599802 ch
1.810645E-10 sec
S.Dev = 1.013519E-11 sec

T1 = 9.95573 ch
2.731339E-10 sec
S.Dev = 4.7791E-11 sec
T2 = 120.1684 ch
3.296802E-09 sec
S.Dev = 1.831221E-11 sec

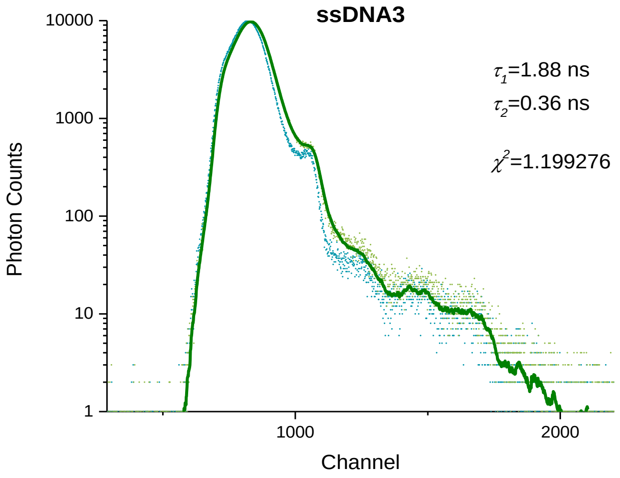
A = 0.4604738
S.Dev = 4.542185E-02

B1 = 0.0435243
[27.41 Rel.Ampl]
S.Dev = 3.832381E-04
B2 = 9.551069E-03
[72.59 Rel.Ampl]
S.Dev = 3.619752E-05

CHISQ = 1.199973
[1535 degrees of freedom]

Chi-squared Probability = 8.9980E-06%
Durbin-Watson Parameter = 1.503305
Negative residuals = 44.51655%
Residuals < 1 s.dev = 66.83971%
Residuals < 2 s.dev = 93.12135%
Residuals < 3 s.dev = 99.0915%
Residuals < 4 s.dev = 99.80532%

ssDNA3:



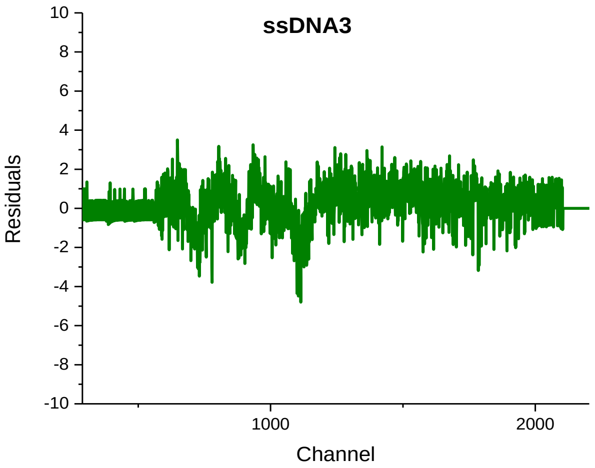


Figure S22. Fluorescence decay (top) and residuals (bottom) of ss**DNA3**.

The initial parameters are:

Shift Value = 0 ch
0 sec
Shift Limit = 100 ch
2.743484E-09 sec

T1 Estimate = 7.850098 ch
2.153662E-10 sec
T2 Estimate = 31.40039 ch
8.614648E-10 sec

A Free
B1 Free
B2 Free

Prompt and decay LO = 289 ch
7.928669E-09 sec
Prompt and decay HI = 2204 ch
6.046639E-08 sec

Background on prompt = 0.9816514
Time calibration = 2.743484E-11 sec/ch

The fitted parameters are:

Hi reduced to: 2104 ch

SHIFT = -2.008504 ch
-5.510298E-11 sec
S.Dev = 2.032537E-12 sec

T1 = 13.19428 ch
3.61983E-10 sec
S.Dev = 1.44578E-11 sec
T2 = 68.51888 ch
1.879805E-09 sec
S.Dev = 5.692604E-11 sec

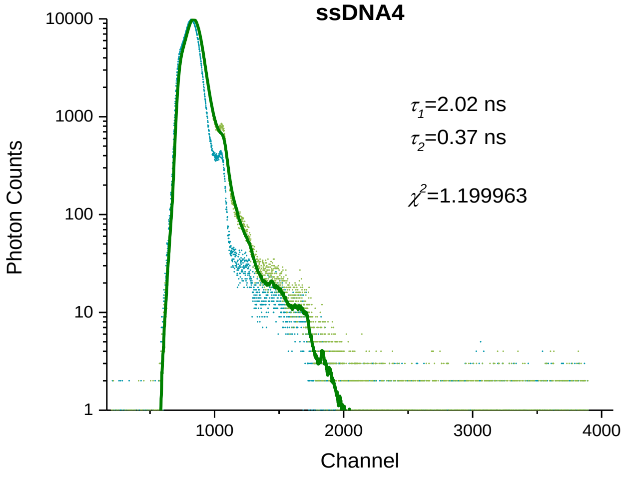
A = 0.5812428
S.Dev = 4.354777E-02

B1 = 7.552148E-02
[92.41 Rel.Ampl]
S.Dev = 1.039623E-04
B2 = 1.194744E-03
[7.59 Rel.Ampl]
S.Dev = 1.579493E-05

CHISQ = 1.199276
[1810 degrees of freedom]

Chi-squared Probability = 8.1037E-07%
Durbin-Watson Parameter = 1.311131
Negative residuals = 40.9141%
Residuals < 1 s.dev = 65.9141%
Residuals < 2 s.dev = 93.39207%
Residuals < 3 s.dev = 99.17401%
Residuals < 4 s.dev = 99.8348%

ssDNA4:



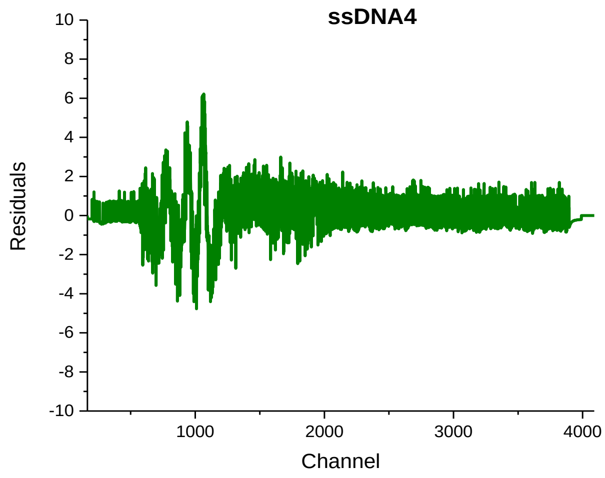


Figure S23. Fluorescence decay (top) and residuals (bottom) of ss**DNA4**.

The initial parameters are:

Shift Value = 0 ch
0 sec
Shift Limit = 100 ch
2.743484E-09 sec

T1 Estimate = 14.62924 ch
4.01351E-10 sec
T2 Estimate = 58.51697 ch
1.605404E-09 sec

A Free
B1 Free
B2 Free

Prompt and decay LO = 165 ch
4.526749E-09 sec
Prompt and decay HI = 4090 ch
1.122085E-07 sec

Background on prompt = 0.4680365
Time calibration = 2.743484E-11 sec/ch

The fitted parameters are:

Hi reduced to: 3990 ch

SHIFT = 1.839861 ch
5.04763E-11 sec
S.Dev = 1.969045E-12 sec

T1 = 13.44109 ch
3.687542E-10 sec
S.Dev = 1.038676E-11 sec
T2 = 73.75643 ch
2.023496E-09 sec
S.Dev = 1.648723E-11 sec

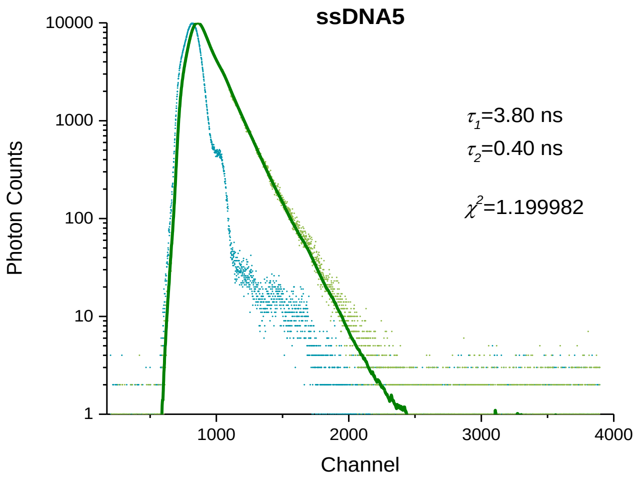
A = 0.1763385
S.Dev = 0.0207223

B1 = 6.847446E-02
[79.58 Rel.Ampl]
S.Dev = 1.018623E-04
B2 = 3.201199E-03
[20.42 Rel.Ampl]
S.Dev = 1.559716E-05

CHISQ = 1.199963
[3820 degrees of freedom]

Chi-squared Probability = 9.8556E-15%
Durbin-Watson Parameter = 0.9851762
Negative residuals = 48.90225%
Residuals < 1 s.dev = 74.93465%
Residuals < 2 s.dev = 93.701%
Residuals < 3 s.dev = 97.5954%
Residuals < 4 s.dev = 99.05907%

ssDNA5:



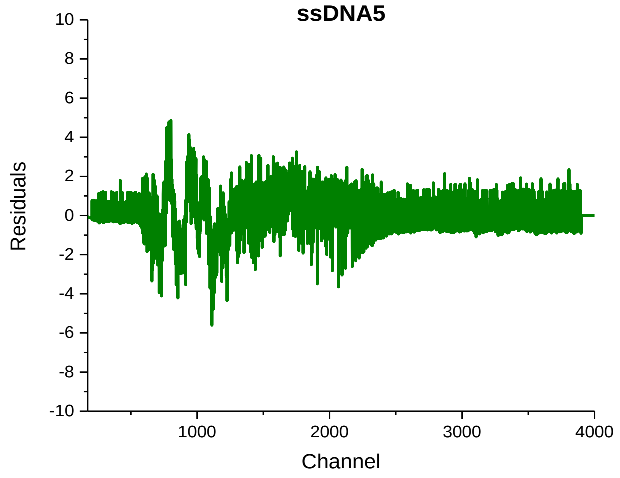


Figure S24. Fluorescence decay (top) and residuals (bottom) of ss**DNA5**.

The initial parameters are:

Shift Value = 0 ch
0 sec
Shift Limit = 100 ch
2.743484E-09 sec

T1 Estimate = 57.06097 ch
1.565459E-09 sec
T2 Estimate = 228.2439 ch
6.261835E-09 sec

A Free
B1 Free
B2 Free

Prompt and decay LO = 174 ch
4.773663E-09 sec
Prompt and decay HI = 4000 ch
1.097394E-07 sec

Background on prompt = 0.7523148
Time calibration = 2.743484E-11 sec/ch

The fitted parameters are:

Hi reduced to: 3900 ch

SHIFT = 4.338104 ch
1.190152E-10 sec
S.Dev = 3.287051E-12 sec

T1 = 14.4518 ch
3.96483E-10 sec
S.Dev = 3.055324E-11 sec
T2 = 138.6282 ch
3.803243E-09 sec
S.Dev = 5.571962E-12 sec

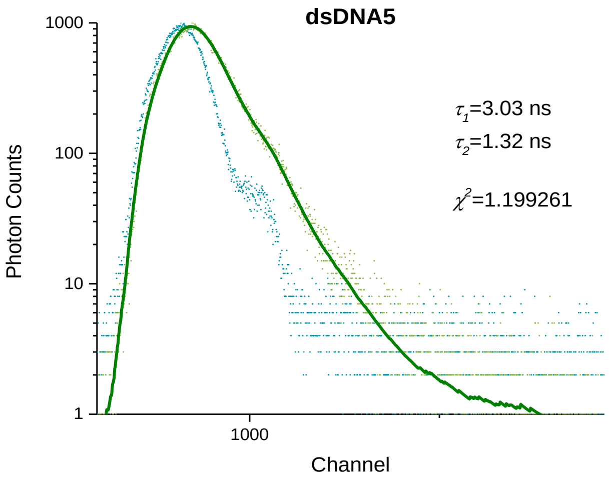
A = 0.1127336
S.Dev = 2.315319E-02

B1 = 2.848977E-02
[24.18 Rel.Ampl]
S.Dev = 8.036877E-05
B2 = 9.313257E-03
[75.82 Rel.Ampl]
S.Dev = 9.885355E-06

CHISQ = 1.199982
[3721 degrees of freedom]

Chi-squared Probability = 2.3987E-14%
Durbin-Watson Parameter = 1.222757
Negative residuals = 42.39334%
Residuals < 1 s.dev = 72.90046%
Residuals < 2 s.dev = 93.02388%
Residuals < 3 s.dev = 98.17548%
Residuals < 4 s.dev = 99.67802%

dsDNA5:



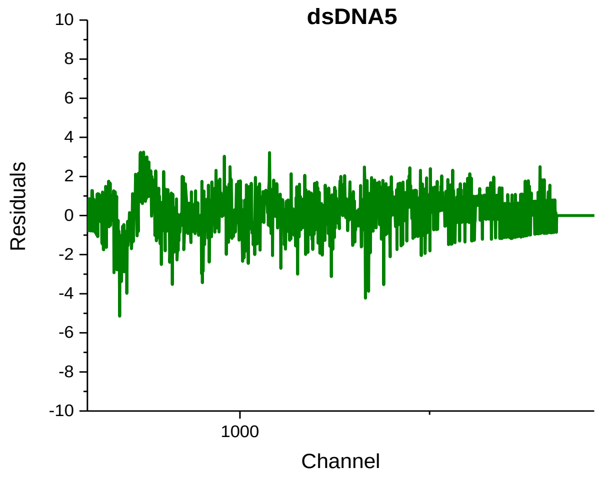


Figure S25. Fluorescence decay (top) and residuals (bottom) of ds**DNA5**.

The initial parameters are:

Shift Value = 0 ch
0 sec
Shift Limit = 100 ch
2.743484E-09 sec

T1 Estimate = 26.46875 ch
7.26166E-10 sec
T2 Estimate = 105.875 ch
2.904664E-09 sec

A Free
B1 Free
B2 Free

Prompt and decay LO = 598 ch
1.640604E-08 sec
Prompt and decay HI = 1934 ch
5.305899E-08 sec

Background on prompt = 5.20339
Time calibration = 2.743484E-11 sec/ch

The fitted parameters are:

Hi reduced to: 1834 ch

SHIFT = -11.35791 ch
-3.116025E-10 sec
S.Dev = 6.53122E-12 sec

T1 = 48.29184 ch
1.324879E-09 sec
S.Dev = 5.699959E-11 sec
T2 = 110.4252 ch
3.029499E-09 sec
S.Dev = 9.572362E-11 sec

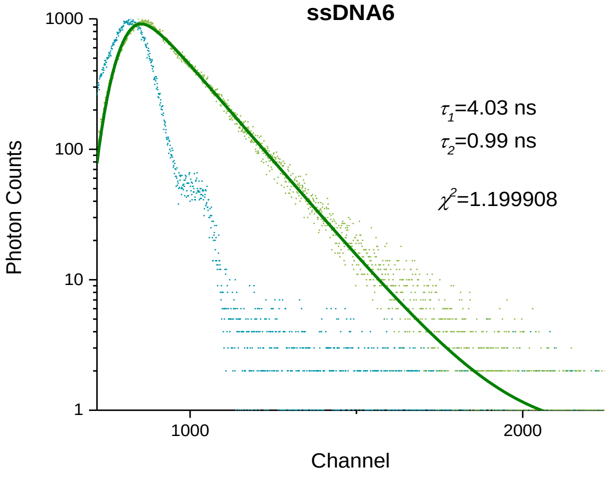
A = 0.756856
S.Dev = 5.665885E-02

B1 = 2.189004E-02
[79.50 Rel.Ampl]
S.Dev = 1.152353E-04
B2 = 2.468913E-03
[20.50 Rel.Ampl]
S.Dev = 4.625874E-05

CHISQ = 1.199261
[1231 degrees of freedom]

Chi-squared Probability = 1.5788E-04%
Durbin-Watson Parameter = 1.610313
Negative residuals = 43.2498%
Residuals < 1 s.dev = 63.2983%
Residuals < 2 s.dev = 94.82619%
Residuals < 3 s.dev = 98.78739%
Residuals < 4 s.dev = 99.83832%

ssDNA6:



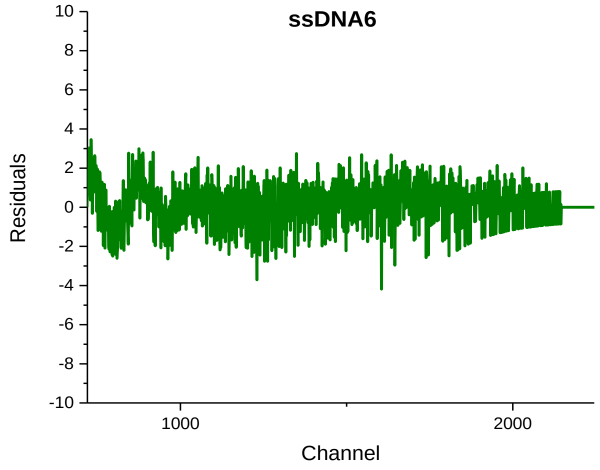


Figure S26. Fluorescence decay (top) and residuals (bottom) of ss**DNA6**.

The initial parameters are:

Shift Value = 0 ch
0 sec
Shift Limit = 100 ch
2.743484E-09 sec

T1 Estimate = 67.72549 ch
1.858038E-09 sec
T2 Estimate = 270.902 ch
7.432153E-09 sec

A Free
B1 Free
B2 Free

Prompt and decay LO = 720 ch
1.975309E-08 sec
Prompt and decay HI = 2245 ch
6.159122E-08 sec

Background on prompt = 270
Time calibration = 2.743484E-11 sec/ch

The fitted parameters are:

Hi reduced to: 2145 ch

SHIFT = -52.62615 ch
-1.44379E-09 sec
S.Dev = 3.266522E-11 sec

T1 = 36.25599 ch
9.946773E-10 sec
S.Dev = 2.543734E-11 sec
T2 = 146.9474 ch
4.031478E-09 sec
S.Dev = 1.297158E-11 sec

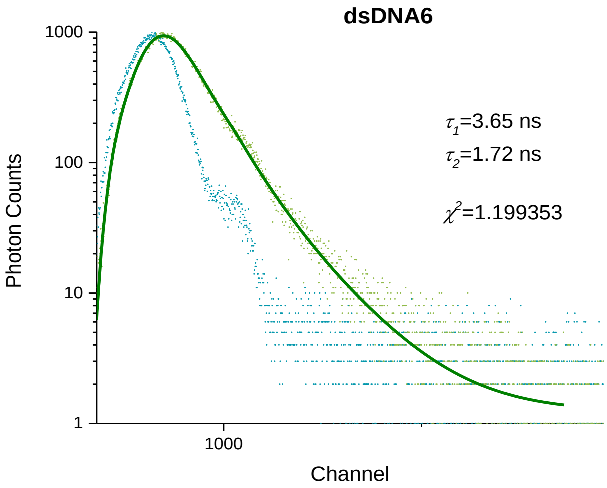
A = 0.6629046
S.Dev = 5.884882E-02

B1 = -3.079218E-02
[-33.10 Rel.Ampl]
S.Dev = 1.922266E-04
B2 = 3.055112E-02
[133.10 Rel.Ampl]
S.Dev = 7.656286E-05

CHISQ = 1.199908
[1420 degrees of freedom]

Chi-squared Probability = 2.5772E-05%
Durbin-Watson Parameter = 1.645394
Negative residuals = 42.35624%
Residuals < 1 s.dev = 63.81487%
Residuals < 2 s.dev = 93.26788%
Residuals < 3 s.dev = 99.7195%
Residuals < 4 s.dev = 99.92987%

dsDNA6:



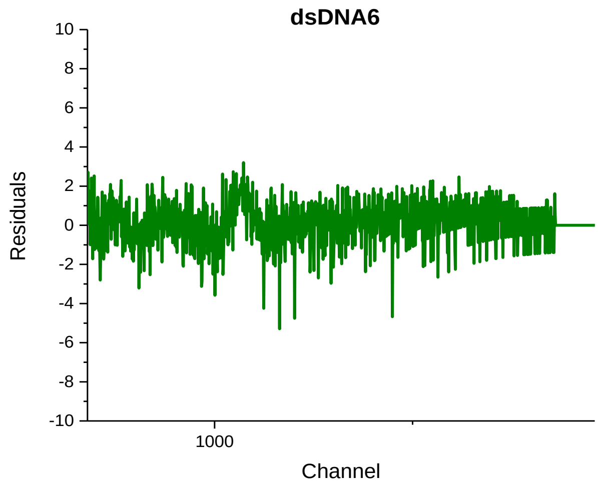


Figure S27. Fluorescence decay (top) and residuals (bottom) of ds**DNA6**.

The initial parameters are:

Shift Value = 0 ch
0 sec
Shift Limit = 100 ch
2.743484E-09 sec

T1 Estimate = 34.71695 ch
9.52454E-10 sec
T2 Estimate = 138.8678 ch
3.809816E-09 sec

A Free
B1 Free
B2 Free

Prompt and decay LO = 679 ch
1.862826E-08 sec
Prompt and decay HI = 1960 ch
5.377229E-08 sec

Background on prompt = 33
Time calibration = 2.743484E-11 sec/ch

The fitted parameters are:

Hi reduced to: 1860 ch

SHIFT = -15.17089 ch
-4.162111E-10 sec
S.Dev = 6.508744E-12 sec

T1 = 62.64719 ch
1.718716E-09 sec
S.Dev = 6.815119E-11 sec
T2 = 133.0079 ch
3.649052E-09 sec
S.Dev = 9.523141E-11 sec

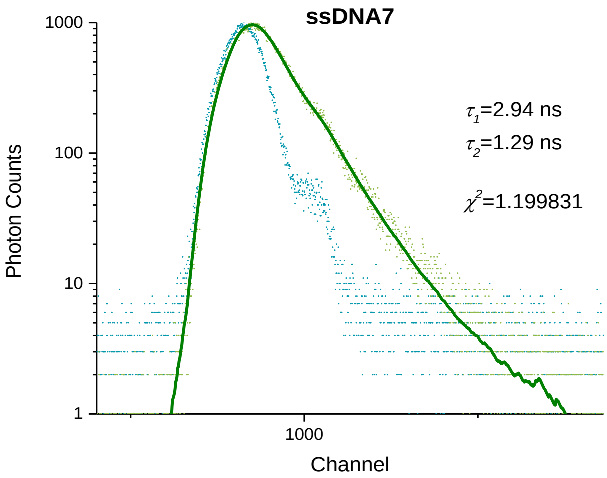
A = 1.235477
S.Dev = 7.240191E-02

B1 = 1.766665E-02
[72.36 Rel.Ampl]
S.Dev = 9.916998E-05
B2 = 3.17808E-03
[27.64 Rel.Ampl]
S.Dev = 4.468079E-05

CHISQ = 1.199353
[1176 degrees of freedom]

Chi-squared Probability = 2.5673E-04%
Durbin-Watson Parameter = 1.635764
Negative residuals = 39.42471%
Residuals < 1 s.dev = 63.45178%
Residuals < 2 s.dev = 94.75465%
Residuals < 3 s.dev = 99.32318%
Residuals < 4 s.dev = 99.66159%

ssDNA7:



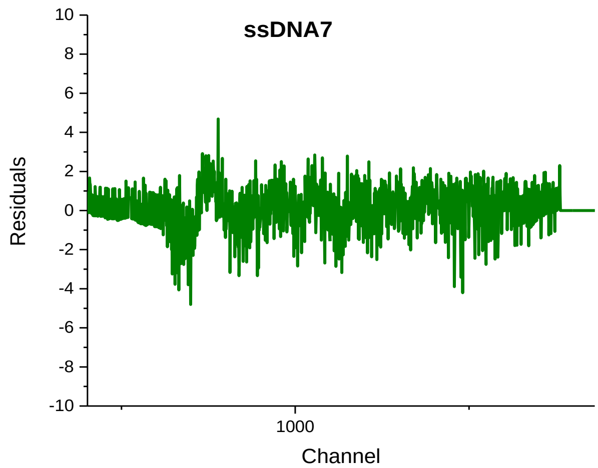


Figure S28. Fluorescence decay (top) and residuals (bottom) of ss**DNA7**.

The initial parameters are:

Shift Value = 0 ch
0 sec
Shift Limit = 100 ch
2.743484E-09 sec

T1 Estimate = 30.84464 ch
8.462177E-10 sec
T2 Estimate = 123.3785 ch
3.384871E-09 sec

A Free
B1 Free
B2 Free

Prompt and decay LO = 402 ch
1.102881E-08 sec
Prompt and decay HI = 1862 ch
5.108368E-08 sec

Background on prompt = 3.957692
Time calibration = 2.743484E-11 sec/ch

The fitted parameters are:

Hi reduced to: 1762 ch

SHIFT = -15.35995 ch
-4.213979E-10 sec
S.Dev = 7.603721E-12 sec

T1 = 46.84391 ch
1.285155E-09 sec
S.Dev = 1.103939E-10 sec
T2 = 107.2317 ch
2.941886E-09 sec
S.Dev = 3.759248E-11 sec

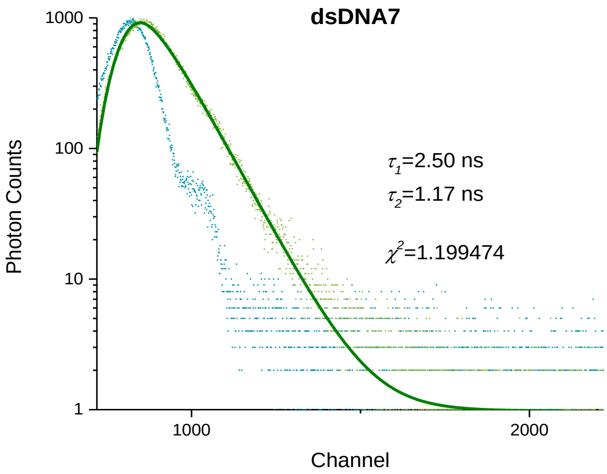
A = 1.168434E-02
S.Dev = 5.223098E-02

B1 = 0.0148905
[46.43 Rel.Ampl]
S.Dev = 1.387272E-04
B2 = 7.504016E-03
[53.57 Rel.Ampl]
S.Dev = 6.150384E-05

CHISQ = 1.199831
[1355 degrees of freedom]

Chi-squared Probability = 4.7577E-05%
Durbin-Watson Parameter = 1.57371
Negative residuals = 44.01176%
Residuals < 1 s.dev = 66.64217%
Residuals < 2 s.dev = 94.04849%
Residuals < 3 s.dev = 98.97134%
Residuals < 4 s.dev = 99.7061%

dsDNA7:



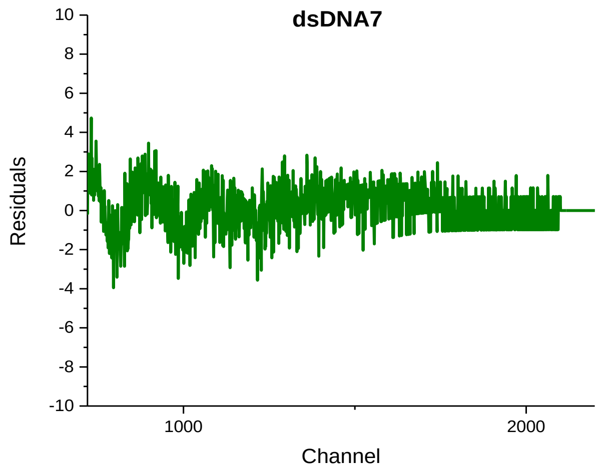


Figure S29. Fluorescence decay (top) and residuals (bottom) of ds**DNA7**.

The initial parameters are:

Shift Value = 0 ch
0 sec
Shift Limit = 100 ch
2.743484E-09 sec

T1 Estimate = 43.21747 ch
1.185664E-09 sec
T2 Estimate = 172.8699 ch
4.742658E-09 sec

A Free
B1 Free
B2 Free

Prompt and decay LO = 720 ch
1.975309E-08 sec
Prompt and decay HI = 2200 ch
6.035665E-08 sec

Background on prompt = 200
Time calibration = 2.743484E-11 sec/ch

The fitted parameters are:

Hi reduced to: 2100 ch

SHIFT = -53.72655 ch
-1.473979E-09 sec
S.Dev = 2.737418E-11 sec

T1 = 42.5616 ch
1.167671E-09 sec
S.Dev = 2.660255E-11 sec
T2 = 91.13138 ch
2.500175E-09 sec
S.Dev = 1.027668E-11 sec

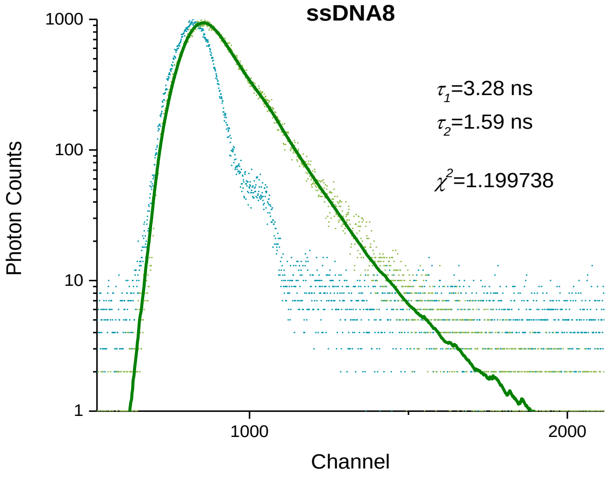
A = 0.9787993
S.Dev = 4.635355E-02

B1 = -5.045155E-02
[-88.20 Rel.Ampl]
S.Dev = 2.689535E-04
B2 = 0.050277
[188.20 Rel.Ampl]
S.Dev = 1.593001E-04

CHISQ = 1.199474
[1375 degrees of freedom]

Chi-squared Probability = 4.1327E-05%
Durbin-Watson Parameter = 1.297447
Negative residuals = 42.14338%
Residuals < 1 s.dev = 63.79435%
Residuals < 2 s.dev = 94.27951%
Residuals < 3 s.dev = 99.27589%
Residuals < 4 s.dev = 99.92759%

ssDNA8:



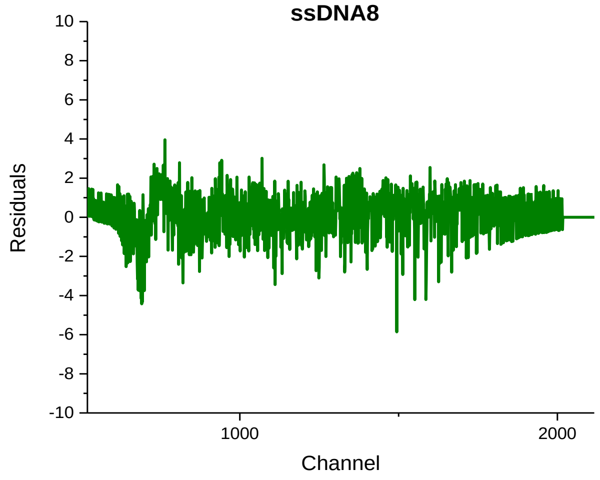


Figure S30. Fluorescence decay (top) and residuals (bottom) of ss**DNA8**.

The initial parameters are:

Shift Value = 0 ch
0 sec
Shift Limit = 100 ch
2.743484E-09 sec

T1 Estimate = 41.18469 ch
1.129896E-09 sec
T2 Estimate = 164.7388 ch
4.519582E-09 sec

A Free
B1 Free
B2 Free

Prompt and decay LO = 520 ch
1.426612E-08 sec
Prompt and decay HI = 2116 ch
5.805213E-08 sec

Background on prompt = 5.832061
Time calibration = 2.743484E-11 sec/ch

The fitted parameters are:

Hi reduced to: 2016 ch

SHIFT = -16.61835 ch
-4.559217E-10 sec
S.Dev = 8.037188E-12 sec

T1 = 57.95068 ch
1.589868E-09 sec
S.Dev = 1.79345E-10 sec
T2 = 119.8267 ch
3.287427E-09 sec
S.Dev = 3.734778E-11 sec

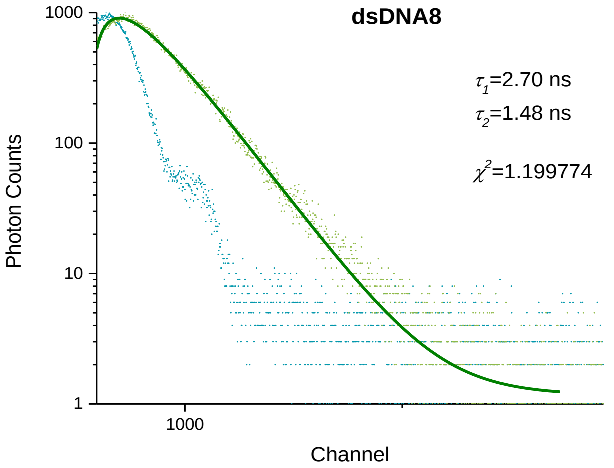
A = -0.169827
S.Dev = 5.101821E-02

B1 = 9.74207E-03
[34.88 Rel.Ampl]
S.Dev = 1.260712E-04
B2 = 8.795408E-03
[65.12 Rel.Ampl]
S.Dev = 6.349591E-05

CHISQ = 1.199738
[1491 degrees of freedom]

Chi-squared Probability = 1.3869E-05%
Durbin-Watson Parameter = 1.694077
Negative residuals = 40.68136%
Residuals < 1 s.dev = 65.39746%
Residuals < 2 s.dev = 94.32198%
Residuals < 3 s.dev = 98.7308%
Residuals < 4 s.dev = 99.5992%

dsDNA8:



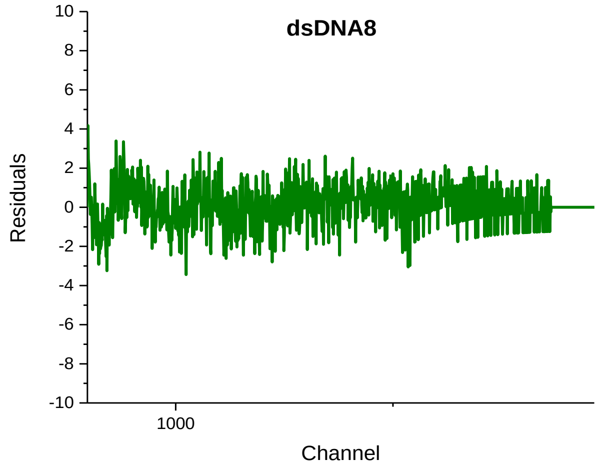


Figure S31. Fluorescence decay (top) and residuals (bottom) of ds**DNA8**.

The initial parameters are:

Shift Value = 0 ch
0 sec
Shift Limit = 100 ch
2.743484E-09 sec

T1 Estimate = 58.90509 ch
1.616052E-09 sec
T2 Estimate = 235.6204 ch
6.464207E-09 sec

A Free
B1 Free
B2 Free

Prompt and decay LO = 797 ch
2.186557E-08 sec
Prompt and decay HI = 1963 ch
5.38546E-08 sec

Background on prompt = 823
Time calibration = 2.743484E-11 sec/ch

The fitted parameters are:

Hi reduced to: 1863 ch

SHIFT = -44.90597 ch
-1.231988E-09 sec
S.Dev = 7.713335E-11 sec

T1 = 53.83774 ch
1.47703E-09 sec
S.Dev = 3.127762E-11 sec
T2 = 98.44467 ch
2.700814E-09 sec
S.Dev = 1.143306E-11 sec

A = 1.172085
S.Dev = 6.695937E-02

B1 = -1.03747
[-120.94 Rel.Ampl]
S.Dev = 5.353337E-03
B2 = 1.03653
[220.94 Rel.Ampl]
S.Dev = 3.319057E-03

CHISQ = 1.199774
[1061 degrees of freedom]

Chi-squared Probability = 7.1653E-04%
Durbin-Watson Parameter = 1.521631
Negative residuals = 41.98688%
Residuals < 1 s.dev = 61.48079%
Residuals < 2 s.dev = 94.37675%
Residuals < 3 s.dev = 99.34396%
Residuals < 4 s.dev = 99.90628%

ssDNA9:

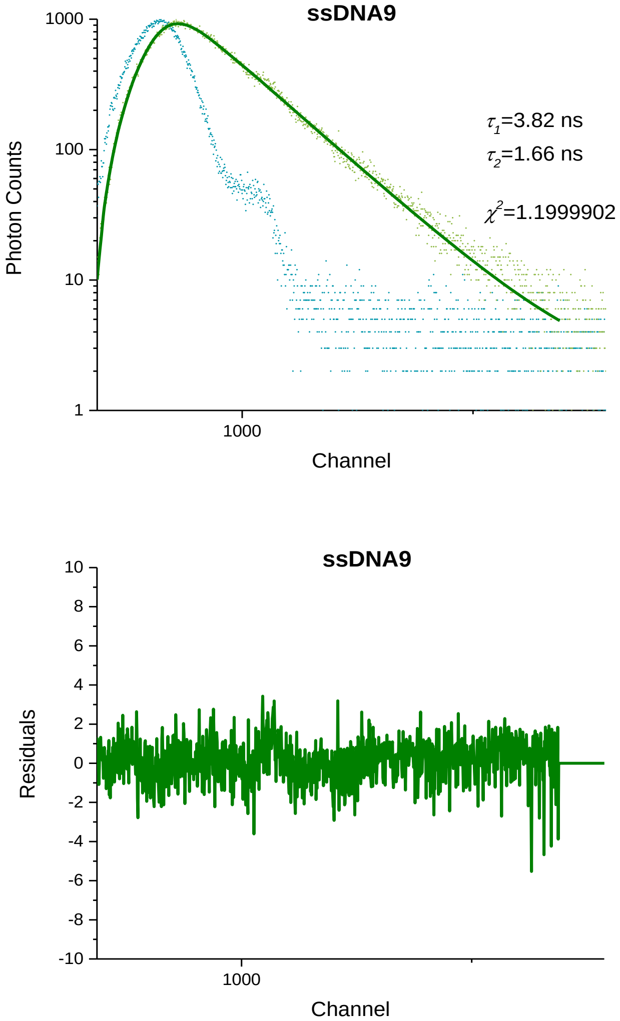


Figure S32. Fluorescence decay (top) and residuals (bottom) of ss**DNA9**.

The initial parameters are:

Shift Value = 0 ch
0 sec
Shift Limit = 100 ch
2.743484E-09 sec

T1 Estimate = 58.20059 ch
1.596724E-09 sec
T2 Estimate = 232.8024 ch
6.386896E-09 sec

A Free
B1 Free
B2 Free

Prompt and decay LO = 686 ch
1.88203E-08 sec
Prompt and decay HI = 1788 ch
4.90535E-08 sec

Background on prompt = 37
Time calibration = 2.743484E-11 sec/ch

The fitted parameters are:

Hi reduced to: 1688 ch

SHIFT = -17.33445 ch
-4.755679E-10 sec
S.Dev = 1.009941E-11 sec

T1 = 60.42396 ch
1.657722E-09 sec
S.Dev = 1.165802E-10 sec
T2 = 139.1989 ch
3.818899E-09 sec
S.Dev = 3.463184E-11 sec

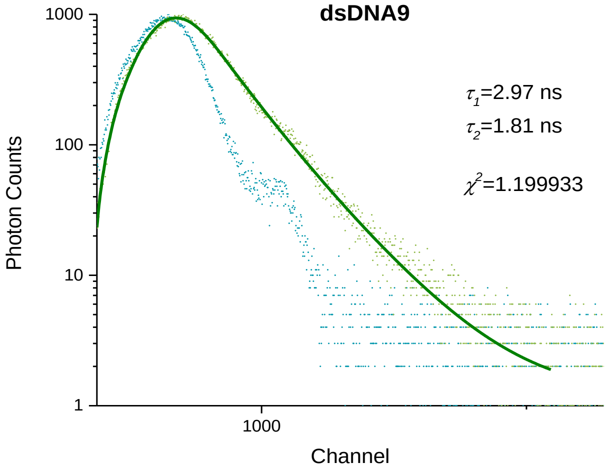
A = 1.68504
S.Dev = 0.1783364

B1 = -2.846797E-05
[-0.09 Rel.Ampl]
S.Dev = 1.209101E-04
B2 = 1.410179E-02
[100.09 Rel.Ampl]
S.Dev = 6.320419E-05

CHISQ = 1.199902
[997 degrees of freedom]

Chi-squared Probability = 1.2817E-03%
Durbin-Watson Parameter = 1.718134
Negative residuals = 43.27019%
Residuals < 1 s.dev = 65.70289%
Residuals < 2 s.dev = 93.91824%
Residuals < 3 s.dev = 99.20239%
Residuals < 4 s.dev = 99.7009%

dsDNA9:



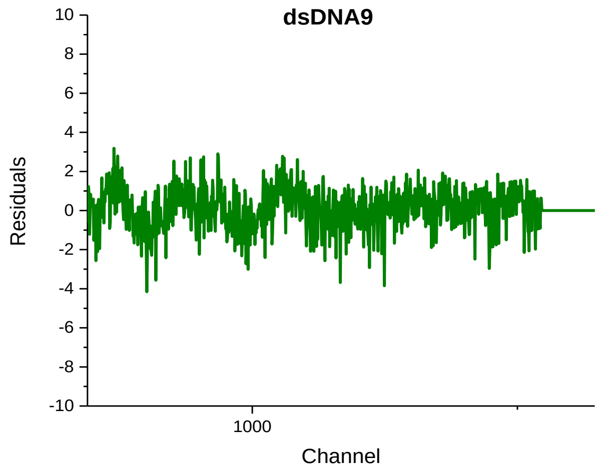


Figure S33. Fluorescence decay (top) and residuals (bottom) of ds**DNA9**.

The initial parameters are:

Shift Value = 0 ch
0 sec
Shift Limit = 100 ch
2.743484E-09 sec

T1 Estimate = 28.38708 ch
7.787952E-10 sec
T2 Estimate = 113.5483 ch
3.115181E-09 sec

A Free
B1 Free
B2 Free

Prompt and decay LO = 689 ch
1.890261E-08 sec
Prompt and decay HI = 1646 ch
4.515775E-08 sec

Background on prompt = 78
Time calibration = 2.743484E-11 sec/ch

The fitted parameters are:

Hi reduced to: 1546 ch

SHIFT = -25.49063 ch
-6.993313E-10 sec
S.Dev = 7.029621E-12 sec

T1 = 66.13319 ch
1.814354E-09 sec
S.Dev = 1.223507E-10 sec
T2 = 108.1708 ch
2.967648E-09 sec
S.Dev = 1.050616E-10 sec

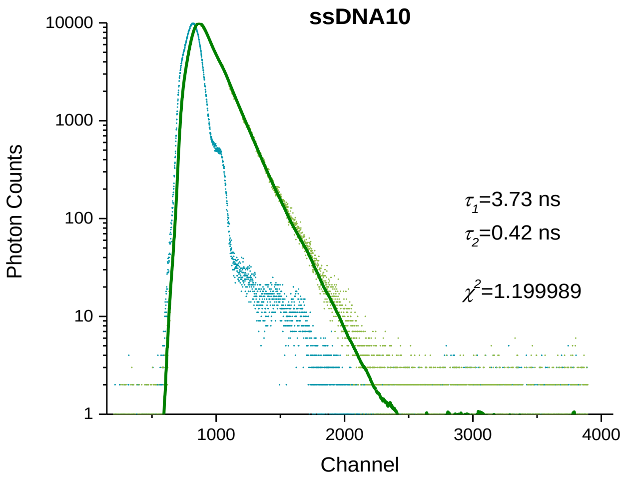
A = 1.205835
S.Dev = 0.1218205

B1 = 1.517045E-02
[60.87 Rel.Ampl]
S.Dev = 1.563469E-04
B2 = 5.963195E-03
[39.13 Rel.Ampl]
S.Dev = 9.767997E-05

CHISQ = 1.199933
[852 degrees of freedom]

Chi-squared Probability = 4.8965E-03%
Durbin-Watson Parameter = 1.476346
Negative residuals = 41.84149%
Residuals < 1 s.dev = 65.15151%
Residuals < 2 s.dev = 93.47319%
Residuals < 3 s.dev = 99.3007%
Residuals < 4 s.dev = 99.88345%

ssDNA10:



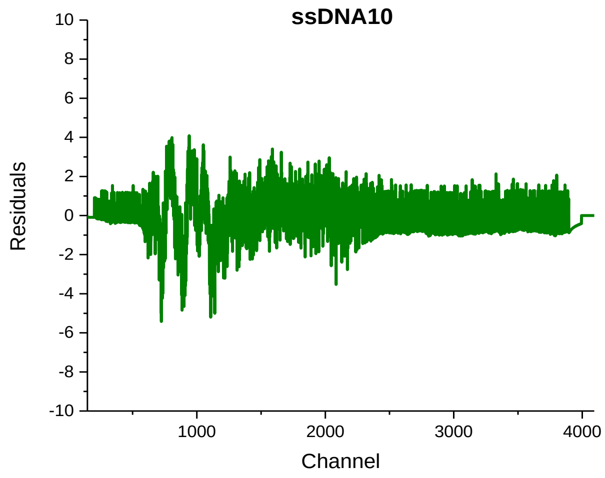


Figure S34. Fluorescence decay (top) and residuals (bottom) of ss**DNA10**.

The initial parameters are:

Shift Value = 0 ch
0 sec
Shift Limit = 100 ch
2.743484E-09 sec

T1 Estimate = 61.49338 ch
1.687061E-09 sec
T2 Estimate = 245.9735 ch
6.748245E-09 sec

A Free
B1 Free
B2 Free

Prompt and decay LO = 148 ch
4.060356E-09 sec
Prompt and decay HI = 4094 ch
1.123182E-07 sec

Background on prompt = 0.6513158
Time calibration = 2.743484E-11 sec/ch

The fitted parameters are:

Hi reduced to: 3994 ch

SHIFT = 6.439065 ch
1.766547E-10 sec
S.Dev = 3.892315E-12 sec

T1 = 15.18804 ch
4.166816E-10 sec
S.Dev = 4.421856E-11 sec
T2 = 135.8171 ch
3.726121E-09 sec
S.Dev = 5.141317E-12 sec

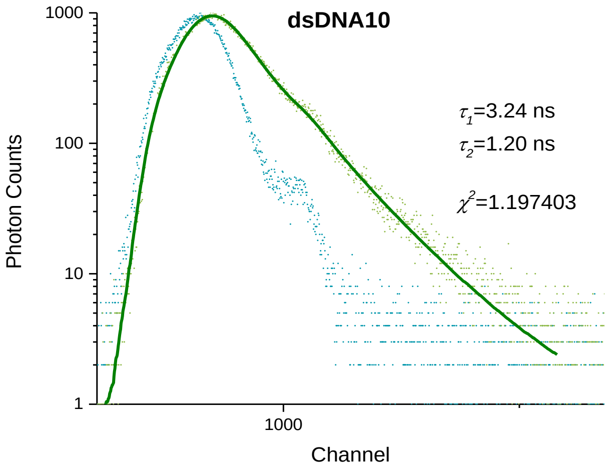
A = 8.845718E-02
S.Dev = 2.269959E-02

B1 = 1.909779E-02
[16.70 Rel.Ampl]
S.Dev = 7.685415E-05
B2 = 1.065247E-02
[83.30 Rel.Ampl]
S.Dev = 1.060617E-05

CHISQ = 1.199989
[3841 degrees of freedom]

Chi-squared Probability = 8.1595E-15%
Durbin-Watson Parameter = 1.160567
Negative residuals = 42.55264%
Residuals < 1 s.dev = 72.34209%
Residuals < 2 s.dev = 93.42345%
Residuals < 3 s.dev = 97.99844%
Residuals < 4 s.dev = 99.61008%

dsDNA10:



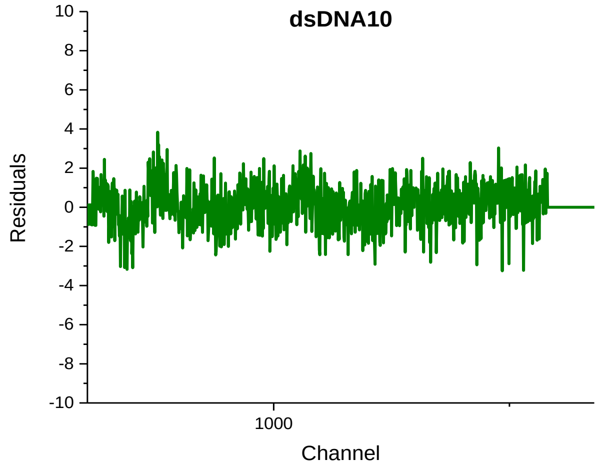


Figure S35. Fluorescence decay (top) and residuals (bottom) of ds**DNA10**.

The initial parameters are:

Shift Value = 0 ch
0 sec
Shift Limit = 100 ch
2.743484E-09 sec

T1 Estimate = 34.13016 ch
9.363555E-10 sec
T2 Estimate = 136.5206 ch
3.745422E-09 sec

A Free
B1 Free
B2 Free

Prompt and decay LO = 605 ch
1.659808E-08 sec
Prompt and decay HI = 1680 ch
4.609053E-08 sec

Background on prompt = 4.788462
Time calibration = 2.743484E-11 sec/ch

The fitted parameters are:

Hi reduced to: 1580 ch

SHIFT = -9.808468 ch
-2.690938E-10 sec
S.Dev = 7.625179E-12 sec

T1 = 43.80527 ch
1.201791E-09 sec
S.Dev = 8.513679E-11 sec
T2 = 117.9182 ch
3.235067E-09 sec
S.Dev = 4.38411E-11 sec

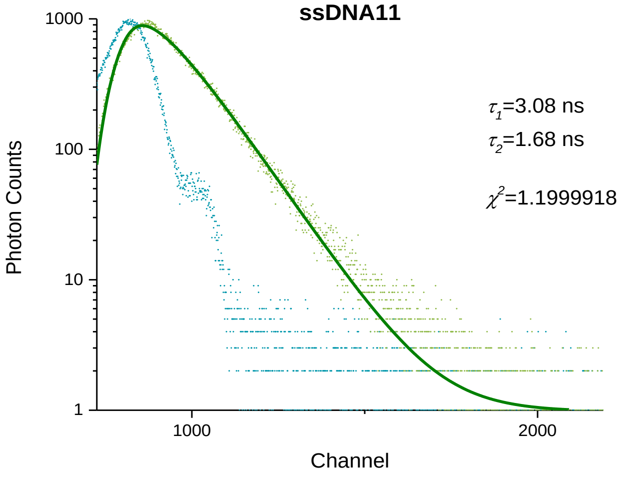
A = 0.8482031
S.Dev = 0.1089867

B1 = 1.752216E-02
[52.69 Rel.Ampl]
S.Dev = 1.252485E-04
B2 = 5.845251E-03
[47.31 Rel.Ampl]
S.Dev = 4.769505E-05

CHISQ = 1.197403
[970 degrees of freedom]

Chi-squared Probability = 2.0198E-03%
Durbin-Watson Parameter = 1.704324
Negative residuals = 44.46721%
Residuals < 1 s.dev = 65.77869%
Residuals < 2 s.dev = 94.2623%
Residuals < 3 s.dev = 99.07787%
Residuals < 4 s.dev = 100%

ssDNA11:



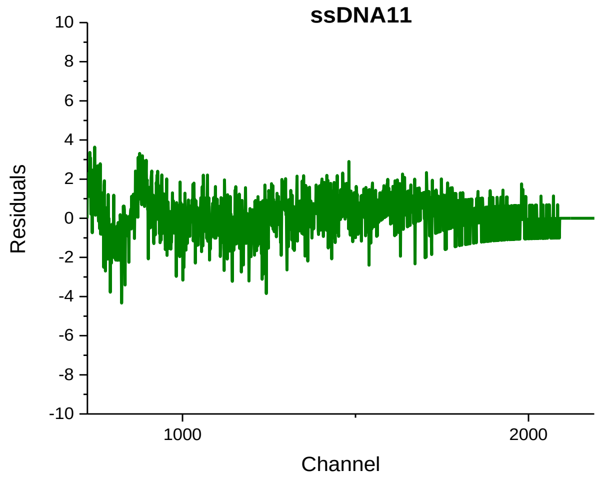


Figure S36. Fluorescence decay (top) and residuals (bottom) of ss**DNA11**.

The initial parameters are:

Shift Value = 0 ch
0 sec
Shift Limit = 100 ch
2.743484E-09 sec

T1 Estimate = 59.74802 ch
1.639177E-09 sec
T2 Estimate = 238.9921 ch
6.55671E-09 sec

A Free
B1 Free
B2 Free

Prompt and decay LO = 725 ch
1.989026E-08 sec
Prompt and decay HI = 2190 ch
6.008231E-08 sec

Background on prompt = 323
Time calibration = 2.743484E-11 sec/ch

The fitted parameters are:

Hi reduced to: 2090 ch

SHIFT = -55.75471 ch
-1.529622E-09 sec
S.Dev = 2.872733E-11 sec

T1 = 61.24899 ch
1.680357E-09 sec
S.Dev = 1.476286E-11 sec
T2 = 112.0862 ch
3.075066E-09 sec
S.Dev = 1.181068E-11 sec

A = 0.9781677
S.Dev = 5.407171E-02

B1 = -7.179778E-02
[-120.97 Rel.Ampl]
S.Dev = 2.90841E-04
B2 = 0.0716667
[220.97 Rel.Ampl]
S.Dev = 2.025364E-04

CHISQ = 1.199918
[1360 degrees of freedom]

Chi-squared Probability = 4.4612E-05%
Durbin-Watson Parameter = 1.405217
Negative residuals = 45.31479%
Residuals < 1 s.dev = 61.20058%
Residuals < 2 s.dev = 93.33821%
Residuals < 3 s.dev = 98.9019%
Residuals < 4 s.dev = 99.9268%

dsDNA11:

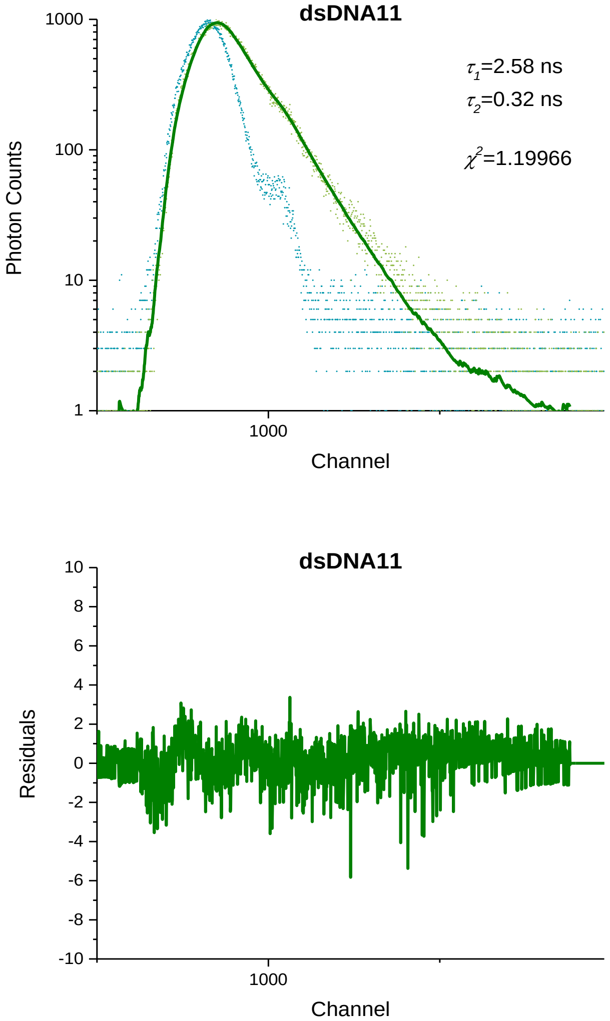


Figure S37. Fluorescence decay (top) and residuals (bottom) of ds**DNA11**.

The initial parameters are:

Shift Value = 0 ch
0 sec
Shift Limit = 100 ch
2.743484E-09 sec

T1 Estimate = 32.89313 ch
9.024178E-10 sec
T2 Estimate = 131.5725 ch
3.609671E-09 sec

A Free
B1 Free
B2 Free

Prompt and decay LO = 500 ch
1.371742E-08 sec
Prompt and decay HI = 1980 ch
5.432099E-08 sec

Background on prompt = 3.753012
Time calibration = 2.743484E-11 sec/ch

The fitted parameters are:

Hi reduced to: 1880 ch

SHIFT = -6.894238 ch
-1.891423E-10 sec
S.Dev = 1.133173E-11 sec

T1 = 11.71957 ch
3.215245E-10 sec
S.Dev = 4.696774E-11 sec
T2 = 94.05235 ch
2.580311E-09 sec
S.Dev = 1.678147E-11 sec

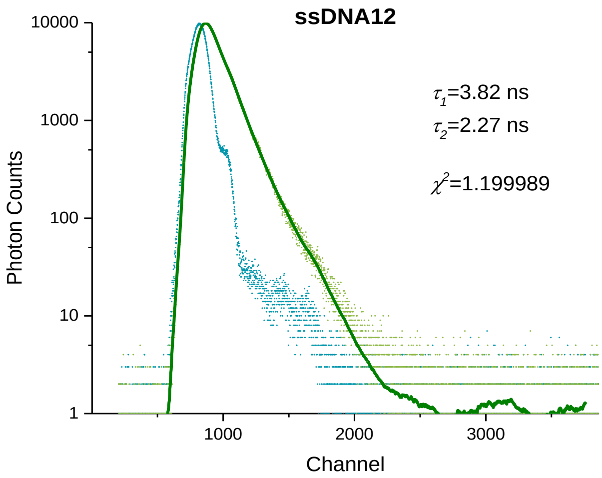
A = 0.6672095
S.Dev = 5.234806E-02

B1 = 0.0313203
[24.97 Rel.Ampl]
S.Dev = 3.665343E-04
B2 = 1.172977E-02
[75.03 Rel.Ampl]
S.Dev = 5.098569E-05

CHISQ = 1.19966
[1375 degrees of freedom]

Chi-squared Probability = 4.0421E-05%
Durbin-Watson Parameter = 1.674751
Negative residuals = 40.62274%
Residuals < 1 s.dev = 63.07024%
Residuals < 2 s.dev = 94.06227%
Residuals < 3 s.dev = 99.05865%
Residuals < 4 s.dev = 99.78277%

ssDNA12:



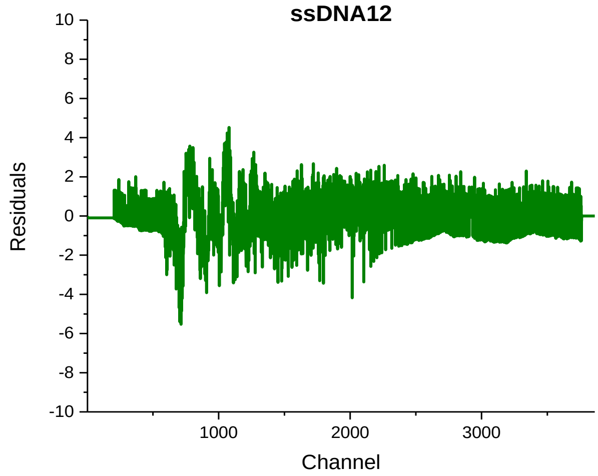


Figure S38. Fluorescence decay (top) and residuals (bottom) of ss**DNA12**.

The initial parameters are:

Shift Value = 0 ch
0 sec
Shift Limit = 100 ch
2.743484E-09 sec

T1 Estimate = 53.54553 ch
1.469013E-09 sec
T2 Estimate = 214.1821 ch
5.876053E-09 sec

A Free
B1 Free
B2 Free

Prompt and decay LO = 2 ch
5.486969E-11 sec
Prompt and decay HI = 3861 ch
1.059259E-07 sec

Background on prompt = 0.8630363
Time calibration = 2.743484E-11 sec/ch

The fitted parameters are:

Hi reduced to: 3761 ch

SHIFT = -3.796562 ch
-1.041581E-10 sec
S.Dev = 2.269347E-12 sec

T1 = 82.77507 ch
2.270921E-09 sec
S.Dev = 7.665973E-11 sec
T2 = 139.3546 ch
3.823171E-09 sec
S.Dev = 1.827265E-11 sec

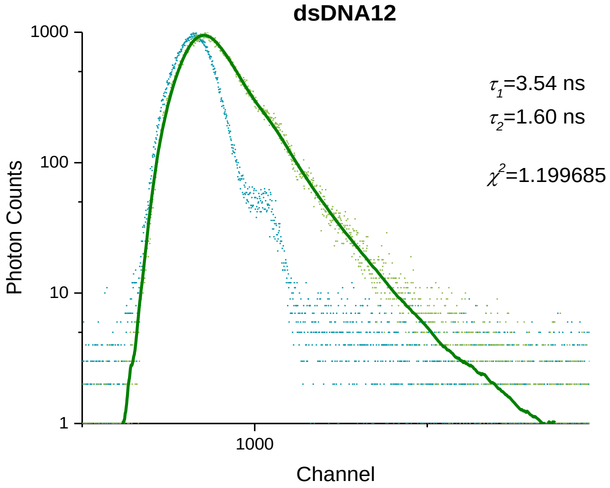
A = 9.366913E-02
S.Dev = 2.407943E-02

B1 = 1.046916E-02
[51.19 Rel.Ampl]
S.Dev = 3.3098E-05
B2 = 5.93029E-03
[48.81 Rel.Ampl]
S.Dev = 1.959281E-05

CHISQ = 1.199989
[3754 degrees of freedom]

Chi-squared Probability = 1.7659E-14%
Durbin-Watson Parameter = 1.306689
Negative residuals = 47.23404%
Residuals < 1 s.dev = 64.9734%
Residuals < 2 s.dev = 93.51064%
Residuals < 3 s.dev = 98.37766%
Residuals < 4 s.dev = 99.73404%

dsDNA12:



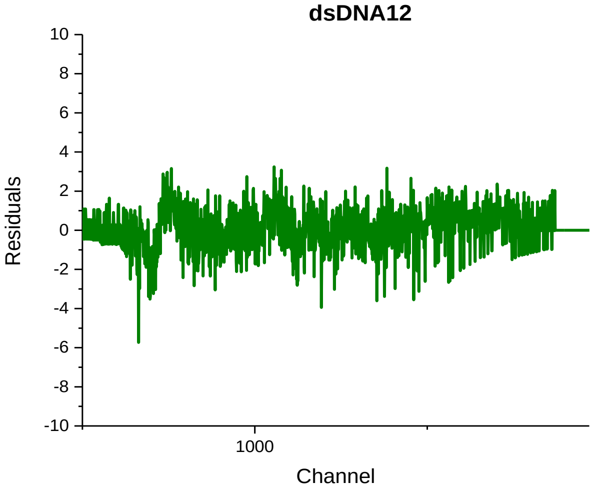


Figure S39. Fluorescence decay (top) and residuals (bottom) of ds**DNA12**.

The initial parameters are:

Shift Value = 0 ch
0 sec
Shift Limit = 100 ch
2.743484E-09 sec

T1 Estimate = 36.58762 ch
1.003776E-09 sec
T2 Estimate = 146.3505 ch
4.015102E-09 sec

A Free
B1 Free
B2 Free

Prompt and decay LO = 500 ch
1.371742E-08 sec
Prompt and decay HI = 1970 ch
5.404664E-08 sec

Background on prompt = 3.753012
Time calibration = 2.743484E-11 sec/ch

The fitted parameters are:

Hi reduced to: 1870 ch

SHIFT = -15.3005 ch
-4.197668E-10 sec
S.Dev = 7.14499E-12 sec

T1 = 58.30676 ch
1.599637E-09 sec
S.Dev = 1.424307E-10 sec
T2 = 128.9734 ch
3.538364E-09 sec
S.Dev = 5.363263E-11 sec

A = 0.4119495
S.Dev = 5.782321E-02

B1 = 1.497738E-02
[57.85 Rel.Ampl]
S.Dev = 1.058001E-04
B2 = 4.93406E-03
[42.15 Rel.Ampl]
S.Dev = 4.741007E-05

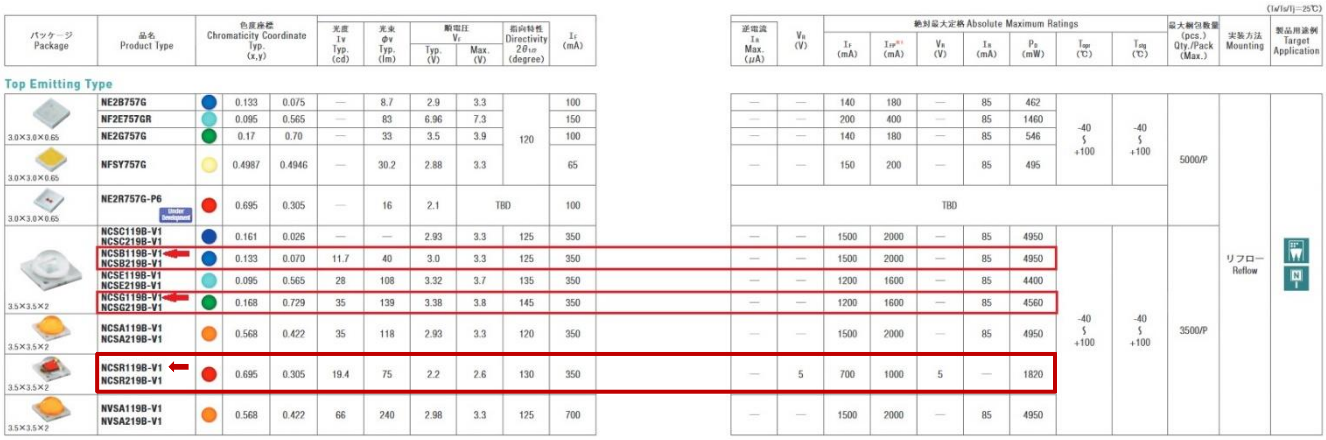
CHISQ = 1.199685
[1365 degrees of freedom]

Chi-squared Probability = 4.4162E-05%
Durbin-Watson Parameter = 1.627788
Negative residuals = 41.06491%
Residuals < 1 s.dev = 64.47849%
Residuals < 2 s.dev = 93.94602%
Residuals < 3 s.dev = 98.76003%
Residuals < 4 s.dev = 99.92706%

9. Photostability of ssDNAs

The photoreactor *FRITZ* with built-in temperature controller and built-in air cooling was used for the irradiation experiments. This photoreactor was developed under the guidance of *M. Weinberger* and carried out from the central fine-mechanical and electronic workshop of the *Department of Chemistry* at the *University of Regensburg*. LEDs from *Nichia* with a wavelength of λ_{LED} = 468 and 520 nm were used for the irradiation experiments, and the temperature was kept constant at 20 °C. For singlet-oxygen sensitization with rose bengal, a LED from *Nichia* was used with a wavelength of λ_{LED} = 637 nm

A solution consisting of 2.5 µM respective dye-DNA bioconjugate, 10 mM NaP_i buffer (pH 7) and 250 mM NaCl in *Millipore* water was introduced into a quartz glass cuvette and irradiated in the photoreactor *FRITZ* in certain cycles. Between each cycle absorption, emission and excitation spectra were recorded. After a total of four half-lives the irradiation experiment was finished and the half-lives were determined as single-exponential decays in all cases.



(Ia/Is/Tj=25℃)

パッケージ Package	品名 Product Type	色度座標 Chromaticity Coordinate Typ. x	y	光度 Iv Typ. (cd)	光束 φv Typ. (lm)	順電圧 VF Typ. (V)	VF Max. (V)	指向特性 Directivity 2θ1/2 (degree)	IF (mA)	逆電流 IR Max. (µA)	VR (V)	絶対最大定格 Absolute Maximum Ratings IF (mA)	IFP*1 (mA)	VR (V)	IR (mA)	PD (mW)	Topr (℃)	Tstg (℃)	最大梱包数量 (pcs.) Qty./Pack (Max.)	実装方法 Mounting	製品用途例 Target Application
Top Emitting Type																					
3.0×3.0×0.65	NE2B757G	0.133	0.075	—	8.7	2.9	3.3	120	100	—	—	140	180	—	85	462	-40 ∫ +100	-40 ∫ +100	5000/P	リフロー Reflow	
	NF2E757GR	0.095	0.565	—	83	6.96	7.3		150	—	—	200	400	—	85	1460					
	NE2G757G	0.17	0.70	—	33	3.5	3.9		100	—	—	140	180	—	85	546					
3.0×3.0×0.65	NFSY757G	0.4987	0.4946	—	30.2	2.88	3.3		65	—	—	150	200	—	85	495					
3.0×3.0×0.65	NE2R757G-P6 Under Development	0.695	0.305	—	16	2.1	TBD		100	TBD											
3.5×3.5×2	NCSC119B-V1 NCSC219B-V1	0.161	0.026	—	—	2.93	3.3	125	350	—	—	1500	2000	—	85	4950	-40 ∫ +100	-40 ∫ +100	3500/P		
	NCSB119B-V1 NCSB219B-V1	0.133	0.070	11.7	40	3.0	3.3	125	350	—	—	1500	2000	—	85	4950					
	NCSE119B-V1 NCSE219B-V1	0.095	0.565	28	108	3.32	3.7	135	350	—	—	1200	1600	—	85	4400					
	NCSG119B-V1 NCSG219B-V1	0.168	0.729	35	139	3.38	3.8	145	350	—	—	1200	1600	—	85	4560					
3.5×3.5×2	NCSA119B-V1 NCSA219B-V1	0.568	0.422	35	118	2.93	3.3	120	350	—	—	1500	2000	—	85	4950					
3.5×3.5×2	NCSR119B-V1 NCSR219B-V1	0.695	0.305	19.4	75	2.2	2.6	130	350	—	5	700	1000	5	—	1820					
3.5×3.5×2	NVSA119B-V1 NVSA219B-V1	0.568	0.422	66	240	2.98	3.3	125	700	—	—	1500	2000	—	85	4950					

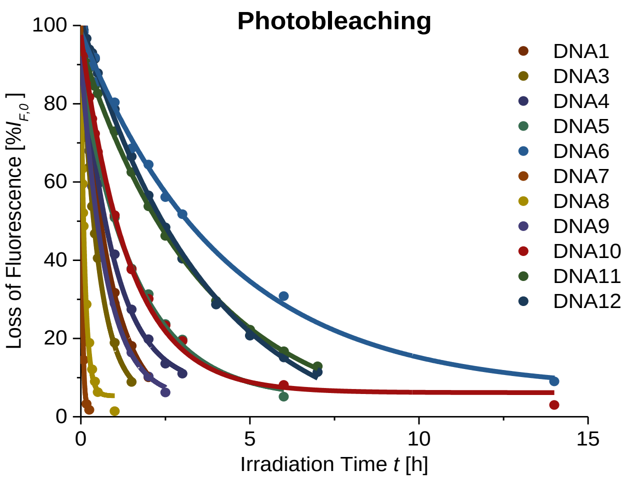
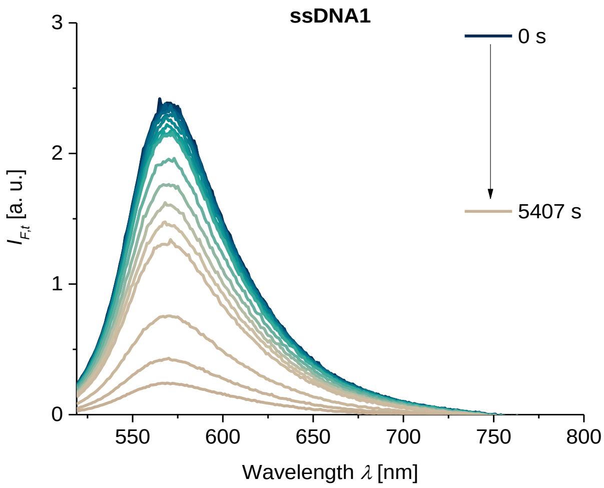


Figure S40. Abstract of the specification sheet of the used LEDs (top) and

photobleaching as loss of fluorescence of ss**DNA1**-**12** during irradiation with a 468 nm LED (bottom).

ssDNA1:



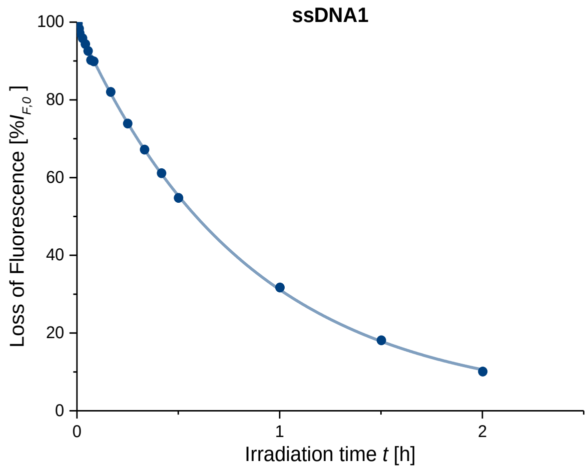


Figure S41. Emission spectra of ss**DNA1** during irradiation with a 468 nm LED (top) and photobleaching (bottom).

Table S11. Fit parameters for the photobleaching of **DNA1**.

Model	ExpDec1
Equation	y = A1*exp(-x/t1) + y0
y0	0.01622 ± 0.00888
A1	0.9768 ± 0.00849
t1	3010.61191 ± 59.59218
Reduced Chi-Sqr	3.34E+00
R-Square(COD)	0.99964
Adj. R-Square	0.9996

ssDNA2:

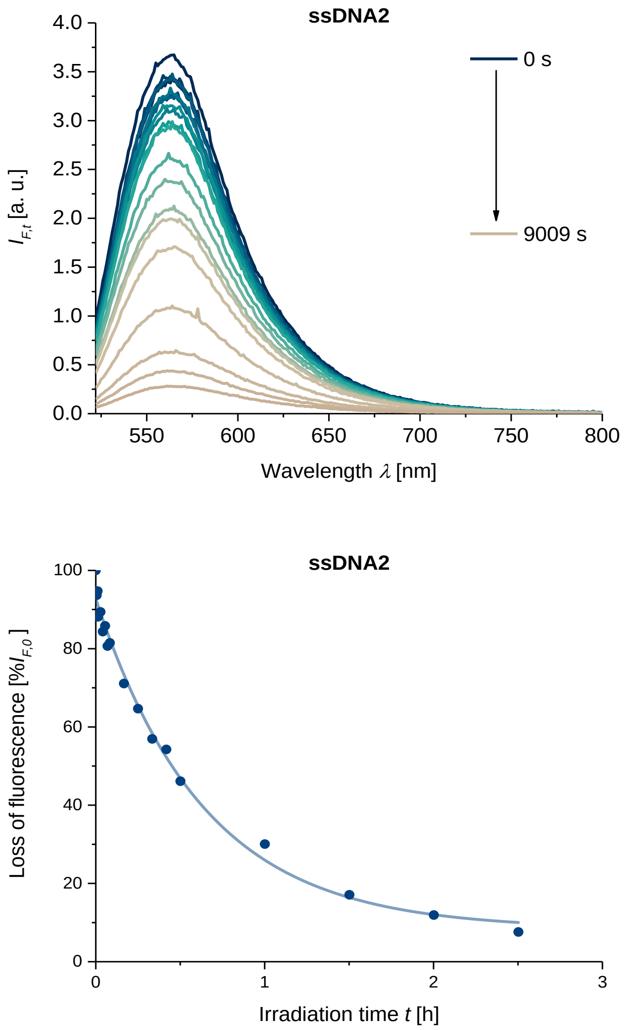
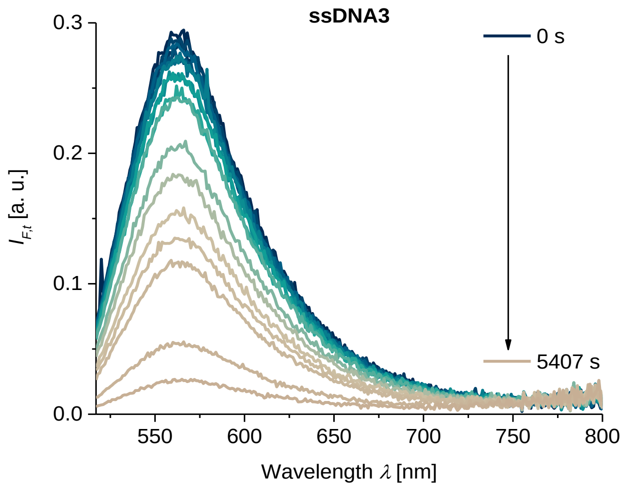


Figure S42. Emission spectra of ss**DNA2** during irradiation with a 468 nm LED (top) and photobleaching (bottom).

Table S12. Fit parameters for the photobleaching of **DNA2**.

Model	ExpDec1
Equation	y = A1*exp(-x/t1) + y0
y0	0.08316 ± 0.02368
A1	0.84443 ± 0.02357
t1	2300.99417 ± 178.66944
Reduced Chi-Sqr	0.00085
R-Square(COD)	0.99146
Adj. R-Square	0.99045

ssDNA3:



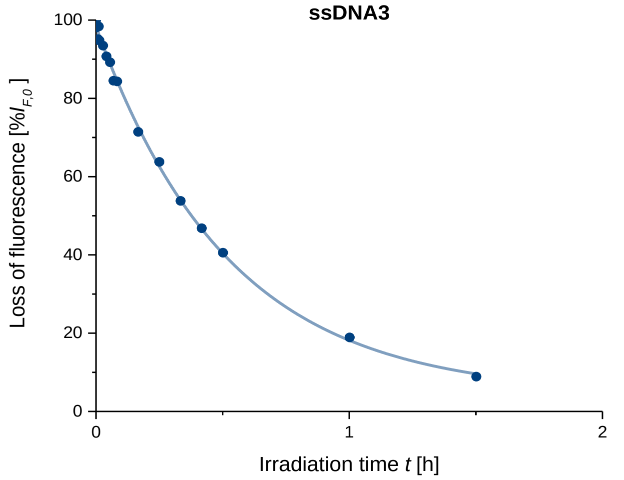


Figure S43. Emission spectra of ss**DNA3** during irradiation with a 468 nm LED (top) and photobleaching (bottom).

Table S13. Fit parameters for the photobleaching of **DNA3**.

Model	ExpDec1
Equation	y = A1*exp(-x/t1) + y0
y0	0.04246 ± 0.01541
A1	0.94107 ± 0.01492
t1	1883.4316 ± 68.18575
Reduced Chi-Sqr	1.43E-4
R-Square(COD)	0.99848
Adj. R-Square	0.99827

ssDNA4:

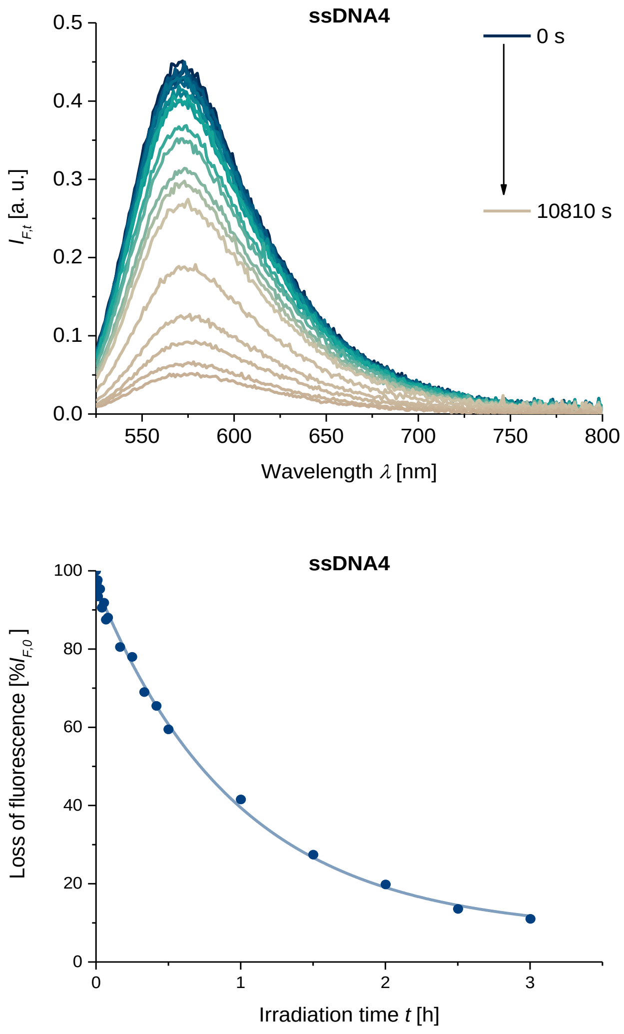


Figure S44. Emission spectra of ss**DNA4** during irradiation with a 468 nm LED (top) and photobleaching (bottom).

Table S14. Fit parameters for the photobleaching of **DNA4**.

Model	ExpDec1
Equation	y = A1*exp(-x/t1) + y0
y0	0.0763 ± 0.01801
A1	0.88693 ± 0.0173
t1	3513.11211 ± 187.68752
Reduced Chi-Sqr	3.15E+01
R-Square(COD)	0.99693
Adj. R-Square	0.99659

ssDNA5:

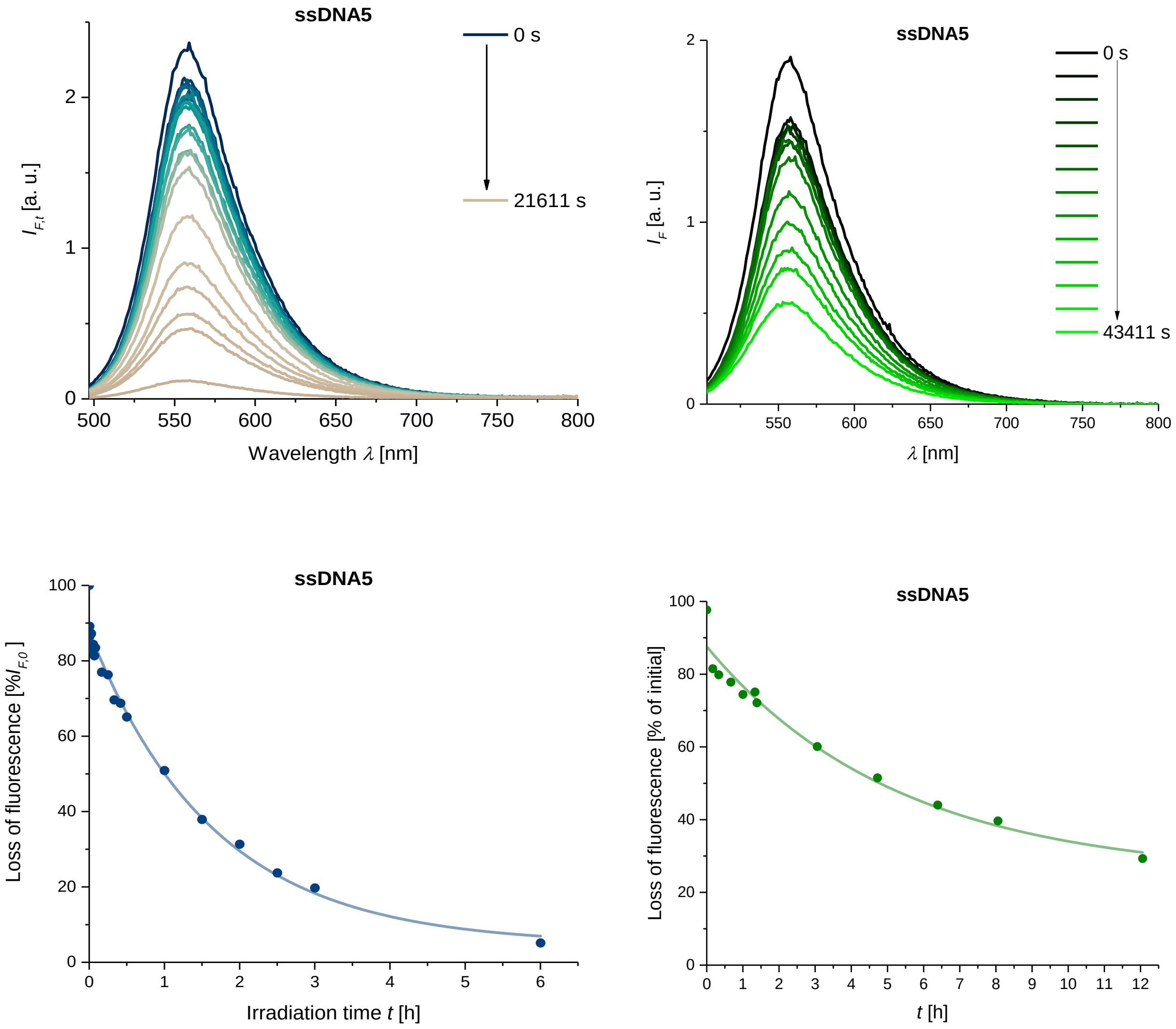
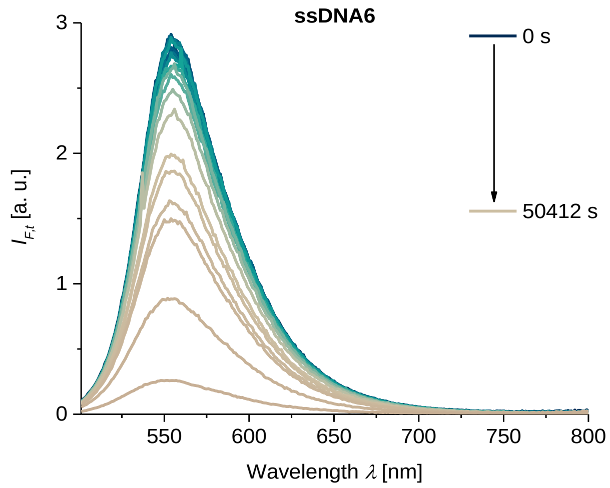


Figure S45. Emission spectra of ss**DNA5** during irradiation with a 468 nm LED (top left) / 520 nm LED (top right) and photobleaching curves of the corresponding irradiation experiment (bottom; left: 468 nm, right: 520 nm).

Table S15. Fit parameters for the photobleaching of **DNA5** with the 468nm (left) and 520 nm LED (right).

Model	ExpDec1	ExpDec1
Equation	y = A1*exp(-x/t1) + y0	y = A1*exp(-x/t1) + y0
y0	0.04703 ± 0.03706	24.56979 ± 7.76237
A1	0.8301 ± 0.03618	63.01303 ± 7.10235
t1	5970.3772 ± 620.60935	18989.99688 ± 5217.05724
Reduced Chi-Sqr	0.00111	17.12687
R-Square(COD)	0.98601	0.96593
Adj. R-Square	0.98454	0.95836

ssDNA6:



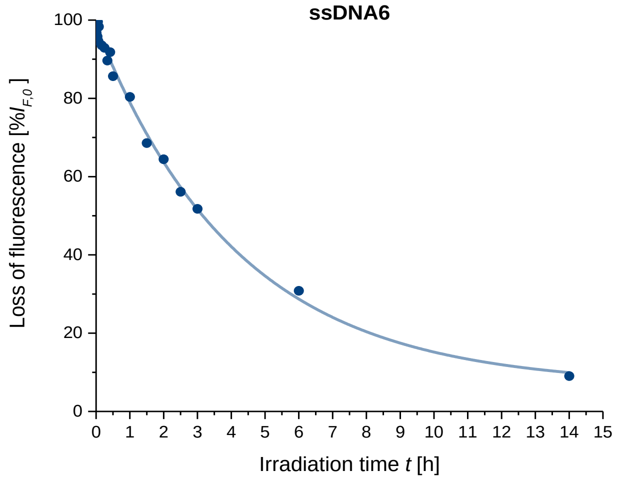


Figure S46. Emission spectra of ss**DNA6** during irradiation with a 468 nm LED (top) and photobleaching (bottom).

Table S16. Fit parameters for the photobleaching of **DNA6**.

Model	ExpDec1
Equation	y = A1*exp(-x/t1) + y0
y0	0.06596 ± 0.02203
A1	0.91749 ± 0.02178
t1	15181.6269 ± 769.96682
Reduced Chi-Sqr	3.22E+01
R-Square(COD)	0.99515
Adj. R-Square	0.99467

ssDNA7:

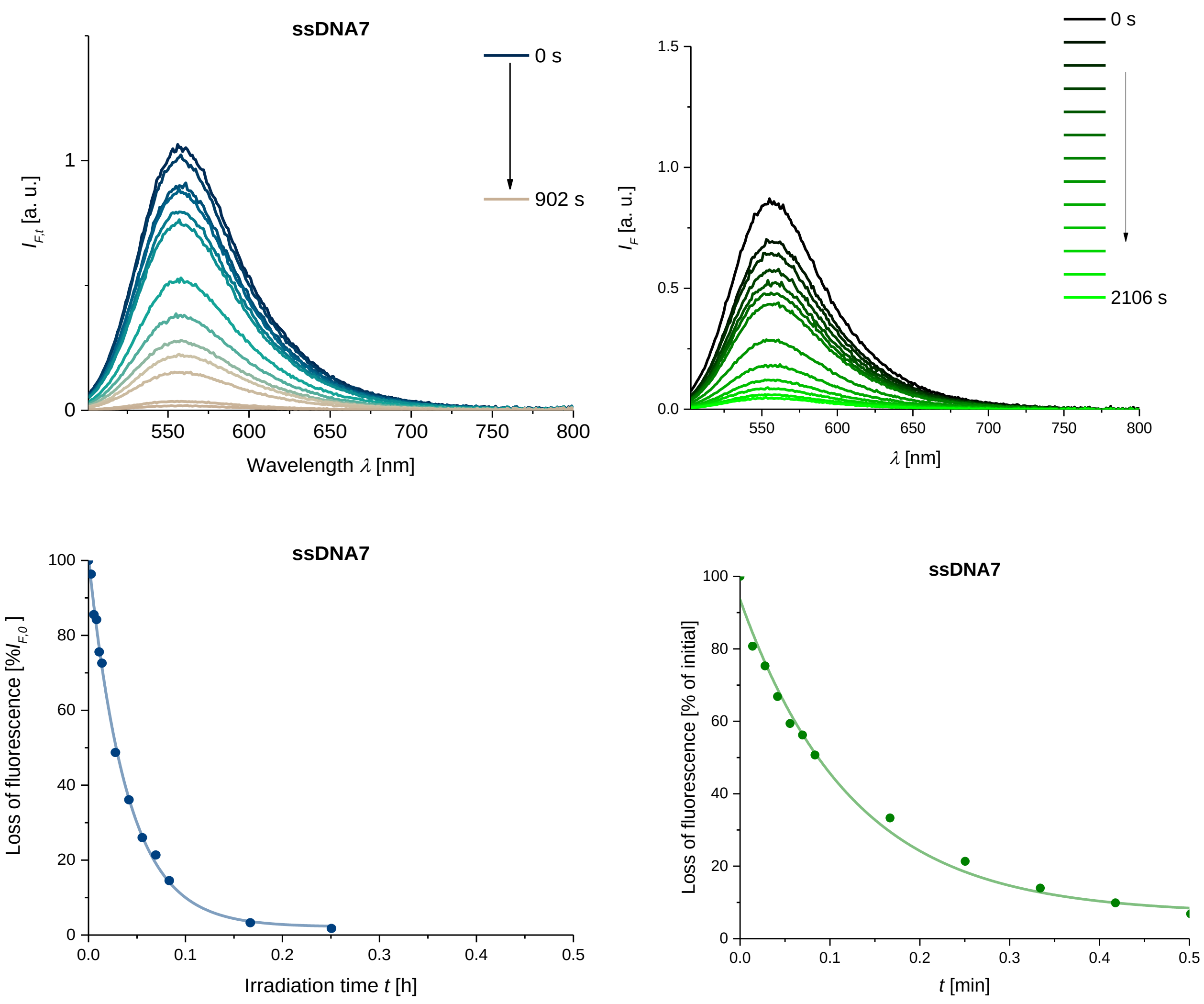
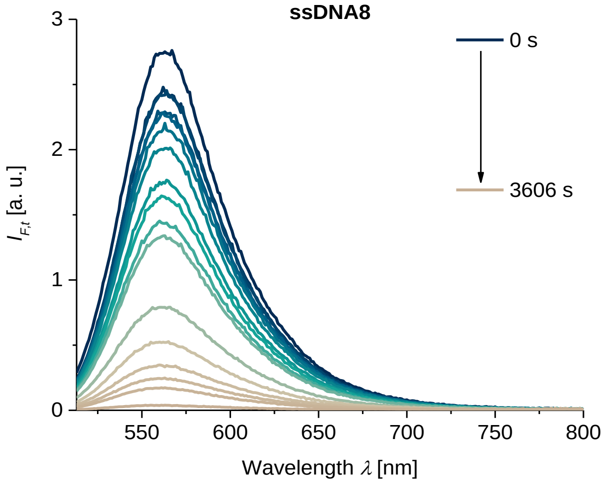


Figure S47. Emission spectra of ss**DNA7** during irradiation with a 468 nm LED (top left) / 520 nm LED (top right) and photobleaching curves of the corresponding irradiation experiment (bottom; left: 468 nm, right: 520 nm).

Table S17. Fit parameters for the photobleaching of **DNA7** with the 468nm (left) and 520 nm LED (right).

Model	ExpDec1	ExpDec1
Equation	y = A1*exp(-x/t1) + y0	y = A1*exp(-x/t1) + y0
y0	0.02179 ± 0.01226	6.87416 ± 2.04612
A1	0.98667 ± 0.01386	86.72925 ± 2.53324
t1	141.96676 ± 5.55527	447.3989981 ± 39.89981
Reduced Chi-Sqr	2.89E+01	10.13899
R-Square(COD)	0.99815	0.99154
Adj. R-Square	0.99777	0.98985

ssDNA8:



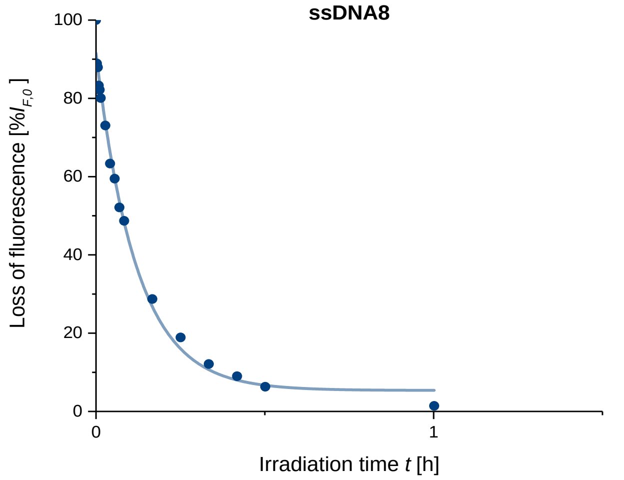
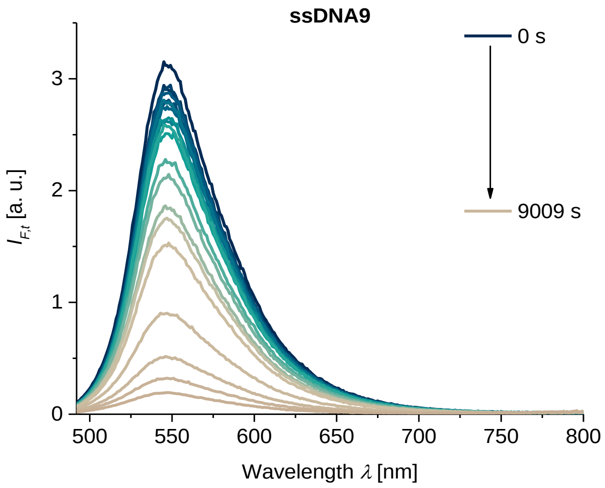


Figure S48. Emission spectra of ss**DNA8** during irradiation with a 468 nm LED (top) and photobleaching (bottom).

Table S18. Fit parameters for the photobleaching of **DNA8**.

Model	ExpDec1
Equation	y = A1*exp(-x/t1) + y0
y0	0.05349 ± 0.01792
A1	0.86198 ± 0.02003
t1	431.43873 ± 31.44897
Reduced Chi-Sqr	9.13E+01
R-Square(COD)	0.99289
Adj. R-Square	0.99188

ssDNA9:



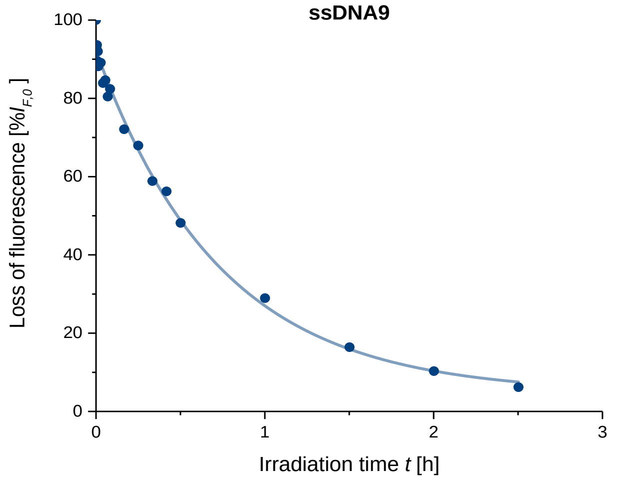
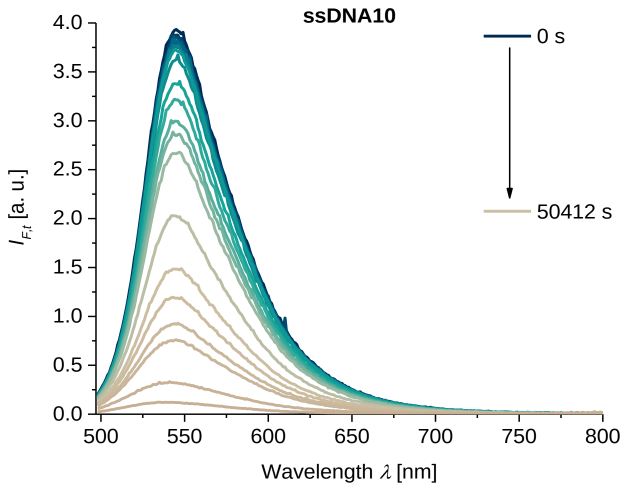


Figure S49. Emission spectra of ss**DNA9** during irradiation with a 468 nm LED (top) and photobleaching (bottom).

Table S19. Fit parameters for the photobleaching of **DNA9**.

Model	ExpDec1
Equation	y = A1*exp(-x/t1) + y0
y0	0.04629 ± 0.02513
A1	0.87549 ± 0.0245
t1	2637.70232 ± 200.12188
Reduced Chi-Sqr	7.25E+01
R-Square(COD)	0.99277
Adj. R-Square	0.99192

ssDNA10:



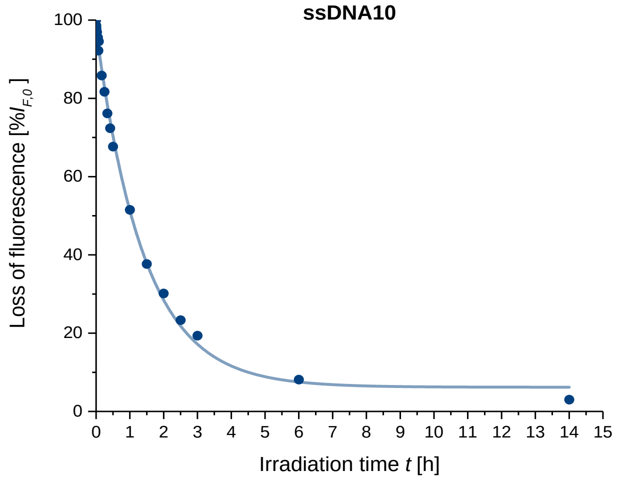
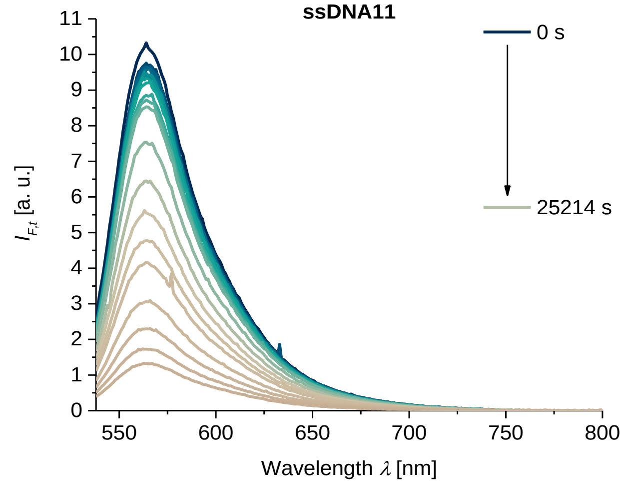


Figure S50. Emission spectra of ss**DNA10** during irradiation with a 468 nm LED (top) and photobleaching (bottom).

Table S20. Fit parameters for the photobleaching of **DNA10**.

Model	ExpDec1
Equation	y = A1*exp(-x/t1) + y0
y0	0.06172 ± 0.01216
A1	0.91388 ± 0.01244
t1	5104.4804 ± 191.59491
Reduced Chi-Sqr	3.04E+01
R-Square(COD)	0.99748
Adj. R-Square	0.99723

ssDNA11:



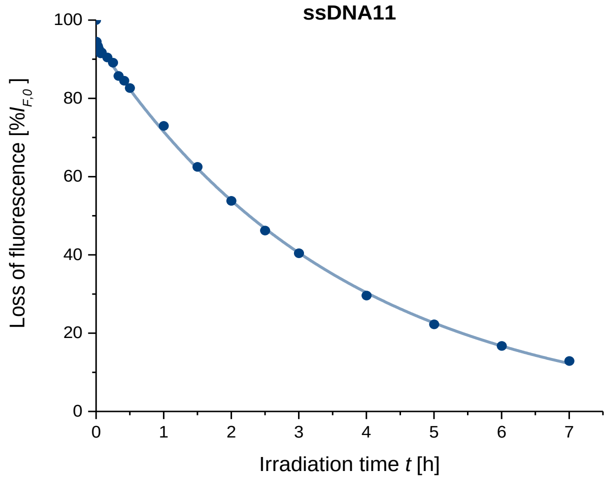


Figure S51. Emission spectra of ss**DNA11** during irradiation with a 468 nm LED (top) and photobleaching (bottom).

Table S21. Fit parameters for the photobleaching of **DNA11**.

Model	ExpDec1
Equation	y = A1*exp(-x/t1) + y0
y0	-0.02015 ± 0.02634
A1	0.96636 ± 0.02549
t1	13166.33283 ± 701.83799
Reduced Chi-Sqr	1.89E+01
R-Square(COD)	0.99784
Adj. R-Square	0.99764

ssDNA12:

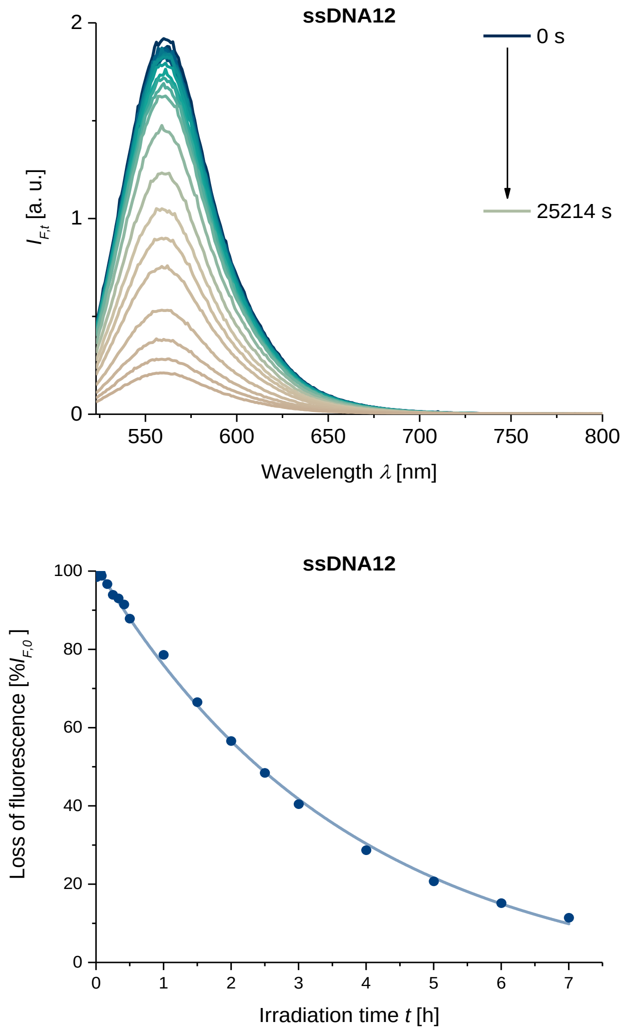


Figure S52. Emission spectra of ss**DNA12** during irradiation with a 468 nm LED (top) and photobleaching (bottom).

Table S22. Fit parameters for the photobleaching of **DNA12**.

Model	ExpDec1
Equation	y = A1*exp(-x/t1) + y0
y0	-0.06756 ± 0.02484
A1	1.08158 ± 0.02405
t1	13458.89786 ± 597.81922
Reduced Chi-Sqr	1.56E+01
R-Square(COD)	0.99854
Adj. R-Square	0.99841

10. Nucleophilicity-Dependent Photostability of ssDNAs

To identify the nucleophilicity-dependence, the measured photobleaching half-life times $t_{1/2}$ were plotted against the calculated nucleophilicity parameter N_{calc}:

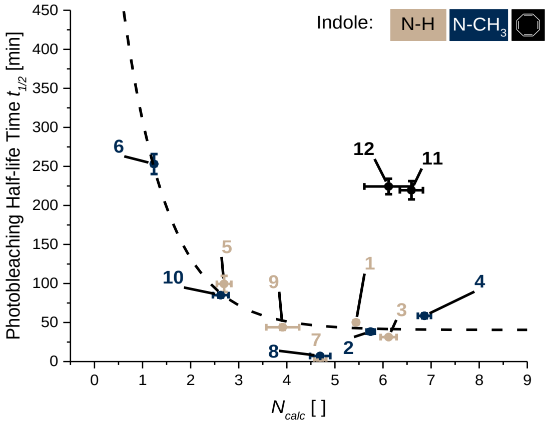


Figure S53. Unreferenced nucleophilicity-dependent photobleaching half-life times of ss**DNA1**-**12**.

Table S23. Fit parameters for the not-referenced nucleophilicity-dependent photobleaching of **DNA1**-**12**.

y0		A1		t1		Statistics	**Statistics**
Value	Standard Error	Value	Standard Error	Value	Standard Error	Reduced Chi-Sqr	**Adj. R-Square**
2432.68726	323.65276	47004.18422	35746.14391	0.93326	0.34028	35.65825	**0.61125**

The bromo-subsituted dyes on ss**DNA7** and ss**DNA8** as well as the COT-conjugates on ss**DNA11** and ss**DNA12** show a strikingly different behavior. **DNA7** and **DNA8** bleach much faster as expected due to the heavy atom effect of the bromo-substitutents and ss**DNA11** and ss**DNA12** bleach slower due to quenched triplet states. The other dye-DNA conjugates (ss**DNA1**-ss**DNA6** and ss**DNA9**-ss**DNA10**) follow the exponential function – although the statistics are not so good.

Taking into account that the dyes do not absorb not the same amount of excitation light, the spectral overlap between the respective absorbances of the single-stranded DNAs and the excitation light source (LED with λ_{exc} = 468 nm) was calculated and all half-life times $t_{1/2}$ were referenced on them.

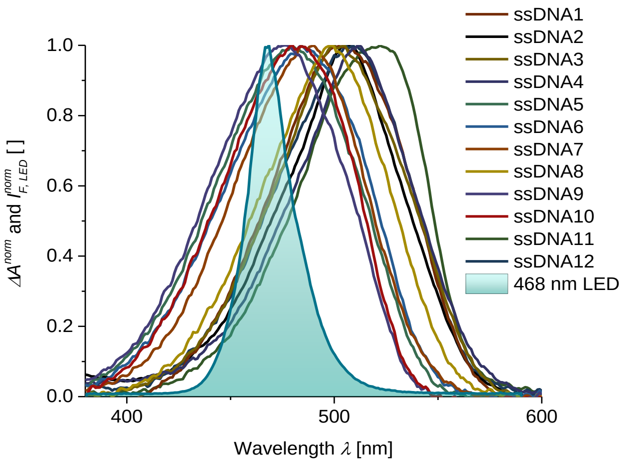


Figure S54. Normalized absorbances of ss**DNA1**-**12** and emission spectra of the 468 nm LED.

The spectral overlap of the appropriate dye absorbances and LED emission are calculated by using following equation:

$$J = \int_{380nm}^{600nm} \varepsilon \cdot \lambda^4 \cdot I_{F,LED}^{norm}\, d\lambda$$

where ε is the absorbance spectra divided by the DNA concentration (2.5 µM) and the diameter of the cuvette (1 cm), and the LED emission spectra is normalized that its integral between 380 nm and 600 nm is 1.

Then the appropriate spectral overlap J was multiplied with the photobleaching half-life time $t_{1/2}$ and divided by 10^{15}:

$$t_{1/2}^{ref} = \int_{380nm}^{600nm} \varepsilon \cdot \lambda^4 \cdot I_{F,LED}^{norm}\, d\lambda \cdot \frac{1}{10^{15} \cdot \mathrm{M}^{-1} \cdot \mathrm{cm}^{-1} \cdot \mathrm{nm}^4} \cdot t_{1/2} = \frac{J}{10^{15}} \cdot t_{1/2}$$

Table S24. Spectral overlap *J* of **DNA1**-**12** and the 468 nm LED, photobleaching ($t_{1/2}$) and referenced photobleaching half-life times ($t_{1/2}^{ref}$).

ssDNA	*J* [$M^{-1}cm^{-1}nm^4$]	$t_{1/2}$ [s]	$\Delta t_{1/2}$ [s]	$t_{1/2}^{ref}$ [s]	$\Delta t_{1/2}^{ref}$ [s]
1	1.35E+15	3011	60	4050	80
2	1.64E+15	2301	179	3781	294
3	1.47E+15	1883	68	2771	100
4	1.32E+15	3513	188	4622	247
5	1.63E+15	5970	621	9720	1010
6	1.44E+15	15182	770	21819	1107
7	1.73E+15	142	5.56	246	9.63
8	1.23E+15	431	31.4	533	38.8
9	1.64E+15	2638	200	4334	329
10	1.52E+15	5104	192	7763	291
11	1.24E+15	13166	702	16360	872
12	1.32E+15	13459	598	17745	788

Plotting the referenced photobleaching half-life times $t_{1/2}^{ref}$ against the calculated nucleophilicity parameter N_{calc} resulted in a far better exponential dependence:

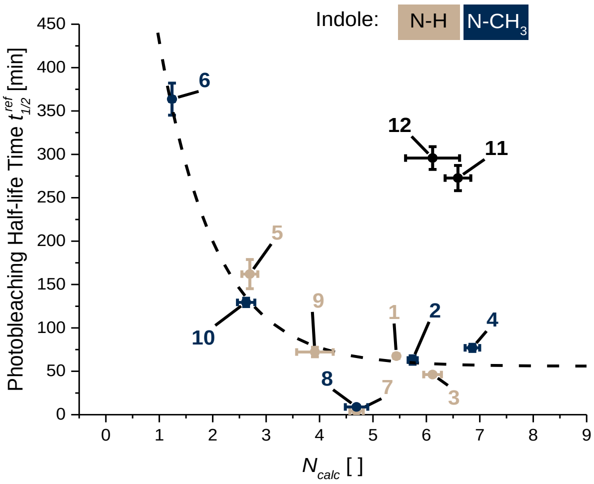


Figure S55. Referenced nucleophilicity-dependent photobleaching half-life times of ss**DNA1**-**12**.

Table S25. Fit parameters for the referenced nucleophilicity-dependent photobleaching of **DNA1**-**12**.

y0		A1		t1		Statistics	**Statistics**
Value	Standard Error	Value	Standard Error	Value	Standard Error	Reduced Chi-Sqr	**Adj. R-Square**
3348.54019	430.20283	58205.95473	33415.66984	1.04946	0.31902	21.58239	**0.75289**

11. Thermal Bleaching Experiments

For thermal bleaching experiments a solution containing:

16 µL 500 µM solution of the respective dye in ethanol (100%)
16 µL 50 mM sodium molybdate
80 µL 100 mM NaP_i (pH 9)
and 672 µl *Millipore* water

was equilibrated for 15 min at 20°C in a closed cuvette.

Afterwards 16 µL 2.5 M hydrogen peroxide was added and the closed cuvette was shaken. One minute after addition, the time-dependent acquisition of absorbance spectra was started. The appropriate absorbance in the absorption maxima was then plotted against the time. Since there is a background reaction with hydrogen peroxide, the same experiment was performed, in which sodium molybdate was substituted by *Millipore* water.

From both, molybdate-catalyzed reaction (Thermal Bleaching Product 1 and 2; TBP1 and TBP2) and reaction with hydrogen peroxide (Thermal Bleaching Product 2; TBP 2), the rate constants were determined. The rate constant for the singlet oxygen reactivity was then determined by subtraction of the hydrogen peroxide background rate constant. In addition, a control experiment with sodium molybdate solely was performed to exclude a second side reaction. Therefore, hydrogen peroxide was substituted by *Millipore* water.

Singlet oxygen reaction:

$$\text{Dye} + {}^1O_2 \rightarrow \text{TBP1}$$

with the parallel reaction

$$\text{Dye} + H_2O_2 \rightarrow \text{TBP2}$$

$$\frac{d[A]}{dt} = k_{TBP1}[A] + k_{TBP2}[A] \Rightarrow \ln\left(\frac{[A]_0}{[A]}\right) = (k_{TBP1} + k_{TBP2})t$$

$$\frac{d}{dt}\left[\ln\left(\frac{[A]_0}{[A]}\right)\right] = k_{TBP1} + k_{TBP2} \Rightarrow k_{TBP1} = \frac{d}{dt}\left[\ln\left(\frac{[A]_0}{[A]}\right)\right] - k_{TBP2}$$

Hydrogen peroxide reaction: $\text{Dye} + H_2O_2 \rightarrow \text{TBP2}$

$$\frac{d[A]}{dt} = k_{TBP2}[A] \Rightarrow k_{TBP2} = \frac{d}{dt}\left[\ln\left(\frac{[A]_0}{[A]}\right)\right]$$

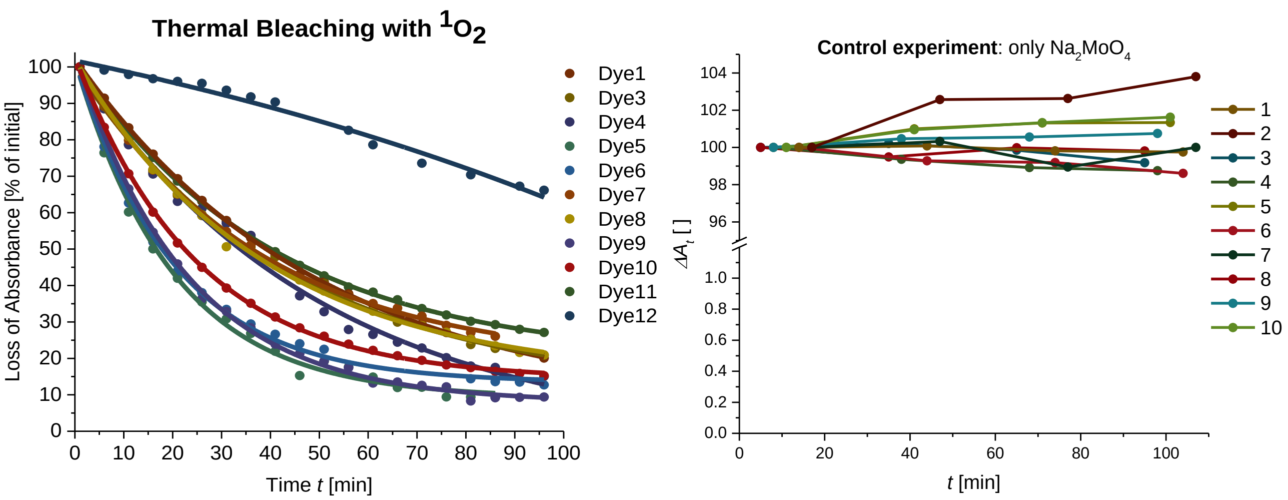


Figure S56. Thermal bleaching curves of dye **1**-**12** and the control experiment with sodium molybdate.

Dye1:

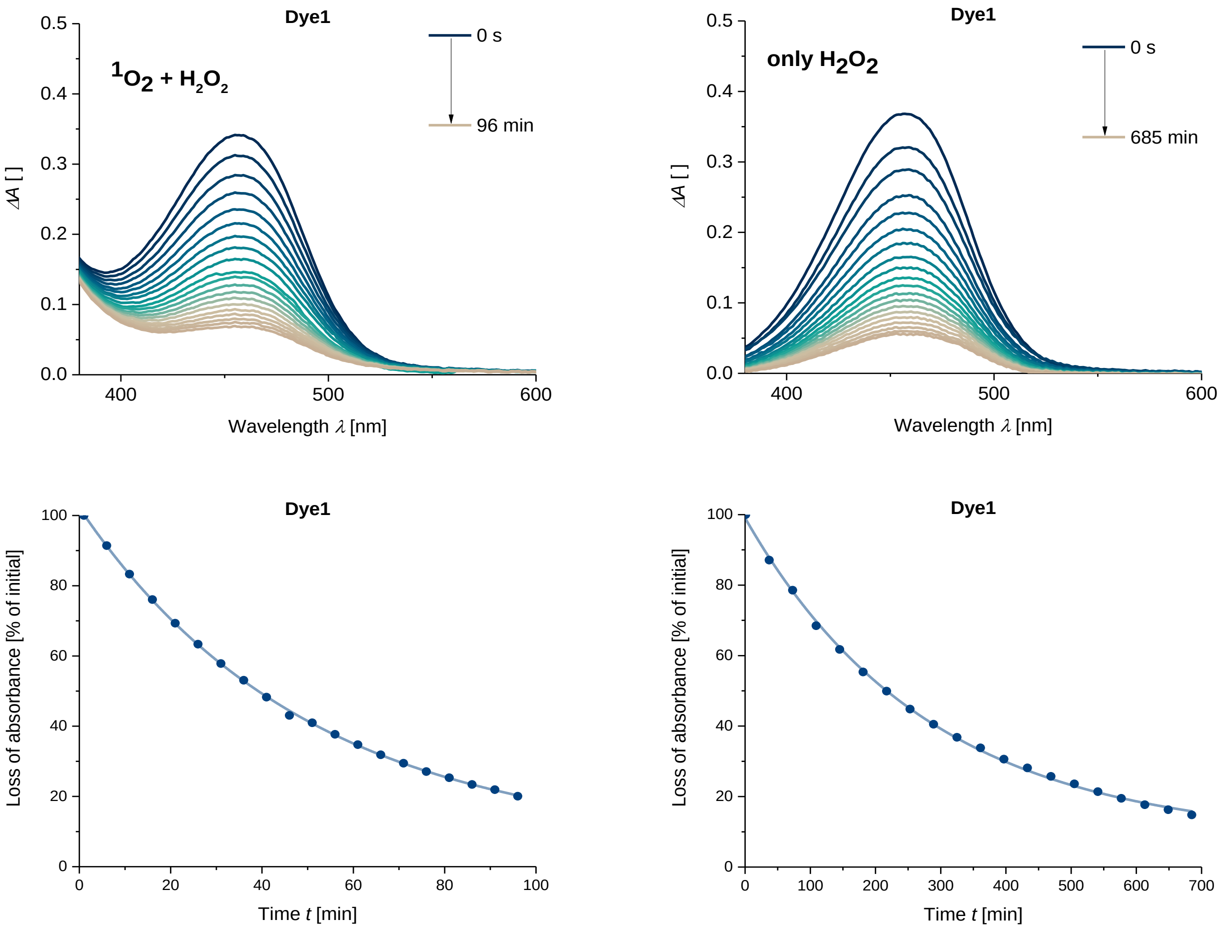


Figure S57. Time course of the thermal Bleaching of dye **1** with $^1O_2$ (left), H_2O_2 (right) and the corresponding bleaching curve (bottom).

Table S26. Fit parameters for the uncorrected thermal bleaching of dye **1** with $^1O_2$ (top) and H_2O_2 (bottom).

$^1O_2$	Equation	y = A1*exp(-x/t1) + y0							
+	y0		A1		t1		**k**		Statistics
H_2O_2	Value	Standard Error	Value	Standard Error	Value	Standard Error	**Value**	**Standard Error**	Adj. R-Square
Dye1	6.32788	0.61437	95.86688	0.51775	49.81723	0.73532	**0.02007**	**2.96E-04**	0.99977

only	Equation	y = A1*exp(-x/t1) + y0							
H_2O_2	y0		A1		t1		**k**		Statistics
	Value	Standard Error	Value	Standard Error	Value	Standard Error	**Value**	**Standard Error**	Adj. R-Square
Dye1	7.81881	0.75995	91.24161	0.68987	281.3672	6.29746	**0.00355**	**7.95E-05**	0.99923

***k*= 2.75E-04 ± 6.26E-06 s^{-1}**

$t_{1/2}$= 2518 ± 57 s

Dye2:

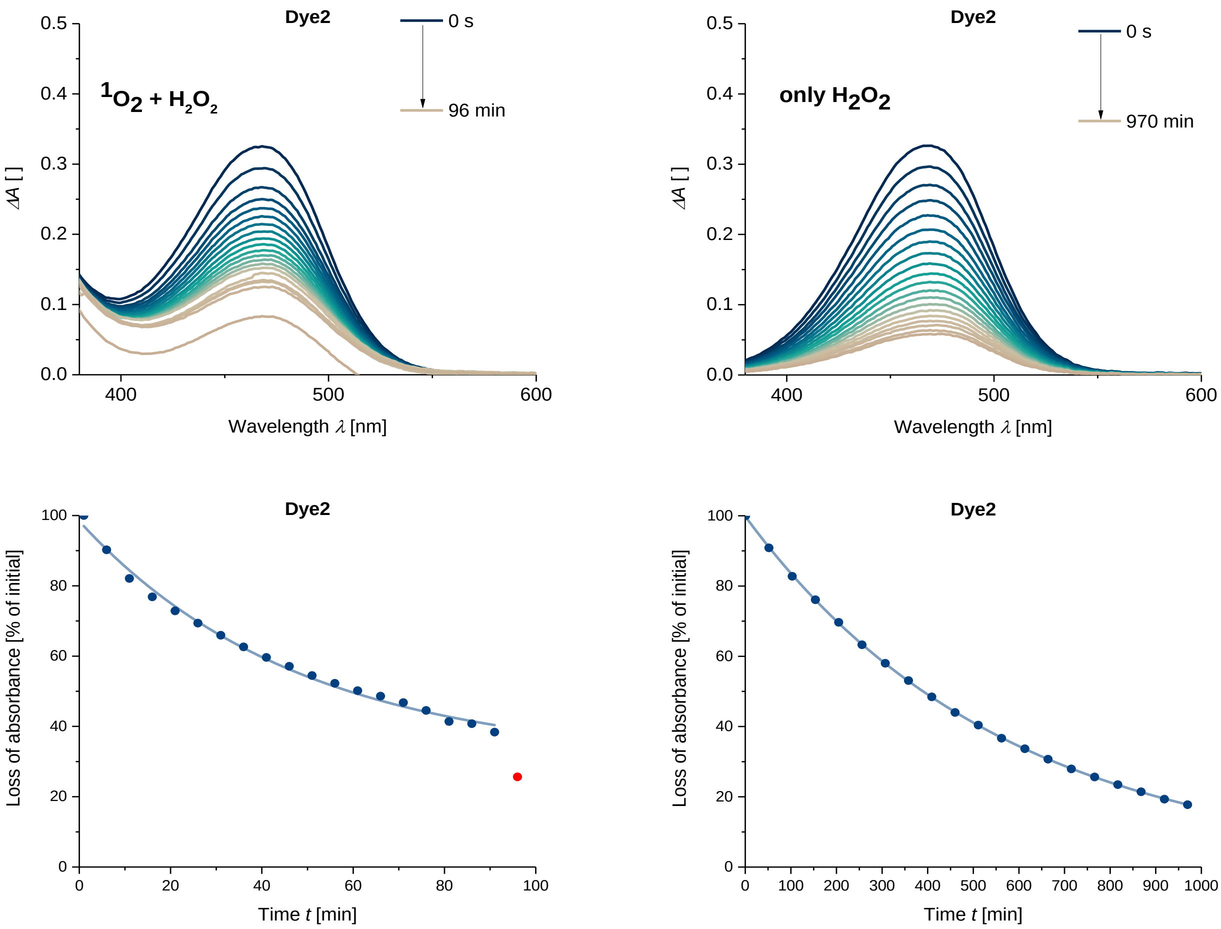


Figure S58. Time course of the thermal Bleaching of dye **2** with $^1O_2$ (left), H_2O_2 (right) and the corresponding bleaching curve (bottom).

Table S27. Fit parameters for the uncorrected thermal bleaching of dye **2** with $^1O_2$ (top) and H_2O_2 (bottom).

$^1O_2$	Equation	y = A1*exp(-x/t1) + y0							
+	y0		A1		t1		**k**		Statistics
H_2O_2	Value	Standard Error	Value	Standard Error	Value	Standard Error	**Value**	**Standard Error**	Adj. R-Square
Dye2	30.2476	2.49638	68.16408	2.10649	47.72132	3.997	**0.02095**	**0.00176**	0.99315

only	Equation	y = A1*exp(-x/t1) + y0							
H_2O_2	y0		A1		t1		**k**		Statistics
	Value	Standard Error	Value	Standard Error	Value	Standard Error	**Value**	**Standard Error**	Adj. R-Square
Dye2	-0.29931	0.3649	100.1519	0.31523	566.21253	4.35049	**0.00177**	**1.357E-05**	0.99995

k= 3.20E-04 ± 2.96E-05 s^{-1}

$t_{1/2}$= 2168 ± 201 s

Dye3:

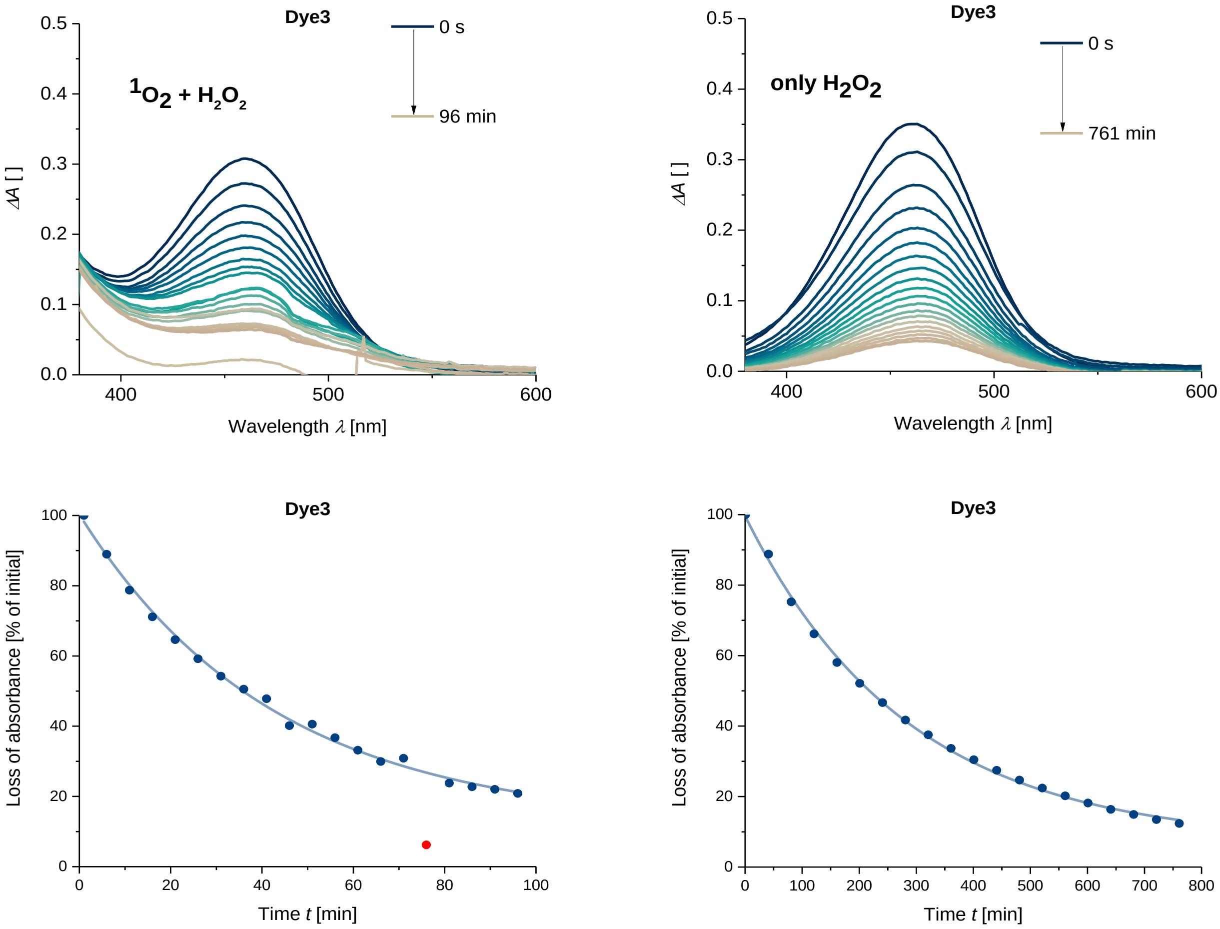


Figure S59. Time course of the thermal Bleaching of dye **3** with $^1O_2$ (left), H_2O_2 (right) and the corresponding bleaching curve (bottom).

Table S28. Fit parameters for the uncorrected thermal bleaching of dye **3** with $^1O_2$ (top) and H_2O_2 (bottom).

$^1O_2$	Equation	y = A1*exp(-x/t1) + y0							
+	y0		A1		t1		**k**		Statistics
H_2O_2	Value	Standard Error	Value	Standard Error	Value	Standard Error	**Value**	**Standard Error**	Adj. R-Square
Dye3	12.05196	1.79326	88.25758	1.5587	42.41596	2.19364	**0.02358**	**0.00122**	0.99646

only	Equation	y = A1*exp(-x/t1) + y0							
H_2O_2	y0		A1		t1		**k**		Statistics
	Value	Standard Error	Value	Standard Error	Value	Standard Error	**Value**	**Standard Error**	Adj. R-Square
Dye3	6.91935	0.87229	92.69969	0.84088	284.54058	7.71798	**0.00351**	**9.53E-05**	0.9987

***k*= 3.35E-04 ± 2.19E-05 s^{-1}**

$t_{1/2}$= 2072 ± 136 s

Dye4:

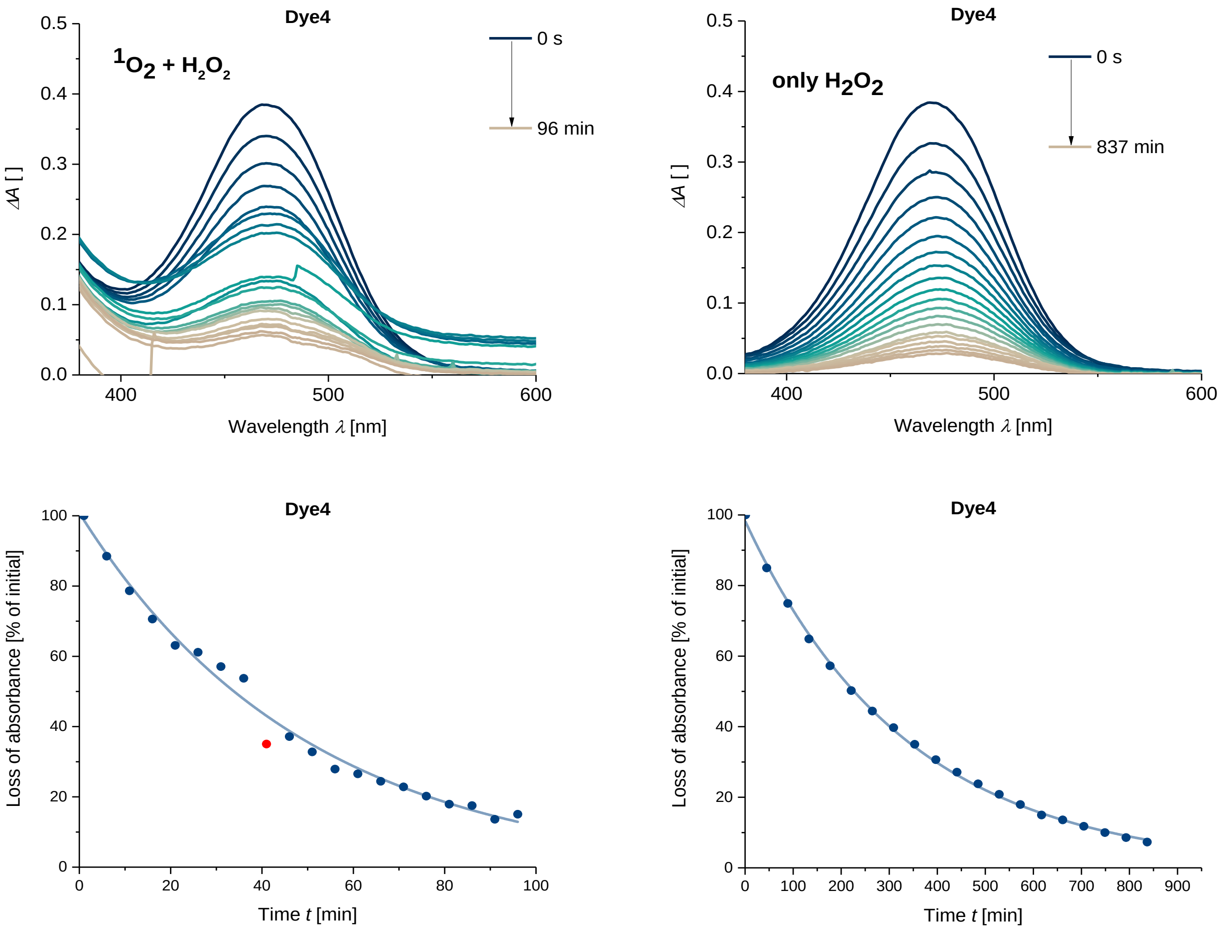


Figure S60. Time course of the thermal Bleaching of dye **4** with $^1O_2$ (left), H_2O_2 (right) and the corresponding bleaching curve (bottom).

Table S29. Fit parameters for the uncorrected thermal bleaching of dye **4** with $^1O_2$ (top) and H_2O_2 (bottom).

$^1O_2$	Equation	y = A1*exp(-x/t1) + y0							
+	y0		A1		t1		**k**		Statistics
H_2O_2	Value	Standard Error	Value	Standard Error	Value	Standard Error	**Value**	**Standard Error**	Adj. R-Square
Dye4	-2.01467	4.19889	102.81758	3.52143	49.699	4.73115	**0.02012**	**0.00192**	0.99162

only	Equation	y = A1*exp(-x/t1) + y0							
H_2O_2	y0		A1		t1		**k**		Statistics
	Value	Standard Error	Value	Standard Error	Value	Standard Error	**Value**	**Standard Error**	Adj. R-Square
Dye4	-0.29534	0.8716	98.63788	0.8007	336.5802	8.11525	**0.00297**	**7.16E-05**	0.99908

***k*= 2.86E-04 ± 3.32E-05 s^{-1}**

$t_{1/2}$= 2425 ± 282 s

Dye5:

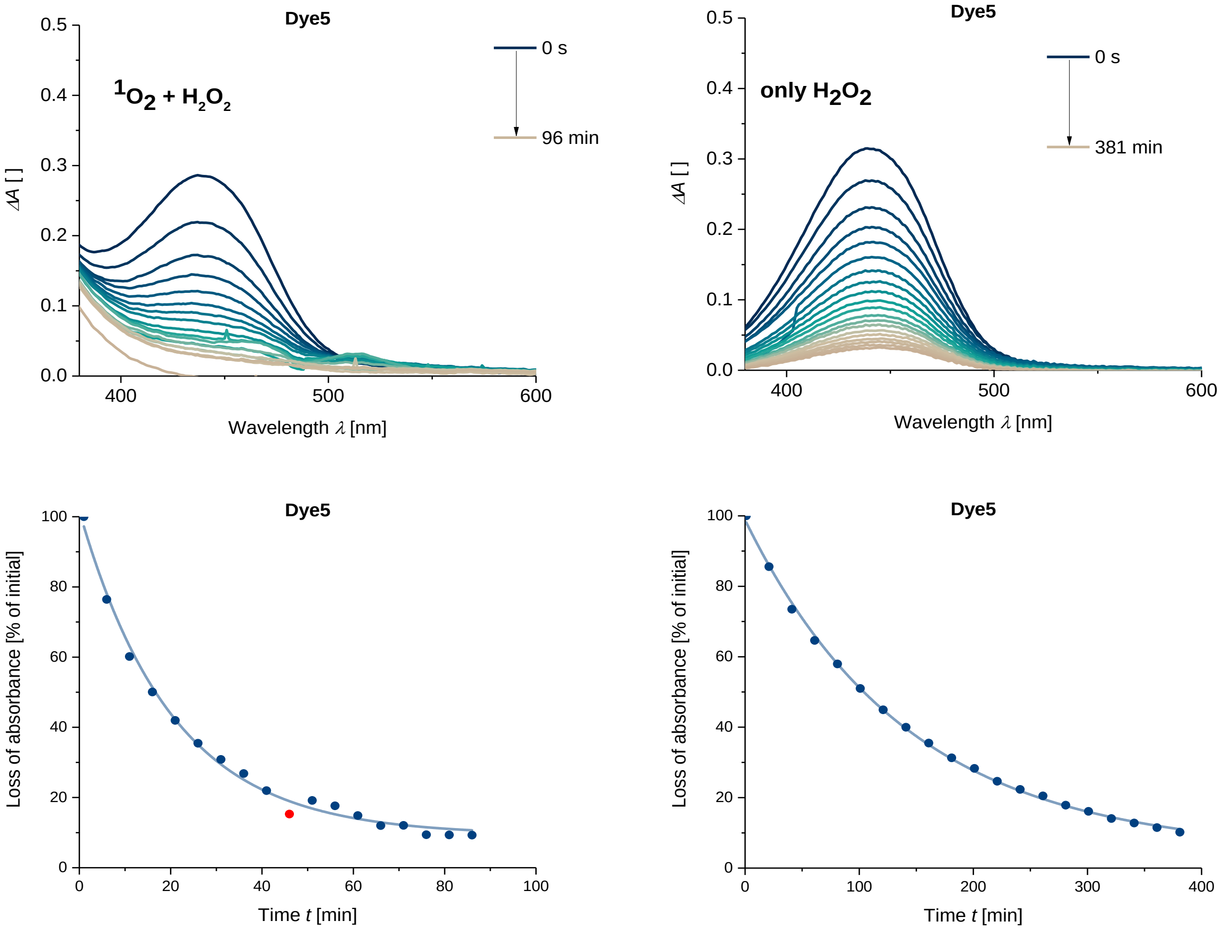


Figure S61. Time course of the thermal Bleaching of dye **5** with $^1O_2$ (left), H_2O_2 (right) and the corresponding bleaching curve (bottom).

Table S30. Fit parameters for the uncorrected thermal bleaching of dye **5** with $^1O_2$ (top) and H_2O_2 (bottom).

$^1O_2$	Equation	y = A1*exp(-x/t1) + y0							
+	y0		A1		t1		**k**		Statistics
H_2O_2	Value	Standard Error	Value	Standard Error	Value	Standard Error	**Value**	**Standard Error**	Adj. R-Square
Dye5	9.29211	0.9888	92.34466	1.68323	20.37088	0.91678	**0.04909**	**0.00221**	0.99495

only	Equation	y = A1*exp(-x/t1) + y0							
H_2O_2	y0		A1		t1		**k**		Statistics
	Value	Standard Error	Value	Standard Error	Value	Standard Error	**Value**	**Standard Error**	Adj. R-Square
Dye5	4.49113	0.77801	94.3365	0.74786	142.65217	3.39626	**0.00701**	**1.67E-04**	0.999

***k*= 7.01E-04 ± 3.96E-05 s^{-1}**

***t*$_{1/2}$= 988 ± 56 s**

Dye6:

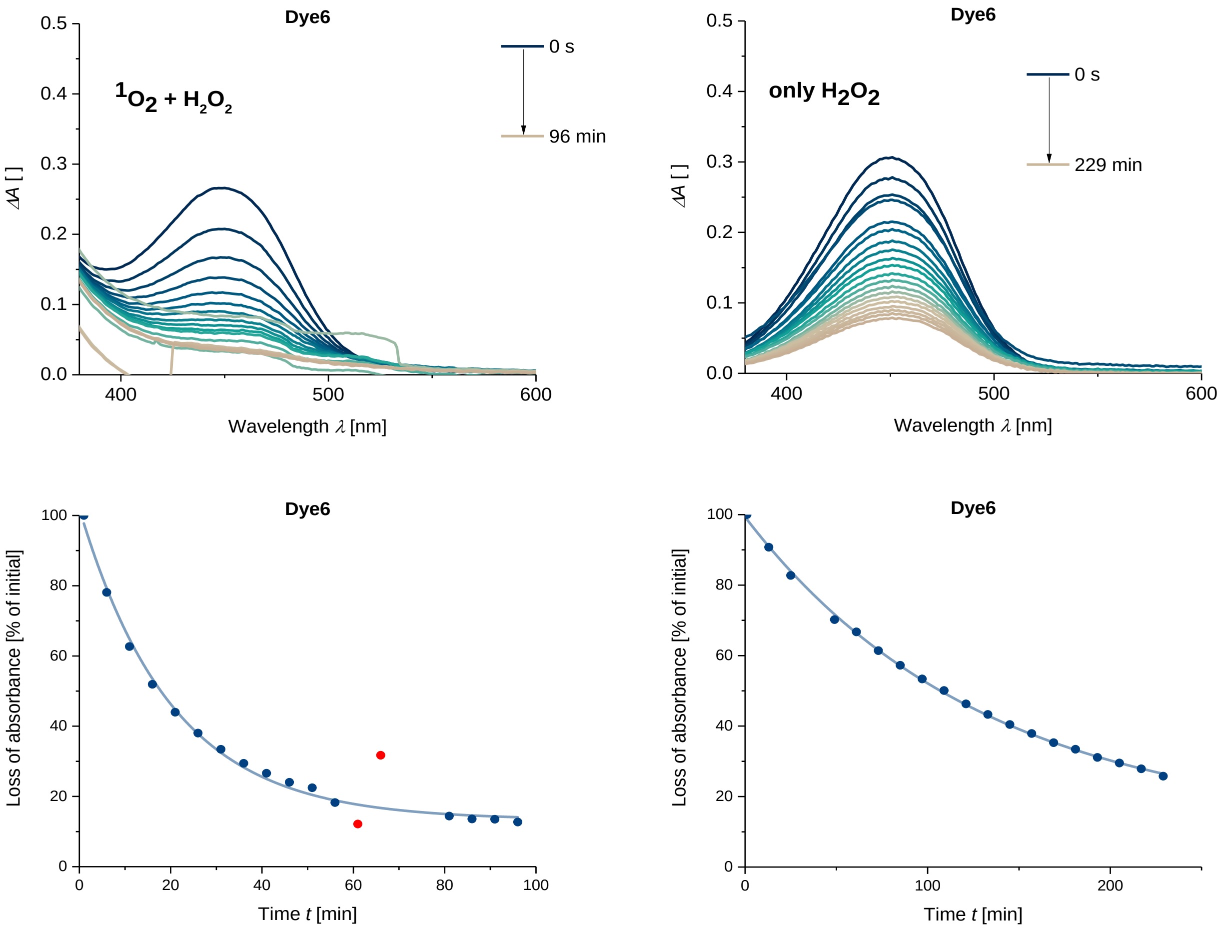


Figure S62. Time course of the thermal Bleaching of dye **6** with $^1O_2$ (left), H_2O_2 (right) and the corresponding bleaching curve (bottom).

Table S31. Fit parameters for the uncorrected thermal bleaching of dye **6** with $^1O_2$ (top) and H_2O_2 (bottom).

$^1O_2$	Equation	y = A1*exp(-x/t1) + y0							
+	y0		A1		t1		**k**		Statistics
H_2O_2	Value	Standard Error	Value	Standard Error	Value	Standard Error	**Value**	**Standard Error**	Adj. R-Square
Dye6	13.29931	0.804	88.71641	1.39715	20.22539	0.73757	**0.04944**	**0.0018**	0.99645

only	Equation	y = A1*exp(-x/t1) + y0							
H_2O_2	y0		A1		t1		**k**		Statistics
	Value	Standard Error	Value	Standard Error	Value	Standard Error	**Value**	**Standard Error**	Adj. R-Square
Dye6	11.29805	1.29813	88.01571	1.12943	130.20227	4.1231	**0.00768**	**2.43E-04**	0.99908

***k*= 6.96E-04 ± 3.41E-05 s^{-1}**

$t_{1/2}$= 996 ± 49 s

Dye7:

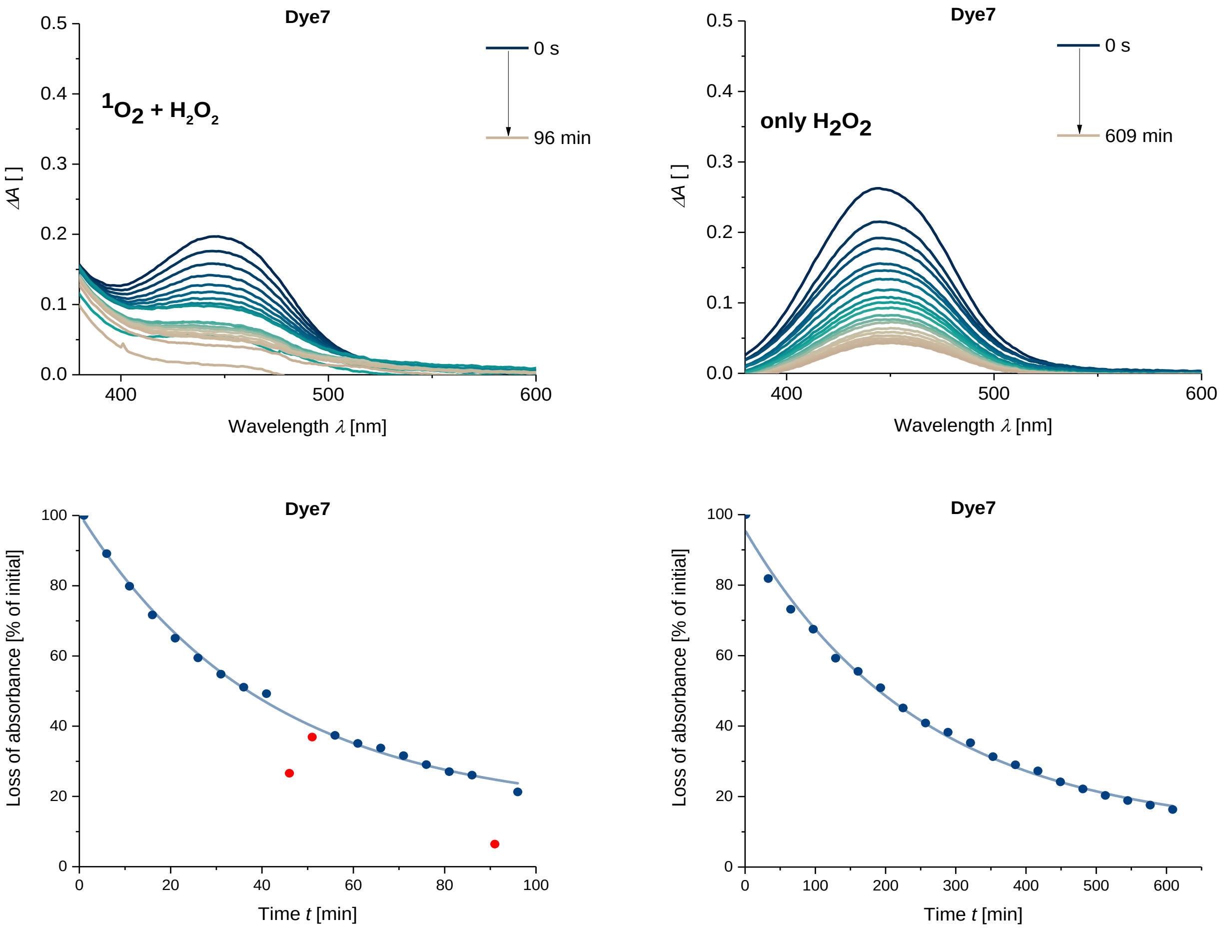


Figure S63. Time course of the thermal Bleaching of dye **7** with $^1O_2$ (left), H_2O_2 (right) and the corresponding bleaching curve (bottom).

Table S32. Fit parameters for the uncorrected thermal bleaching of dye **7** with $^1O_2$ (top) and H_2O_2 (bottom).

$^1O_2$	Equation	y = A1*exp(-x/t1) + y0							
+	y0		A1		t1		**k**		Statistics
H_2O_2	Value	Standard Error	Value	Standard Error	Value	Standard Error	**Value**	**Standard Error**	Adj. R-Square
Dye7	15.63243	1.6694	84.89177	1.43185	40.85394	2.11608	**0.02448**	**0.00127**	0.99707

only	Equation	y = A1*exp(-x/t1) + y0							
H_2O_2	y0		A1		t1		**k**		Statistics
	Value	Standard Error	Value	Standard Error	Value	Standard Error	**Value**	**Standard Error**	Adj. R-Square
Dye7	9.52566	2.01331	86.01119	1.81599	253.23417	15.78982	**0.00395**	**2.46E-04**	0.99415

***k*= 3.42E-04 ± 2.53E-05 s^{-1}**

$t_{1/2}$= 2026 ± 150 s

Dye8:

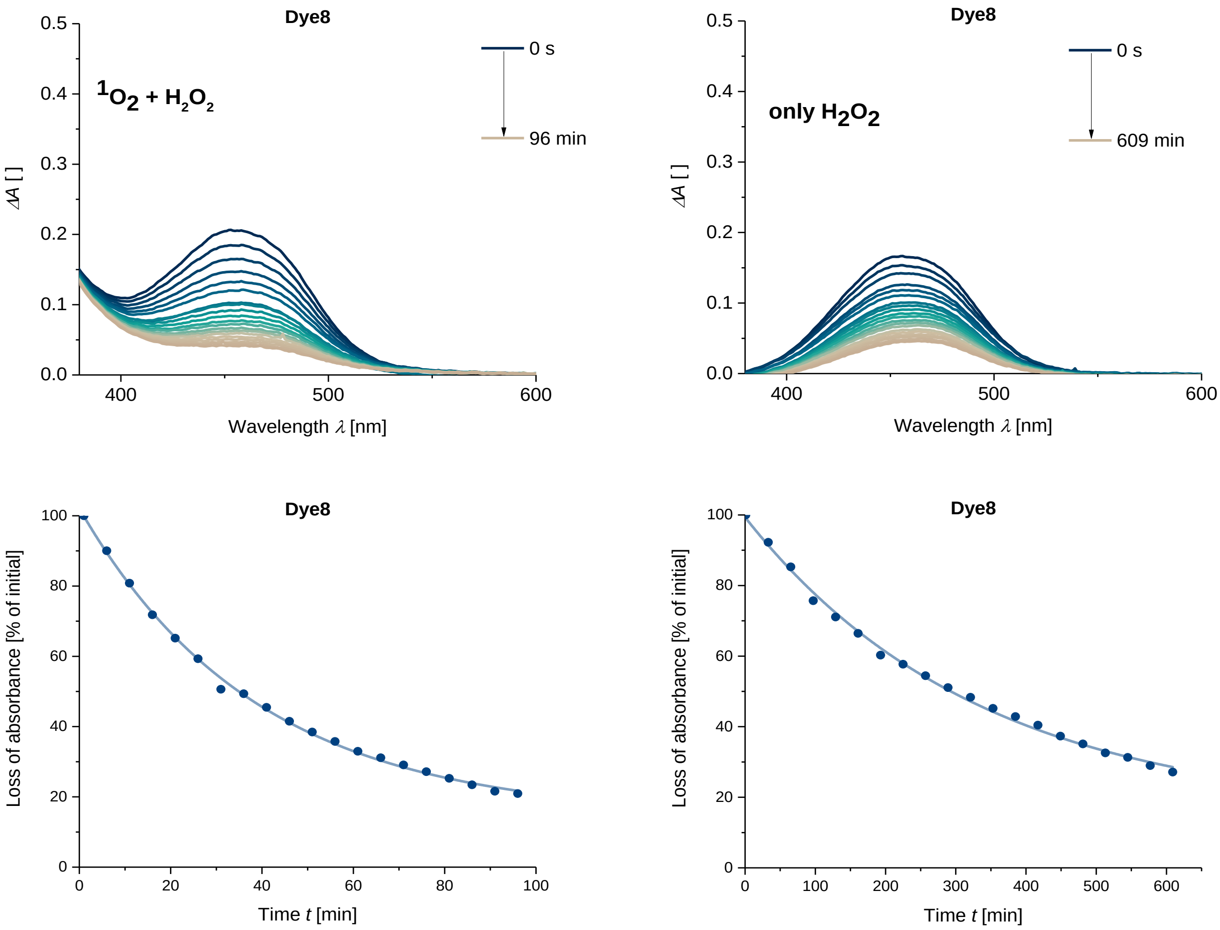


Figure S64. Time course of the thermal Bleaching of dye **8** with $^1O_2$ (left), H_2O_2 (right) and the corresponding bleaching curve (bottom).

Table S33. Fit parameters for the uncorrected thermal bleaching of dye **8** with $^1O_2$ (top) and H_2O_2 (bottom).

$^1O_2$	Equation	y = A1*exp(-x/t1) + y0							
+	y0		A1		t1		**k**		Statistics
H_2O_2	Value	Standard Error	Value	Standard Error	Value	Standard Error	**Value**	**Standard Error**	Adj. R-Square
Dye8	14.33047	1.0449	87.76358	0.94155	38.77407	1.27574	**0.02579**	**8.49E-04**	0.99831

only	Equation	y = A1*exp(-x/t1) + y0							
H_2O_2	y0		A1		t1		**k**		Statistics
	Value	Standard Error	Value	Standard Error	Value	Standard Error	**Value**	**Standard Error**	Adj. R-Square
Dye8	14.98252	2.09649	84.37199	1.80081	333.06456	18.20875	**0.003**	**1.64E-04**	0.99708

k= 3.80E-04 ± 1.69E-05 s^{-1}

$t_{1/2}$= 1825 ± 81 s

Dye9:

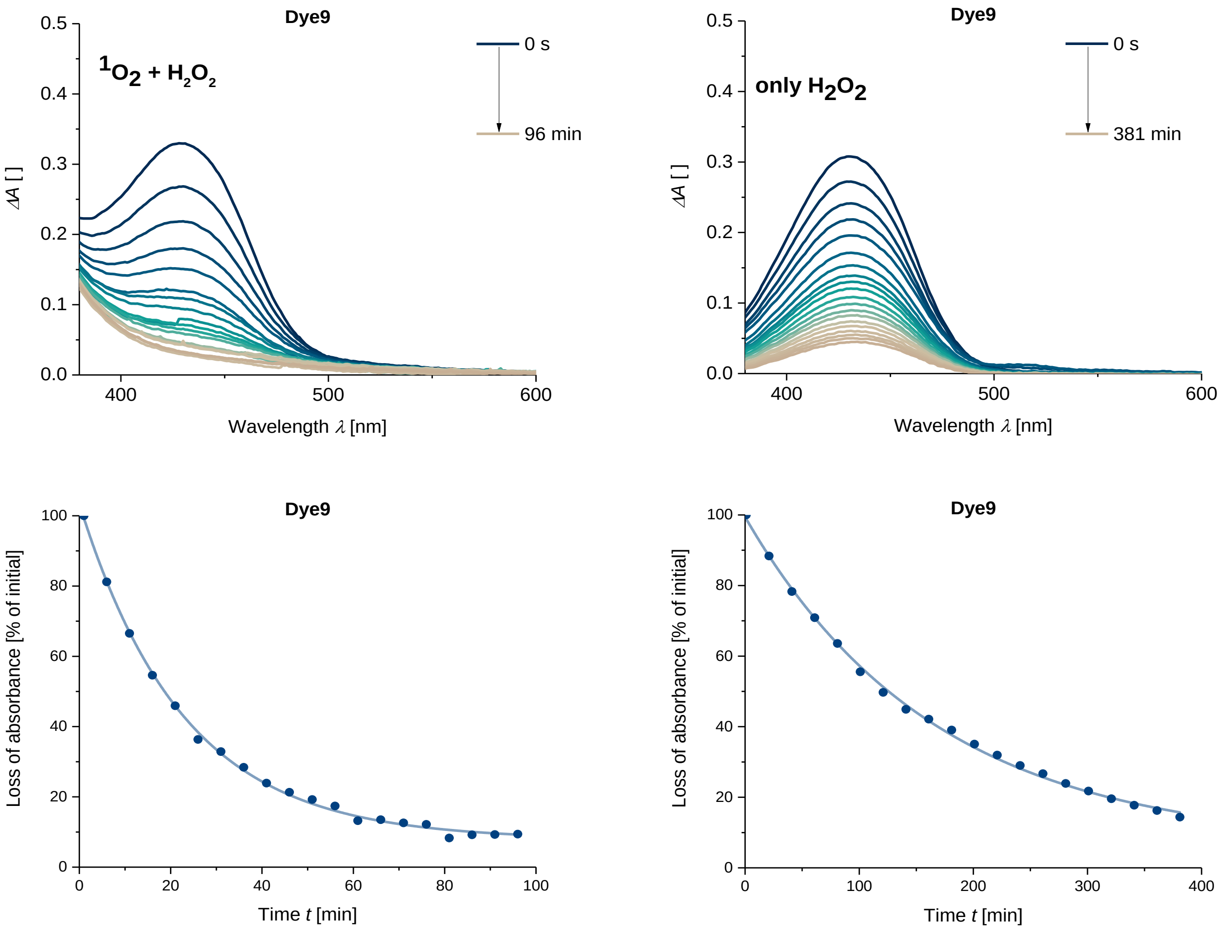


Figure S65. Time course of the thermal Bleaching of dye **9** with $^1O_2$ (left), H_2O_2 (right) and the corresponding bleaching curve (bottom).

Table S34. Fit parameters for the uncorrected thermal bleaching of dye **9** with $^1O_2$ (top) and H_2O_2 (bottom).

$^1O_2$	Equation	y = A1*exp(-x/t1) + y0							
+	y0		A1		t1		**k**		Statistics
H_2O_2	Value	Standard Error	Value	Standard Error	Value	Standard Error	**Value**	**Standard Error**	Adj. R-Square
Dye9	7.83268	0.53317	95.61779	0.90354	22.7861	0.53412	**0.04389**	**0.00103**	0.99838

only	Equation	y = A1*exp(-x/t1) + y0							
H_2O_2	y0		A1		t1		**k**		Statistics
	Value	Standard Error	Value	Standard Error	Value	Standard Error	**Value**	**Standard Error**	Adj. R-Square
Dye9	6.30706	1.20035	93.12539	1.05937	166.1168	5.51781	**0.00602**	**2.00E-04**	0.99845

k= 6.31E-04 ± 2.05E-05 s^{-1}

$t_{1/2}$= 1098 ± 36 s

Dye10:

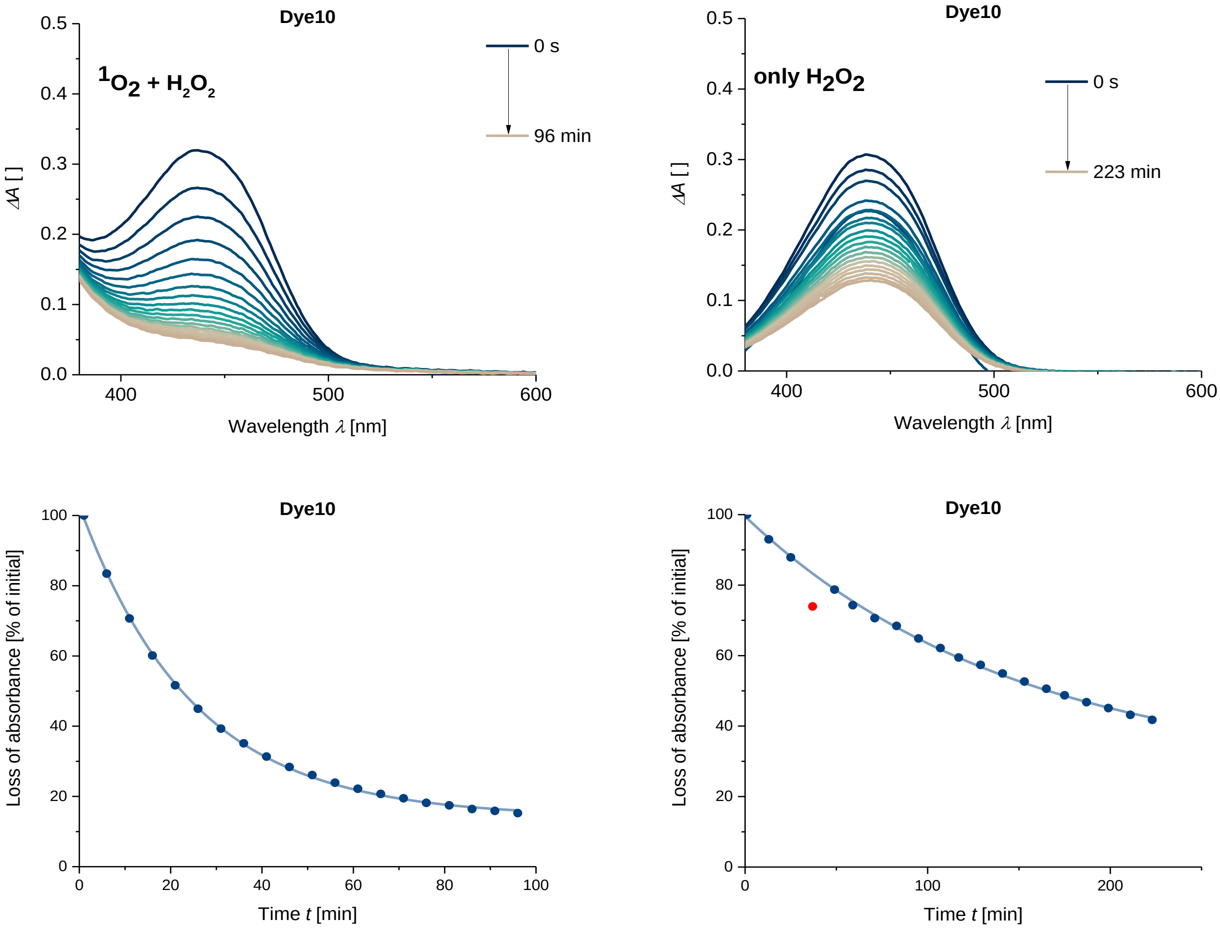


Figure S66. Time course of the thermal bleaching of dye **10** with $^1O_2$ (left), H_2O_2 (right) and the corresponding bleaching curve (bottom).

Table S35. Fit parameters for the uncorrected thermal bleaching of dye **10** with $^1O_2$ (top) and H_2O_2 (bottom).

$^1O_2$	Equation	y = A1*exp(-x/t1) + y0							
+	y0		A1		t1		**k**		Statistics
H_2O_2	Value	Standard Error	Value	Standard Error	Value	Standard Error	**Value**	**Standard Error**	Adj. R-Square
Dye10	14.15909	2.61E-01	88.6404	0.39374	24.76108	0.28751	**0.04039**	**4.69E-04**	0.99963

only	Equation	y = A1*exp(-x/t1) + y0							
H_2O_2	y0		A1		t1		**k**		Statistics
	Value	Standard Error	Value	Standard Error	Value	Standard Error	**Value**	**Standard Error**	Adj. R-Square
Dye10	25.88877	1.48E+00	73.6135	1.305	148.71092	5.8239	**0.00672**	**2.63E-04**	0.99892

k= 5.61E-04 ± 1.22E-05 s^{-1}

$t_{1/2}$= 1235 ± 27 s

Control Experiment with Rose Bengal:

To test the reactivity of the dyes towards singlet oxygen, a solution containing 2 µM rose bengal (RB) and 25 µM of the corresponding dye in ethanol was irradiated with a 620 nm LED.

For this experiment, the singlet oxygen trap 1,3-diphenylbenzoisofuran (DPBF) served as positive control:

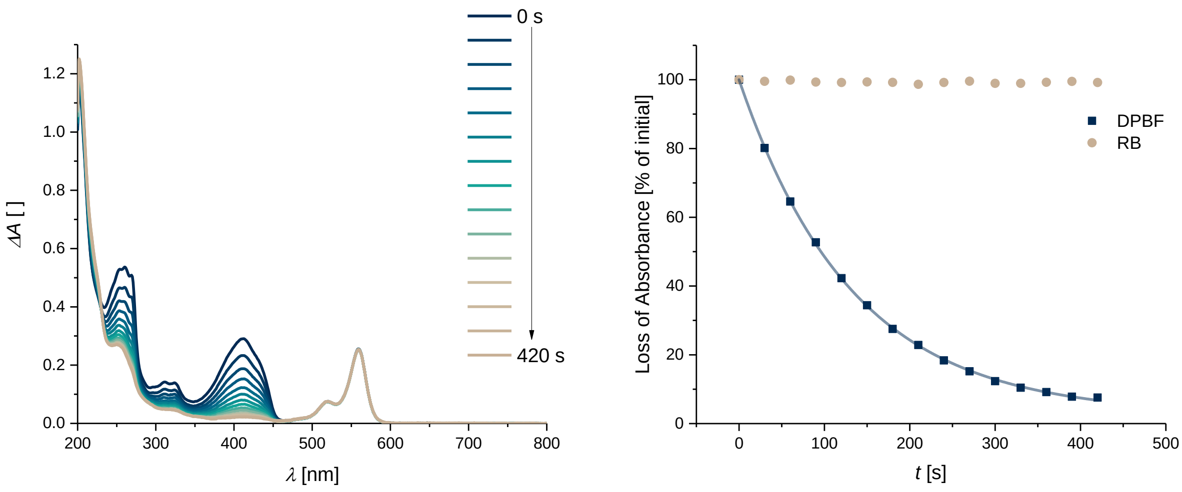


Figure S67. Time course of the thermal bleaching of dye **DPBF** with $^1O_2$ sensitized by RB (left) and the corresponding bleaching curve (right).

The dyes **3** and **5** were chosen as representatives (**3** shows a good stability in previous experiments and **5** not) for this control experiment:

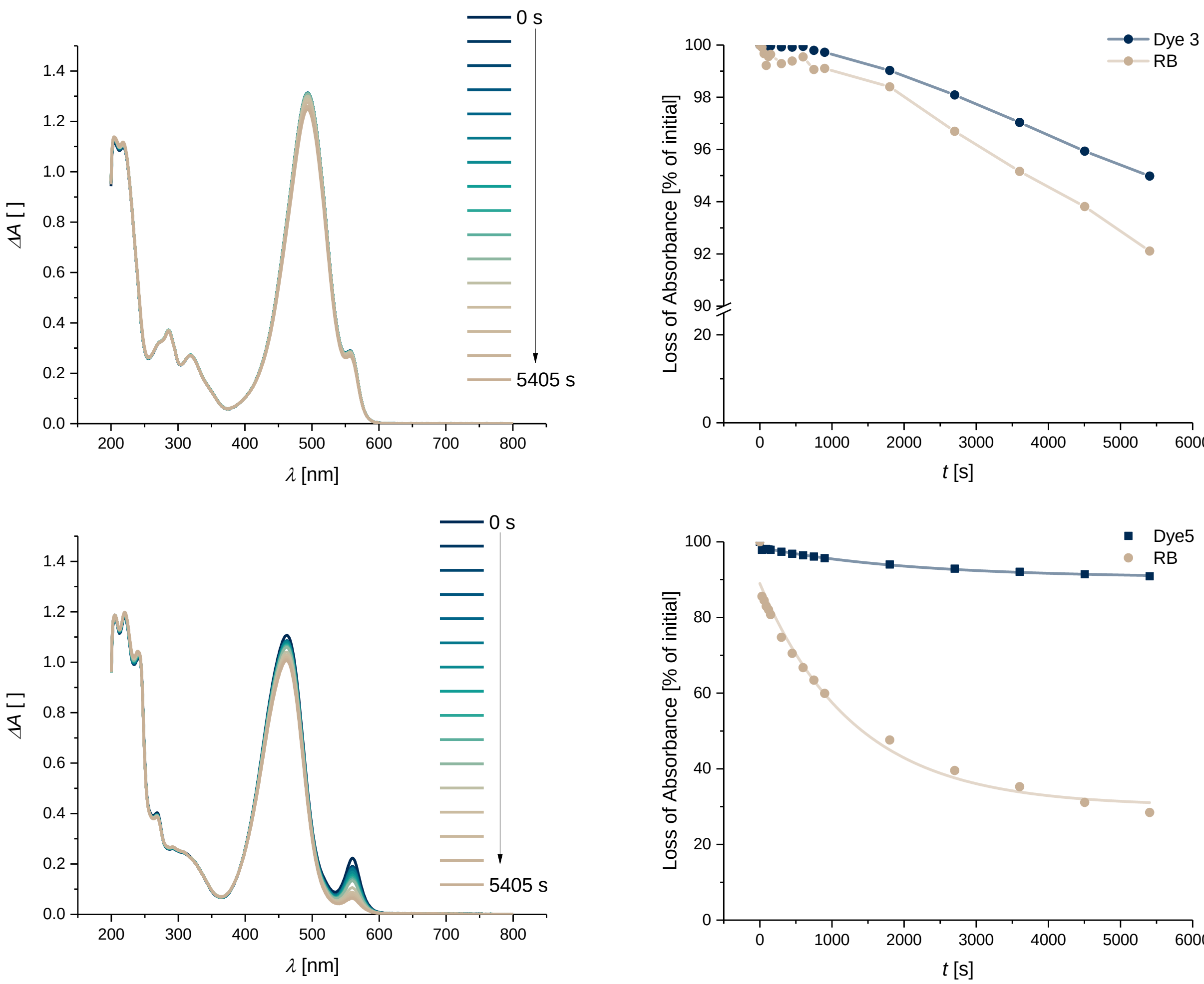


Figure S68. Time course of the thermal bleaching of dye **3** and **5** with $^1O_2$ sensitized by RB (left) and the corresponding bleaching curve (right).

These different bleaching profiles of RB are very likely due to electron transfer with RB as donor and dye **5** as acceptor and could be confirmed by emission spectroscopy.

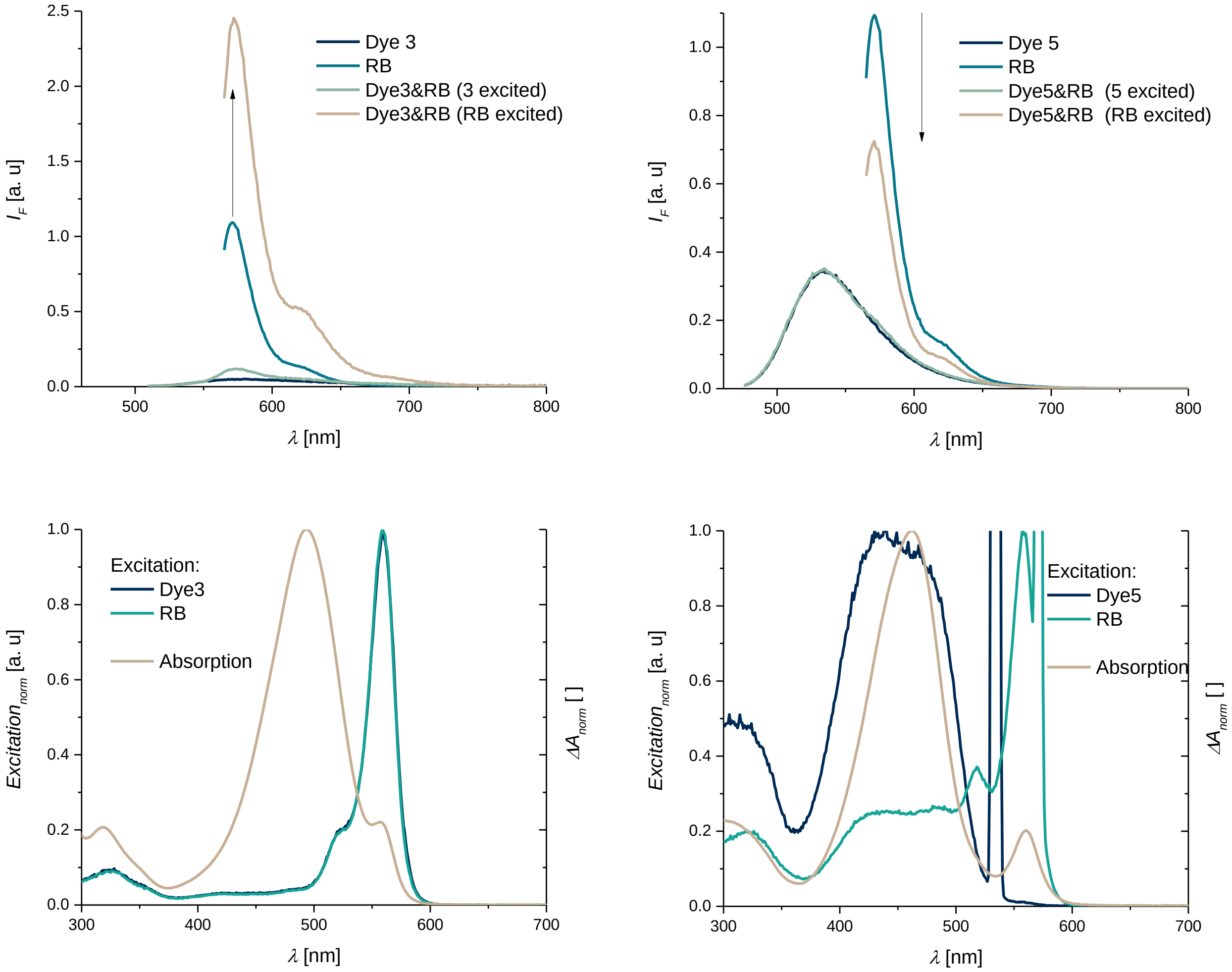


Figure S69. Emission and excitation spectra of dye **3**, **5** and in combination with RB.

Since the excitation spectra of the longer wavelength emission (RB) does not resemble the absorption spectra, a ground state interaction can be assumed, which leads to a loss of sensitizer control in this experiment. In case of dye **5**, both emissive entities emit at the same wavelength and therefore the excitation spectra show the same profile. Nevertheless, the excitation of RB shows an increased fluorescence which can be attributed partially to a crosstalk of **5**, but is higher than the summed up spectra and a interaction of **5** and **RB** cannot be excluded. Therefore, RB cannot function successfully as singlet oxygen sensitizer for thermal bleaching experiments of cationic cyanine styryl dyes, because excited state lifetimes of RB are influenced in a different extend by different dyes.

12. Nucleophilicity-Dependent Thermal Bleaching

The determined corrected half-life times $t_{1/2}$ from the singlet-oxygen thermal bleaching experiments (see Section 11) were plotted against the calculated nucleophilicity parameter N_{calc}.

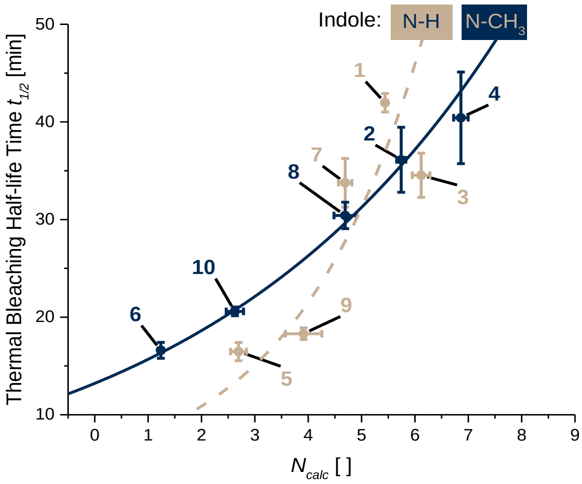


Figure S70. Corrected nucleophilicity-dependent thermal bleaching half-life times of dye **1**-**12**.

The nonlinear curve fit for the methylated dyes (blue curve, **2**, **4**, **6**, **8** and **10**) show a clear nucleophilicity dependence:

Table S36. Fit parameters for the corrected thermal bleaching of the methylated dyes **2**, **4**, **6**, **8**, and **10** with $^1O_2$.

y0		x0		A1		t1		Statistics	
Value	Standard Error	Value	Standard Error	Value	Standard Error	Value	Standard Error	Reduced Chi-Sqr	**Adj. R-Square**
20.3065	757.68421	0.45073	--	836.23622	--	5.71085	3.02058	0.92709	**0.96809**

The shown nonlinear curve fit (exponential growth) for the unmethylated dyes (beige curve, **1**, **3**, **5**, **7**, and **9**) did not converge and the parameter and statistics data is not shown, but altogether an exponential dependence can be assumed.

13. MTT-Assay

To elucidate the influence on metabolic activity of the dyes towards HeLa cells, the *CellTiter 96® Non-Radioactive Cell Proliferation Assay* (*Promega*) was deployed. This test is based on the intracellular colorchange caused by the reduction of a tetrazolium salt (yellow) into a formazan product (blue), which only takes place in metabolic active cells. At wavelengths between 630–750 nm the absorbance of the formazan product can be detected and used as a direct measure for the viability of the cells.

For the experimental setup a 96 well plate (*Cstar 3596*, 96 Well Cell Culture Cluster, sterile) was seeded with 1 x 104 HeLa cells/well in 100 µl Dulbecco's modified Eagle's medium (DMEM, high glucose, gibco) supplemented with 10% fetal calf serum (FCS, PAA), and 1 U/mL Penicillin/Streptomycin at 37°C, 5% CO2 and 95% humidity. After 24 h, 8 wells were respectively treated with a final concentration of 1 µM, 5 µM, 10 µM, 20 µM and 50 µM of each dye (2 mM stock solutions in ethanol) and incubated for 72 h. As a negative control, a set of cells was kept untreated, whereas cells treated with 5 µl of 20% Triton X served as a positive control. Subsequently, 15 µl of the tetrazolium dye solution were added to each well and incubated for 4 h before the reaction was stopped and the generated formazan solubilized with 100 µl Solubilization Solution/Stop Mix, according to the manufacturer's manual. After 24 h incubation, the absorbance at 595 nm using a 96-well plate reader (*SpectraMax M2 Microplate Reader*, *Molecular Devices*) was measured. Data were averaged and the multiple determination of each substance and concentration made it possible to calculate the standard deviation.

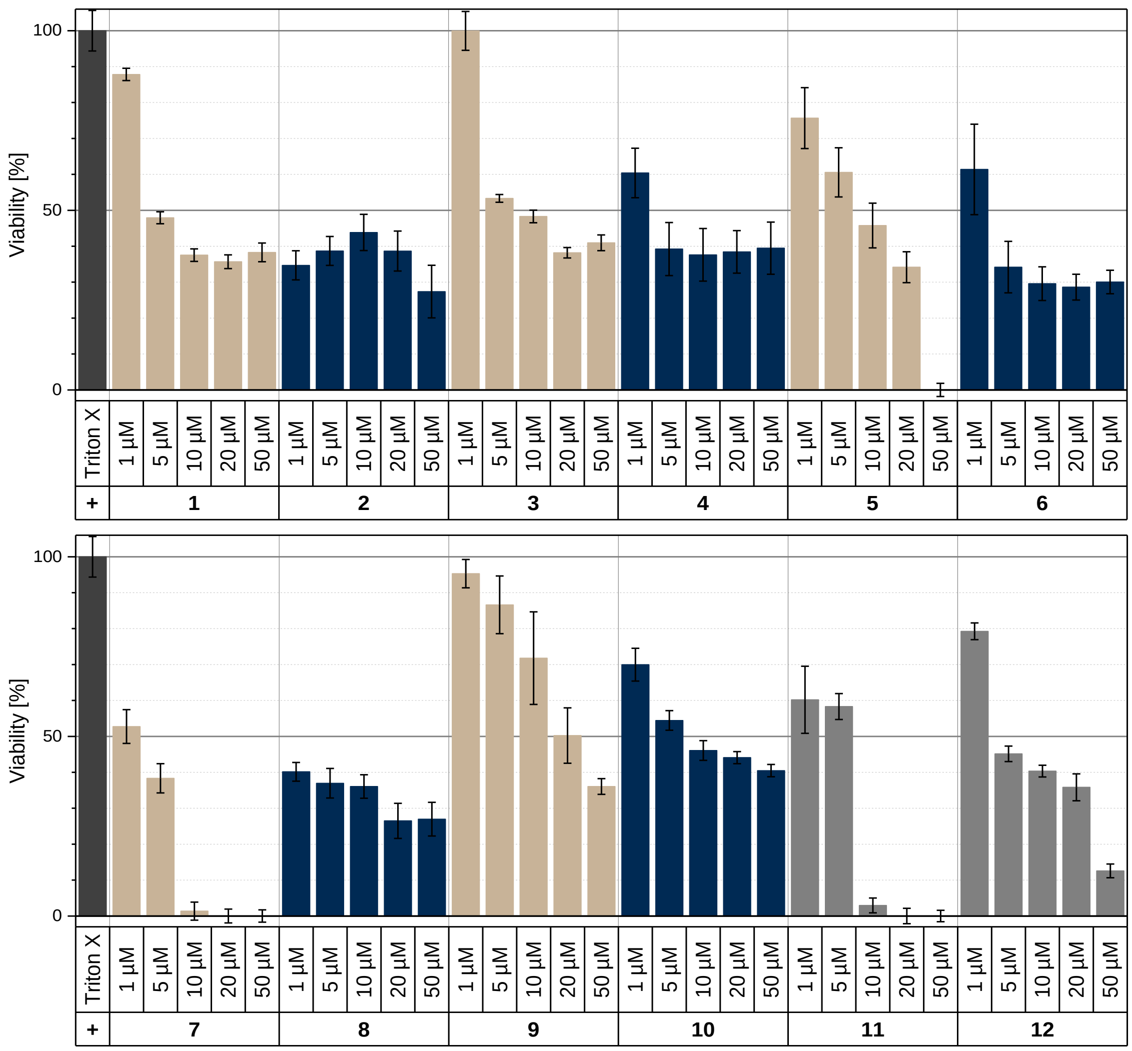


Figure S71. HeLa cell-viability of dye **1**-**12** at different dye concentrations.

14. Cell Culture and Live Cell Confocal Fluorescent Microscopy

2 × 10^4 HeLa (human cervix carcinoma) cells were seeded into each well of an 8-well µ-slide (µ Slide 8 well ibiTreat, IBIDI), and cultured for 24 h in 200 µL of Dulbecco's modified Eagle's medium (DMEM, high glucose, *Invitrogen*) supplemented with 60 µg/ml penicillin, 100 µg/ml streptomycin and 10 % fetal calf serum (FCS, *Sigma-Aldrich*) under sterile conditions at 37°C, 5% CO_2, and 95% humidity. Subsequently, cells were incubated at a final concentration of 10 µM of the respective dye (2 mM stock solution in ethanol) diluted with Dulbecco's modified Eagle's medium to a final incubation volume of 200 µl. After 24 h, cells were washed 3 times with PBS (Phosphate buffered saline, *Gibco*) before cellular uptake of the dyes was measured by live cell confocal fluorescence microscopy.

Visualization of the intracellular localization of the dyes was achieved by confocal microscopy using a *Leica TCS-SP8*, equipped with a *Leica DMI8-CS* invers microscope and a *HCPL APO CS2 40x/1.10 WATER* objective. Dyes were excited using a 488 nm line of an argon ion laser (λ_{exc} = 488 nm) and the fluorescent emission was detected at 500 – 530 nm (λ_{em} = 500-530 nm), complemented with a brightfield image. Image acquisition was performed at a lateral resolution of 1024 × 1024 pixels and 8 bit depth using *LAS-AF 1.1.0.12420* software.

For transfection experiments, 2 × 10^4 HeLa cells were treated with *ScreenFect® A* transfection reagent (*ScreenFect GmbH*) and a final concentration of 75 nM of the respective dye modified oligonucleotides. Therefor, 0.85 µl *ScreenFect® A* were diluted in 20 µl Dilution Buffer (*ScreenFect GmbH*) and mixed with 6 µl of the respective DNA (2.5 µM stock solution in phosphate buffer), which was freshly diluted with 14 µl of Dilution Buffer. After 30 min complex formation at room temperature, 160 µl DMEM was added to the transfection mixture, transferred to the cells of each well and subsequently incubated for 24 h at 37°C and 5% CO_2. Eventually, cells were washed 3 times with DMEM before measuring cellular uptake by live cell confocal fluorescence microscopy.

For colocalization experiments, 2 × 10^4 HeLa cells were incubated for 24 h at 37°C and 5% CO_2 at a final concentration of 10 µM of **6** diluted with Dulbecco's modified Eagle's medium to a final incubation volume of 200 µl. After 24 h, cells were washed 3 times with PBS (Phosphate buffered saline, *Gibco*). Subsequently, cells were incubated for 1 h at 37°C and 5% CO_2at a final concentration of 125 nM of MitoTracker® Red FM (1 mM stock solution in DMSO, *Thermo Fisher Scientific*) diluted with Dulbecco's modified Eagle's medium to a final incubation volume of 200 µl. The cells were washed 3 times with DMEM before measuring cellular uptake by live cell confocal fluorescence microscopy.

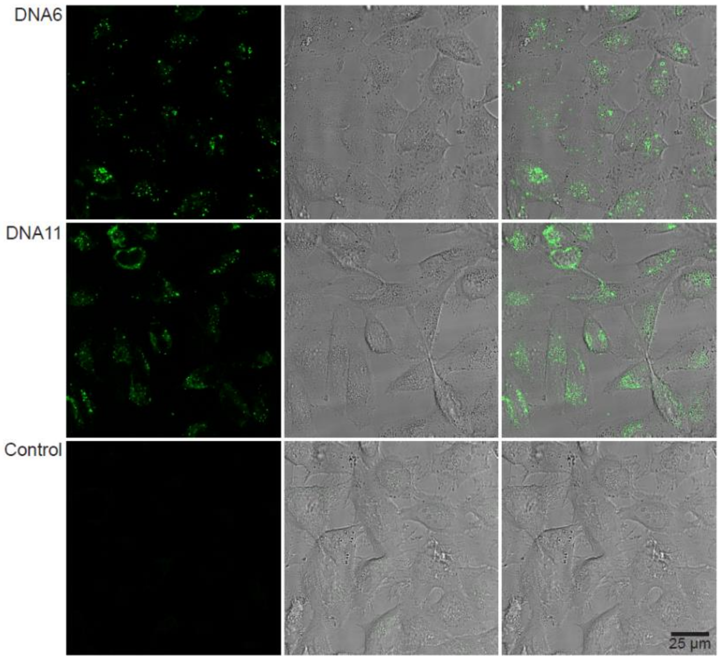


Figure S72. Transfection of ss**DNA6**, ss**DNA11** and control without transfection of any fluorescent DNA-probe.

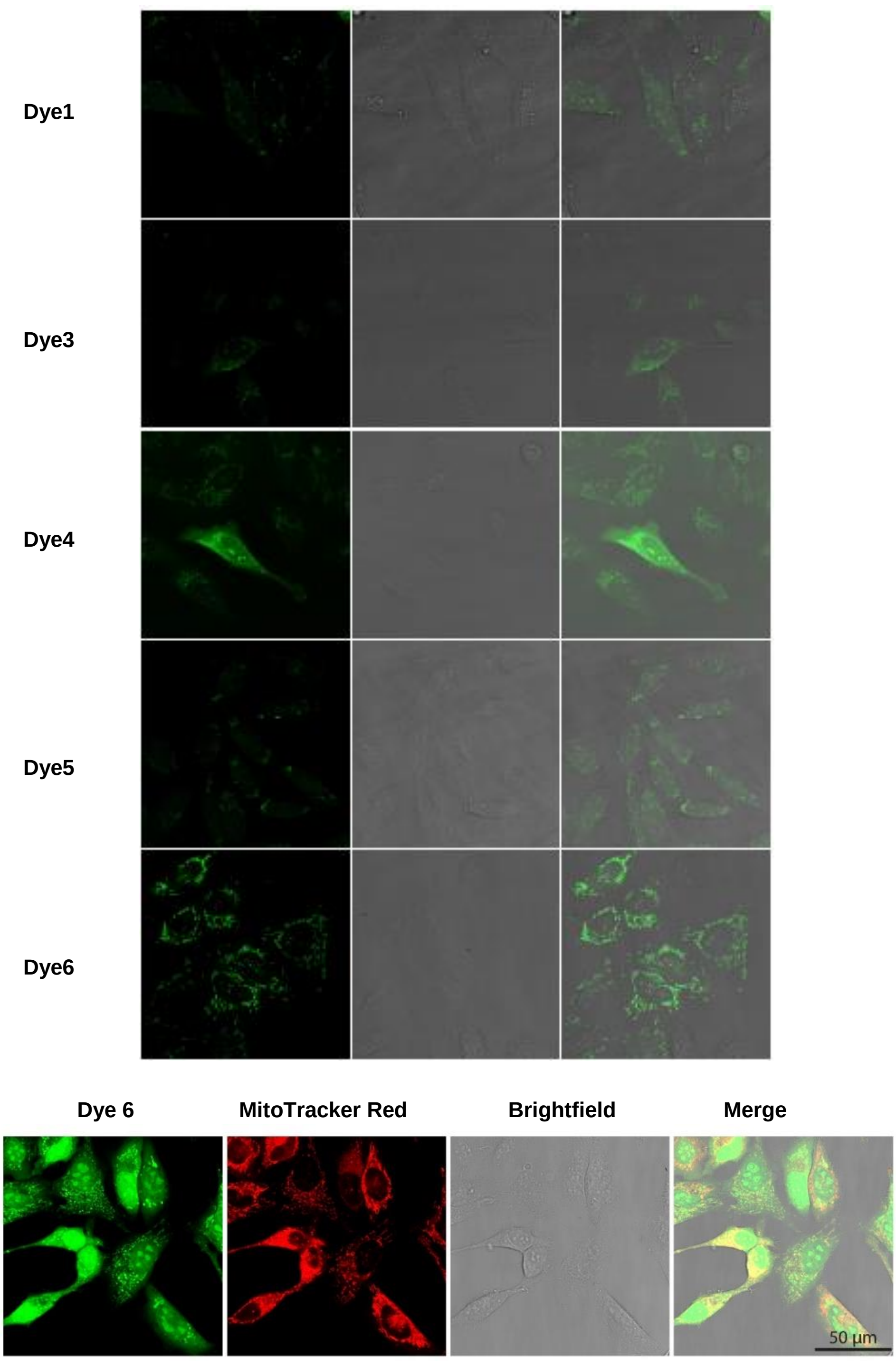
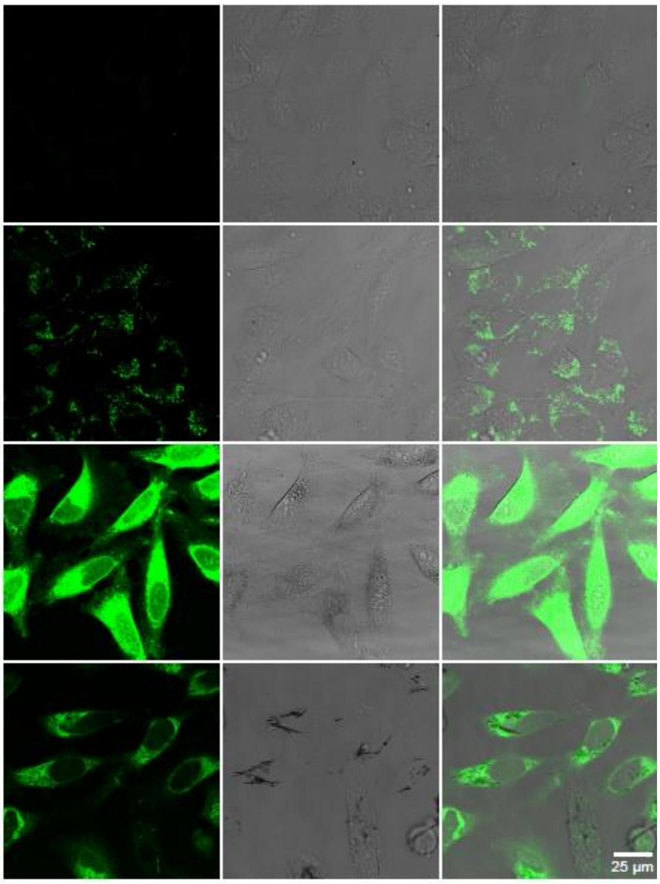


Figure S73. HeLa cell penetration, live cell confocal fluorescent microscopy of dye **1** and **3**-**6** and colocalization of dye **6** and MitoTracker Red.



Dye9

Dye10

Dye11

Dye12

Figure S74. HeLa cell penetration and live cell confocal fluorescent microscopy of dye **9**-**12**.

15. Analytics

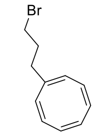
a. Analytics of 13 and the Quinolinium Salts 14 and 15

The analytics of the compounds **13**-**15** are shown in earlier publications of our working group.[1-2]

b. Analytics of 17 and the Indoles 18-28

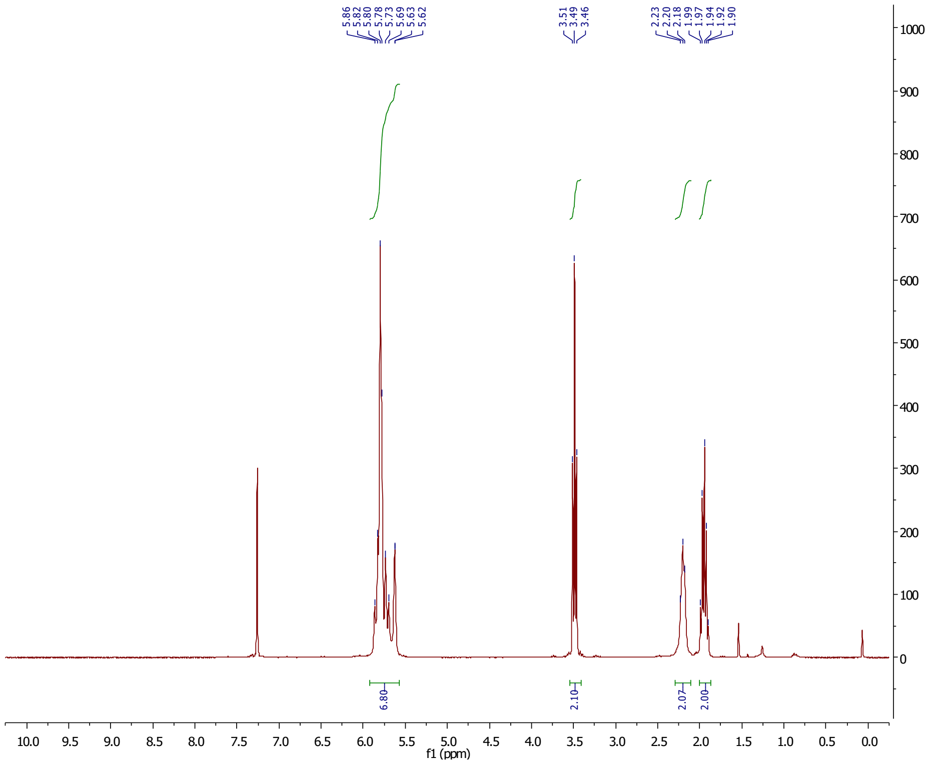
The compounds **19**-**22** are commercially available, and therefore their analytics are not shown here. The analytics of compound **16** can be found in the publication of Altman et al.[3] and compound **23** is described in earlier publications of our group.[2]

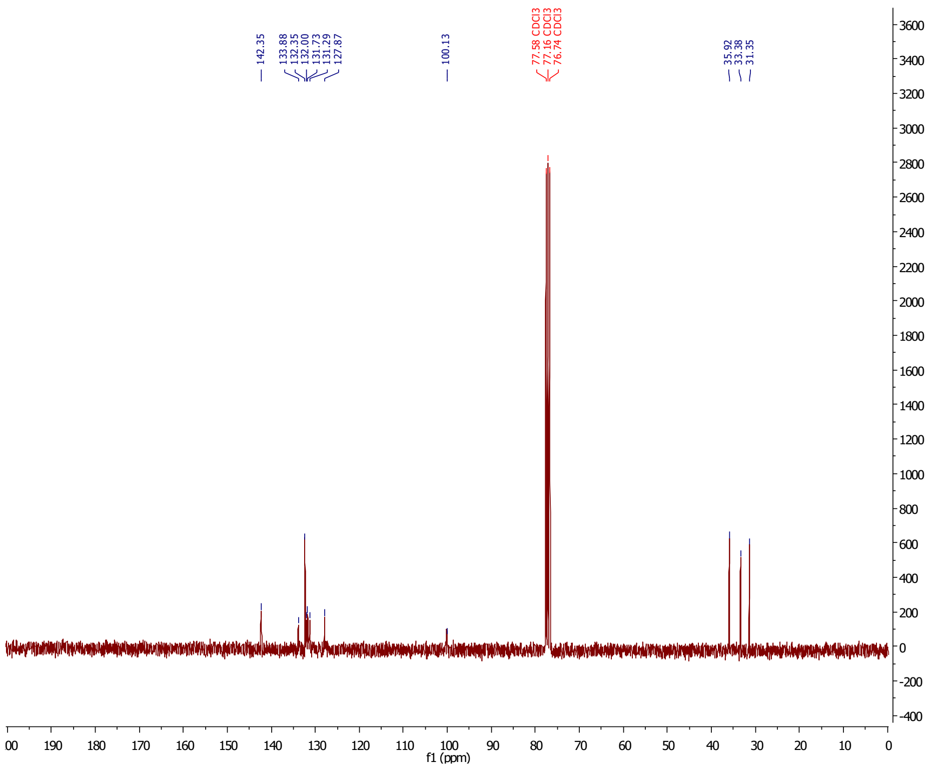
(1*Z*,3*Z*,5*Z*,7*Z*)-1-(3-bromopropyl)cycloocta-1,3,5,7-tetraene (17):

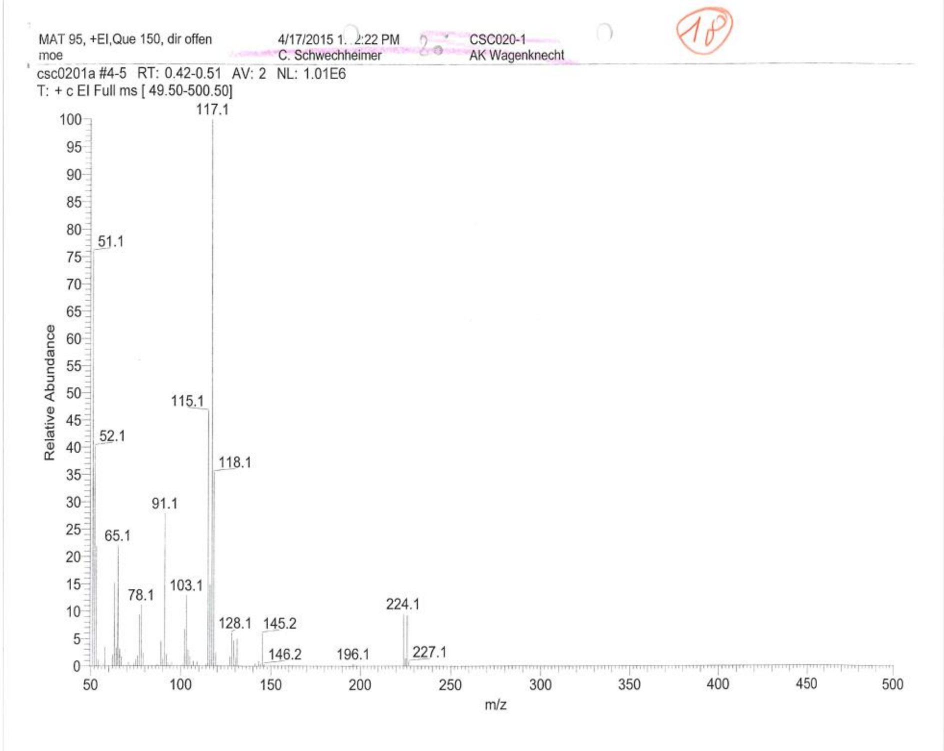


17

$C_{11}H_{13}Br$
225.1290 g/mol






MAT 95, +EI,Que 150, dir offen
moe
4/17/2015 1. 2:22 PM
C. Schwechheimer
CSC020-1
AK Wagenknecht
18
csc0201a #4-5 RT: 0.42-0.51 AV: 2 NL: 1.01E6
T: + c EI Full ms [49.50-500.50]
Relative Abundance
m/z
117.1
51.1
115.1
52.1
118.1
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65.1
78.1
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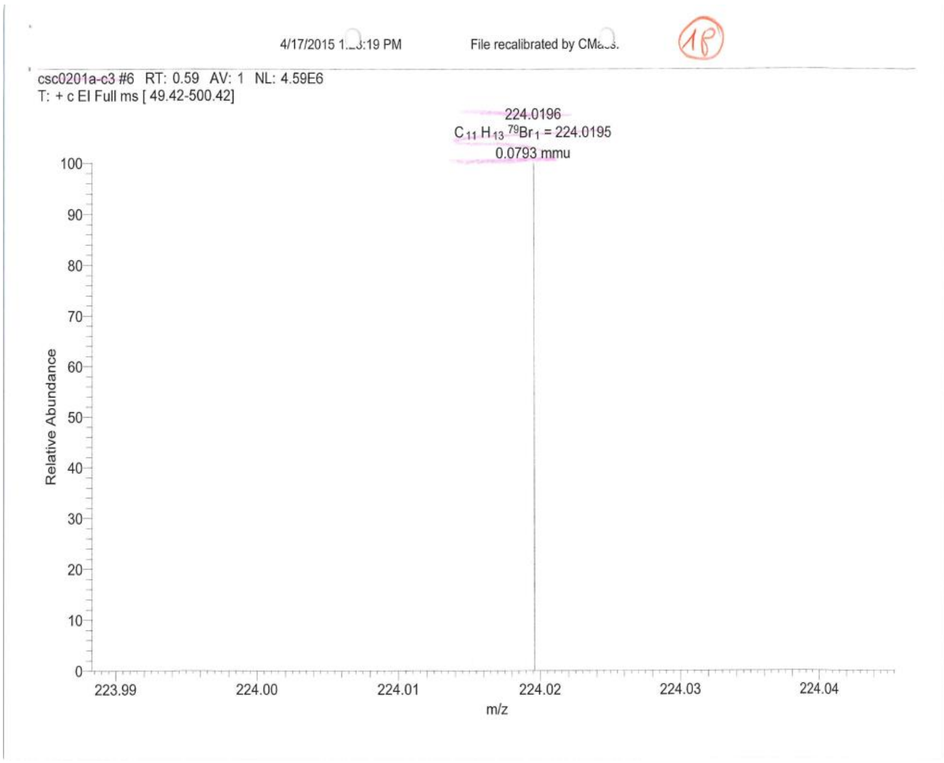
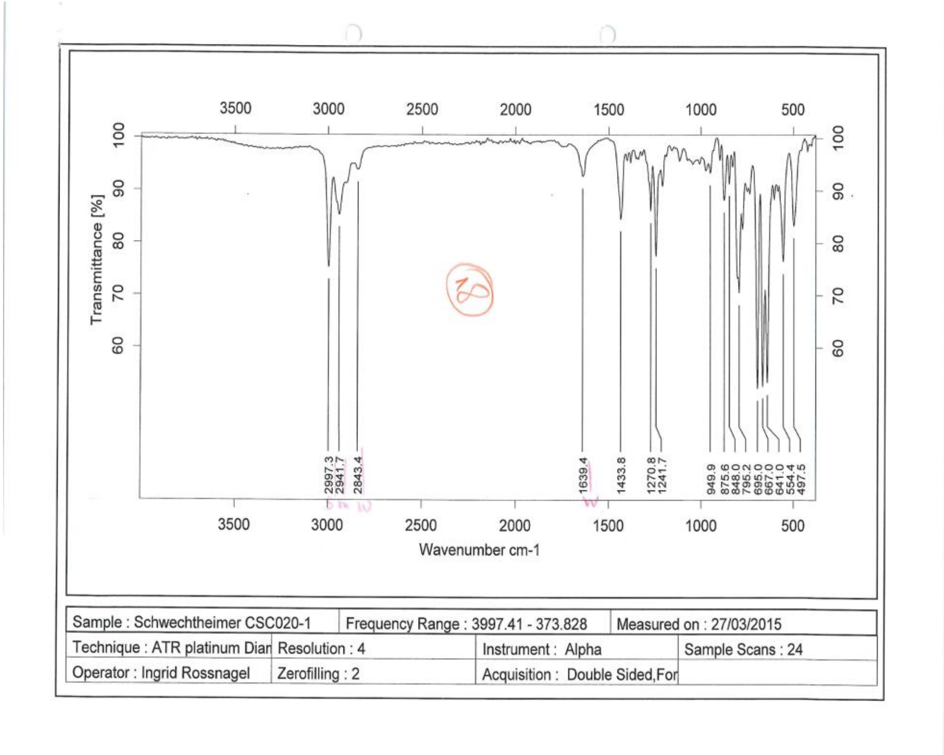
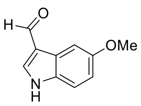
128.1
145.2
146.2
196.1
227.1


4/17/2015
File recalibrated by CMass.
18
csc0201a-c3 #6 RT: 0.59 AV: 1 NL: 4.59E6
T: + c EI Full ms [49.42-500.42]
224.0196
C11 H13 79Br1 = 224.0195
0.0793 mmu
Relative Abundance
m/z

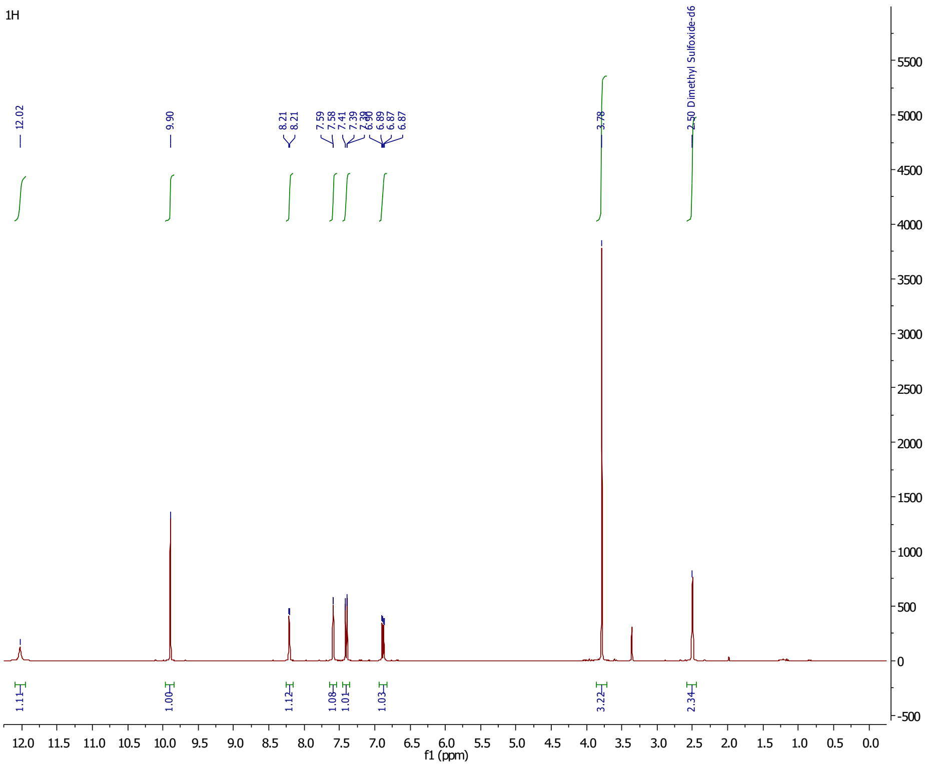


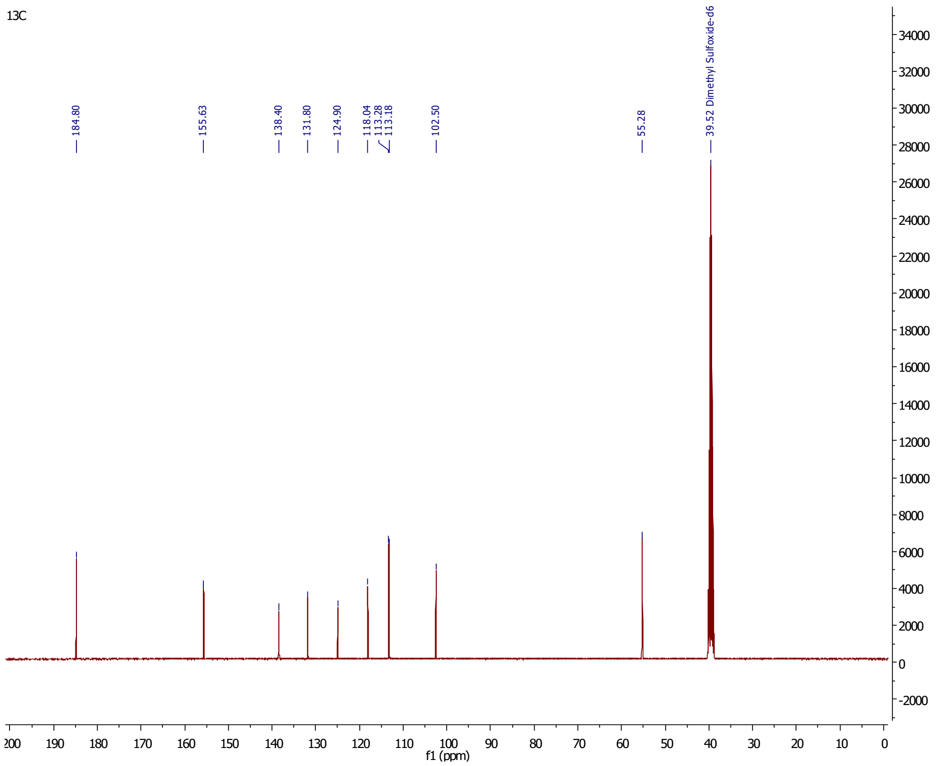
5-methoxy-1*H*-indole-3-carbaldehyde (18):

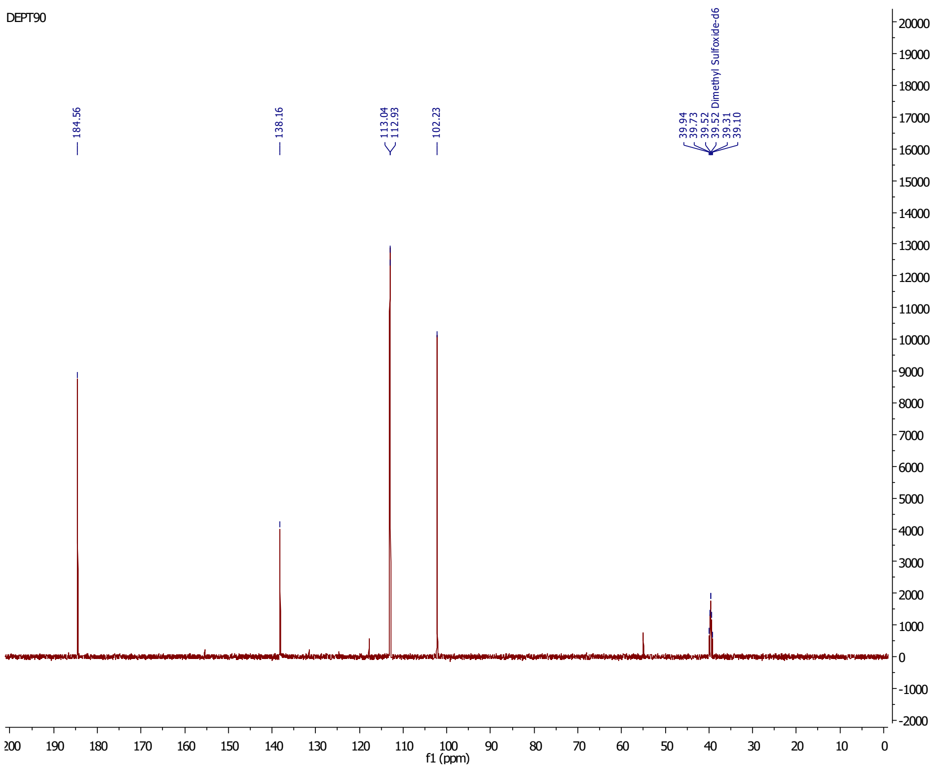


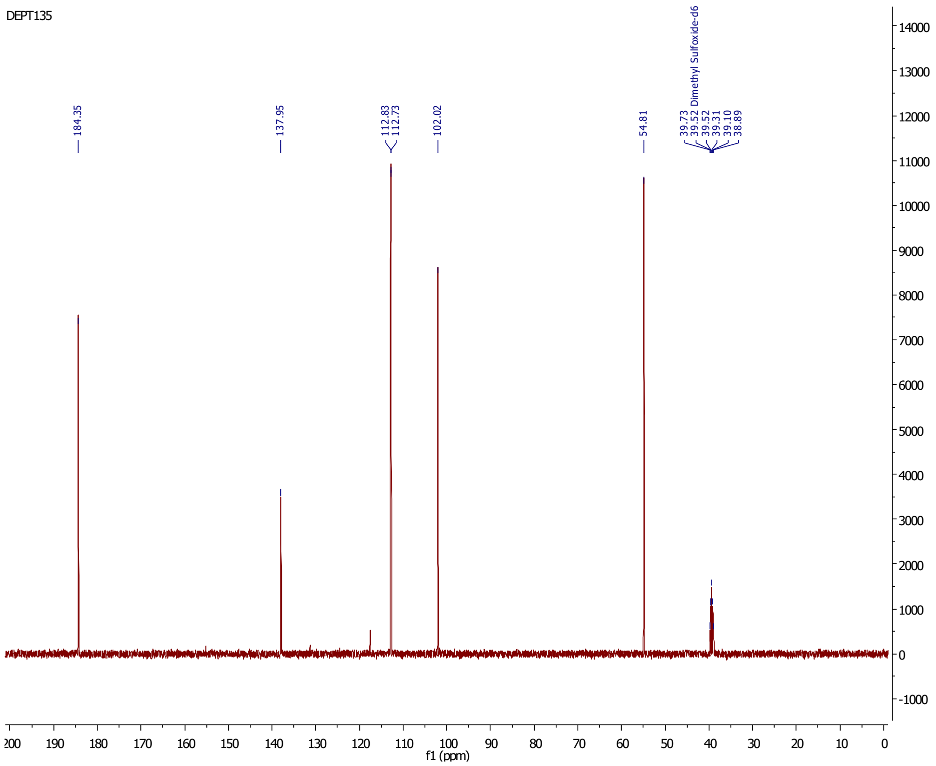
18

$C_{10}H_9NO_2$
175.1870 g/mol




13C
184.80
155.63
138.40
131.80
124.90
118.04
113.28
113.18
102.50
55.28
39.52 Dimethyl Sulfoxide-d6
f1 (ppm)


DEPT90
184.56
138.16
113.04
112.93
102.23
39.94
39.73
39.52
39.52 Dimethyl Sulfoxide-d6
39.31
39.10
f1 (ppm)


DEPT135
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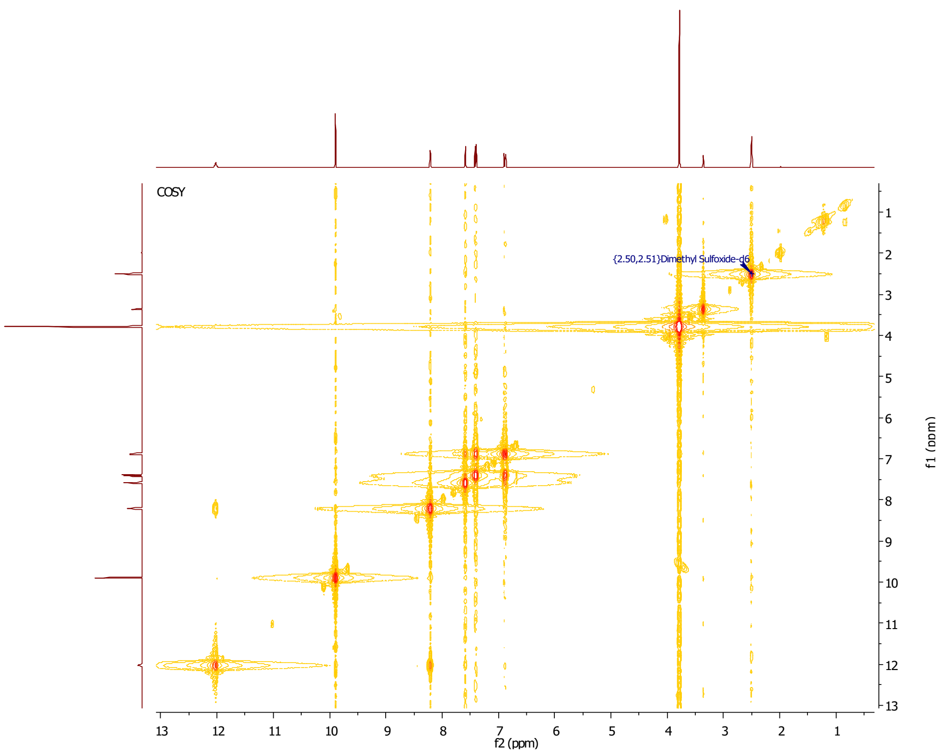
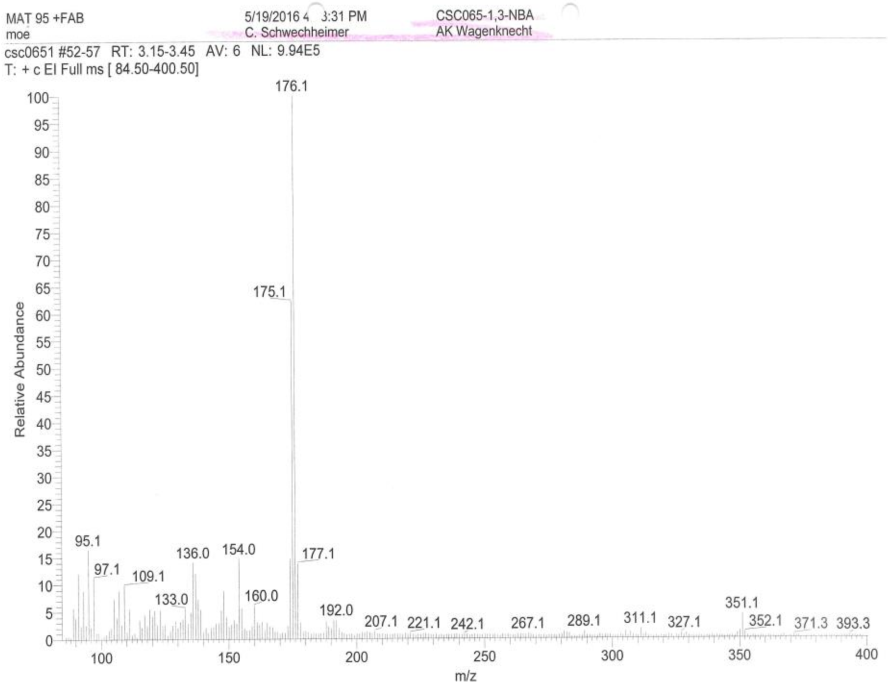
137.95
112.83
112.73
102.02
54.81
Dimethyl Sulfoxide-d6
39.73
39.52
39.52
39.31
39.10
38.89
f1 (ppm)


COSY
{2.50,2.51}Dimethyl Sulfoxide-d6
f2 (ppm)
f1 (ppm)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moe
5/19/2016 4 3:31 PM
C. Schwechheimer
CSC065-1,3-NBA
AK Wagenknecht
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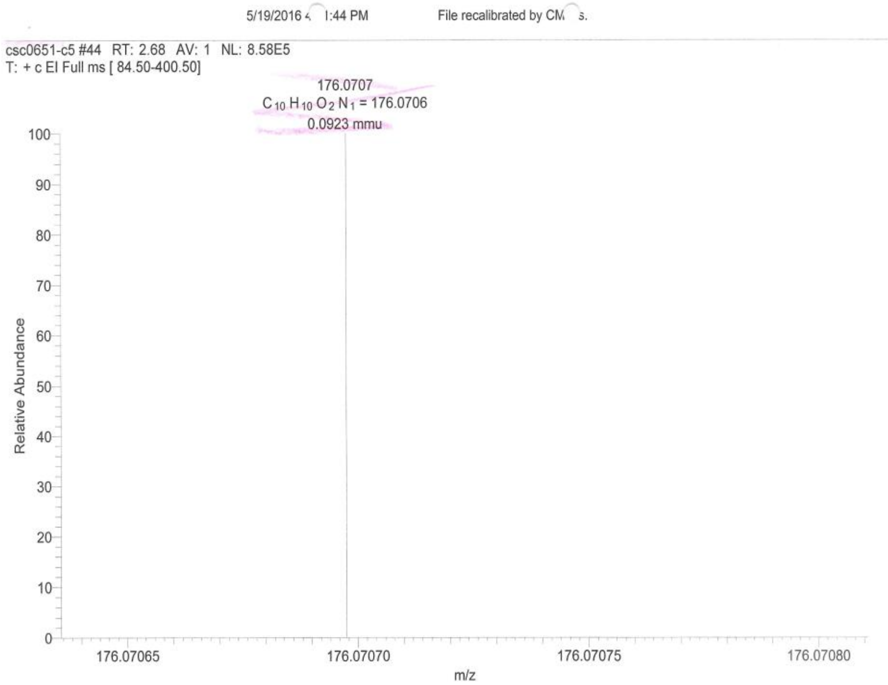
T: + c EI Full ms [84.50-400.50]
Relative Abundance
m/z


5/19/2016 4 1:44 PM
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csc0651-c5 #44 RT: 2.68 AV: 1 NL: 8.58E5
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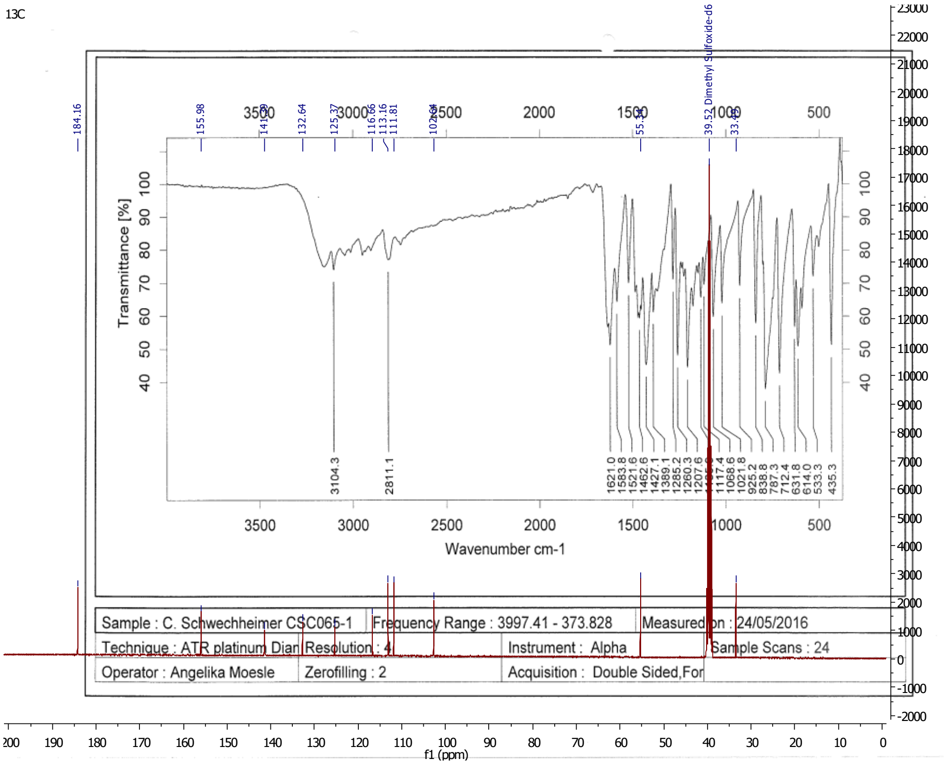
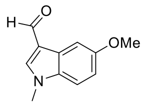
176.0707
C 10 H 10 O 2 N 1 = 176.0706
0.0923 mmu
Relative Abundance
m/z



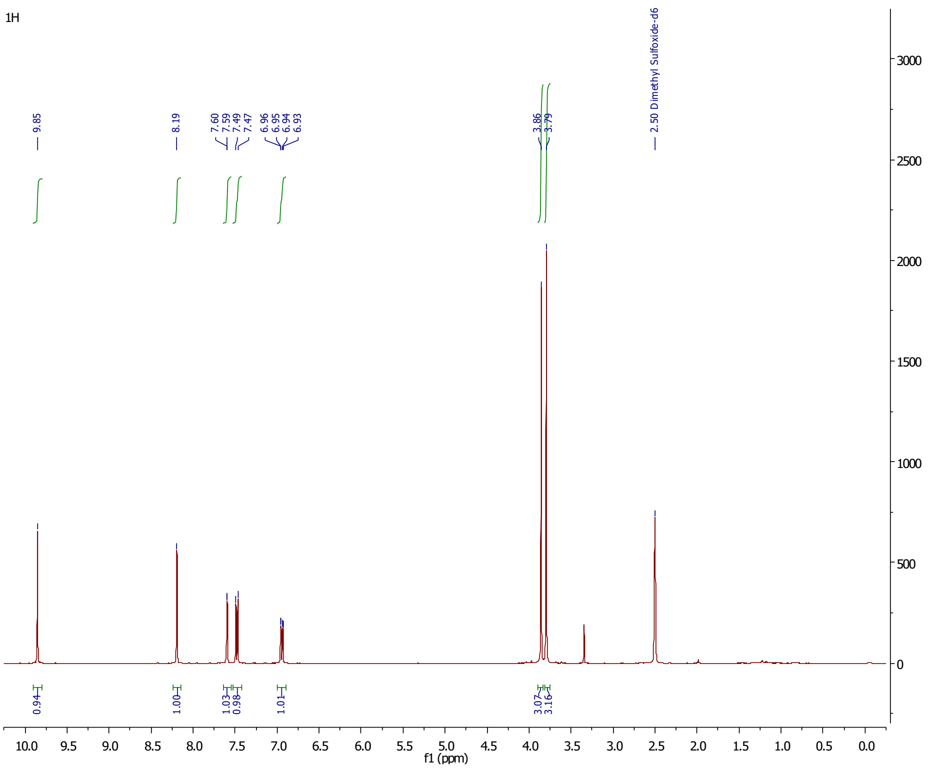
5-methoxy-1-methyl-1*H*-indole-3-carbaldehyde (24):

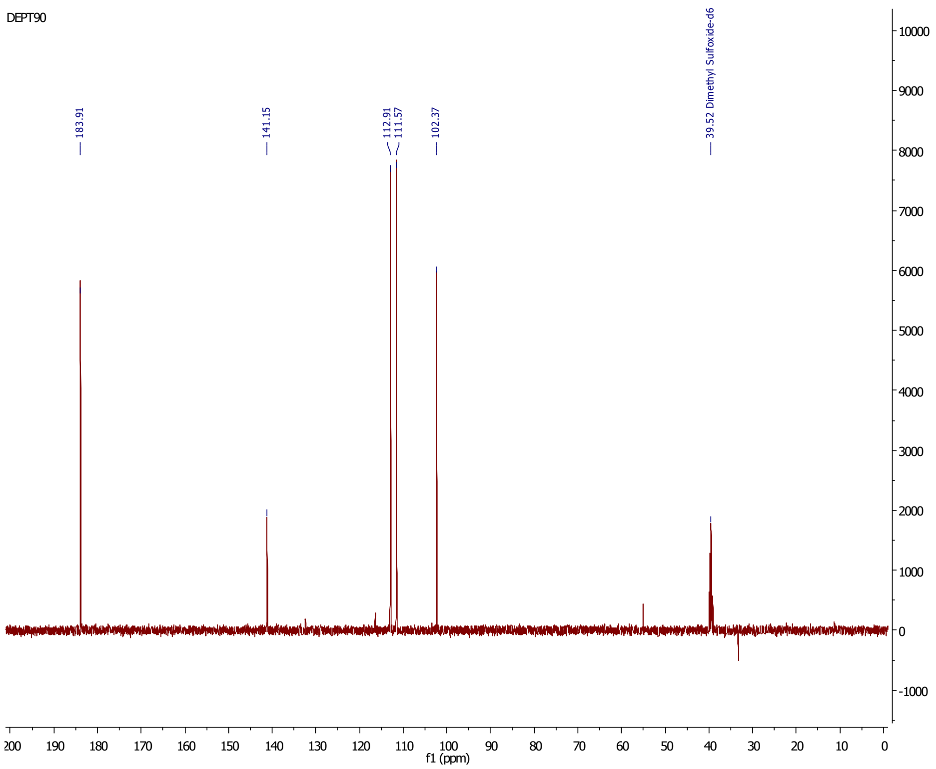


24

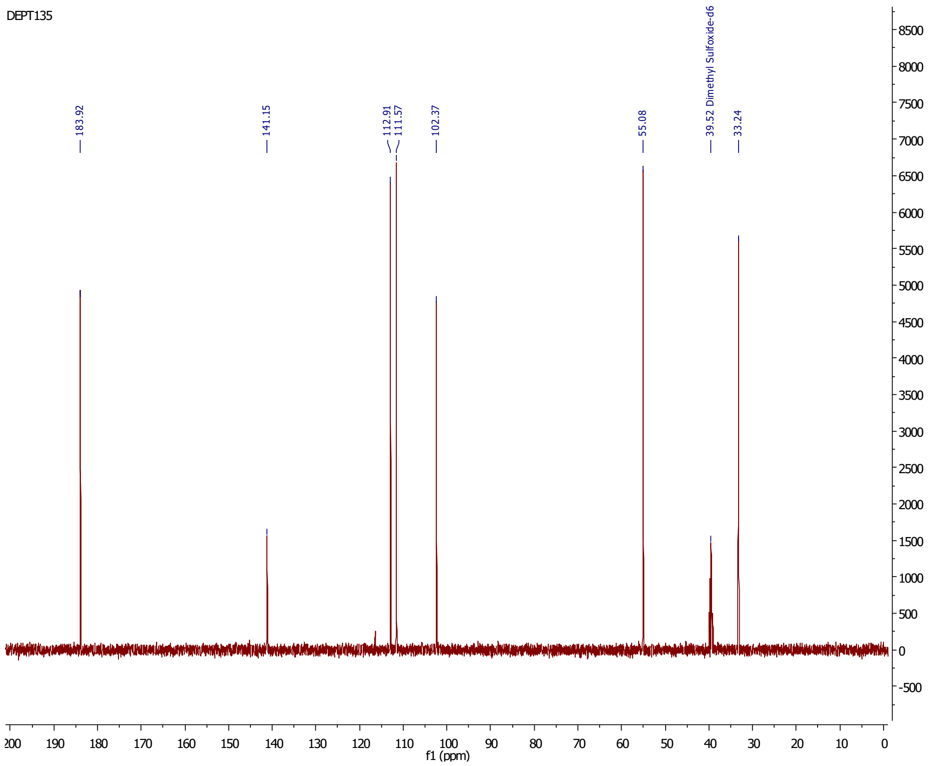
$C_{11}H_{11}NO_2$

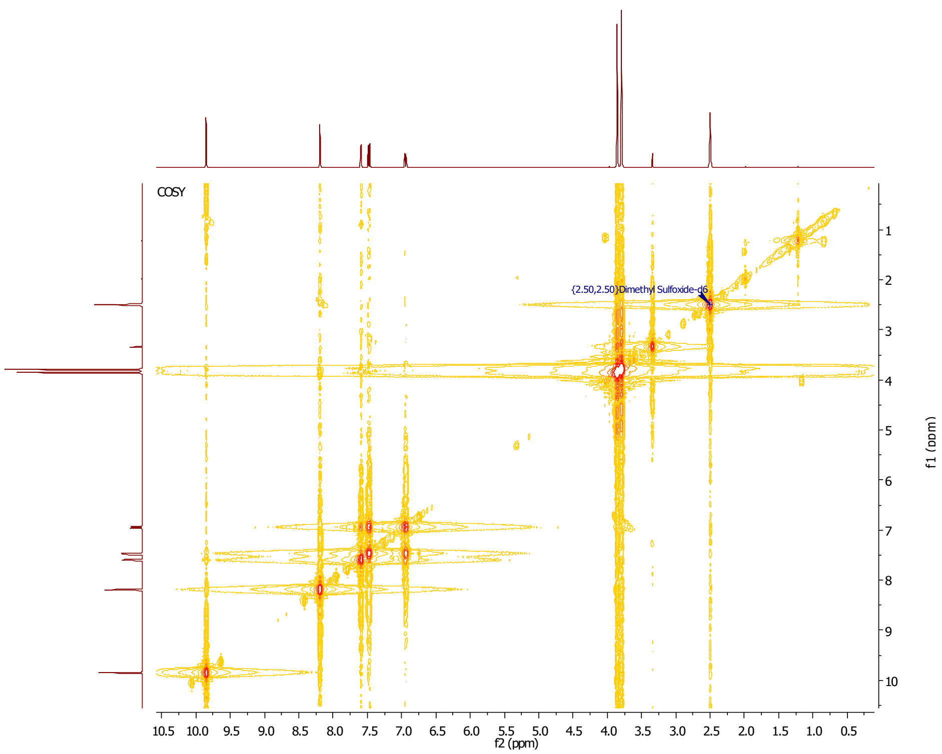
189.2140 g/mol

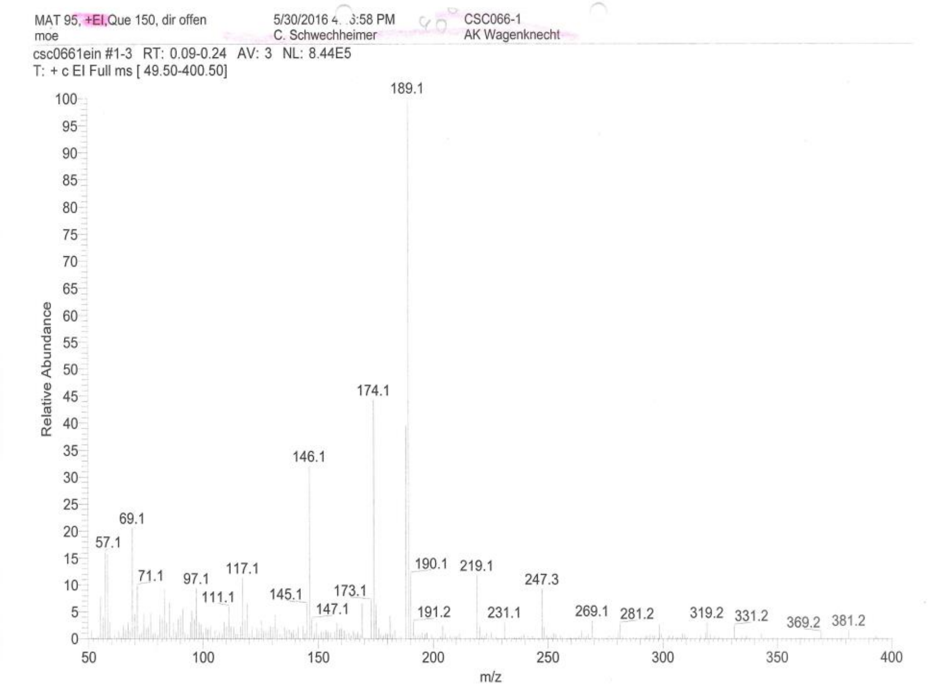


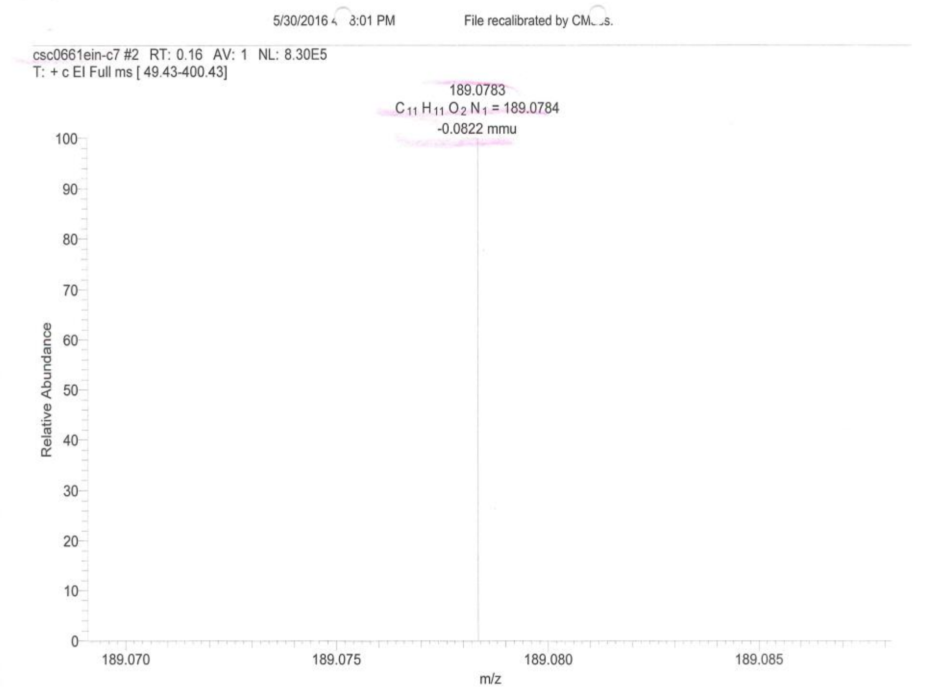


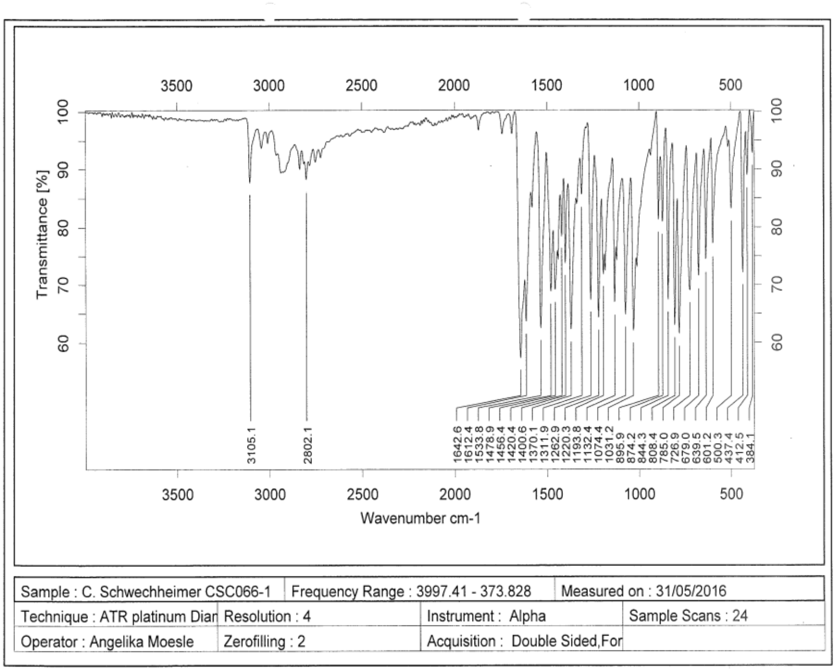
DEPT90
183.91
141.15
112.91
111.57
102.37
39.52 Dimethyl Sulfoxide-d6
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


DEPT135
183.92
141.15
112.91
111.57
102.37
55.08
39.52 Dimethyl Sulfoxide-d6
33.24
f1 (ppm)

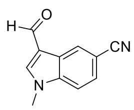

COSY
{2.50,2.50} Dimethyl Sulfoxide-d6
f2 (ppm)
f1 (ppm)


MAT 95, +EI,Que 150, dir offen
moe
5/30/2016 4:..:58 PM
C. Schwechheimer
CSC066-1
AK Wagenknecht
csc0661ein #1-3 RT: 0.09-0.24 AV: 3 NL: 8.44E5
T: + c EI Full ms [49.50-400.50]
Relative Abundance
m/z
189.1
174.1
146.1
69.1
57.1
71.1
97.1
117.1
111.1
145.1
147.1
173.1
190.1
219.1
247.3
191.2
231.1
269.1
281.2
319.2
331.2
369.2
381.2


5/30/2016 ..:01 PM
File recalibrated by CM...s.
csc0661ein-c7 #2 RT: 0.16 AV: 1 NL: 8.30E5
T: + c EI Full ms [49.43-400.43]
189.0783
C11 H11 O2 N1 = 189.0784
-0.0822 mmu
Relative Abundance
m/z

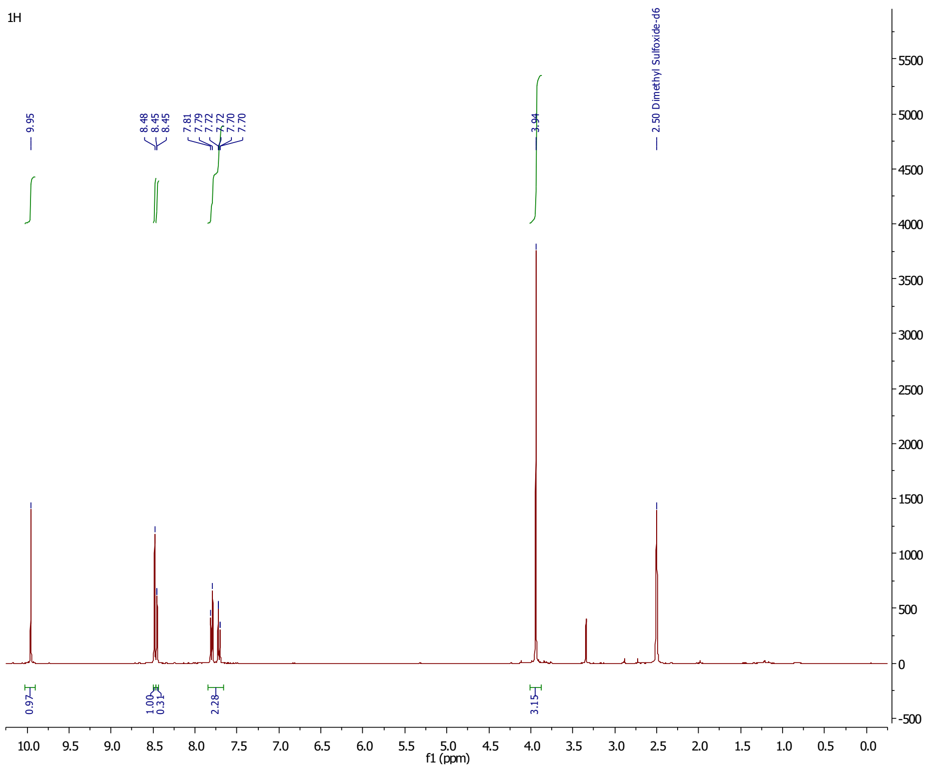


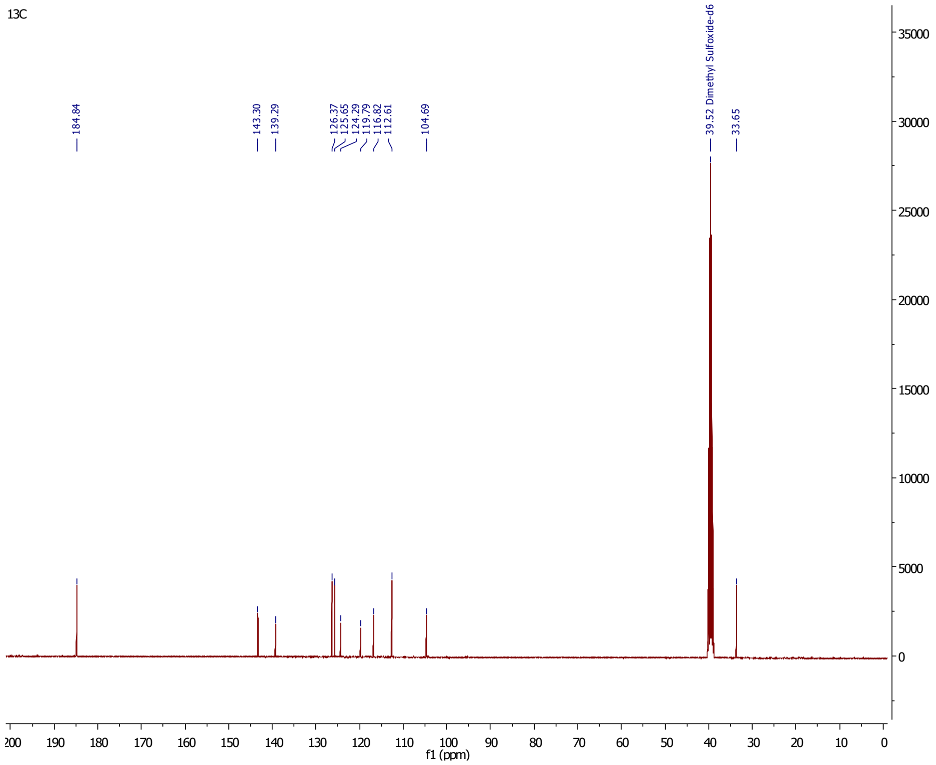
3-formyl-1-methyl-1*H*-indole-5-carbonitrile (25):

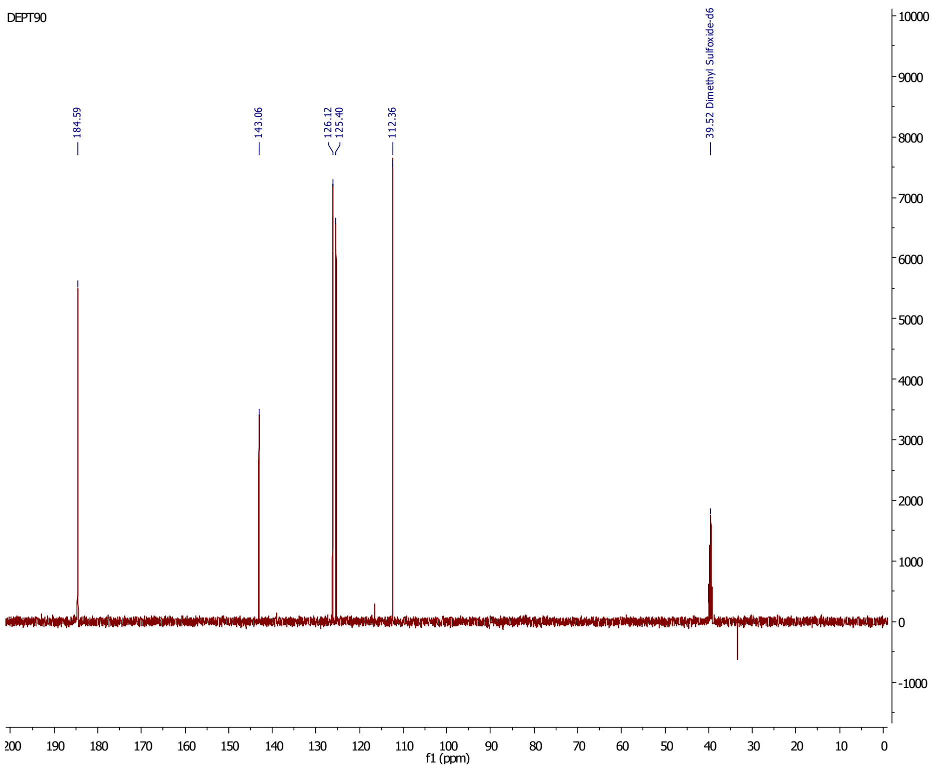


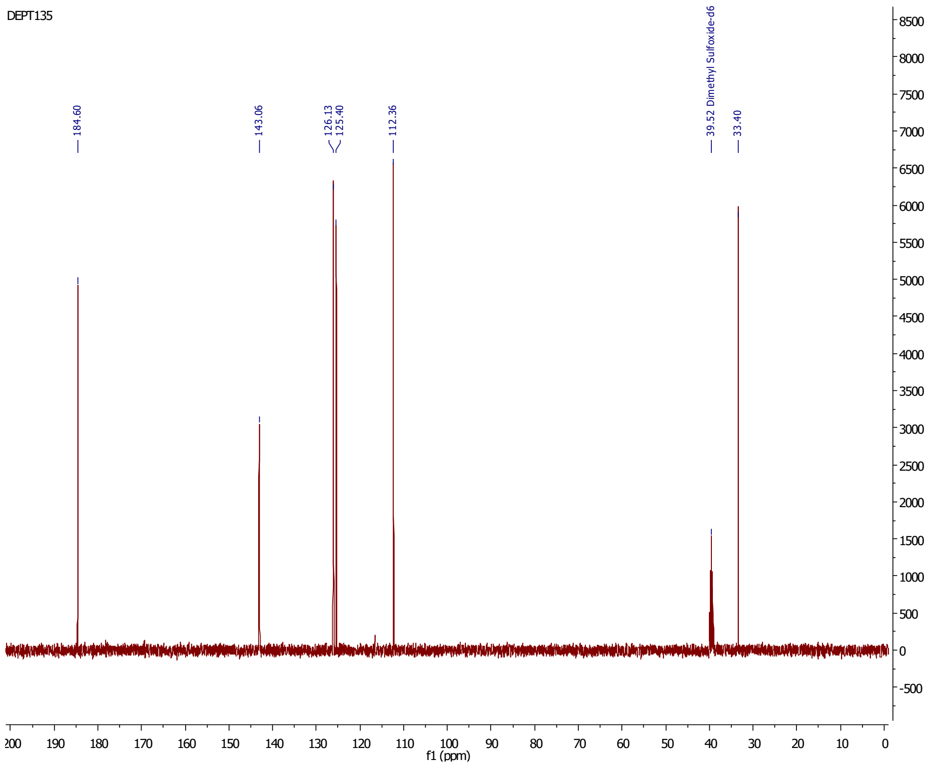
25

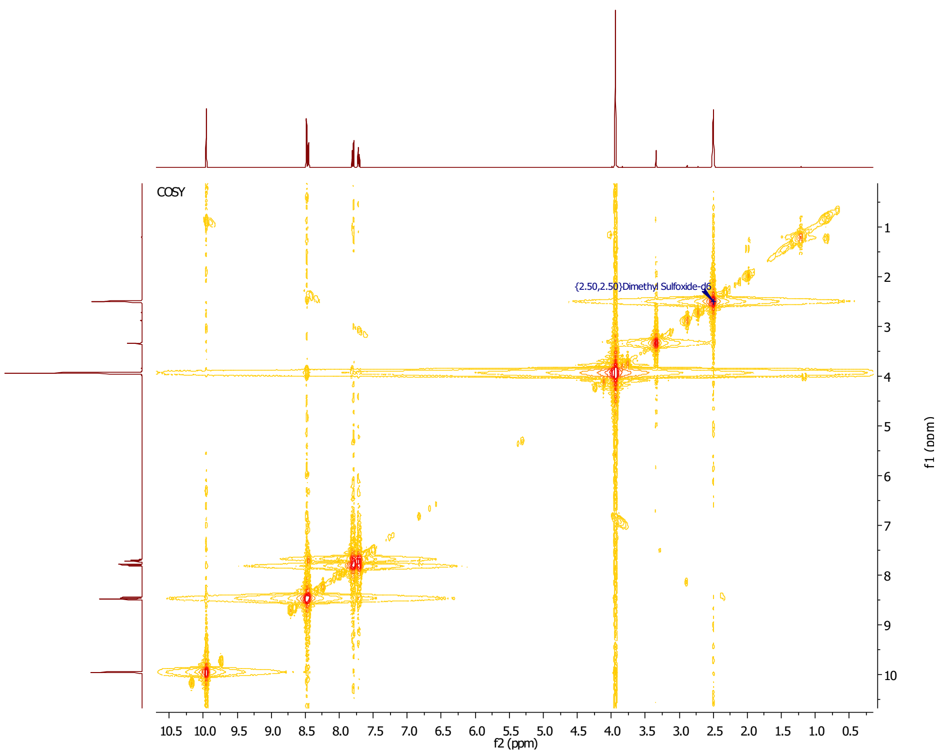
$C_{11}H_8N_2O$
184.1980 g/mol

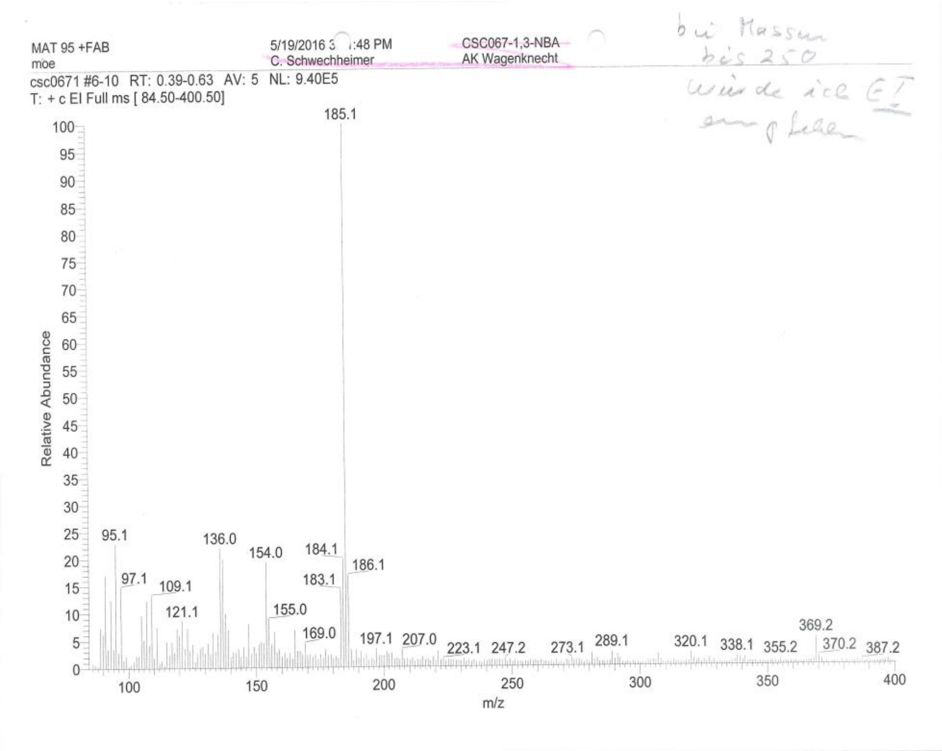


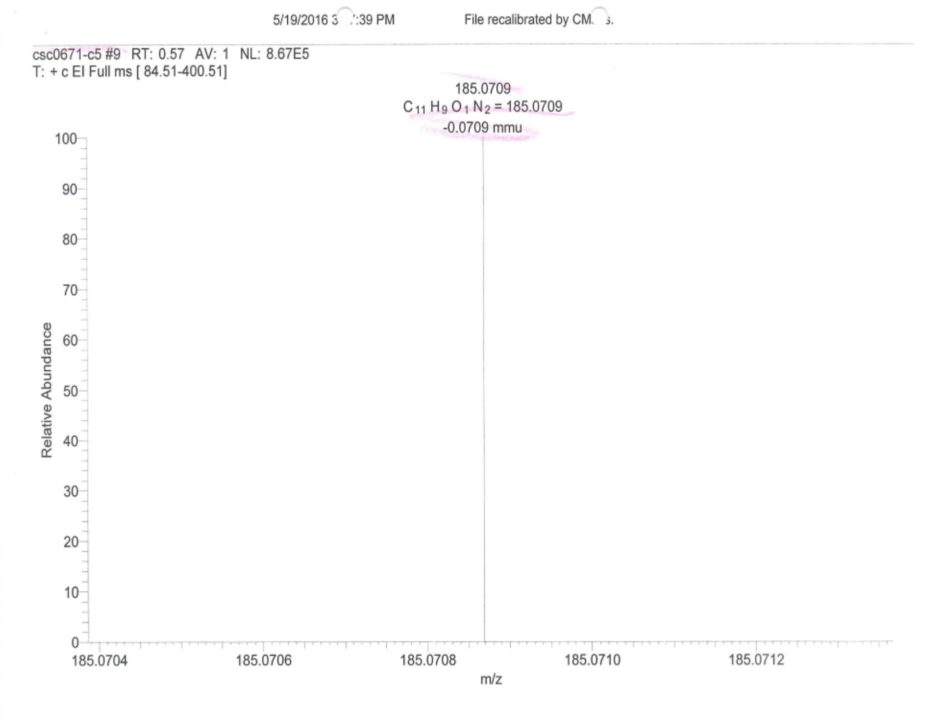

13C
184.84
143.30
139.29
126.37
125.65
124.29
119.79
116.82
112.61
104.69
39.52 Dimethyl Sulfoxide-d6
33.65
f1 (ppm)

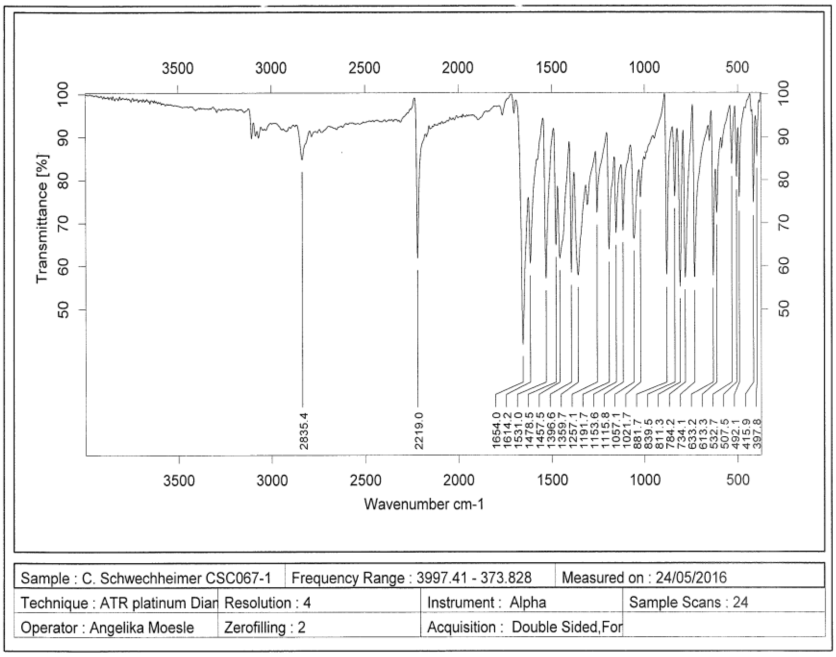

DEPT90
184.59
143.06
126.12
125.40
112.36
39.52 Dimethyl Sulfoxide-d6
f1 (ppm)


DEPT135
184.60
143.06
126.13
125.40
112.36
39.52 Dimethyl Sulfoxide-d6
33.40
f1 (ppm)

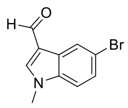

COSY
{2.50,2.50}Dimethyl Sulfoxide-d6
f2 (ppm)
f1 (ppm)


MAT 95 +FAB
moe
5/19/2016 3 :48 PM
C. Schwechheimer
CSC067-1,3-NBA
AK Wagenknecht
csc0671 #6-10 RT: 0.39-0.63 AV: 5 NL: 9.40E5
T: + c EI Full ms [84.50-400.50]
bei Massen bis 250 würde ich EI empfehlen
Relative Abundance
m/z
185.1
95.1
136.0
154.0
184.1
186.1
97.1
109.1
183.1
121.1
155.0
169.0
197.1
207.0
223.1
247.2
273.1
289.1
320.1
338.1
355.2
369.2
370.2
387.2


5/19/2016 3 :39 PM
File recalibrated by CM. s.
csc0671-c5 #9 RT: 0.57 AV: 1 NL: 8.67E5
T: + c EI Full ms [84.51-400.51]
185.0709
C 11 H 9 O 1 N 2 = 185.0709
-0.0709 mmu
Relative Abundance
m/z
185.0704
185.0706
185.0708
185.0710
185.0712



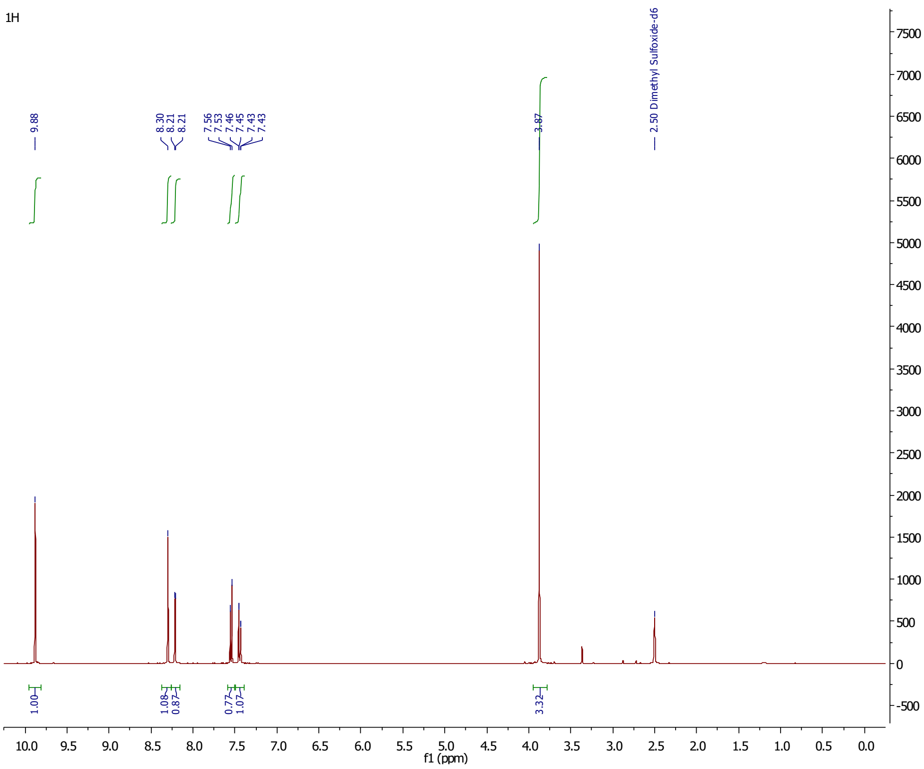
5-bromo-1-methyl-1*H*-indole-3-carbaldehyde (26):

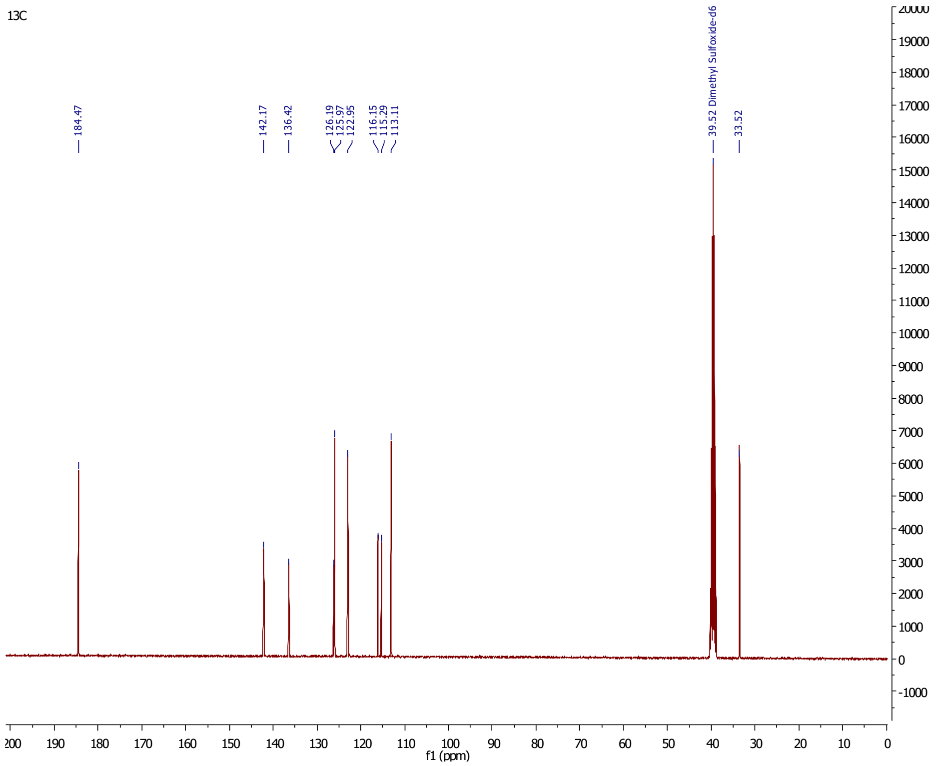


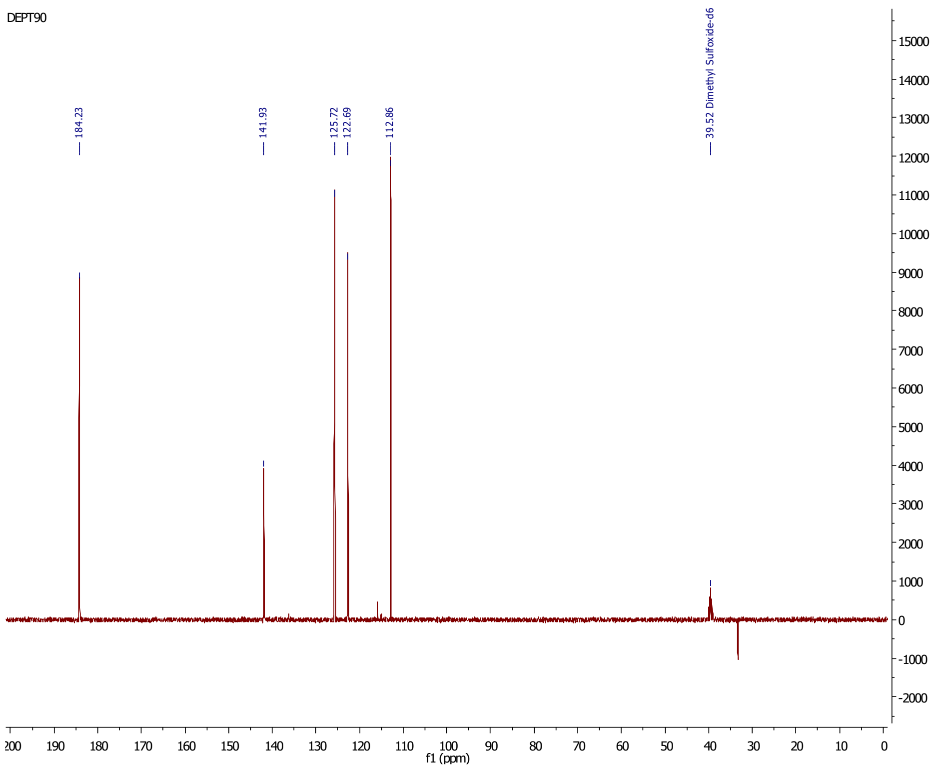
26

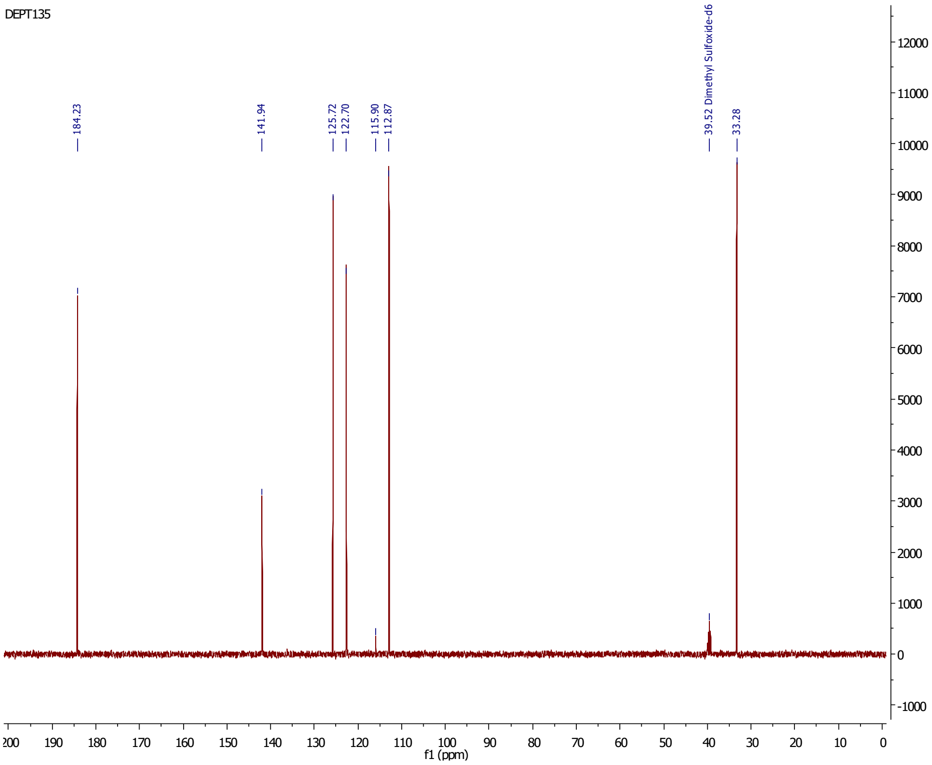
$C_{10}H_8BrNO$

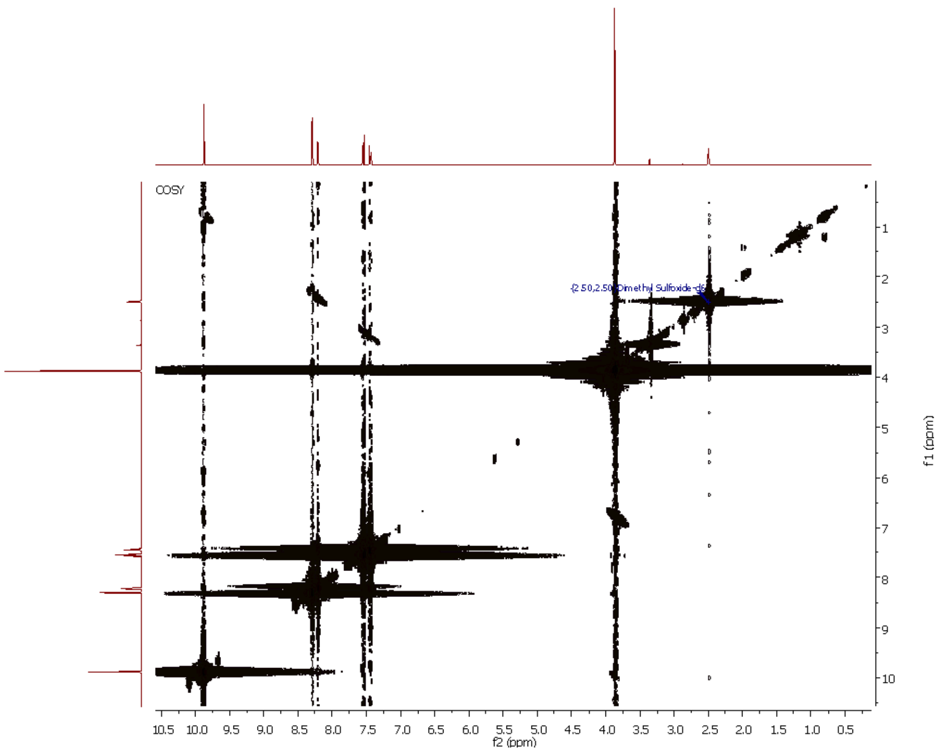
238.0840 g/mol

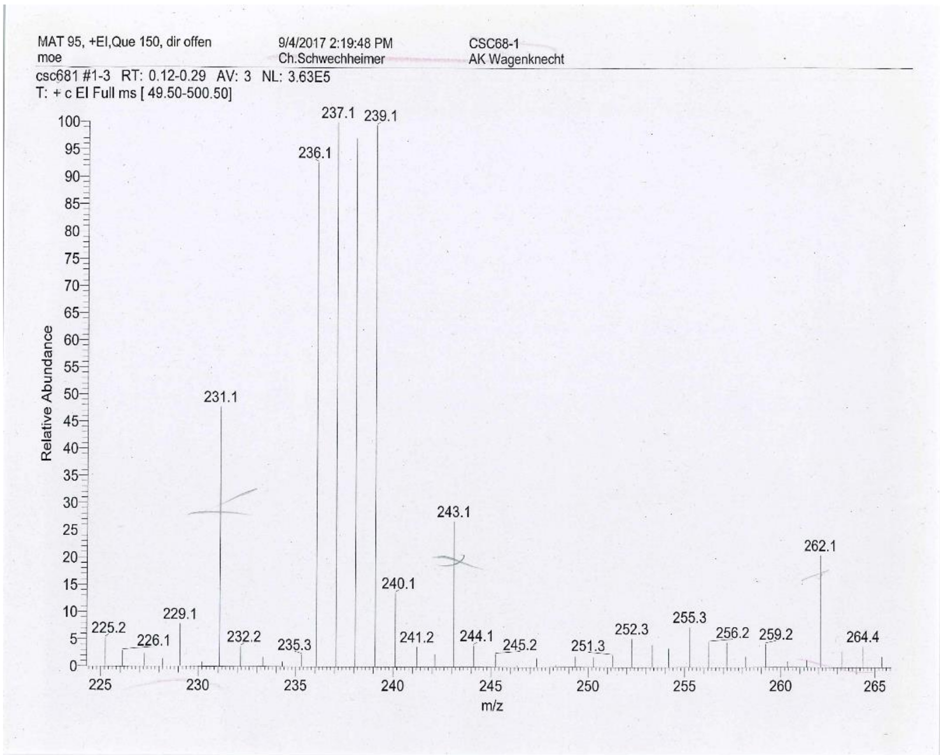



13C
184.47
142.17
136.42
126.19
125.97
122.95
116.15
115.29
113.11
39.52 Dimethyl Sulfoxide-d6
33.52
f1 (ppm)

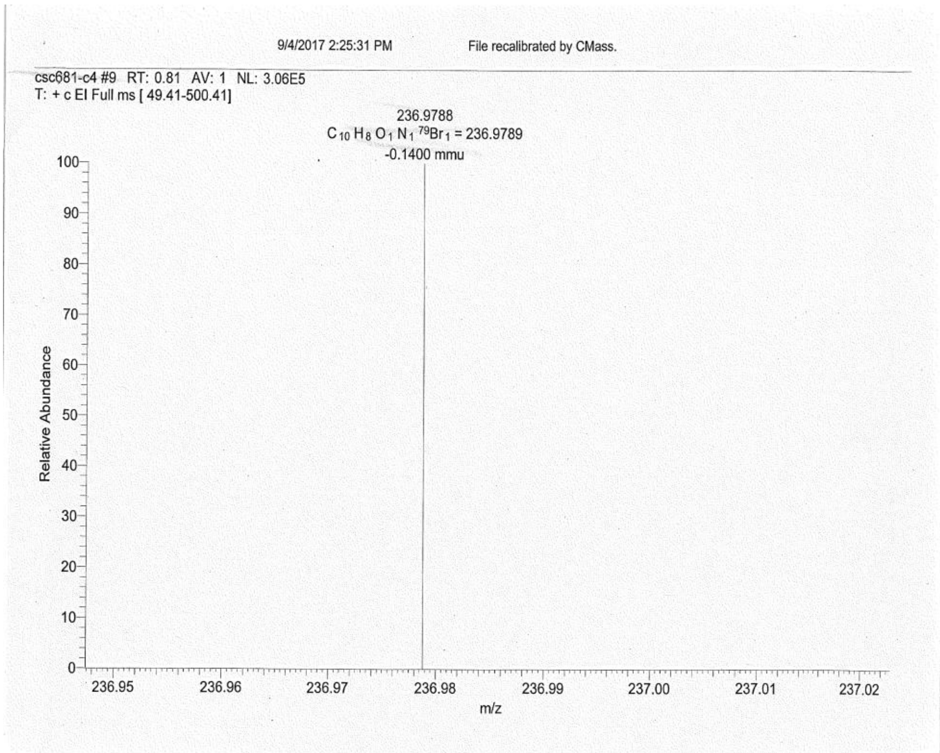

DEPT90
184.23
141.93
125.72
122.69
112.86
39.52 Dimethyl Sulfoxide-d6
f1 (ppm)


DEPT135
184.23
141.94
125.72
122.70
115.90
112.87
39.52 Dimethyl Sulfoxide-d6
33.28
f1 (ppm)

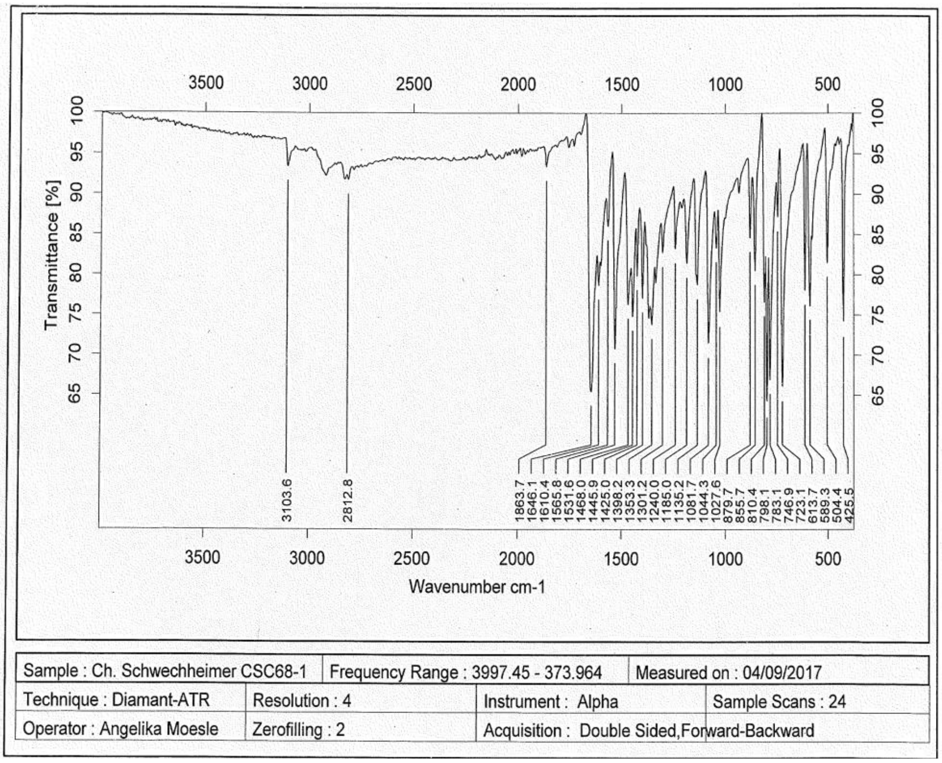

COSY
(2.50,2.50) Dimethyl Sulfoxide-d6
f2 (ppm)
f1 (ppm)



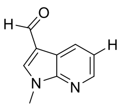
MAT 95, +EI,Que 150, dir offen
moe
9/4/2017 2:19:48 PM
Ch.Schwechheimer
CSC68-1
AK Wagenknecht
csc681 #1-3 RT: 0.12-0.29 AV: 3 NL: 3.63E5
T: + c EI Full ms [49.50-500.50]
Relative Abundance
m/z
237.1
239.1
236.1
231.1
243.1
262.1
240.1
229.1
225.2
226.1
232.2
235.3
241.2
244.1
245.2
251.3
252.3
255.3
256.2
259.2
264.4



9/4/2017 2:25:31 PM
File recalibrated by CMass.
csc681-c4 #9 RT: 0.81 AV: 1 NL: 3.06E5
T: + c EI Full ms [49.41-500.41]
236.9788
C10 H8 O1 N1 79Br1 = 236.9789
-0.1400 mmu
Relative Abundance
m/z



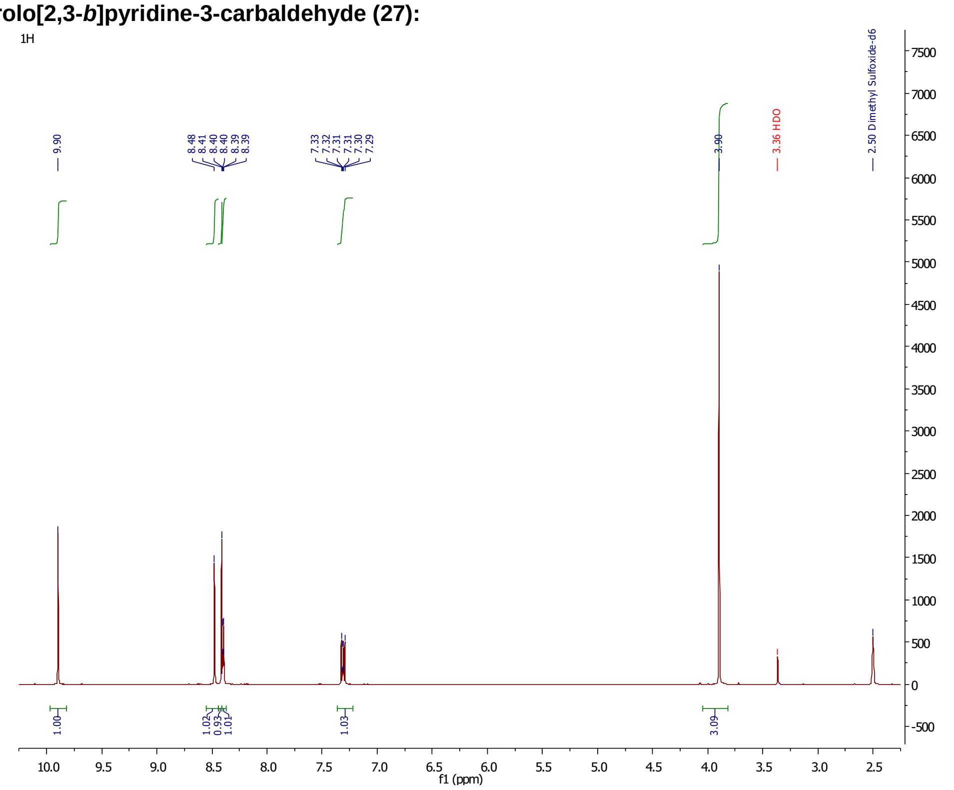
1-methyl-1*H*-pyrrolo[2,3-*b*]pyridine-3-carbaldehyde (27):

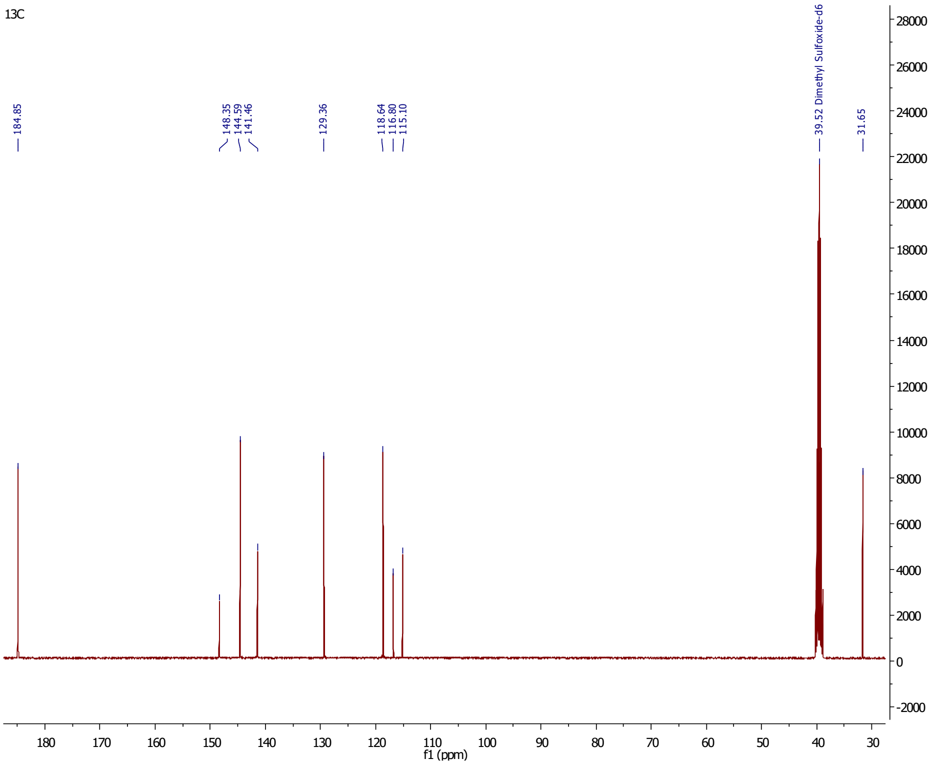


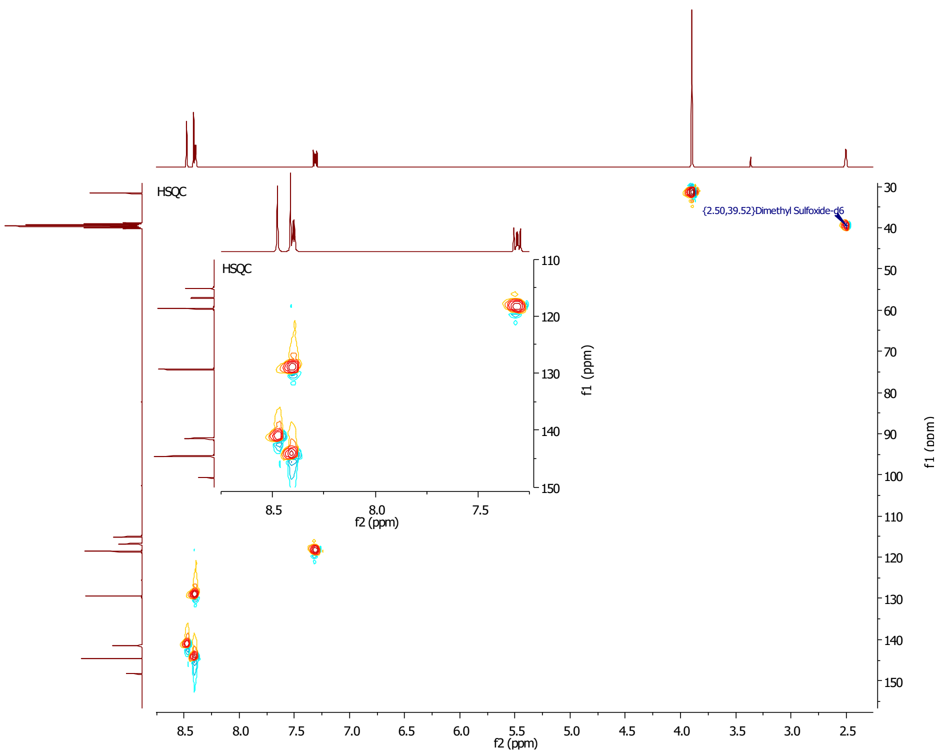
27

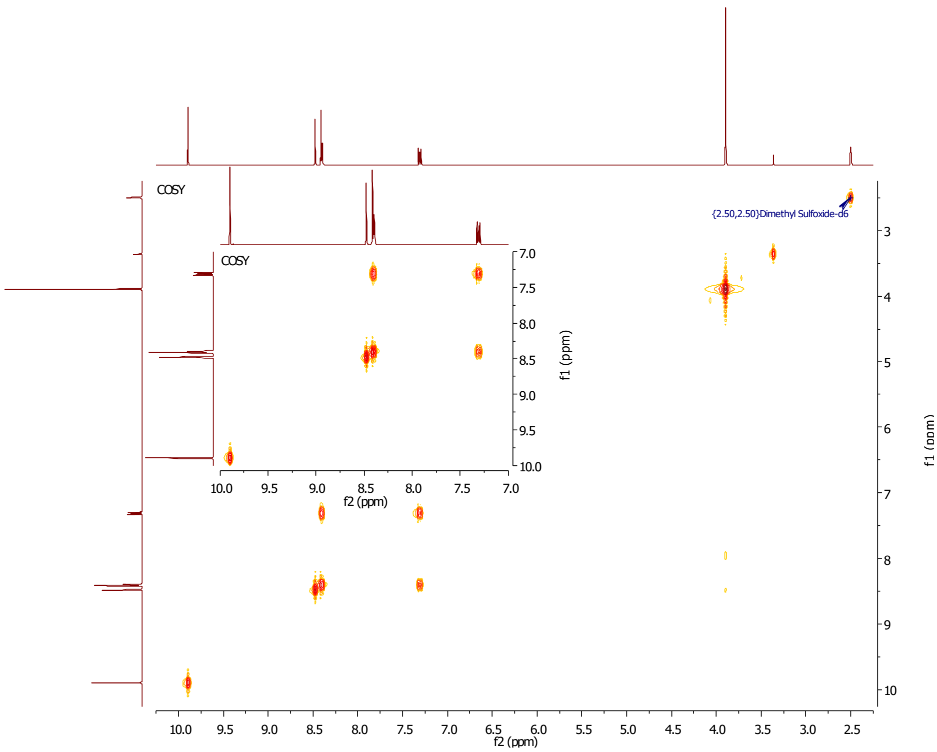
$C_9H_8N_2O$

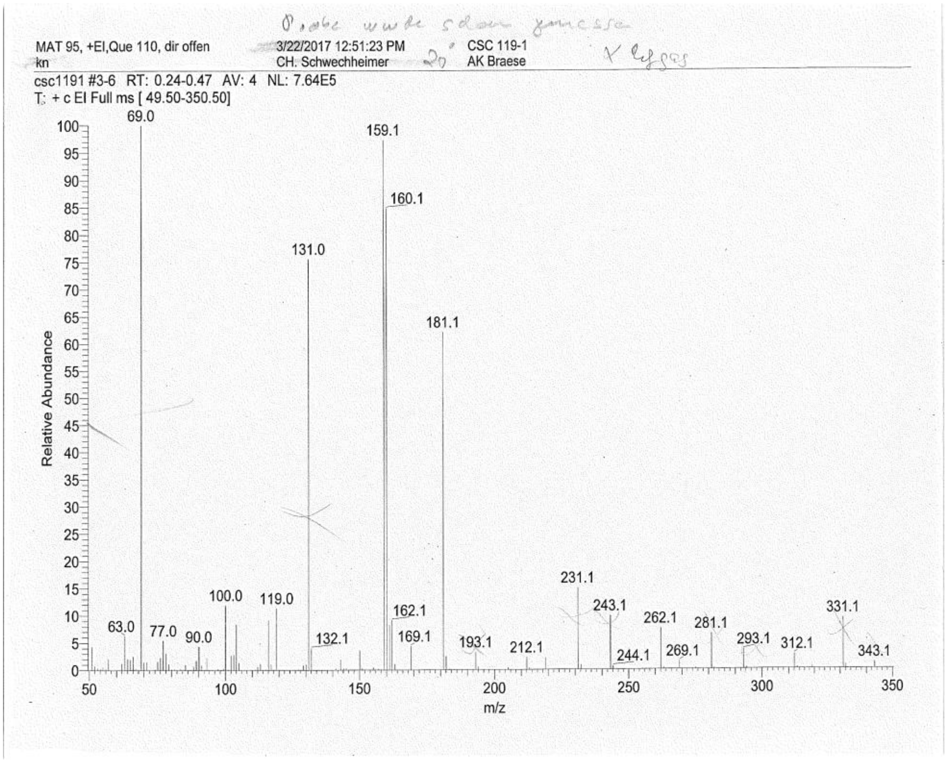
160.1760 g/mol

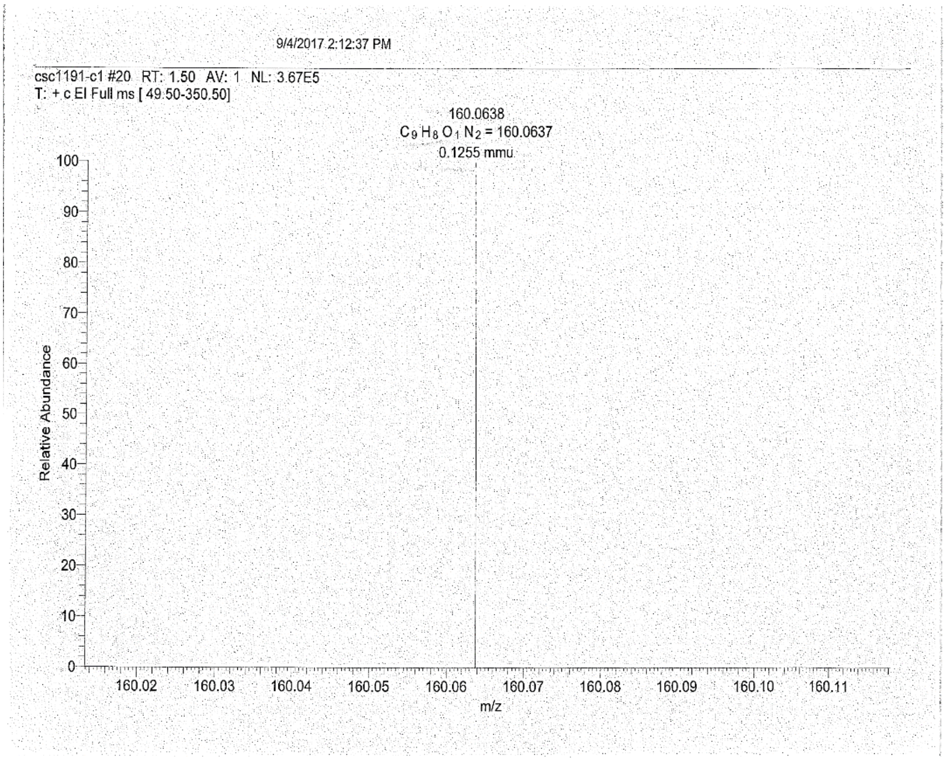


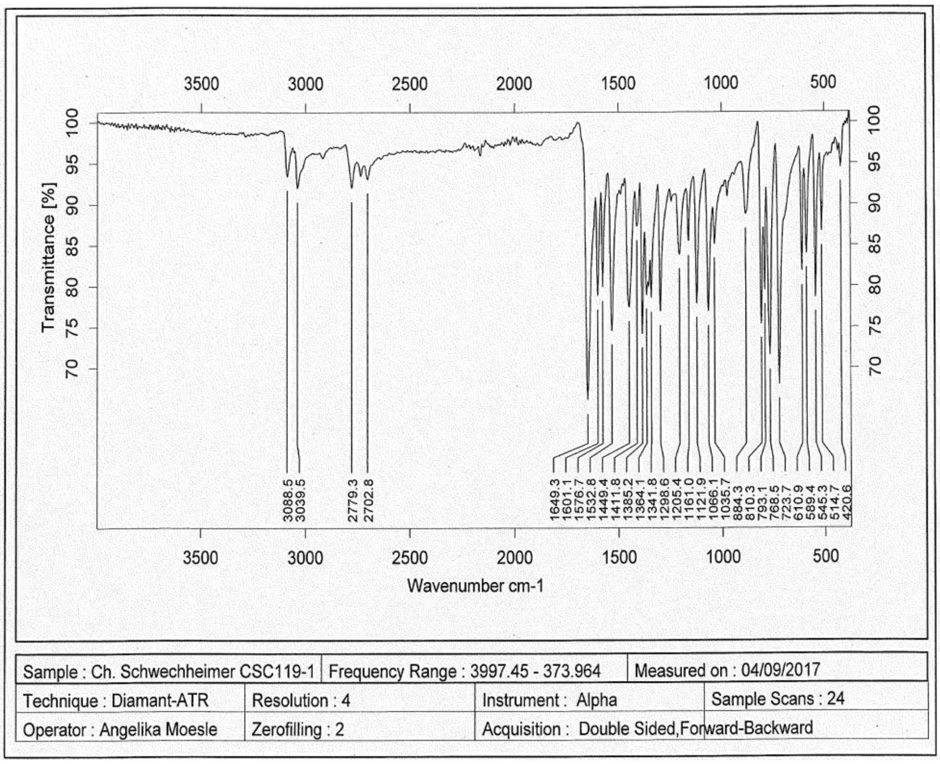

13C
184.85
148.35
144.59
141.46
129.36
118.64
116.80
115.10
39.52 Dimethyl Sulfoxide-d6
31.65
f1 (ppm)


HSQC
{2.50,39.52}Dimethyl Sulfoxide-d6
f1 (ppm)
f2 (ppm)

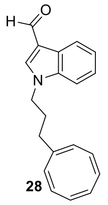

COSY
{2.50,2.50}Dimethyl Sulfoxide-d6
f2 (ppm)
f1 (ppm)


MAT 95, +EI,Que 110, dir offen
kn
3/22/2017 12:51:23 PM
CH. Schwechheimer
CSC 119-1
AK Braese
csc1191 #3-6 RT: 0.24-0.47 AV: 4 NL: 7.64E5
T: + c EI Full ms [49.50-350.50]
Relative Abundance
m/z


9/4/2017 2:12:37 PM
csc1191-c1 #20 RT: 1.50 AV: 1 NL: 3.67E5
T: + c EI Full ms [49.50-350.50]
160.0638
C9 H8 O1 N2 = 160.0637
0.1255 mmu
Relative Abundance
m/z

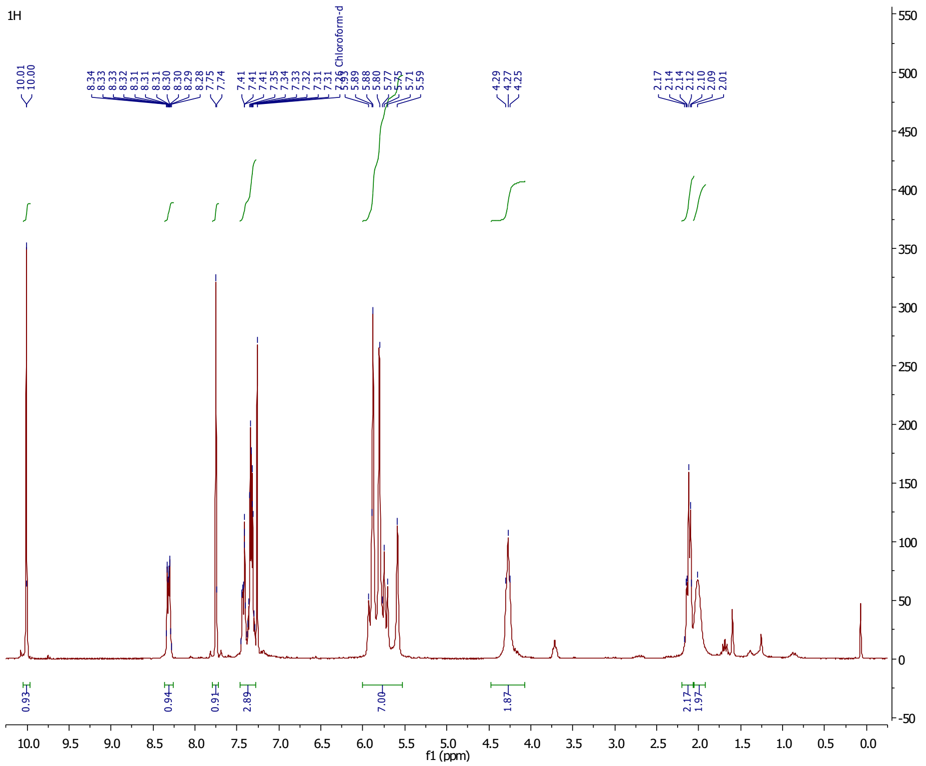

Transmittance [%]
Wavenumber cm-1
3088.5
3039.5
2779.3
2702.8
1649.3
1601.1
1576.7
1532.8
1449.4
1411.8
1385.2
1364.1
1341.8
1298.6
1205.4
1161.0
1121.9
1066.1
1035.7
884.3
810.3
793.1
768.5
723.7
610.9
589.4
545.3
514.7
420.6
Sample : Ch. Schwechheimer CSC119-1
Frequency Range : 3997.45 - 373.964
Measured on : 04/09/2017
Technique : Diamant-ATR
Resolution : 4
Instrument : Alpha
Sample Scans : 24
Operator : Angelika Moesle
Zerofilling : 2
Acquisition : Double Sided,Forward-Backward

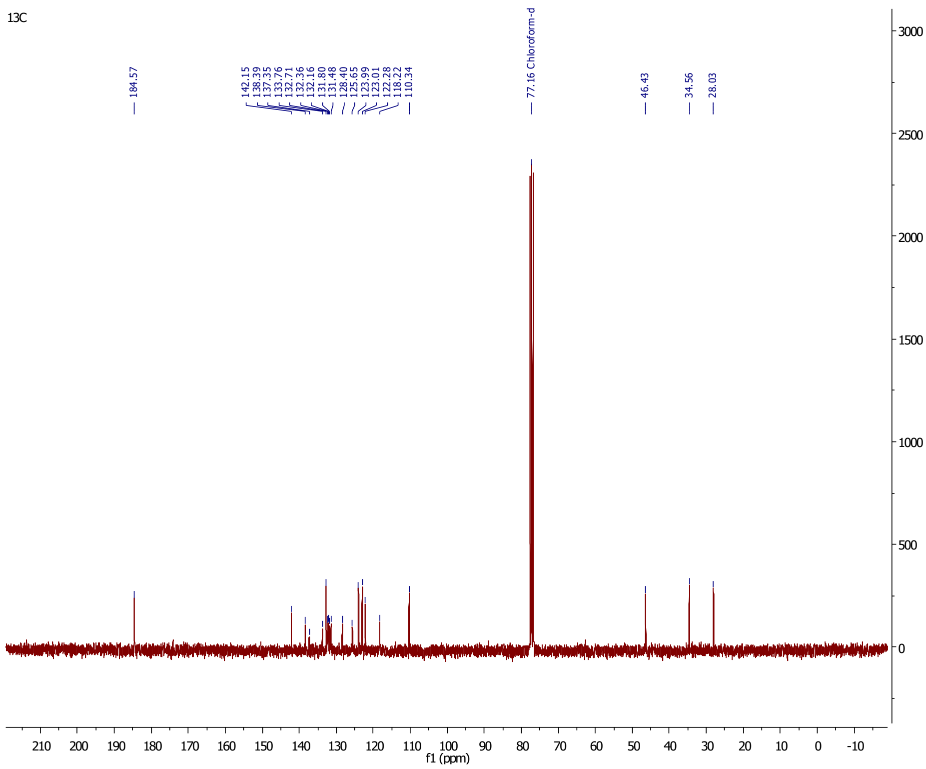
1-(3-((1*Z*,3*Z*,5*Z*,7*Z*)-cycloocta-1,3,5,7-tetraen-1-yl)propyl)-1*H*-indole-3-carbaldehyde (28):

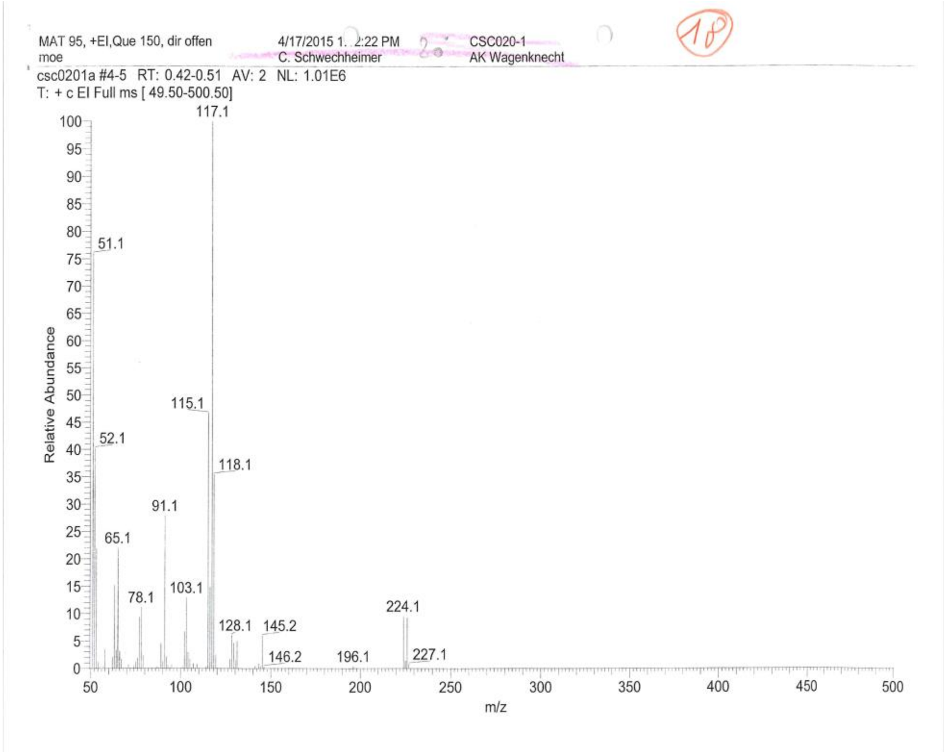


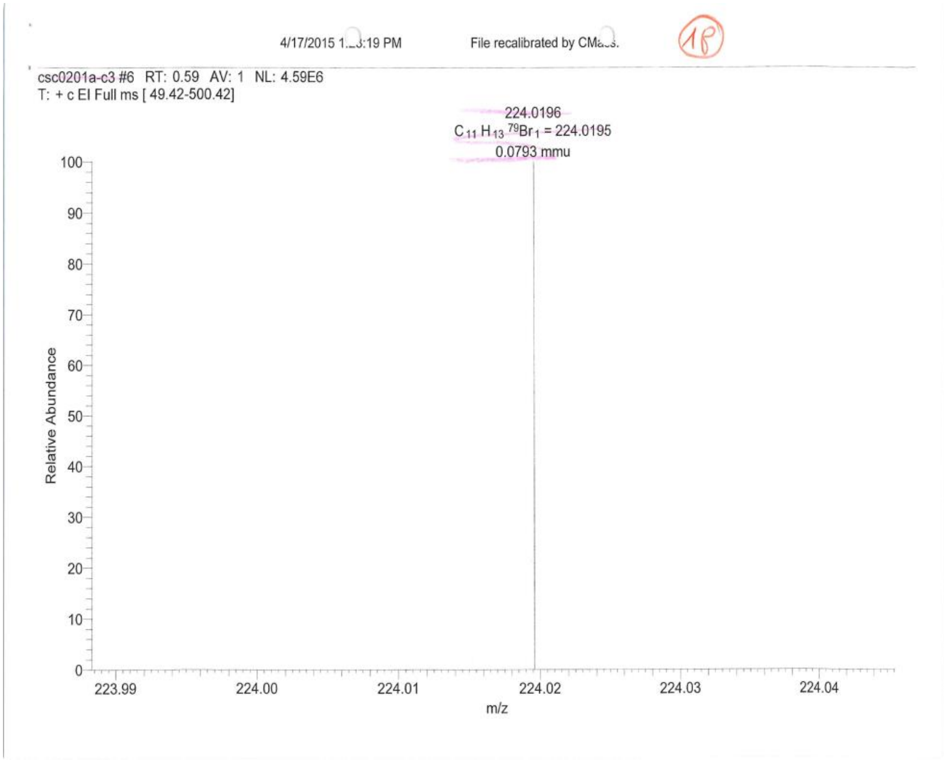
28

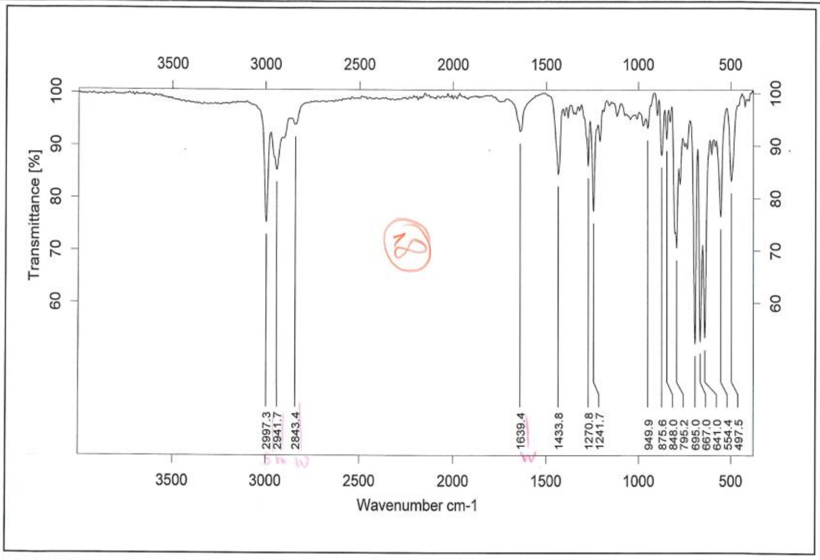
$C_{20}H_{19}NO$
289.3780 g/mol






MAT 95, +EI,Que 150, dir offen
moe
4/17/2015 1. 2:22 PM
C. Schwechheimer
CSC020-1
AK Wagenknecht
18
csc0201a #4-5 RT: 0.42-0.51 AV: 2 NL: 1.01E6
T: + c EI Full ms [49.50-500.50]
117.1
51.1
115.1
52.1
118.1
91.1
65.1
103.1
78.1
224.1
128.1
145.2
146.2
196.1
227.1
Relative Abundance
m/z


4/17/2015
File recalibrated by CMass.
18
csc0201a-c3 #6 RT: 0.59 AV: 1 NL: 4.59E6
T: + c EI Full ms [49.42-500.42]
224.0196
C 11 H 13 79Br 1 = 224.0195
0.0793 mmu
Relative Abundance
m/z

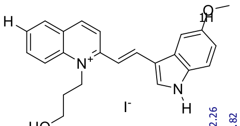


Sample : Schwechtheimer CSC020-1	Frequency Range : 3997.41 - 373.828		Measured on : 27/03/2015
Technique : ATR platinum Diar	Resolution : 4	Instrument : Alpha	Sample Scans : 24
Operator : Ingrid Rossnagel	Zerofilling : 2	Acquisition : Double Sided,For	

c. Analytics of the Dyes 1-12

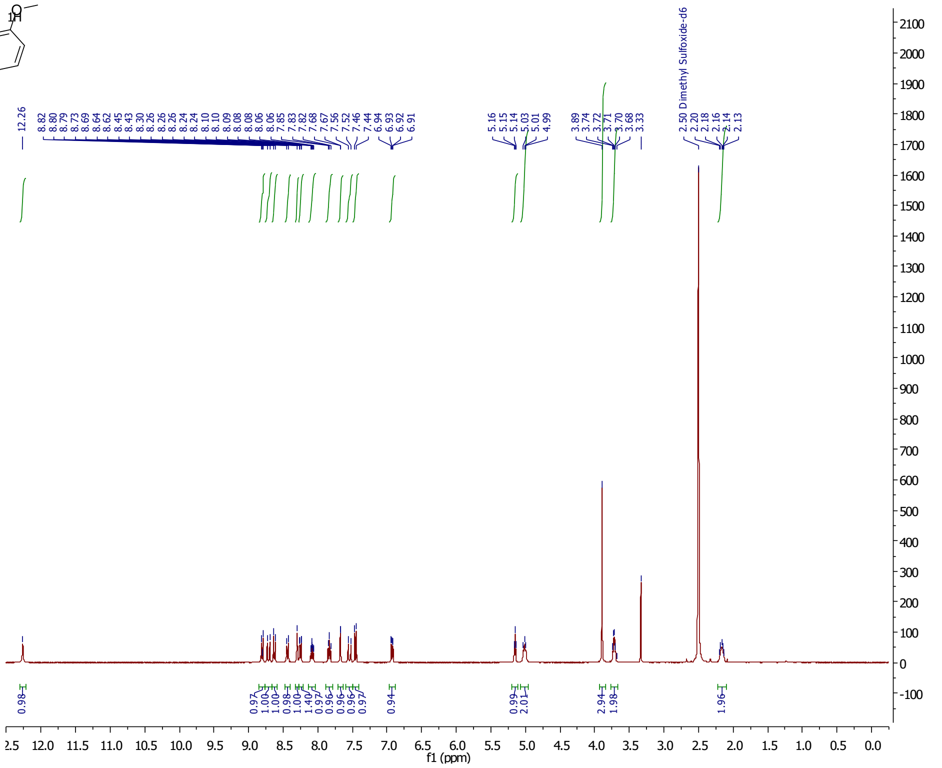
The analytics of the compounds **1** and **2** are described in earlier publications of our working group.[1-2]

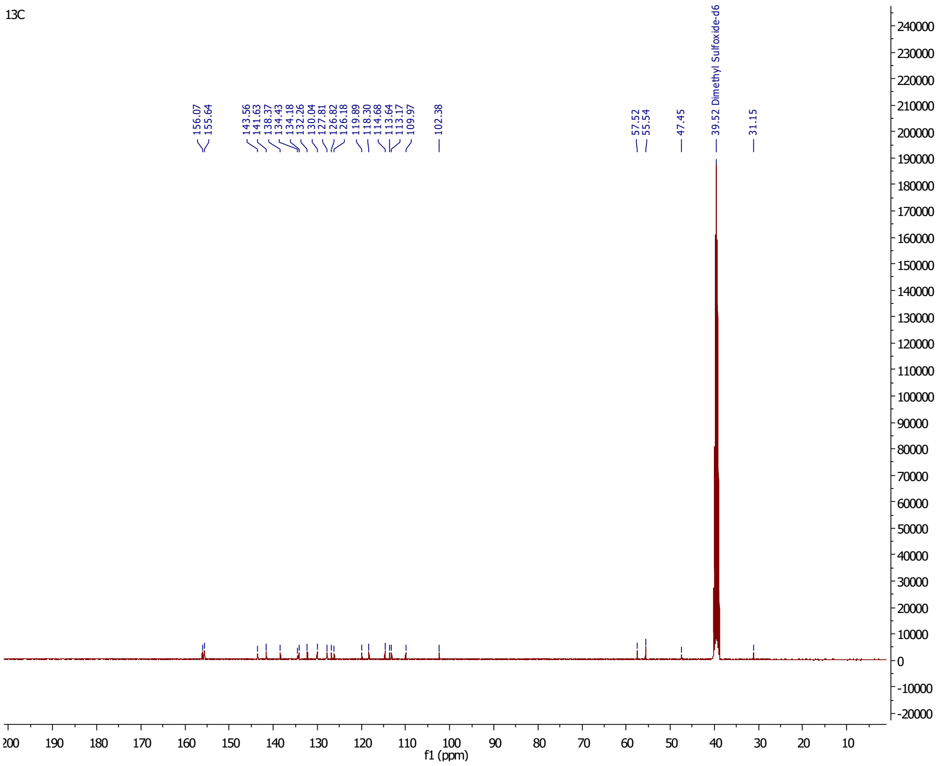
(*E*)-1-(3-hydroxypropyl)-2-(2-(5-methoxy-1*H*-indol-3-yl)vinyl)quinolin-1-ium iodide (3):

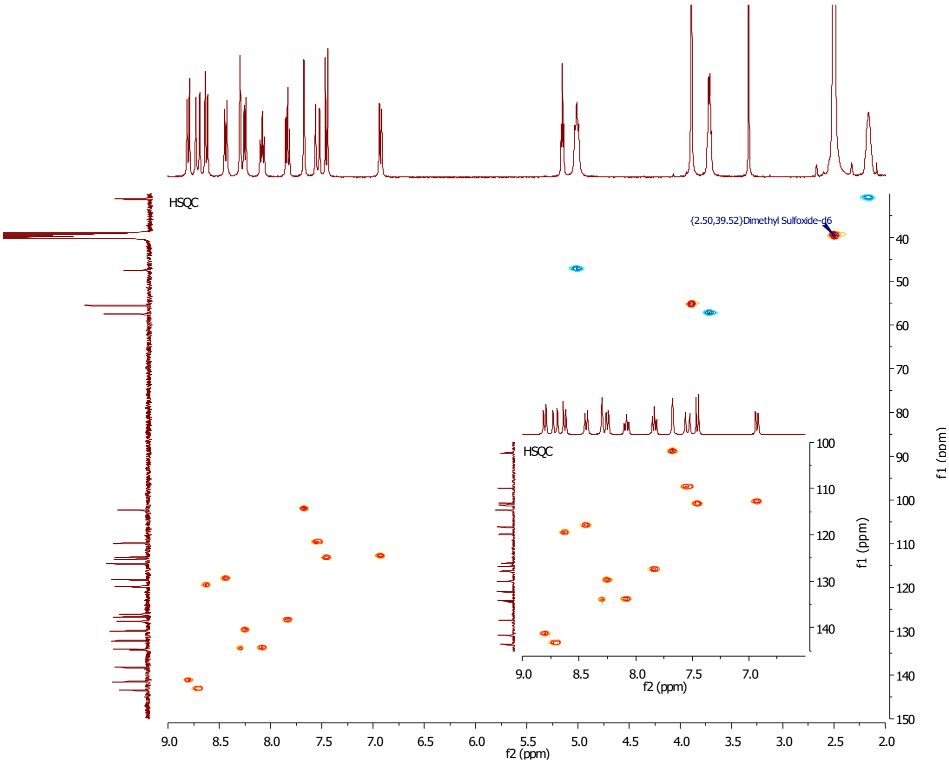


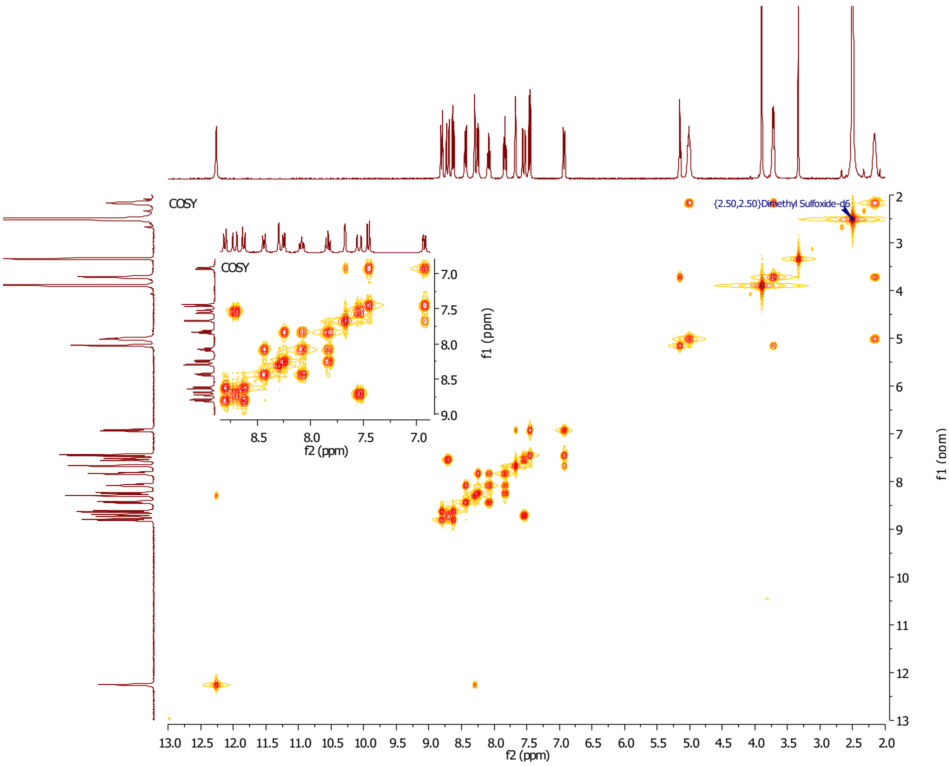
3

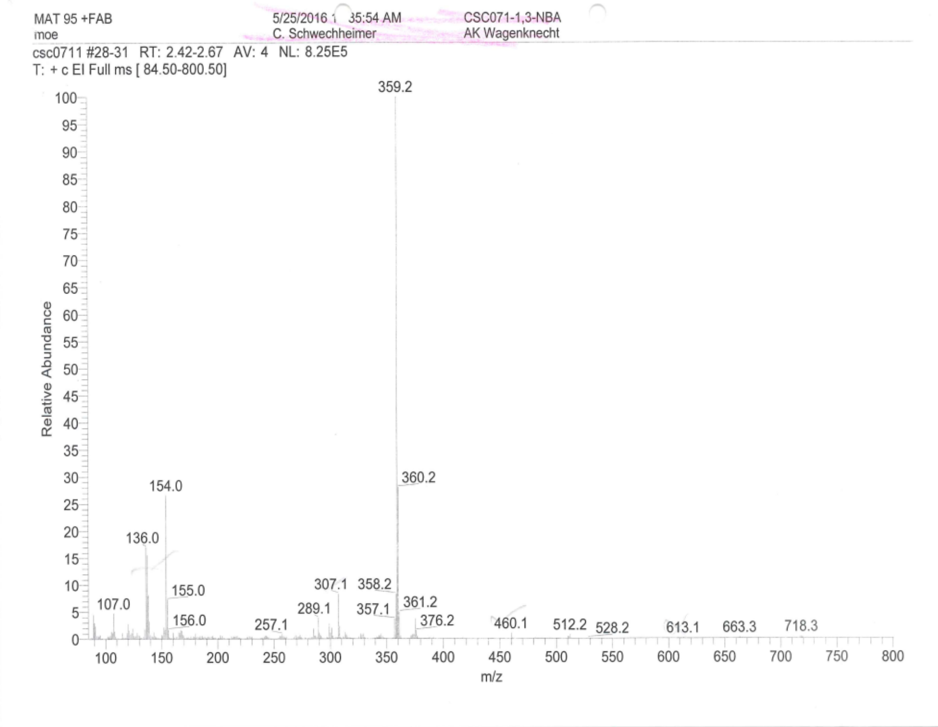
$C_{23}H_{23}IN_2O_2$
486.3535 g/mol



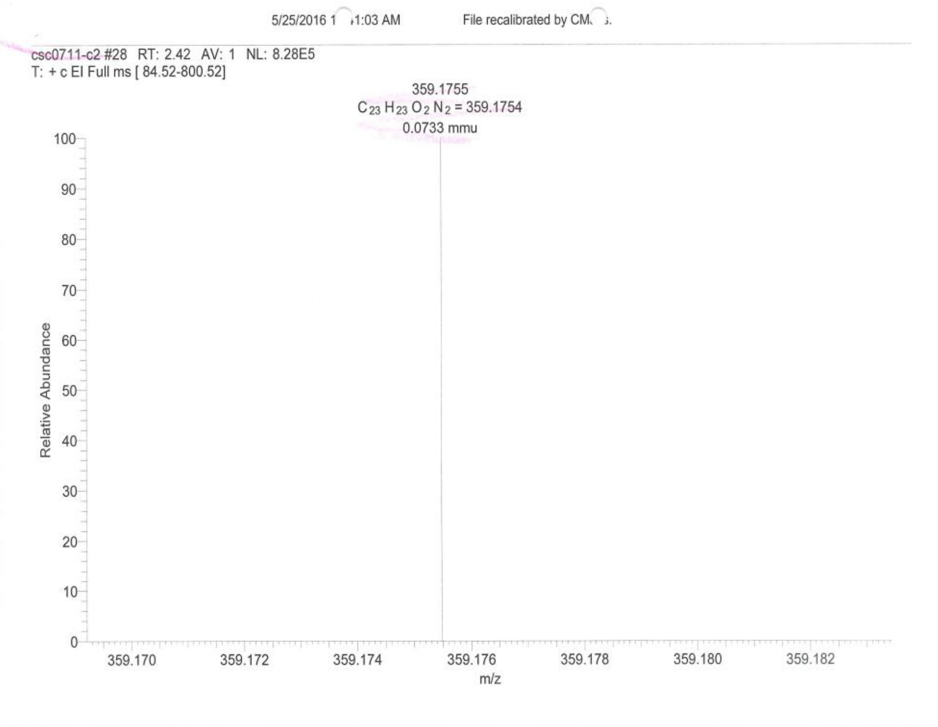



HSQC
{2.50,39.52}Dimethyl Sulfoxide-d6
HSQC
f2 (ppm)
f1 (ppm)

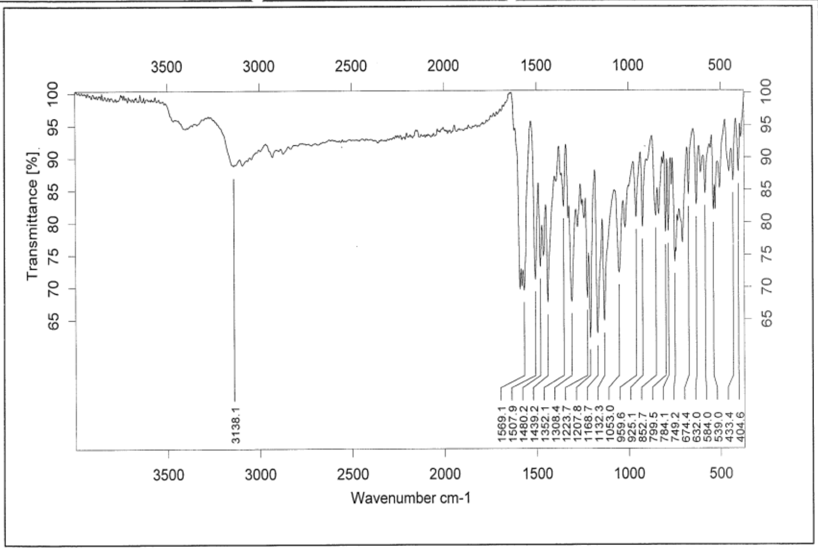

COSY
{2.50,2.50}Dimethyl Sulfoxide-d6
COSY
f2 (ppm)
f1 (ppm)



MAT 95 +FAB
moe
5/25/2016 1 35:54 AM
C. Schwechheimer
CSC071-1,3-NBA
AK Wagenknecht
csc0711 #28-31 RT: 2.42-2.67 AV: 4 NL: 8.25E5
T: + c EI Full ms [84.50-800.50]
Relative Abundance
m/z
359.2
360.2
154.0
136.0
155.0
156.0
107.0
257.1
289.1
307.1
358.2
357.1
361.2
376.2
460.1
512.2
528.2
613.1
663.3
718.3



5/25/2016 1 1:03 AM
File recalibrated by CM.
csc0711-c2 #28 RT: 2.42 AV: 1 NL: 8.28E5
T: + c EI Full ms [84.52-800.52]
359.1755
C23 H23 O2 N2 = 359.1754
0.0733 mmu
Relative Abundance
m/z



Sample : C. Schwechheimer CSC 071-1	Frequency Range : 3997.41 - 373.828		Measured on : 02/06/2016
Technique : ATR platinum Diar	Resolution : 4	Instrument : Alpha	Sample Scans : 24
Operator : Angelika Moesle	Zerofilling : 2	Acquisition : Double Sided,For	

ELEMENTARANALYSE

Auftraggeber:

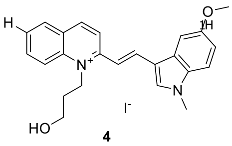
Christian Schwechheimer, Tel.: 47212, Raum 205, AK Wagenknecht

Substanzbezeichnung: CSC 071-1

Summenformel: $C_{23}H_{23}IN_2O_2$

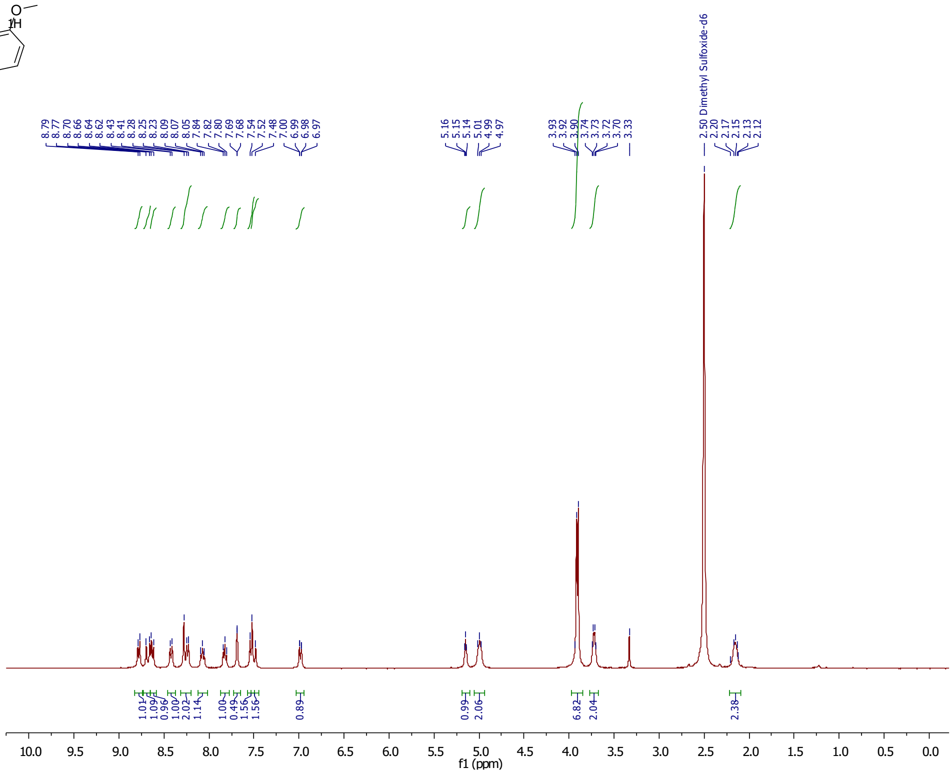
Berechnet:	N:	5.76	C:	56.80
	H:	4.77	~~S:~~	I: 26.09 O: 6.58
Gefunden:	N:	5,75	C:	56,56
x / e	H:	4,71	S:	
	N:	5,72	C:	56,68
	H:	4,71	S:	

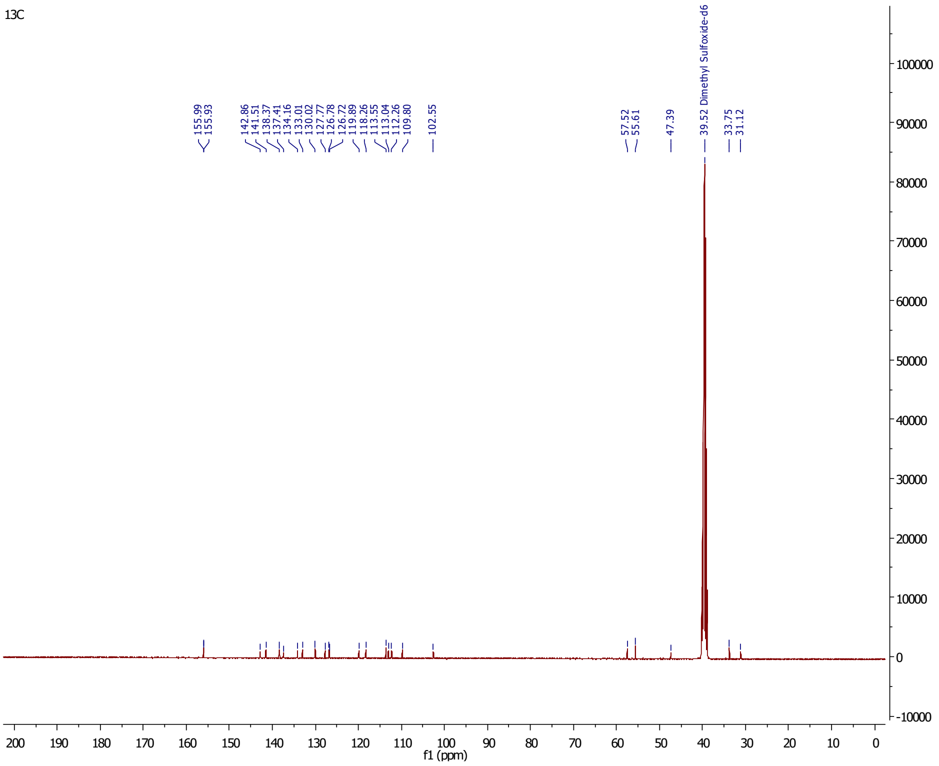
(*E*)-1-(3-hydroxypropyl)-2-(2-(5-methoxy-1-methyl-1*H*-indol-3-yl)vinyl)quinolin-1-ium iodide (4):

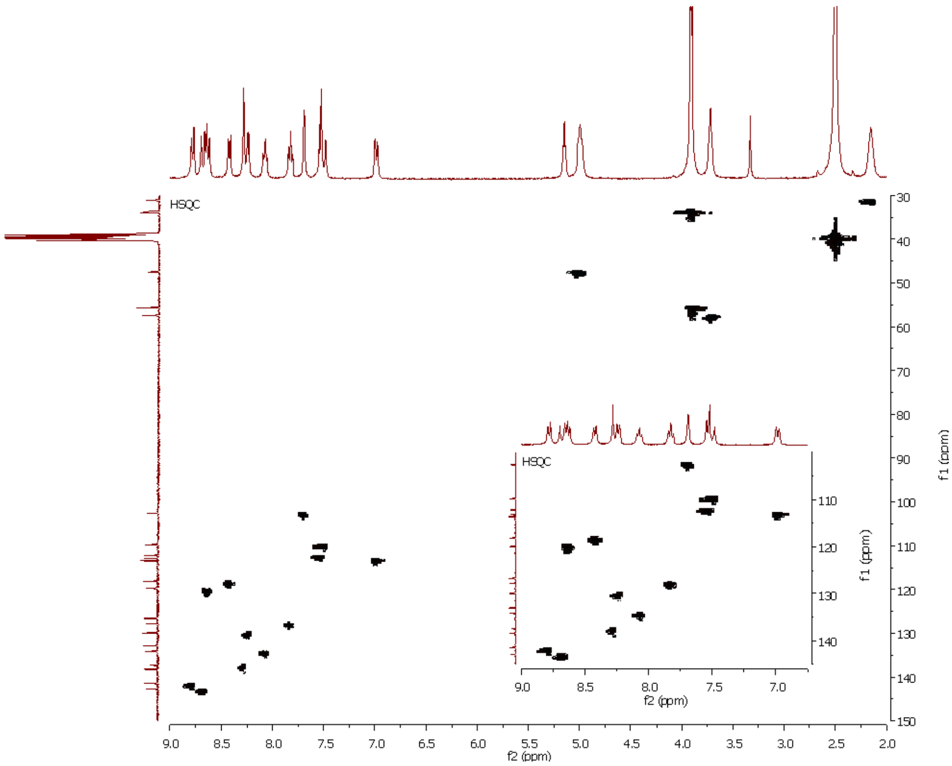


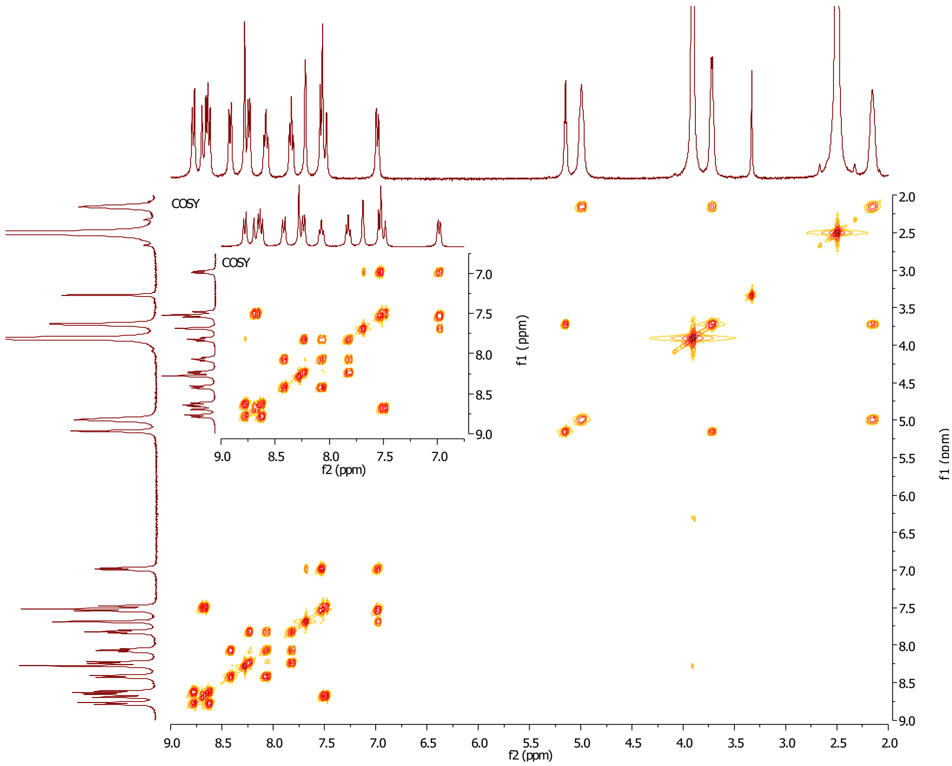
4

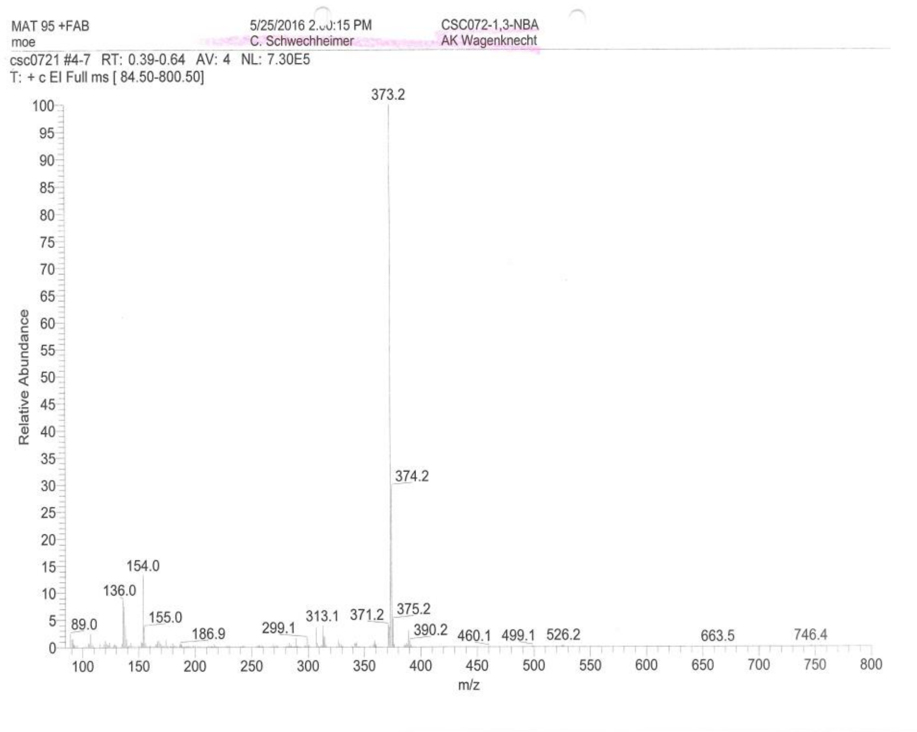
$C_{24}H_{25}IN_2O_2$
500.3805 g/mol

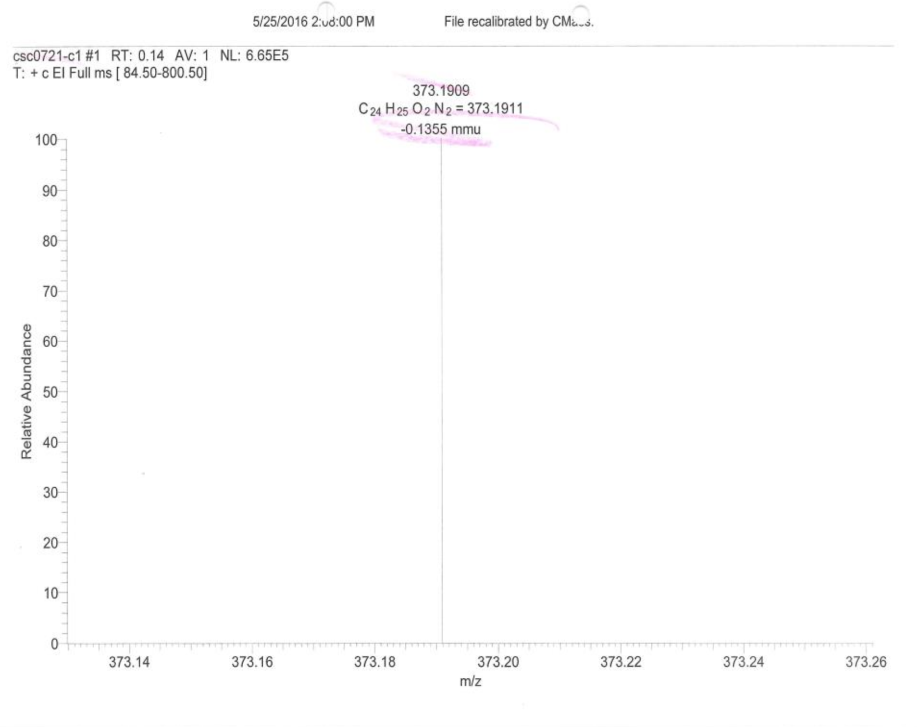


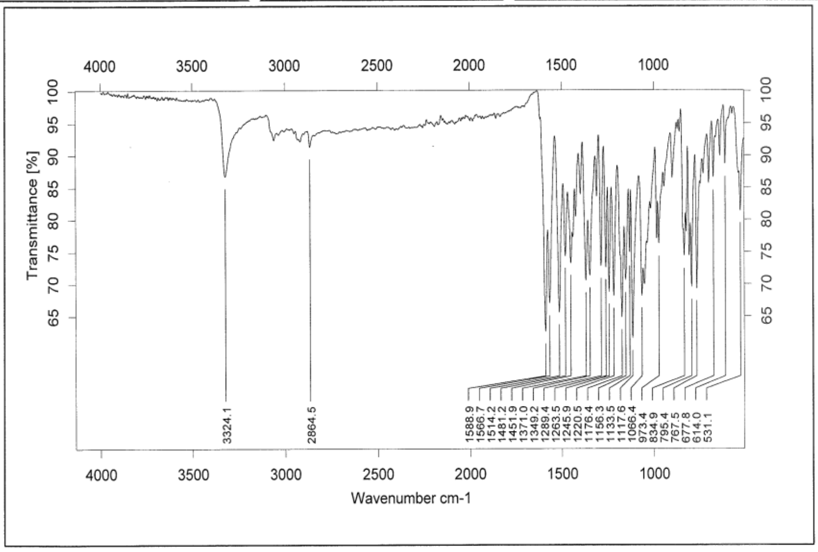



HSQC
f1 (ppm)
f2 (ppm)


COSY
f1 (ppm)
f2 (ppm)


MAT 95 +FAB
moe
5/25/2016 2:00:15 PM
C. Schwechheimer
CSC072-1,3-NBA
AK Wagenknecht
csc0721 #4-7 RT: 0.39-0.64 AV: 4 NL: 7.30E5
T: + c EI Full ms [84.50-800.50]
Relative Abundance
m/z
373.2
374.2
154.0
136.0
155.0
89.0
186.9
299.1
313.1
371.2
375.2
390.2
460.1
499.1
526.2
663.5
746.4


5/25/2016 2:08:00 PM
File recalibrated by CMass.
csc0721-c1 #1 RT: 0.14 AV: 1 NL: 6.65E5
T: + c EI Full ms [84.50-800.50]
373.1909
$C_{24}H_{25}O_2N_2$ = 373.1911
-0.1355 mmu
Relative Abundance
m/z



Sample : C. Schwechheimer CSC 072-1	Frequency Range : 3997.41 - 373.828		Measured on : 01/06/2016
Technique : ATR platinum Dian	Resolution : 4	Instrument : Alpha	Sample Scans : 24
Operator : Angelika Moesle	Zerofilling : 2	Acquisition : Double Sided,For	

ELEMENTARANALYSE

Auftraggeber:

Christian Schwechheimer, Tel.: 47212, Raum 205, AK Wagenknecht

Substanzbezeichnung: CSC072-1

Summenformel: $C_{24}H_{25}IN_2O_2$

Berechnet: N: 5.60 C: 57.61

H: 5.04 ~~S:~~ I: 25.36 O: 6.39

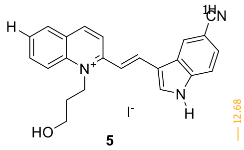
Gefunden: N: 5,59 C: 57,55

H: 4,97 S:

N: 5,57 C: 57,48

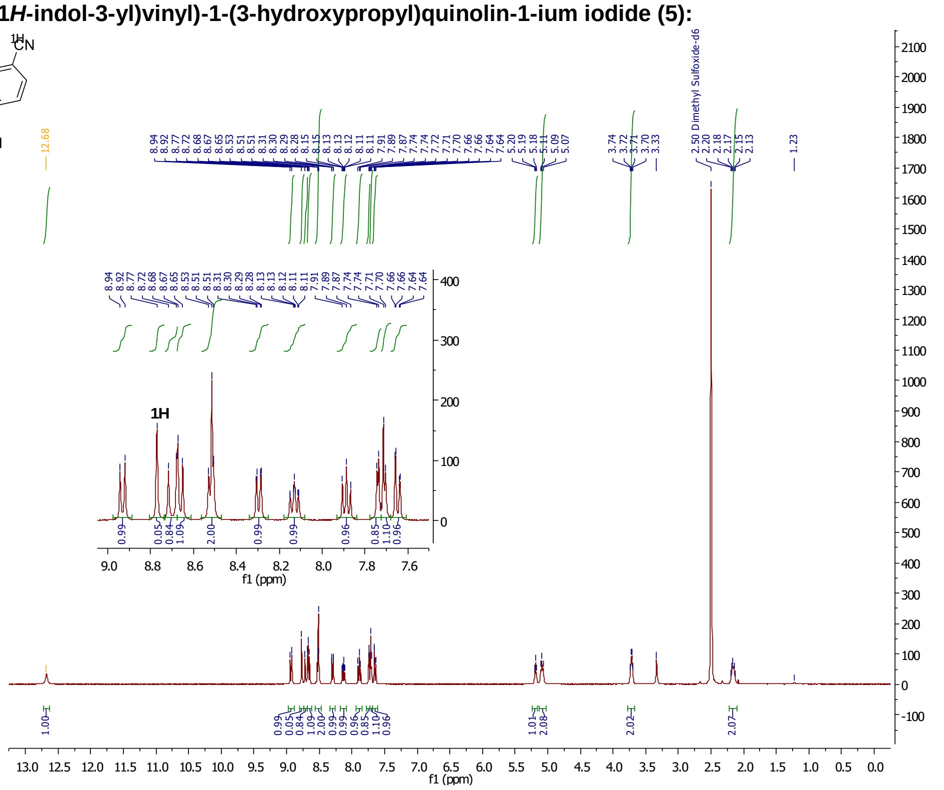
H: 5,00 S:

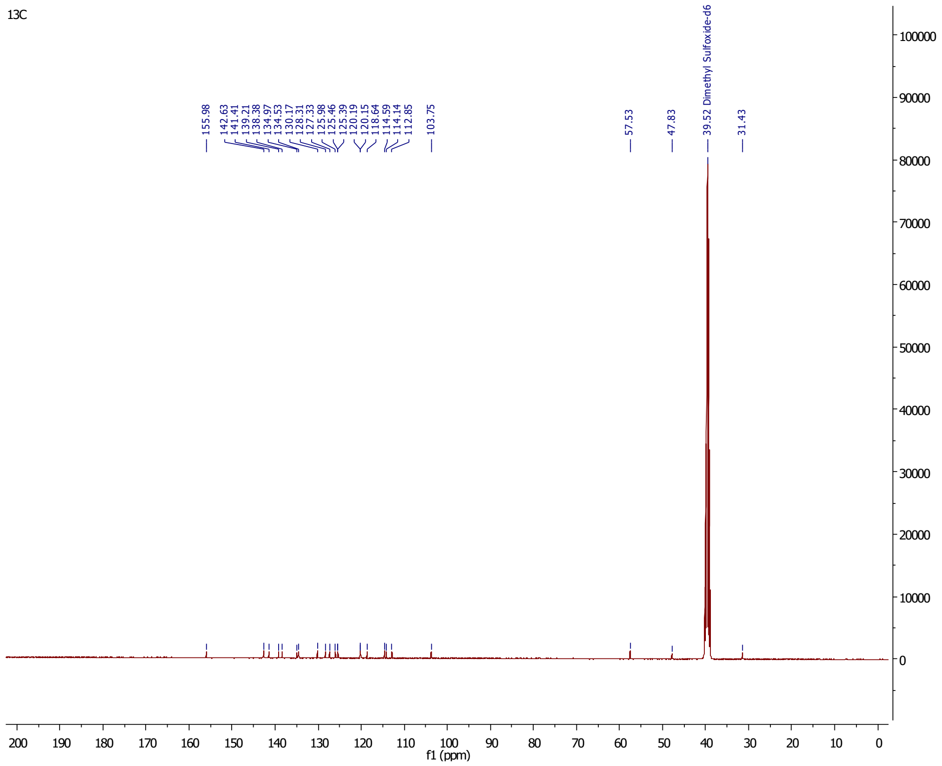
(*E*)-2-(2-(5-cyano-1*H*-indol-3-yl)vinyl)-1-(3-hydroxypropyl)quinolin-1-ium iodide (5):

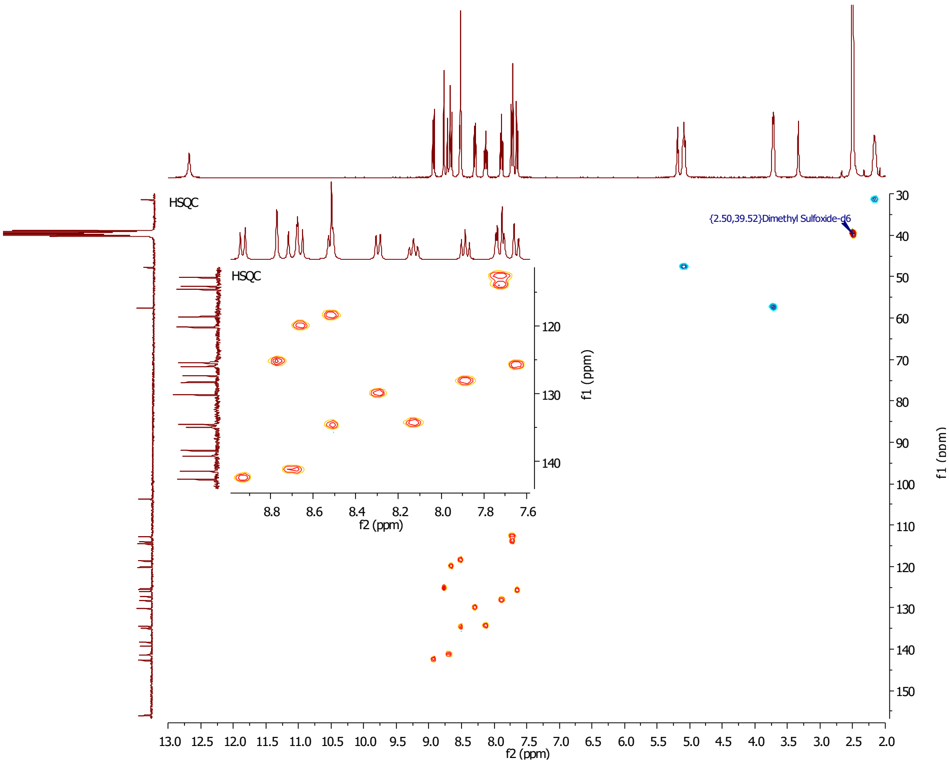


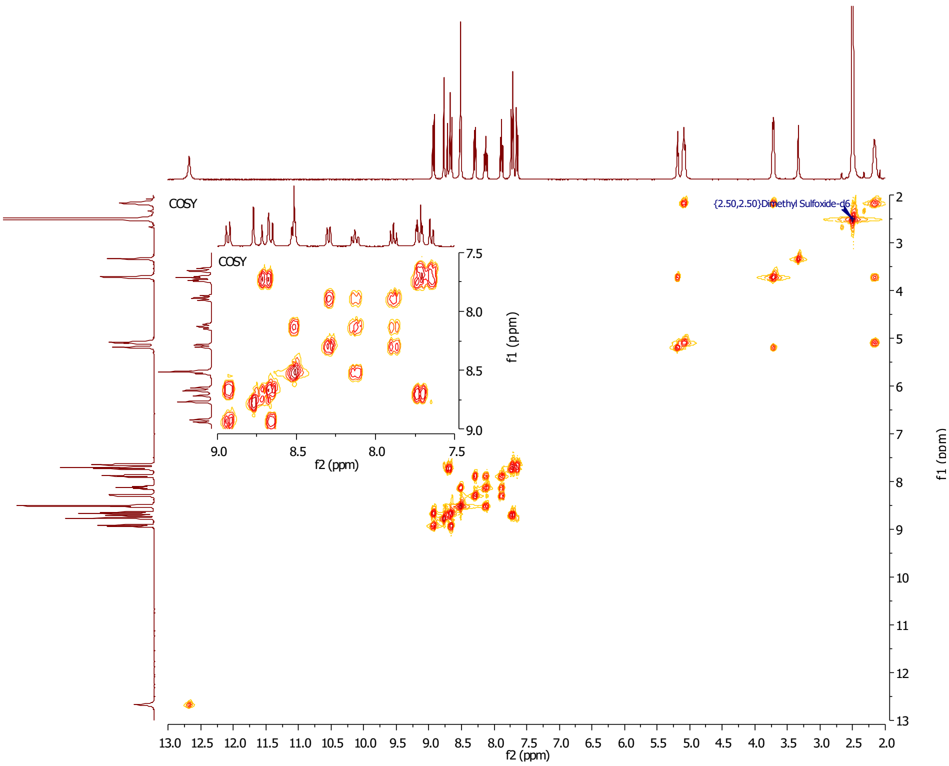
5

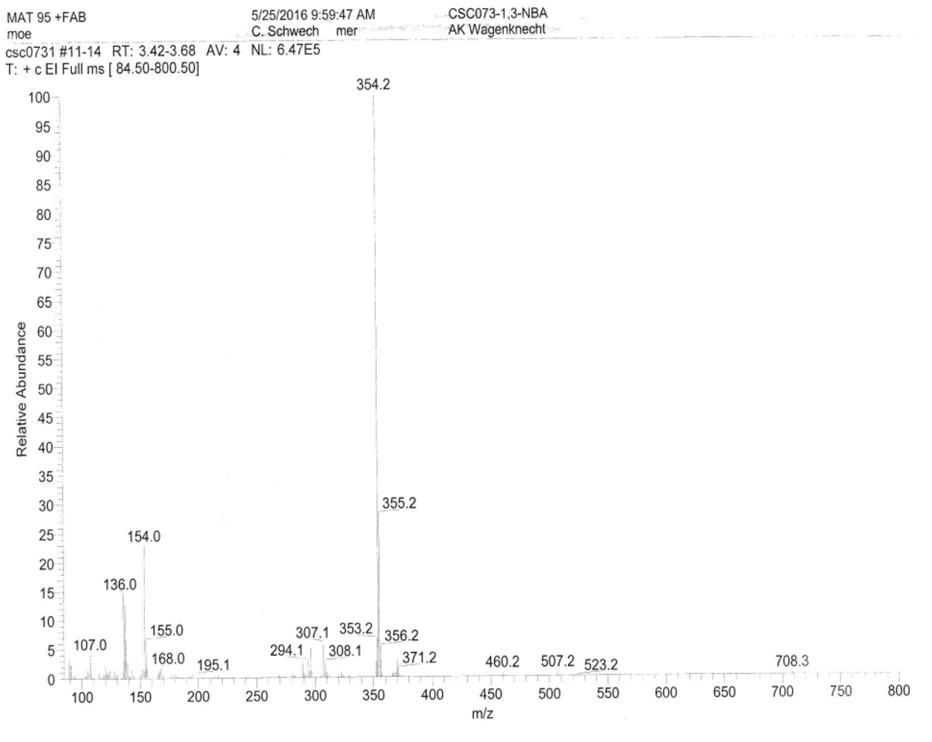
$C_{23}H_{20}IN_3O$
481.3375 g/mol

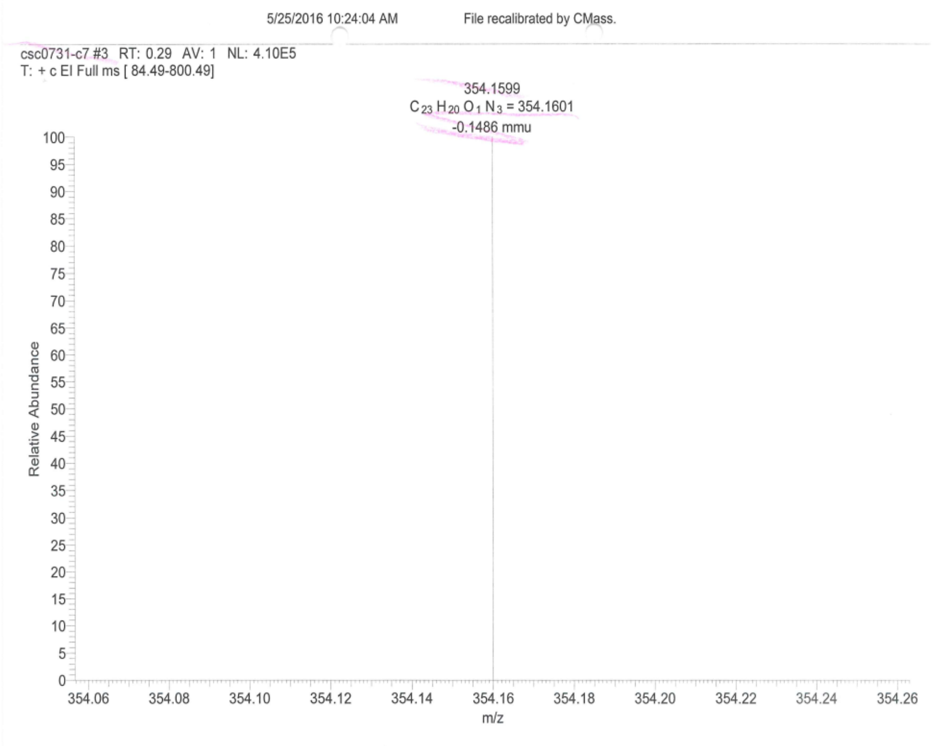


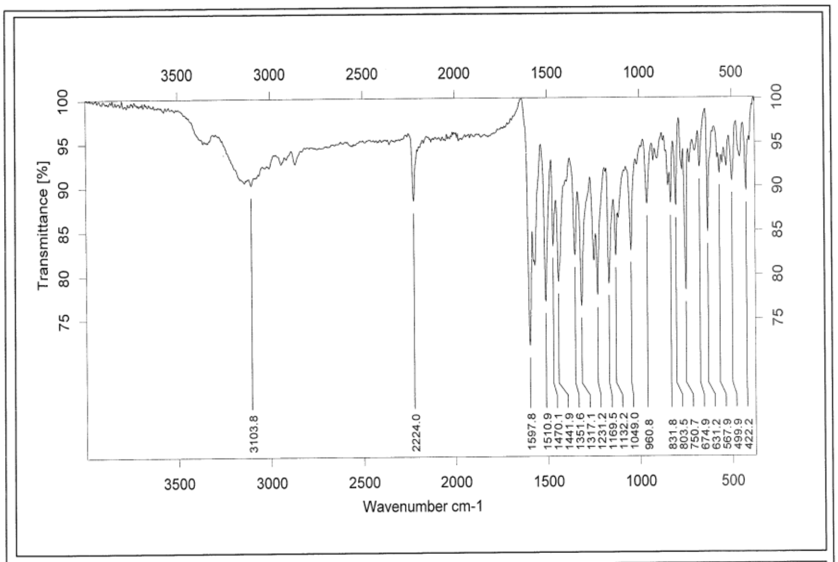



HSQC
{2.50,39.52}Dimethyl Sulfoxide-d6
f2 (ppm)
f1 (ppm)


COSY
{2.50,2.50}Dimethyl Sulfoxide-d6
f2 (ppm)
f1 (ppm)


MAT 95 +FAB
moe
5/25/2016 9:59:47 AM
C. Schwech mer
CSC073-1,3-NBA
AK Wagenknecht
csc0731 #11-14 RT: 3.42-3.68 AV: 4 NL: 6.47E5
T: + c EI Full ms [84.50-800.50]
354.2
355.2
154.0
136.0
107.0
155.0
168.0
195.1
294.1
307.1
308.1
353.2
356.2
371.2
460.2
507.2
523.2
708.3
Relative Abundance
m/z


5/25/2016 10:24:04 AM
File recalibrated by CMass.
csc0731-c7 #3 RT: 0.29 AV: 1 NL: 4.10E5
T: + c EI Full ms [84.49-800.49]
354.1599
C23 H20 O1 N3 = 354.1601
-0.1486 mmu
Relative Abundance
m/z



Sample : C. Schwechheimer CSC 073-1	Frequency Range : 3997.41 - 373.828	Measured on : 02/06/2016
Technique : ATR platinum Diar	Resolution : 4	Instrument : Alpha	Sample Scans : 24
Operator : Angelika Moesle	Zerofilling : 2	Acquisition : Double Sided,For

ELEMENTARANALYSE

Auftraggeber:

Christian Schwechheimer, Tel.: 47212, Raum 205, AK Wagenknecht

Substanzbezeichnung: CSC073-1

Summenformel: $C_{23}H_{20}IN_{3}O$

Berechnet: N: 8.73 C: 57.39

H: 4.19 ~~S:~~ I: 26.36

O: 3.32

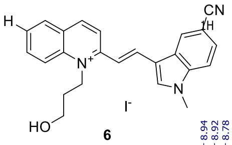
Gefunden: N: 8,68 C: 57,47

H: 4,05 S:

N: 8,75 C: 57,53

H: 4,10 S:

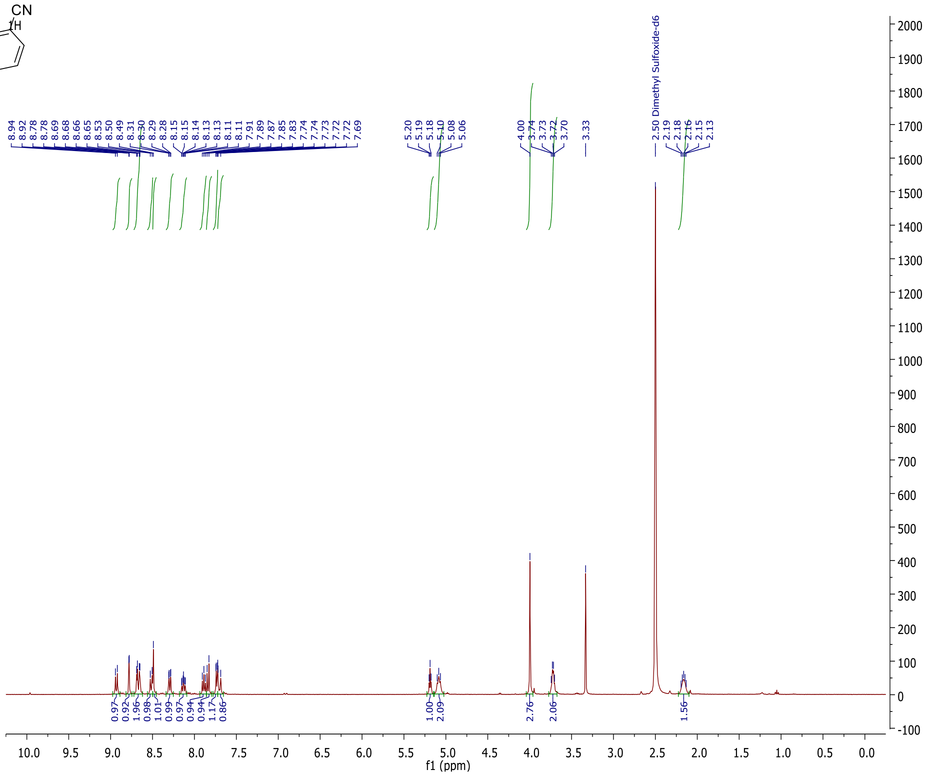
E)-2-(2-(5-cyano-1-methyl-1*H*-indol-3-yl)vinyl)-1-(3-hydroxypropyl)quinolin-1-ium iodide (6):

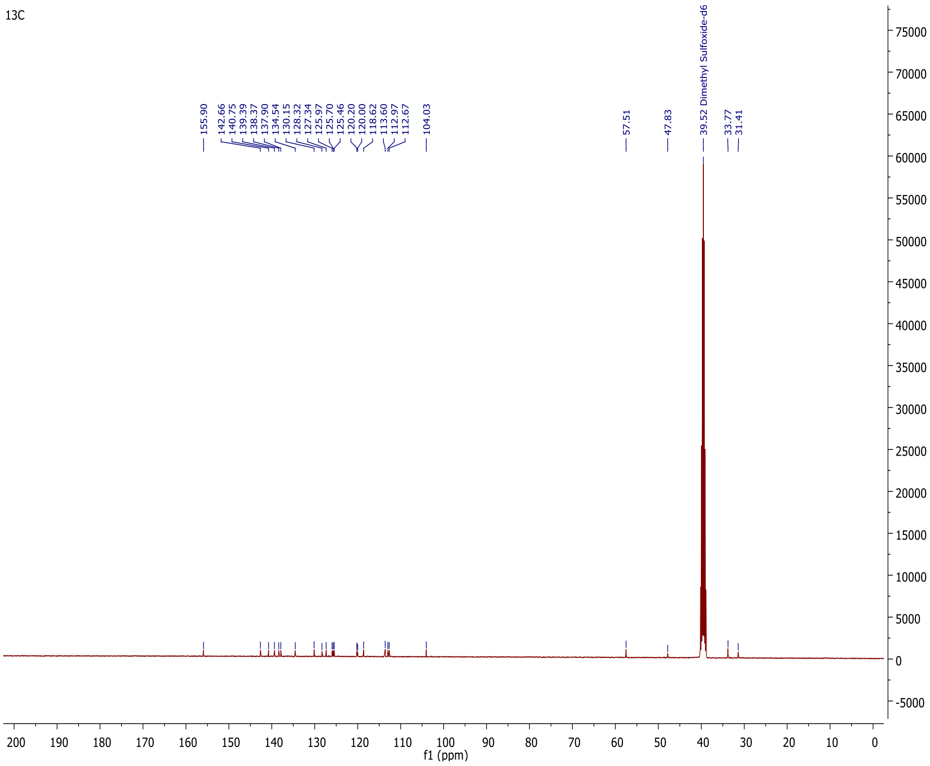


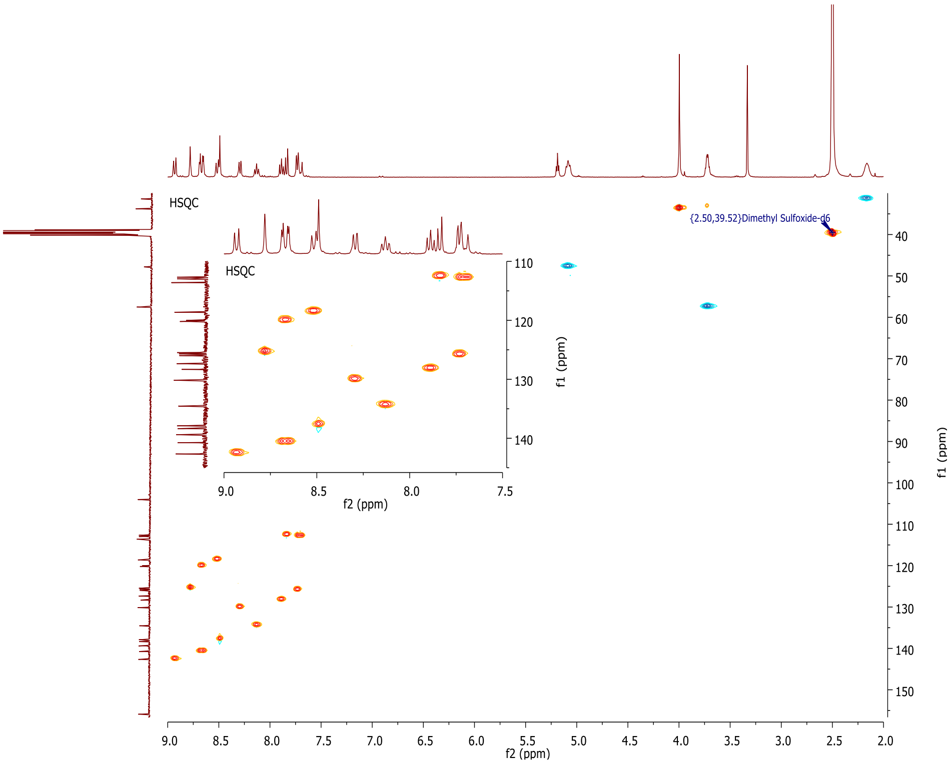
6

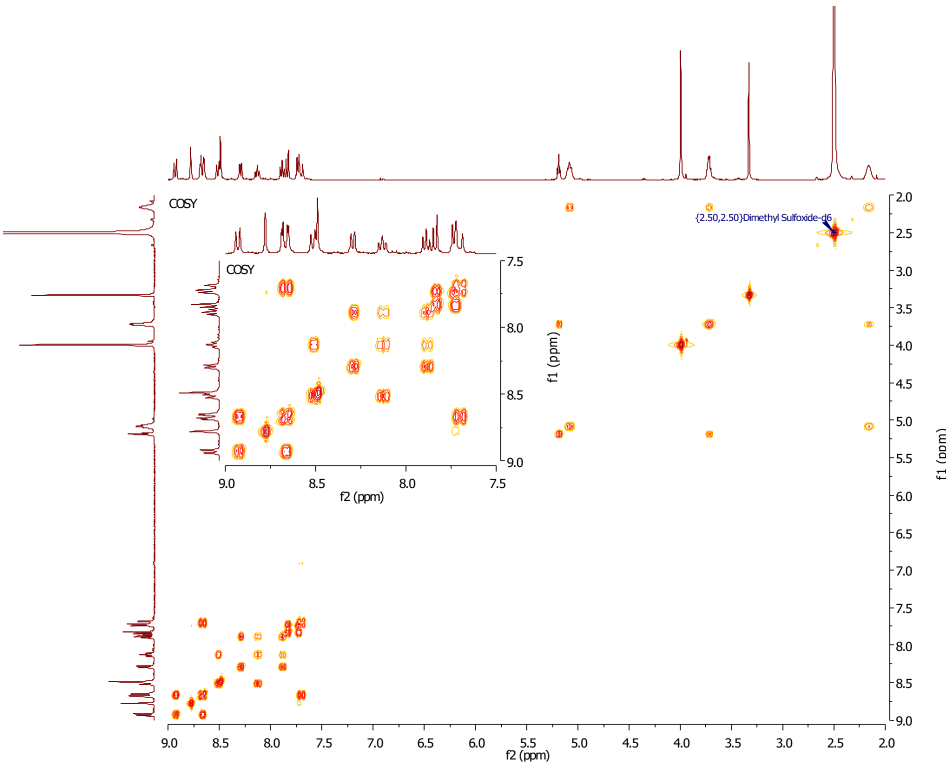
$C_{24}H_{22}IN_3O$

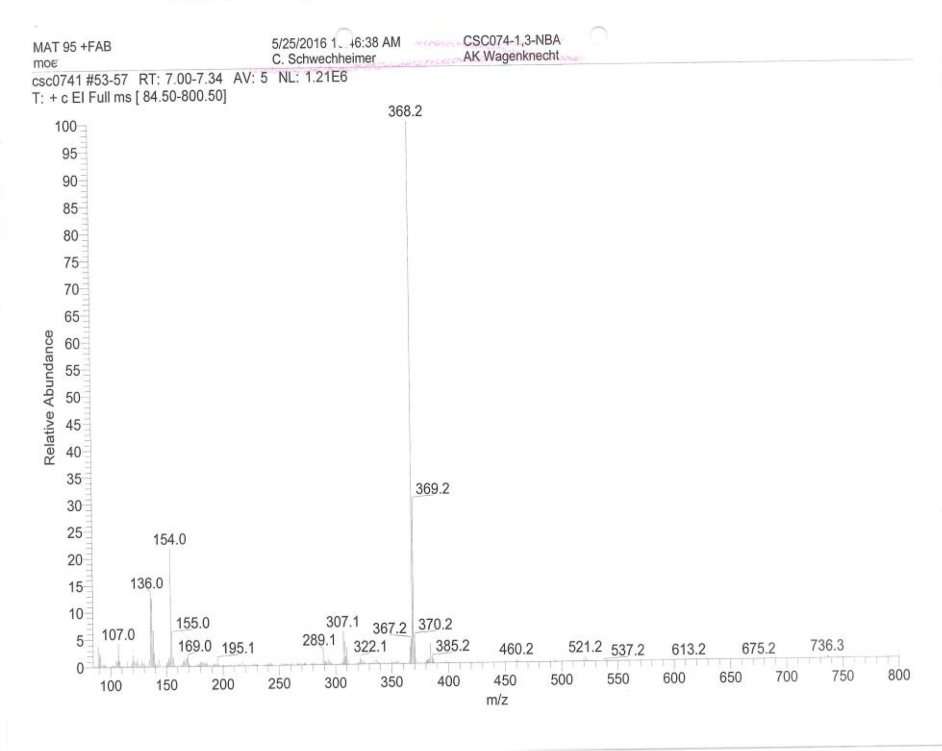
495.3645 g/mol



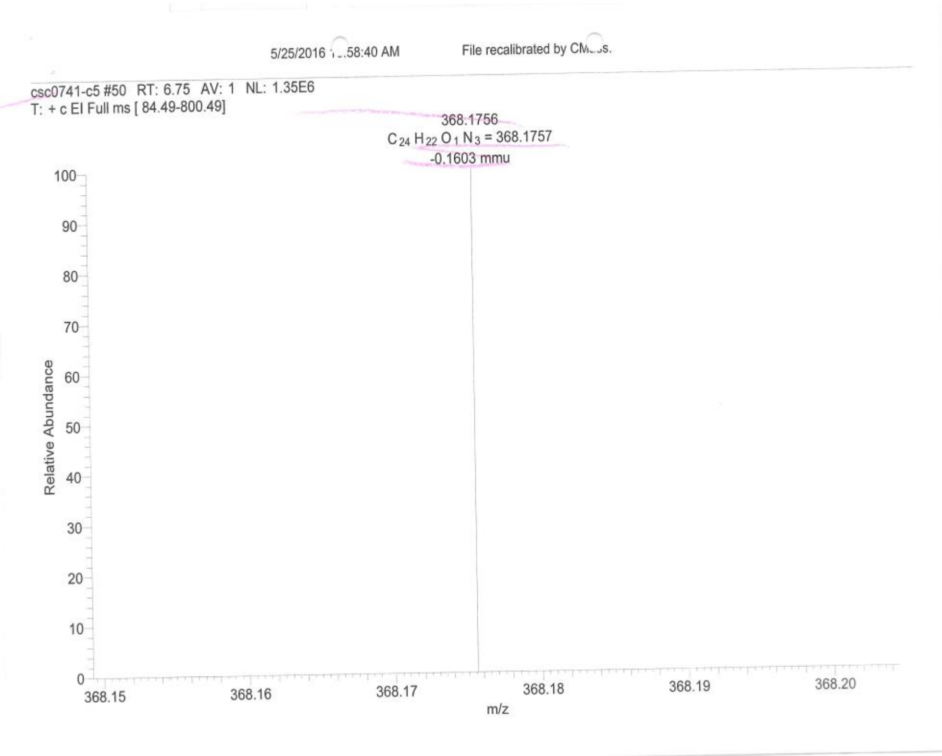



HSQC
{2.50,39.52}Dimethyl Sulfoxide-d6
f1 (ppm)
f2 (ppm)

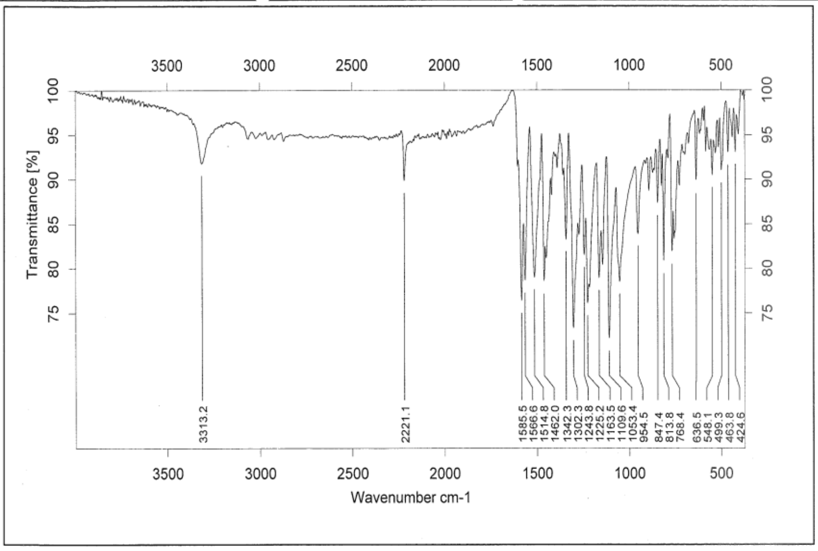

COSY
{2.50,2.50}Dimethyl Sulfoxide-d6
f1 (ppm)
f2 (ppm)



MAT 95 +FAB
moe
5/25/2016 1.46:38 AM
C. Schwechheimer
CSC074-1,3-NBA
AK Wagenknecht
csc0741 #53-57 RT: 7.00-7.34 AV: 5 NL: 1.21E6
T: + c EI Full ms [84.50-800.50]
368.2
369.2
154.0
136.0
107.0
155.0
169.0
195.1
289.1
307.1
322.1
367.2
370.2
385.2
460.2
521.2
537.2
613.2
675.2
736.3
Relative Abundance
m/z



5/25/2016 1.58:40 AM
File recalibrated by CM..s.
csc0741-c5 #50 RT: 6.75 AV: 1 NL: 1.35E6
T: + c EI Full ms [84.49-800.49]
368.1756
C24 H22 O1 N3 = 368.1757
-0.1603 mmu
Relative Abundance
m/z



Sample : C. Schwechheimer CSC 074-1	Frequency Range : 3997.41 - 373.828	Measured on : 02/06/2016	
Technique : ATR platinum Dian	Resolution : 4	Instrument : Alpha	Sample Scans : 24
Operator : Angelika Moesle	Zerofilling : 2	Acquisition : Double Sided,For	

ELEMENTARANALYSE

Auftraggeber:

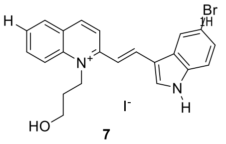
Christian Schwechheimer, Tel.: 47212, Raum 205, AK Wagenknecht

Substanzbezeichnung: CSC074-1

Summenformel: $C_{24}H_{22}IN_3O$

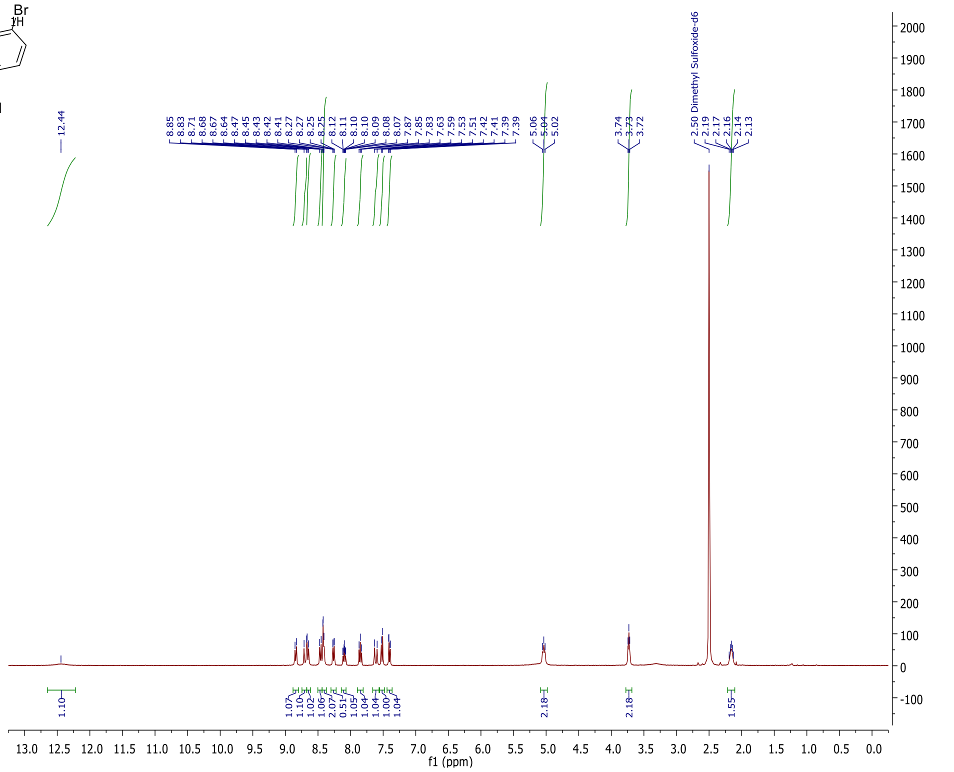
Berechnet:	N: 8.48	C: 58.19
	H: 4.48	~~S:~~ I: 25.62 O: 3.23
Gefunden:	N: 8,42	C: 57,85
	H: 4,40	S:
	N: 8,53	C: 58,18
	H: 4,37	S:

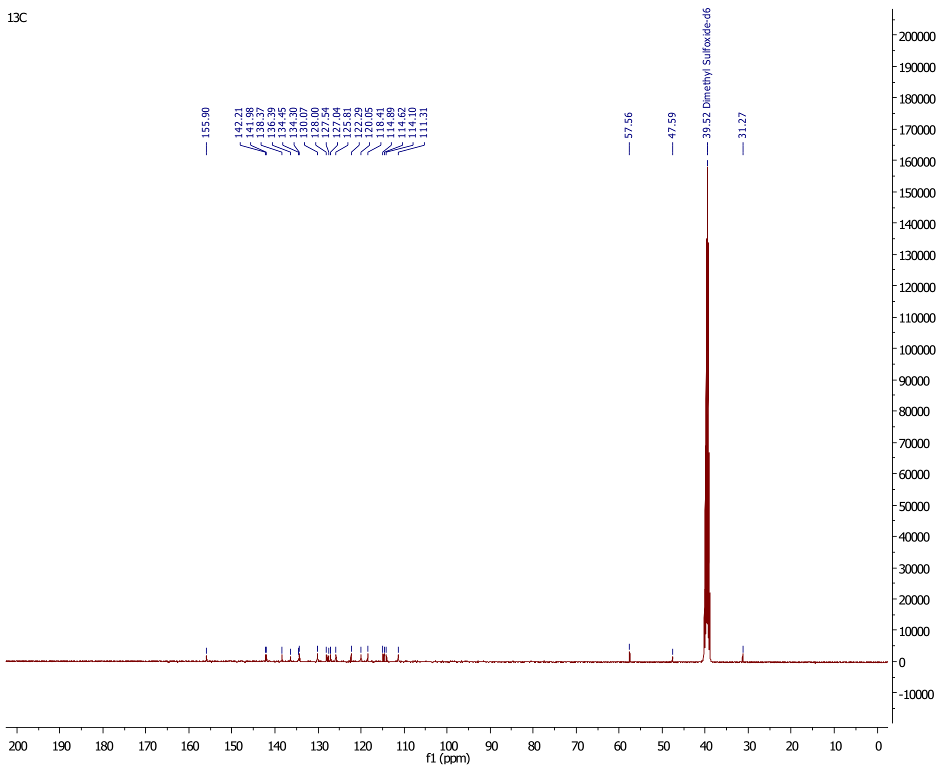
(*E*)-2-(2-(5-bromo-1*H*-indol-3-yl)vinyl)-1-(3-hydroxypropyl)quinolin-1-ium iodide (7):

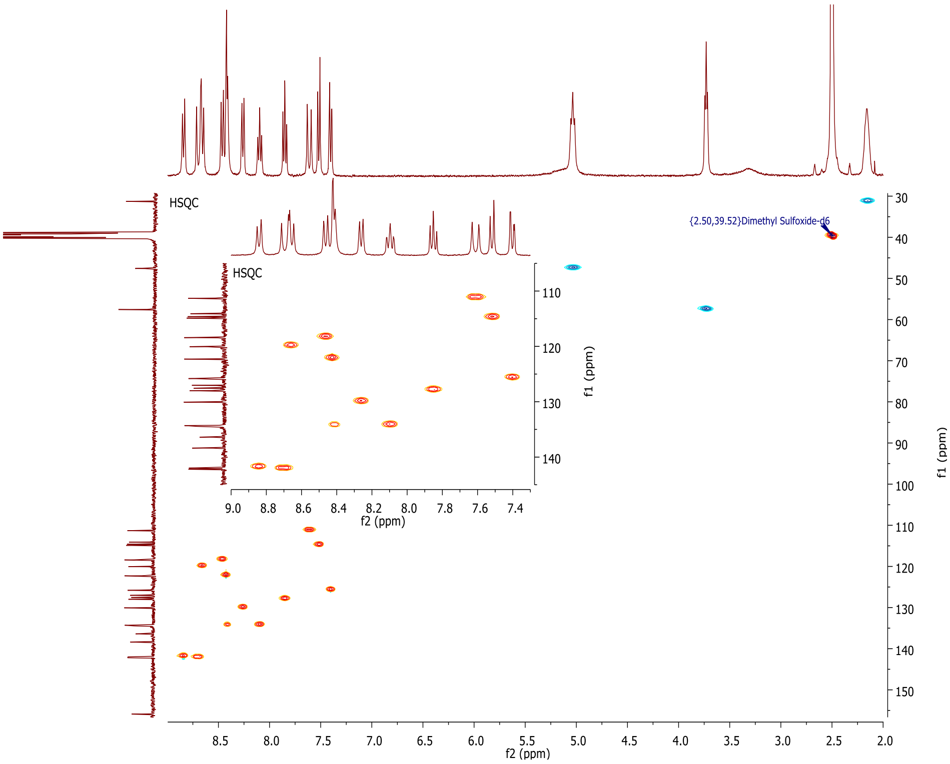


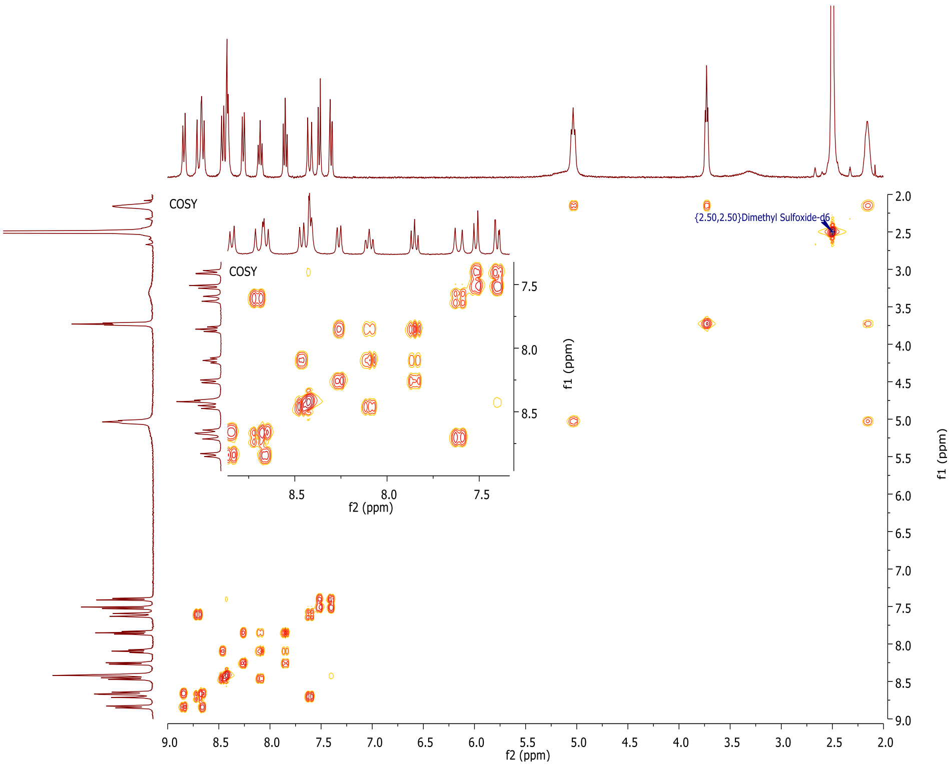
7

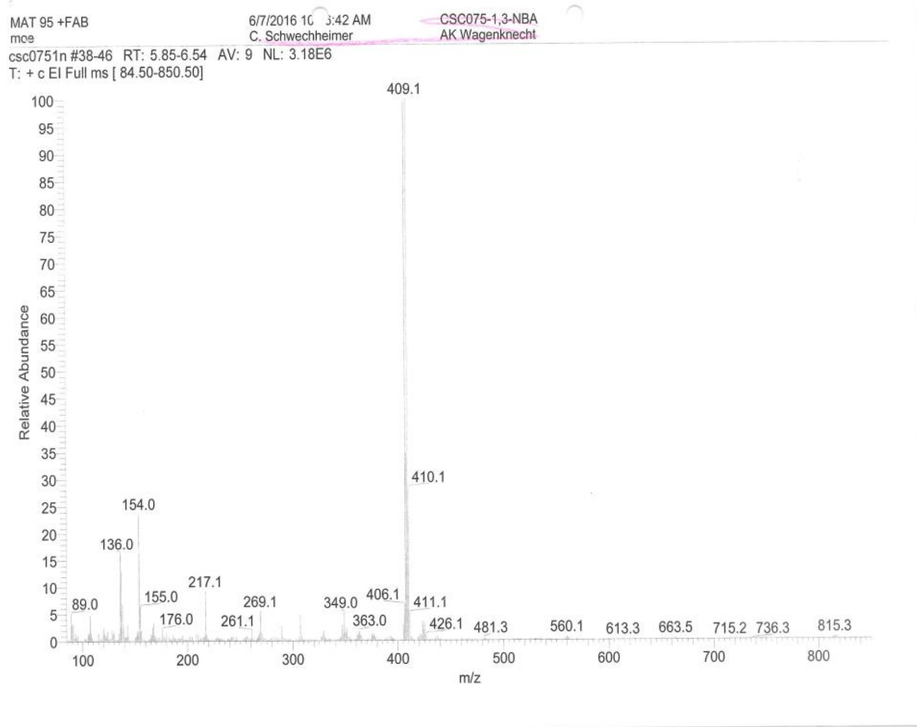
$C_{22}H_{20}BrIN_2O$
535.2235 g/mol

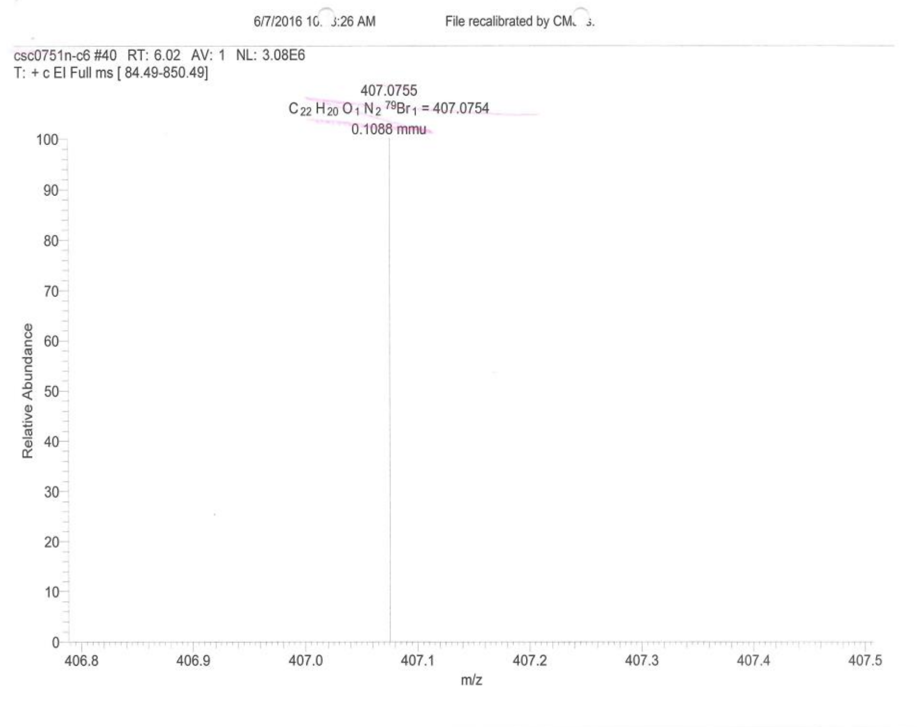


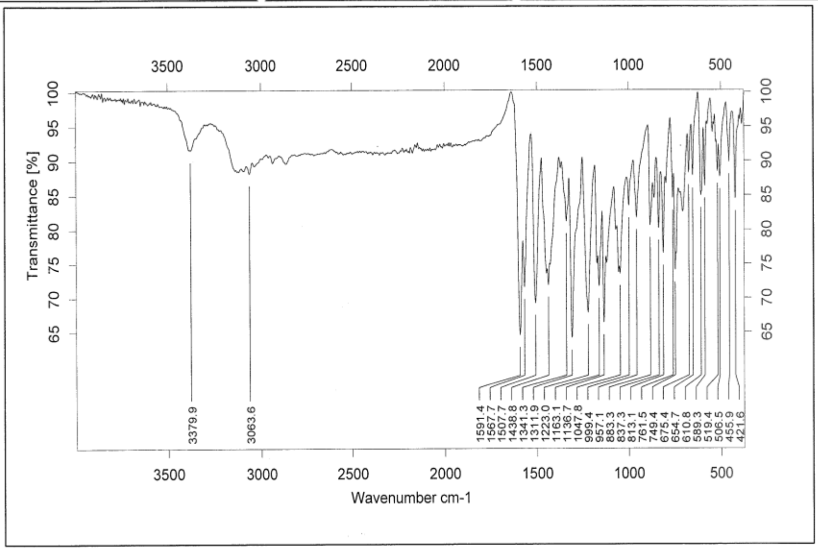



HSQC
{2.50,39.52}Dimethyl Sulfoxide-d6
f2 (ppm)
f1 (ppm)


COSY
{2.50,2.50}Dimethyl Sulfoxide-d6
f2 (ppm)
f1 (ppm)


MAT 95 +FAB
moe
6/7/2016 10:3:42 AM
C. Schwechheimer
CSC075-1,3-NBA
AK Wagenknecht
csc0751n #38-46 RT: 5.85-6.54 AV: 9 NL: 3.18E6
T: + c EI Full ms [84.50-850.50]
Relative Abundance
m/z
409.1
410.1
154.0
136.0
217.1
155.0
269.1
349.0
406.1
411.1
89.0
176.0
261.1
363.0
426.1
481.3
560.1
613.3
663.5
715.2
736.3
815.3


6/7/2016 10:3:26 AM
File recalibrated by CM
csc0751n-c6 #40 RT: 6.02 AV: 1 NL: 3.08E6
T: + c EI Full ms [84.49-850.49]
407.0755
C 22 H 20 O 1 N 2 79Br 1 = 407.0754
0.1088 mmu
Relative Abundance
m/z



Sample : C. Schwechheimer CSC075-1	Frequency Range : 3997.41 - 373.828		Measured on : 10/06/2016
Technique : ATR platinum Dian	Resolution : 4	Instrument : Alpha	Sample Scans : 24
Operator : Angelika Moesle	Zerofilling : 2	Acquisition : Double Sided,For	

T 102

ELEMENTARANALYSE

Auftraggeber:

Christian Schwechheimer, Tel.: 47212, Raum 205, AK Wagenknecht

Substanzbezeichnung: CSC075-1

Summenformel: $C_{22}H_{20}BrIN_2O$

Berechnet: N: 5.23 C: 49.37

H: 3.77 I: 23.71 Br: 14.93 O: 2.99

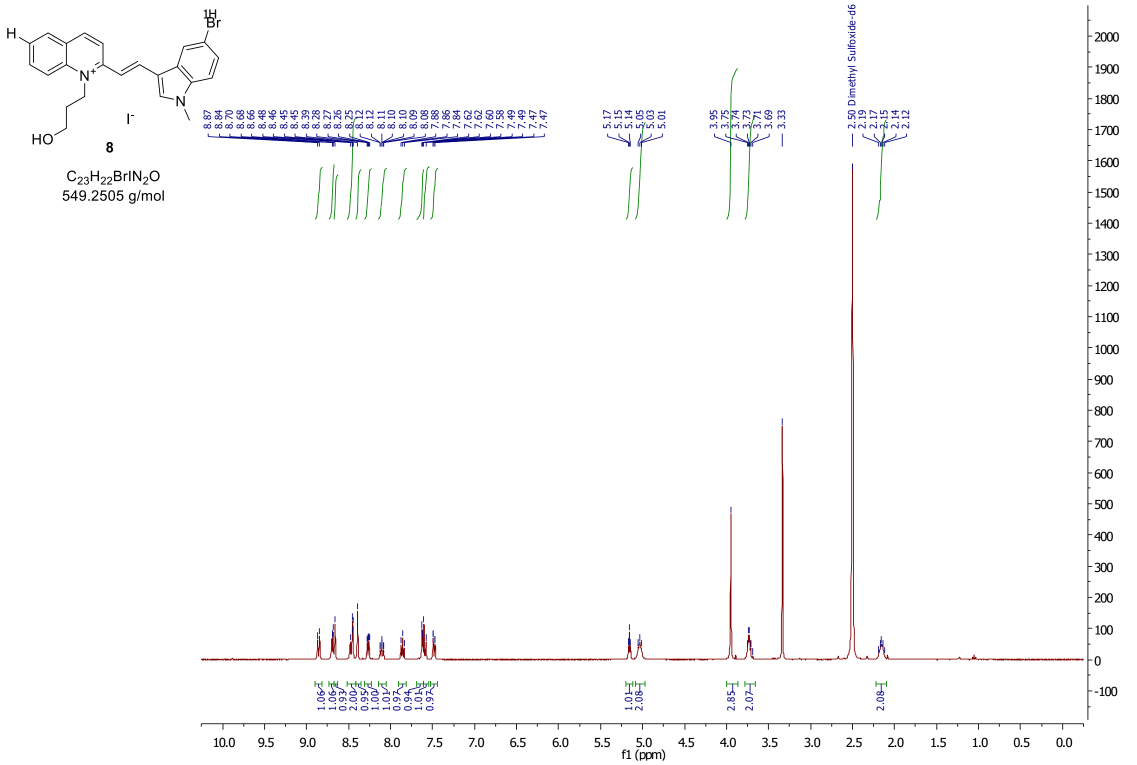
Gefunden: N: 5,20 C: 48,93

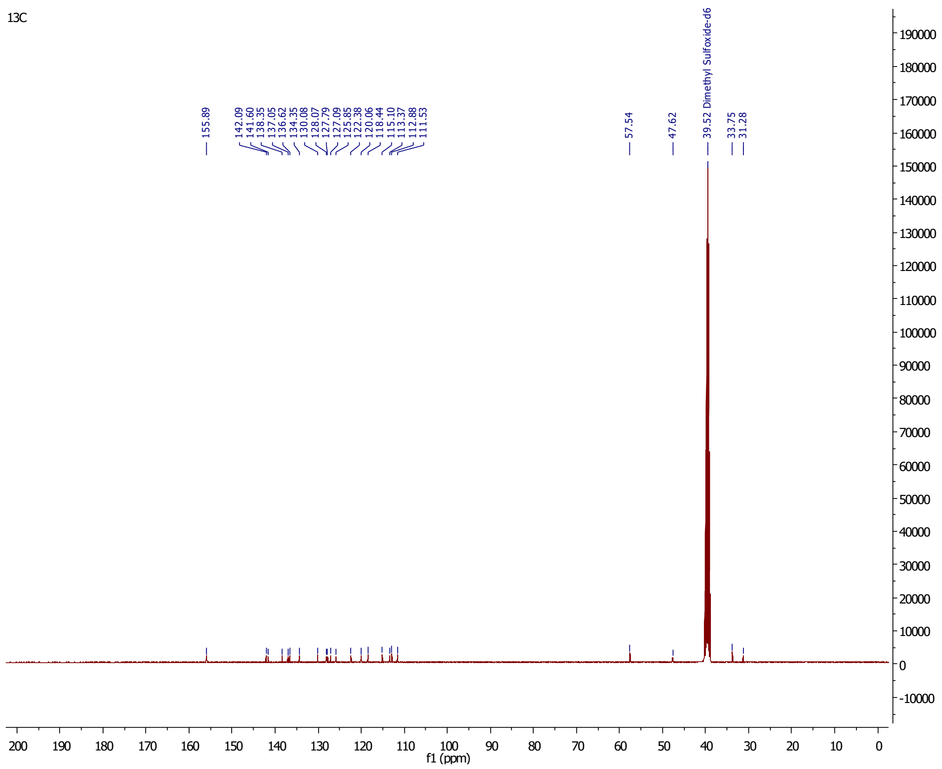
H: 3,68 S:

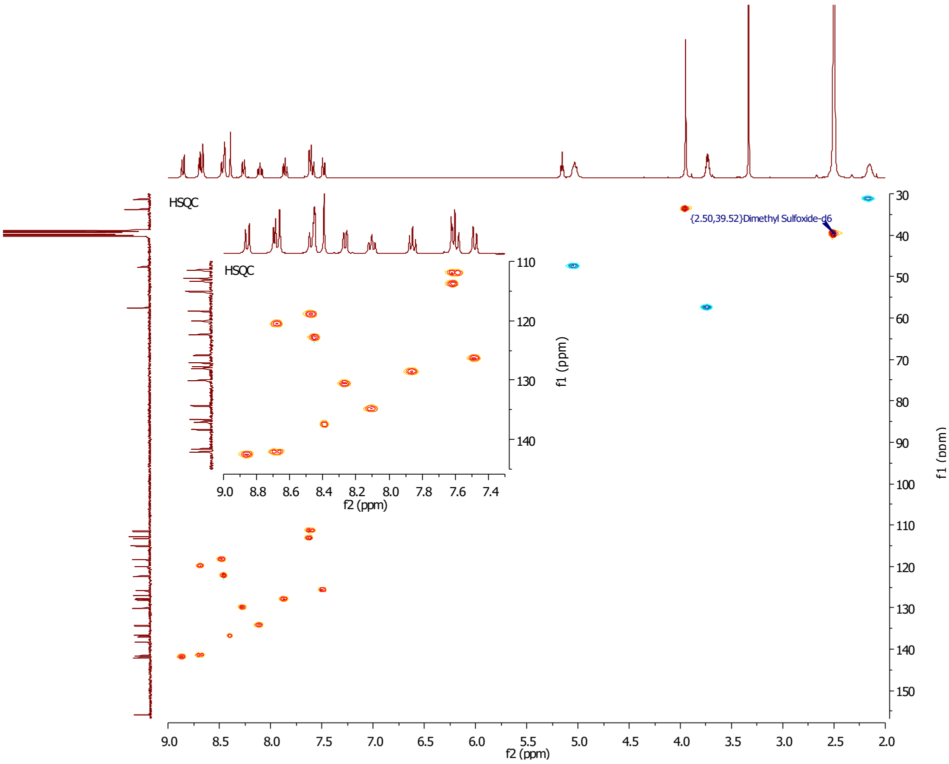
N: 5,19 C: 48,91

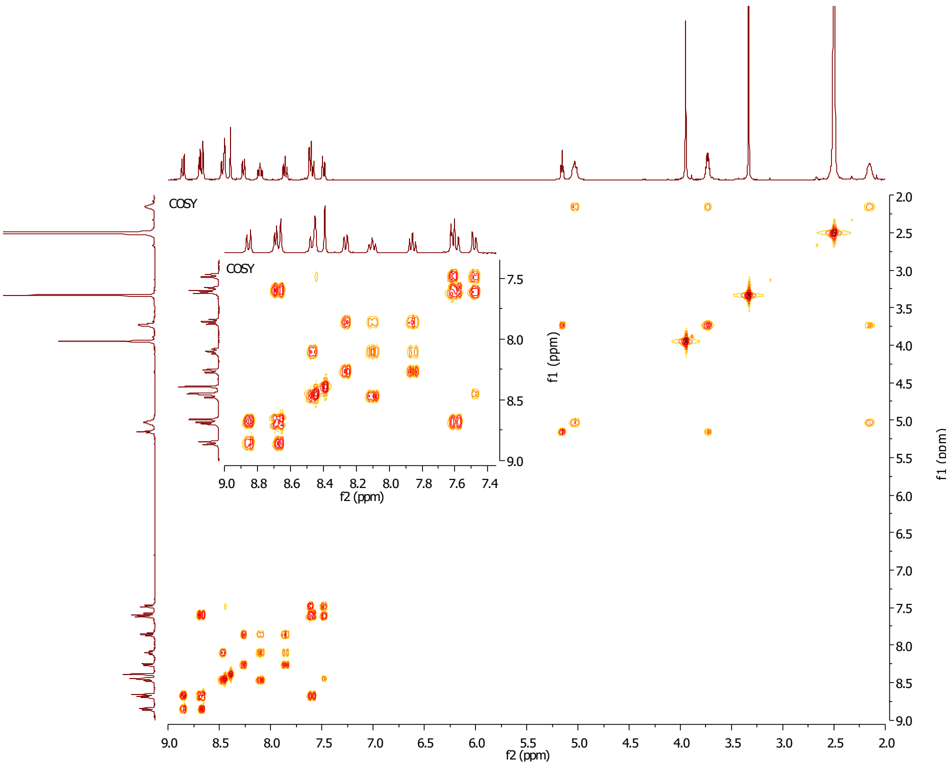
H: 3,65 S:

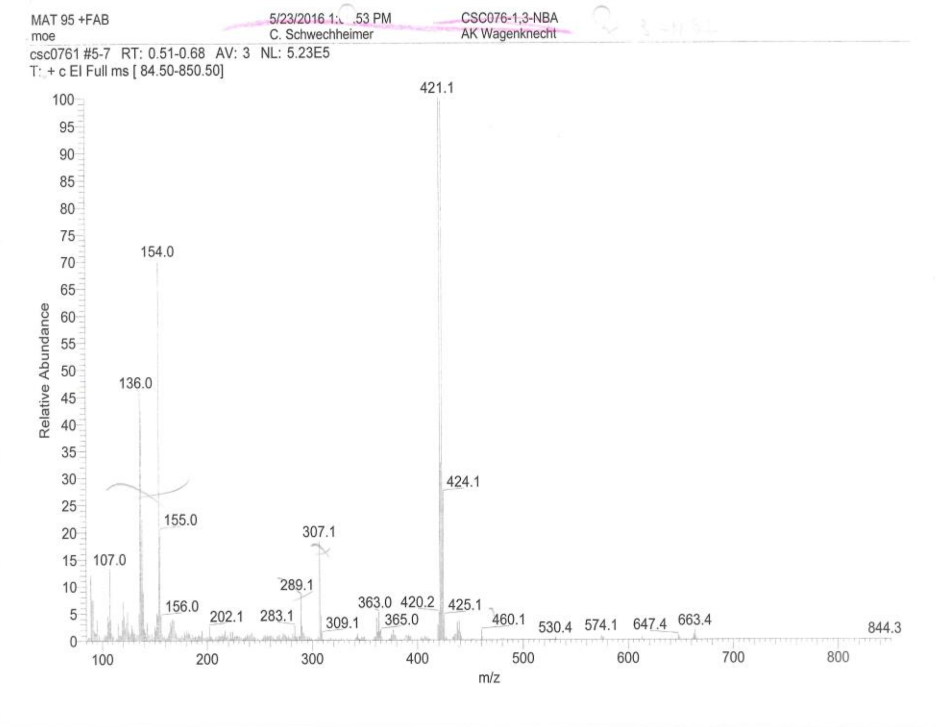
(*E*)-2-(2-(5-bromo-1-methyl-1*H*-indol-3-yl)vinyl)-1-(3-hydroxypropyl)quinolin-1-ium iodide (8):

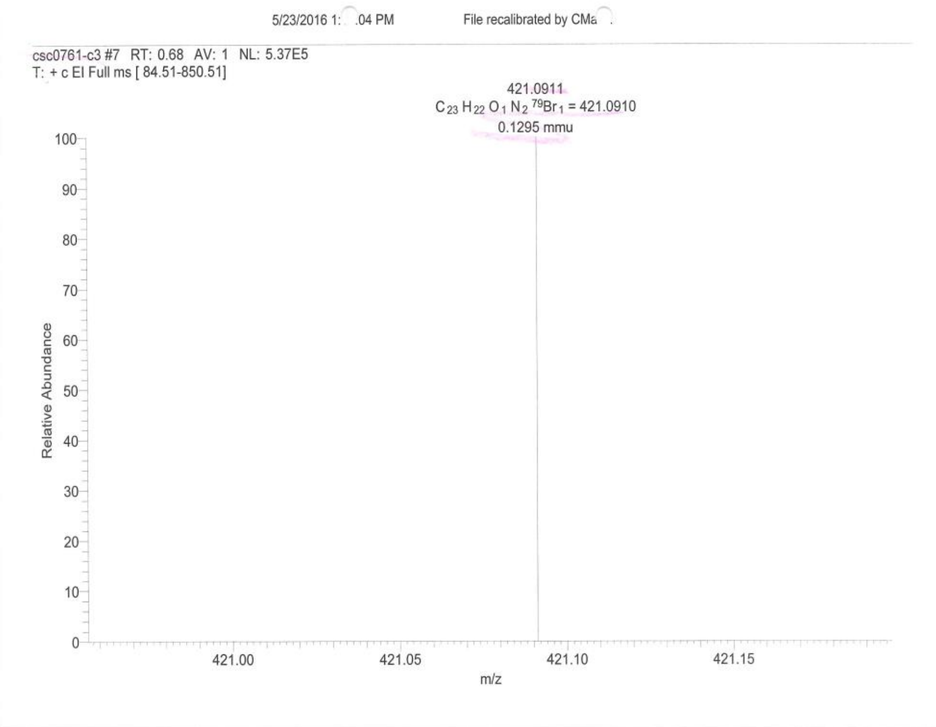


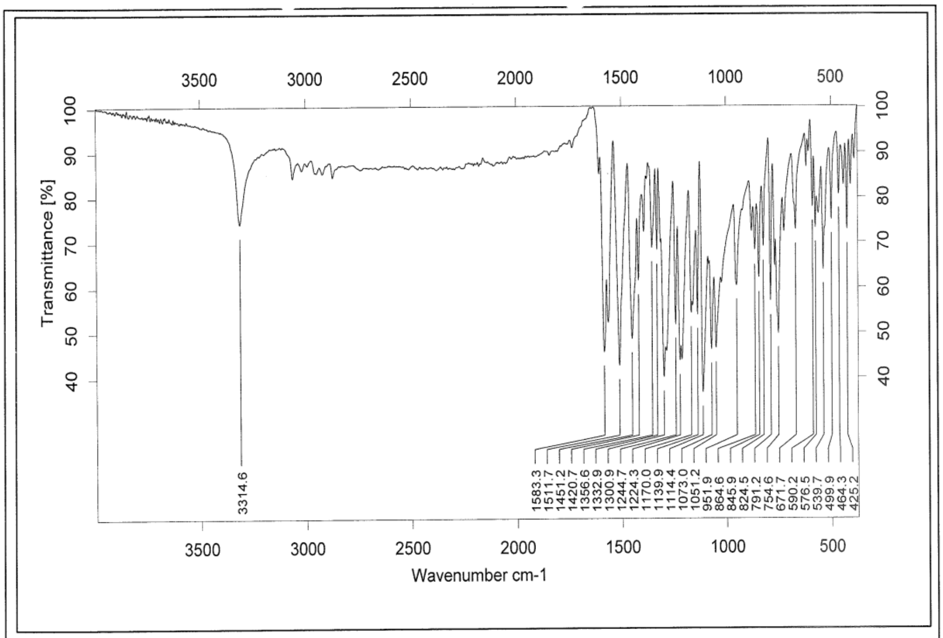



HSQC
{2.50,39.52}Dimethyl Sulfoxide-d6
f2 (ppm)
f1 (ppm)


COSY
f2 (ppm)
f1 (ppm)


MAT 95 +FAB
moe
5/23/2016 1:..53 PM
C. Schwechheimer
CSC076-1,3-NBA
AK Wagenknecht
csc0761 #5-7 RT: 0.51-0.68 AV: 3 NL: 5.23E5
T: + c EI Full ms [84.50-850.50]
421.1
154.0
136.0
424.1
155.0
307.1
107.0
289.1
156.0
202.1
283.1
309.1
363.0
365.0
420.2
425.1
460.1
530.4
574.1
647.4
663.4
844.3
Relative Abundance
m/z


5/23/2016 1:..04 PM
File recalibrated by CMa
csc0761-c3 #7 RT: 0.68 AV: 1 NL: 5.37E5
T: + c EI Full ms [84.51-850.51]
421.0911
C23 H22 O1 N2 79Br1 = 421.0910
0.1295 mmu
Relative Abundance
m/z



Sample : C. Schwechheimer CSC076-1	Frequency Range : 3997.41 - 373.828		Measured on : 25/05/2016
Technique : ATR platinum Dian	Resolution : 4	Instrument : Alpha	Sample Scans : 24
Operator : Angelika Moesle	Zerofilling : 2	Acquisition : Double Sided,For	

ELEMENTARANALYSE

Auftraggeber:

Christian Schwechheimer, Tel.: 47212, Raum 205, AK Wagenknecht

Substanzbezeichnung: CSC076-1

Summenformel: $C_{23}H_{22}BrIN_2O$

Berechnet: N: 5.10 C: 50.30

H: 4.04 ~~S:~~ I: 23.11 Br: 14.55 O: 2.91

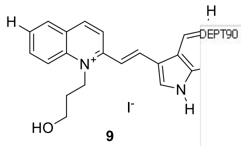
Gefunden: N: 5,09 C: 50,28

H: ~~6,57~~ 4,00 S:

N: 5,12 C: 50,23

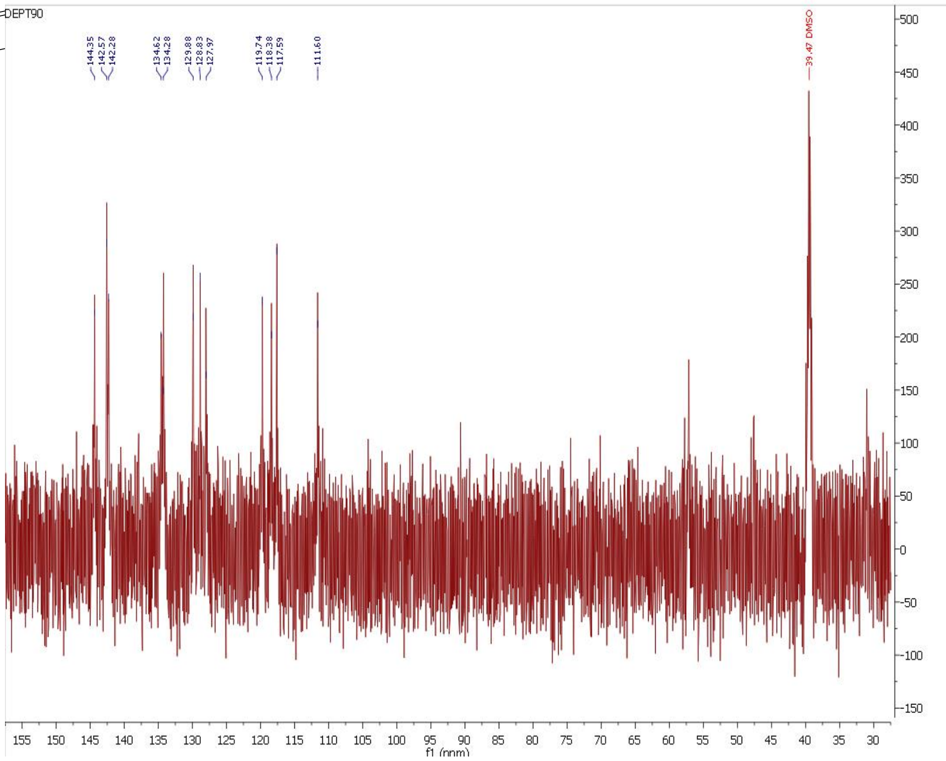
H: 3,98 S:

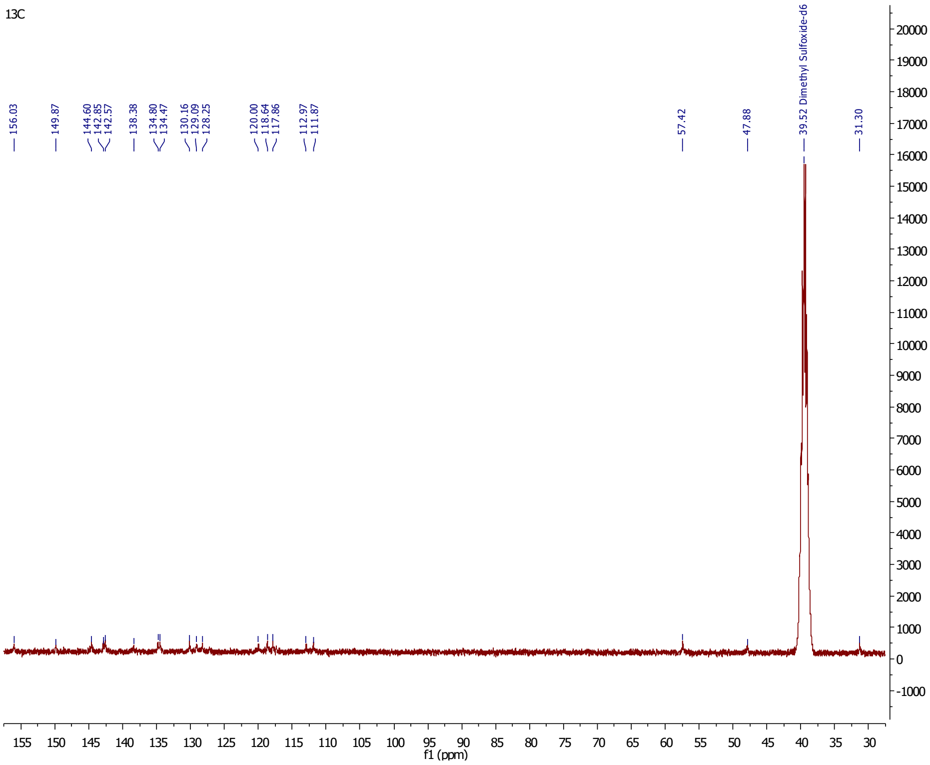
(*E*)-2-(2-(1*H*-pyrrolo[2,3-*b*]pyridin-3-yl)vinyl)-1-(3-hydroxypropyl)quinolin-1-ium iodide (9):

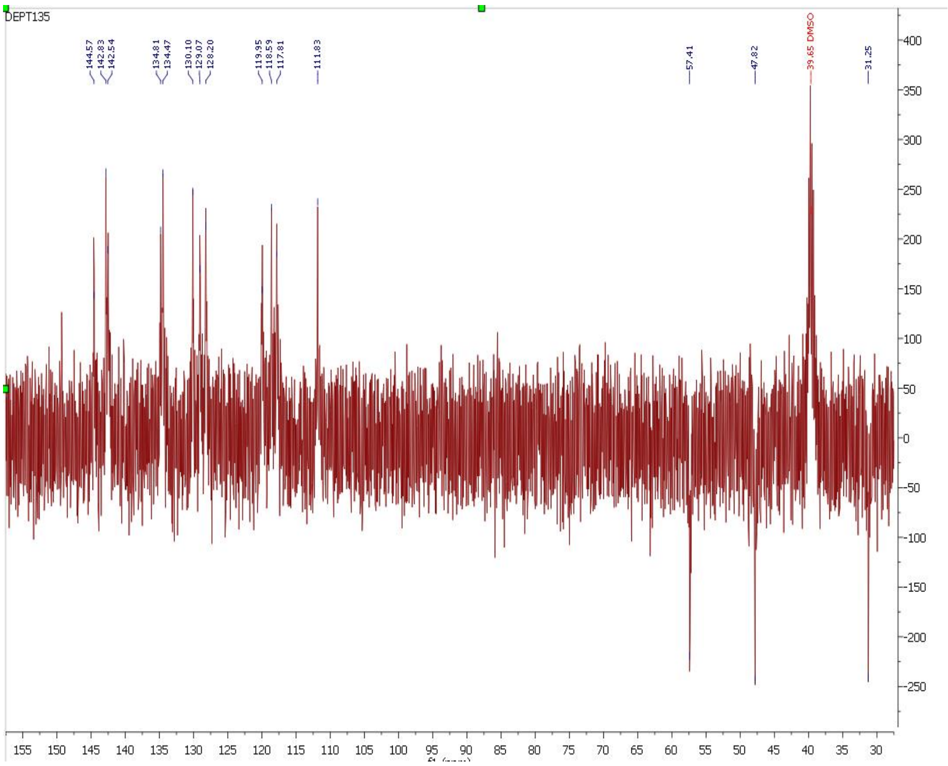


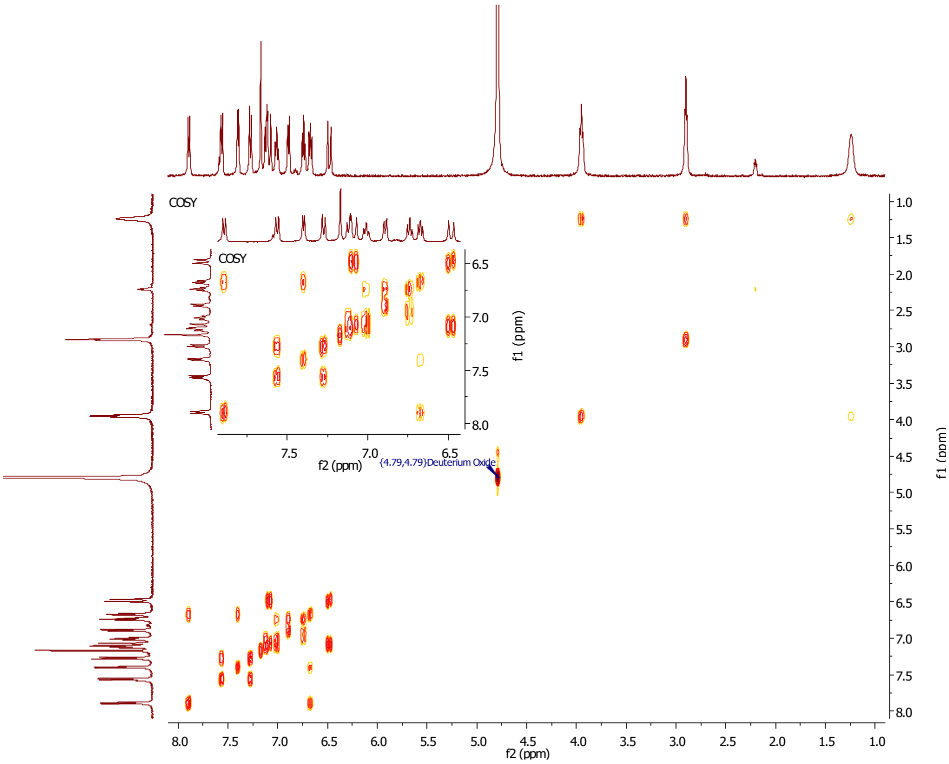
9

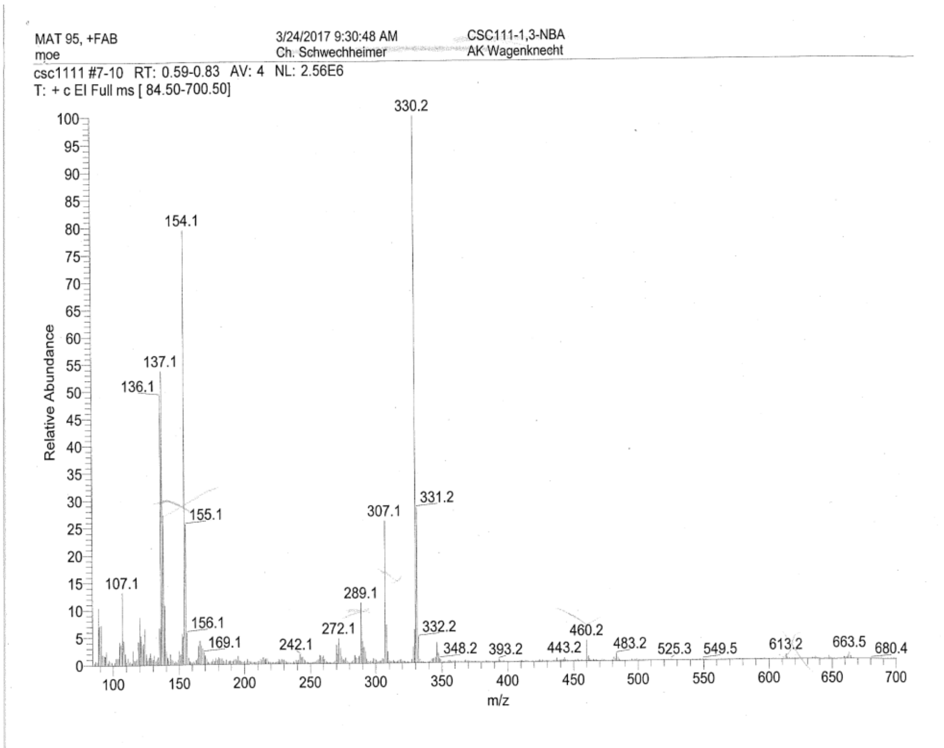
$C_{21}H_{20}IN_3O$
457.3155 g/mol

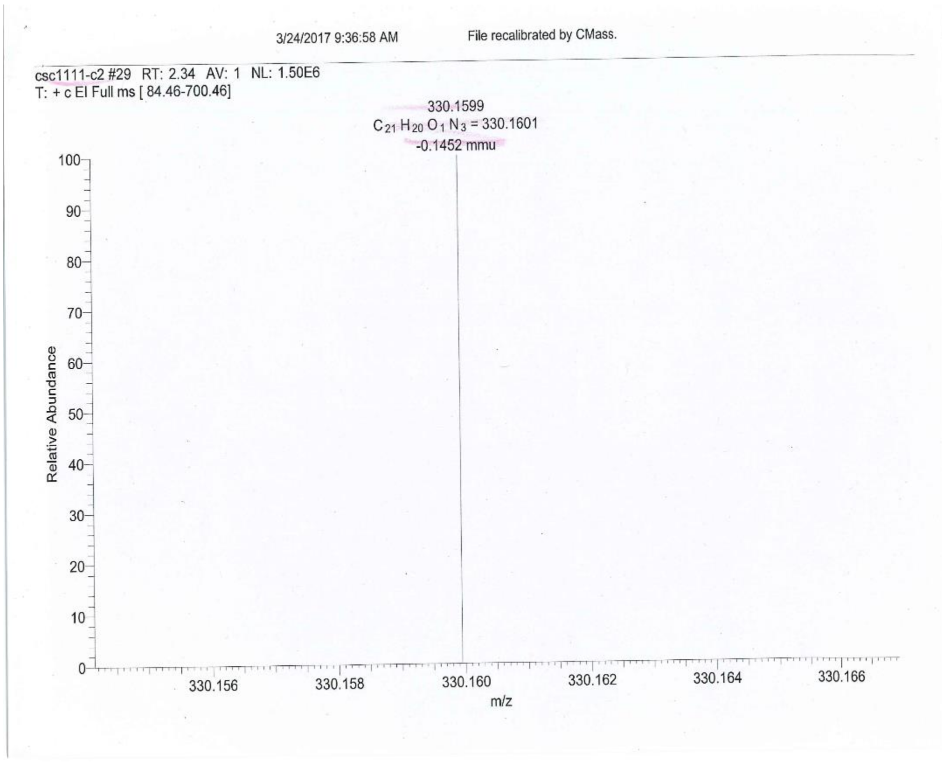


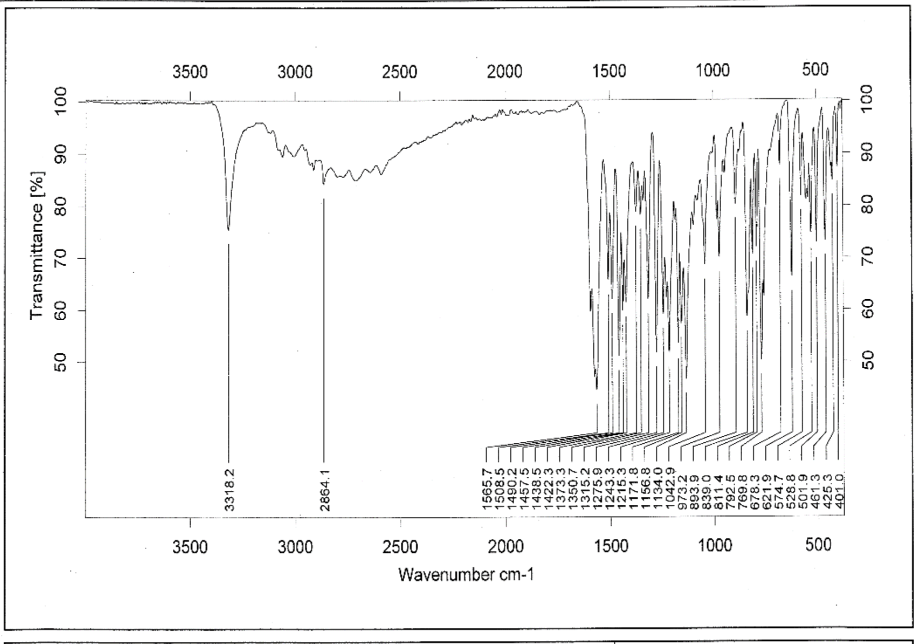



DEPT135
144.57
142.83
142.54
134.81
134.47
130.10
129.07
128.20
119.95
118.59
117.81
111.83
57.41
47.82
39.65 DMSO
31.25


COSY
{4.79,4.79}Deuterium Oxide
f2 (ppm)
f1 (ppm)


MAT 95, +FAB
moe
3/24/2017 9:30:48 AM
Ch. Schwechheimer
CSC111-1,3-NBA
AK Wagenknecht
csc1111 #7-10 RT: 0.59-0.83 AV: 4 NL: 2.56E6
T: + c EI Full ms [84.50-700.50]
Relative Abundance
m/z
330.2
154.1
137.1
136.1
155.1
307.1
331.2
289.1
107.1
272.1
332.2
156.1
169.1
242.1
348.2
393.2
443.2
460.2
483.2
525.3
549.5
613.2
663.5
680.4





Sample : Ch. Schwechheimer CSC111-1	Frequency Range : 3997.41 - 373.828		Measured on : 30/03/2017
Technique : Diamant-ATR	Resolution : 4	Instrument : Alpha	Sample Scans : 24
Operator : Angelika Moesle	Zerofilling : 2	Acquisition : Double Sided,Forward-Backward	

ELEMENTARANALYSE

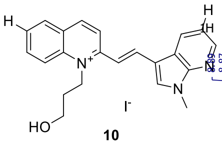
Auftraggeber: Christian Schwechheimer, Tel.: 47281, Raum 007, AK Wagenknecht

Substanzbezeichnung: (KG38) CSC111-1

Summenformel: $C_{21}H_{20}I_1N_3O_1$

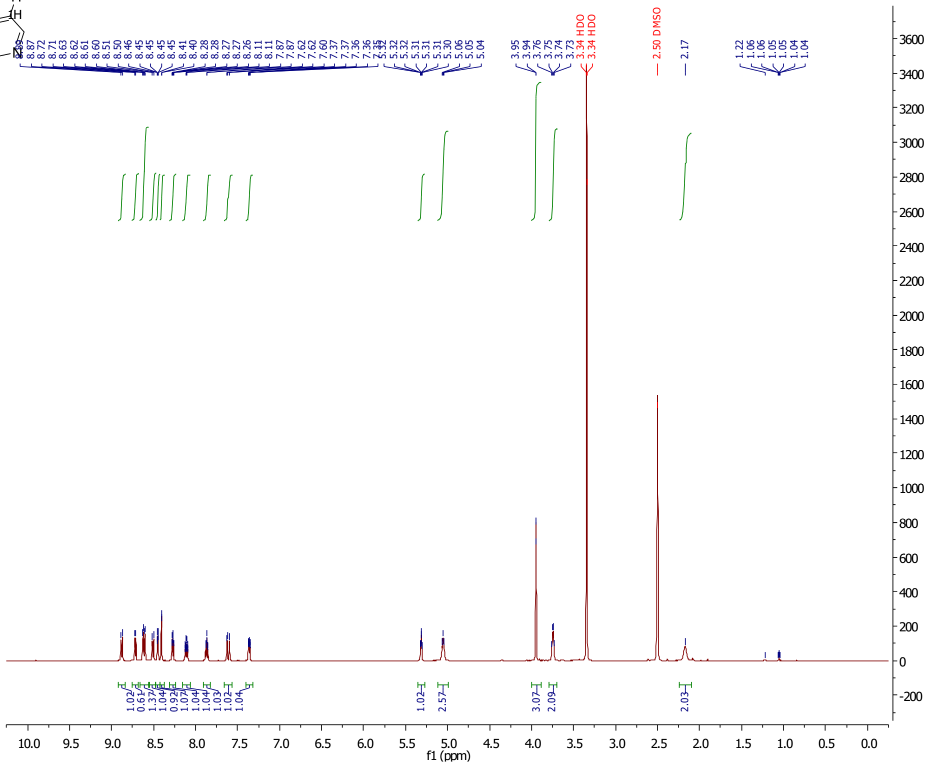
Berechnet:	N	9.19	C	55.15
	H	4.41	O	3.50
	(I 27.75)			
Gefunden:	N	9,55	C	55,34
	H	4,37	O	
	N	9,51	C	55,22
	H	4,44	O	

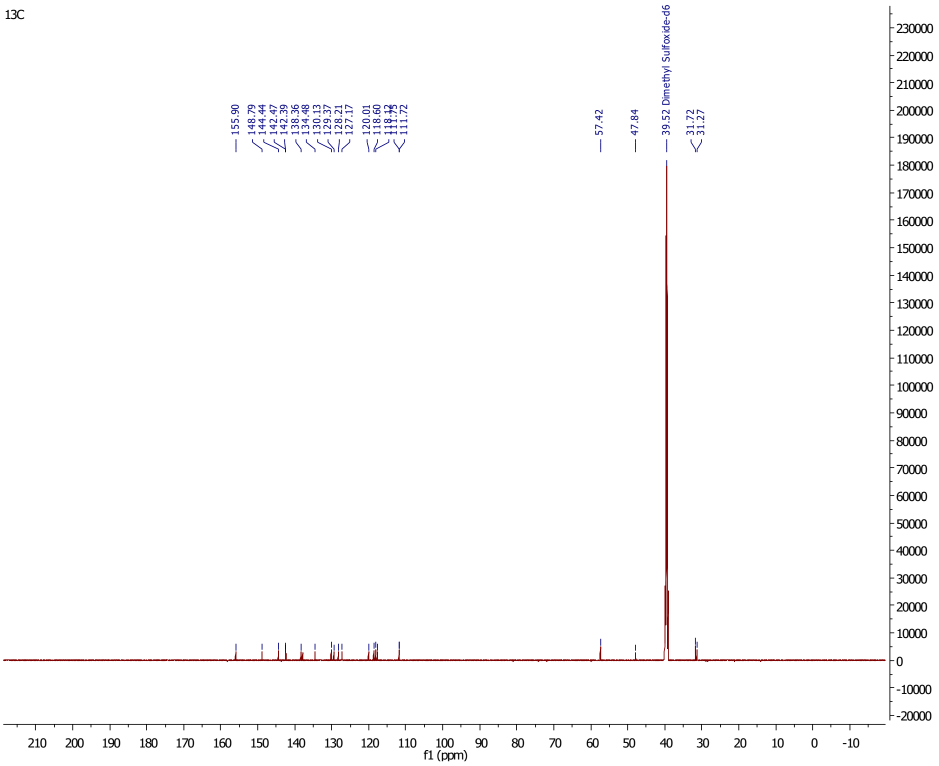
(*E*)-1-(3-hydroxypropyl)-2-(2-(1-methyl-1*H*-pyrrolo[2,3-*b*]pyridin-3-yl)vinyl)quinolin-1-ium iodide (10):

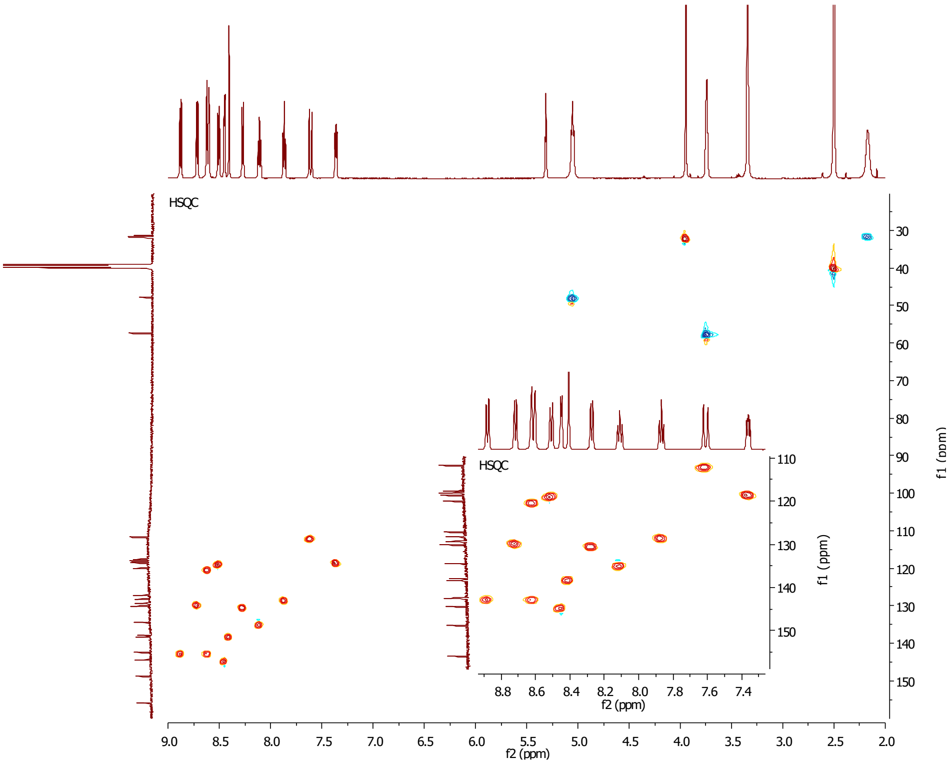


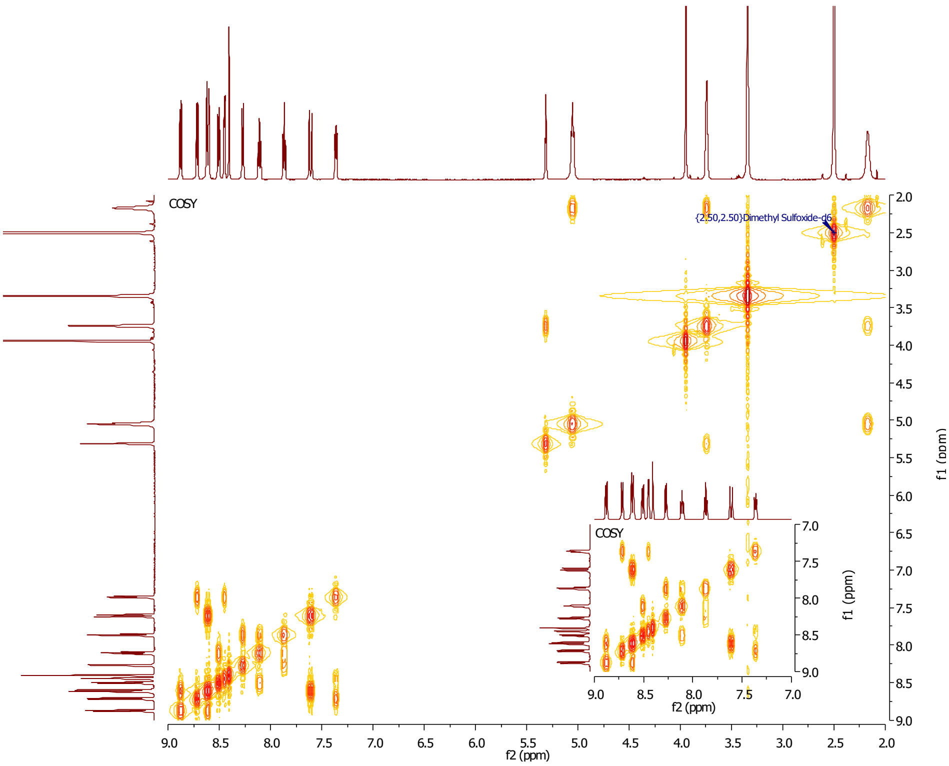
10

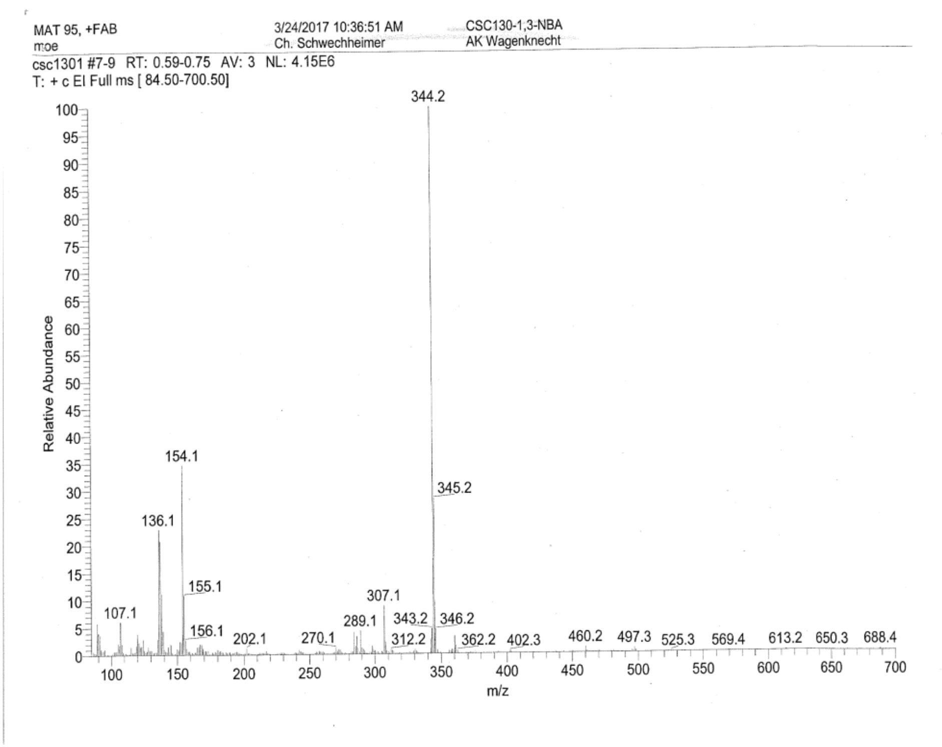
$C_{22}H_{22}IN_3O$
471.3425 g/mol

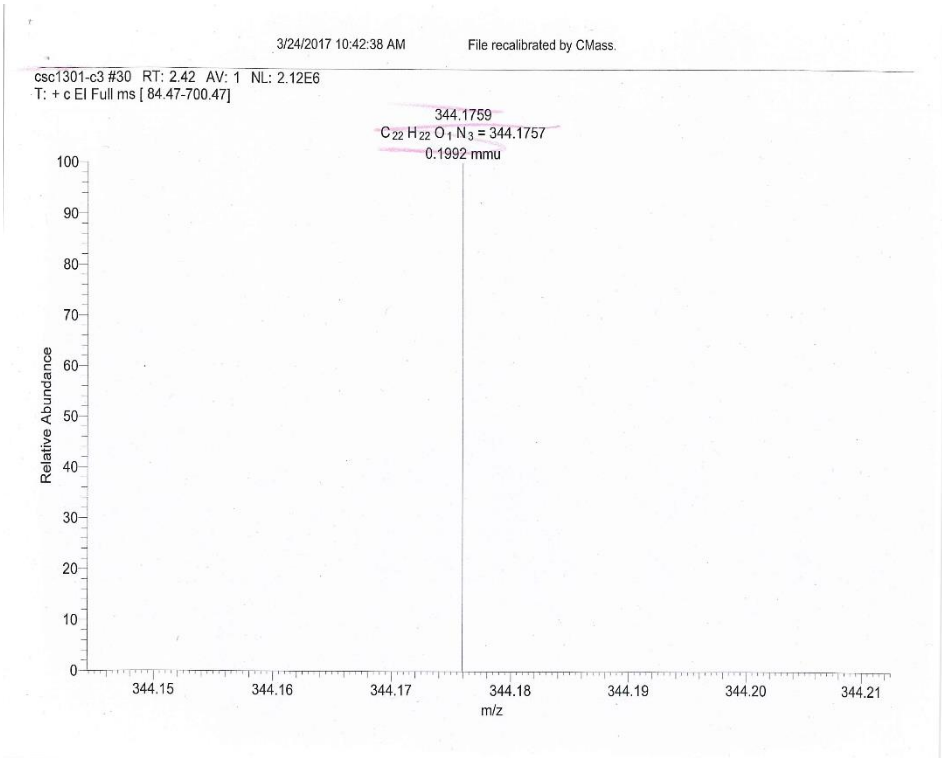


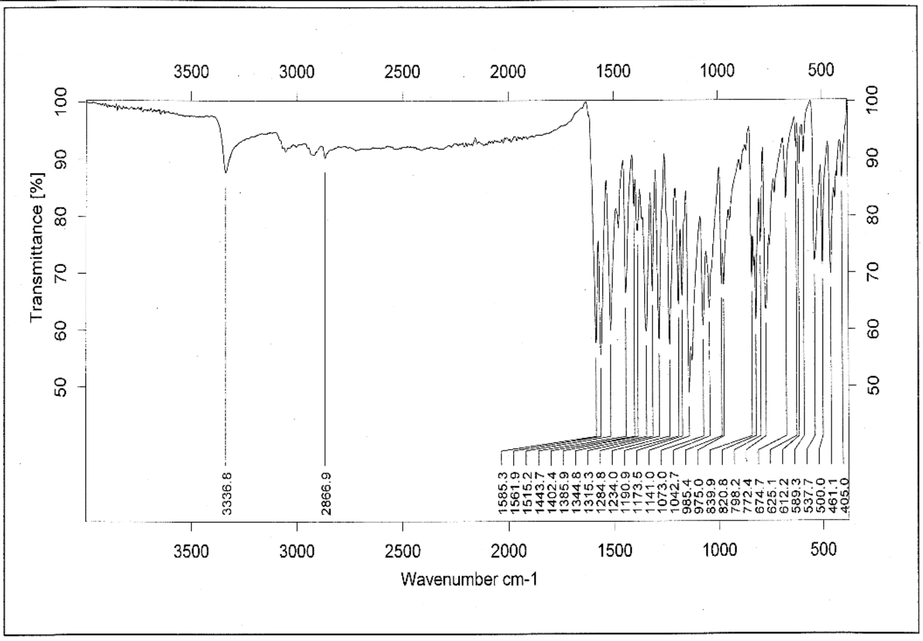



HSQC
HSQC
f1 (ppm)
f2 (ppm)
f1 (ppm)
f2 (ppm)


COSY
(2.50,2.50)Dimethyl Sulfoxide-d6
COSY
f1 (ppm)
f2 (ppm)
f1 (ppm)
f2 (ppm)


MAT 95, +FAB
moe
3/24/2017 10:36:51 AM
Ch. Schwechheimer
CSC130-1,3-NBA
AK Wagenknecht
csc1301 #7-9 RT: 0.59-0.75 AV: 3 NL: 4.15E6
T: + c EI Full ms [84.50-700.50]
Relative Abundance
m/z
344.2
345.2
154.1
136.1
155.1
107.1
156.1
202.1
270.1
289.1
307.1
312.2
343.2
346.2
362.2
402.3
460.2
497.3
525.3
569.4
613.2
650.3
688.4


3/24/2017 10:42:38 AM
File recalibrated by CMass.
csc1301-c3 #30 RT: 2.42 AV: 1 NL: 2.12E6
T: + c EI Full ms [84.47-700.47]
344.1759
C 22 H 22 O 1 N 3 = 344.1757
0.1992 mmu
Relative Abundance
m/z



Sample : Ch.Schwechheimer CSC130-1	Frequency Range : 3997.41 - 373.828	Measured on : 30/03/2017	
Technique : Diamant-ATR	Resolution : 4	Instrument : Alpha	Sample Scans : 24
Operator : Angelika Moesle	Zerofilling : 2	Acquisition : Double Sided,Forward-Backward	

ELEMENTARANALYSE

Auftraggeber: Christian Schwechheimer, Tel.: 47281, Raum 007, AK Wagenknecht

Substanzbezeichnung: 130-1

Summenformel: $C_{22}H_{22}I_1N_3O_1$

Berechnet: N 8.92 C 56.06

H 4.70 O 3.39 (I 26.92)

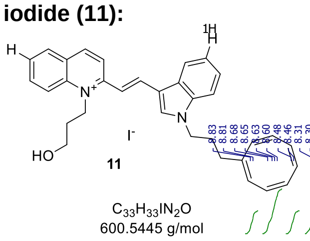
Gefunden: N 8,53 C 54,27

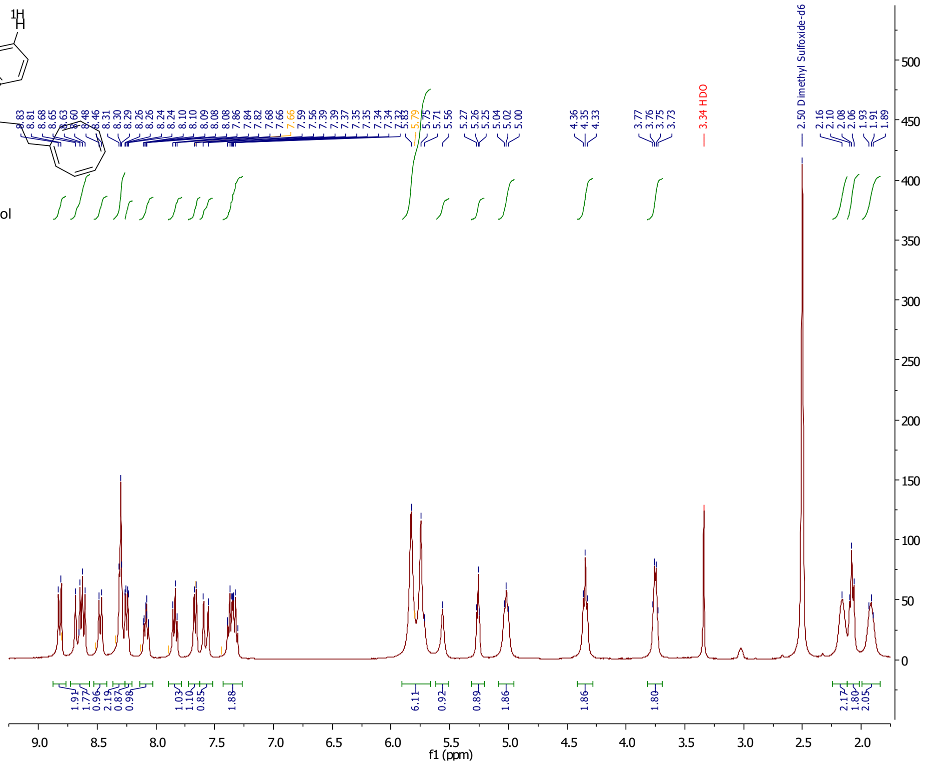
H 4,54 O

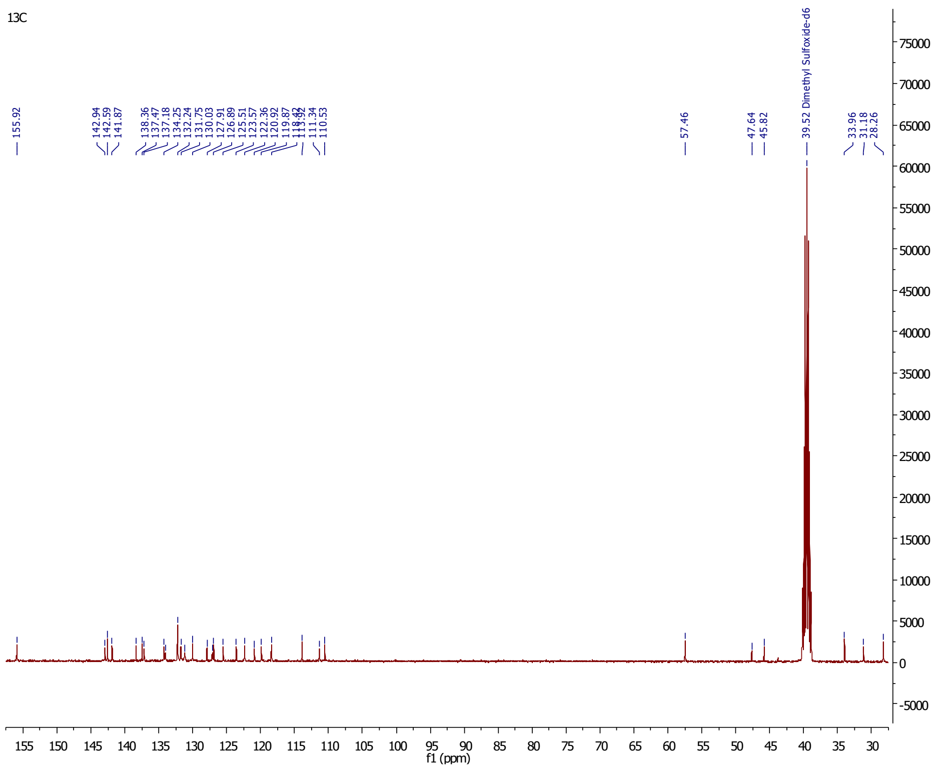
N 8,61 C 54,56

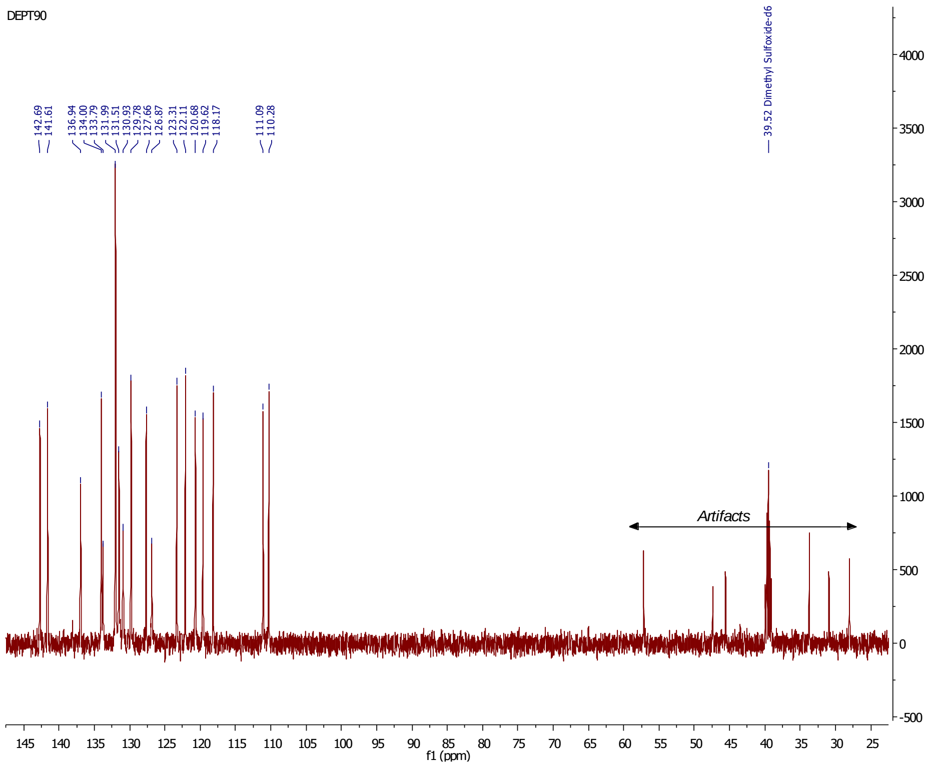
H 4,58 O

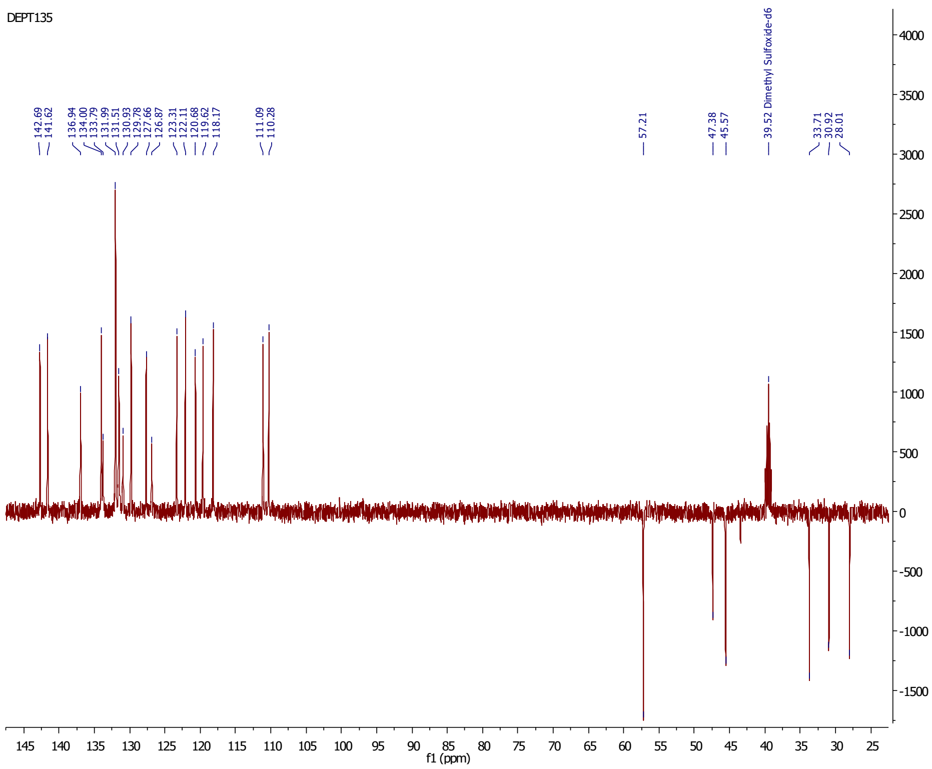
2-((*E*)-2-(1-(3-((1*Z*,3*Z*,5*Z*,7*Z*)-cycloocta-1,3,5,7-tetraen-1-yl)propyl)-1*H*-indol-3-yl)vinyl)-1-(3-hydroxypropyl)quinolin-1-ium iodide (11):

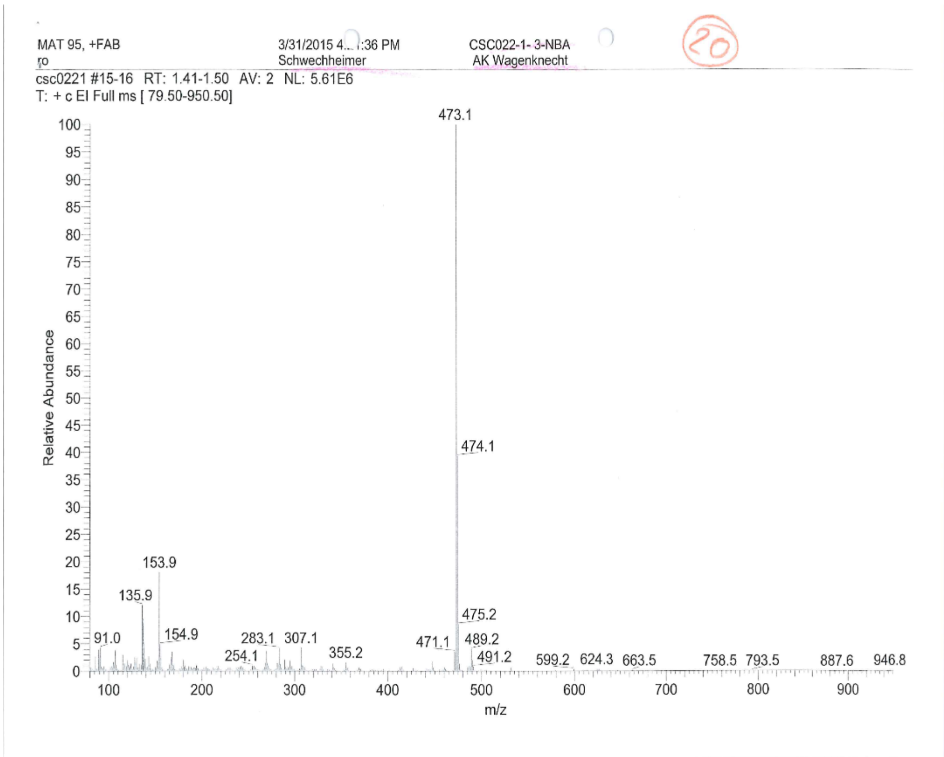


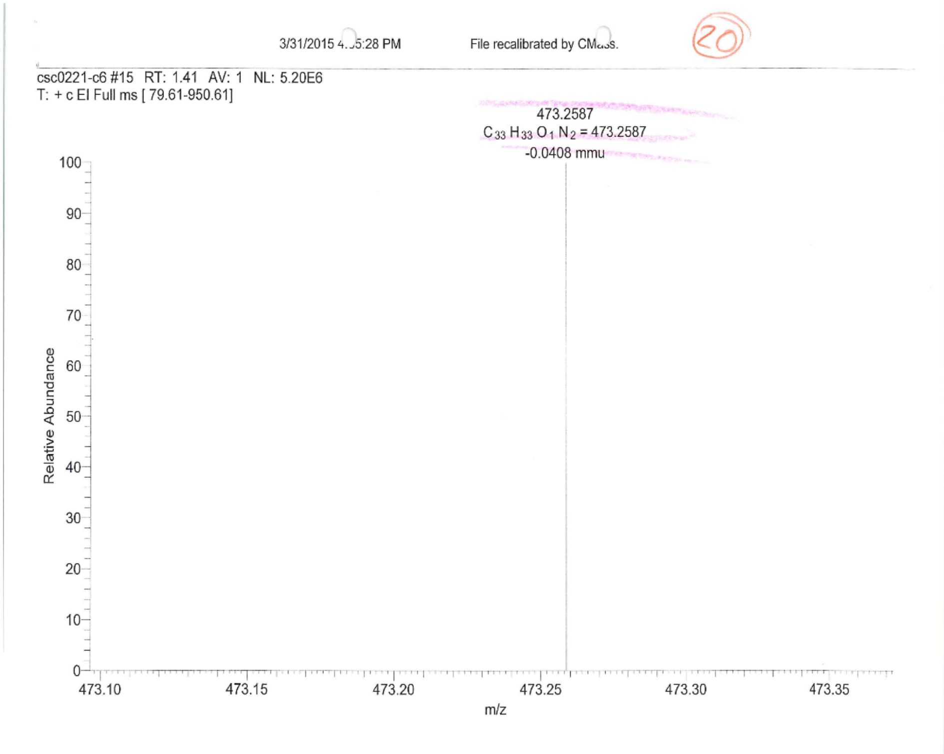


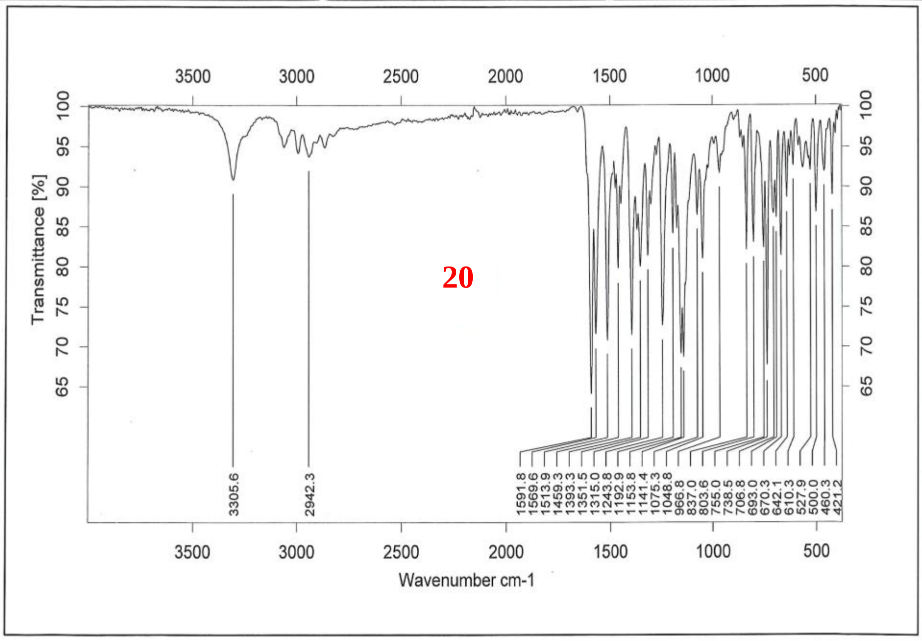



DEPT90
142.69
141.61
136.94
134.00
133.79
131.99
131.51
130.93
129.78
127.66
126.87
123.31
122.11
120.68
119.62
118.17
111.09
110.28
39.52 Dimethyl Sulfoxide-d6
Artifacts
f1 (ppm)


DEPT135
142.69
141.62
136.94
134.00
133.79
131.99
131.51
130.93
129.78
127.66
126.87
123.31
122.11
120.68
119.62
118.17
111.09
110.28
57.21
47.38
45.57
39.52 Dimethyl Sulfoxide-d6
33.71
30.92
28.01
f1 (ppm)


MAT 95, +FAB
ro
3/31/2015
Schwechheimer
CSC022-1-3-NBA
AK Wagenknecht
20
csc0221 #15-16 RT: 1.41-1.50 AV: 2 NL: 5.61E6
T: + c EI Full ms [79.50-950.50]
Relative Abundance
473.1
474.1
153.9
135.9
475.2
91.0
154.9
283.1
307.1
254.1
355.2
471.1
489.2
491.2
599.2
624.3
663.5
758.5
793.5
887.6
946.8
m/z


3/31/2015
File recalibrated by CMass.
20
csc0221-c6 #15 RT: 1.41 AV: 1 NL: 5.20E6
T: + c EI Full ms [79.61-950.61]
473.2587
C33 H33 O1 N2 = 473.2587
-0.0408 mmu
Relative Abundance
m/z



Sample : Ch. Schwechheimer CSC 022-1	Frequency Range : 3997.41 - 373.828		Measured on : 14/04/2015
Technique : ATR platinum Diar	Resolution : 4	Instrument : Alpha	Sample Scans : 24
Operator : Angelika Moesle	Zerofilling : 2	Acquisition : Double Sided,For	

ELEMENTARANALYSE

Name: Ch. Schwechheimer Datum: 7.4.'15

AK: Wagenknecht

Substanzbezeichnung: CSC022-1 (20)

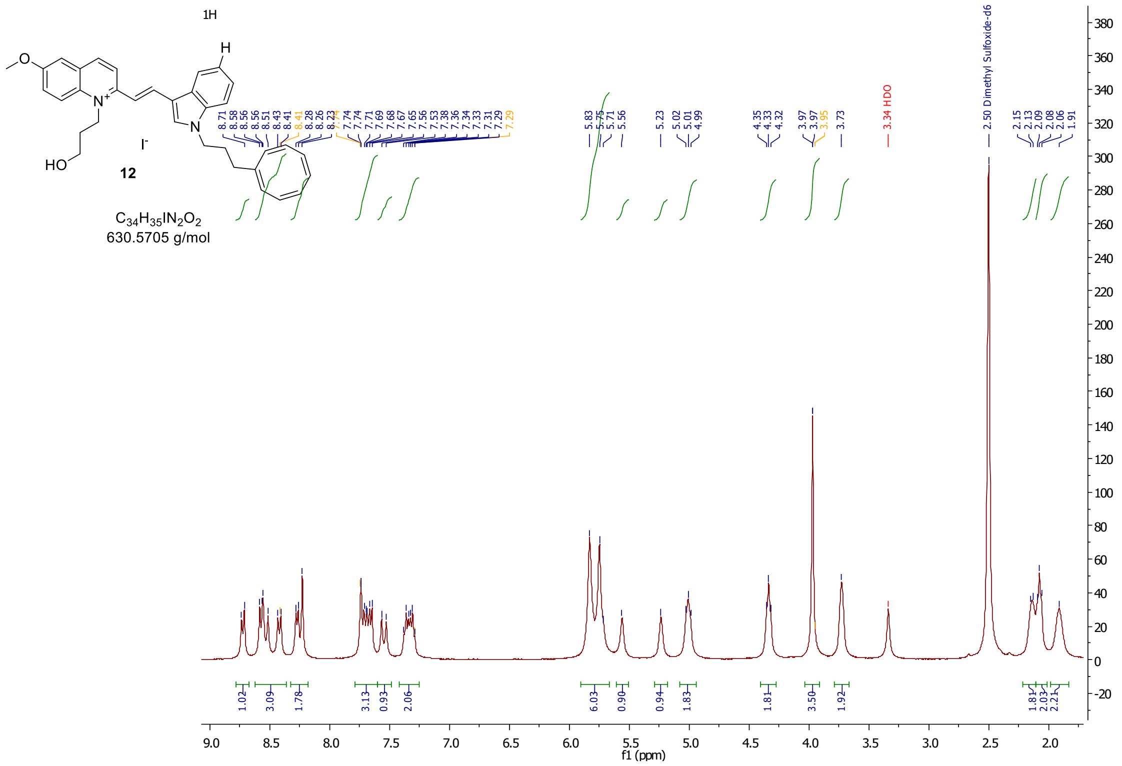
Summenformel: $C_{33}H_{33}IN_2O$

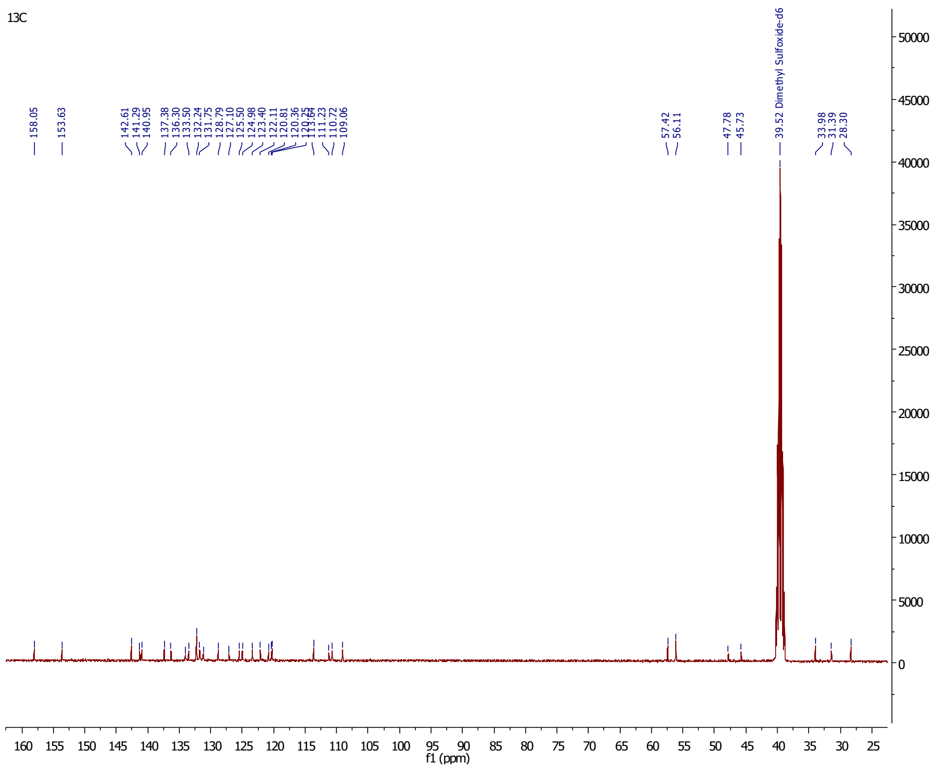
Berechnet: N: 4,66 C: 66,00 H: 5,54 ~~S:~~ (I: 21,13 O: 2,66)

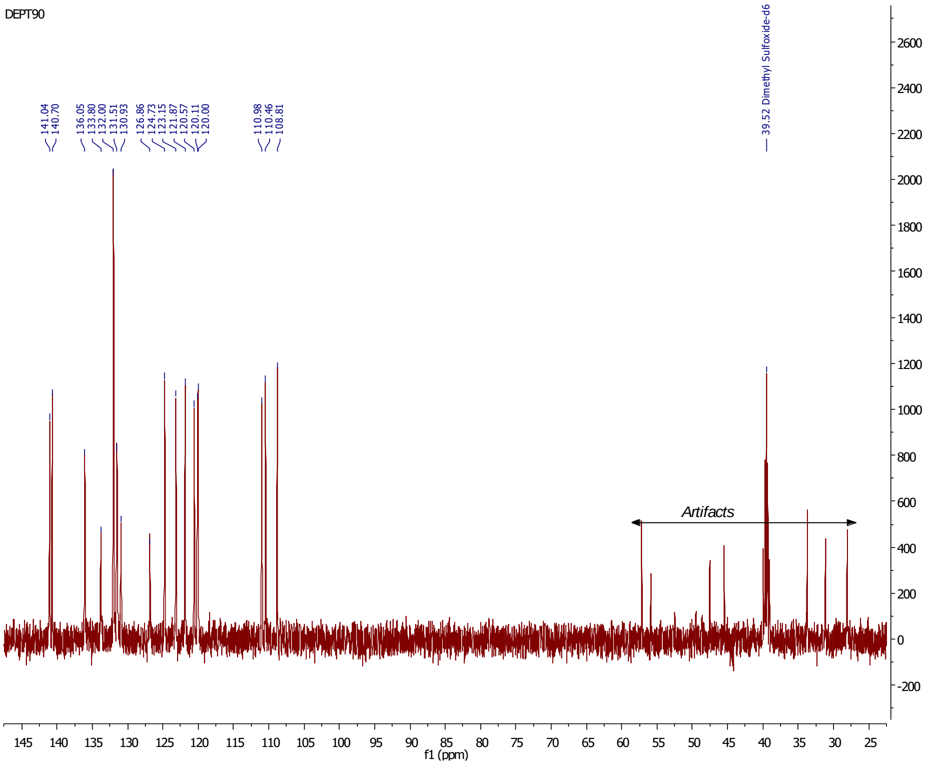
Gefunden: N: 4,77 C: 65,94 H: 5,66 S:

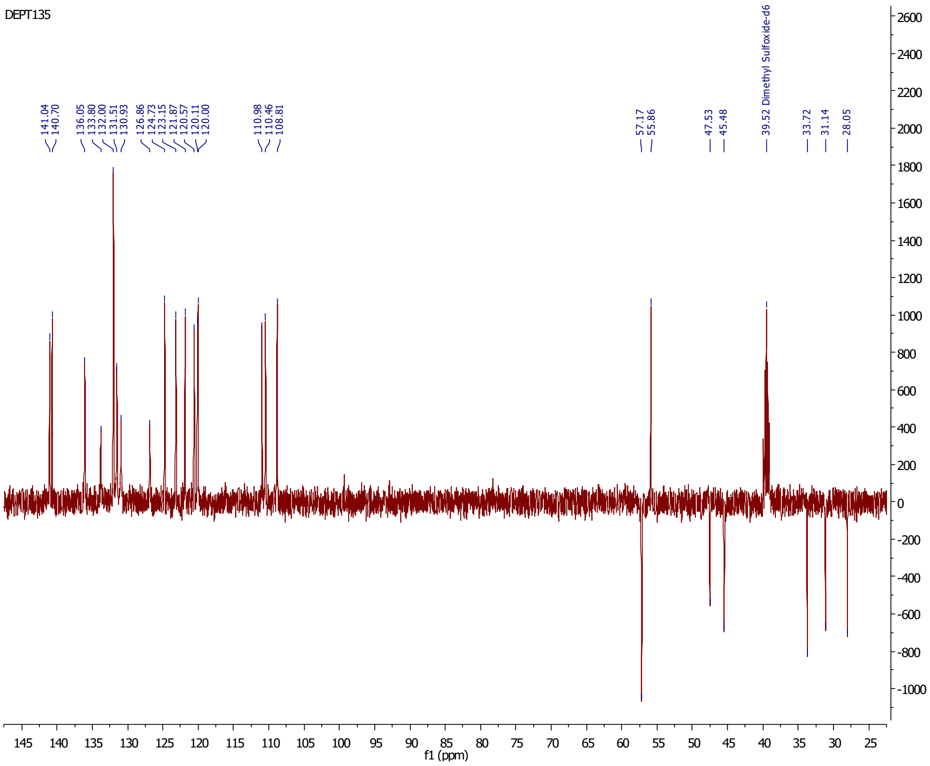
Gefunden: N: 4,73 C: 65,32 H: 5,59 S:

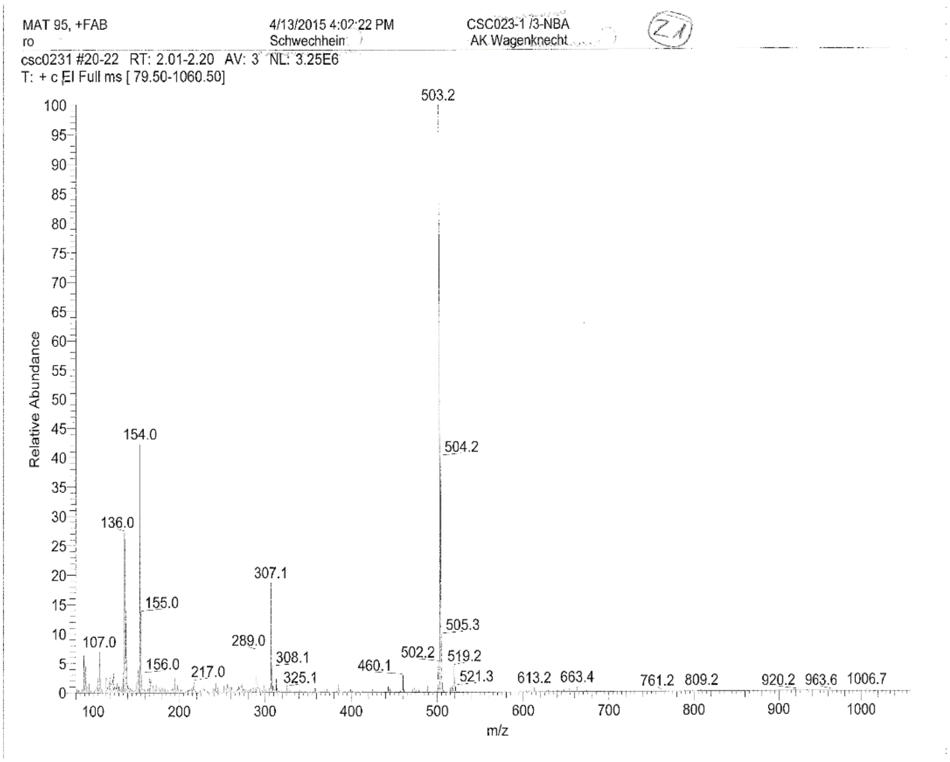
2-((*E*)-2-(1-(3-((1*Z*,3*Z*,5*Z*,7*Z*)-cycloocta-1,3,5,7-tetraen-1-yl)propyl)-1*H*-indol-3-yl)vinyl)-1-(3-hydroxypropyl)-6-methoxyquinolin-1-ium iodide (12):

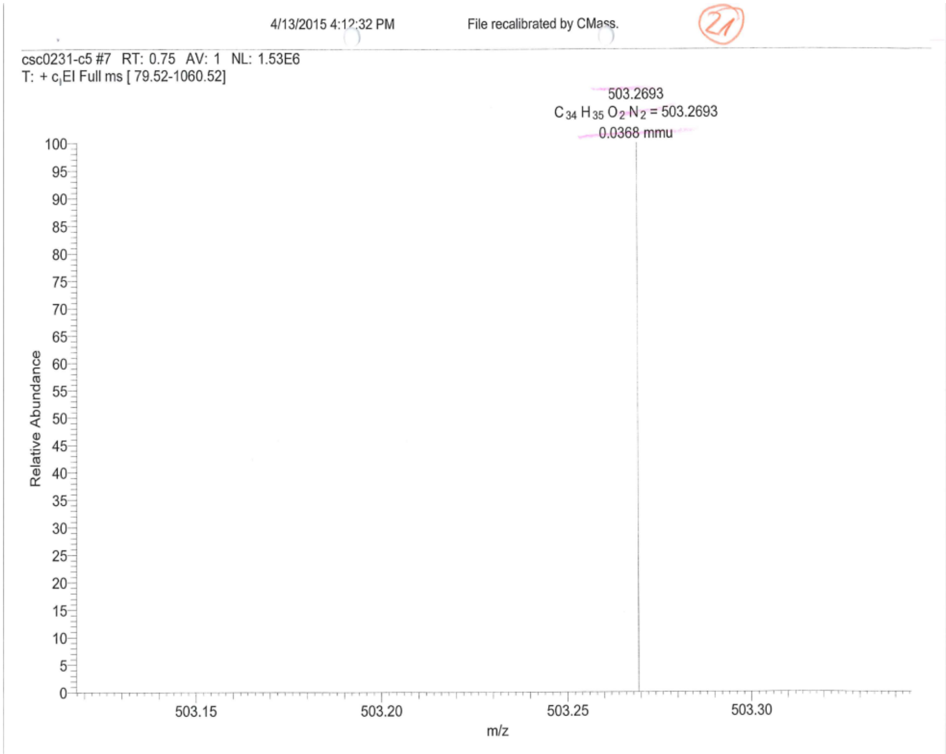


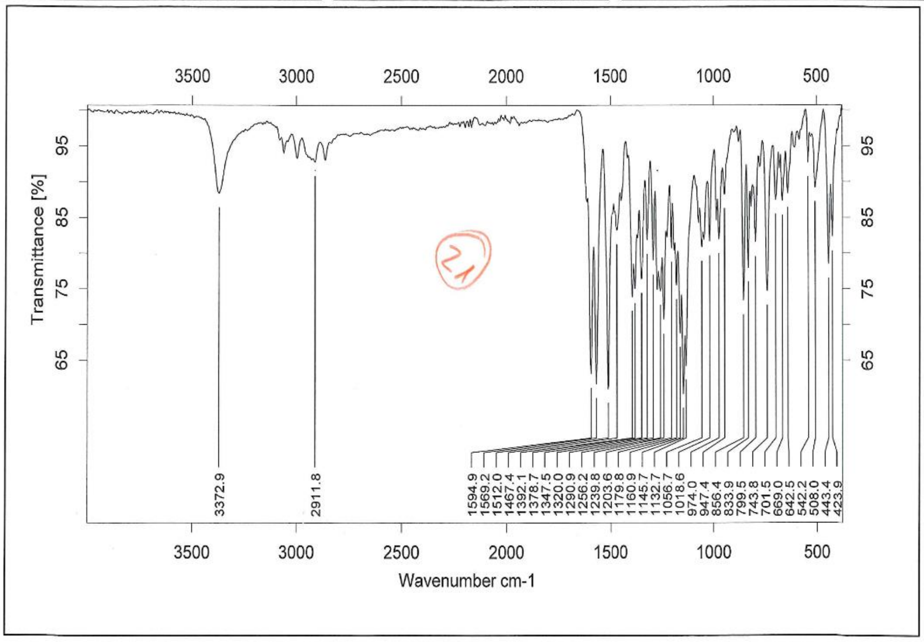



DEPT90
141.04
140.70
136.05
133.80
132.00
131.51
130.93
126.86
124.73
123.15
121.87
120.57
120.11
120.00
110.98
110.46
108.81
39.52 Dimethyl Sulfoxide-d6
Artifacts
f1 (ppm)


DEPT135
141.04
140.70
136.05
133.80
132.00
131.51
130.93
126.86
124.73
123.15
121.87
120.57
120.11
120.00
110.98
110.46
108.81
57.17
55.86
47.53
45.48
39.52 Dimethyl Sulfoxide-d6
33.72
31.14
28.05
f1 (ppm)


MAT 95, +FAB
ro
4/13/2015 4:02:22 PM
Schwechheim
CSC023-1 /3-NBA
AK Wagenknecht
csc0231 #20-22 RT: 2.01-2.20 AV: 3 NL: 3.25E6
T: + c EI Full ms [79.50-1060.50]
Relative Abundance
m/z
503.2
504.2
154.0
136.0
307.1
155.0
505.3
107.0
289.0
308.1
156.0
217.0
325.1
460.1
502.2
519.2
521.3
613.2
663.4
761.2
809.2
920.2
963.6
1006.7


4/13/2015 4:12:32 PM
File recalibrated by CMass.
csc0231-c5 #7 RT: 0.75 AV: 1 NL: 1.53E6
T: + c EI Full ms [79.52-1060.52]
503.2693
C 34 H 35 O 2 N 2 = 503.2693
0.0368 mmu
Relative Abundance
m/z
503.15
503.20
503.25
503.30



Sample : C. Schwechheimer CSC023-1	Frequency Range : 3997.41 - 373.828		Measured on : 20/04/2015
Technique : Diamant-ATR	Resolution : 4	Instrument : Alpha	Sample Scans : 24
Operator : Angelika Moesle	Zerofilling : 2	Acquisition : Double Sided,For	

ELEMENTARANALYSE

Messung gewünscht nochmals abgegeben A. Mösle

Name: Ch. Schwechheimer

Datum: 7.4.15

AK: Wagenknecht

21

Substanzbezeichnung: CSC023-1

Summenformel: $C_{34}H_{35}IN_2O_2$

Berechnet: N: 4,44 C: 64,76 H: 5,59 ~~S:~~ (I: 20,13 O: 5,07)

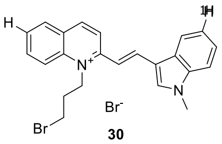
Gefunden: N: 4,34 C: 63,67 H: 5,51 S:

Gefunden: N: C: H: S:

d. Analytics of the Dye-Bromides/-Iodides 29-40

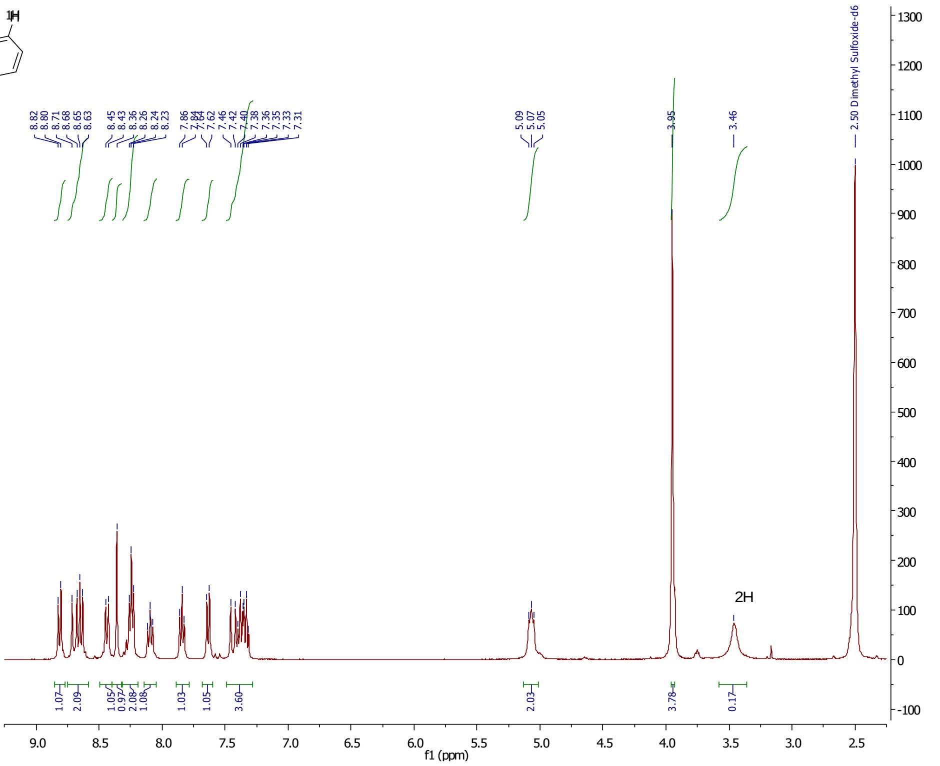
The analytics of compound **29** is described in earlier publications of our working group.[1]

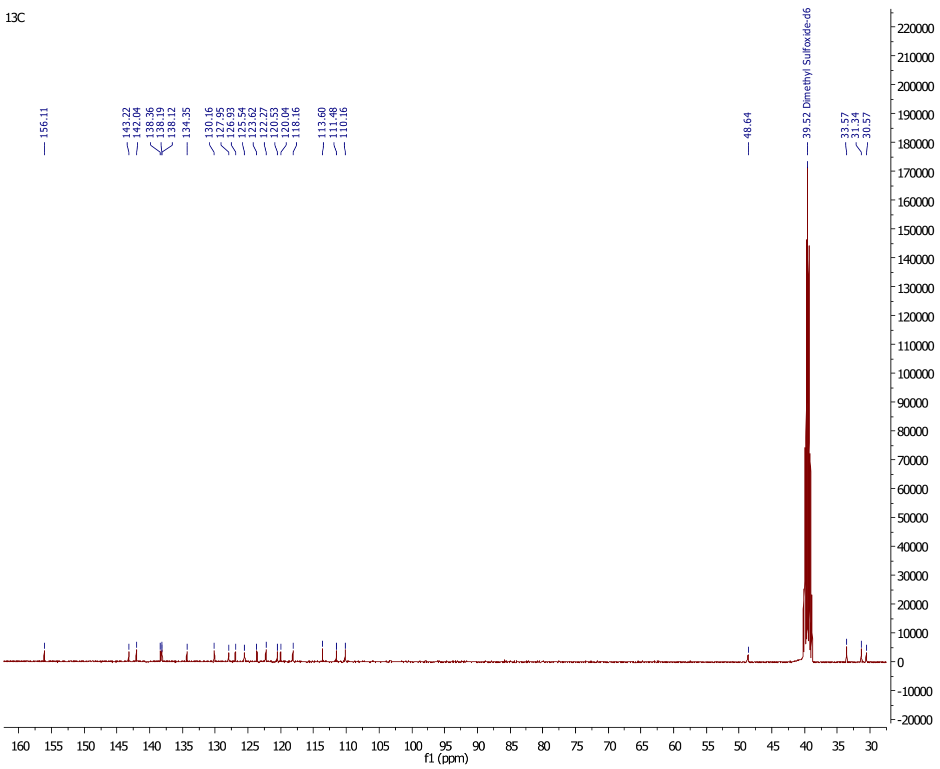
(*E*)-1-(3-iodopropyl)-2-(2-(1-methyl-1*H*-indol-3-yl)vinyl)quinolin-1-ium iodide (30):

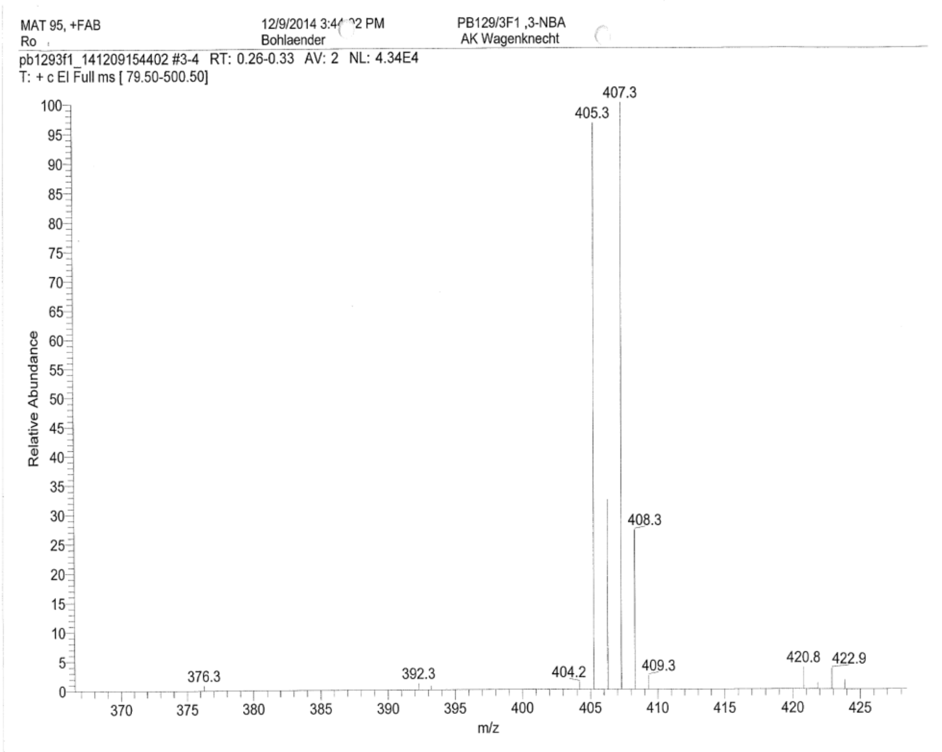


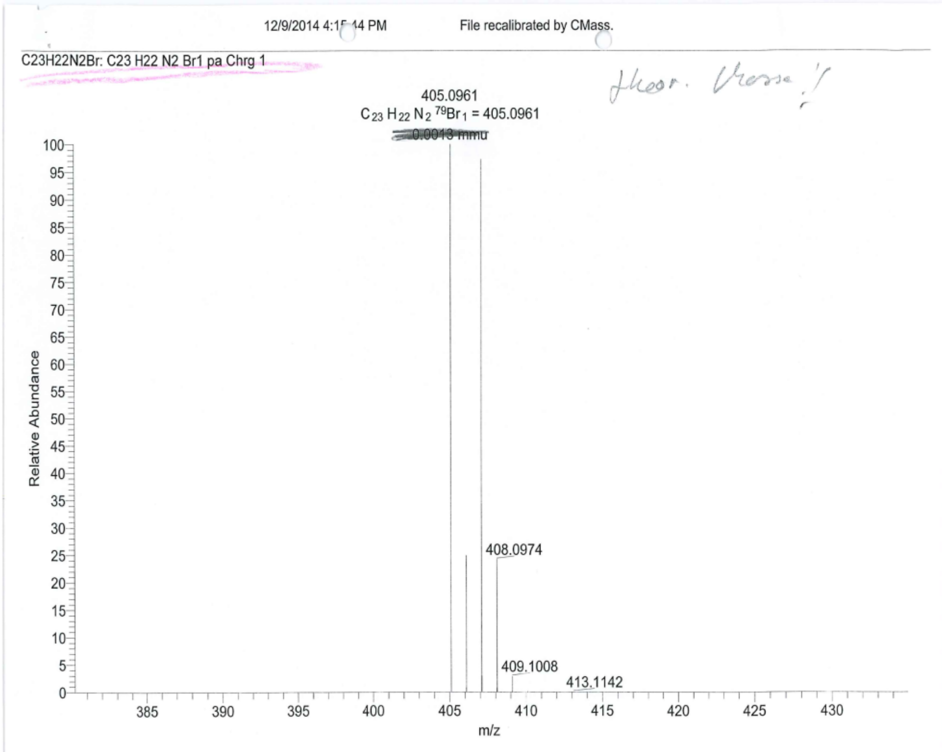
30

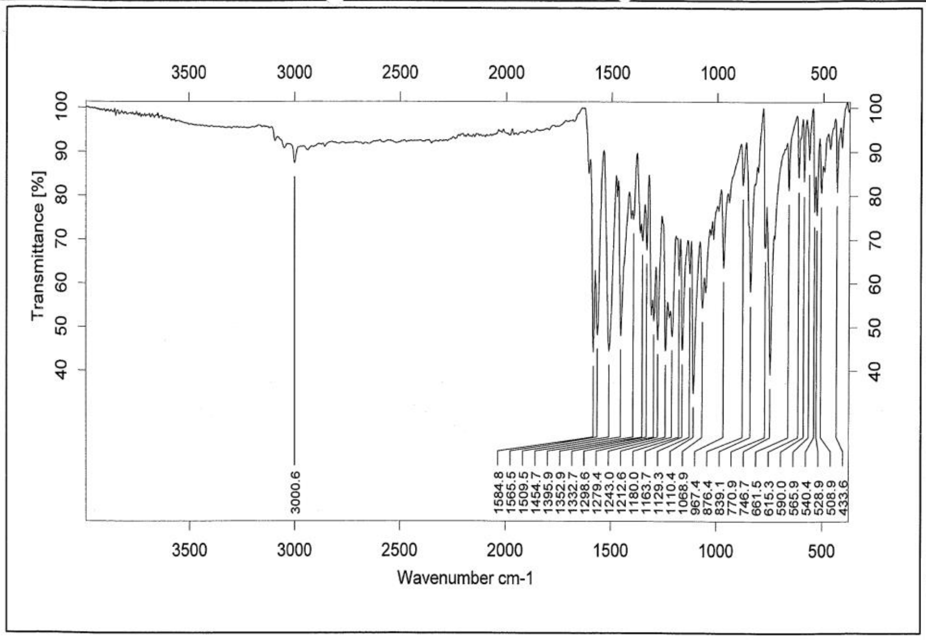
$C_{23}H_{22}Br_2N_2$
486.2510 g/mol





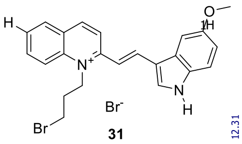

MAT 95, +FAB
Ro
12/9/2014 3:44:02 PM
Bohlaender
PB129/3F1 ,3-NBA
AK Wagenknecht
pb1293f1_141209154402 #3-4 RT: 0.26-0.33 AV: 2 NL: 4.34E4
T: + c EI Full ms [79.50-500.50]
407.3
405.3
408.3
376.3
392.3
404.2
409.3
420.8
422.9
Relative Abundance
m/z


12/9/2014 4:15:44 PM
File recalibrated by CMass.
C23H22N2Br: C23 H22 N2 Br1 pa Chrg 1
405.0961
C23 H22 N2 79Br1 = 405.0961
0.0013 mmu
theor. Masse!
408.0974
409.1008
413.1142
Relative Abundance
m/z



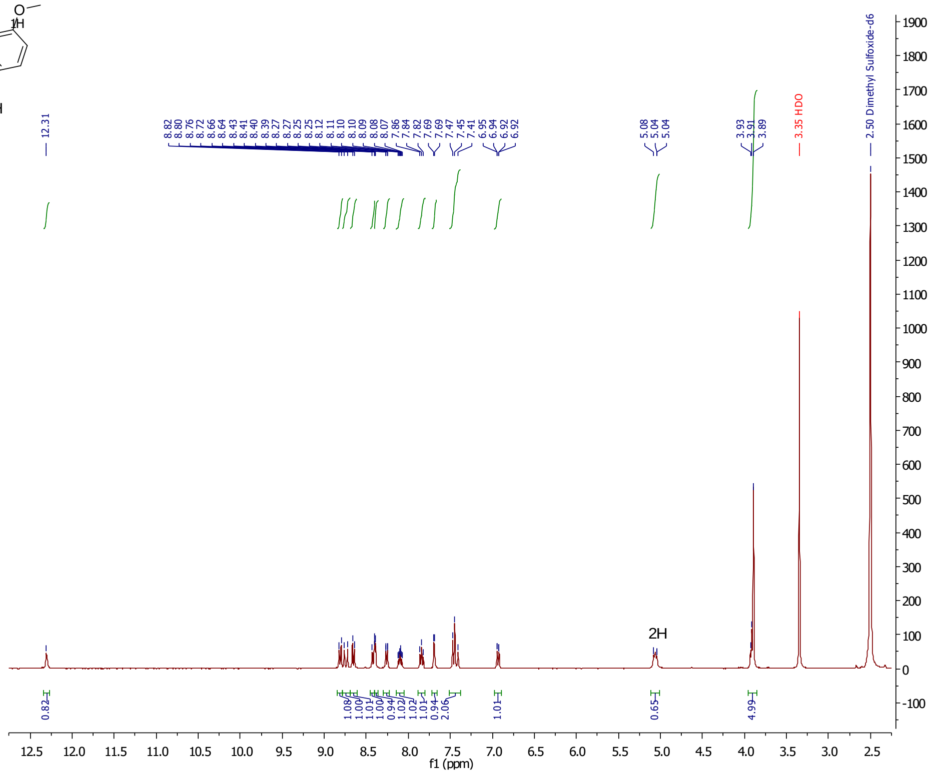
Sample : P.Bohlaender PB 129 F1b	Frequency Range : 3998.39 - 373.92		Measured on : 07/02/2013
Technique : ATR platinum Diar	Resolution : 4	Instrument : Alpha	Sample Scans : 24
Operator : Angelika Kernert	Zerofilling : 2	Acquisition : Double Sided,For	

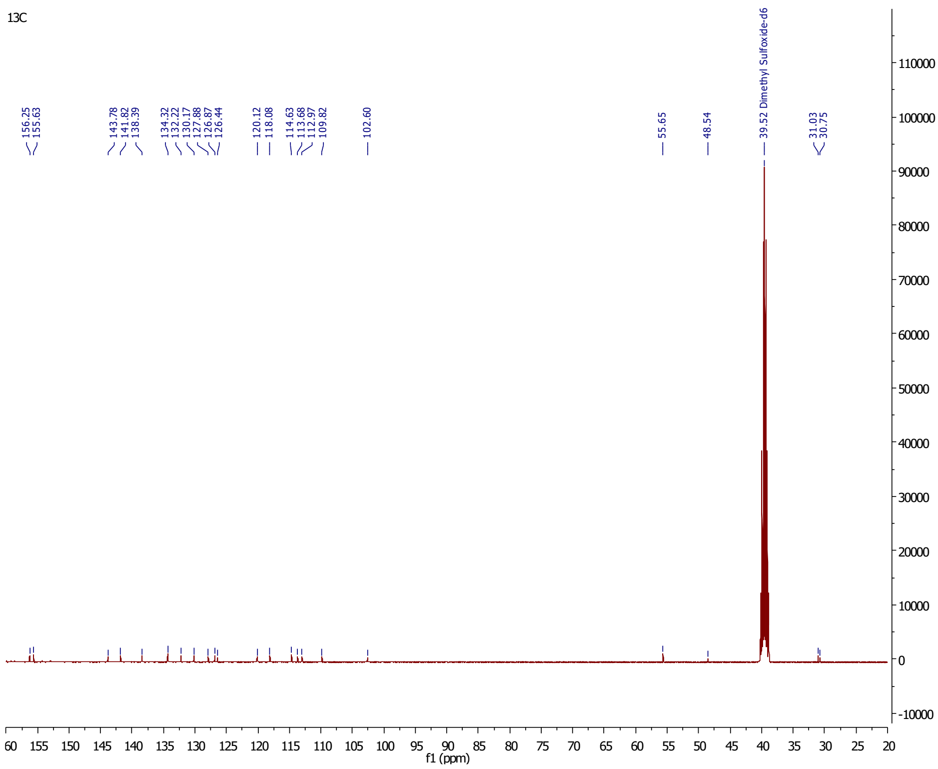
(*E*)-1-(3-bromopropyl)-2-(2-(5-methoxy-1*H*-indol-3-yl)vinyl)quinolin-1-ium bromide (31):

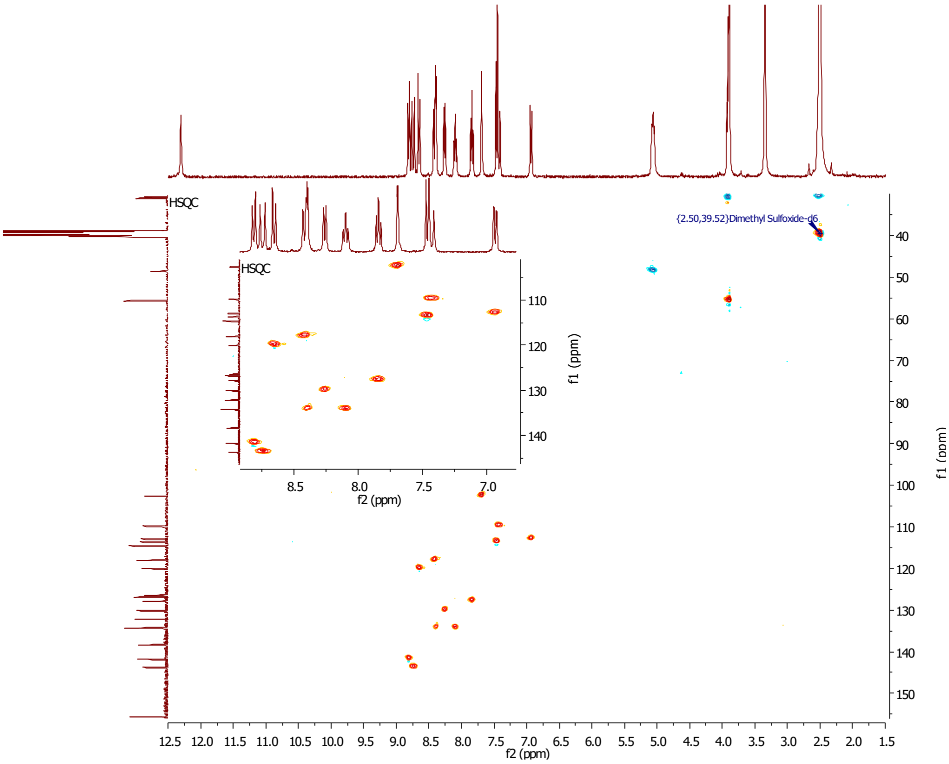


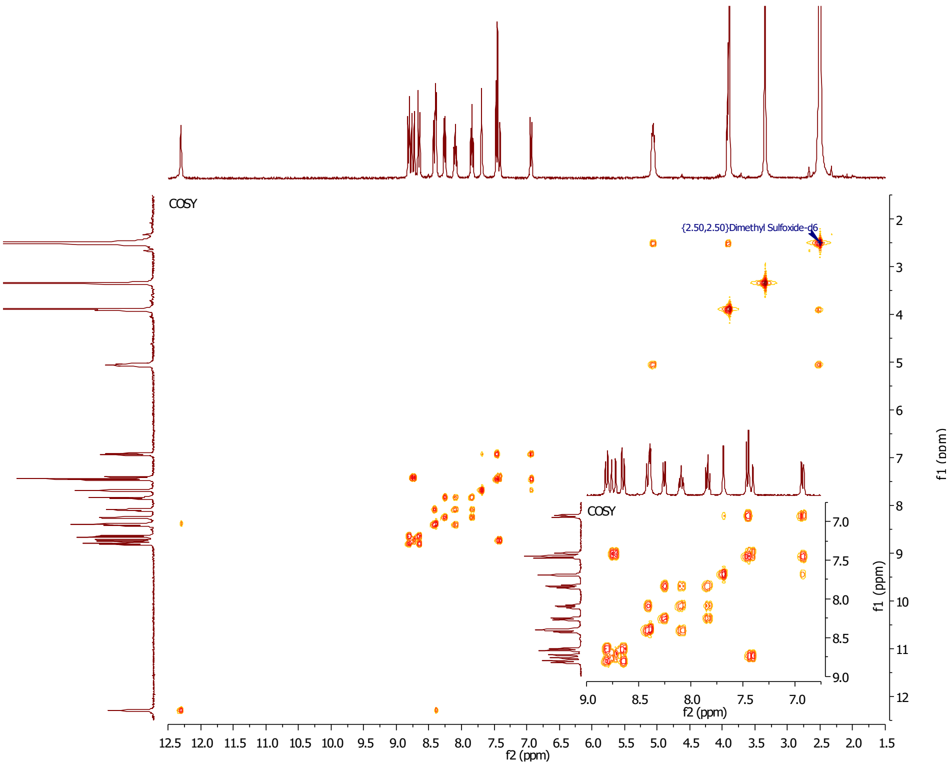
31

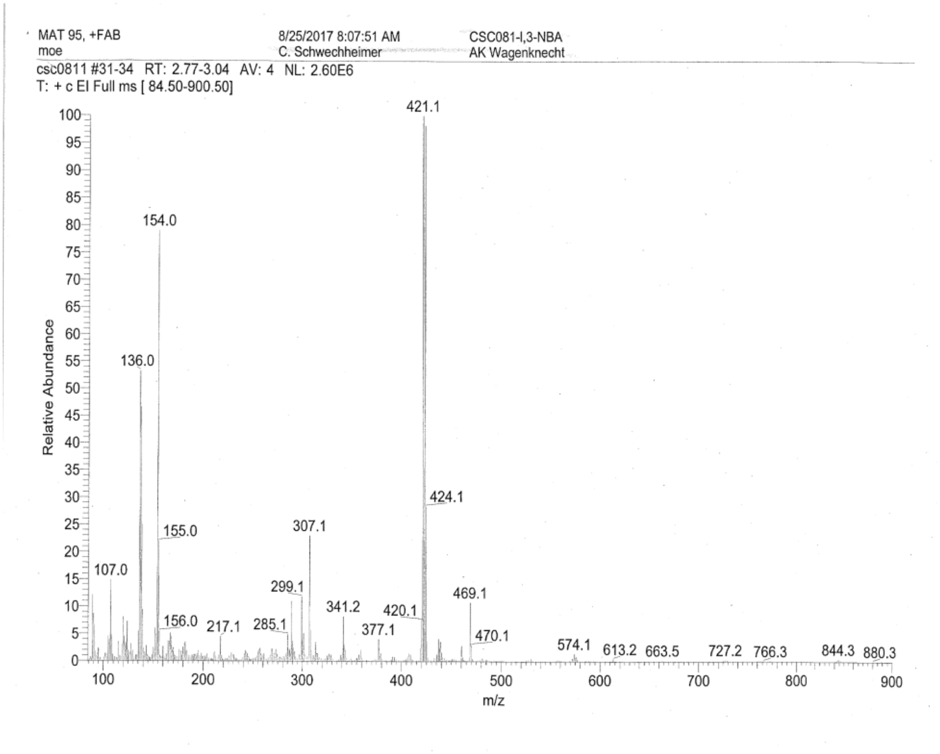
$C_{23}H_{22}Br_2N_2O$
502.2500 g/mol



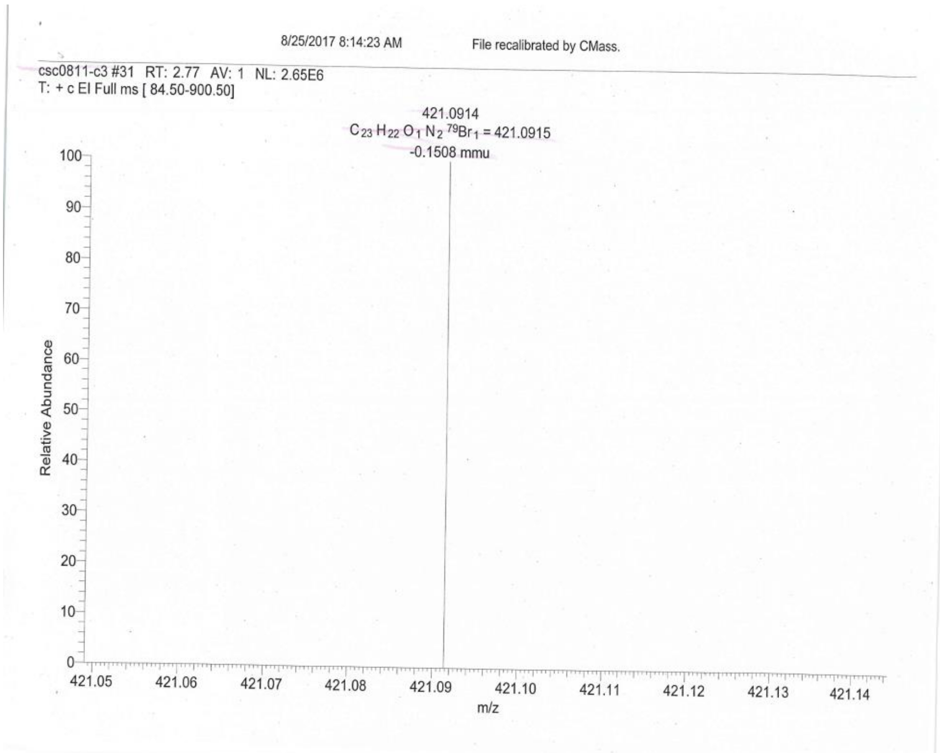



HSQC
{2.50,39.52}Dimethyl Sulfoxide-d6
f2 (ppm)
f1 (ppm)

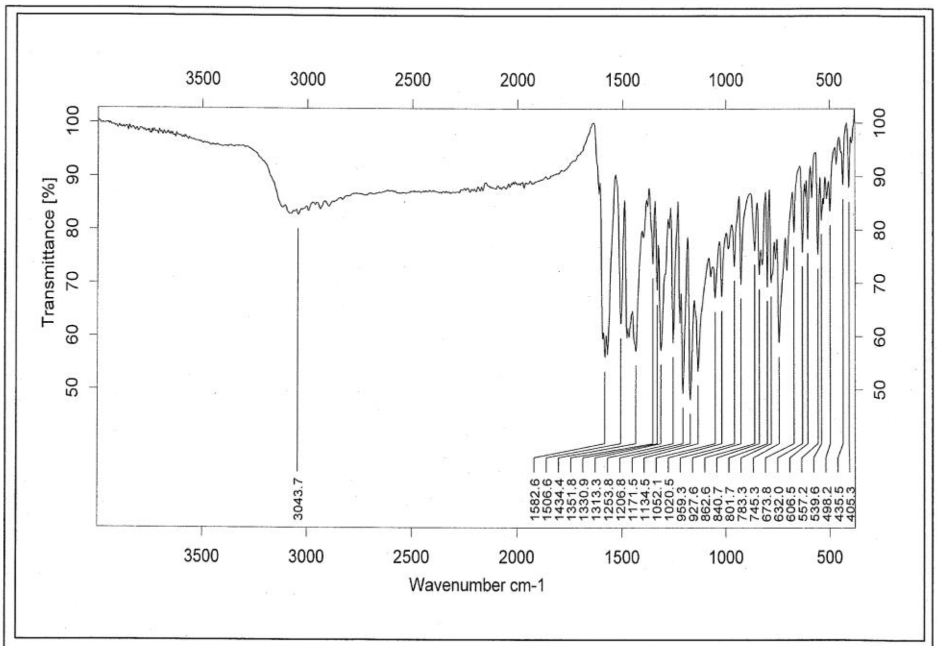

COSY
{2.50,2.50}Dimethyl Sulfoxide-d6
f2 (ppm)
f1 (ppm)



MAT 95, +FAB
moe
8/25/2017 8:07:51 AM
C. Schwechheimer
CSC081-I,3-NBA
AK Wagenknecht
csc0811 #31-34 RT: 2.77-3.04 AV: 4 NL: 2.60E6
T: + c EI Full ms [84.50-900.50]
Relative Abundance
m/z
421.1
154.0
136.0
424.1
155.0
307.1
107.0
299.1
341.2
420.1
469.1
156.0
217.1
285.1
377.1
470.1
574.1
613.2
663.5
727.2
766.3
844.3
880.3

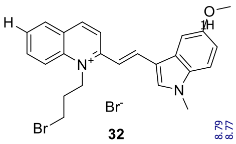


8/25/2017 8:14:23 AM
File recalibrated by CMass.
csc0811-c3 #31 RT: 2.77 AV: 1 NL: 2.65E6
T: + c EI Full ms [84.50-900.50]
421.0914
$C_{23} H_{22} O_1 N_2 {}^{79}Br_1$ = 421.0915
-0.1508 mmu
Relative Abundance
m/z



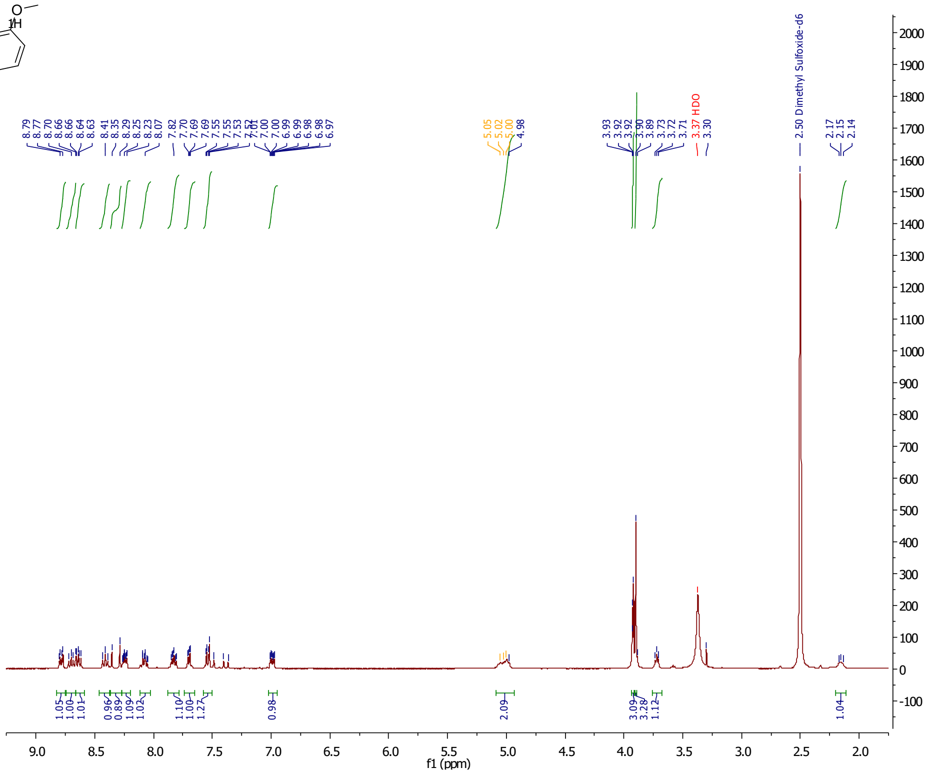
Sample : Ch.Schwechheimer CSC081-1	Frequency Range : 3997.45 - 373.964	Measured on : 28/08/2017	
Technique : ATR platinum Diamond	Resolution : 4	Instrument : Alpha	Sample Scans : 24
Operator : Angelika Moesle	Zerofilling : 2	Acquisition : Double Sided,Forward-Backward	

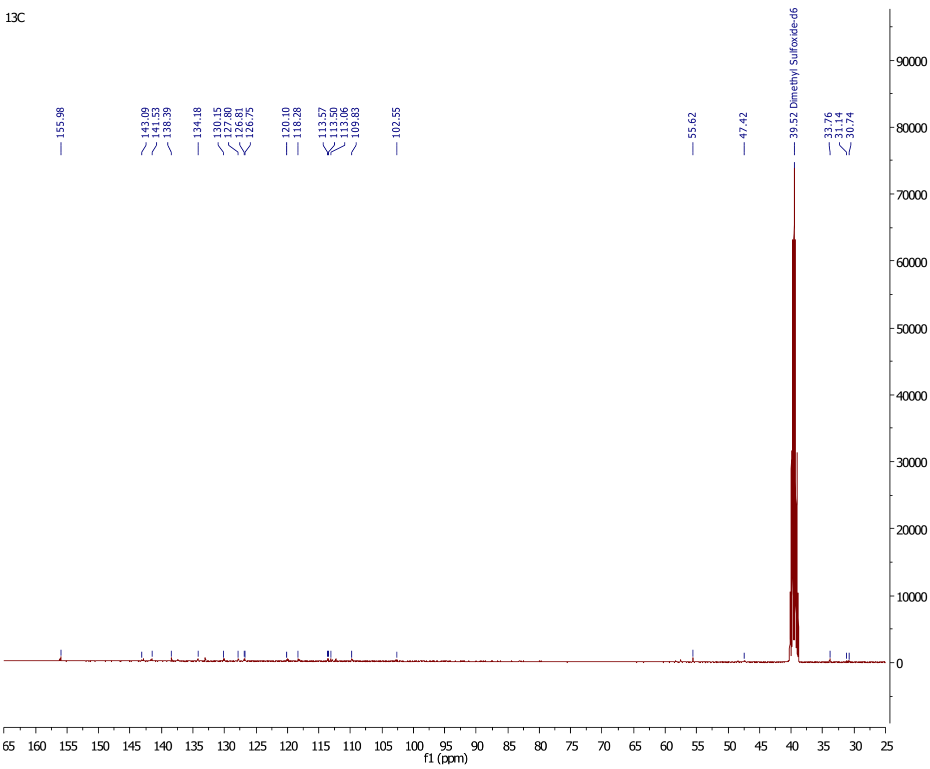
(*E*)-1-(3-bromopropyl)-2-(2-(5-methoxy-1-methyl-1*H*-indol-3-yl)vinyl)quinolin-1-ium bromide (32):

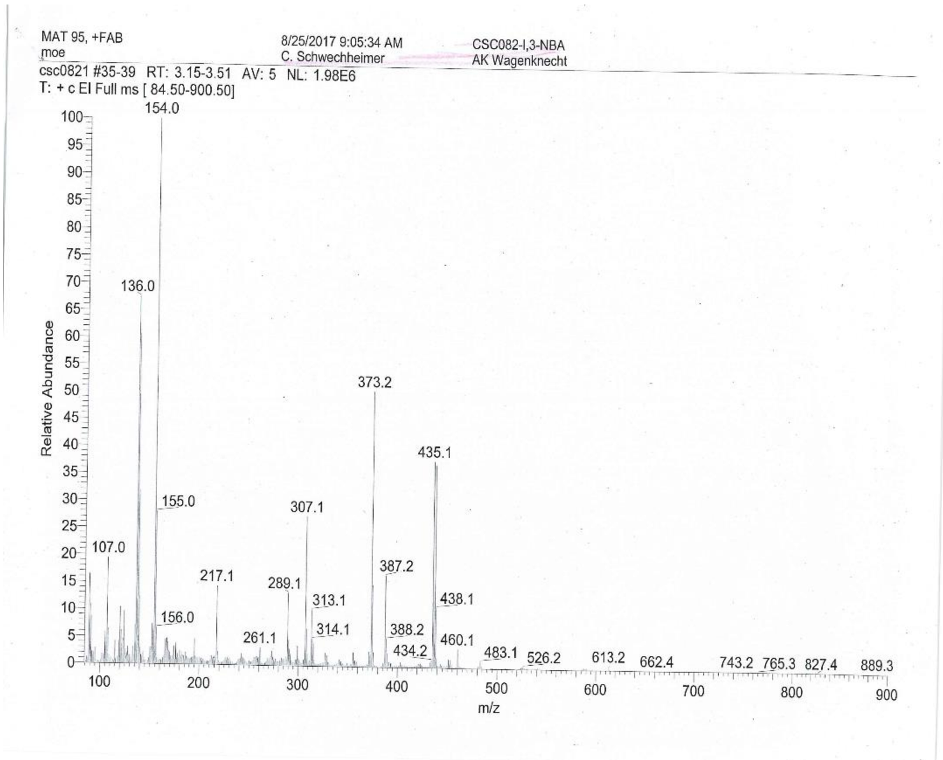


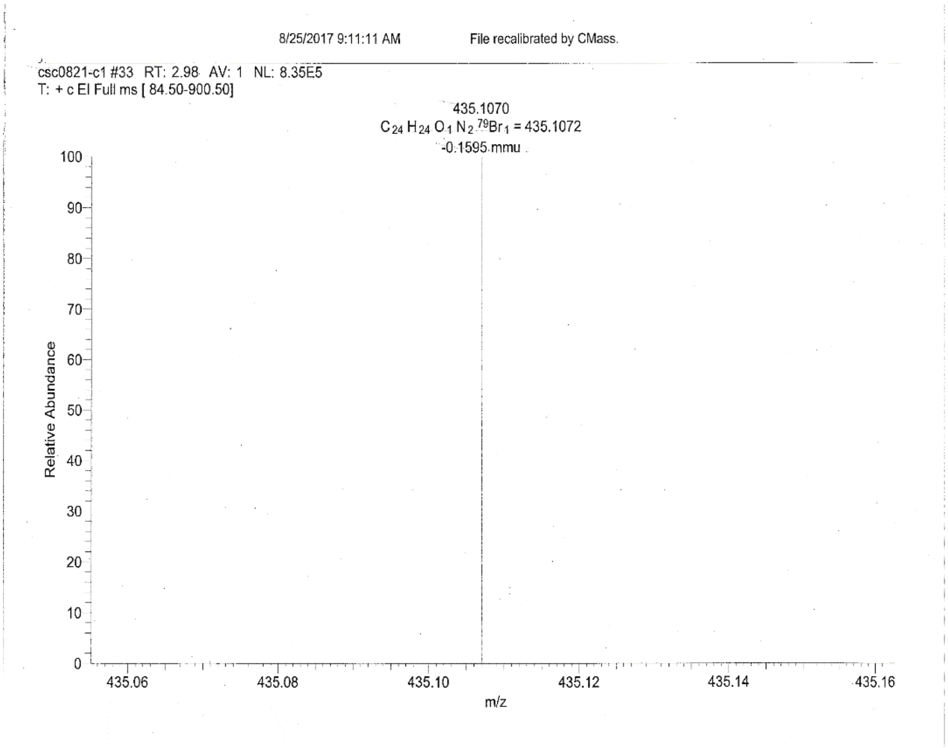
32

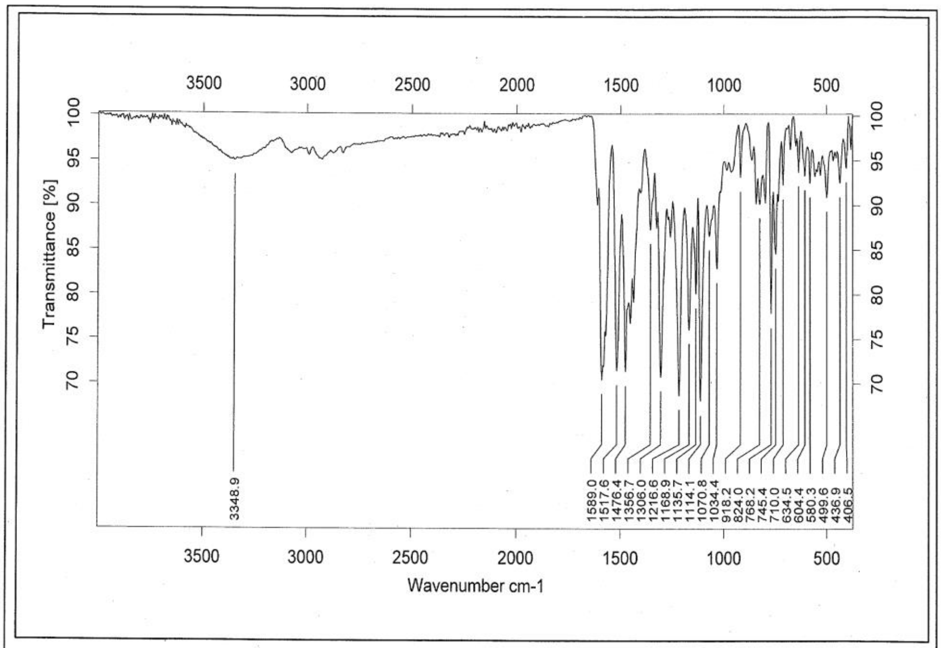
$C_{24}H_{24}Br_2N_2O$
516.2770 g/mol





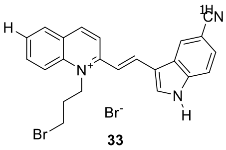

MAT 95, +FAB
moe
8/25/2017 9:05:34 AM
C. Schwechheimer
CSC082-I,3-NBA
AK Wagenknecht
csc0821 #35-39 RT: 3.15-3.51 AV: 5 NL: 1.98E6
T: + c EI Full ms [84.50-900.50]
Relative Abundance
m/z
154.0
136.0
373.2
435.1
155.0
307.1
107.0
387.2
217.1
289.1
438.1
313.1
156.0
314.1
388.2
261.1
460.1
434.2
483.1
526.2
613.2
662.4
743.2
765.3
827.4
889.3


8/25/2017 9:11:11 AM
File recalibrated by CMass.
csc0821-c1 #33 RT: 2.98 AV: 1 NL: 8.35E5
T: + c EI Full ms [84.50-900.50]
435.1070
C 24 H 24 O 1 N 2 79Br 1 = 435.1072
-0.1595 mmu
Relative Abundance
m/z



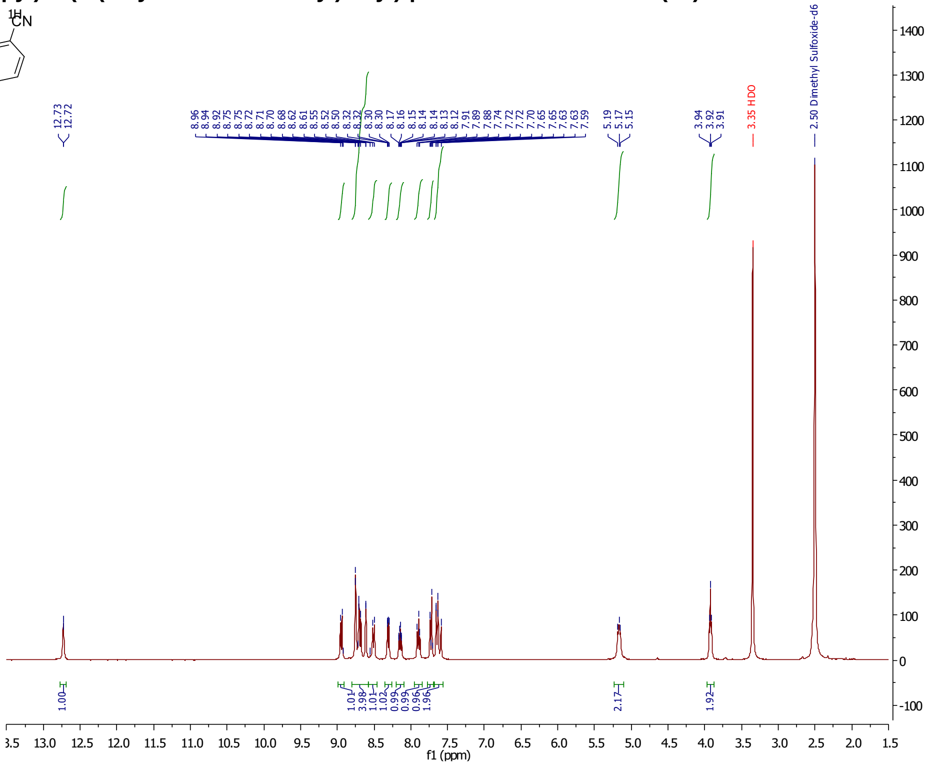
Sample : Ch. Schwechheimer CSC082-1	Frequency Range : 3997.45 - 373.964		Measured on : 25/08/2017
Technique : Diamant-ATR	Resolution : 4	Instrument : Alpha	Sample Scans : 24
Operator : Angelika Moesle	Zerofilling : 2	Acquisition : Double Sided,Forward-Backward	

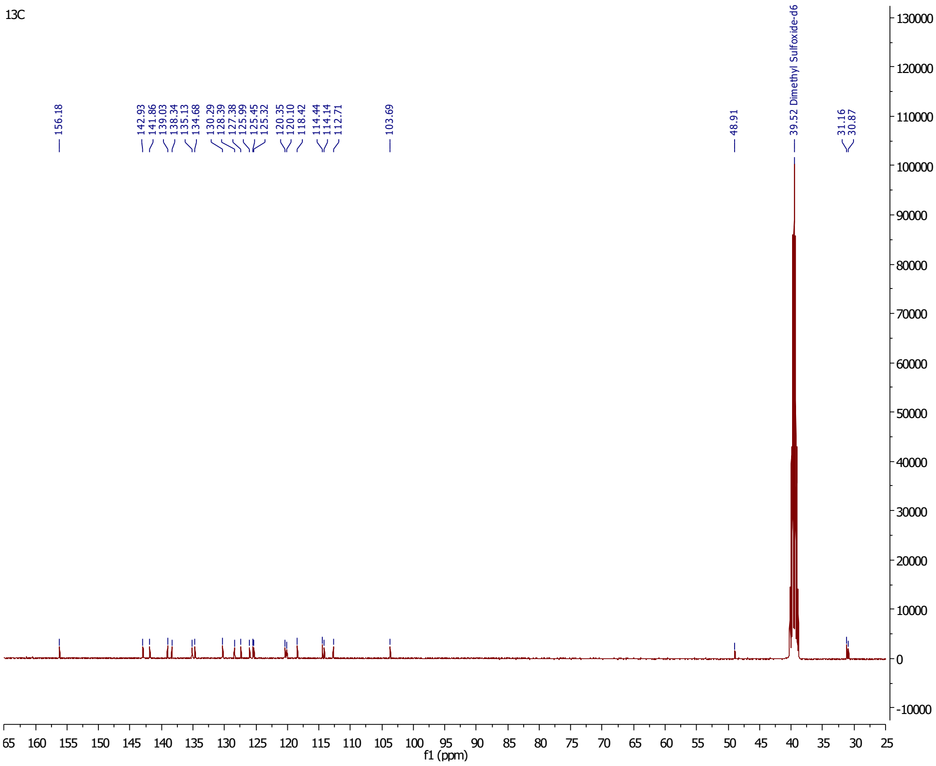
(*E*)-1-(3-bromopropyl)-2-(2-(5-cyano-1*H*-indol-3-yl)vinyl)quinolin-1-ium bromide (33):

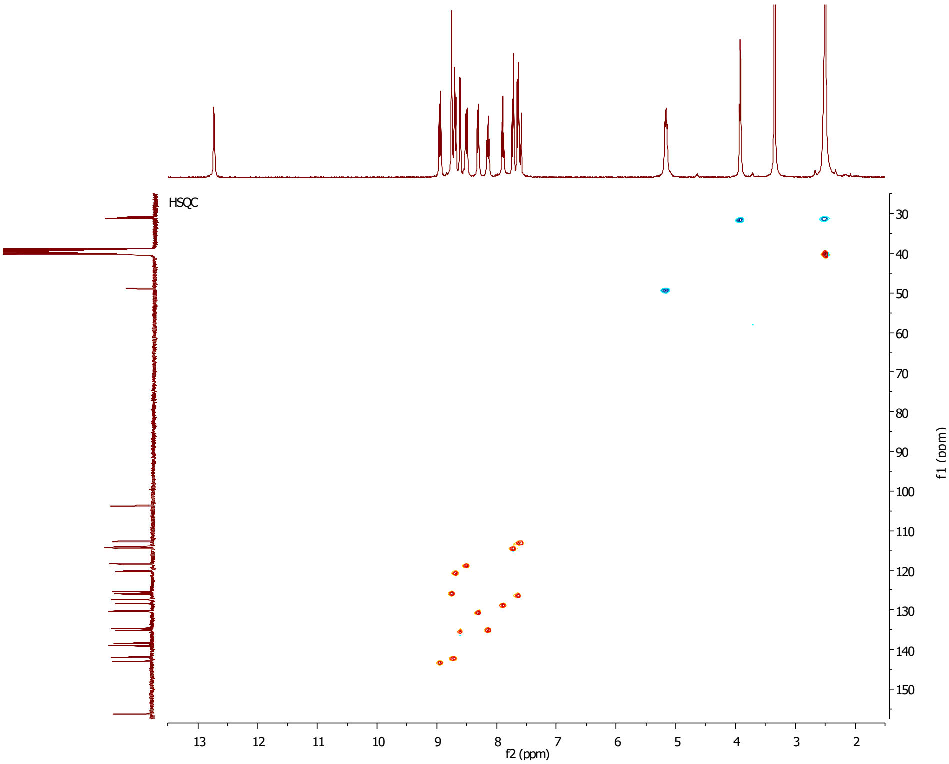


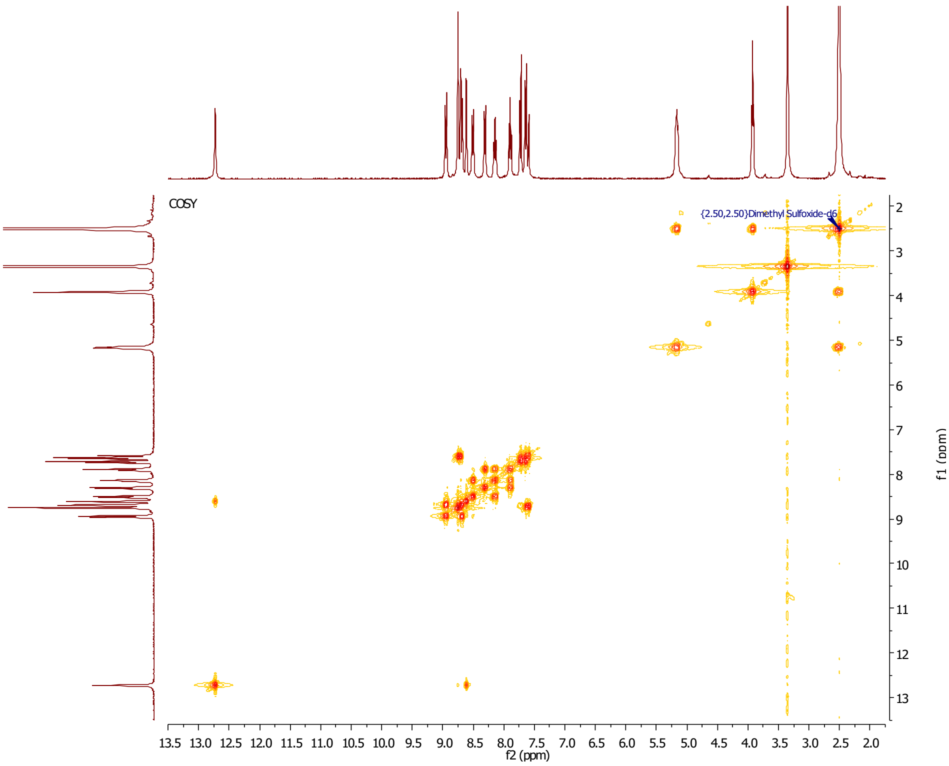
33

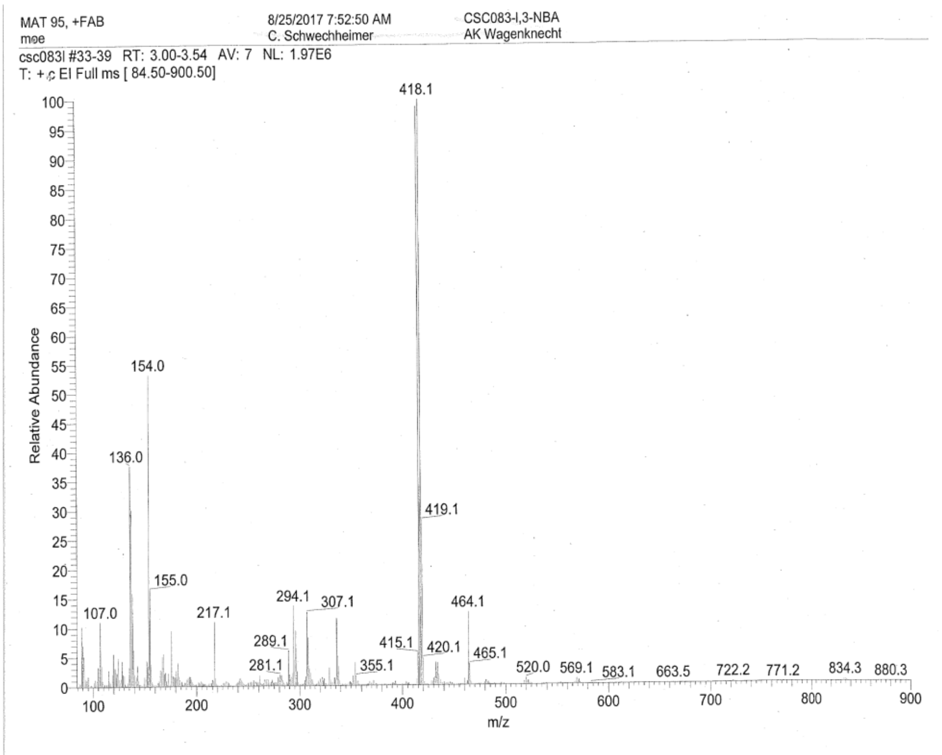
$C_{23}H_{19}Br_2N_3$
497.2340 g/mol

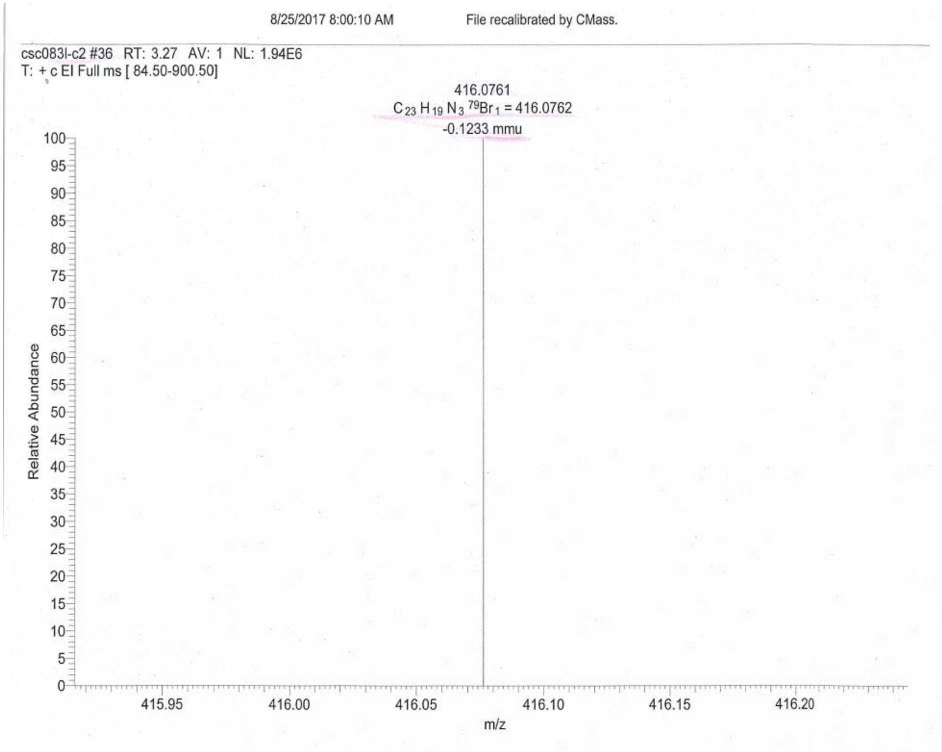


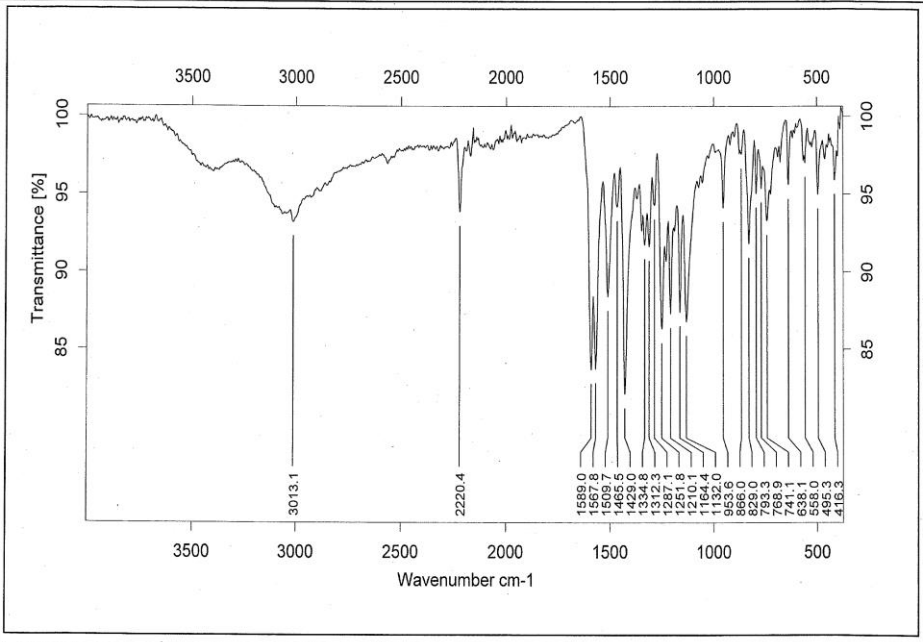



HSQC
f2 (ppm)
f1 (ppm)


COSY
{2.50,2.50}Dimethyl Sulfoxide-d6
f2 (ppm)
f1 (ppm)

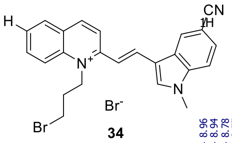

MAT 95, +FAB
8/25/2017 7:52:50 AM
CSC083-I,3-NBA
C. Schwechheimer
AK Wagenknecht
csc083l #33-39 RT: 3.00-3.54 AV: 7 NL: 1.97E6
T: + c EI Full ms [84.50-900.50]
Relative Abundance
m/z
418.1
154.0
136.0
419.1
155.0
107.0
217.1
294.1
307.1
464.1
289.1
281.1
415.1
420.1
465.1
355.1
520.0
569.1
583.1
663.5
722.2
771.2
834.3
880.3


8/25/2017 8:00:10 AM
File recalibrated by CMass.
csc083l-c2 #36 RT: 3.27 AV: 1 NL: 1.94E6
T: + c EI Full ms [84.50-900.50]
416.0761
C23 H19 N3 79Br1 = 416.0762
-0.1233 mmu
Relative Abundance
m/z



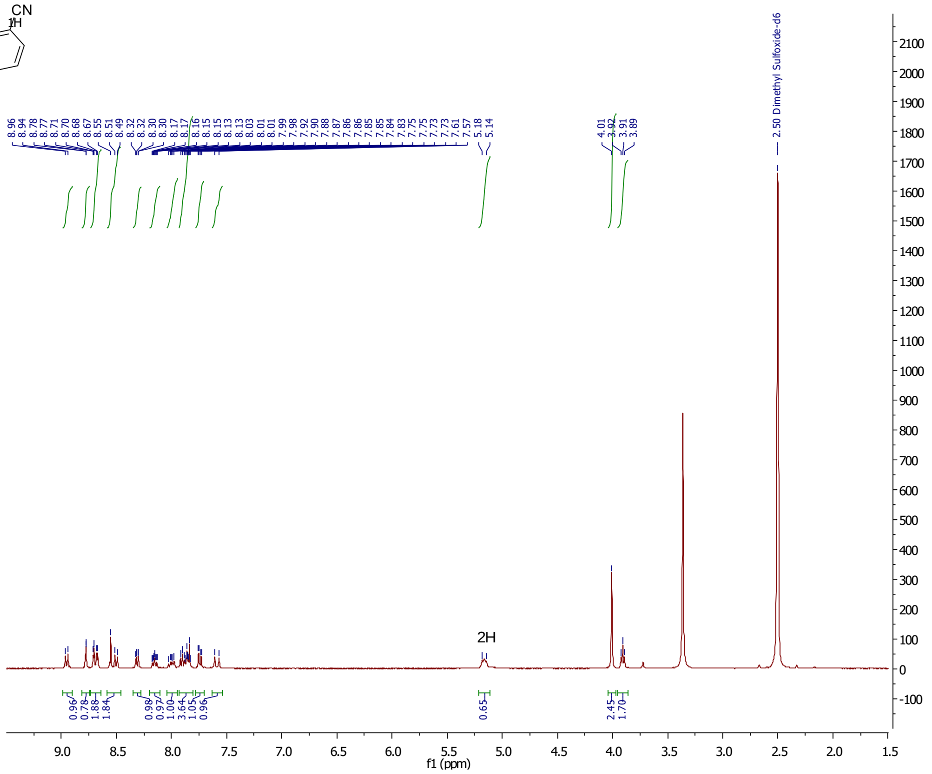
Sample : Ch. Schwechheimer CSC083-1	Frequency Range : 3997.45 - 373.964	Measured on : 25/08/2017	
Technique : Diamant-ATR	Resolution : 4	Instrument : Alpha	Sample Scans : 24
Operator : Angelika Moesle	Zerofilling : 2	Acquisition : Double Sided,Forward-Backward	

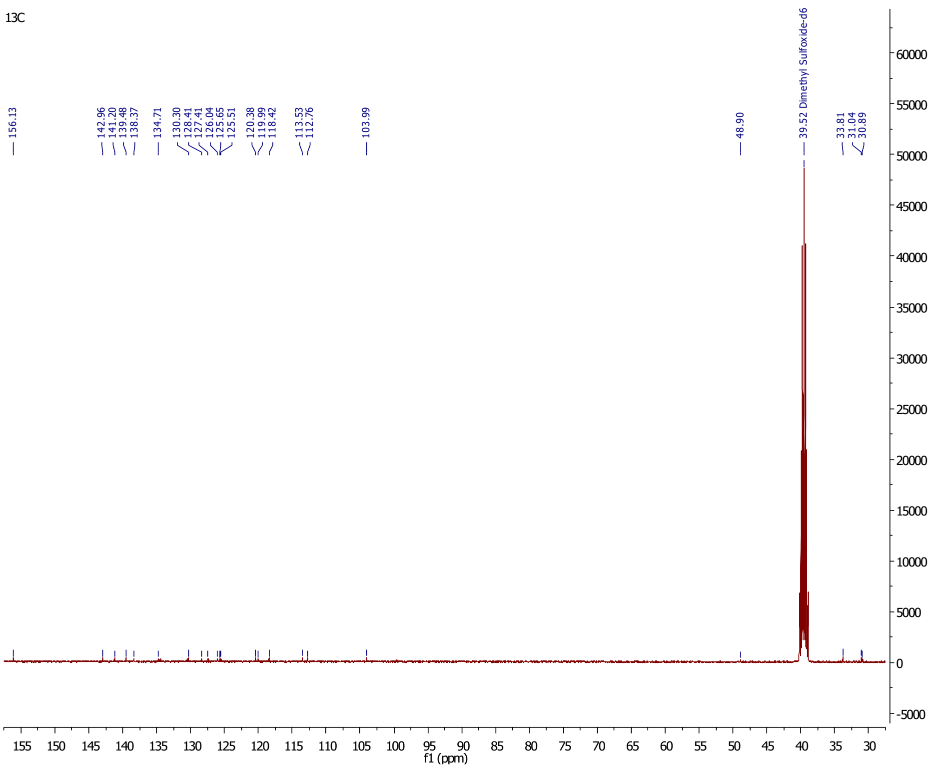
(*E*)-1-(3-bromopropyl)-2-(2-(5-cyano-1-methyl-1*H*-indol-3-yl)vinyl)quinolin-1-ium bromide (34):

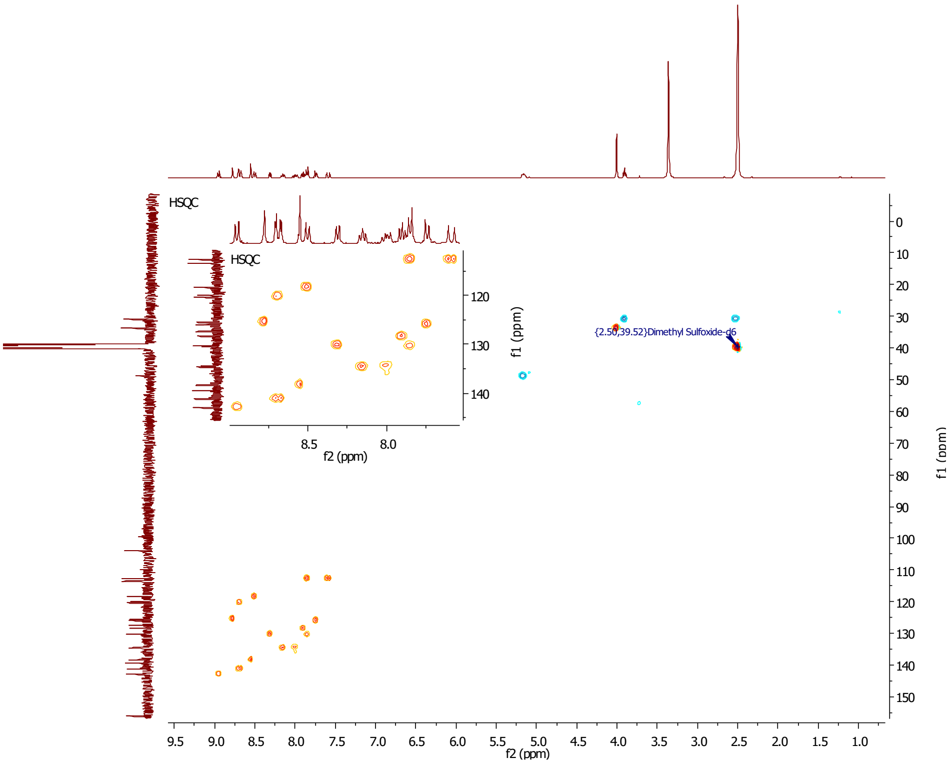


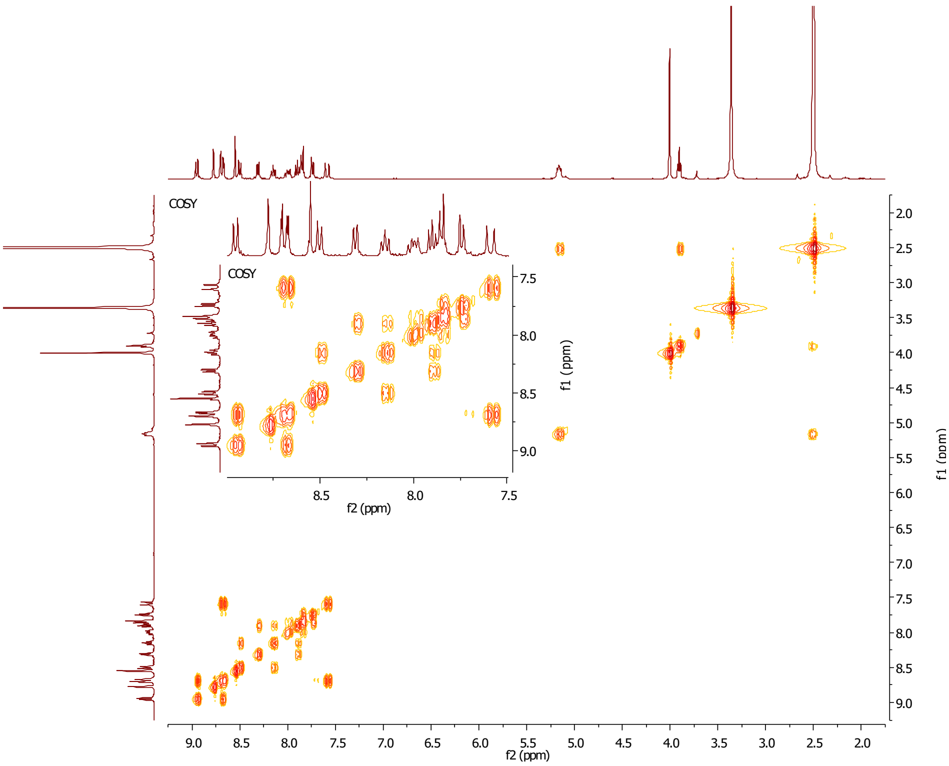
34

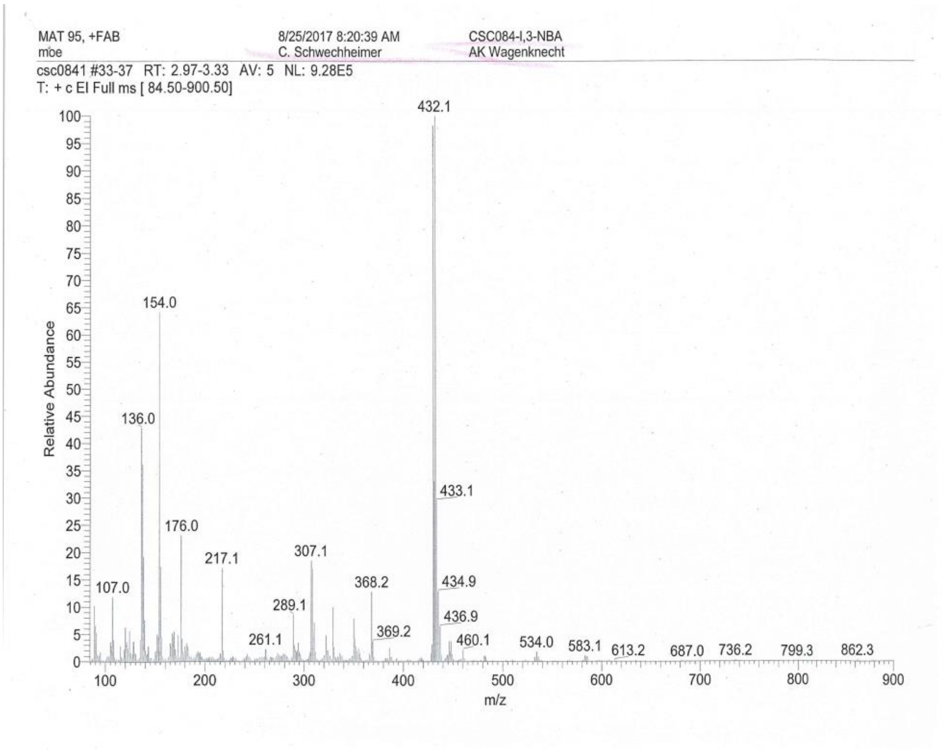
$C_{24}H_{21}Br_2N_3$
511.2610 g/mol

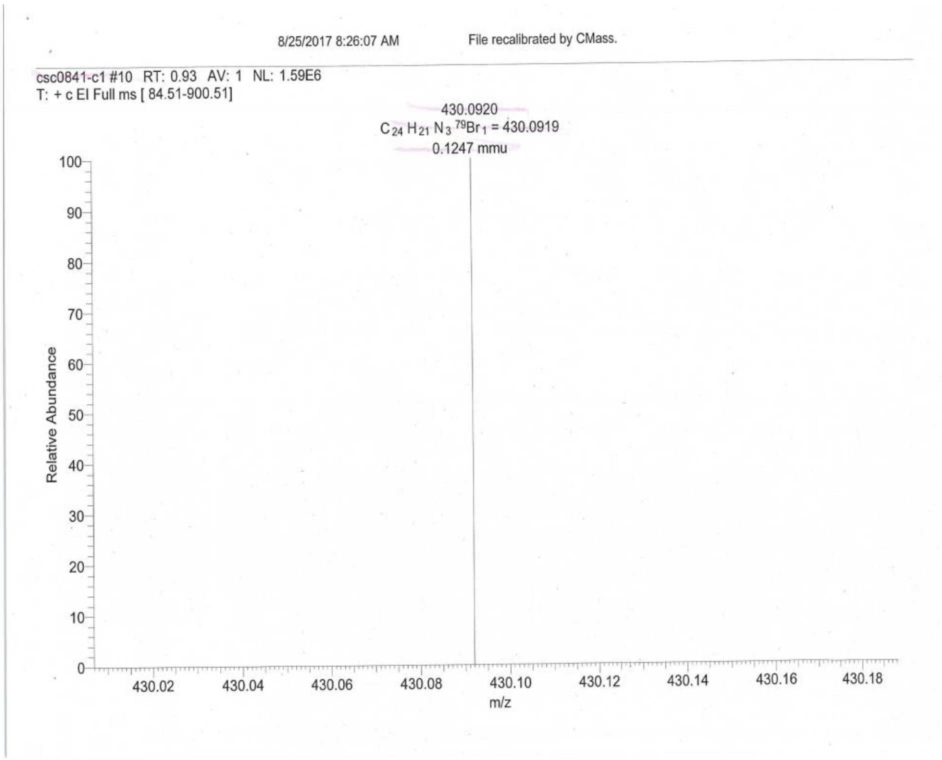


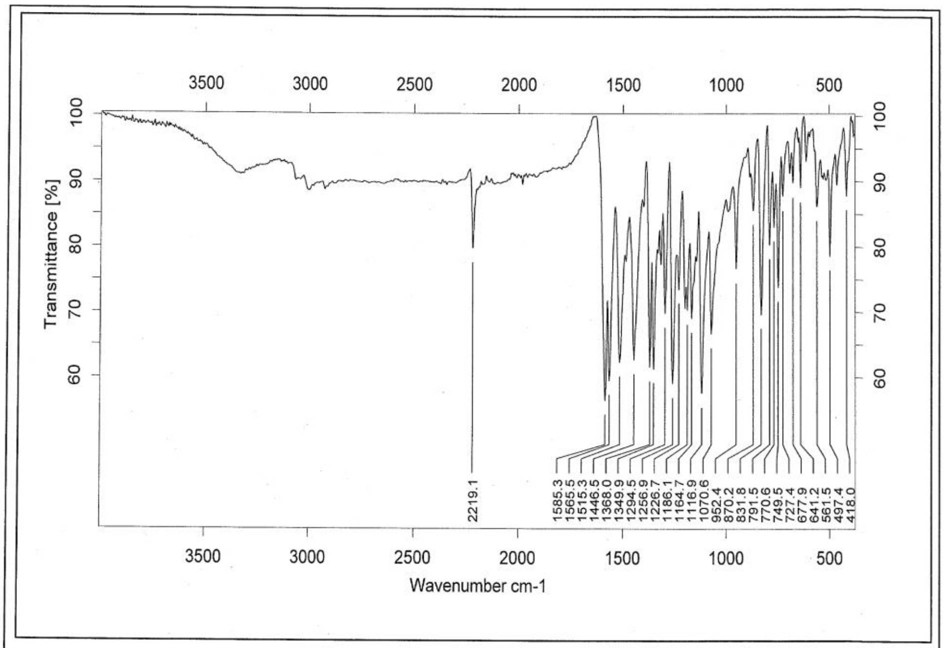



HSQC
{2.50,39.52}Dimethyl Sulfoxide-d6
f2 (ppm)
f1 (ppm)


COSY
f2 (ppm)
f1 (ppm)

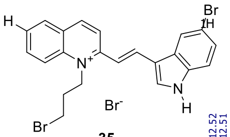

MAT 95, +FAB
mbe
8/25/2017 8:20:39 AM
C. Schwechheimer
CSC084-I,3-NBA
AK Wagenknecht
csc0841 #33-37 RT: 2.97-3.33 AV: 5 NL: 9.28E5
T: + c EI Full ms [84.50-900.50]
432.1
154.0
136.0
433.1
176.0
217.1
307.1
107.0
368.2
434.9
289.1
436.9
261.1
369.2
460.1
534.0
583.1
613.2
687.0
736.2
799.3
862.3
Relative Abundance
m/z


8/25/2017 8:26:07 AM
File recalibrated by CMass.
csc0841-c1 #10 RT: 0.93 AV: 1 NL: 1.59E6
T: + c EI Full ms [84.51-900.51]
430.0920
C 24 H 21 N 3 79Br 1 = 430.0919
0.1247 mmu
Relative Abundance
m/z



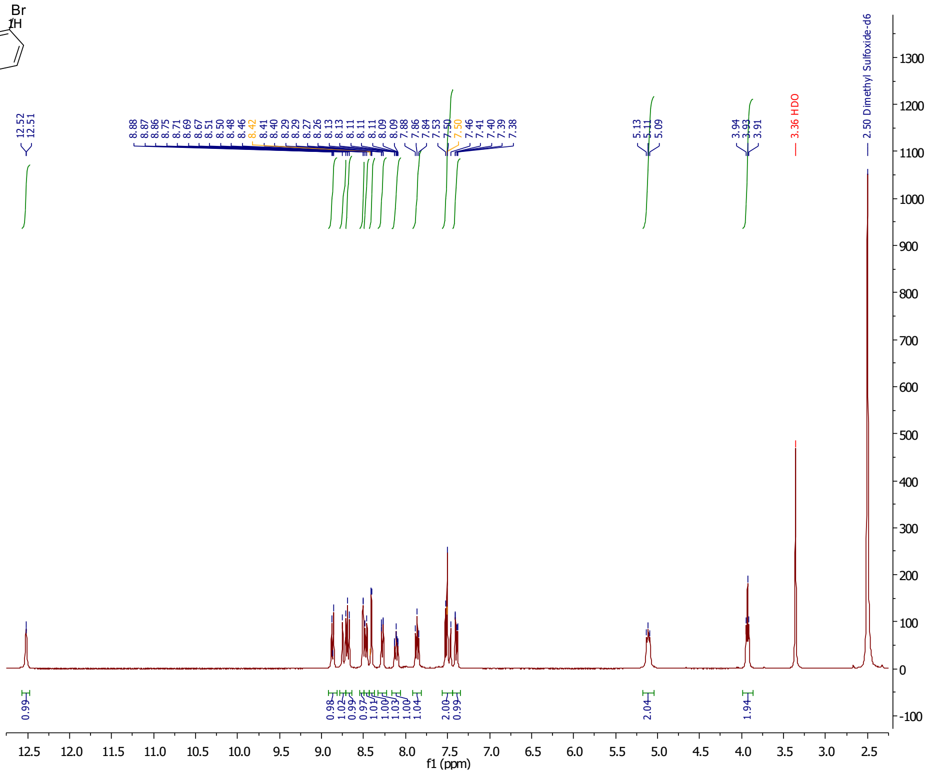
Sample : Ch. Schwechheimer CSC084-1	Frequency Range : 3997.45 - 373.964	Measured on : 25/08/2017	
Technique : Diamant-ATR	Resolution : 4	Instrument : Alpha	Sample Scans : 24
Operator : Angelika Moesle	Zerofilling : 2	Acquisition : Double Sided,Forward-Backward	

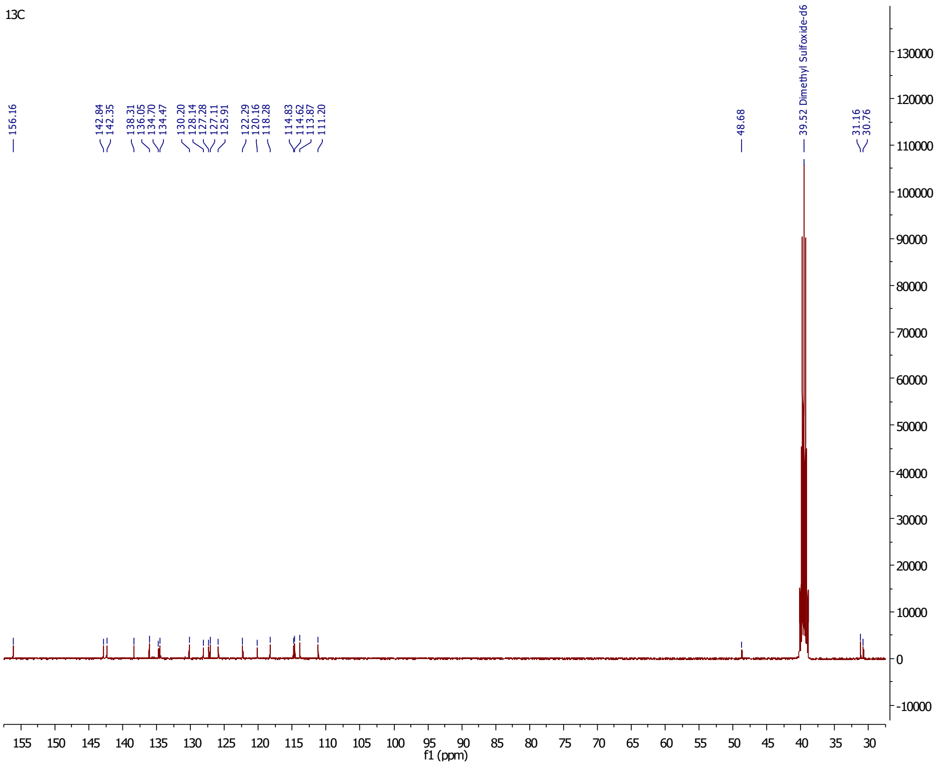
(*E*)-2-(2-(5-bromo-1*H*-indol-3-yl)vinyl)-1-(3-bromopropyl)quinolin-1-ium bromide (35):

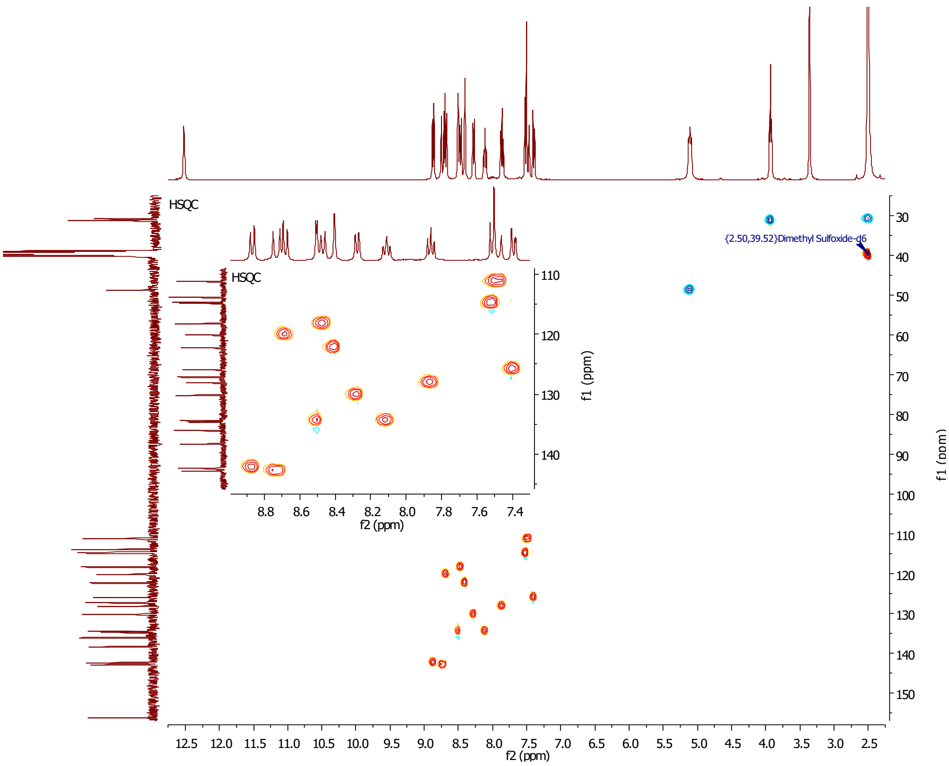


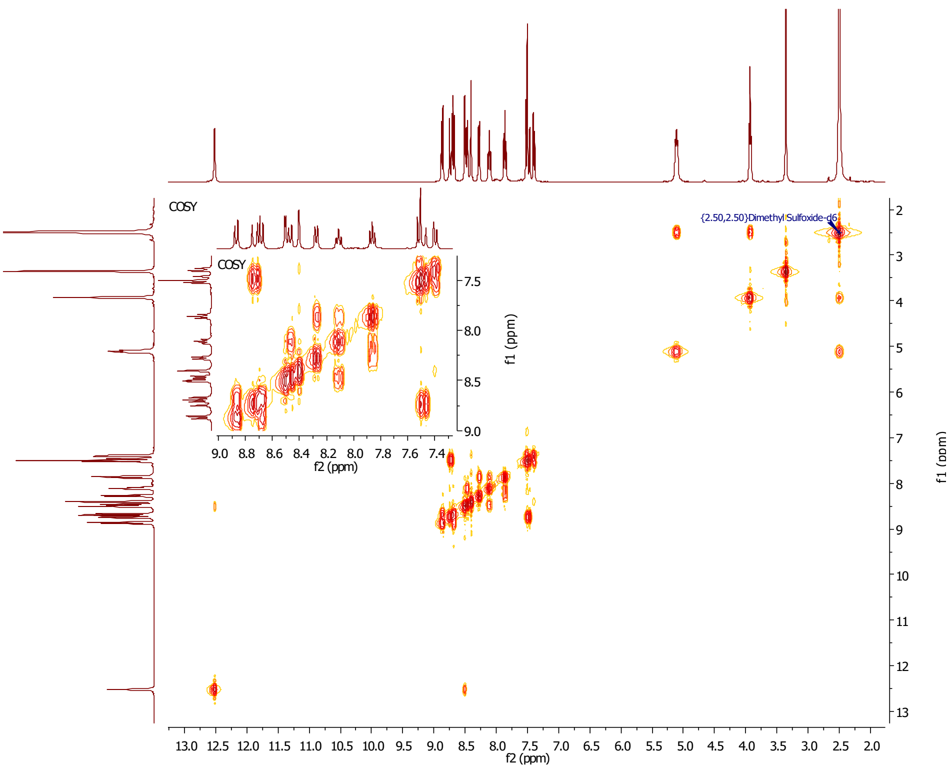
35

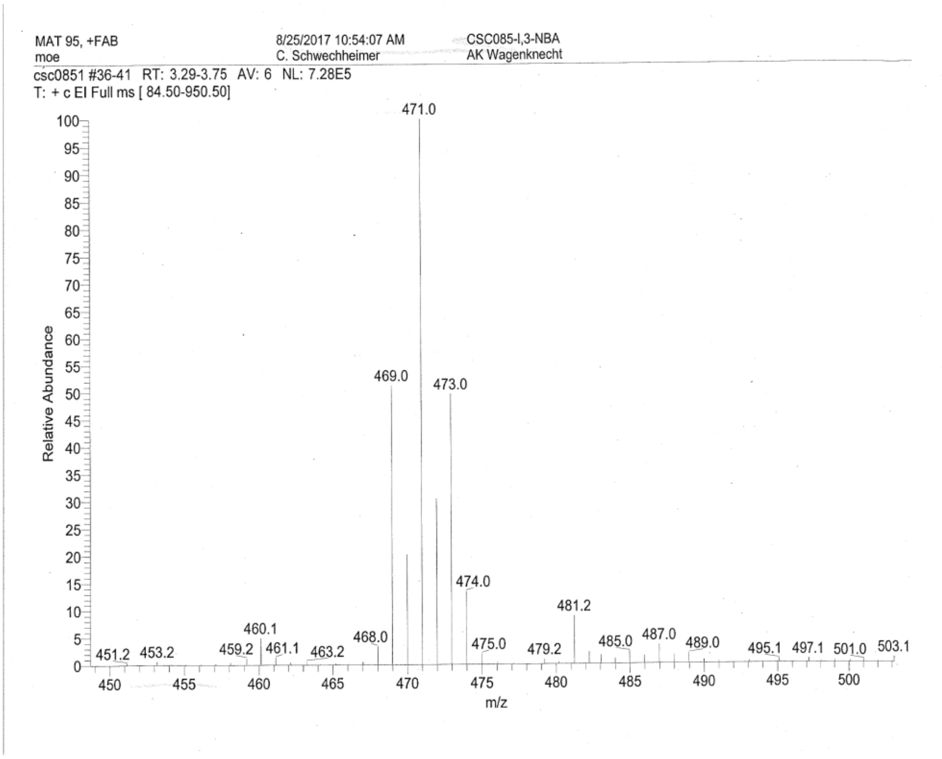
$C_{22}H_{19}Br_3N_2$
551.1200 g/mol

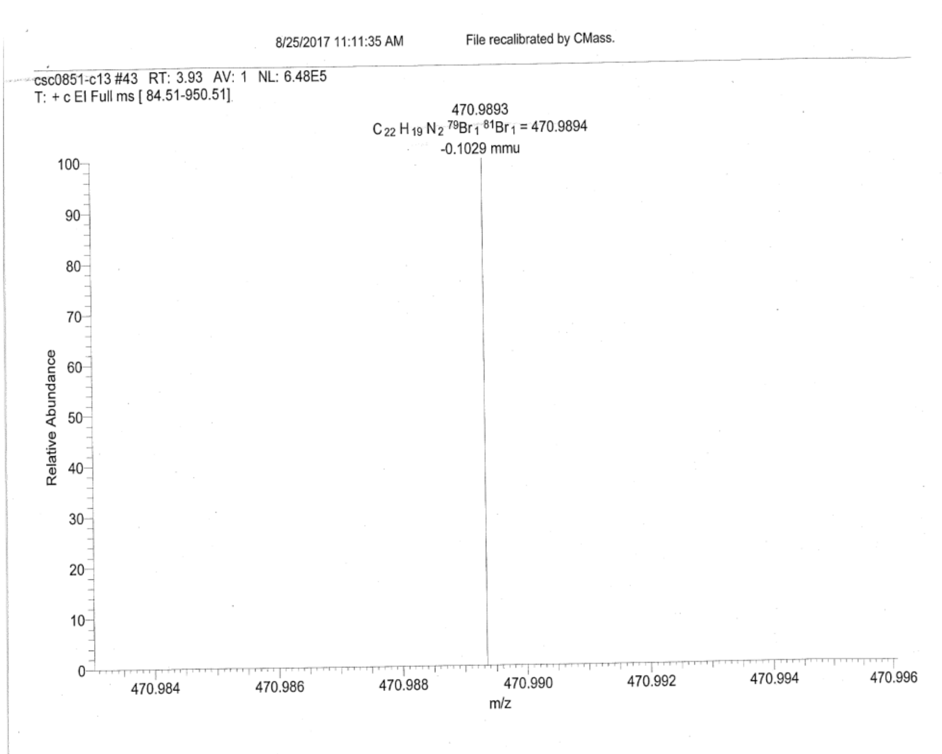


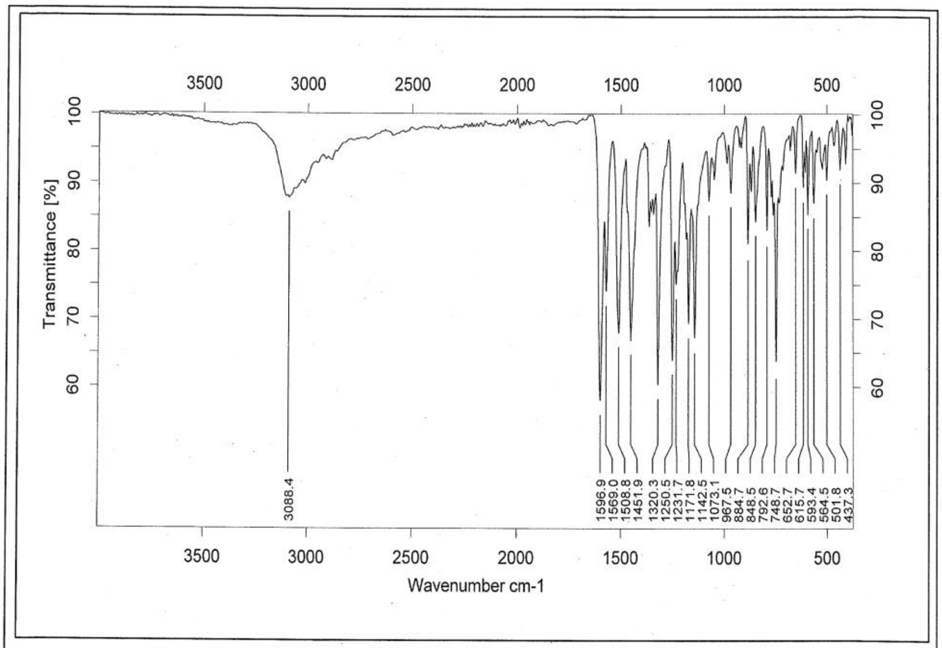



HSQC
{2.50,39.52}Dimethyl Sulfoxide-d6
f1 (ppm)
f2 (ppm)


COSY
{2.50,2.50}Dimethyl Sulfoxide-d6
f1 (ppm)
f2 (ppm)

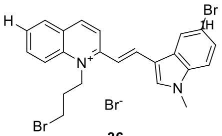

MAT 95, +FAB
moe
8/25/2017 10:54:07 AM
C. Schwechheimer
CSC085-I,3-NBA
AK Wagenknecht
csc0851 #36-41 RT: 3.29-3.75 AV: 6 NL: 7.28E5
T: + c EI Full ms [84.50-950.50]
471.0
469.0
473.0
474.0
481.2
460.1
Relative Abundance
m/z


8/25/2017 11:11:35 AM
File recalibrated by CMass.
csc0851-c13 #43 RT: 3.93 AV: 1 NL: 6.48E5
T: + c EI Full ms [84.51-950.51]
470.9893
C22 H19 N2 79Br1 81Br1 = 470.9894
-0.1029 mmu
Relative Abundance
m/z



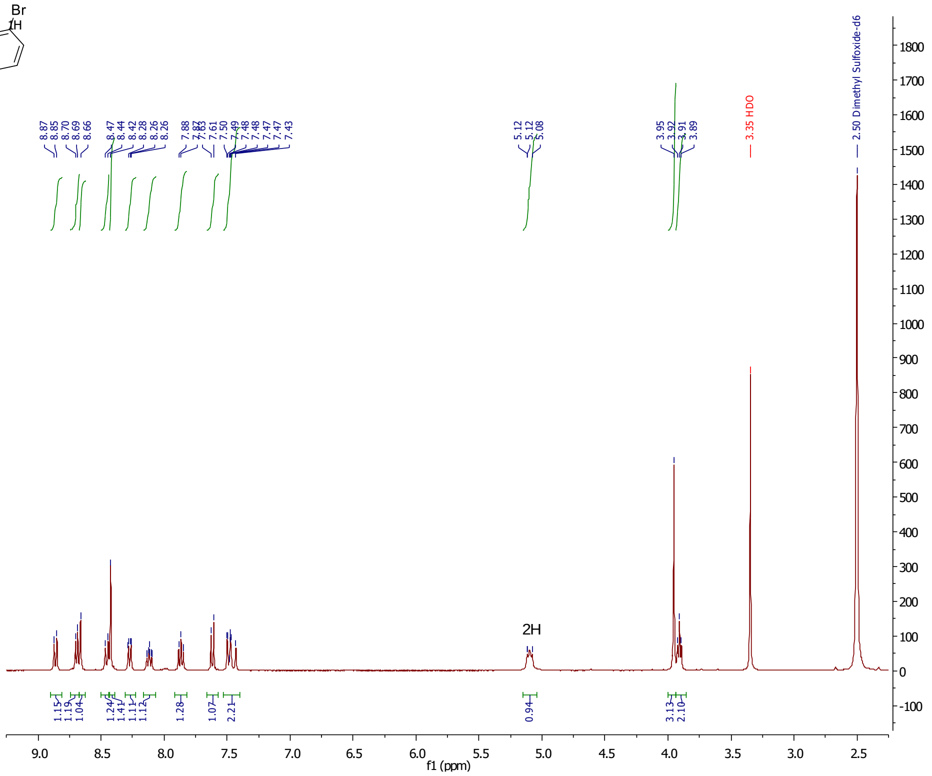
Sample : Ch. Schwechheimer CS0851	Frequency Range : 3997.45 - 373.964	Measured on : 25/08/2017	
Technique : Diamant-ATR	Resolution : 4	Instrument : Alpha	Sample Scans : 24
Operator : Angelika Moesle	Zerofilling : 2	Acquisition : Double Sided,Forward-Backward	

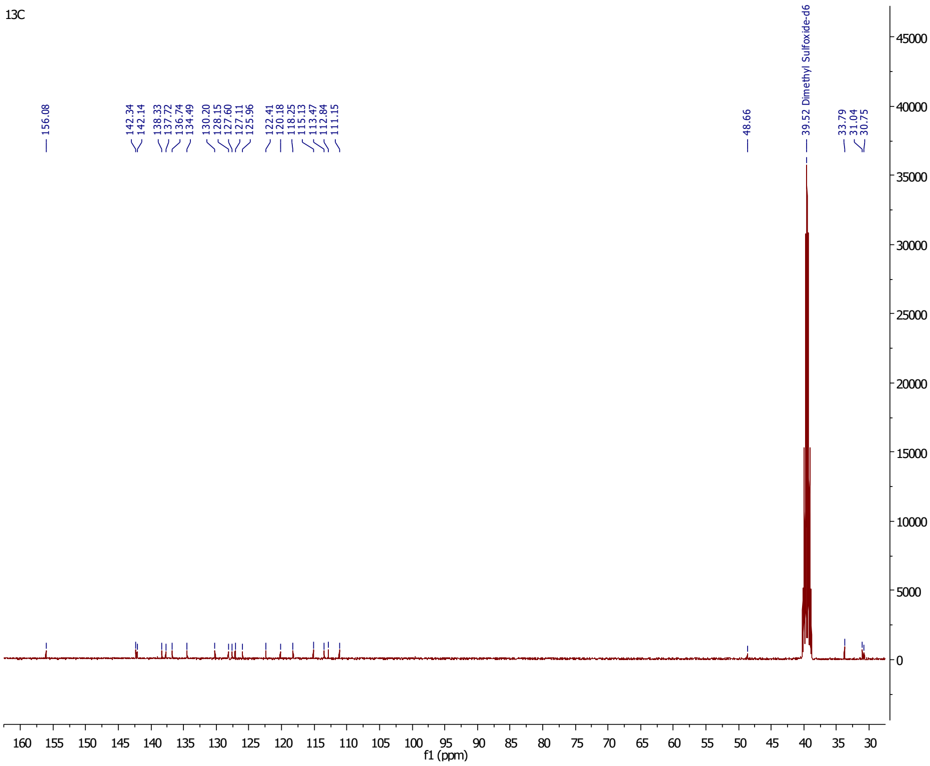
(*E*)-2-(2-(5-bromo-1-methyl-1*H*-indol-3-yl)vinyl)-1-(3-bromopropyl)quinolin-1-ium bromide (36):

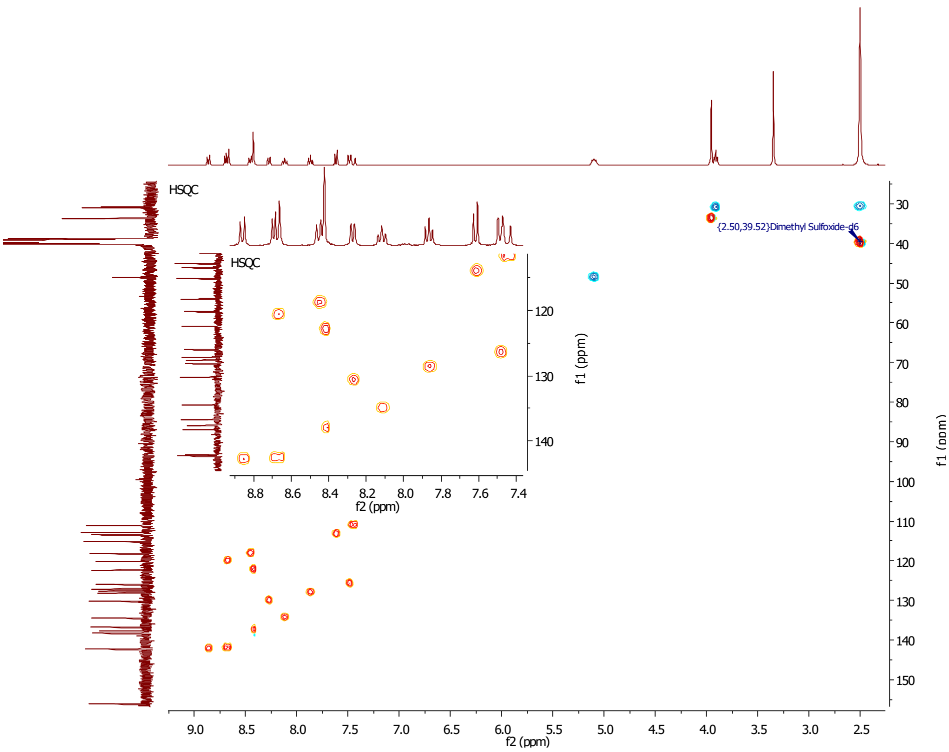


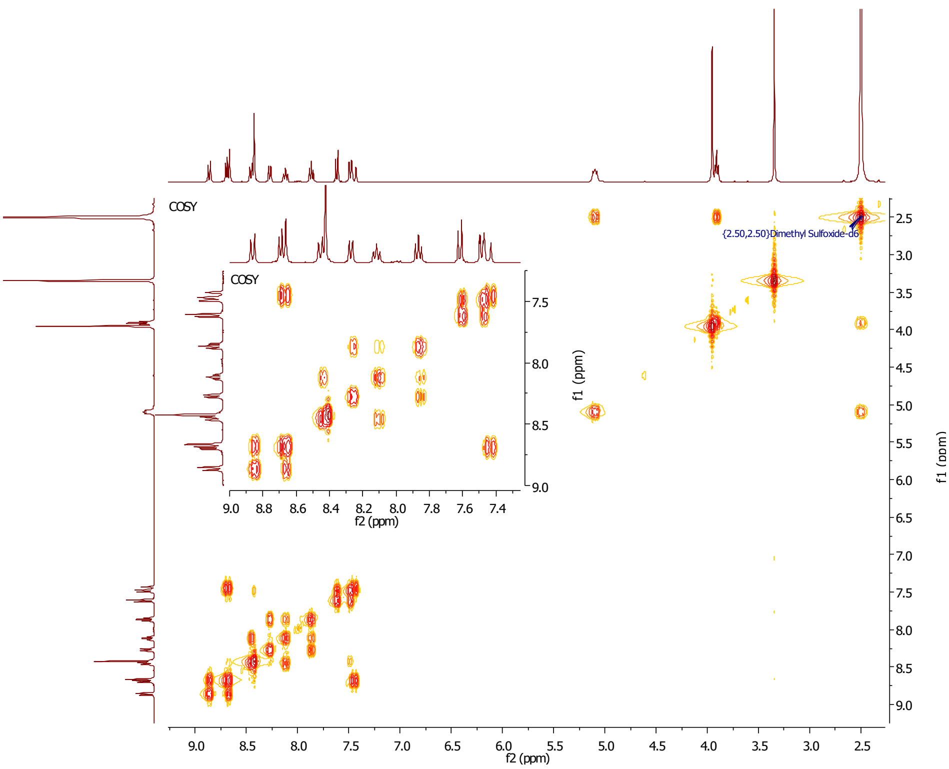
36

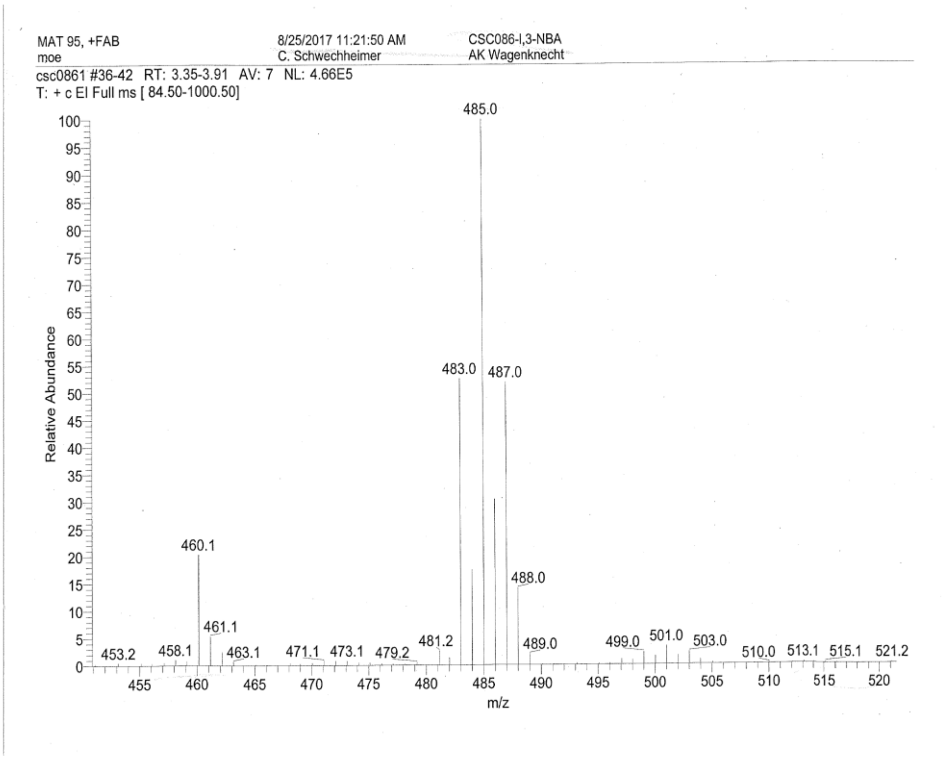
$C_{23}H_{21}Br_3N_2$
565.1470 g/mol

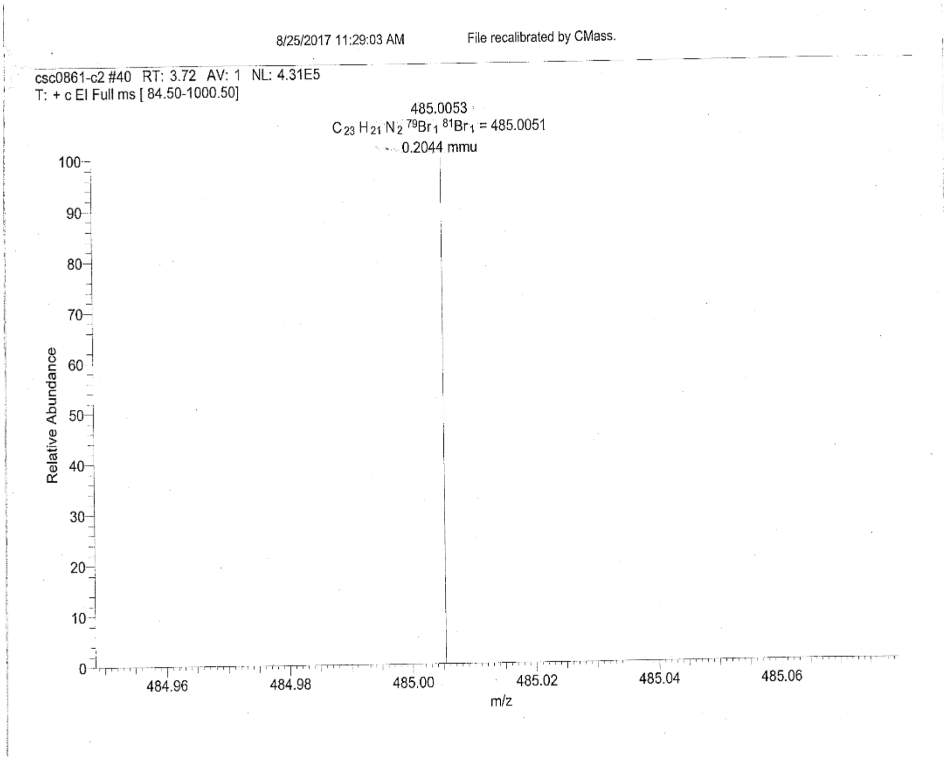


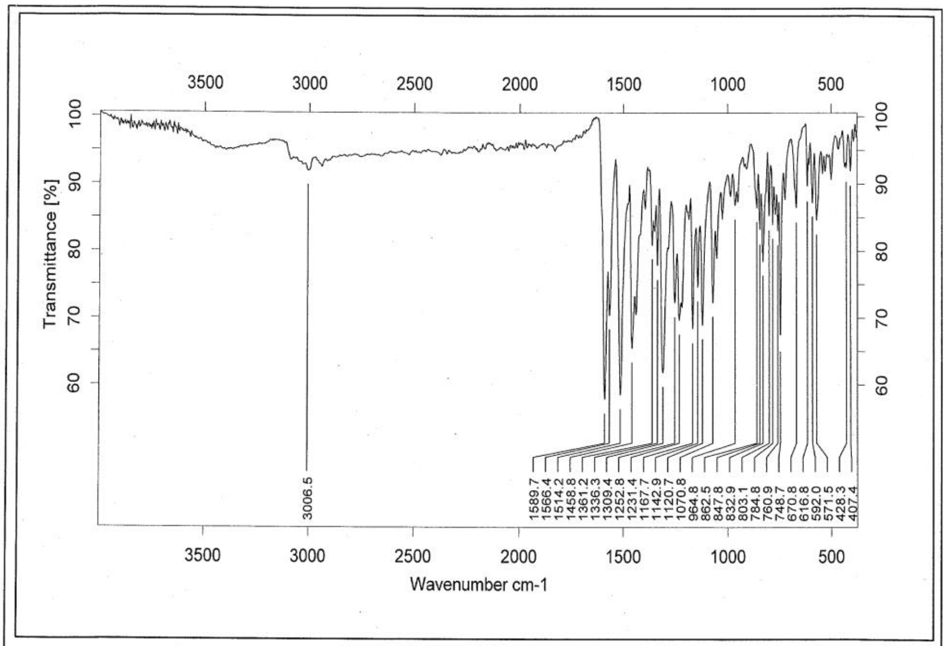



HSQC
{2.50,39.52}Dimethyl Sulfoxide-d6
f2 (ppm)
f1 (ppm)


COSY
{2.50,2.50}Dimethyl Sulfoxide-d6
f2 (ppm)
f1 (ppm)


MAT 95, +FAB
moe
8/25/2017 11:21:50 AM
C. Schwechheimer
CSC086-I,3-NBA
AK Wagenknecht
csc0861 #36-42 RT: 3.35-3.91 AV: 7 NL: 4.66E5
T: + c EI Full ms [84.50-1000.50]
Relative Abundance
m/z

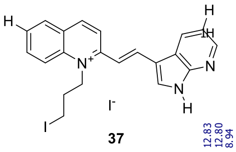

8/25/2017 11:29:03 AM
File recalibrated by CMass.
csc0861-c2 #40 RT: 3.72 AV: 1 NL: 4.31E5
T: + c EI Full ms [84.50-1000.50]
485.0053
C23 H21 N2 79Br1 81Br1 = 485.0051
0.2044 mmu
Relative Abundance
m/z



Sample : Ch. Schwechheimer CSC086-1	Frequency Range : 3997.45 - 373.964	Measured on : 25/08/2017

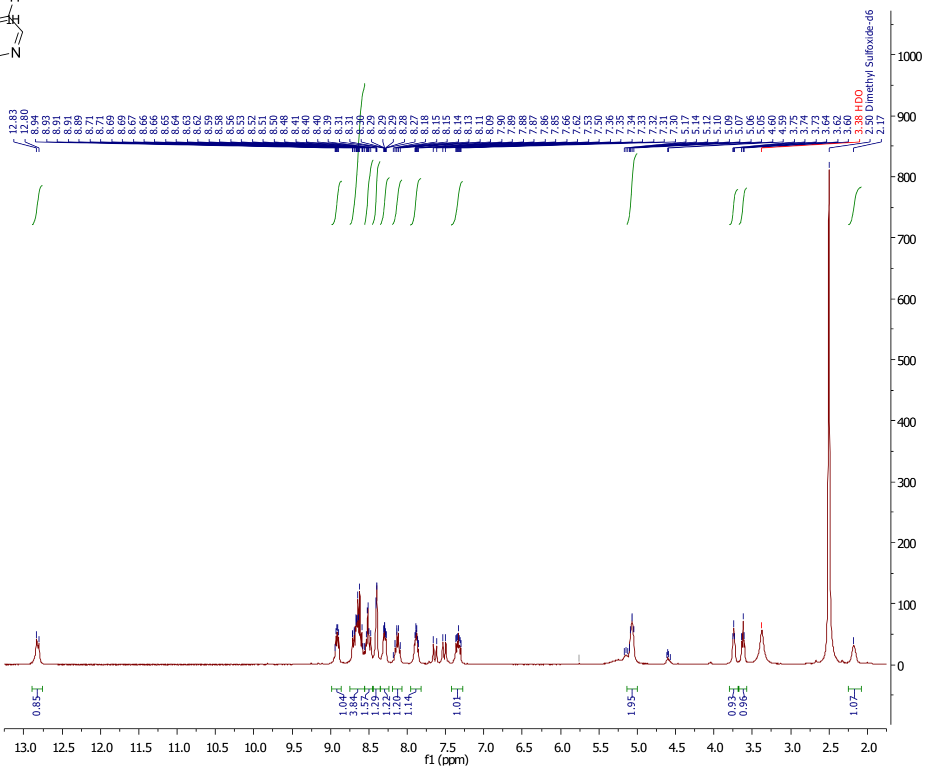
Technique : Diamant-ATR	Resolution : 4	Instrument : Alpha	Sample Scans : 24
Operator : Angelika Moesle	Zerofilling : 2	Acquisition : Double Sided,Forward-Backward	

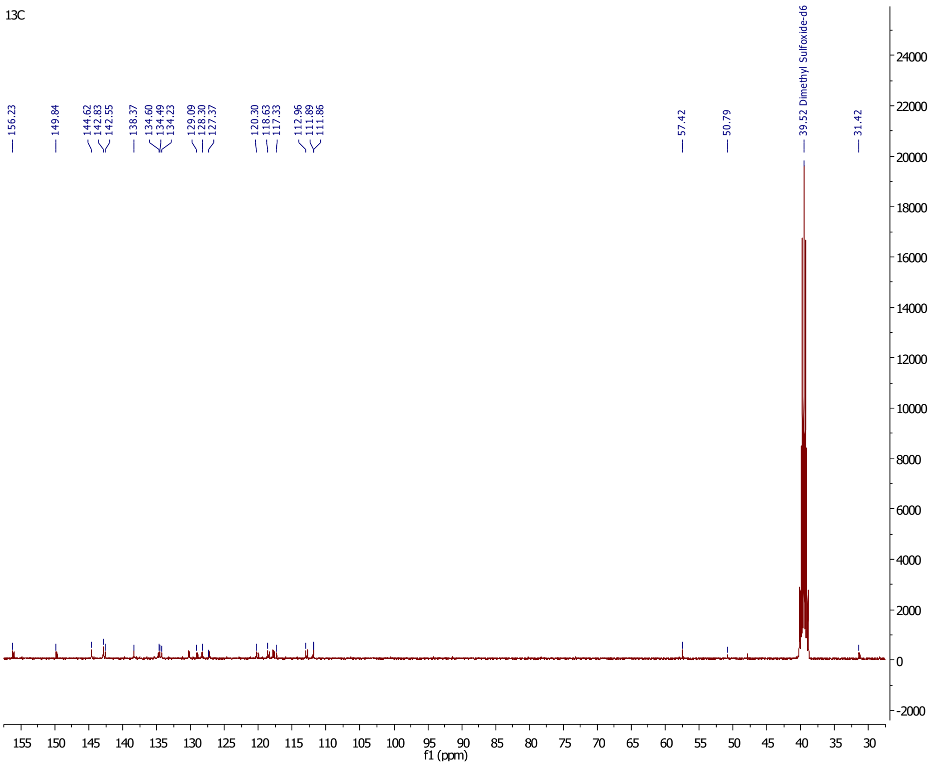
(*E*)-2-(2-(1*H*-pyrrolo[2,3-*b*]pyridin-3-yl)vinyl)-1-(3-iodopropyl)quinolin-1-ium iodide (37):

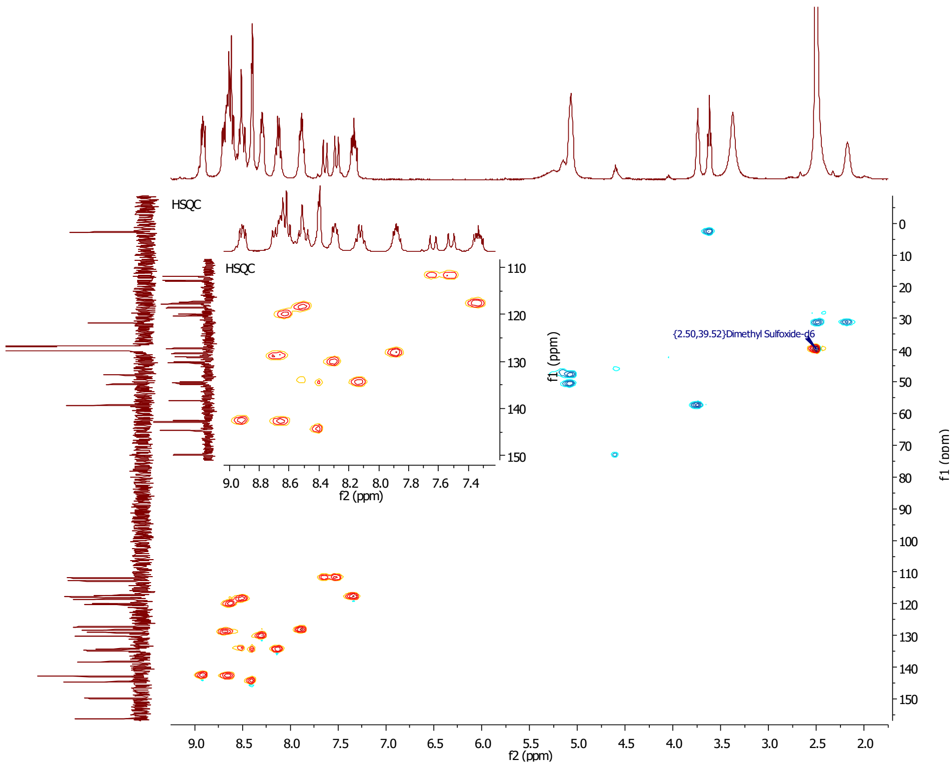


37

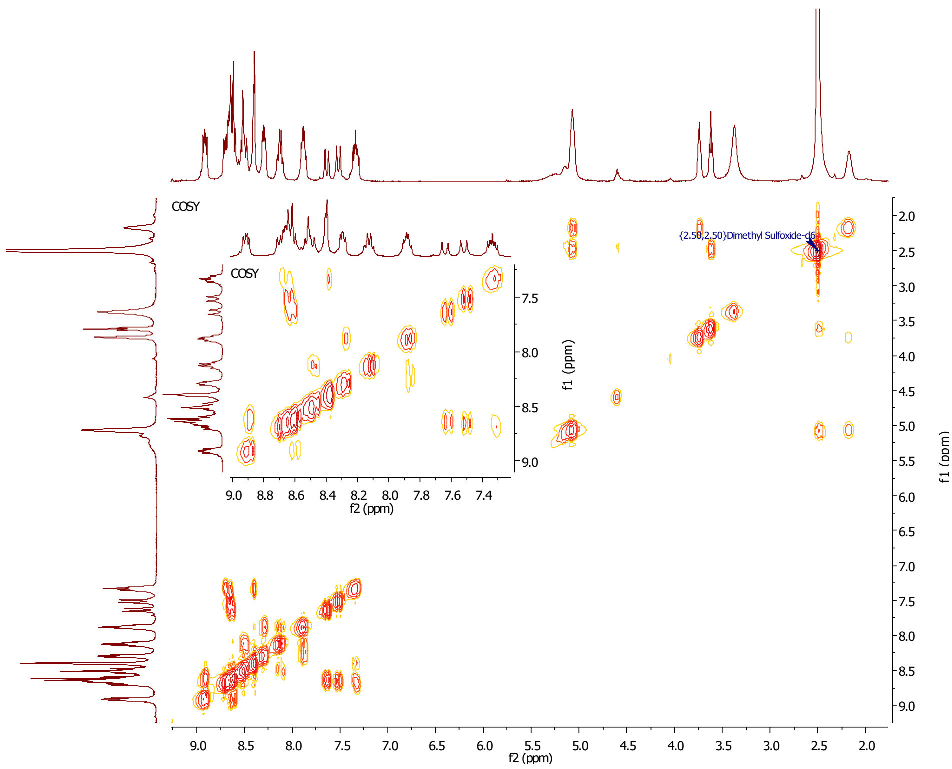
$C_{21}H_{19}I_2N_3$
567.2129 g/mol



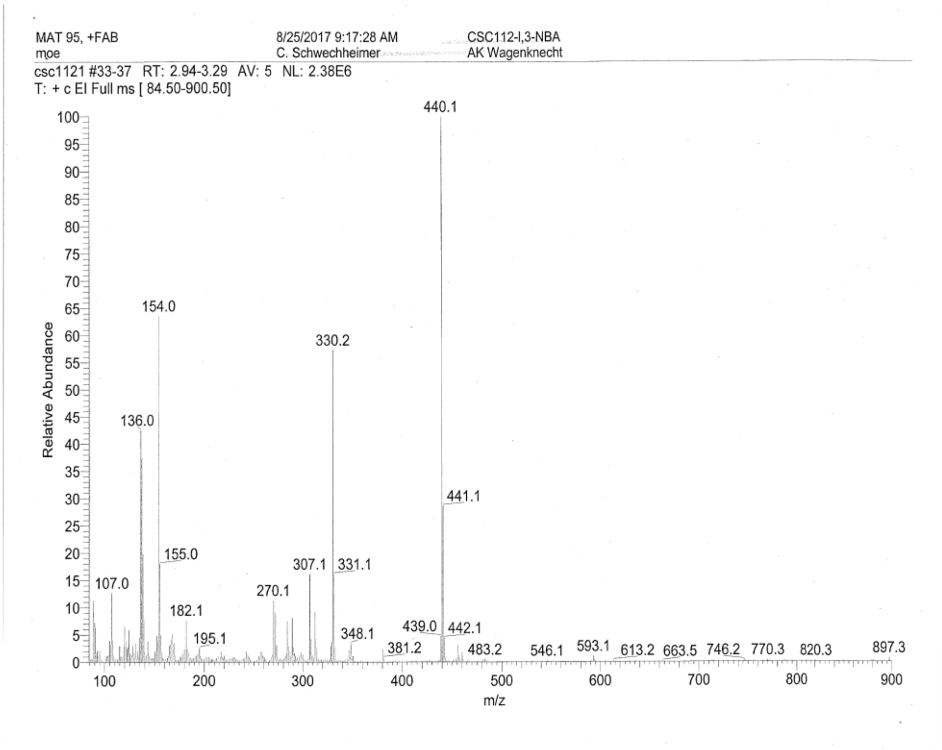


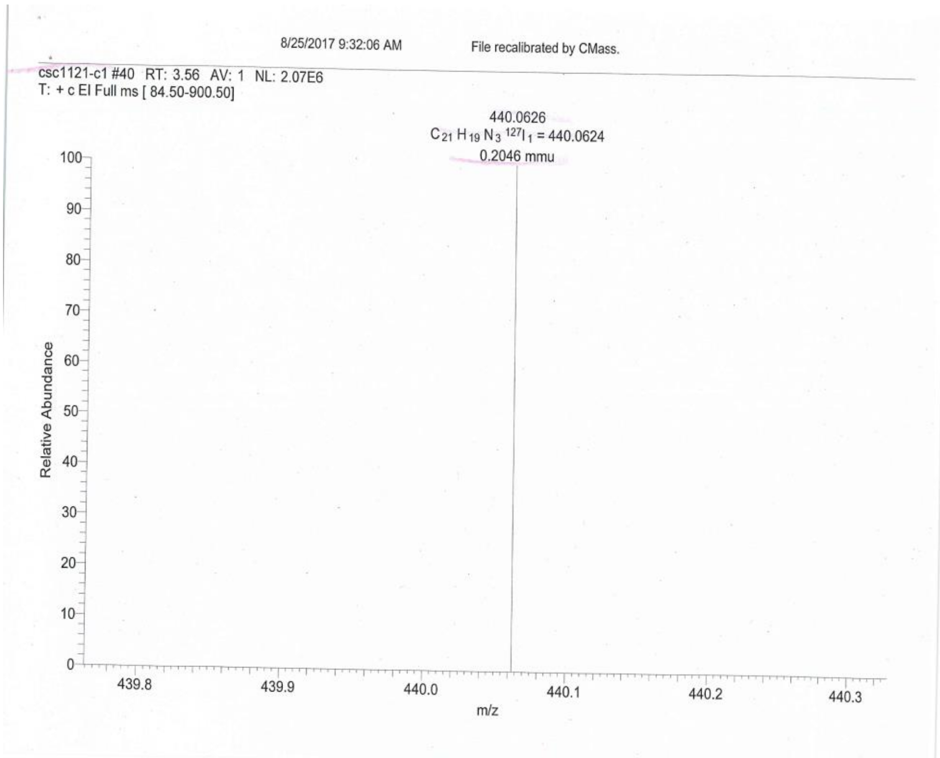


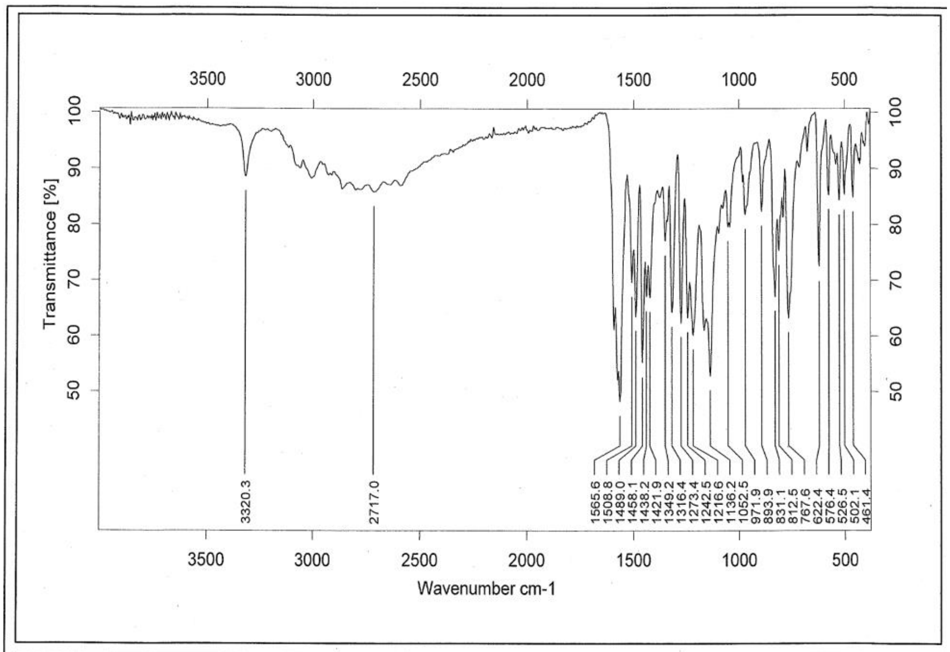
HSQC
HSQC
{2.50,39.52}Dimethyl Sulfoxide-d6
f1 (ppm)
f2 (ppm)
f1 (ppm)
f2 (ppm)



COSY
COSY
{2.50,2.50}Dimethyl Sulfoxide-d6
f1 (ppm)
f2 (ppm)
f1 (ppm)
f2 (ppm)

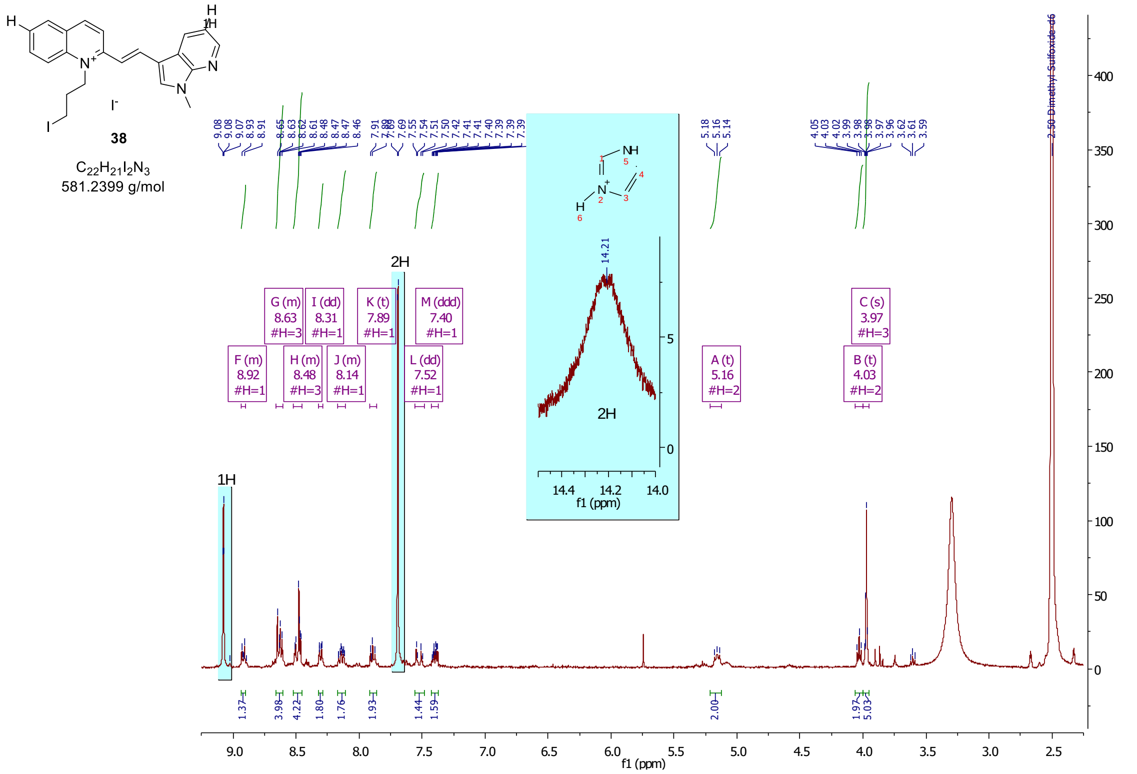

MAT 95, +FAB
moe
8/25/2017 9:17:28 AM
C. Schwechheimer
CSC112-I,3-NBA
AK Wagenknecht
csc1121 #33-37 RT: 2.94-3.29 AV: 5 NL: 2.38E6
T: + c EI Full ms [84.50-900.50]
Relative Abundance
m/z
440.1
154.0
330.2
136.0
441.1
155.0
307.1
331.1
107.0
270.1
182.1
195.1
348.1
439.0
442.1
381.2
483.2
546.1
593.1
613.2
663.5
746.2
770.3
820.3
897.3

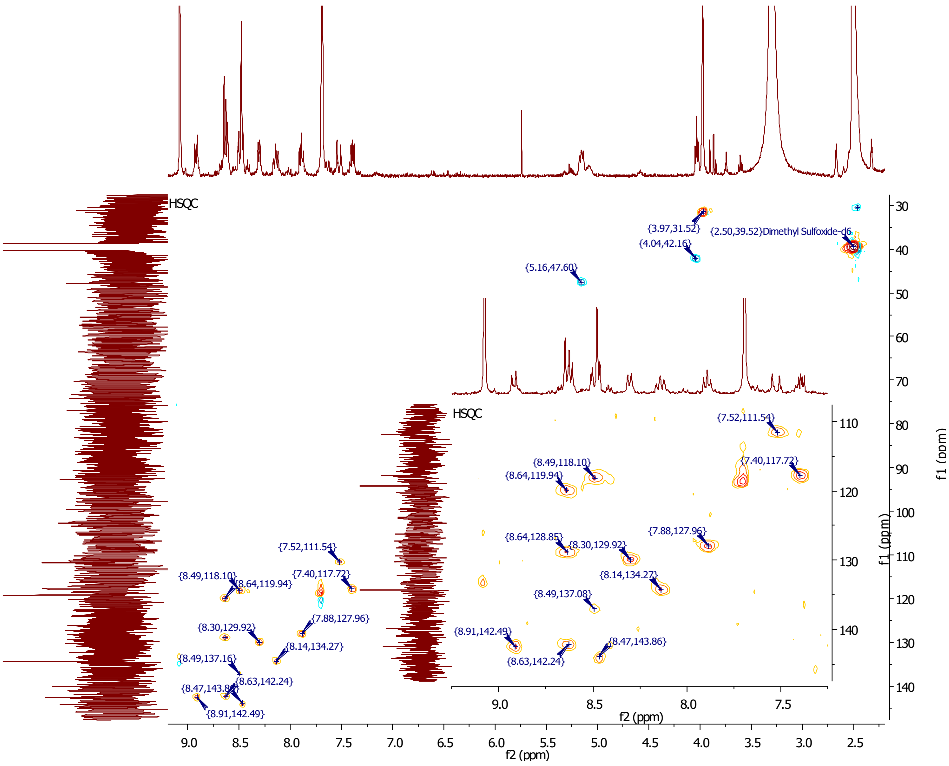

8/25/2017 9:32:06 AM
File recalibrated by CMass.
csc1121-c1 #40 RT: 3.56 AV: 1 NL: 2.07E6
T: + c EI Full ms [84.50-900.50]
440.0626
C21 H19 N3 127I1 = 440.0624
0.2046 mmu
Relative Abundance
m/z

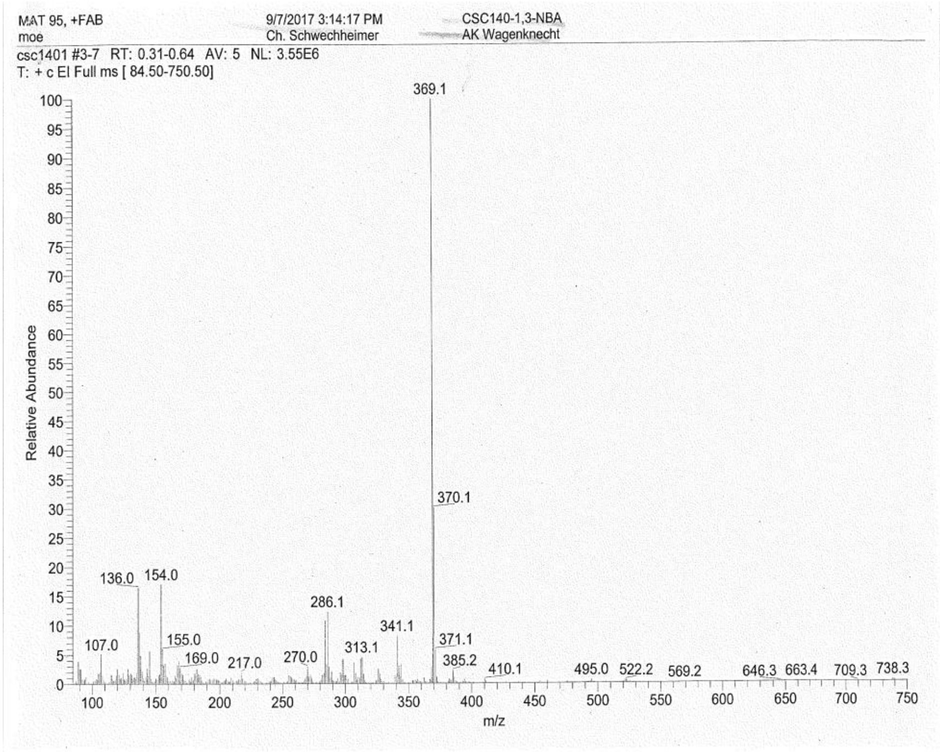


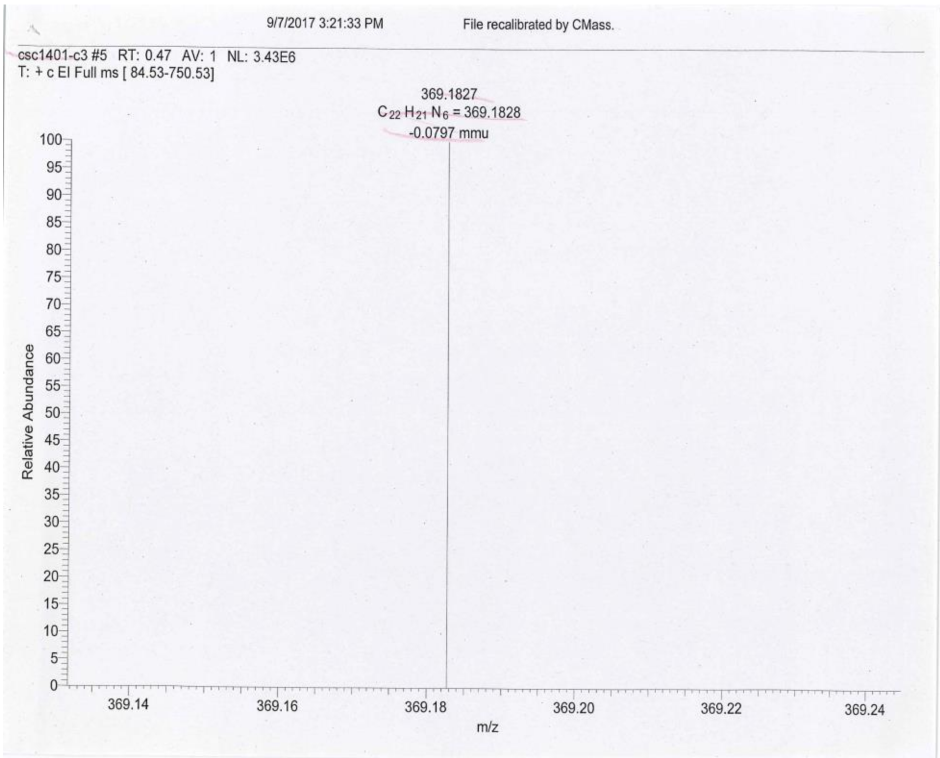
Sample : Ch. Schwechheimer CSC112-1	Frequency Range : 3997.45 - 373.964	Measured on : 25/08/2017	
Technique : Diamant-ATR	Resolution : 4	Instrument : Alpha	Sample Scans : 24
Operator : Angelika Moesle	Zerofilling : 2	Acquisition : Double Sided,Forward-Backward	

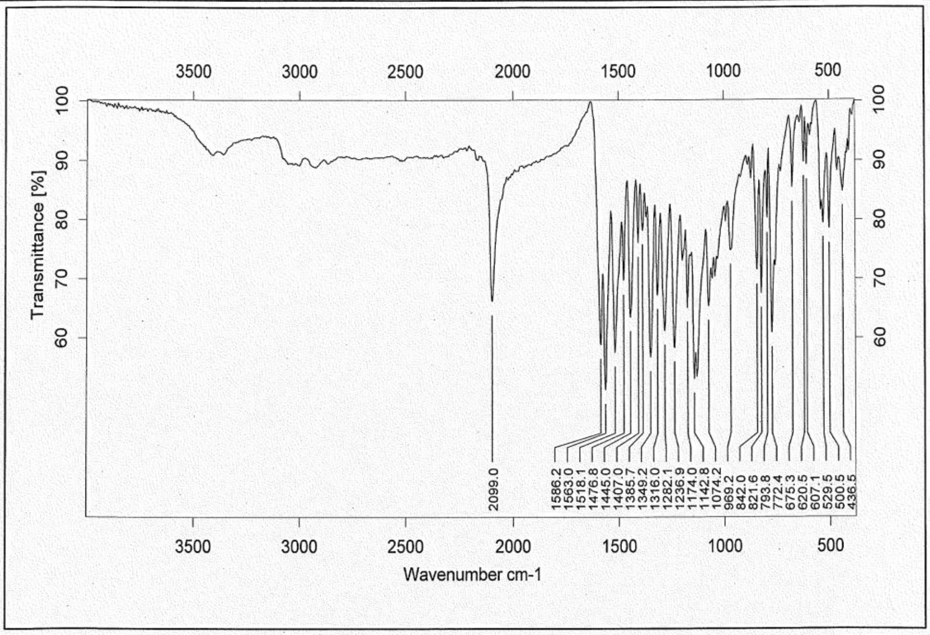
(*E*)-1-(3-iodopropyl)-2-(2-(1-methyl-1*H*-pyrrolo[2,3-*b*]pyridin-3-yl)vinyl)quinolin-1-ium iodide (38):





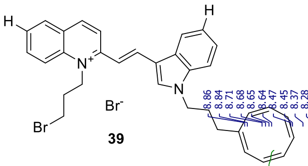

MAT 95, +FAB
moe
9/7/2017 3:14:17 PM
Ch. Schwechheimer
CSC140-1,3-NBA
AK Wagenknecht
csc1401 #3-7 RT: 0.31-0.64 AV: 5 NL: 3.55E6
T: + c EI Full ms [84.50-750.50]
369.1
370.1
136.0
154.0
286.1
341.1
107.0
155.0
169.0
217.0
270.0
313.1
371.1
385.2
410.1
495.0
522.2
569.2
646.3
663.4
709.3
738.3
Relative Abundance
m/z


9/7/2017 3:21:33 PM
File recalibrated by CMass.
csc1401-c3 #5 RT: 0.47 AV: 1 NL: 3.43E6
T: + c EI Full ms [84.53-750.53]
369.1827
C22 H21 N6 = 369.1828
-0.0797 mmu
Relative Abundance
m/z



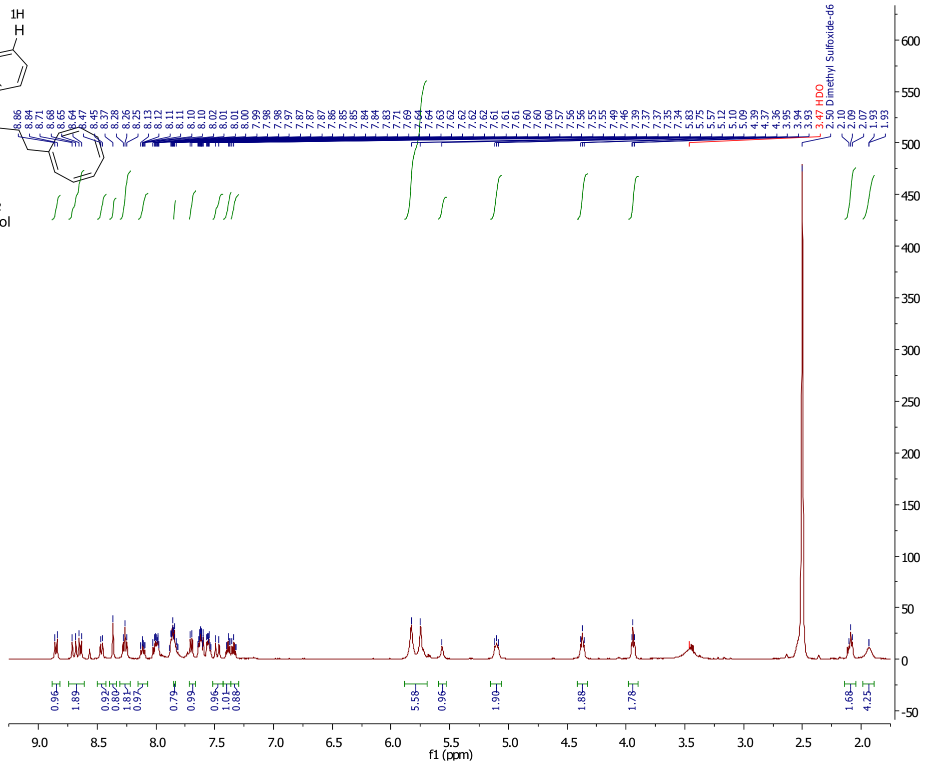
Sample : Ch. Schwechheimer CSC140-1	Frequency Range : 3997.45 - 373.964		Measured on : 07/09/2017
Technique : Diamant-ATR	Resolution : 4	Instrument : Alpha	Sample Scans : 24
Operator : Angelika Moesle	Zerofilling : 2	Acquisition : Double Sided,Forward-Backward	

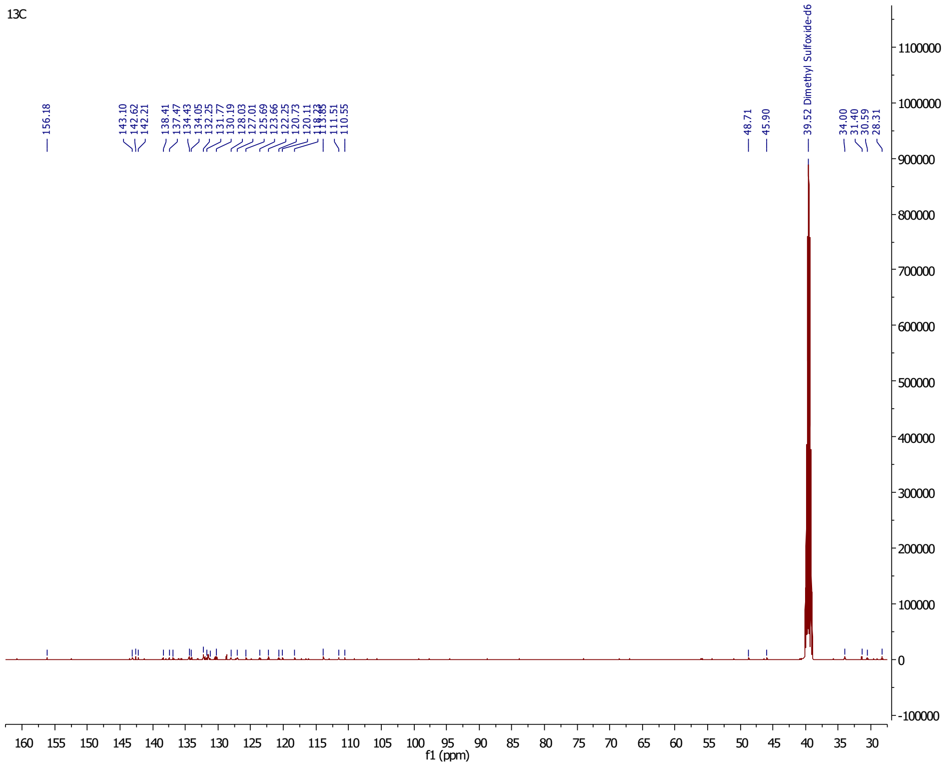
1-(3-bromopropyl)-2-((*E*)-2-(1-(3-((1*Z*,3*Z*,5*Z*,7*Z*)-cycloocta-1,3,5,7-tetraen-1-yl)propyl)-1*H*-indol-3-yl)vinyl)quinolin-1-ium bromide (39):

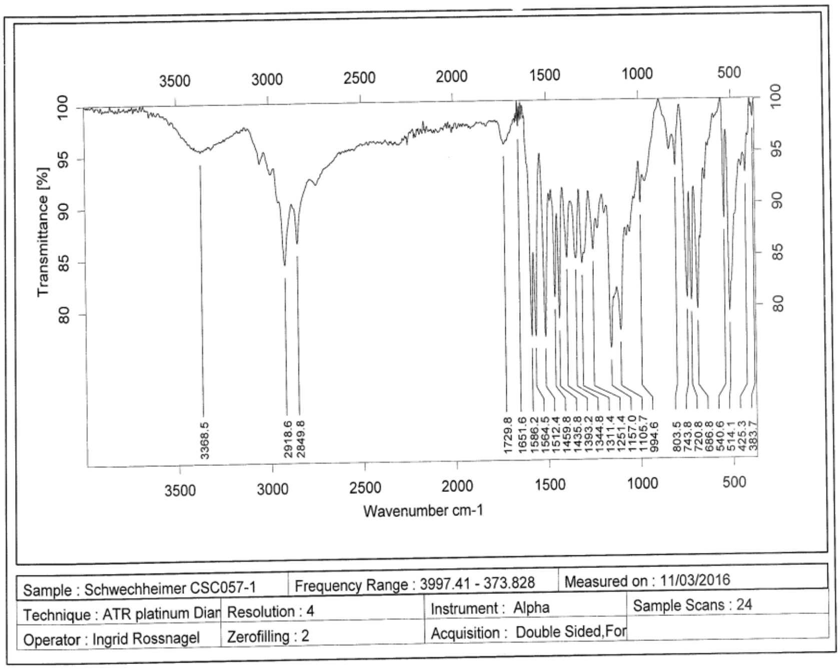


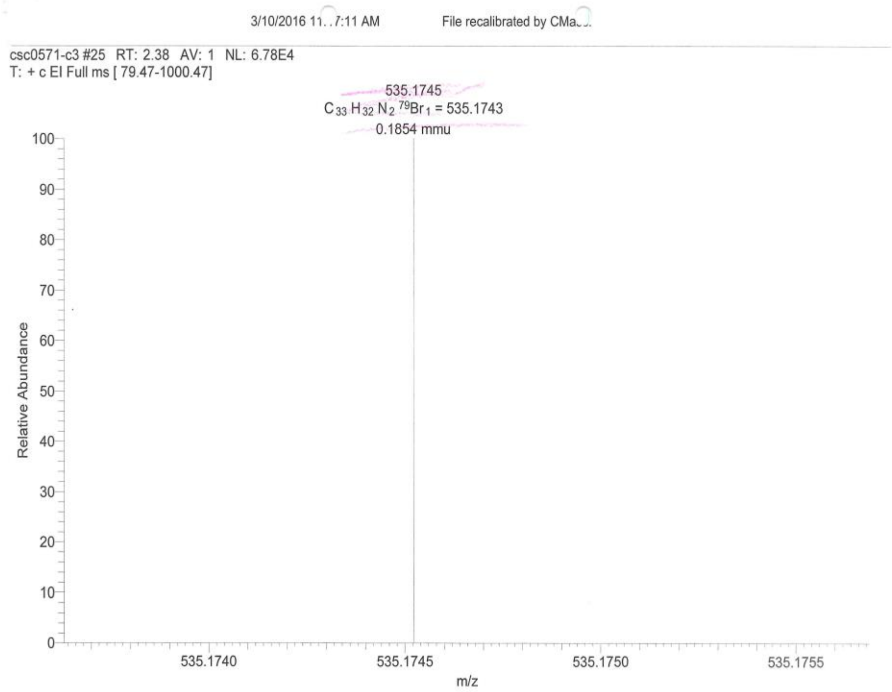
39

$C_{33}H_{32}Br_2N_2$
616.4410 g/mol

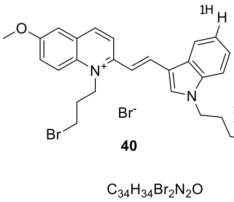





Transmittance [%]
Wavenumber cm-1
3368.5
2918.6
2849.8
1729.8
1651.6
1586.2
1564.5
1512.4
1459.8
1435.8
1393.2
1344.8
1311.4
1251.4
1157.0
1105.7
994.6
803.5
743.8
720.8
686.8
540.6
514.1
425.3
383.7
Sample : Schwechheimer CSC057-1
Frequency Range : 3997.41 - 373.828
Measured on : 11/03/2016
Technique : ATR platinum Diar
Resolution : 4
Instrument : Alpha
Sample Scans : 24
Operator : Ingrid Rossnagel
Zerofilling : 2
Acquisition : Double Sided,For

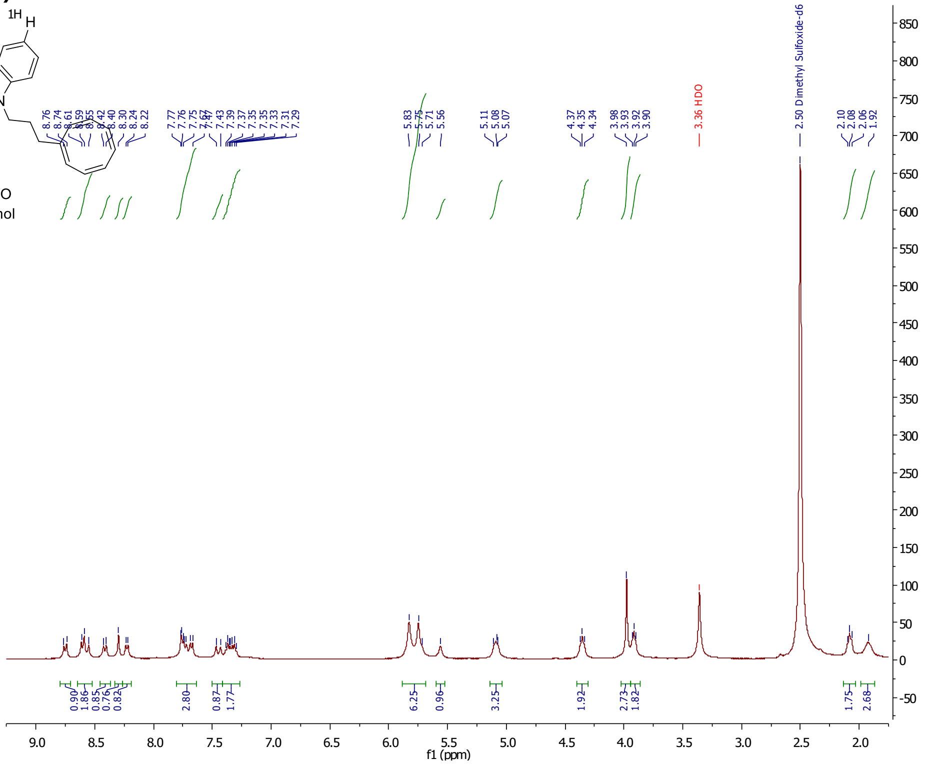

File recalibrated by CMa
csc0571-c3 #25 RT: 2.38 AV: 1 NL: 6.78E4
T: + c EI Full ms [79.47-1000.47]
535.1745
C33 H32 N2 79Br1 = 535.1743
0.1854 mmu
Relative Abundance
m/z

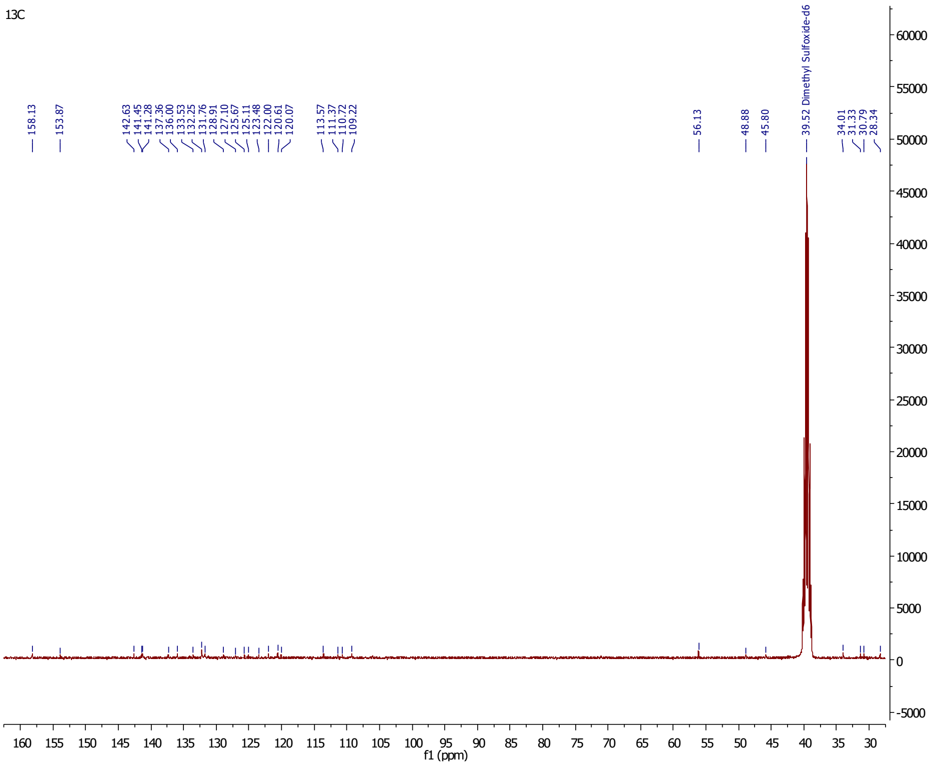
1-(3-bromopropyl)-2-((*E*)-2-(1-(3-((1*Z*,3*Z*,5*Z*,7*Z*)-cycloocta-1,3,5,7-tetraen-1-yl)propyl)-1*H*-indol-3-yl)vinyl)-6-methoxyquinolin-1-ium bromide (40):

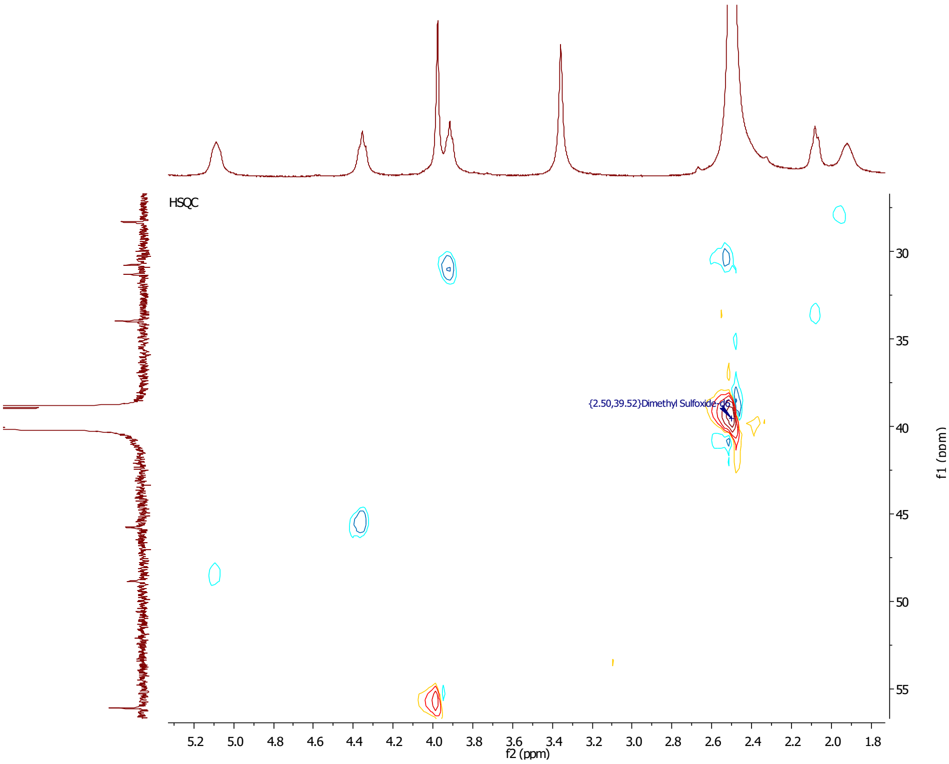


40

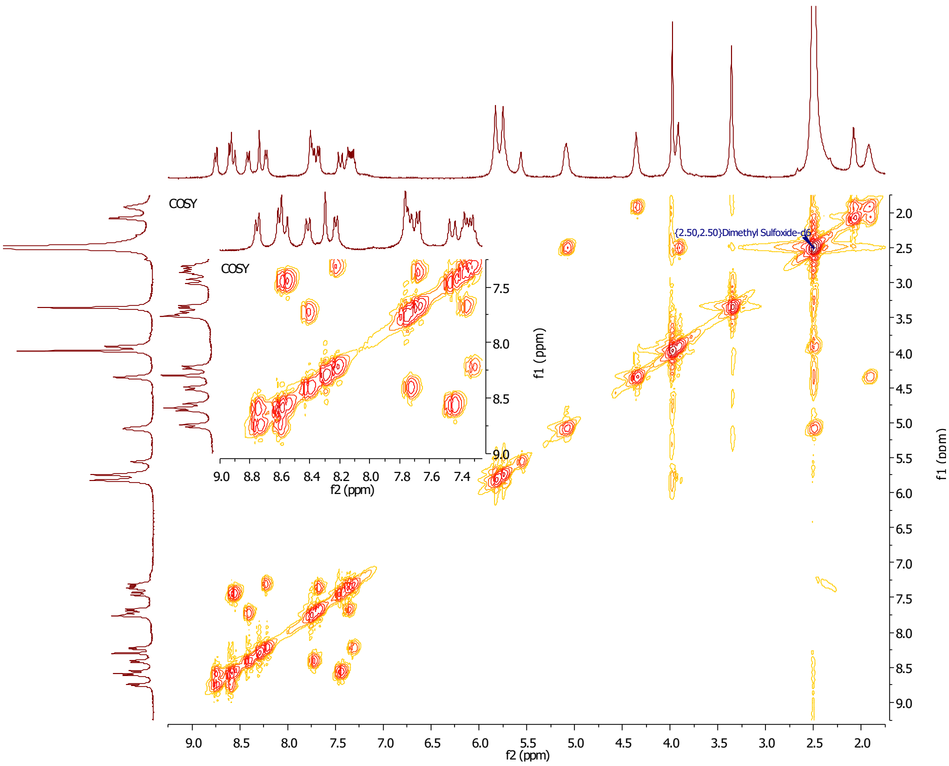
$C_{34}H_{34}Br_2N_2O$
646.4670 g/mol



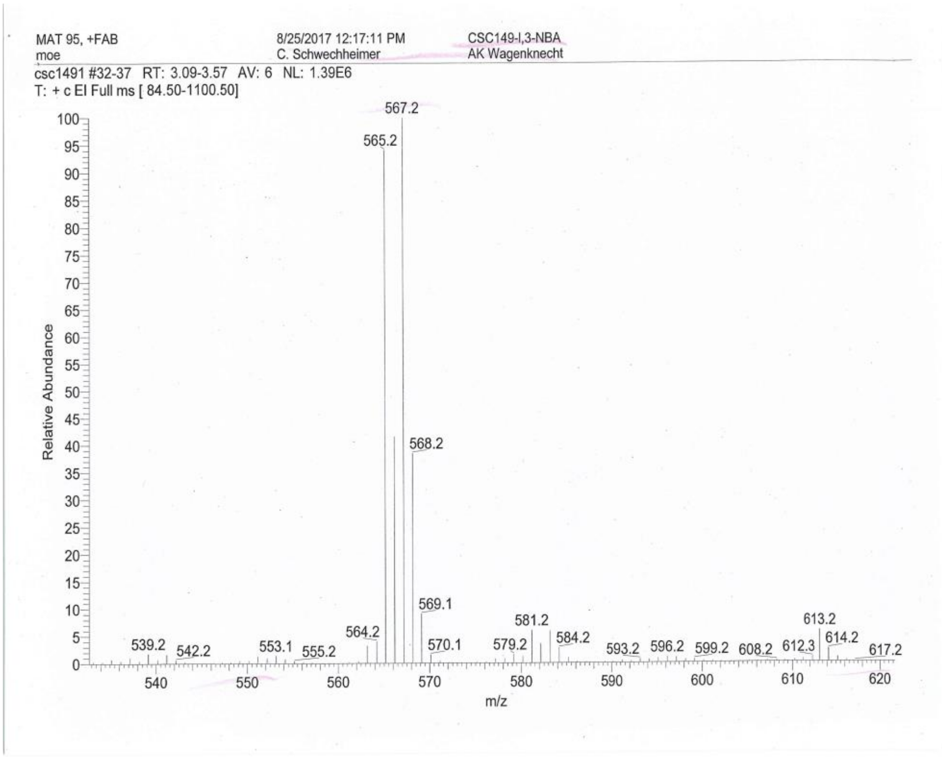




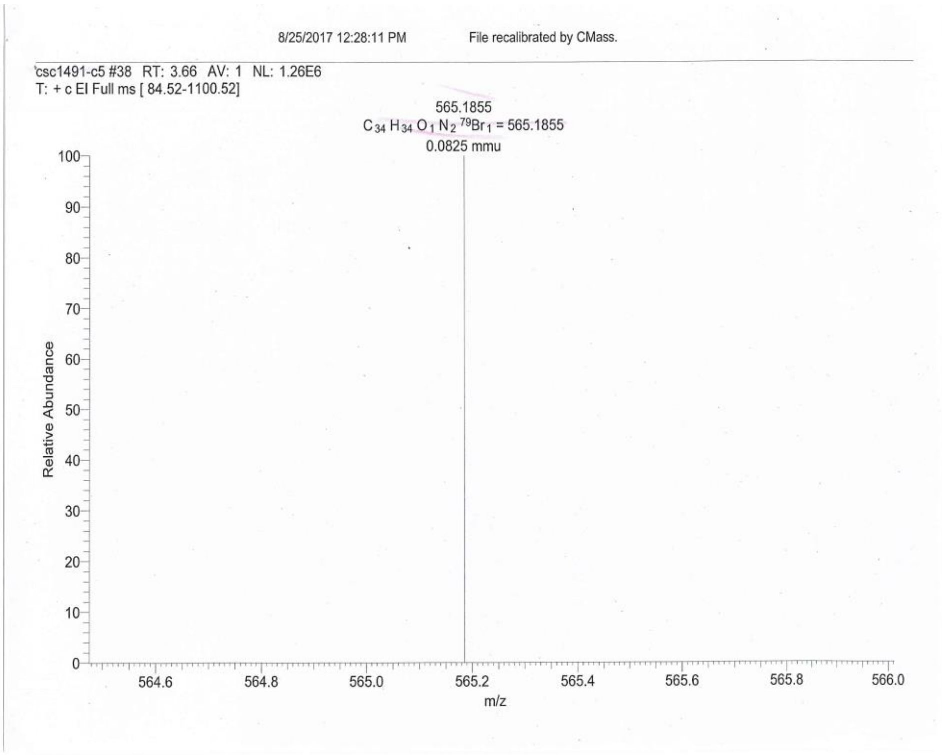
HSQC
{2.50,39.52}Dimethyl Sulfoxide-d6
f2 (ppm)
f1 (ppm)



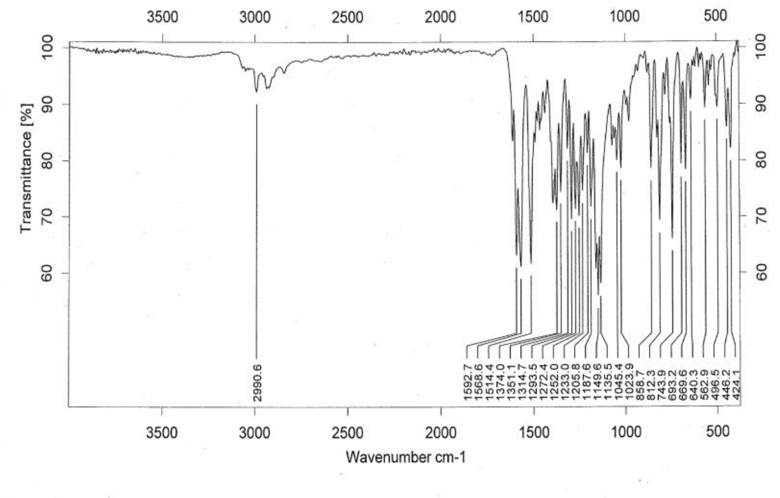
COSY
{2.50,2.50}Dimethyl Sulfoxide-d6
f2 (ppm)
f1 (ppm)



MAT 95, +FAB
moe
8/25/2017 12:17:11 PM
C. Schwechheimer
CSC149-I,3-NBA
AK Wagenknecht
csc1491 #32-37 RT: 3.09-3.57 AV: 6 NL: 1.39E6
T: + c EI Full ms [84.50-1100.50]
Relative Abundance
m/z
567.2
565.2
568.2
569.1
581.2
613.2
564.2
539.2
542.2
553.1
555.2
570.1
579.2
584.2
593.2
596.2
599.2
608.2
612.3
614.2
617.2



8/25/2017 12:28:11 PM
File recalibrated by CMass.
csc1491-c5 #38 RT: 3.66 AV: 1 NL: 1.26E6
T: + c EI Full ms [84.52-1100.52]
565.1855
$C_{34}H_{34}O_1N_2\,^{79}Br_1$ = 565.1855
0.0825 mmu
Relative Abundance
m/z



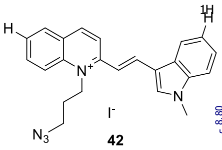
Sample : Ch. Schwechheimer CS149-1	Frequency Range : 3997.45 - 373.964	Measured on : 25/08/2017

Technique : Diamant-ATR	Resolution : 4	Instrument : Alpha	Sample Scans : 24
Operator : Angelika Moesle	Zerofilling : 2	Acquisition : Double Sided,Forward-Backward	

e. Analytics of the Dye-Azides 41-52

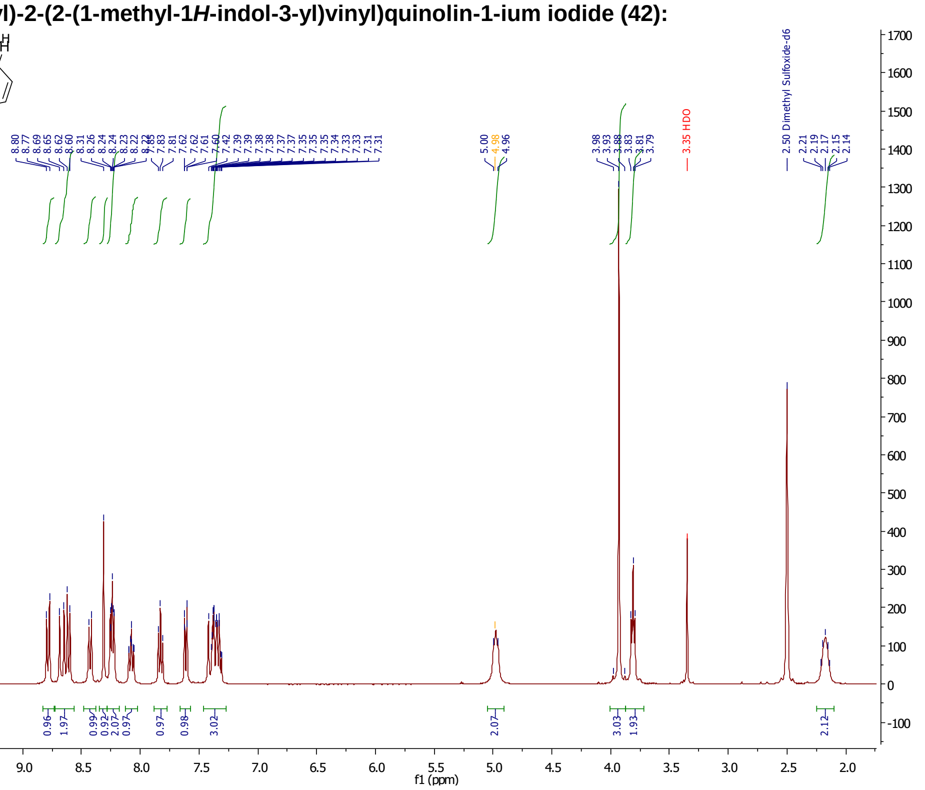
The analytics of compound **41** is described in earlier publications of our working group.[1]

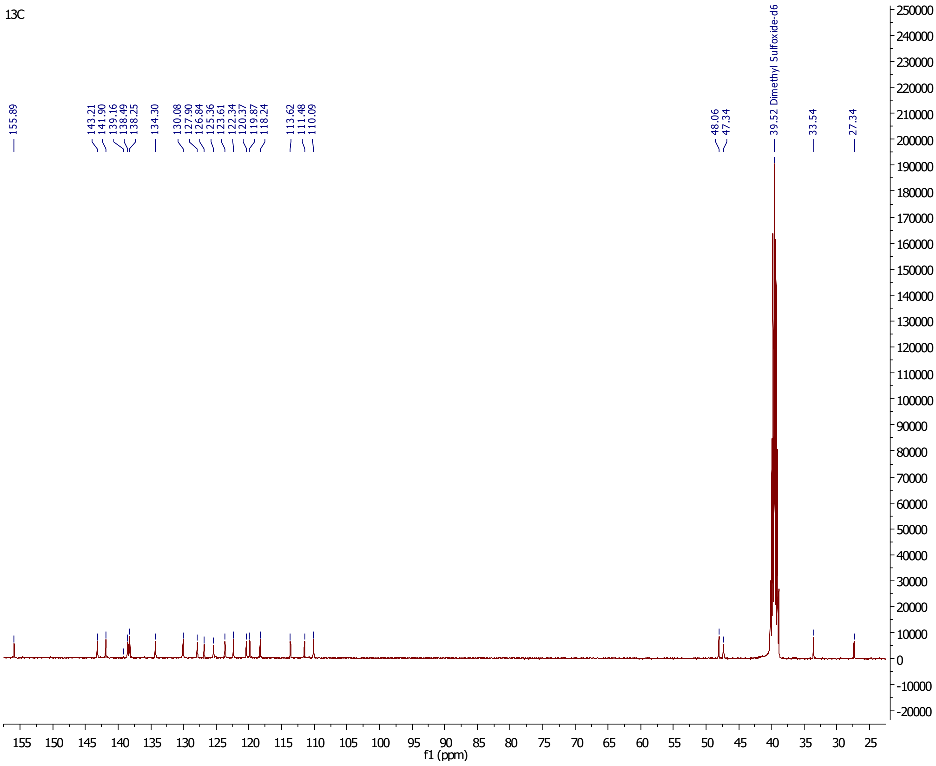
(*E*)-1-(3-azidopropyl)-2-(2-(1-methyl-1*H*-indol-3-yl)vinyl)quinolin-1-ium iodide (42):

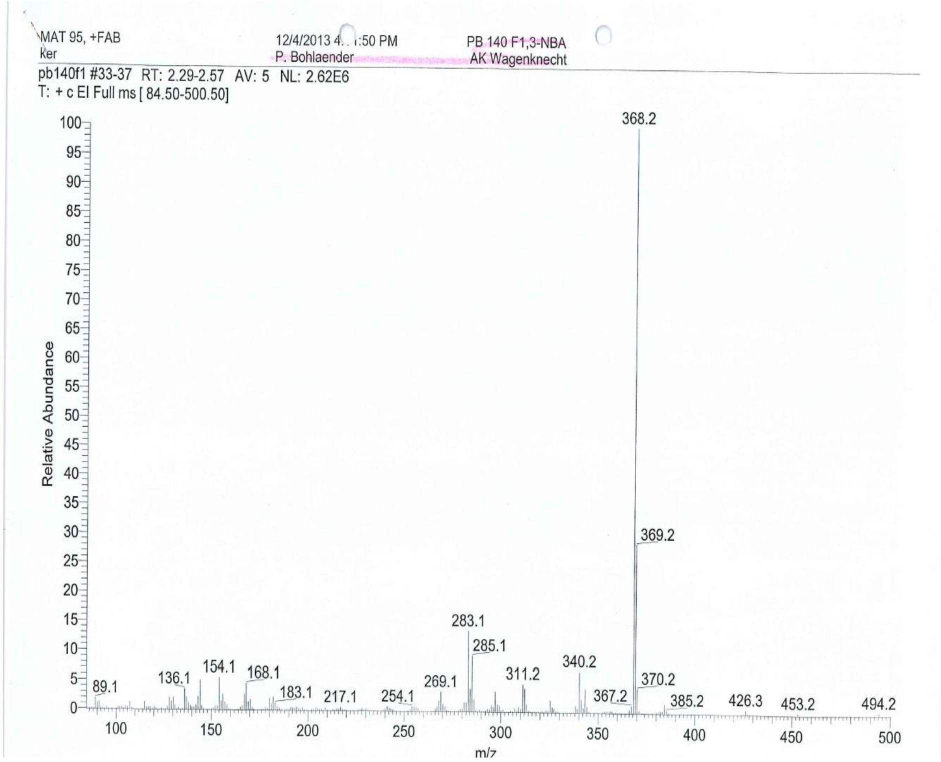


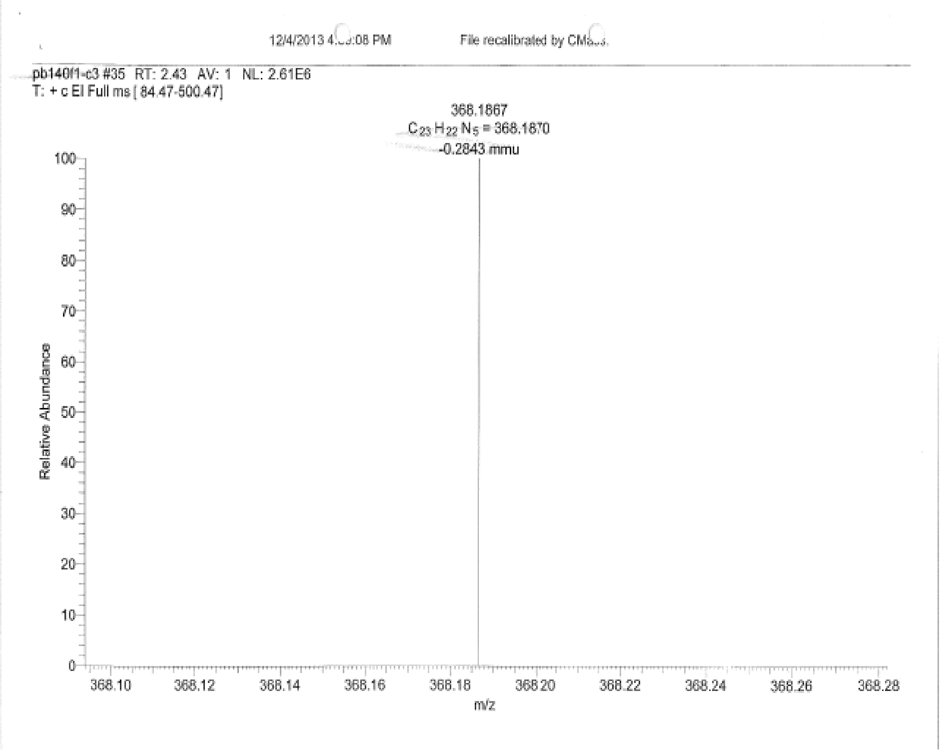
42

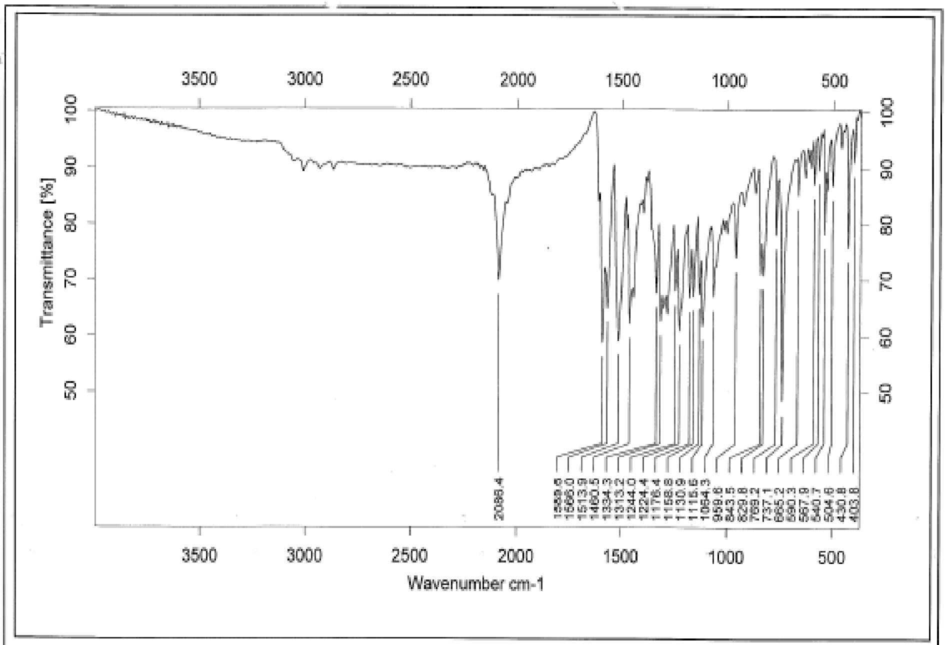
$C_{23}H_{22}IN_5$
495.3685 g/mol





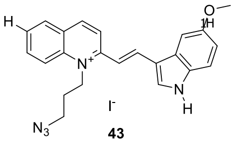

MAT 95, +FAB
ker
12/4/2013 4:‥:50 PM
P. Bohlaender
PB 140 F1,3-NBA
AK Wagenknecht
pb140f1 #33-37 RT: 2.29-2.57 AV: 5 NL: 2.62E6
T: + c EI Full ms [84.50-500.50]
Relative Abundance
m/z
368.2
369.2
283.1
285.1
340.2
311.2
370.2
269.1
154.1
168.1
136.1
89.1
183.1
217.1
254.1
367.2
385.2
426.3
453.2
494.2


File recalibrated by CMass.
pb140f1-c3 #35 RT: 2.43 AV: 1 NL: 2.61E6
T: + c EI Full ms [84.47-500.47]
368.1867
C23 H22 N5 = 368.1870
-0.2843 mmu
Relative Abundance
m/z



Sample : P. Bohlaender PB 140 F1	Frequency Range : 3997.41 - 373.828		Measured on : 11/12/2013
Technique : ATR platinum Diar	Resolution : 4	Instrument : Alpha	Sample Scans : 24
Operator : Angelika Kernert	Zerofilling : 2	Acquisition : Double Sided,For	

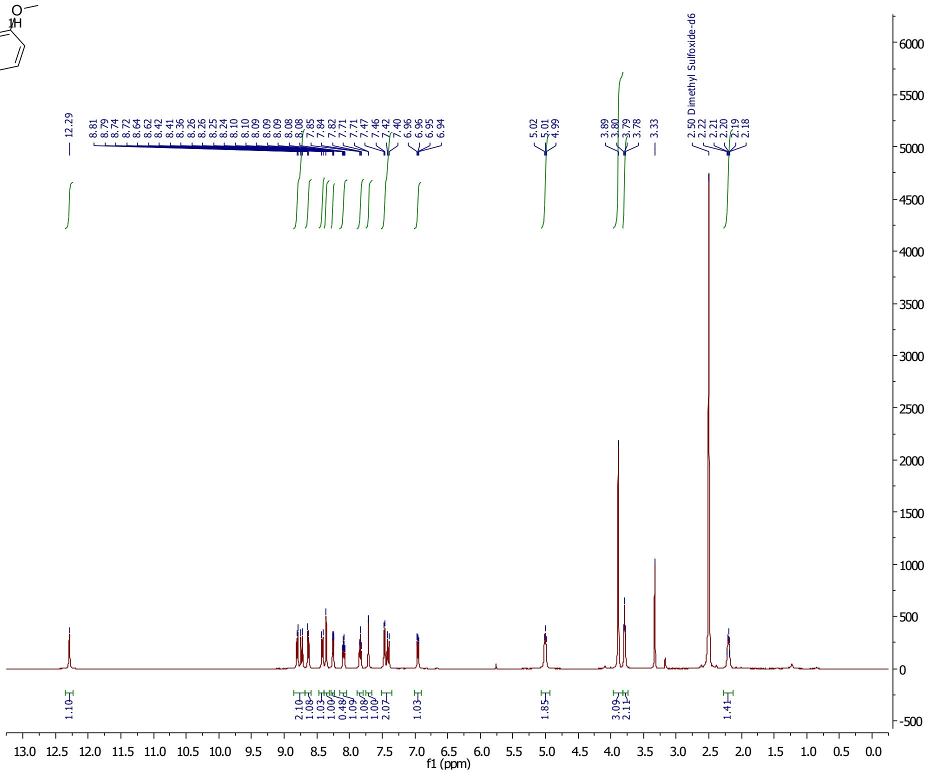
(*E*)-1-(3-azidopropyl)-2-(2-(5-methoxy-1*H*-indol-3-yl)vinyl)quinolin-1-ium iodide (43):

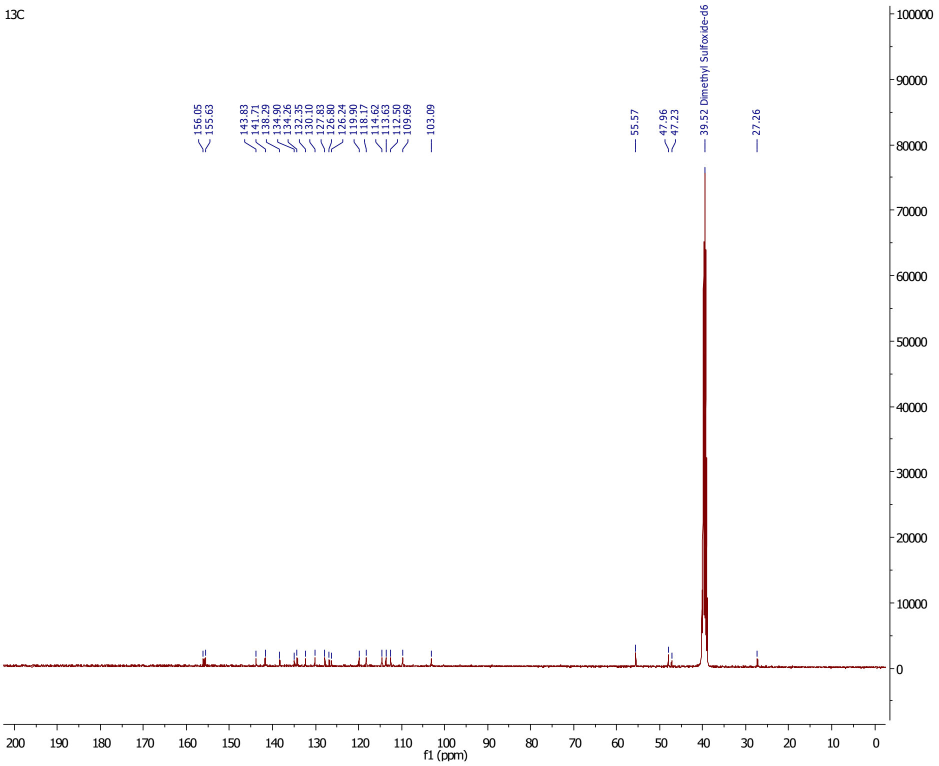


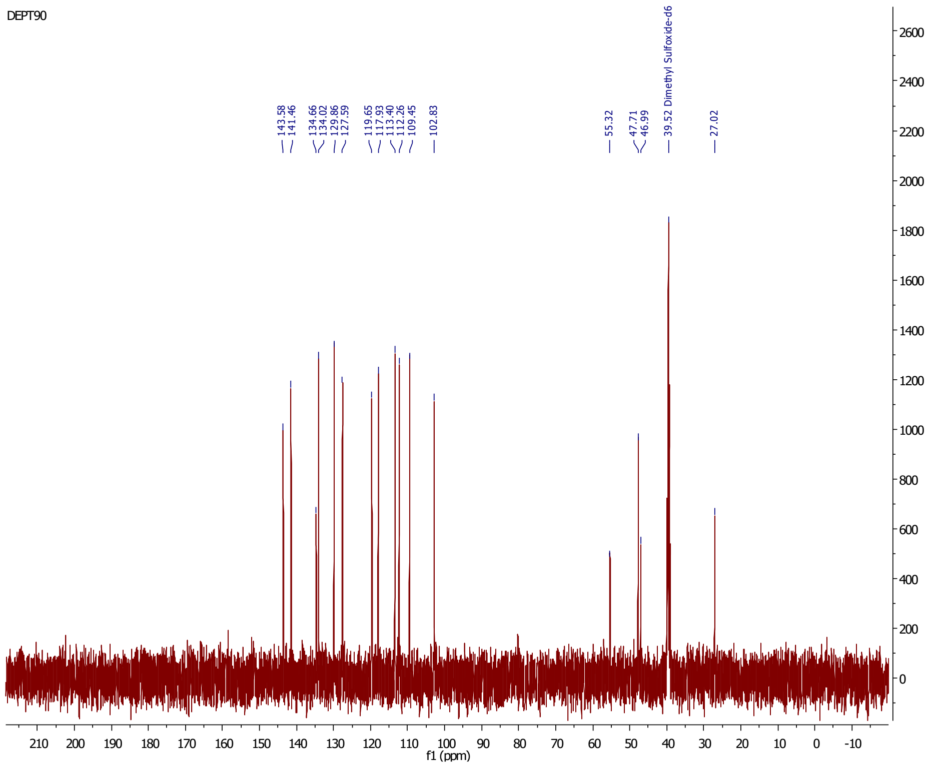
43

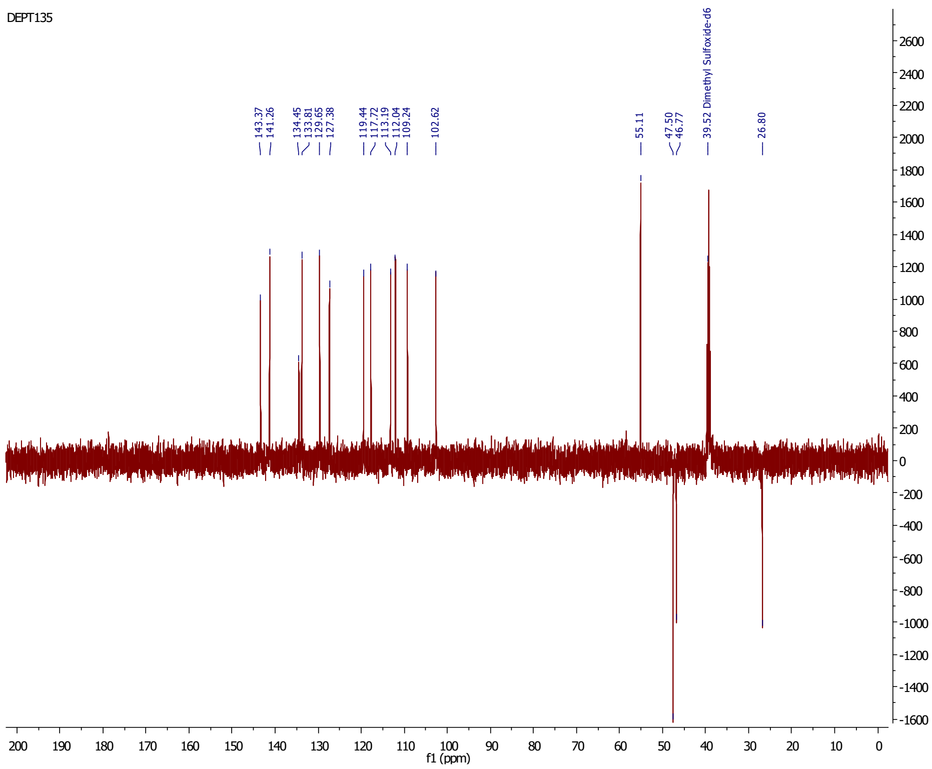
$C_{23}H_{22}IN_5O$

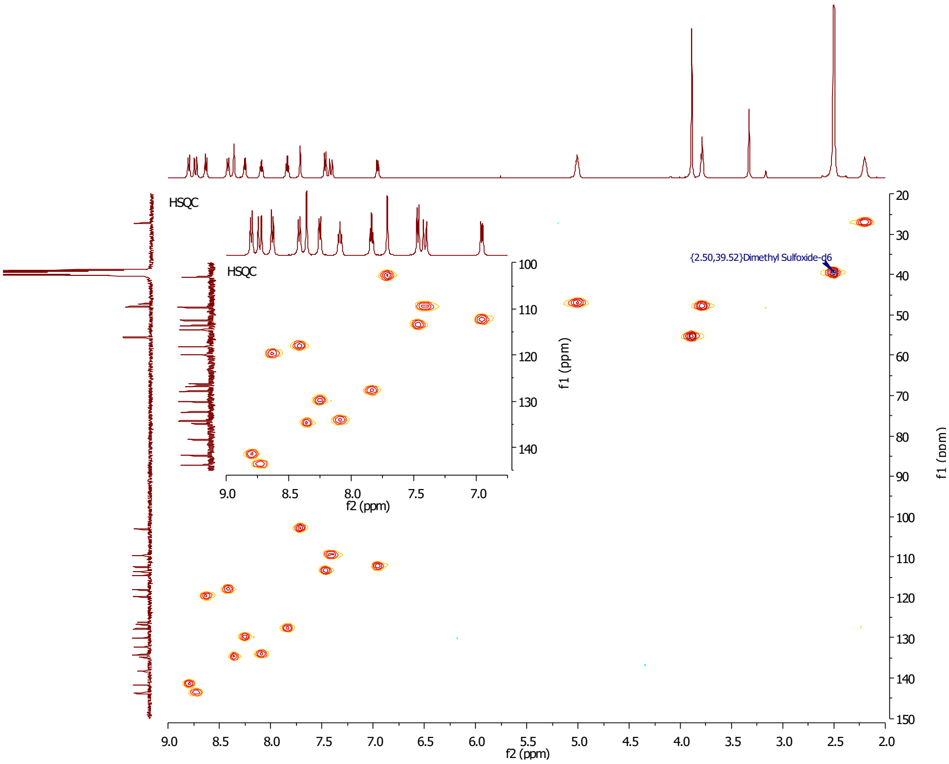
511.3675 g/mol

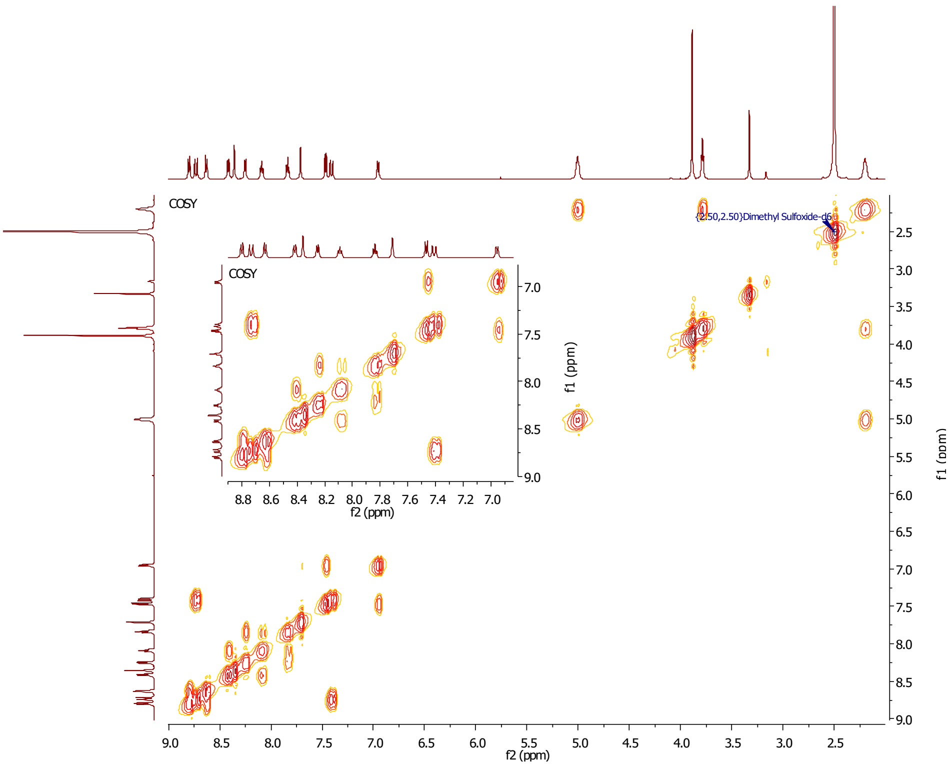


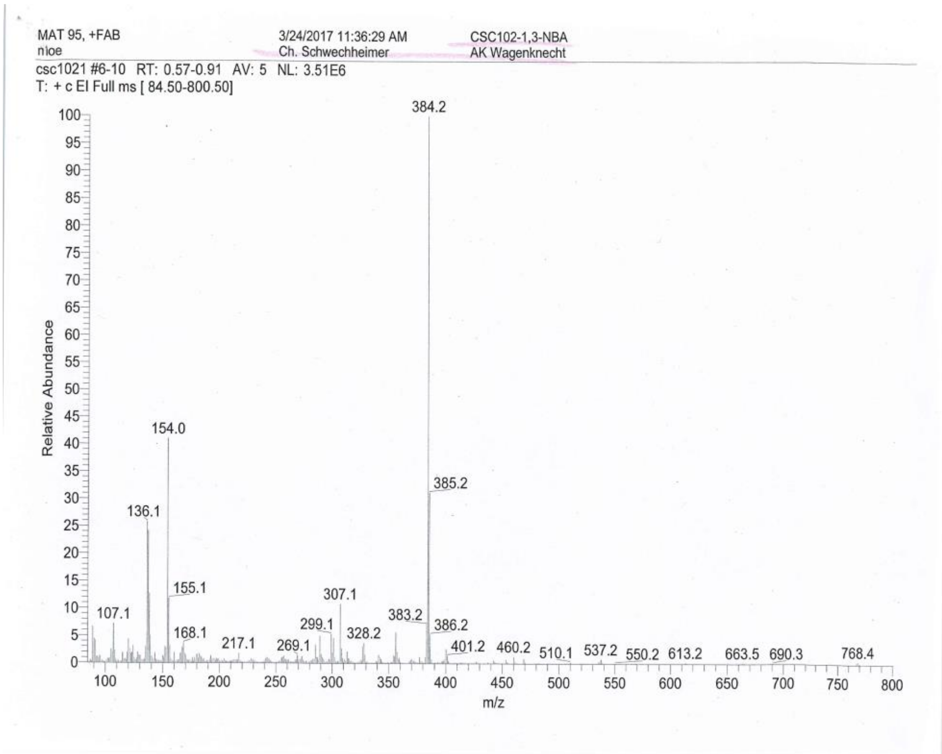


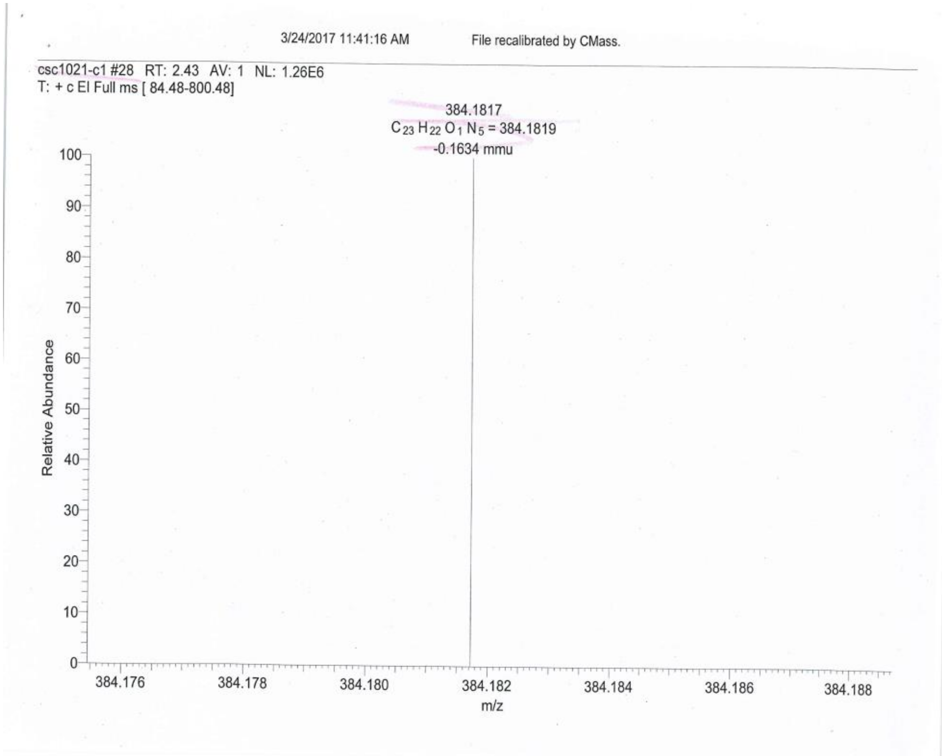

DEPT90
143.58
141.46
134.66
134.02
129.86
127.59
119.65
117.93
113.40
112.26
109.45
102.83
55.32
47.71
46.99
39.52 Dimethyl Sulfoxide-d6
27.02
f1 (ppm)

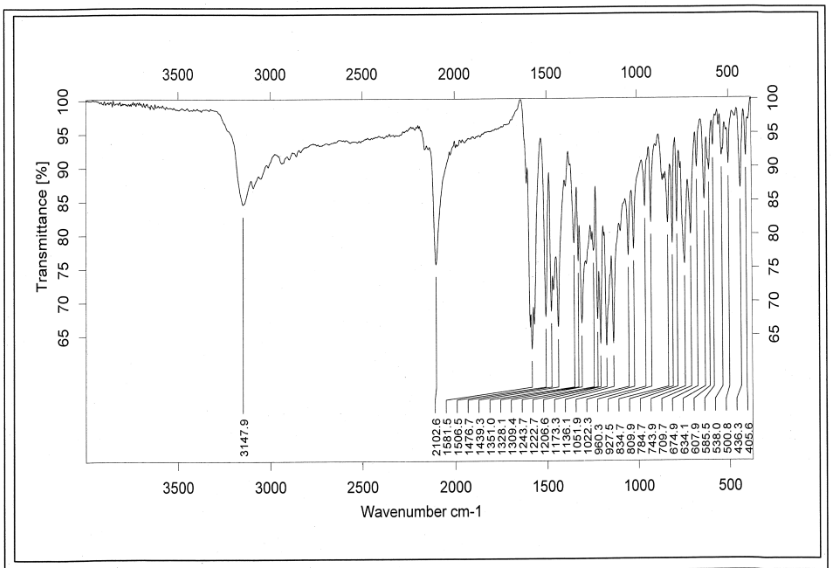

DEPT135
143.37
141.26
134.45
133.81
129.65
127.38
119.44
117.72
113.19
112.04
109.24
102.62
55.11
47.50
46.77
39.52 Dimethyl Sulfoxide-d6
26.80
f1 (ppm)


HSQC
{2.50,39.52}Dimethyl Sulfoxide-d6
f1 (ppm)
f2 (ppm)


COSY
{2.50,2.50}Dimethyl Sulfoxide-d6
f1 (ppm)
f2 (ppm)

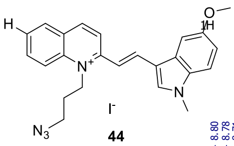

MAT 95, +FAB
nioe
3/24/2017 11:36:29 AM
Ch. Schwechheimer
CSC102-1,3-NBA
AK Wagenknecht
csc1021 #6-10 RT: 0.57-0.91 AV: 5 NL: 3.51E6
T: + c EI Full ms [84.50-800.50]
384.2
154.0
385.2
136.1
155.1
307.1
107.1
383.2
299.1
386.2
168.1
328.2
217.1
269.1
401.2
460.2
510.1
537.2
550.2
613.2
663.5
690.3
768.4
Relative Abundance
m/z


3/24/2017 11:41:16 AM
File recalibrated by CMass.
csc1021-c1 #28 RT: 2.43 AV: 1 NL: 1.26E6
T: + c EI Full ms [84.48-800.48]
384.1817
C23 H22 O1 N5 = 384.1819
-0.1634 mmu
Relative Abundance
m/z



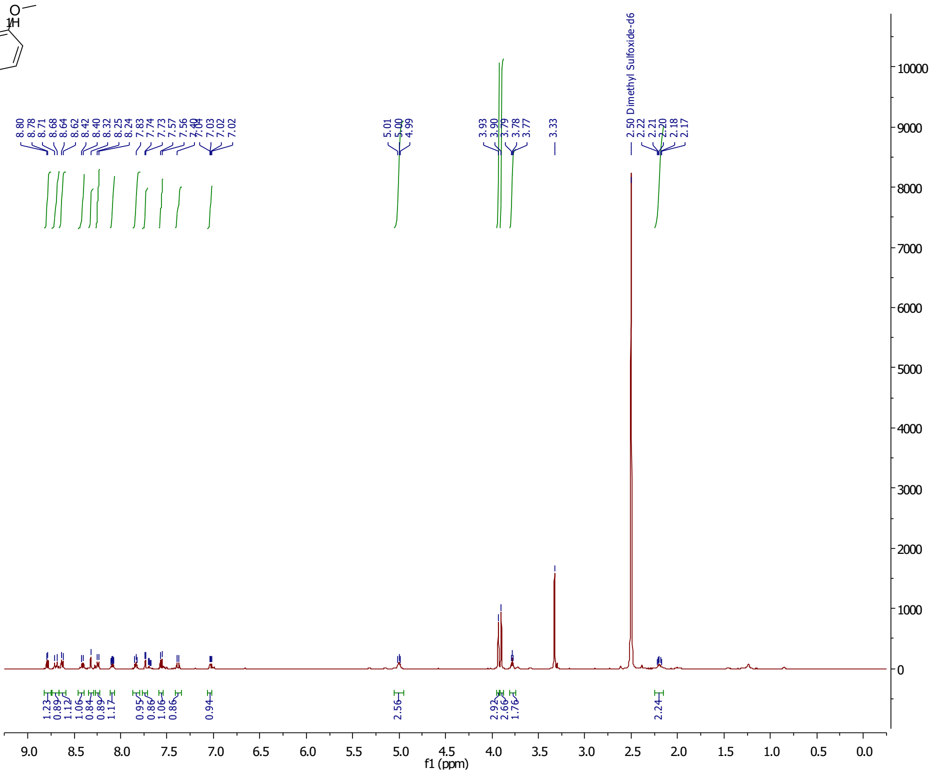
Sample : 102-1	Frequency Range : 3997.41 - 373.828		Measured on : 06/04/2017
Technique : Diamant-ATR	Resolution : 4	Instrument : Alpha	Sample Scans : 24
Operator : Angelika Moesle	Zerofilling : 2	Acquisition : Double Sided,Forward-Backward	

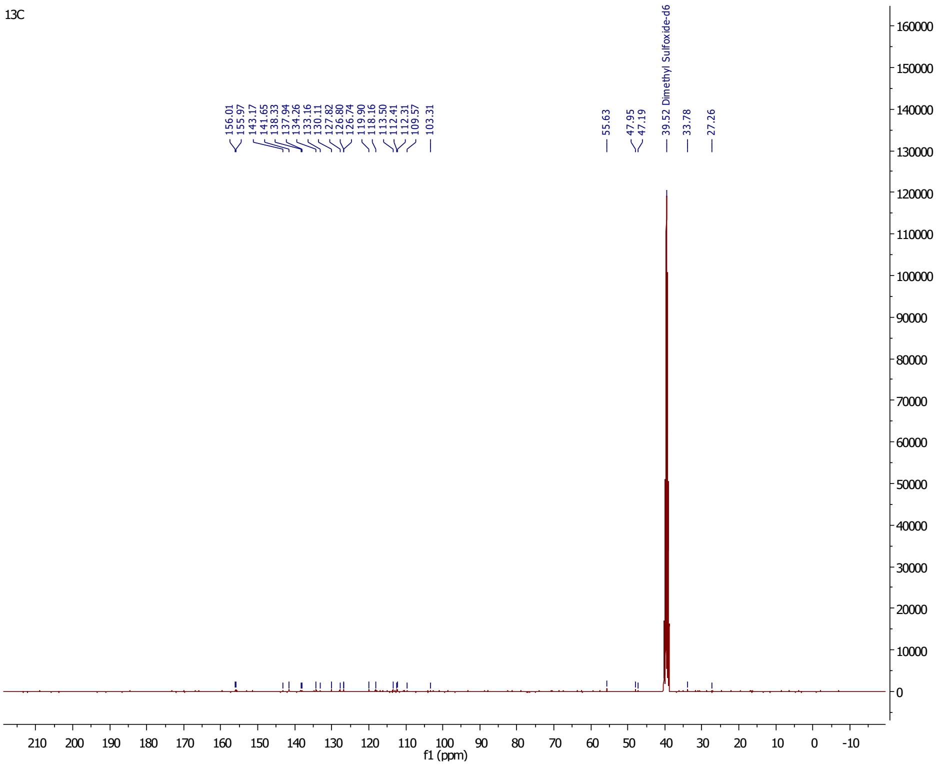
(*E*)-1-(3-azidopropyl)-2-(2-(5-methoxy-1-methyl-1*H*-indol-3-yl)vinyl)quinolin-1-ium iodide (44):

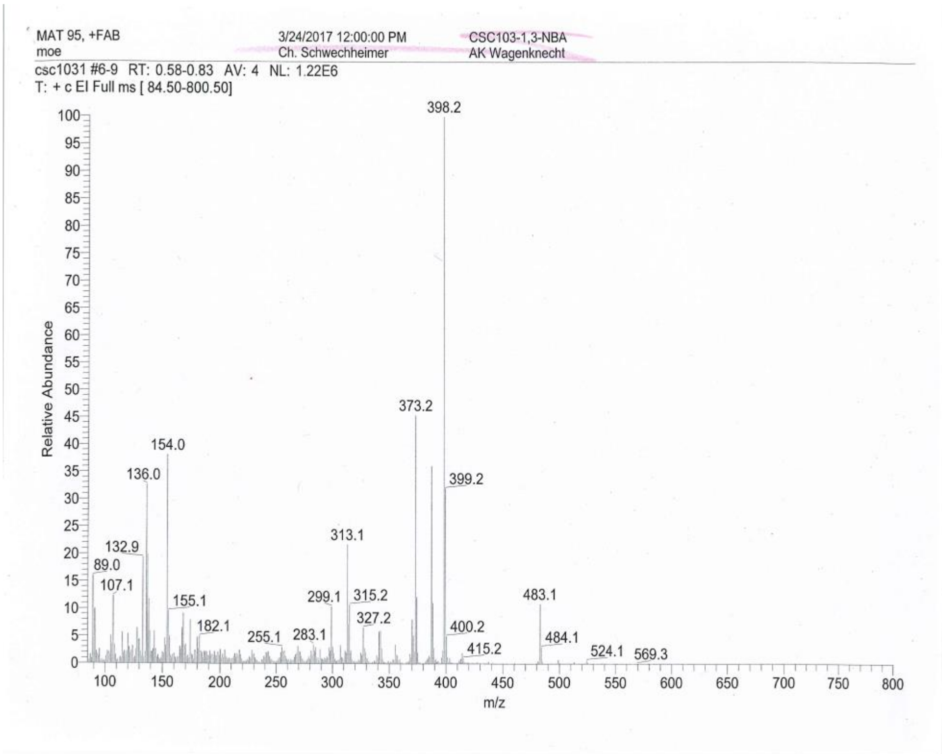


44

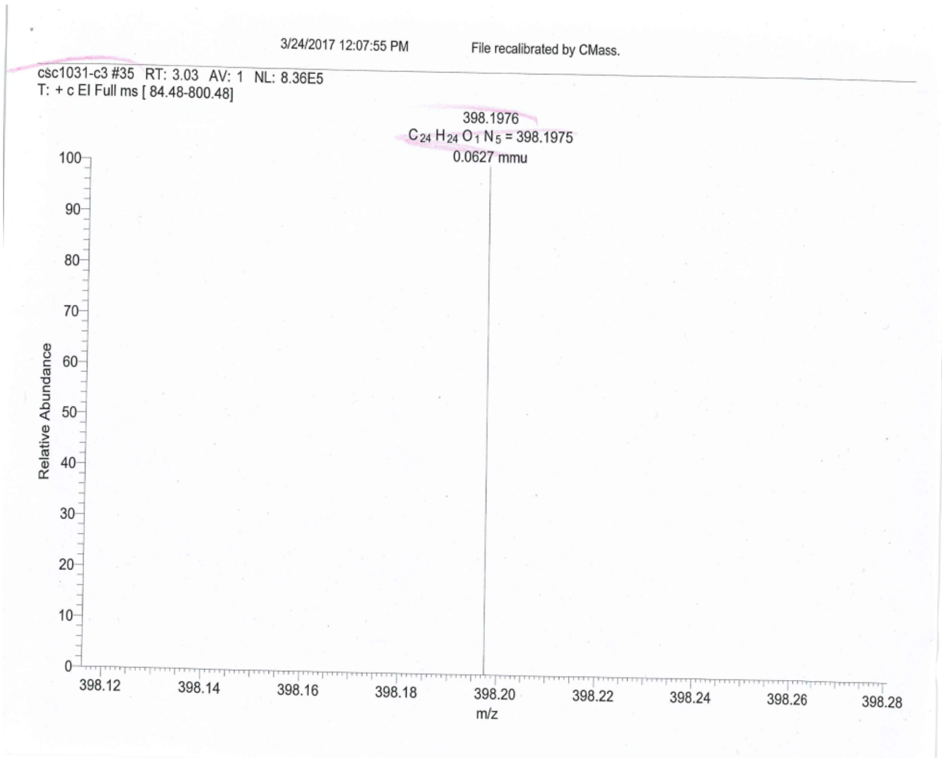
$C_{24}H_{24}IN_5O$
525.3945 g/mol



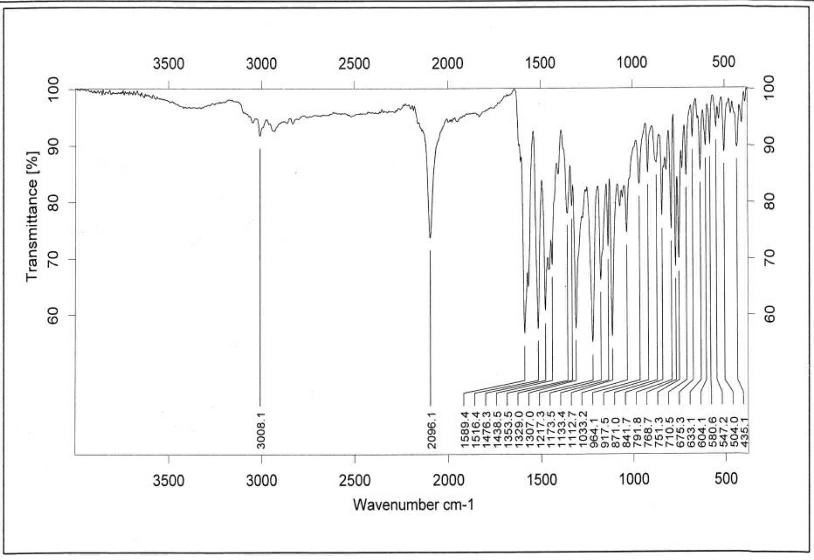




MAT 95, +FAB
moe
3/24/2017 12:00:00 PM
Ch. Schwechheimer
CSC103-1,3-NBA
AK Wagenknecht
csc1031 #6-9 RT: 0.58-0.83 AV: 4 NL: 1.22E6
T: + c EI Full ms [84.50-800.50]
Relative Abundance
m/z
398.2
373.2
154.0
136.0
399.2
313.1
132.9
89.0
107.1
155.1
299.1
315.2
327.2
483.1
182.1
255.1
283.1
400.2
484.1
415.2
524.1
569.3

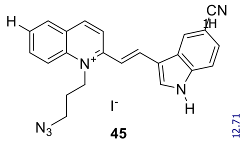


3/24/2017 12:07:55 PM
File recalibrated by CMass.
csc1031-c3 #35 RT: 3.03 AV: 1 NL: 8.36E5
T: + c EI Full ms [84.48-800.48]
398.1976
$C_{24}H_{24}O_1N_5$ = 398.1975
0.0627 mmu
Relative Abundance
m/z



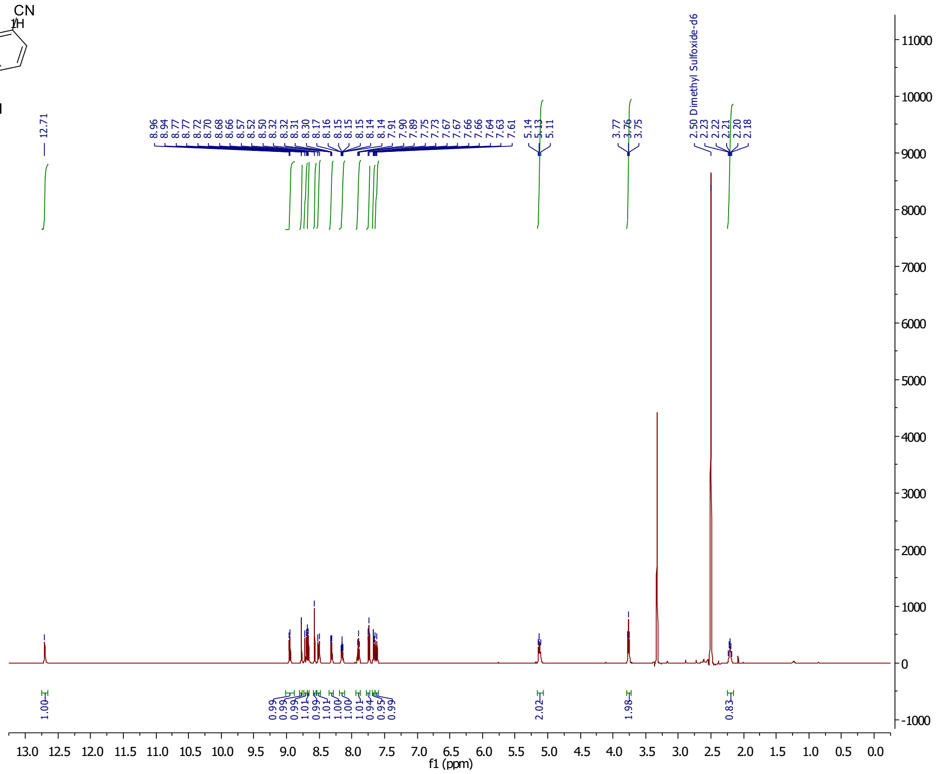
Sample : 103-1F1	Frequency Range : 3997.41 - 373.828	Measured on : 06/04/2017	
Technique : Diamant-ATR	Resolution : 4	Instrument : Alpha	Sample Scans : 24
Operator : Angelika Moesle	Zerofilling : 2	Acquisition : Double Sided,Forward-Backward	

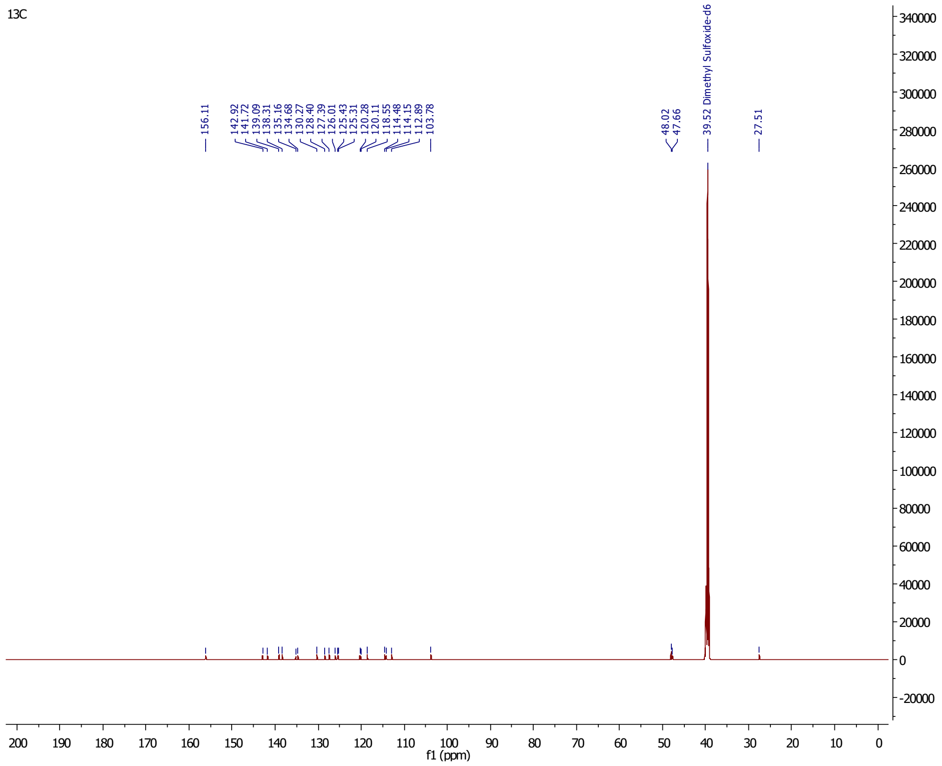
(*E*)-1-(3-azidopropyl)-2-(2-(5-cyano-1*H*-indol-3-yl)vinyl)quinolin-1-ium iodide (45):

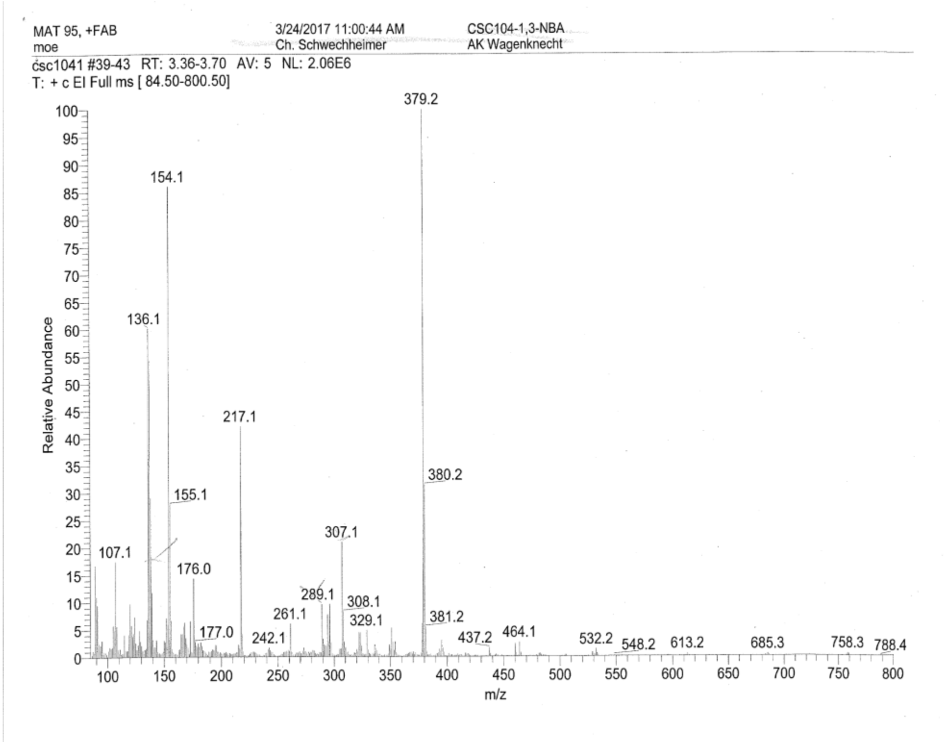


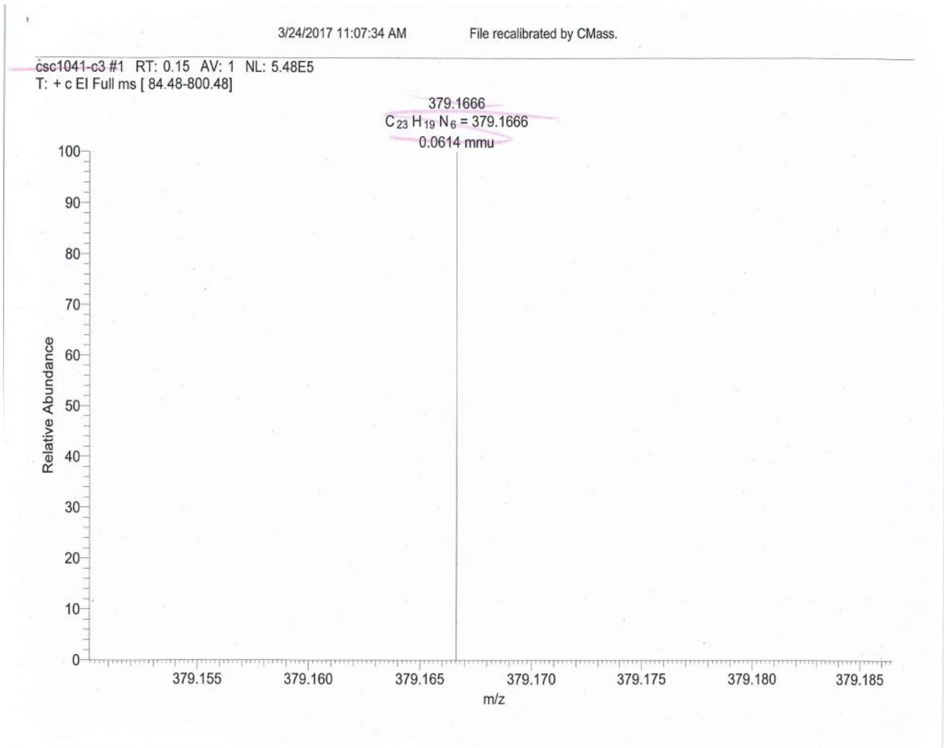
45

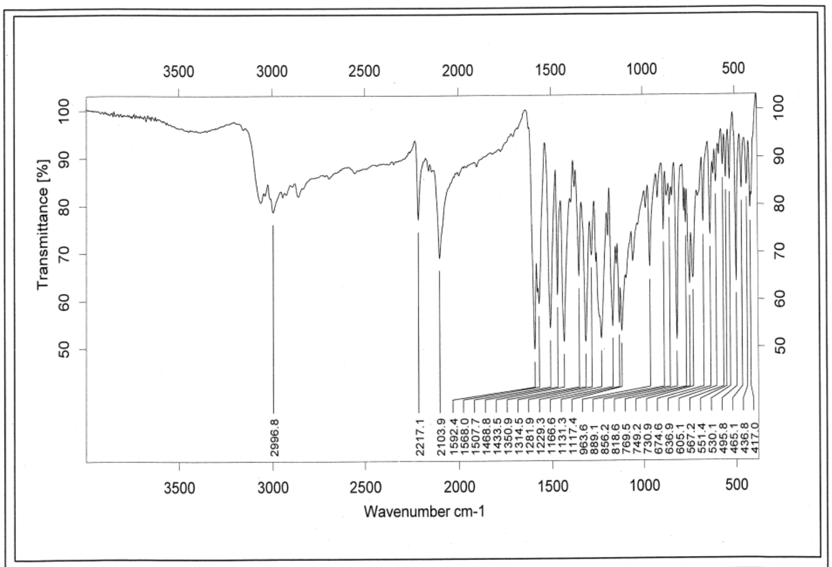
$C_{23}H_{19}IN_6$
506.3515 g/mol





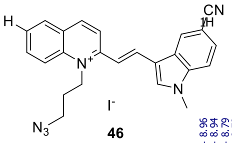

MAT 95, +FAB
moe
3/24/2017 11:00:44 AM
Ch. Schwechheimer
CSC104-1,3-NBA
AK Wagenknecht
csc1041 #39-43 RT: 3.36-3.70 AV: 5 NL: 2.06E6
T: + c EI Full ms [84.50-800.50]
Relative Abundance
m/z
379.2
154.1
136.1
217.1
380.2
155.1
307.1
107.1
176.0
289.1
308.1
261.1
329.1
381.2
177.0
242.1
437.2
464.1
532.2
548.2
613.2
685.3
758.3
788.4


3/24/2017 11:07:34 AM
File recalibrated by CMass.
csc1041-c3 #1 RT: 0.15 AV: 1 NL: 5.48E5
T: + c EI Full ms [84.48-800.48]
379.1666
C 23 H 19 N 6 = 379.1666
0.0614 mmu
Relative Abundance
m/z



Sample : 104-1	Frequency Range : 3997.41 - 373.828		Measured on : 30/03/2017
Technique : Diamant-ATR	Resolution : 4	Instrument : Alpha	Sample Scans : 24
Operator : Angelika Moesle	Zerofilling : 2	Acquisition : Double Sided,Forward-Backward	

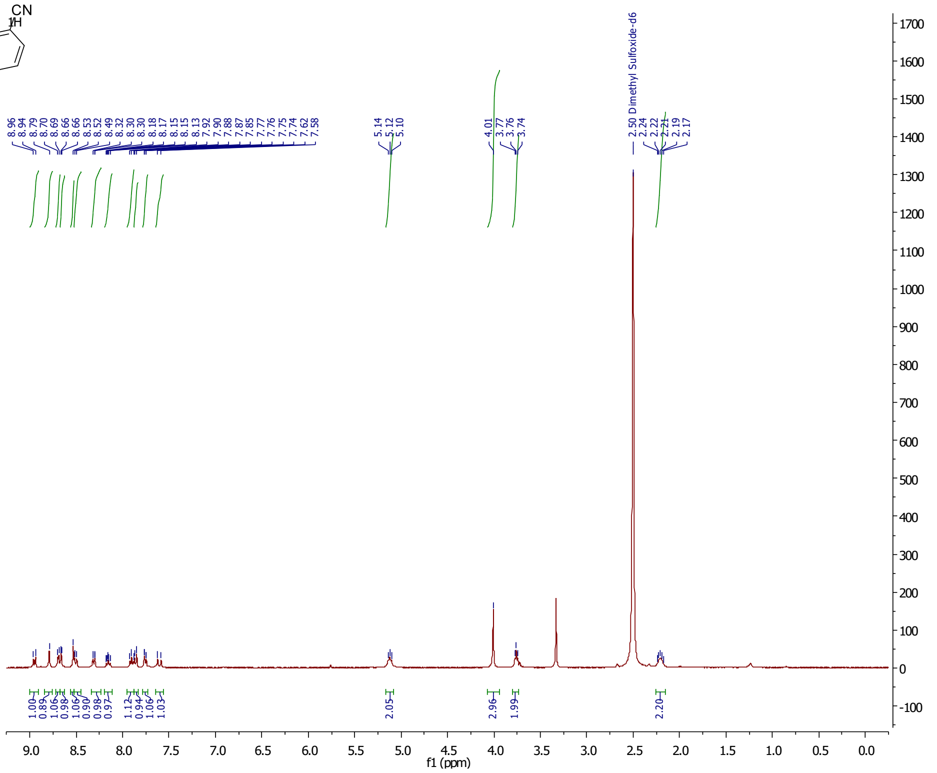
(*E*)-1-(3-azidopropyl)-2-(2-(5-cyano-1-methyl-1*H*-indol-3-yl)vinyl)quinolin-1-ium iodide (46):

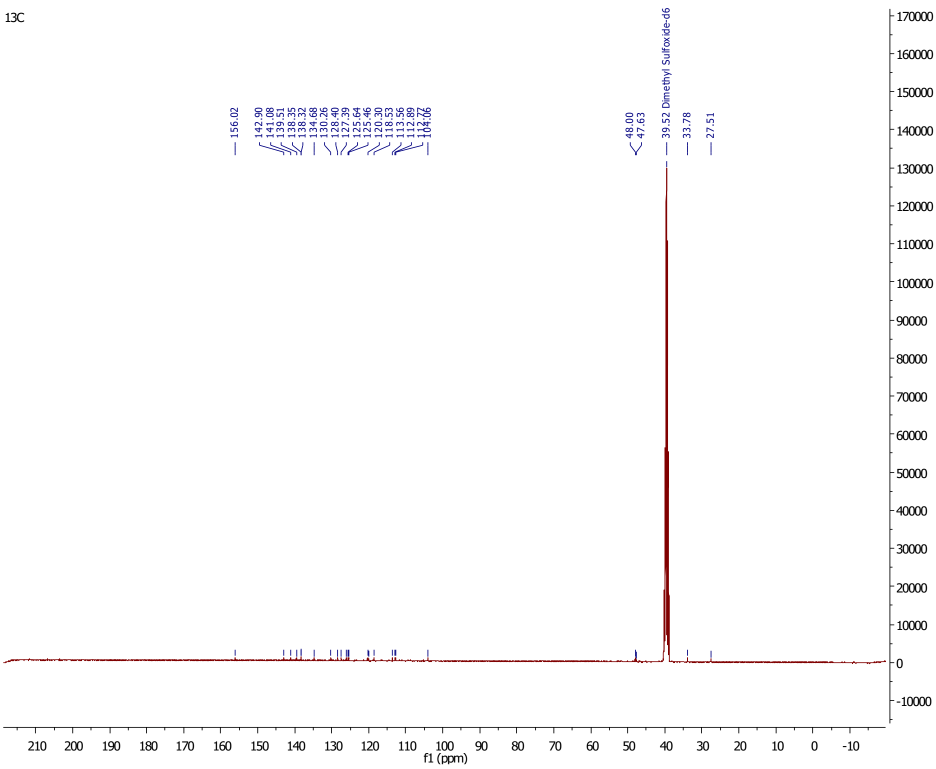


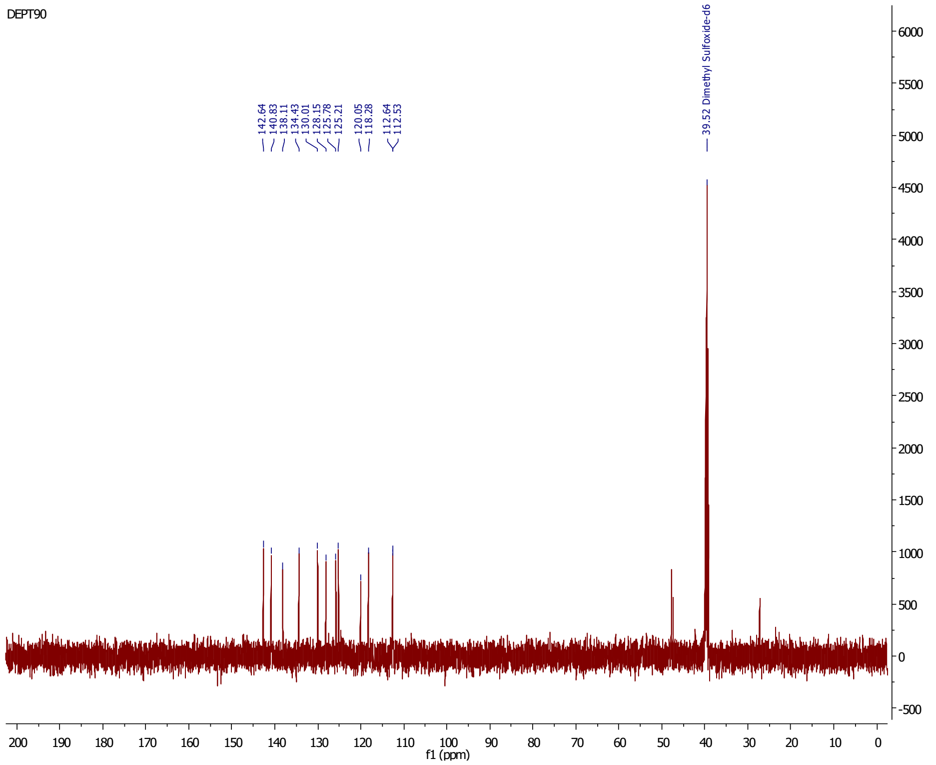
46

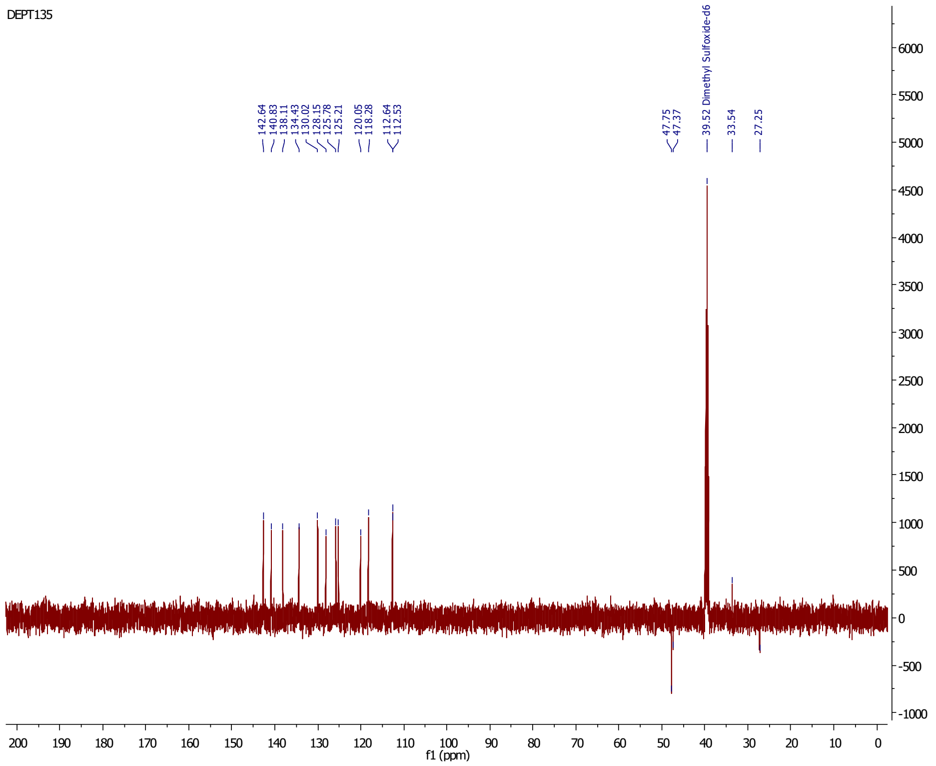
$C_{24}H_{21}IN_6$

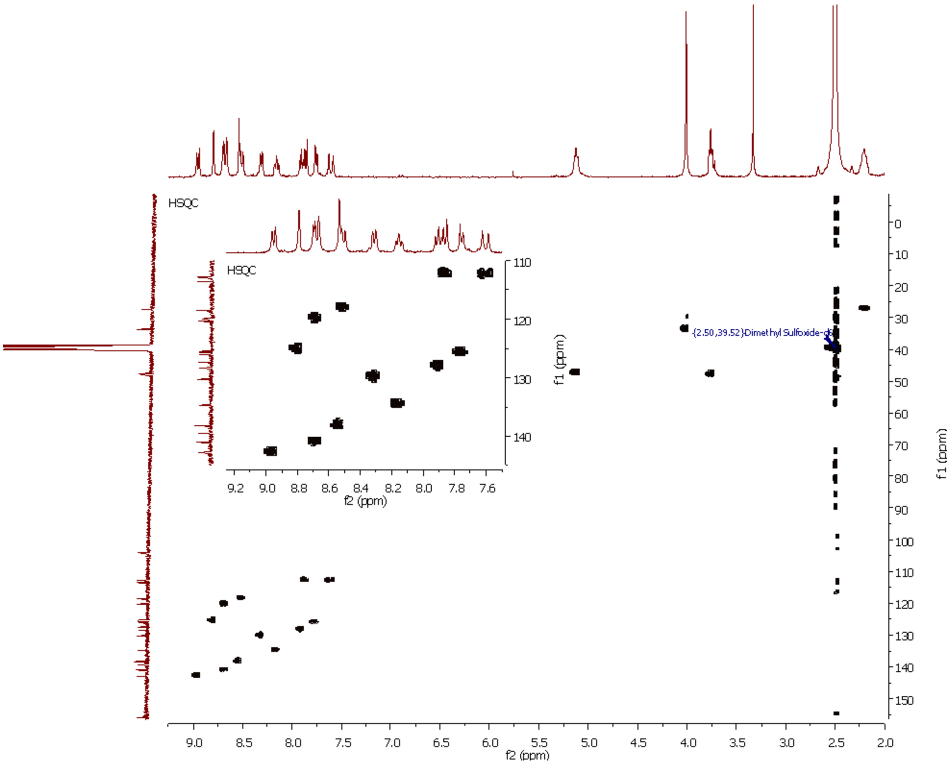
520.3785 g/mol

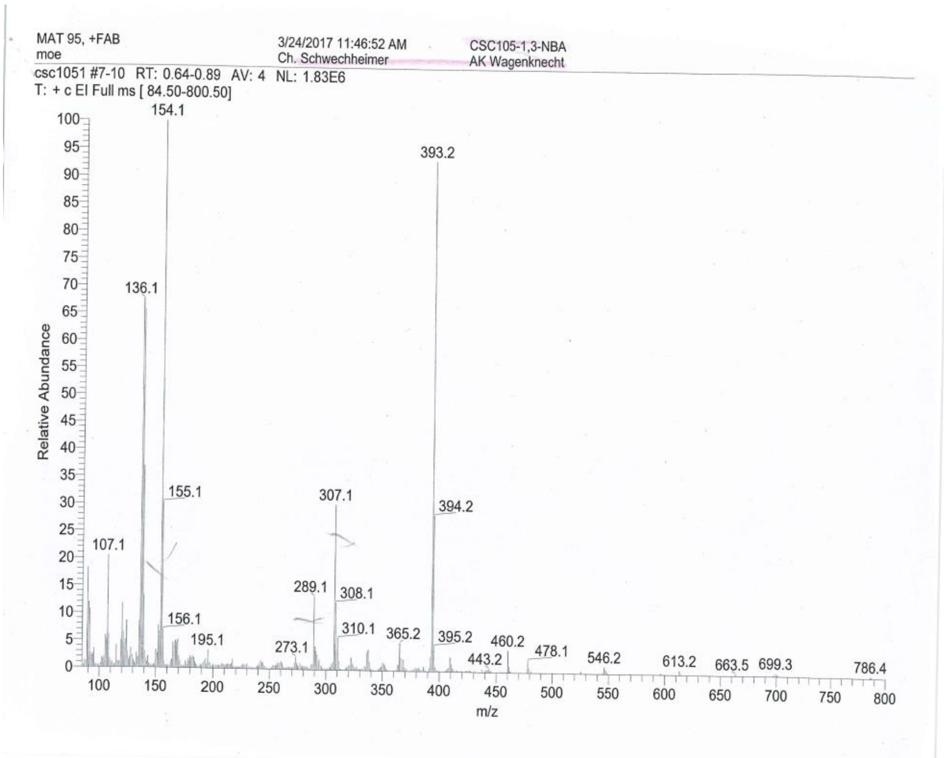


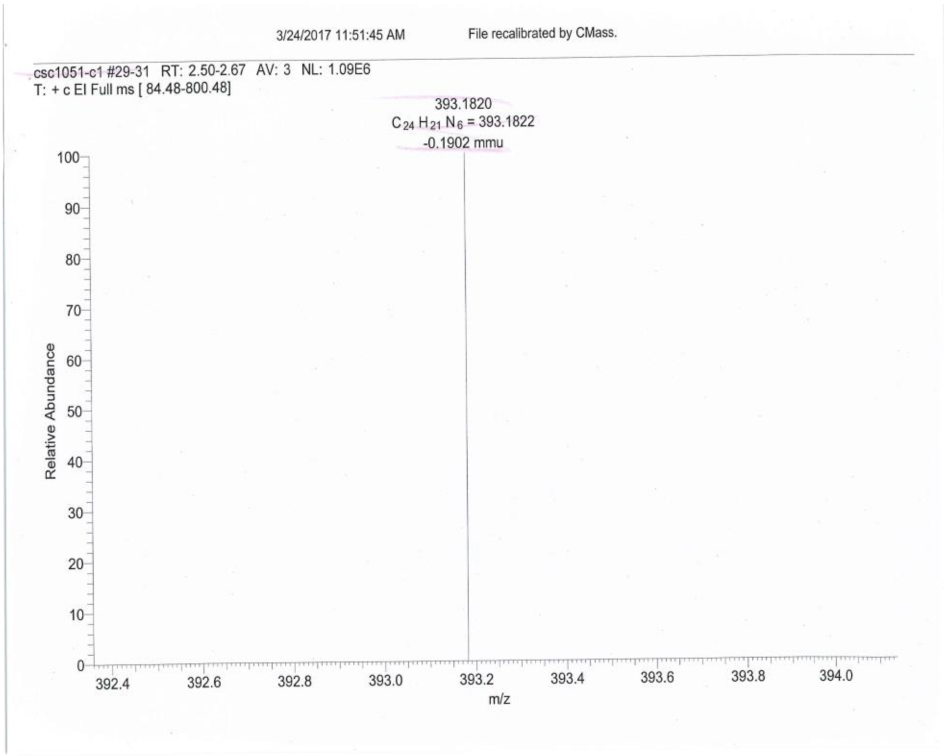


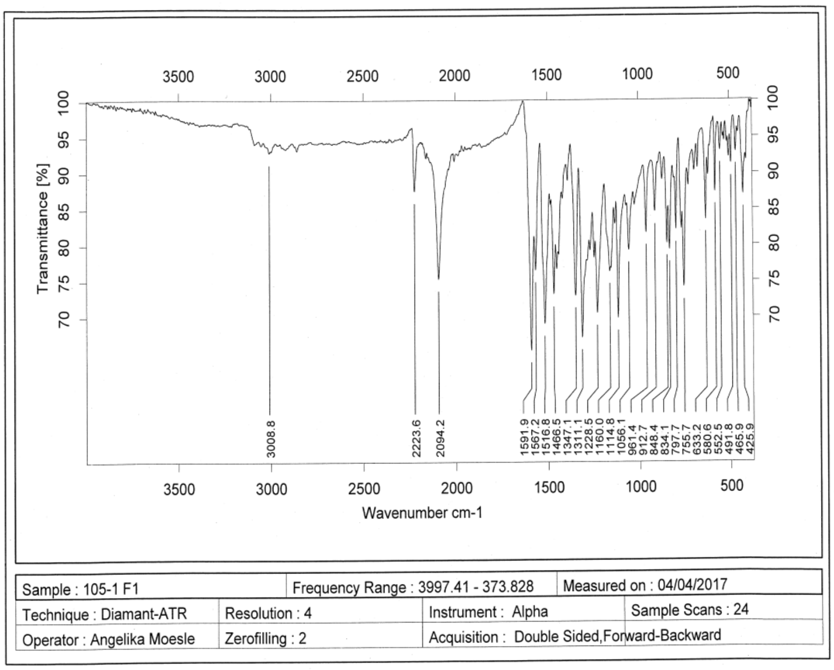

DEPT90
142.64
140.83
138.11
134.43
130.01
128.15
125.78
125.21
120.05
118.28
112.64
112.53
39.52 Dimethyl Sulfoxide-d6
f1 (ppm)


DEPT135
142.64
140.83
138.11
134.43
130.02
128.15
125.78
125.21
120.05
118.28
112.64
112.53
47.75
47.37
39.52 Dimethyl Sulfoxide-d6
33.54
27.25
f1 (ppm)

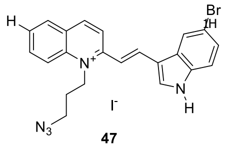

HSQC
f2 (ppm)
f1 (ppm)
(2.50,39.52)Dimethyl Sulfoxide-d6


MAT 95, +FAB
moe
3/24/2017 11:46:52 AM
Ch. Schwechheimer
CSC105-1,3-NBA
AK Wagenknecht
csc1051 #7-10 RT: 0.64-0.89 AV: 4 NL: 1.83E6
T: + c EI Full ms [84.50-800.50]
Relative Abundance
m/z
154.1
393.2
136.1
155.1
307.1
394.2
107.1
289.1
308.1
156.1
310.1
365.2
395.2
460.2
195.1
273.1
443.2
478.1
546.2
613.2
663.5
699.3
786.4


3/24/2017 11:51:45 AM
File recalibrated by CMass.
csc1051-c1 #29-31 RT: 2.50-2.67 AV: 3 NL: 1.09E6
T: + c EI Full ms [84.48-800.48]
393.1820
C 24 H 21 N 6 = 393.1822
-0.1902 mmu
Relative Abundance
m/z

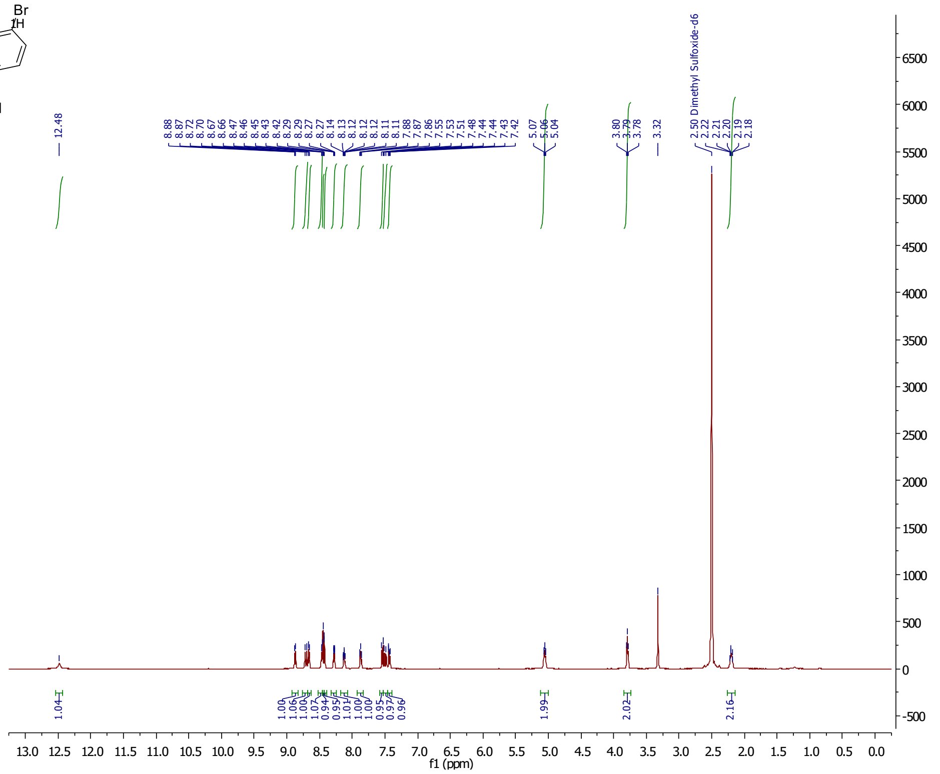

Transmittance [%]
Wavenumber cm-1
3008.8
2223.6
2094.2
1591.9
1567.2
1516.8
1466.5
1347.1
1311.1
1228.5
1160.0
1114.8
1056.1
961.4
912.7
848.4
834.1
797.7
755.7
633.2
580.6
552.5
491.8
465.9
425.9
Sample : 105-1 F1
Frequency Range : 3997.41 - 373.828
Measured on : 04/04/2017
Technique : Diamant-ATR
Resolution : 4
Instrument : Alpha
Sample Scans : 24
Operator : Angelika Moesle
Zerofilling : 2
Acquisition : Double Sided,Forward-Backward

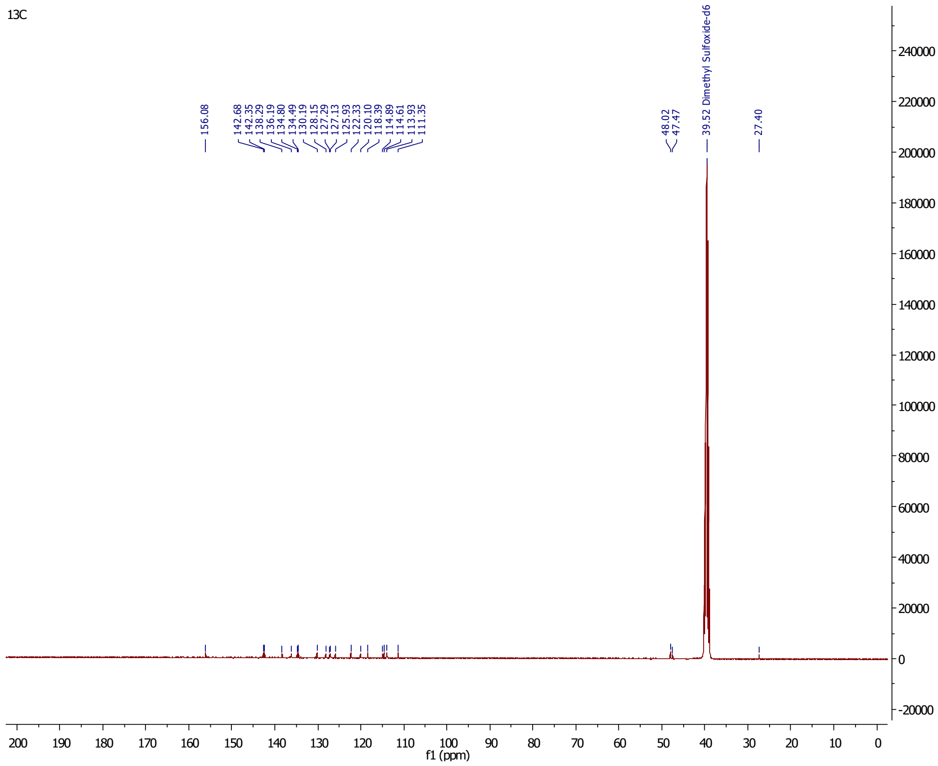
(*E*)-1-(3-azidopropyl)-2-(2-(5-bromo-1*H*-indol-3-yl)vinyl)quinolin-1-ium iodide (47):

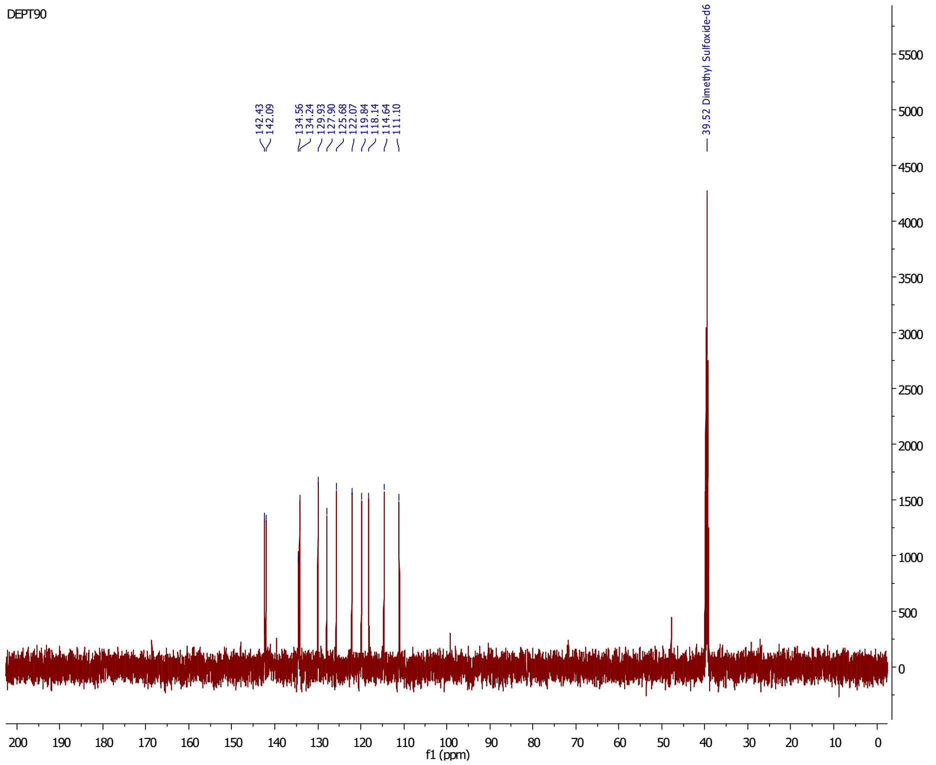


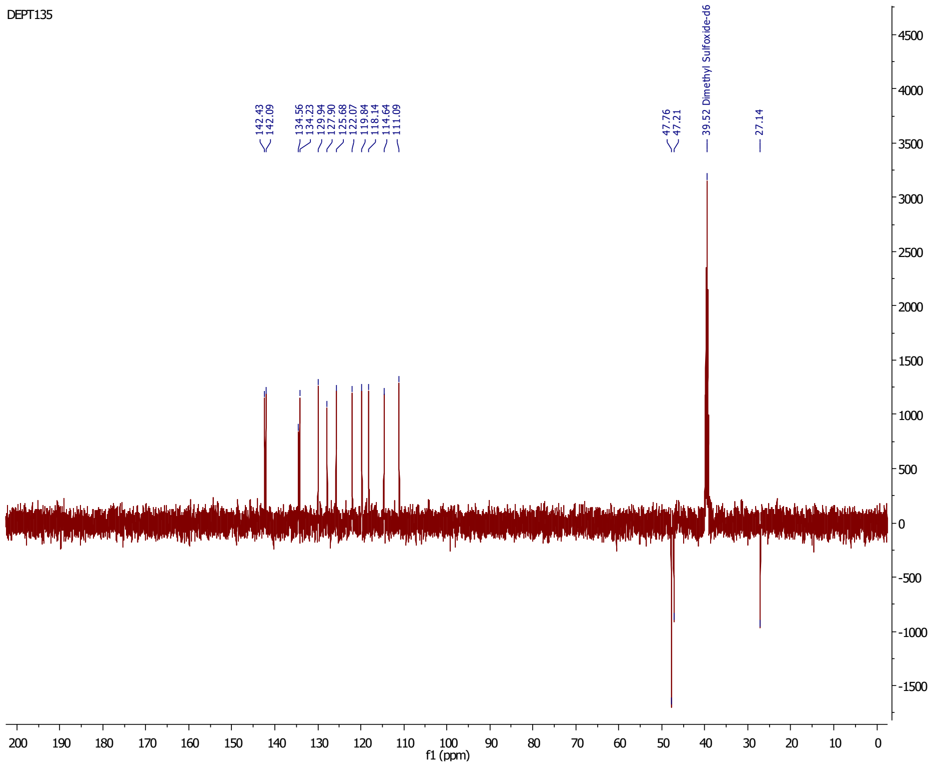
47

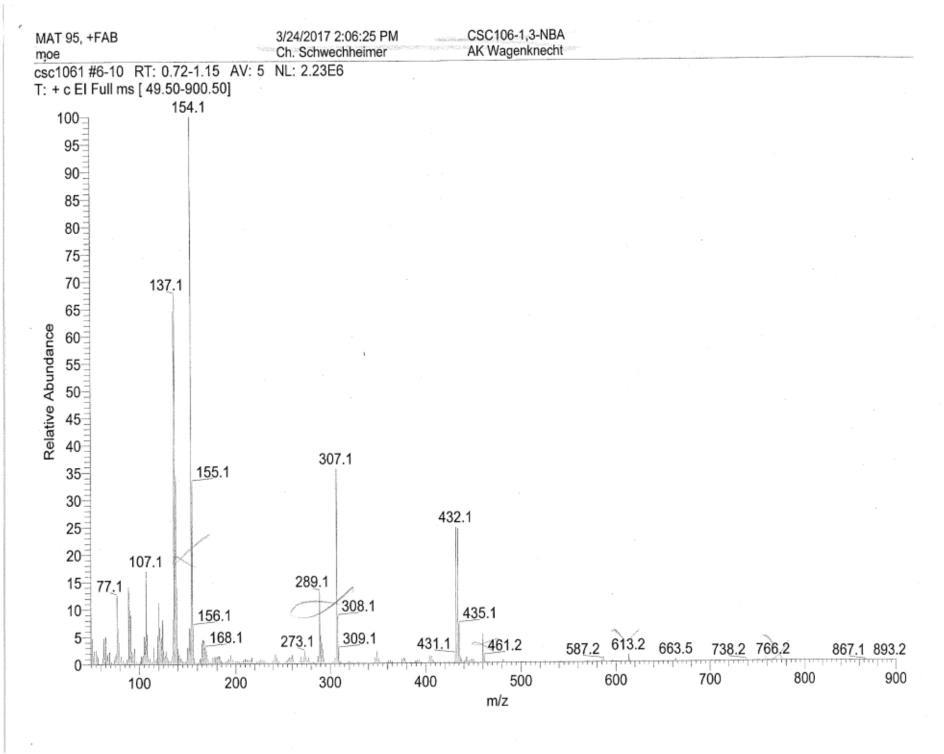
$C_{22}H_{19}BrIN_5$
560.2375 g/mol



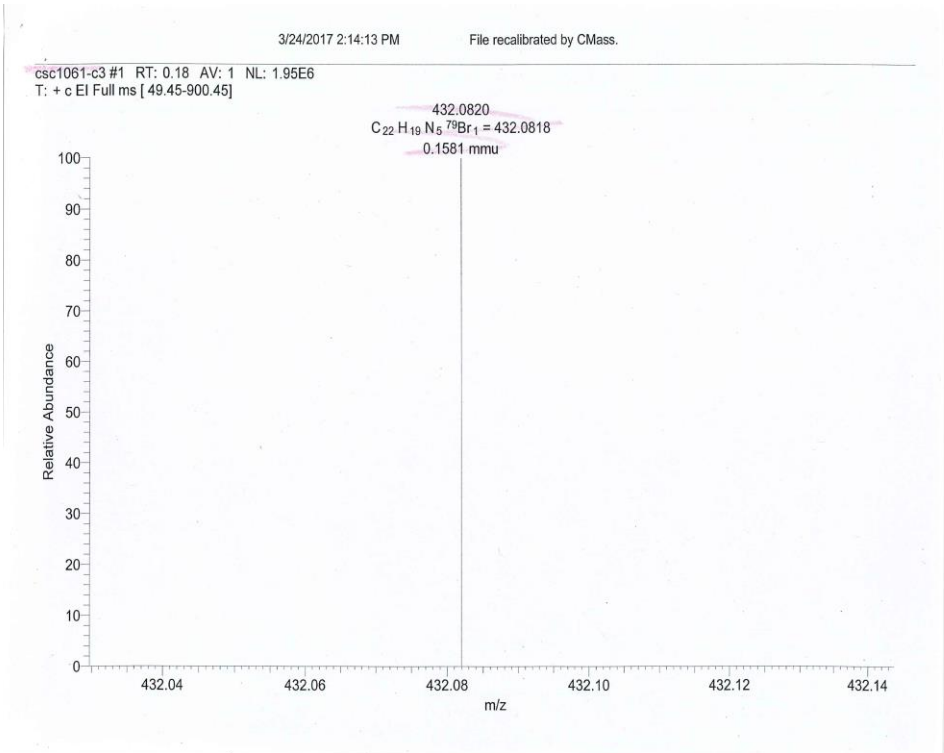



DEPT90
142.43
142.09
134.56
134.24
129.93
127.90
125.68
122.07
119.84
118.14
114.64
111.10
39.52 Dimethyl Sulfoxide-d6
f1 (ppm)

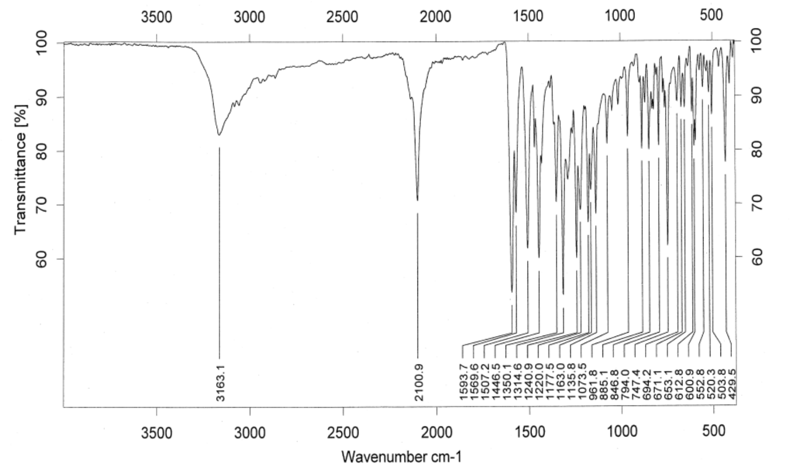

DEPT135
142.43
142.09
134.56
134.23
129.94
127.90
125.68
122.07
119.84
118.14
114.64
111.09
47.76
47.21
39.52 Dimethyl Sulfoxide-d6
27.14
f1 (ppm)



MAT 95, +FAB
moe
3/24/2017 2:06:25 PM
Ch. Schwechheimer
CSC106-1,3-NBA
AK Wagenknecht
csc1061 #6-10 RT: 0.72-1.15 AV: 5 NL: 2.23E6
T: + c EI Full ms [49.50-900.50]
Relative Abundance
m/z
154.1
137.1
307.1
432.1
155.1
107.1
77.1
289.1
308.1
435.1
156.1
168.1
273.1
309.1
431.1
461.2
587.2
613.2
663.5
738.2
766.2
867.1
893.2

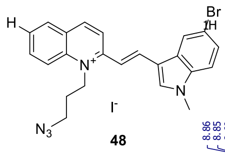


3/24/2017 2:14:13 PM
File recalibrated by CMass.
csc1061-c3 #1 RT: 0.18 AV: 1 NL: 1.95E6
T: + c EI Full ms [49.45-900.45]
432.0820
C22 H19 N5 79Br1 = 432.0818
0.1581 mmu
Relative Abundance
m/z



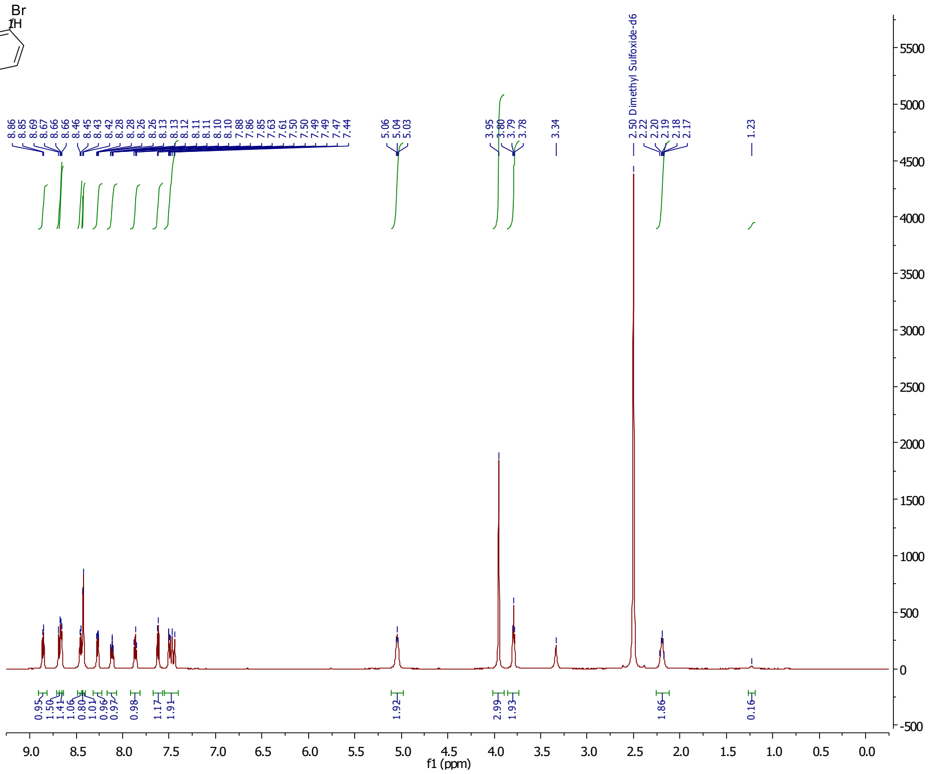
Sample : 106-1	Frequency Range : 3997.41 - 373.828		Measured on : 29/03/2017
Technique : Diamant-ATR	Resolution : 4	Instrument : Alpha	Sample Scans : 24
Operator : Angelika Moesle	Zerofilling : 2	Acquisition : Double Sided,Forward-Backward	

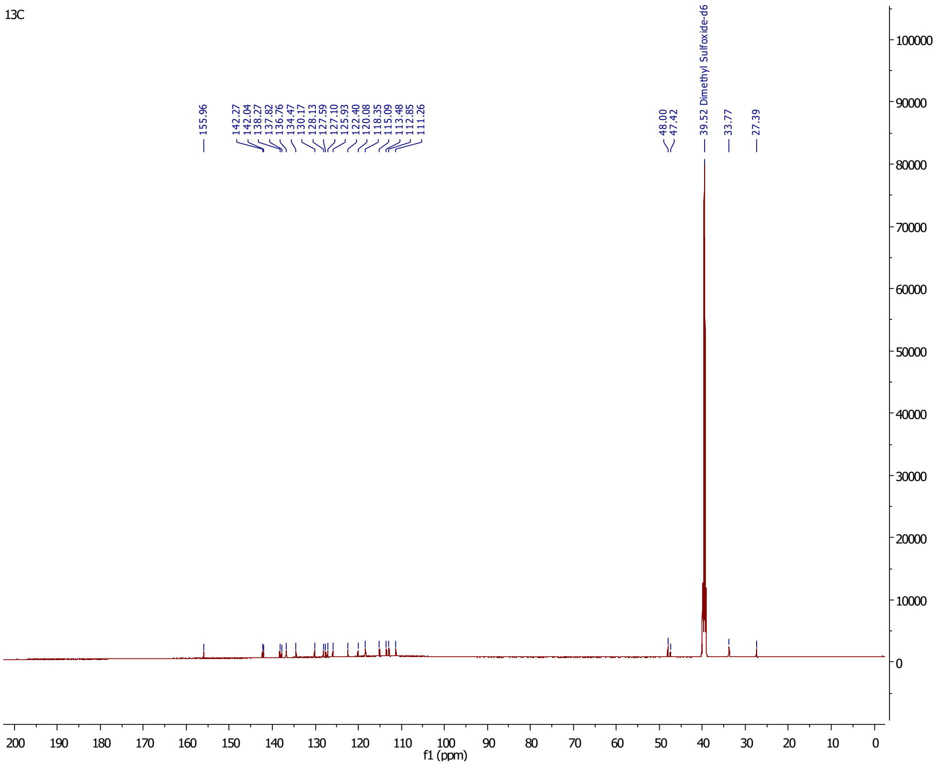
(*E*)-1-(3-azidopropyl)-2-(2-(5-bromo-1-methyl-1*H*-indol-3-yl)vinyl)quinolin-1-ium iodide (48):

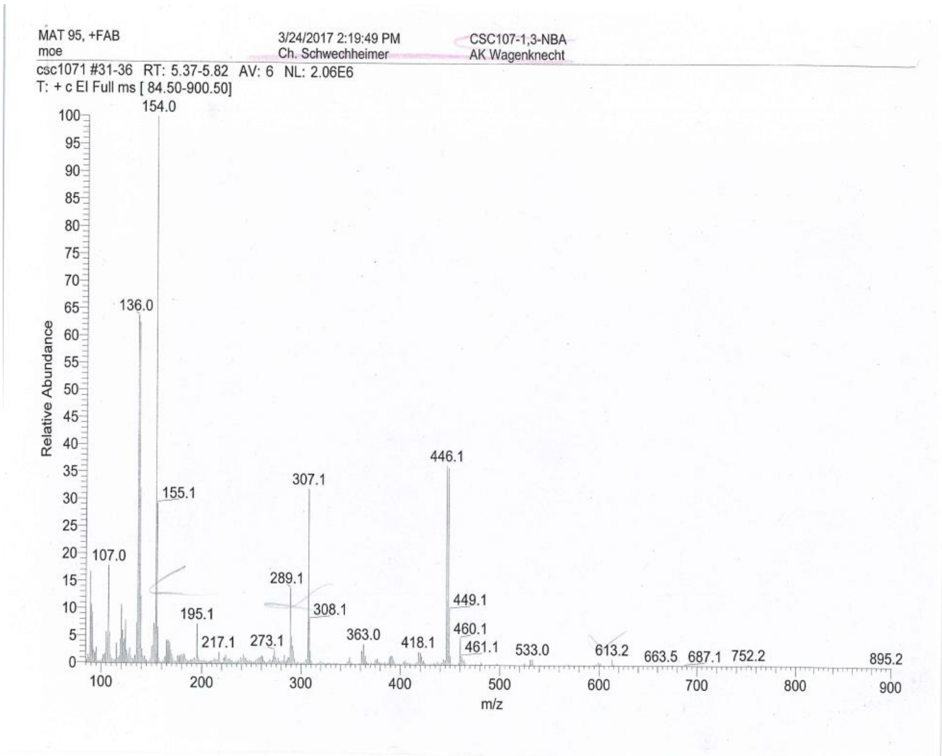


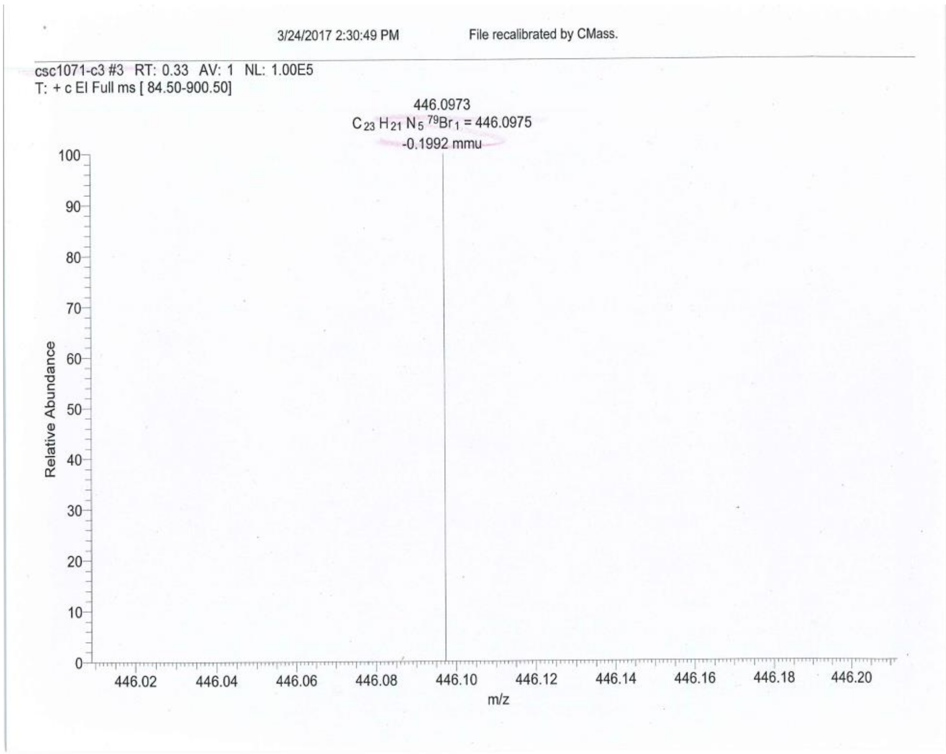
48

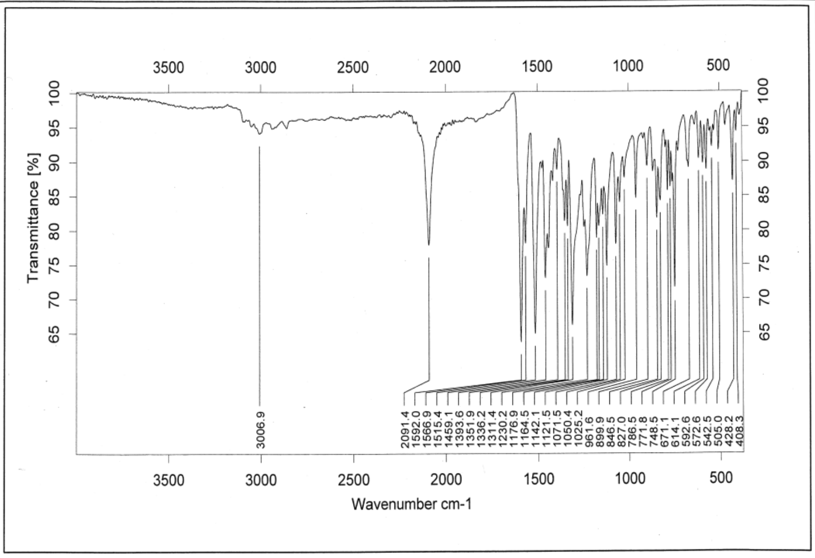
$C_{23}H_{21}BrIN_5$
574.2645 g/mol





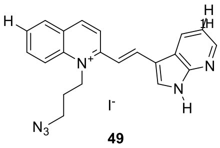

MAT 95, +FAB
moe
3/24/2017 2:19:49 PM
Ch. Schwechheimer
CSC107-1,3-NBA
AK Wagenknecht
csc1071 #31-36 RT: 5.37-5.82 AV: 6 NL: 2.06E6
T: + c EI Full ms [84.50-900.50]
Relative Abundance
m/z


3/24/2017 2:30:49 PM
File recalibrated by CMass.
csc1071-c3 #3 RT: 0.33 AV: 1 NL: 1.00E5
T: + c EI Full ms [84.50-900.50]
446.0973
C23 H21 N5 79Br1 = 446.0975
-0.1992 mmu
Relative Abundance
m/z



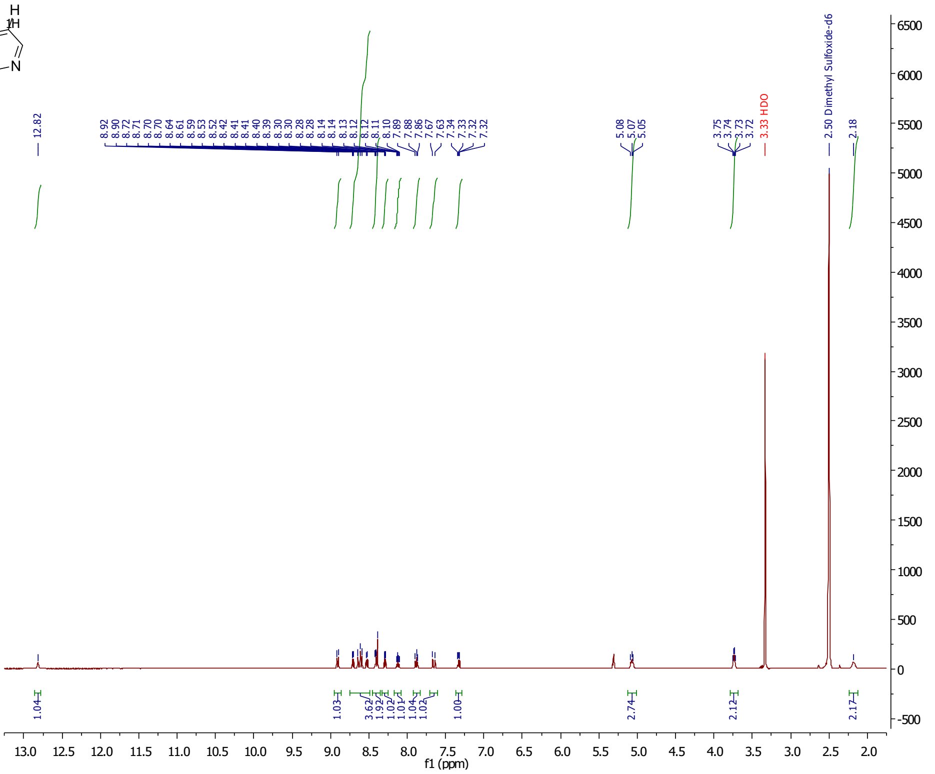
Sample : 107-1		Frequency Range : 3997.41 - 373.828	Measured on : 06/04/2017
Technique : Diamant-ATR	Resolution : 4	Instrument : Alpha	Sample Scans : 24
Operator : Angelika Moesle	Zerofilling : 2	Acquisition : Double Sided,Forward-Backward	

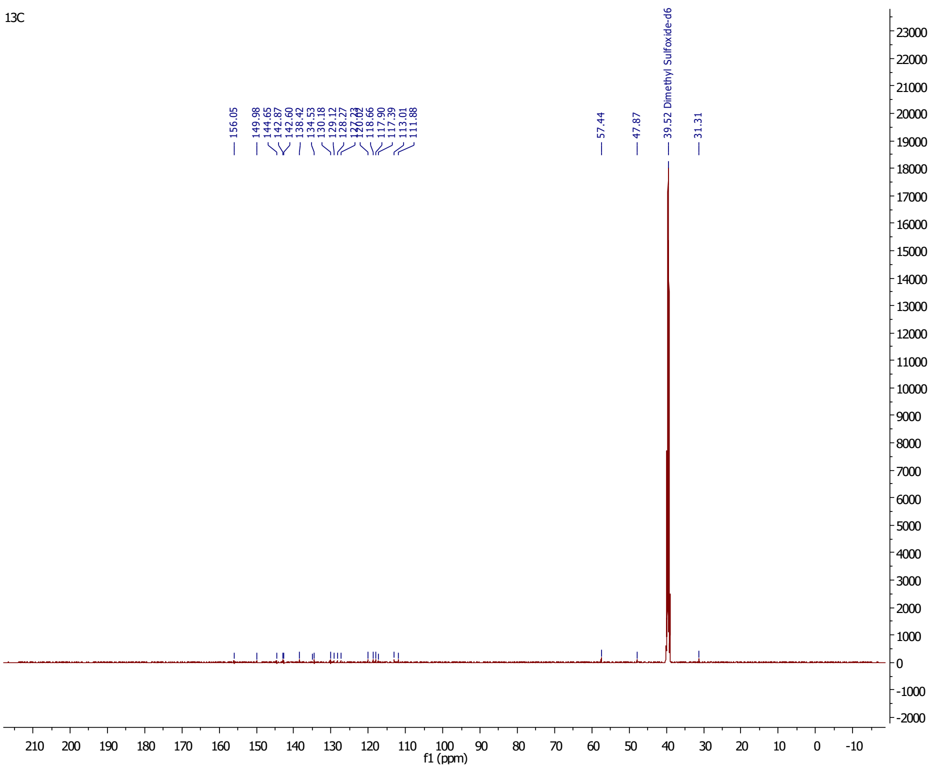
(*E*)-2-(2-(1*H*-pyrrolo[2,3-*b*]pyridin-3-yl)vinyl)-1-(3-azidopropyl)quinolin-1-ium iodide (49):

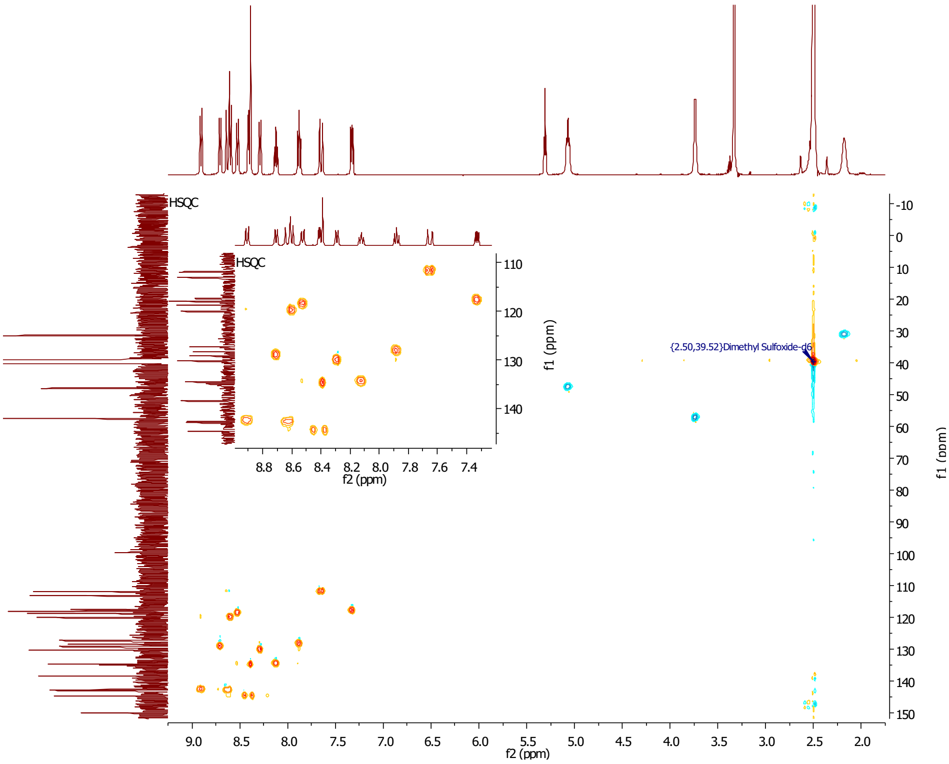


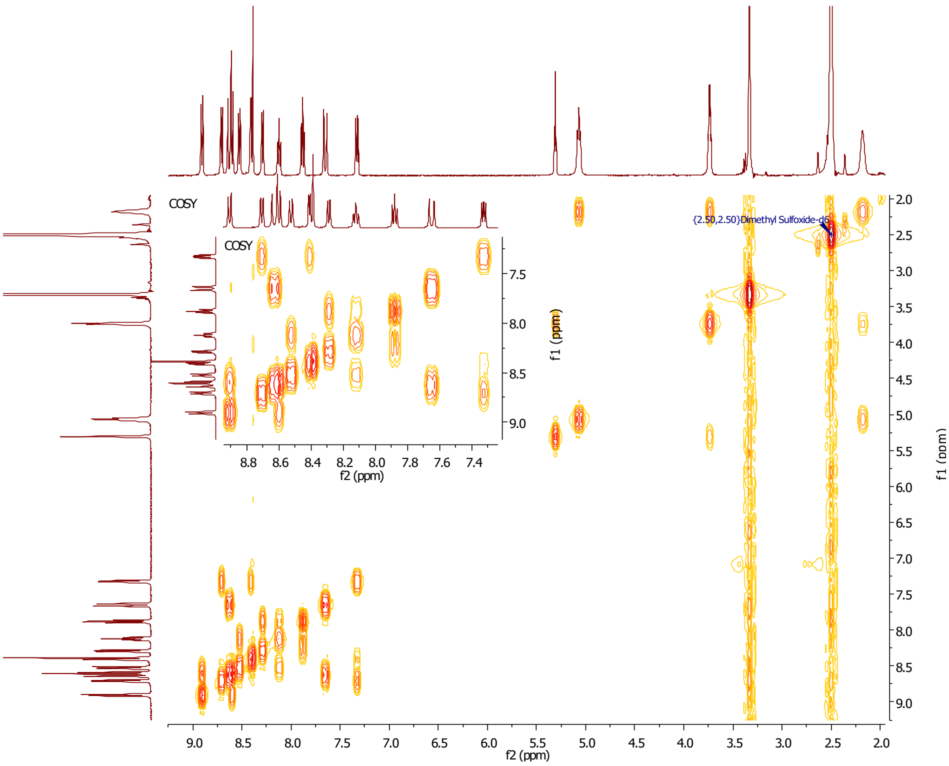
49

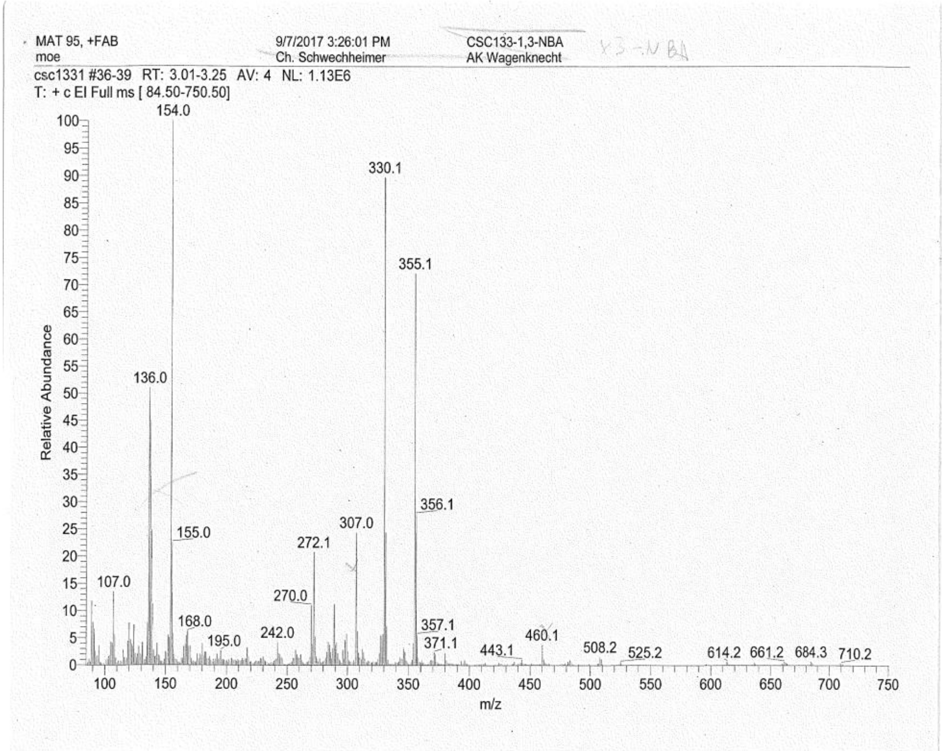
$C_{21}H_{19}IN_6$
482.3295 g/mol

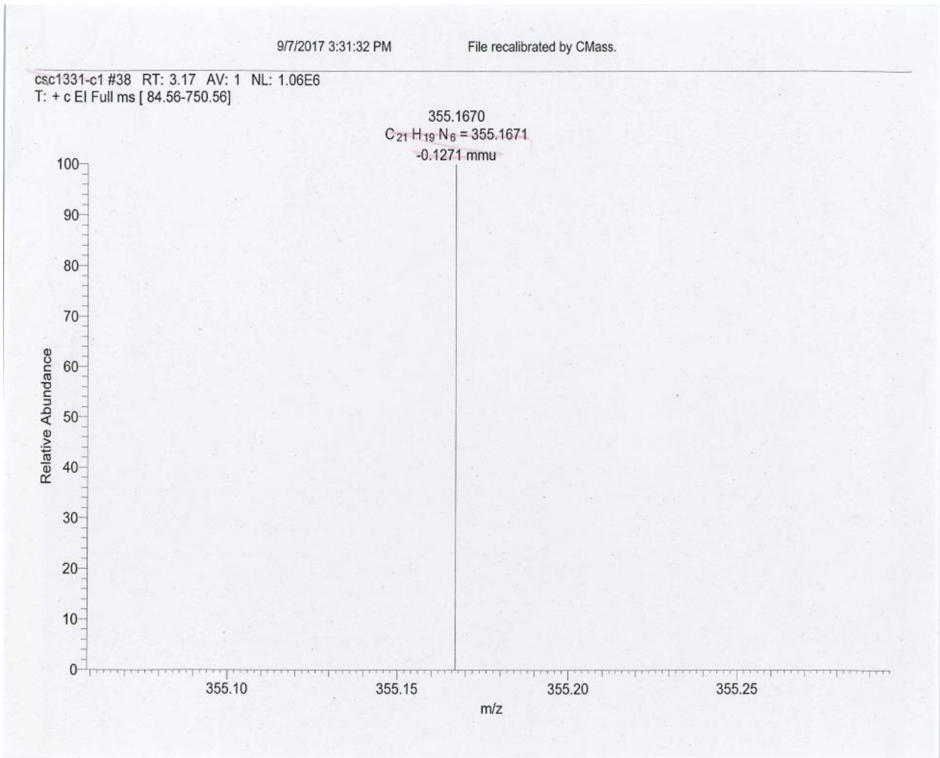


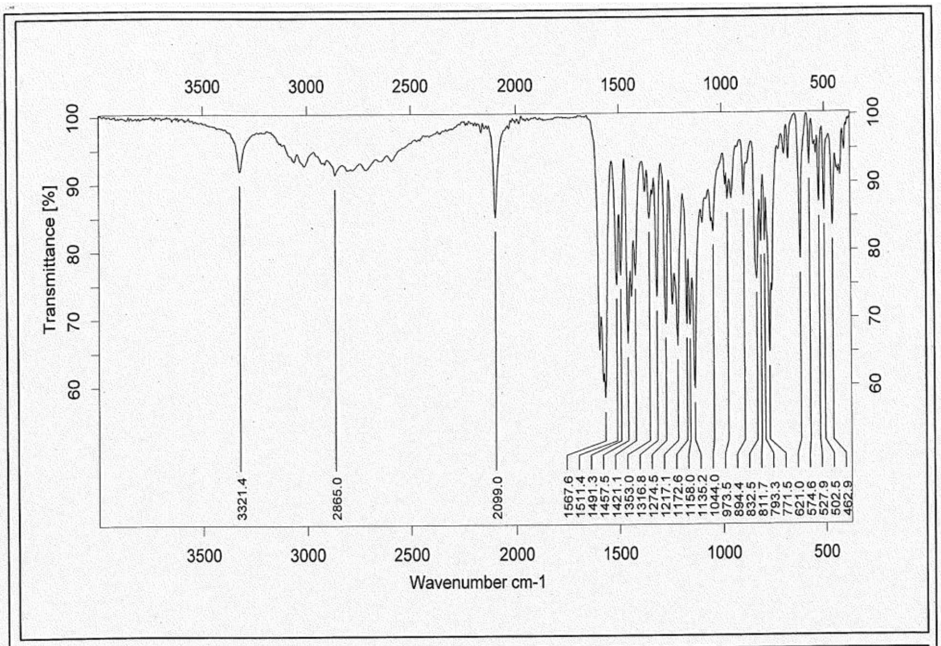



HSQC
(2.50,39.52)Dimethyl Sulfoxide-d6
f2 (ppm)
f1 (ppm)


COSY
(2.50,2.50)Dimethyl Sulfoxide-d6
f2 (ppm)
f1 (ppm)

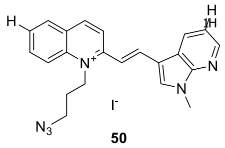

MAT 95, +FAB
moe
9/7/2017 3:26:01 PM
Ch. Schwechheimer
CSC133-1,3-NBA
AK Wagenknecht
csc1331 #36-39 RT: 3.01-3.25 AV: 4 NL: 1.13E6
T: + c EI Full ms [84.50-750.50]
154.0
330.1
355.1
136.0
356.1
307.0
155.0
272.1
107.0
270.0
168.0
357.1
195.0
242.0
460.1
371.1
443.1
508.2
525.2
614.2
661.2
684.3
710.2
Relative Abundance
m/z


9/7/2017 3:31:32 PM
File recalibrated by CMass.
csc1331-c1 #38 RT: 3.17 AV: 1 NL: 1.06E6
T: + c EI Full ms [84.56-750.56]
355.1670
C21 H19 N6 = 355.1671
-0.1271 mmu
Relative Abundance
m/z



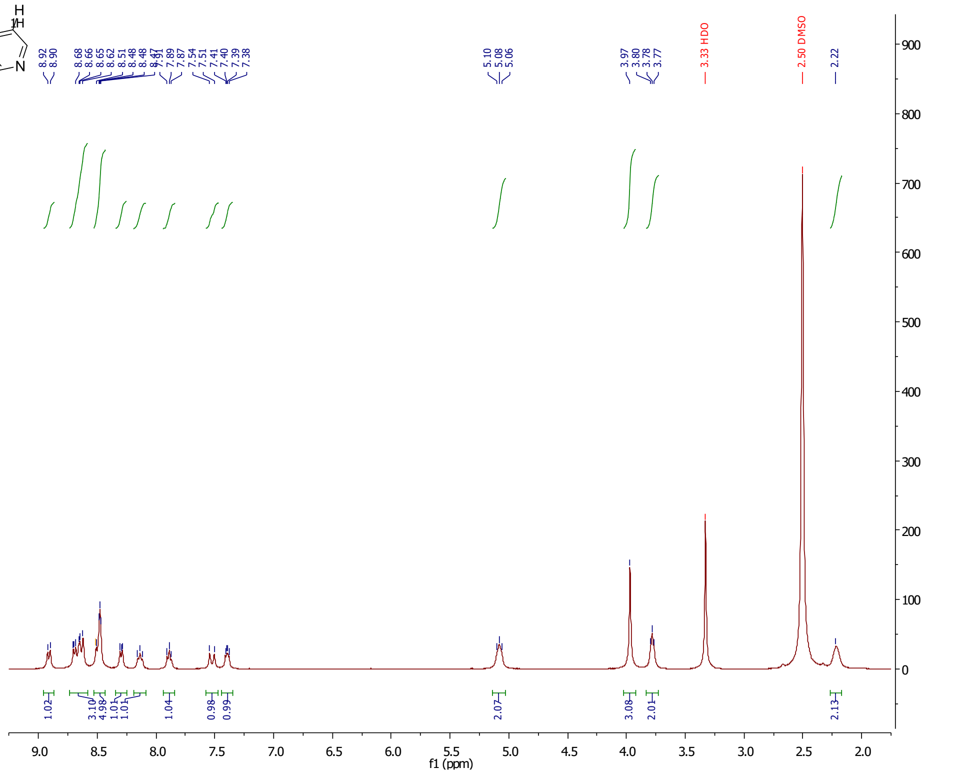
Sample : Ch. Schwechheimer CSC133-1	Frequency Range : 3997.45 - 373.964	Measured on : 07/09/2017	
Technique : Diamant-ATR	Resolution : 4	Instrument : Alpha	Sample Scans : 24
Operator : Angelika Moesle	Zerofilling : 2	Acquisition : Double Sided,Forward-Backward	

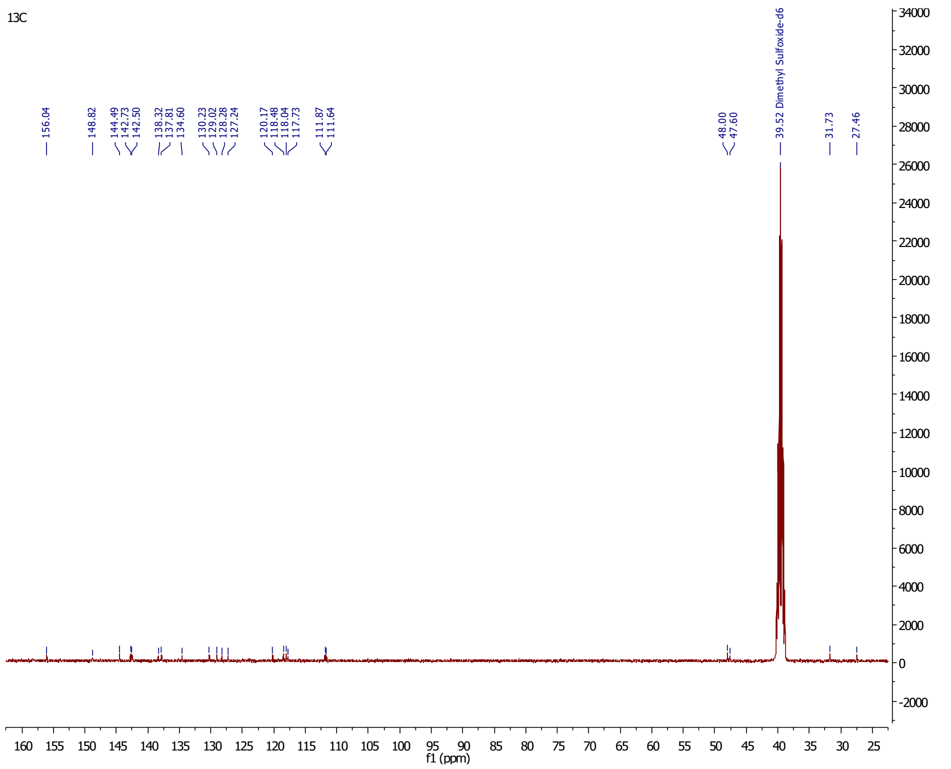
(*E*)-1-(3-azidopropyl)-2-(2-(1-methyl-1*H*-pyrrolo[2,3-*b*]pyridin-3-yl)vinyl)quinolin-1-ium iodide (50):

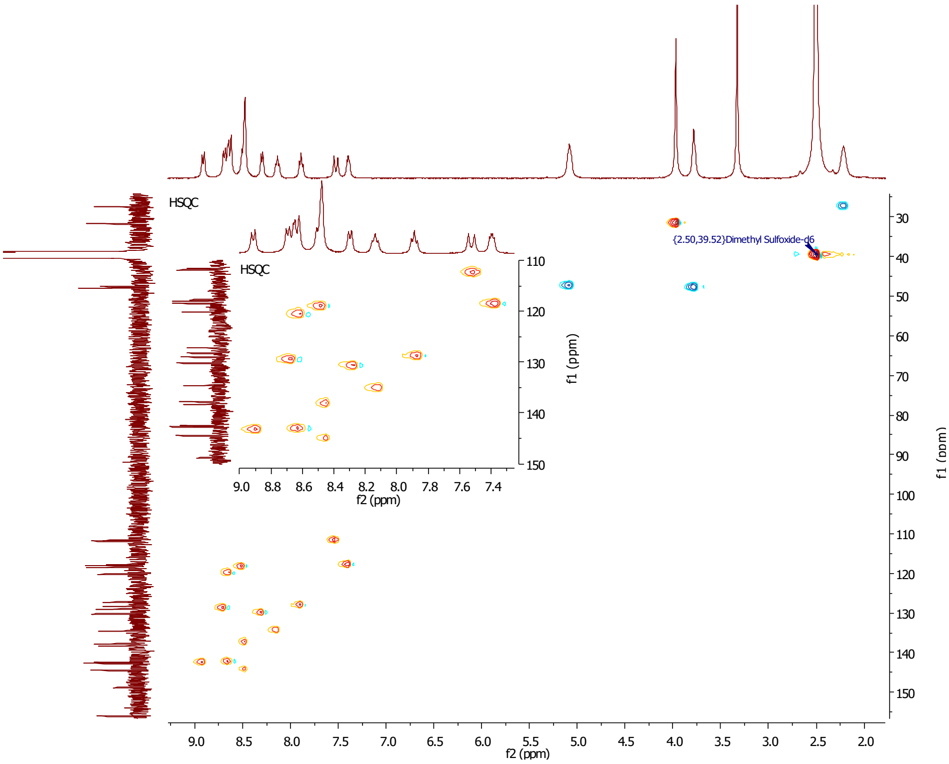


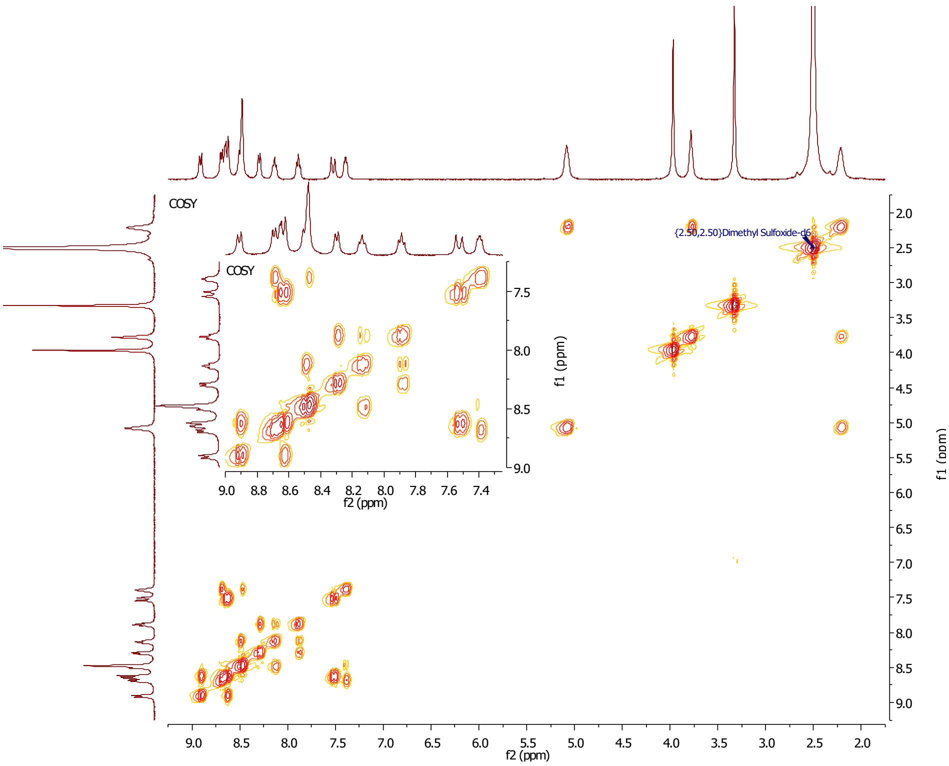
50

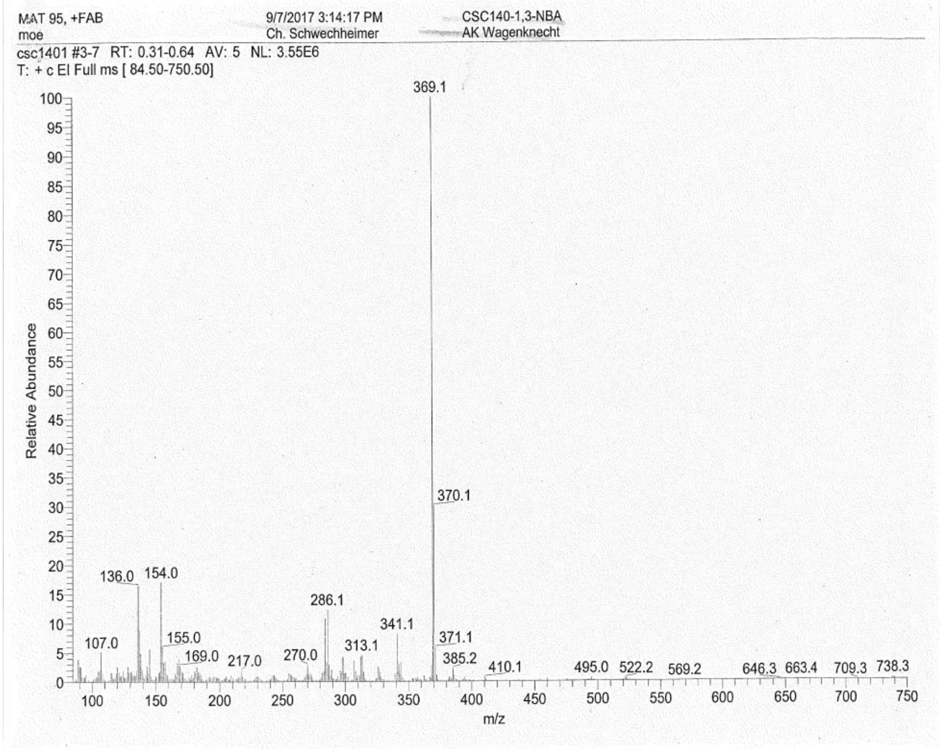
$C_{22}H_{21}IN_6$
496.3565 g/mol

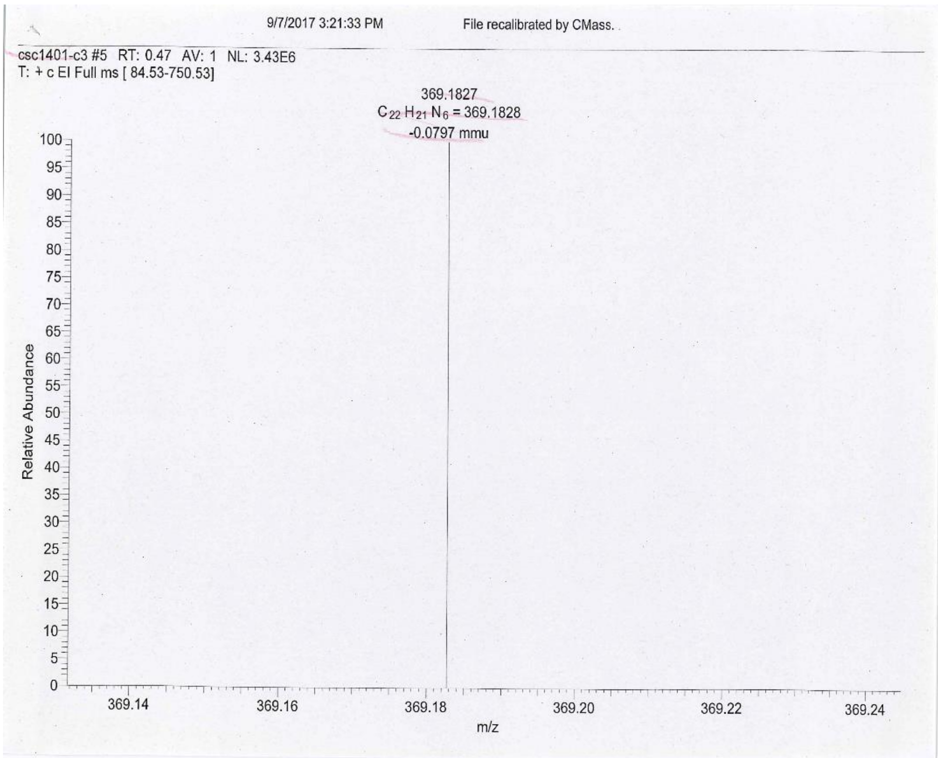


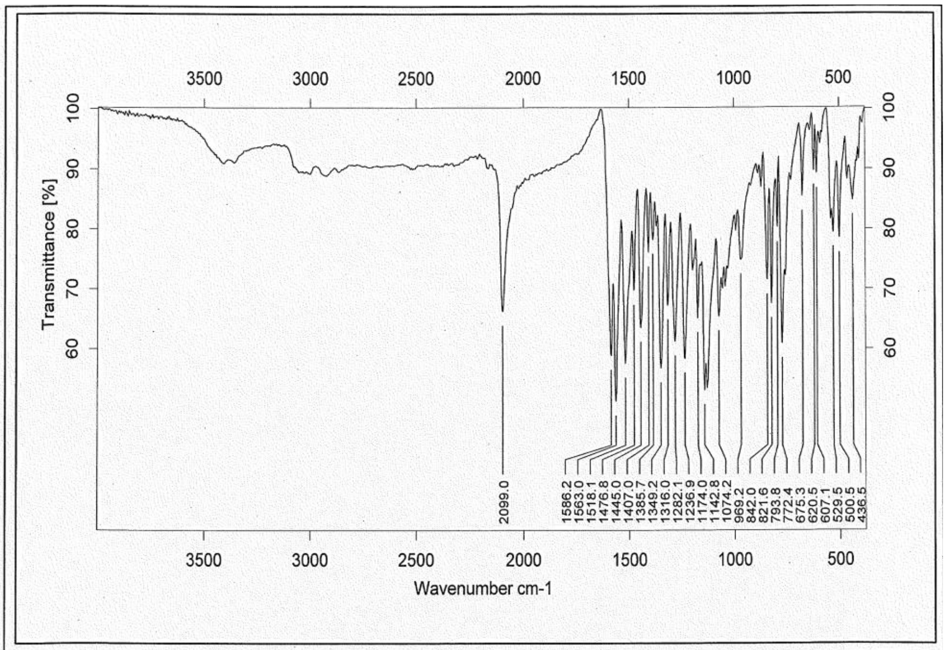



HSQC
{2.50,39.52}Dimethyl Sulfoxide-d6
f2 (ppm)
f1 (ppm)


COSY
{2.50,2.50}Dimethyl Sulfoxide-d6
f2 (ppm)
f1 (ppm)

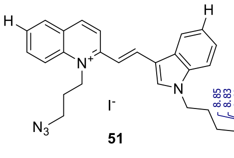

MAT 95, +FAB
moe
9/7/2017 3:14:17 PM
Ch. Schwechheimer
CSC140-1,3-NBA
AK Wagenknecht
csc1401 #3-7 RT: 0.31-0.64 AV: 5 NL: 3.55E6
T: + c EI Full ms [84.50-750.50]
Relative Abundance
m/z
369.1
370.1
136.0
154.0
286.1
341.1
107.0
155.0
169.0
217.0
270.0
313.1
371.1
385.2
410.1
495.0
522.2
569.2
646.3
663.4
709.3
738.3


9/7/2017 3:21:33 PM
File recalibrated by CMass.
csc1401-c3 #5 RT: 0.47 AV: 1 NL: 3.43E6
T: + c EI Full ms [84.53-750.53]
369.1827
$C_{22}H_{21}N_6$ = 369.1828
-0.0797 mmu
Relative Abundance
m/z



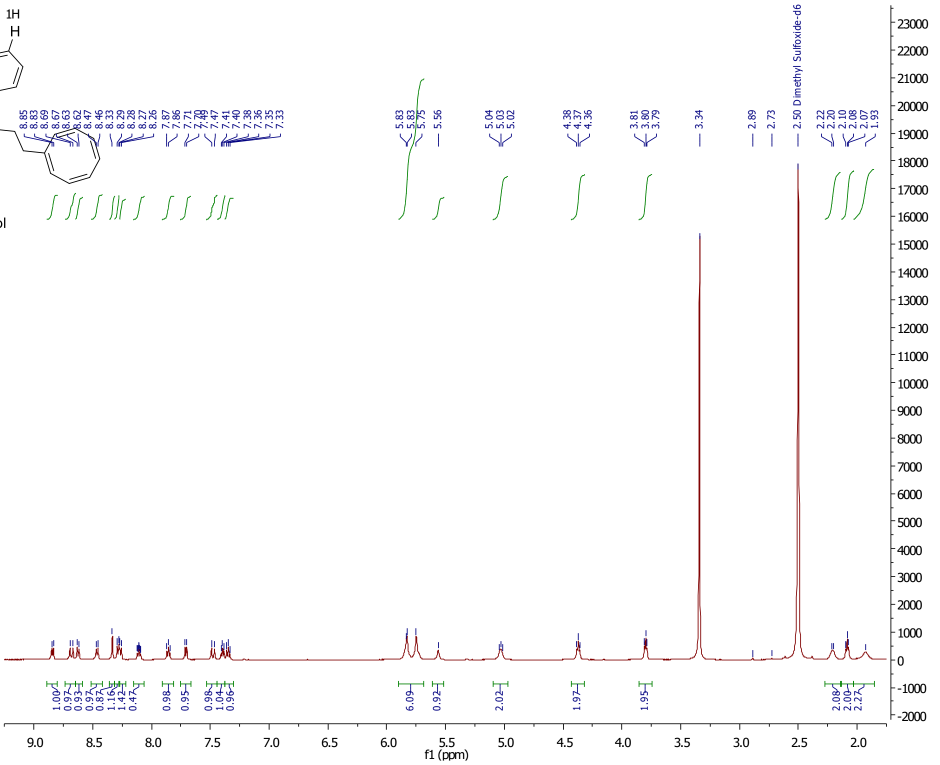
Sample : Ch. Schwechheimer CSC140-1	Frequency Range : 3997.45 - 373.964		Measured on : 07/09/2017
Technique : Diamant-ATR	Resolution : 4	Instrument : Alpha	Sample Scans : 24
Operator : Angelika Moesle	Zerofilling : 2	Acquisition : Double Sided,Forward-Backward	

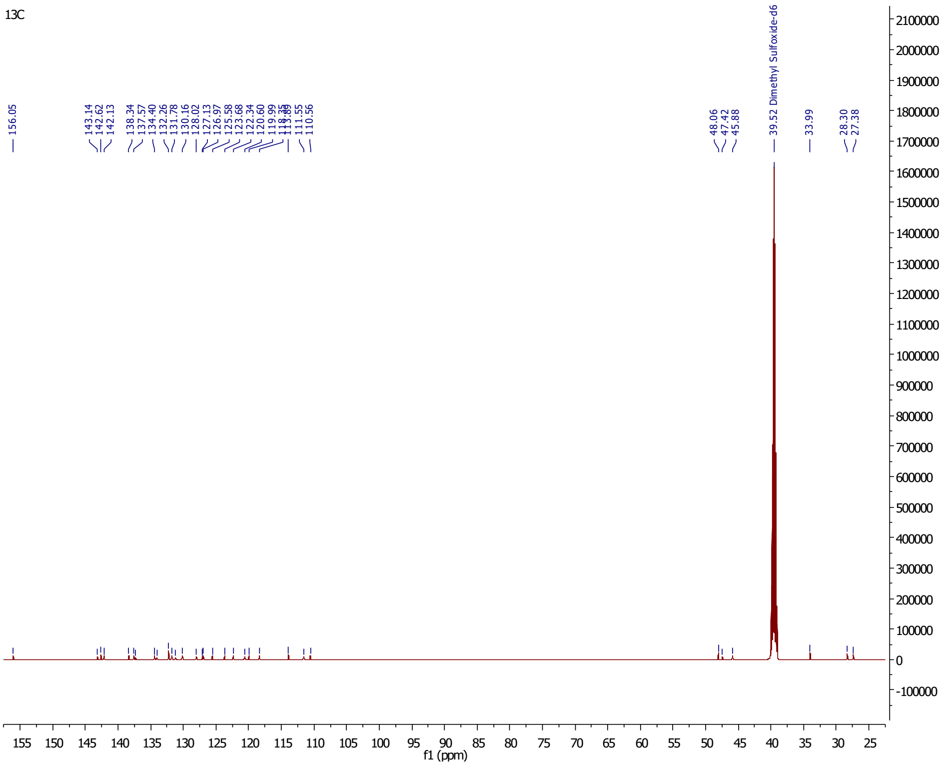
1-(3-azidopropyl)-2-((*E*)-2-(1-(3-((1*Z*,3*Z*,5*Z*,7*Z*)-cycloocta-1,3,5,7-tetraen-1-yl)propyl)-1*H*-indol-3-yl)vinyl)quinolin-1-ium iodide (51):

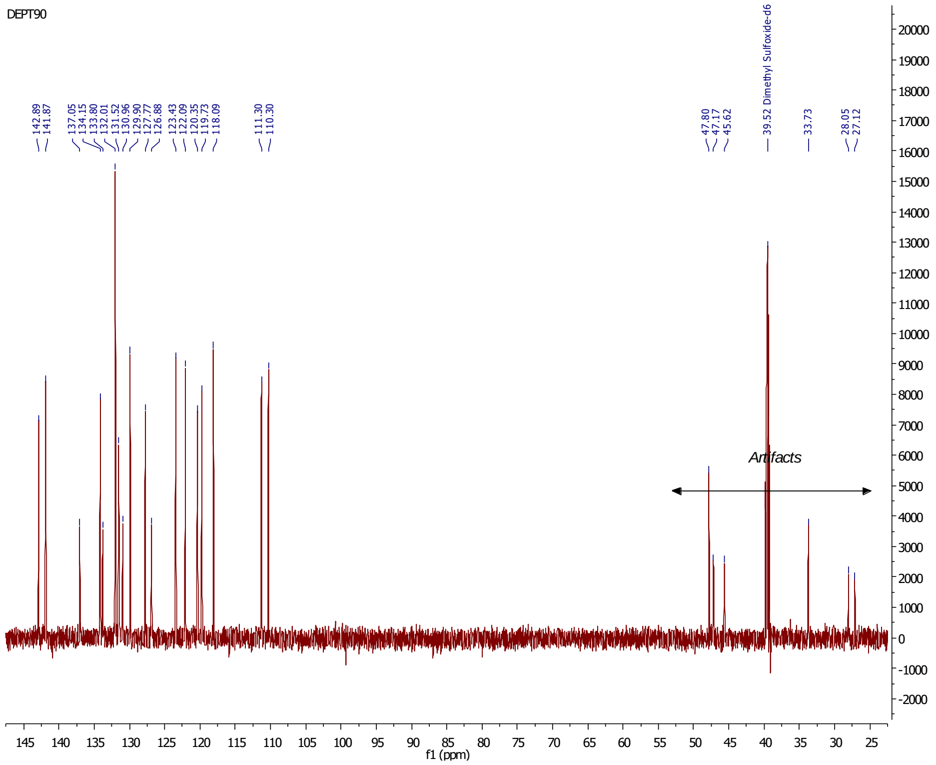


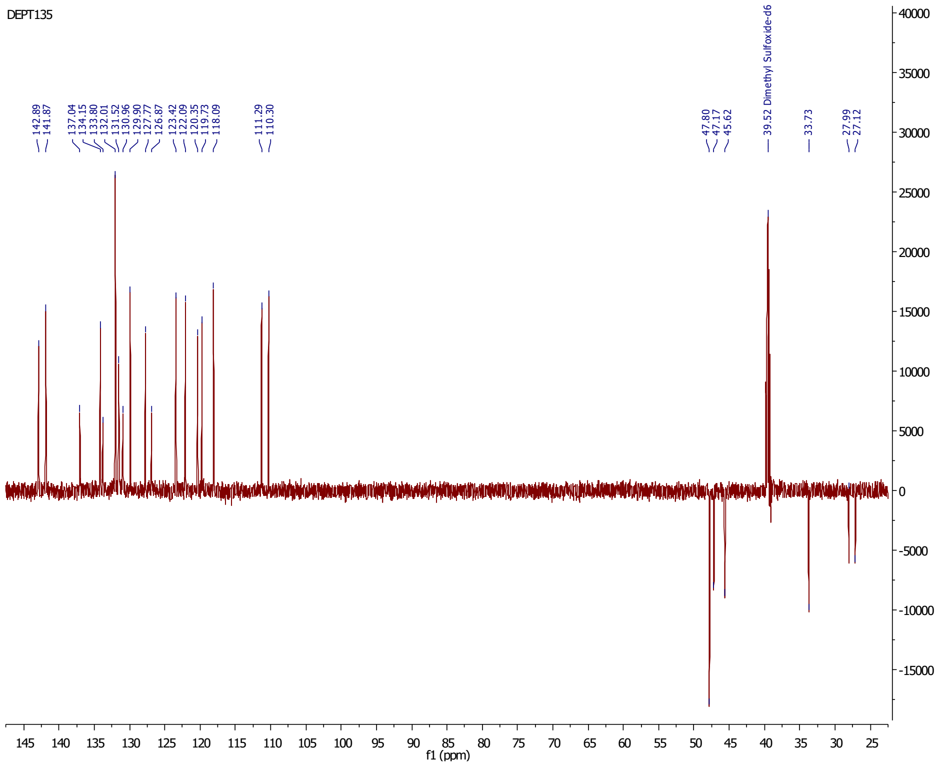
51

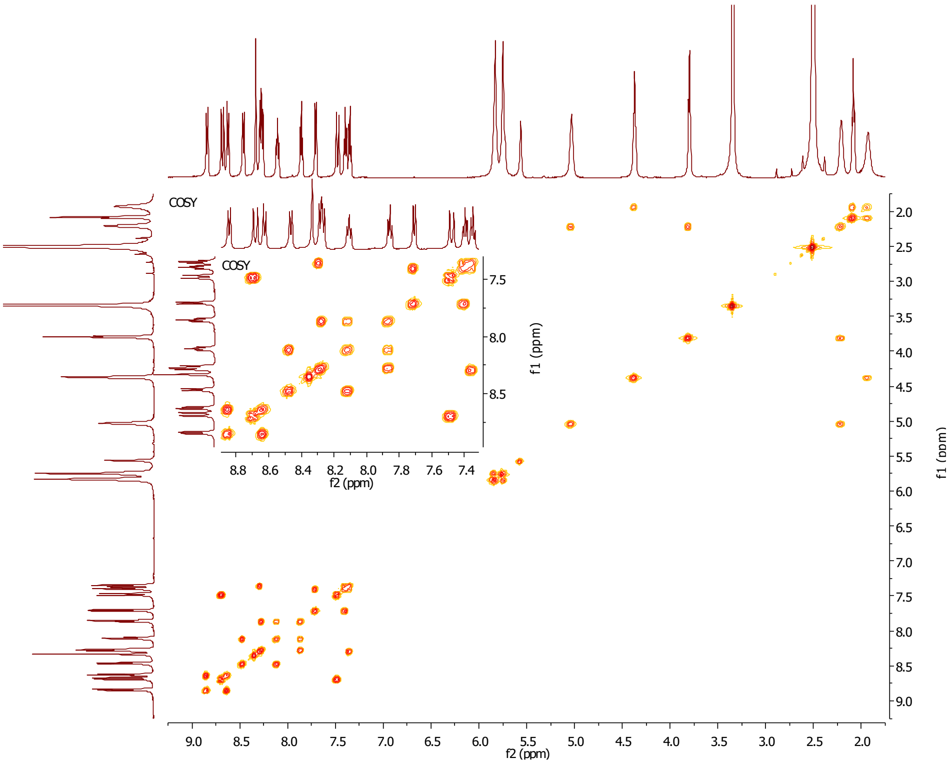
$C_{33}H_{32}IN_5$
625.5585 g/mol

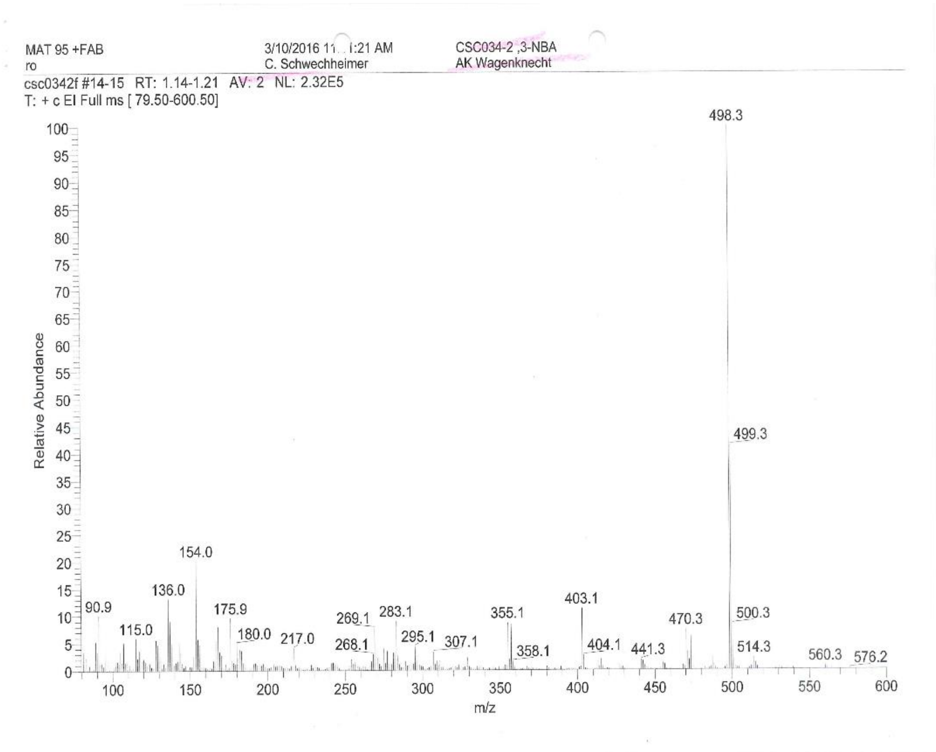


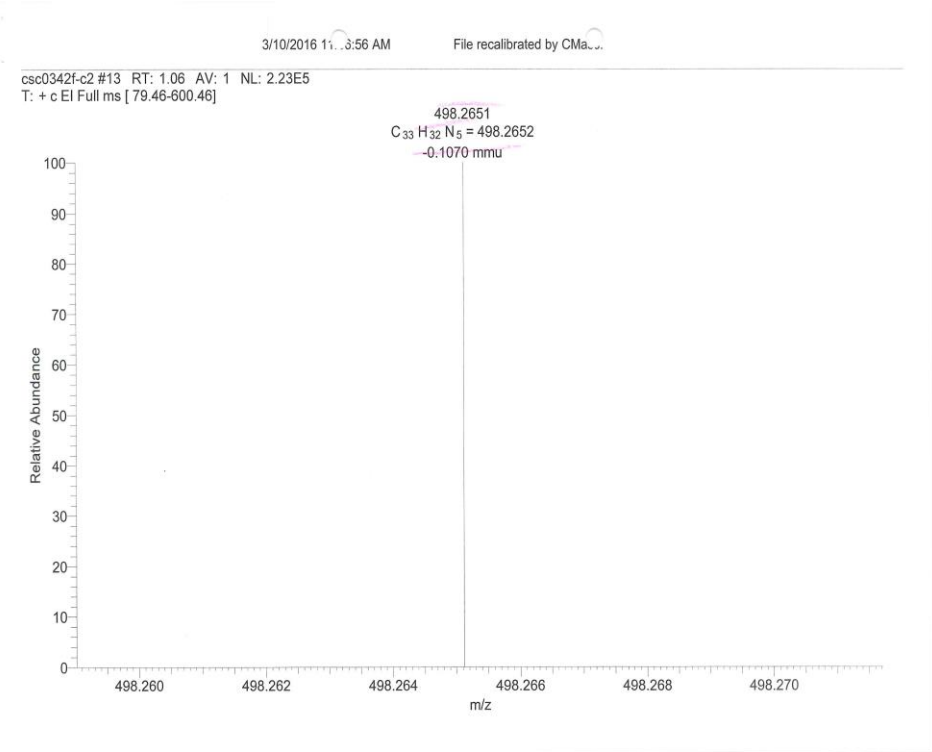


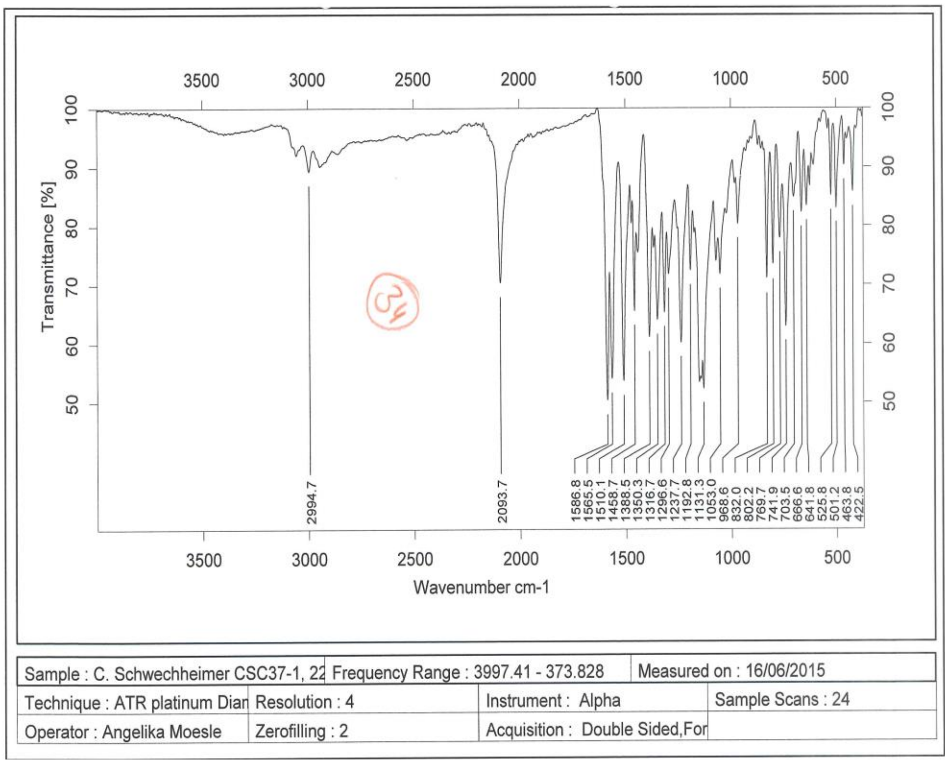

DEPT90
142.89
141.87
137.05
134.15
133.80
132.01
131.52
130.96
129.90
127.77
126.88
123.43
122.09
120.35
119.73
118.09
111.30
110.30
47.80
47.17
45.62
39.52 Dimethyl Sulfoxide-d6
33.73
28.05
27.12
Artifacts
f1 (ppm)


DEPT135
142.89
141.87
137.04
134.15
133.80
132.01
131.52
130.96
129.90
127.77
126.87
123.42
122.09
120.35
119.73
118.09
111.29
110.30
47.80
47.17
45.62
39.52 Dimethyl Sulfoxide-d6
33.73
27.99
27.12
f1 (ppm)

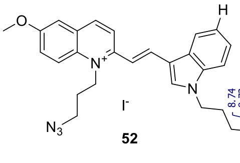

COSY
f2 (ppm)
f1 (ppm)


MAT 95 +FAB
ro
C. Schwechheimer
CSC034-2 ,3-NBA
AK Wagenknecht
csc0342f #14-15 RT: 1.14-1.21 AV: 2 NL: 2.32E5
T: + c EI Full ms [79.50-600.50]
Relative Abundance
m/z
498.3
499.3
154.0
136.0
90.9
115.0
175.9
180.0
217.0
269.1
268.1
283.1
295.1
307.1
355.1
358.1
403.1
404.1
441.3
470.3
500.3
514.3
560.3
576.2


3/10/2016 11..3:56 AM
File recalibrated by CMa...
csc0342f-c2 #13 RT: 1.06 AV: 1 NL: 2.23E5
T: + c EI Full ms [79.46-600.46]
498.2651
$C_{33}H_{32}N_5$ = 498.2652
-0.1070 mmu
Relative Abundance
m/z
498.260
498.262
498.264
498.266
498.268
498.270

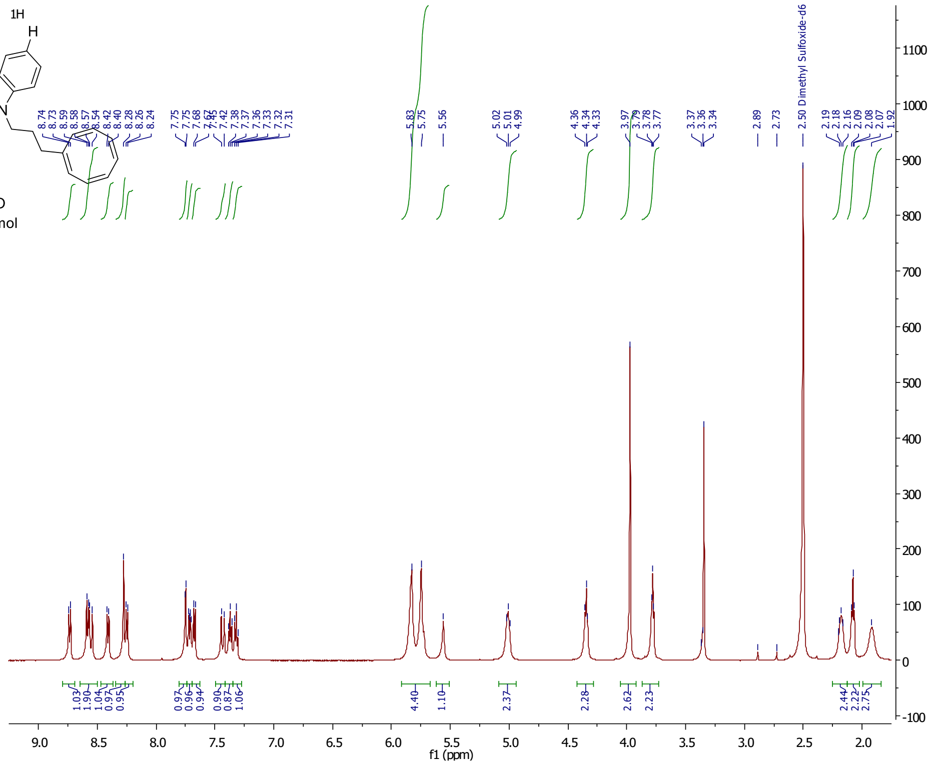

Transmittance [%]
Wavenumber cm-1
2994.7
2093.7
1586.8
1565.5
1510.1
1458.7
1388.5
1350.3
1316.7
1296.6
1237.7
1192.8
1131.3
1053.0
968.6
832.0
802.2
769.7
741.9
703.5
666.6
641.8
525.8
501.2
463.8
422.5
34
Sample : C. Schwechheimer CSC37-1, 22
Frequency Range : 3997.41 - 373.828
Measured on : 16/06/2015
Technique : ATR platinum Dian
Resolution : 4
Instrument : Alpha
Sample Scans : 24
Operator : Angelika Moesle
Zerofilling : 2
Acquisition : Double Sided,For

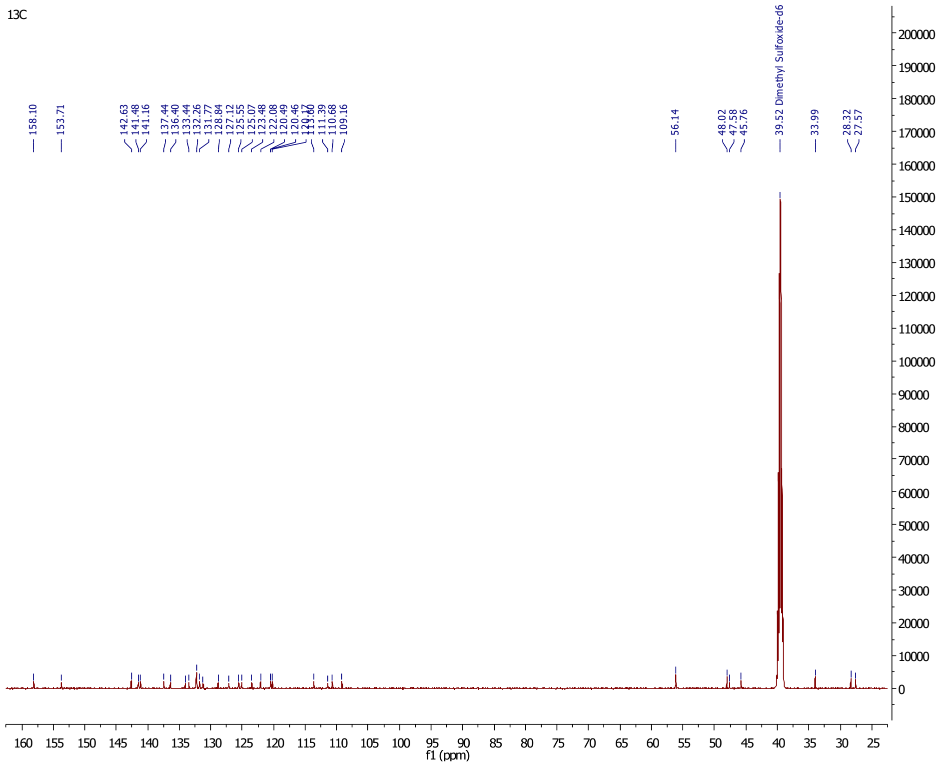
1-(3-azidopropyl)-2-((*E*)-2-(1-(3-((1*Z*,3*Z*,5*Z*,7*Z*)-cycloocta-1,3,5,7-tetraen-1-yl)propyl)-1*H*-indol-3-yl)vinyl)-6-methoxyquinolin-1-ium iodide (52):

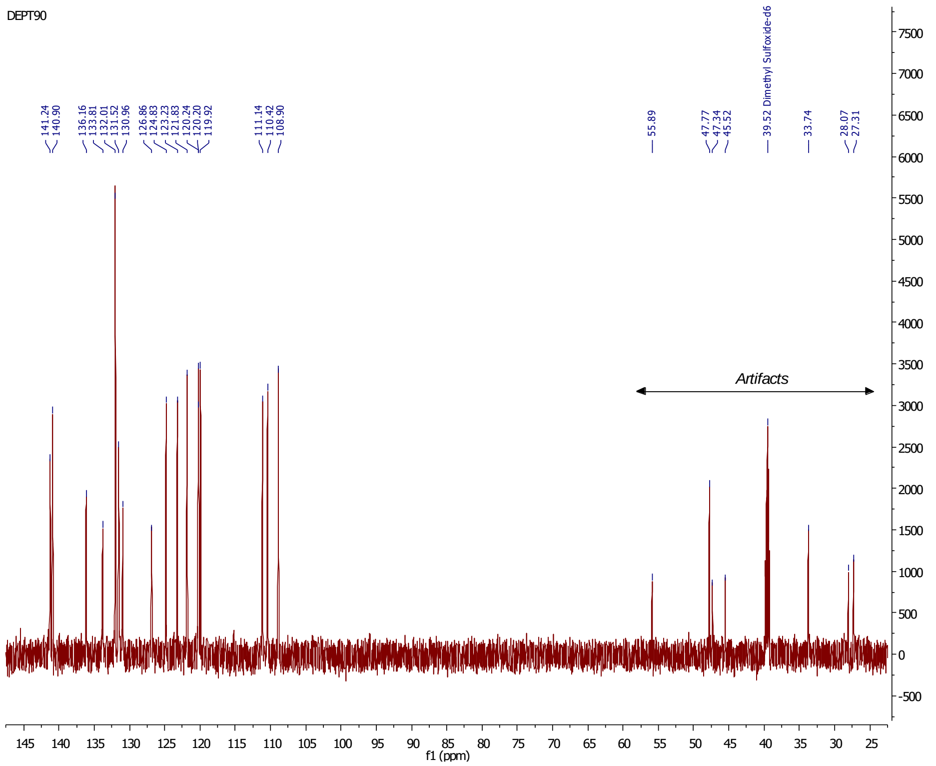


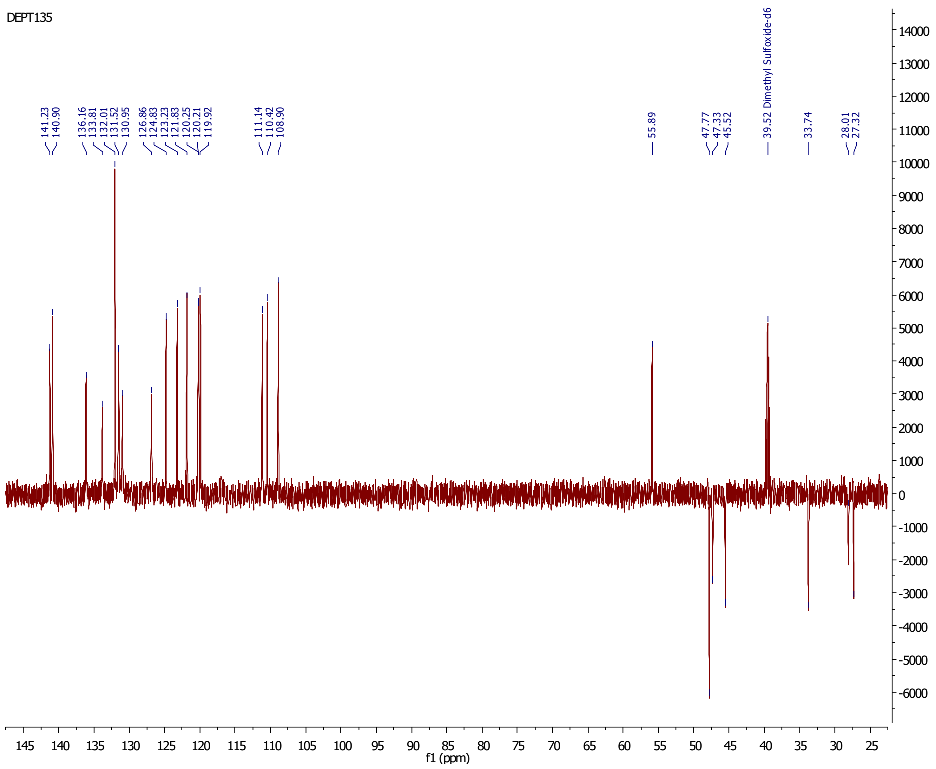
52

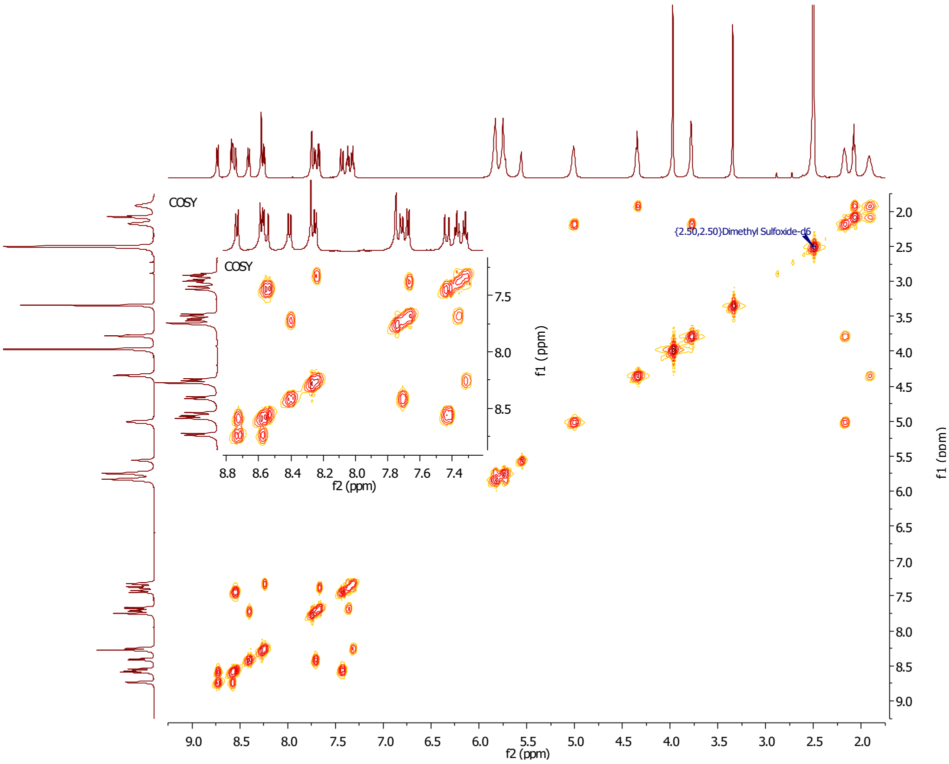
$C_{34}H_{34}IN_5O$
655.5845 g/mol

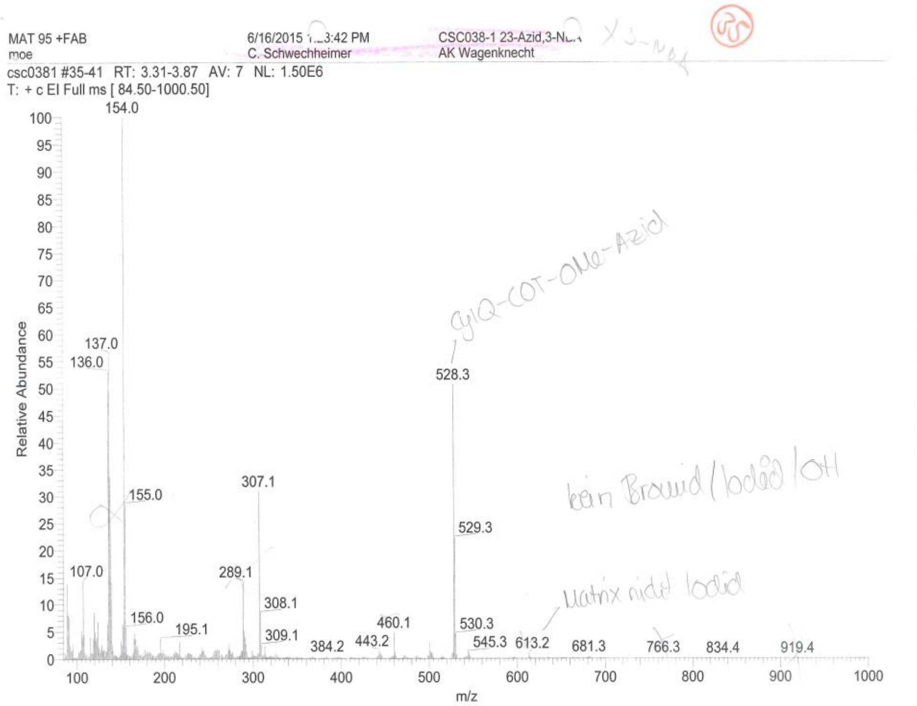


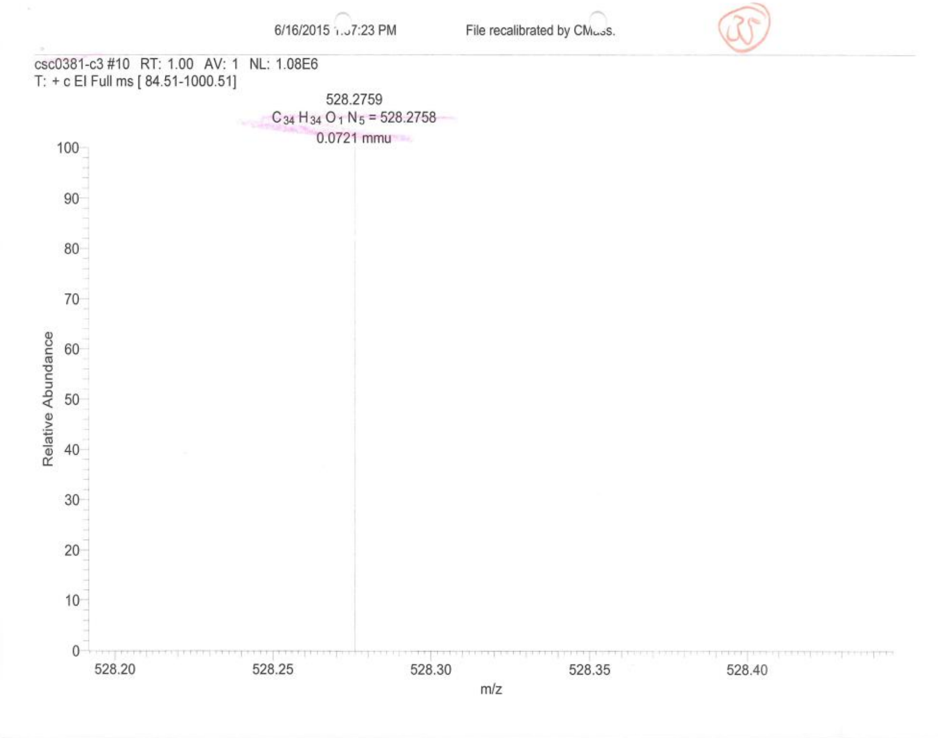


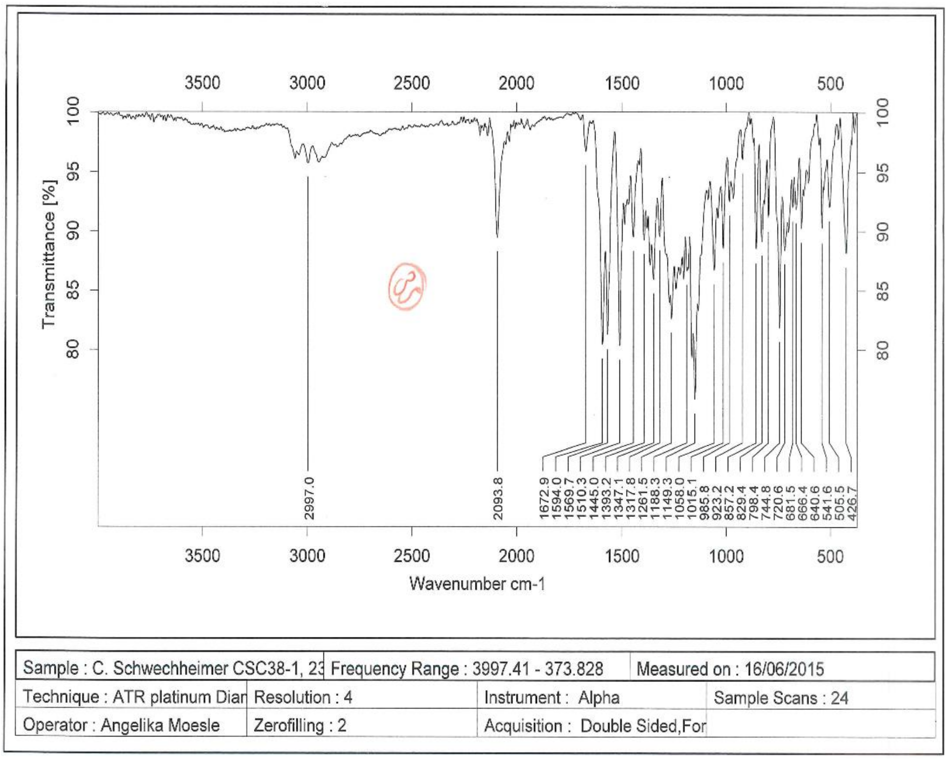

DEPT90
Artifacts
39.52 Dimethyl Sulfoxide-d6
f1 (ppm)


DEPT135
39.52 Dimethyl Sulfoxide-d6
f1 (ppm)


COSY
COSY
{2.50,2.50}Dimethyl Sulfoxide-d6
f1 (ppm)
f2 (ppm)
f1 (ppm)
f2 (ppm)

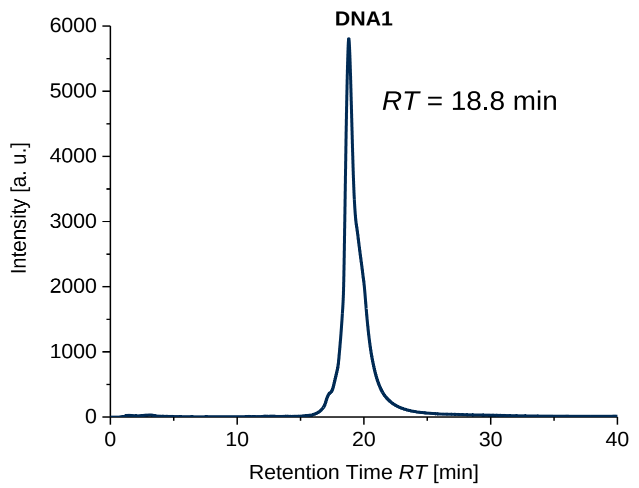

MAT 95 +FAB
moe
C. Schwechheimer
AK Wagenknecht
csc0381 #35-41 RT: 3.31-3.87 AV: 7 NL: 1.50E6
T: + c EI Full ms [84.50-1000.50]
Relative Abundance
m/z
154.0
137.0
136.0
155.0
107.0
156.0
195.1
289.1
307.1
308.1
309.1
384.2
443.2
460.1
528.3
529.3
530.3
545.3
613.2
681.3
766.3
834.4
919.4
Matrix nicht locker
kein Bromid / Iodid / OH

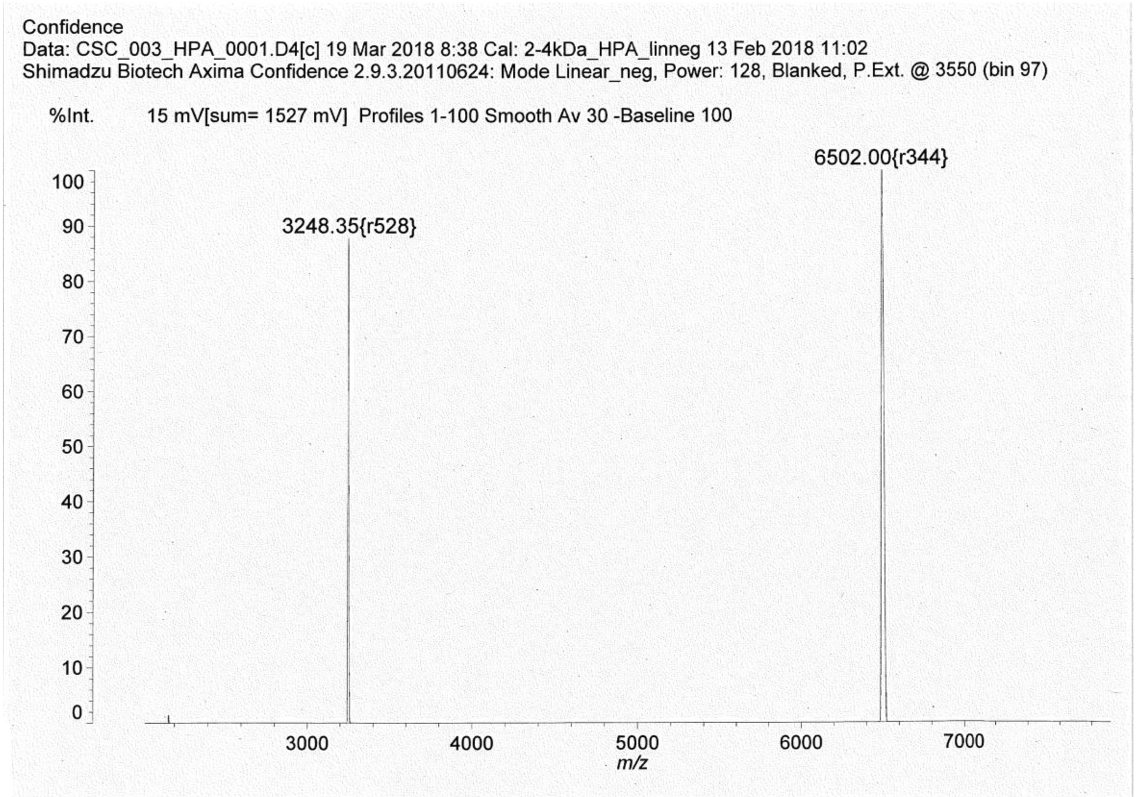

6/16/2015 1:57:23 PM
File recalibrated by CMass.
csc0381-c3 #10 RT: 1.00 AV: 1 NL: 1.08E6
T: + c EI Full ms [84.51-1000.51]
528.2759
C34 H34 O1 N5 = 528.2758
0.0721 mmu
Relative Abundance
m/z


Transmittance [%]
Wavenumber cm-1
2997.0
2093.8
Sample : C. Schwechheimer CSC38-1, 23
Frequency Range : 3997.41 - 373.828
Measured on : 16/06/2015
Technique : ATR platinum Diar
Resolution : 4
Instrument : Alpha
Sample Scans : 24
Operator : Angelika Moesle
Zerofilling : 2
Acquisition : Double Sided,For

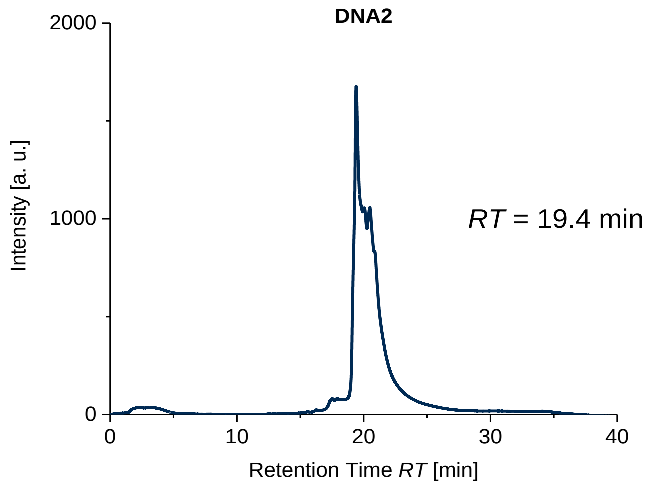
f. Analytics of the DNA-Dye Bioconjugates DNA1-DNA12

DNA1:

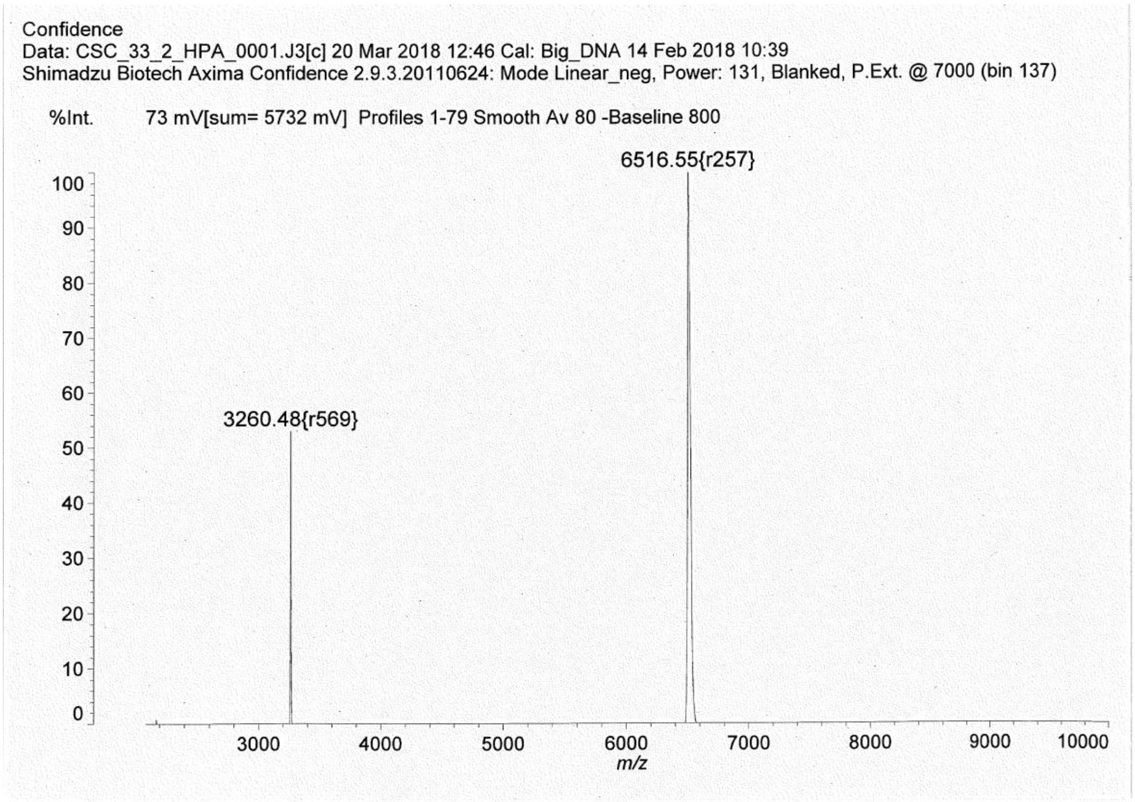




DNA2:

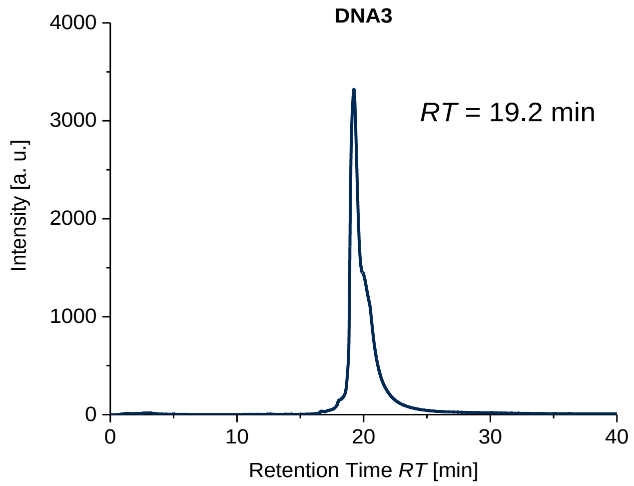


DNA2
2000
1000
0
Intensity [a. u.]
RT = 19.4 min
0
10
20
30
40
Retention Time RT [min]

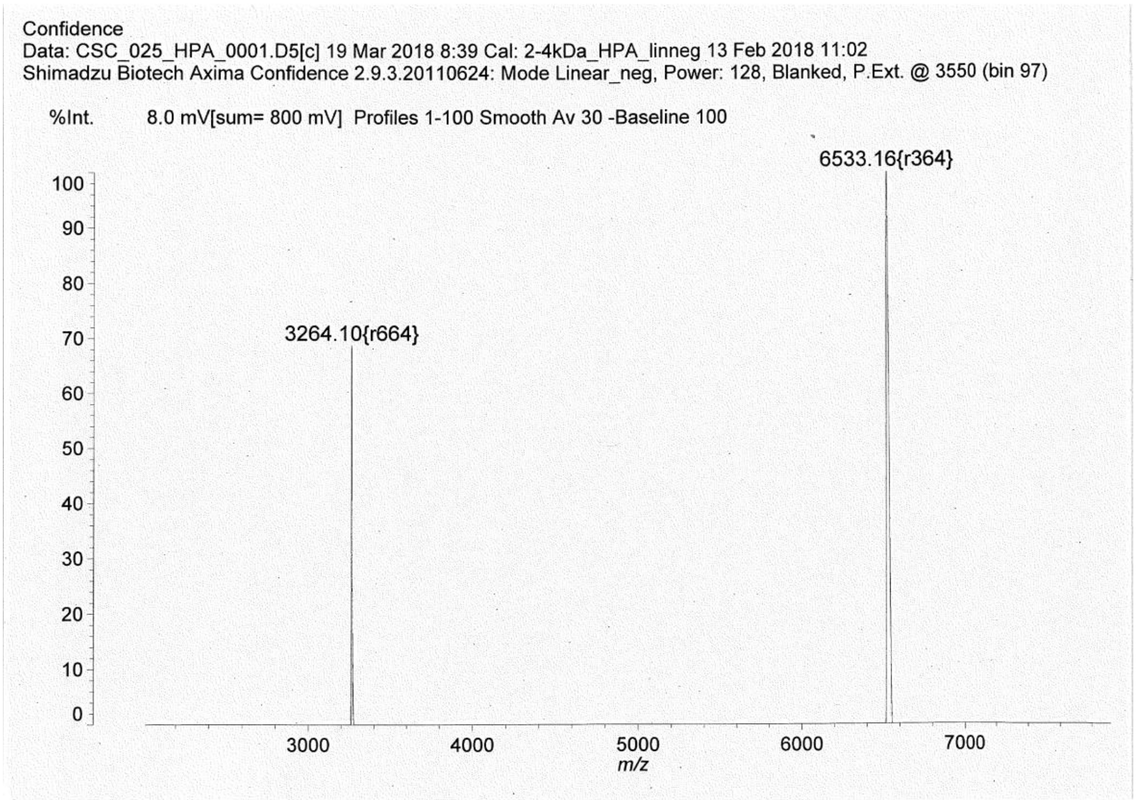


Confidence
Data: CSC_33_2_HPA_0001.J3[c] 20 Mar 2018 12:46 Cal: Big_DNA 14 Feb 2018 10:39
Shimadzu Biotech Axima Confidence 2.9.3.20110624: Mode Linear_neg, Power: 131, Blanked, P.Ext. @ 7000 (bin 137)
%Int.
73 mV[sum= 5732 mV] Profiles 1-79 Smooth Av 80 -Baseline 800
6516.55{r257}
3260.48{r569}
100
90
80
70
60
50
40
30
20
10
0
3000
4000
5000
6000
7000
8000
9000
10000
m/z

DNA3:

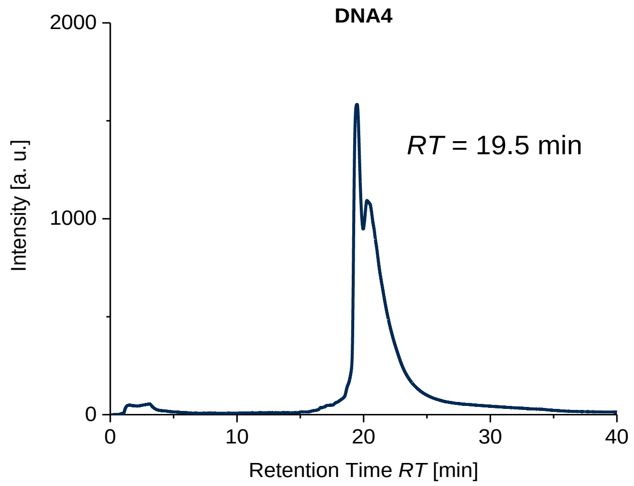


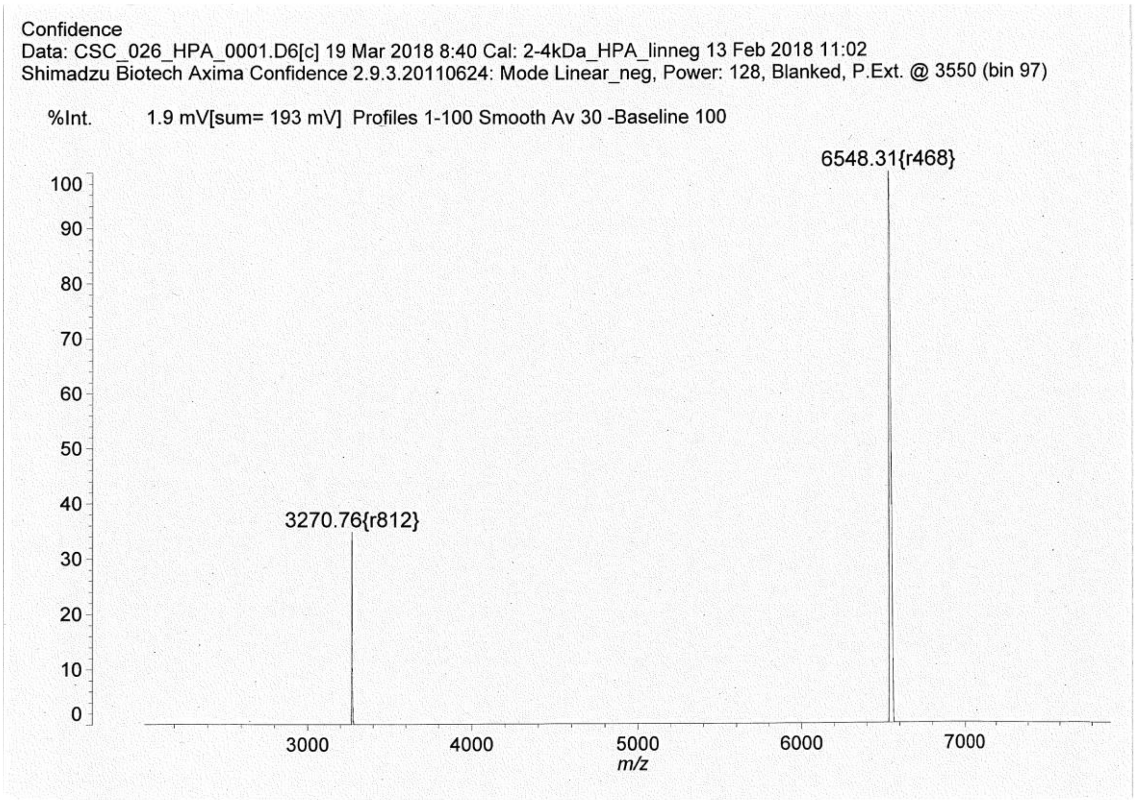
DNA3
RT = 19.2 min
Intensity [a. u.]
4000
3000
2000
1000
0
0
10
20
30
40
Retention Time RT [min]



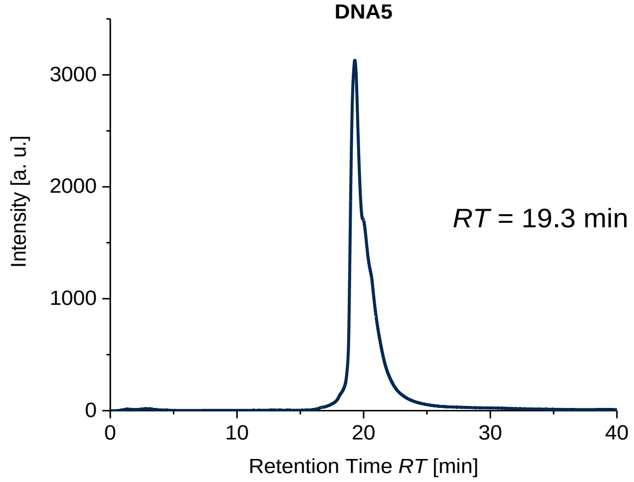
Confidence
Data: CSC_025_HPA_0001.D5[c] 19 Mar 2018 8:39 Cal: 2-4kDa_HPA_linneg 13 Feb 2018 11:02
Shimadzu Biotech Axima Confidence 2.9.3.20110624: Mode Linear_neg, Power: 128, Blanked, P.Ext. @ 3550 (bin 97)
%Int.
8.0 mV[sum= 800 mV] Profiles 1-100 Smooth Av 30 -Baseline 100
6533.16{r364}
3264.10{r664}
100
90
80
70
60
50
40
30
20
10
0
3000
4000
5000
6000
7000
m/z

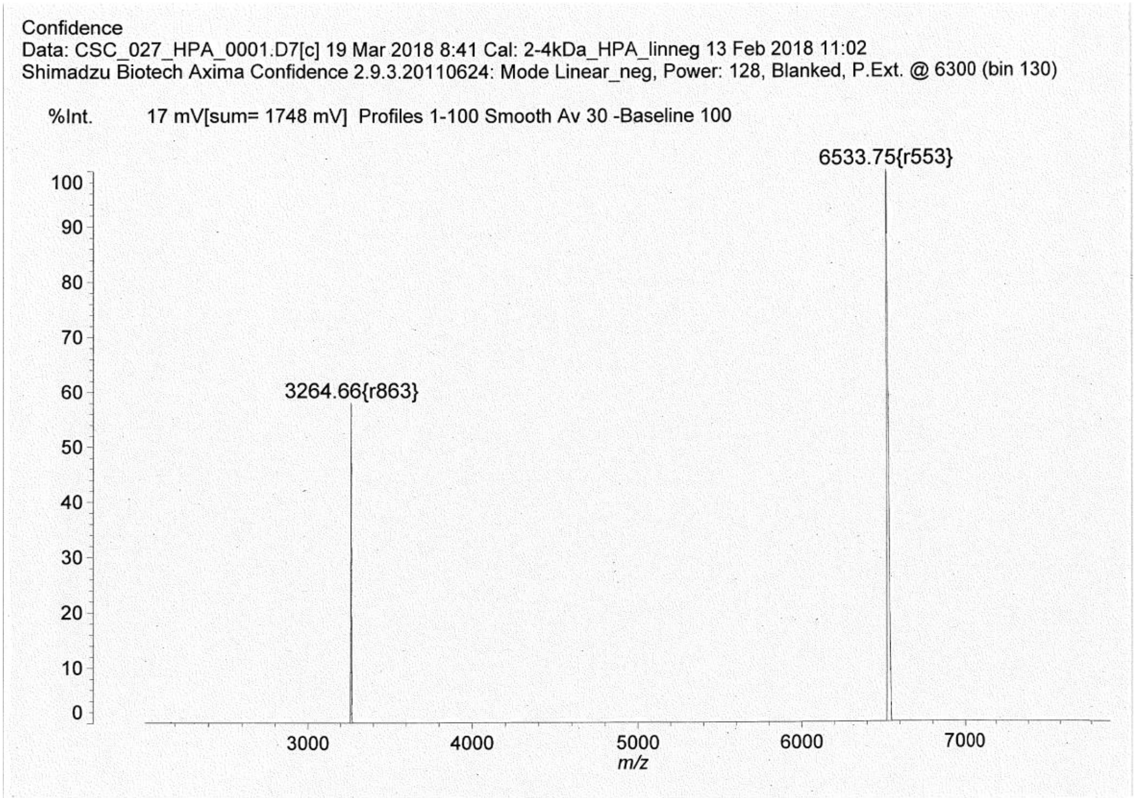
DNA4:


DNA4
RT = 19.5 min
Intensity [a. u.]
2000
1000
0
0
10
20
30
40
Retention Time RT [min]

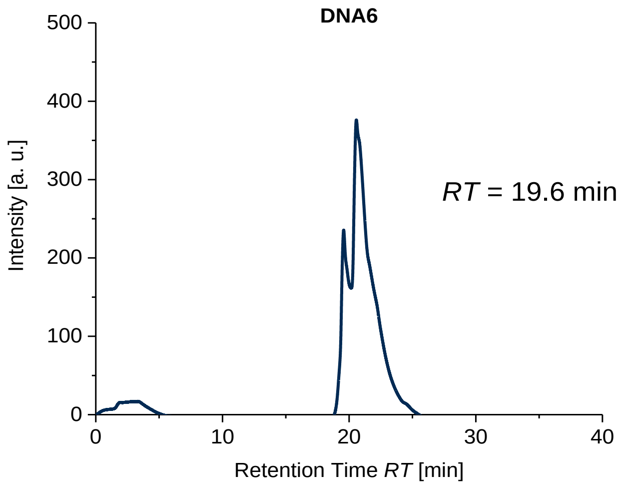

Confidence
Data: CSC_026_HPA_0001.D6[c] 19 Mar 2018 8:40 Cal: 2-4kDa_HPA_linneg 13 Feb 2018 11:02
Shimadzu Biotech Axima Confidence 2.9.3.20110624: Mode Linear_neg, Power: 128, Blanked, P.Ext. @ 3550 (bin 97)
%Int.
1.9 mV[sum= 193 mV] Profiles 1-100 Smooth Av 30 -Baseline 100
6548.31{r468}
3270.76{r812}
100
90
80
70
60
50
40
30
20
10
0
3000
4000
5000
6000
7000
m/z

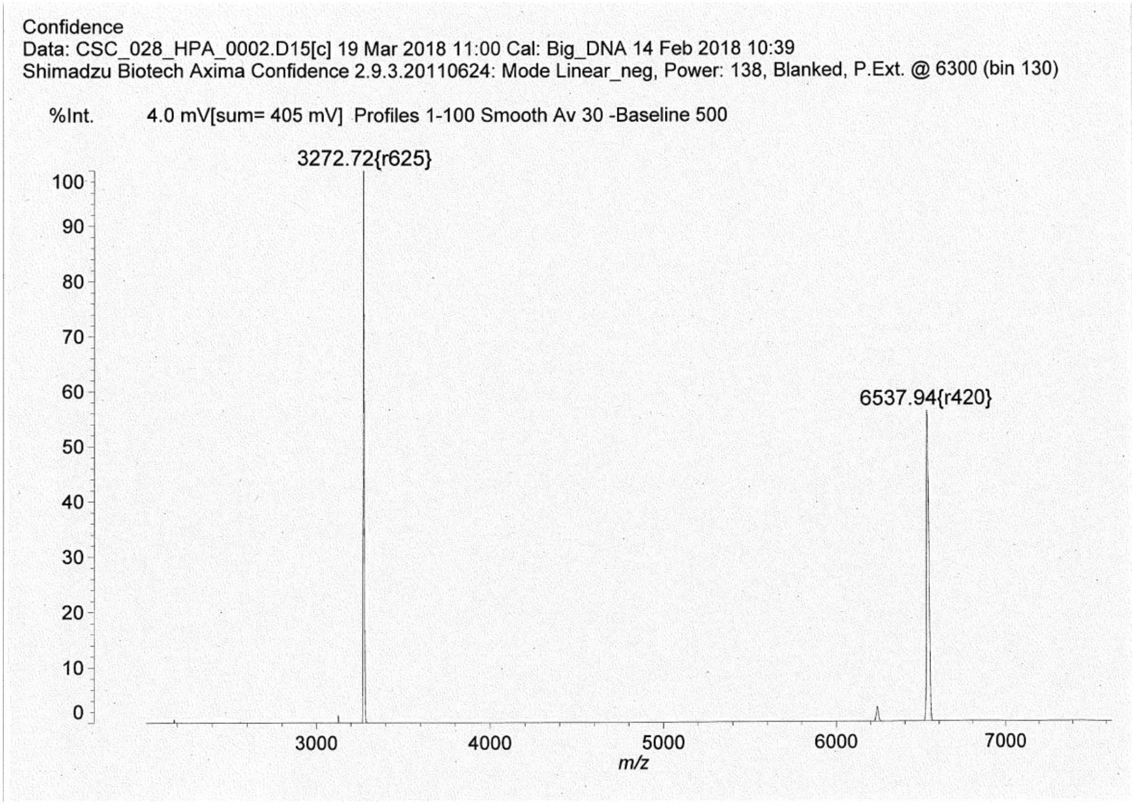
DNA5:


DNA5
3000
2000
1000
0
Intensity [a. u.]
RT = 19.3 min
0
10
20
30
40
Retention Time RT [min]

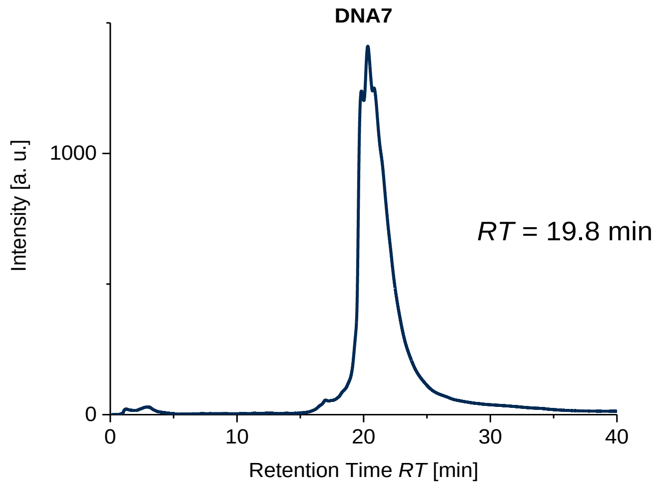

Confidence
Data: CSC_027_HPA_0001.D7[c] 19 Mar 2018 8:41 Cal: 2-4kDa_HPA_linneg 13 Feb 2018 11:02
Shimadzu Biotech Axima Confidence 2.9.3.20110624: Mode Linear_neg, Power: 128, Blanked, P.Ext. @ 6300 (bin 130)
%Int.
17 mV[sum= 1748 mV] Profiles 1-100 Smooth Av 30 -Baseline 100
6533.75{r553}
3264.66{r863}
100
90
80
70
60
50
40
30
20
10
0
3000
4000
5000
6000
7000
m/z

DNA6:

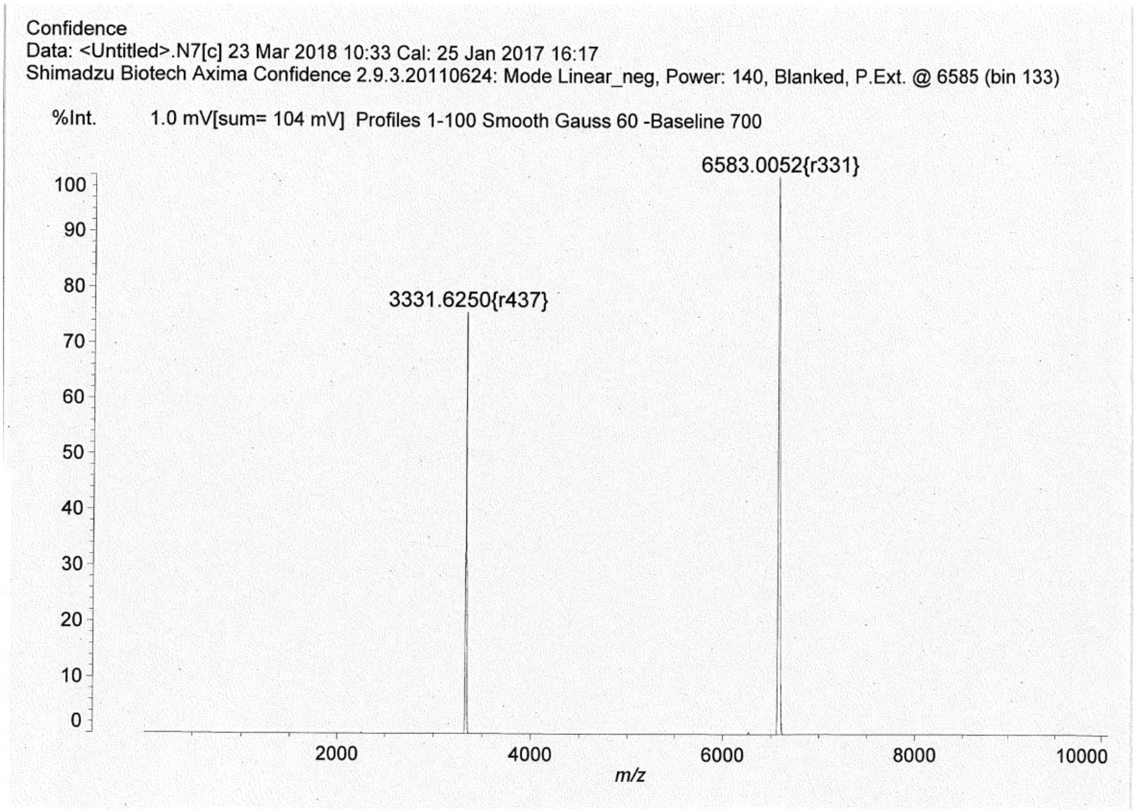

DNA6
500
400
300
200
100
0
Intensity [a. u.]
RT = 19.6 min
0
10
20
30
40
Retention Time RT [min]


Confidence
Data: CSC_028_HPA_0002.D15[c] 19 Mar 2018 11:00 Cal: Big_DNA 14 Feb 2018 10:39
Shimadzu Biotech Axima Confidence 2.9.3.20110624: Mode Linear_neg, Power: 138, Blanked, P.Ext. @ 6300 (bin 130)
%Int.
4.0 mV[sum= 405 mV] Profiles 1-100 Smooth Av 30 -Baseline 500
3272.72{r625}
6537.94{r420}
100
90
80
70
60
50
40
30
20
10
0
3000
4000
5000
6000
7000
m/z

DNA7:

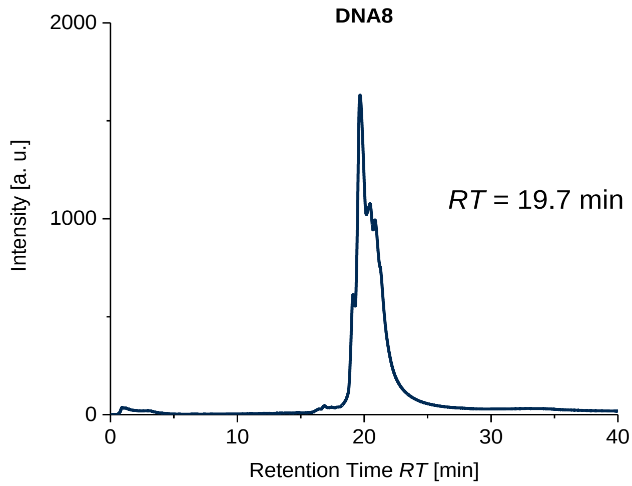


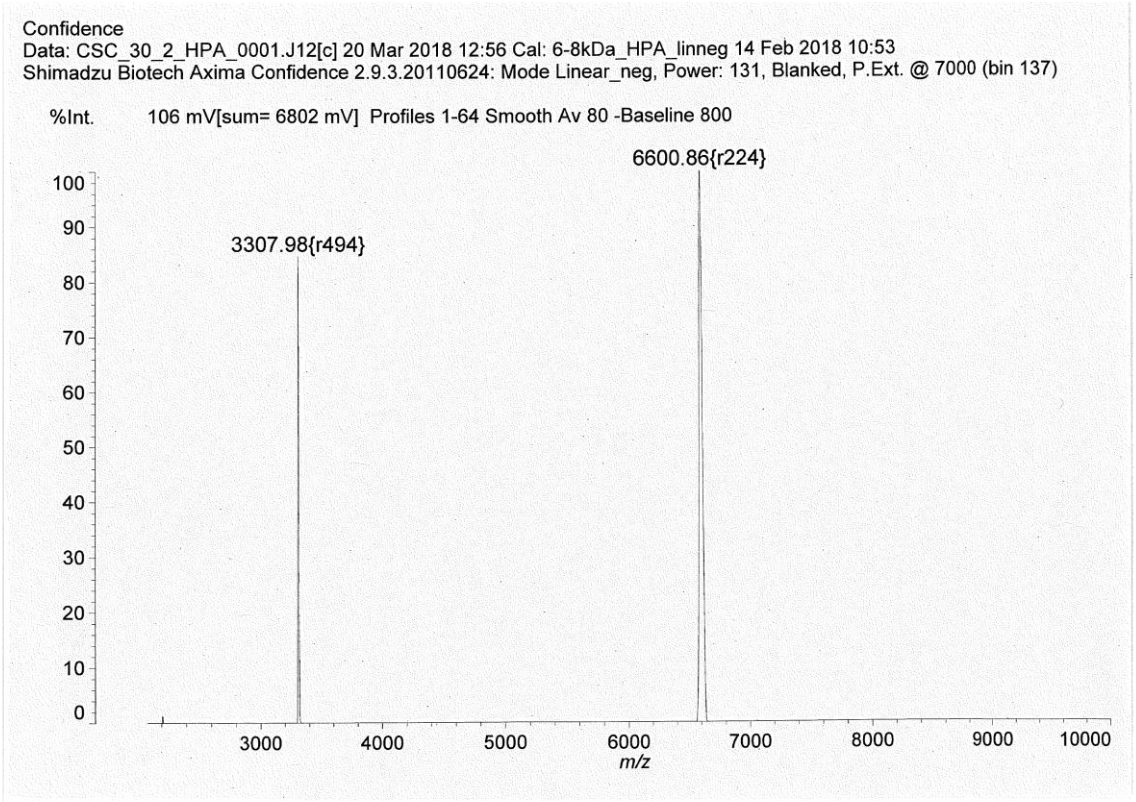
DNA7
Intensity [a. u.]
1000
0
0
10
20
30
40
Retention Time RT [min]
RT = 19.8 min



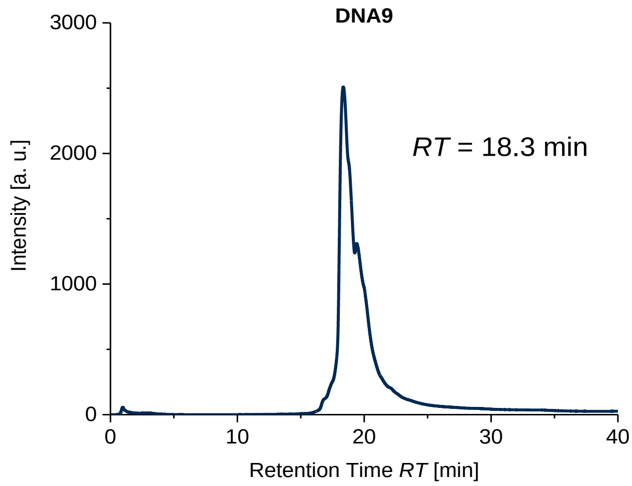
Confidence
Data: <Untitled>.N7[c] 23 Mar 2018 10:33 Cal: 25 Jan 2017 16:17
Shimadzu Biotech Axima Confidence 2.9.3.20110624: Mode Linear_neg, Power: 140, Blanked, P.Ext. @ 6585 (bin 133)
%Int.
1.0 mV[sum= 104 mV] Profiles 1-100 Smooth Gauss 60 -Baseline 700
6583.0052{r331}
3331.6250{r437}
100
90
80
70
60
50
40
30
20
10
0
2000
4000
6000
8000
10000
m/z

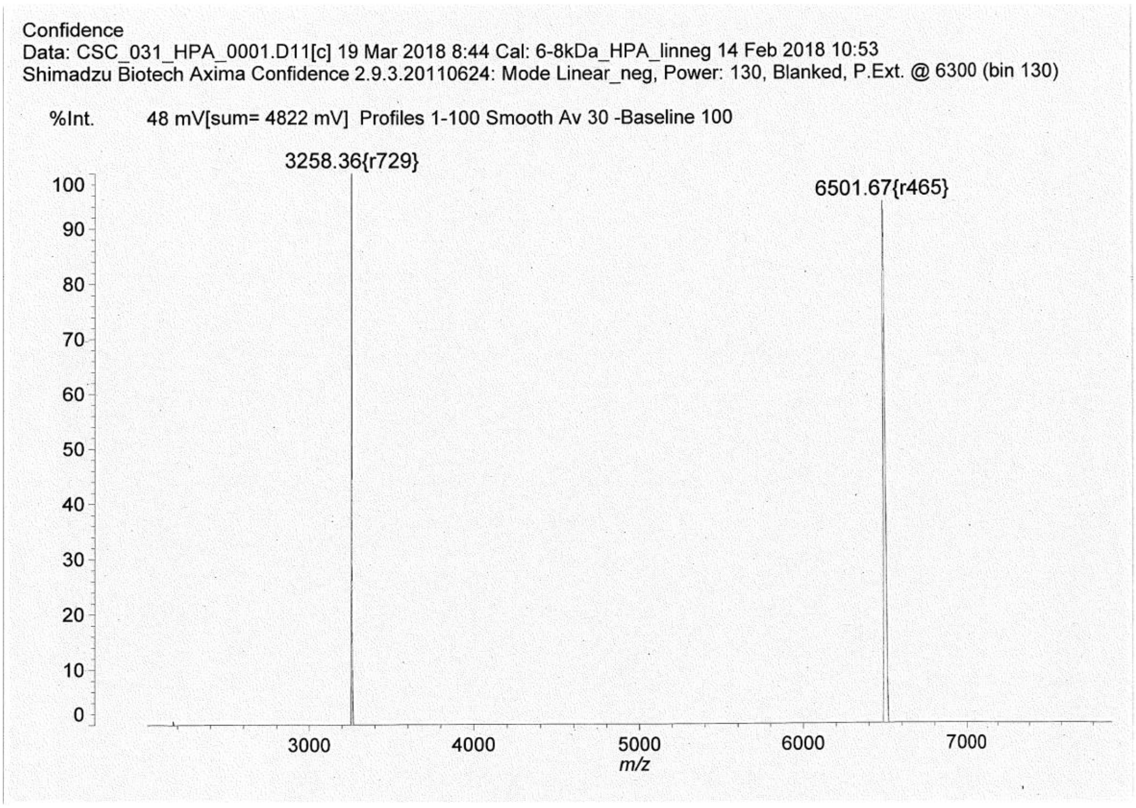
DNA8:


DNA8
RT = 19.7 min
Intensity [a. u.]
Retention Time RT [min]
0
1000
2000
0
10
20
30
40

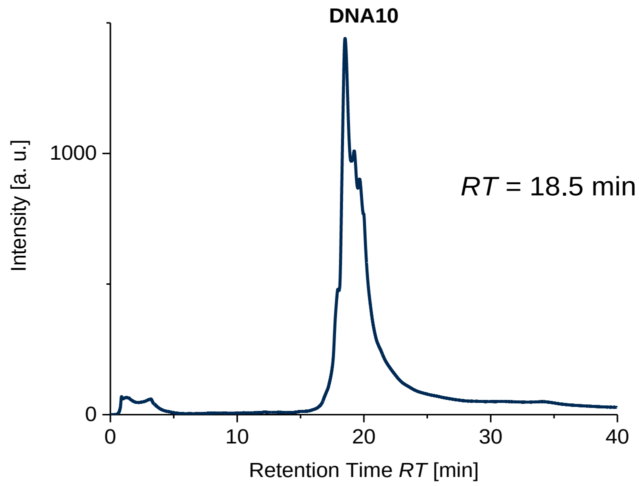

Confidence
Data: CSC_30_2_HPA_0001.J12[c] 20 Mar 2018 12:56 Cal: 6-8kDa_HPA_linneg 14 Feb 2018 10:53
Shimadzu Biotech Axima Confidence 2.9.3.20110624: Mode Linear_neg, Power: 131, Blanked, P.Ext. @ 7000 (bin 137)
%Int.
106 mV[sum= 6802 mV] Profiles 1-64 Smooth Av 80 -Baseline 800
6600.86{r224}
3307.98{r494}
m/z

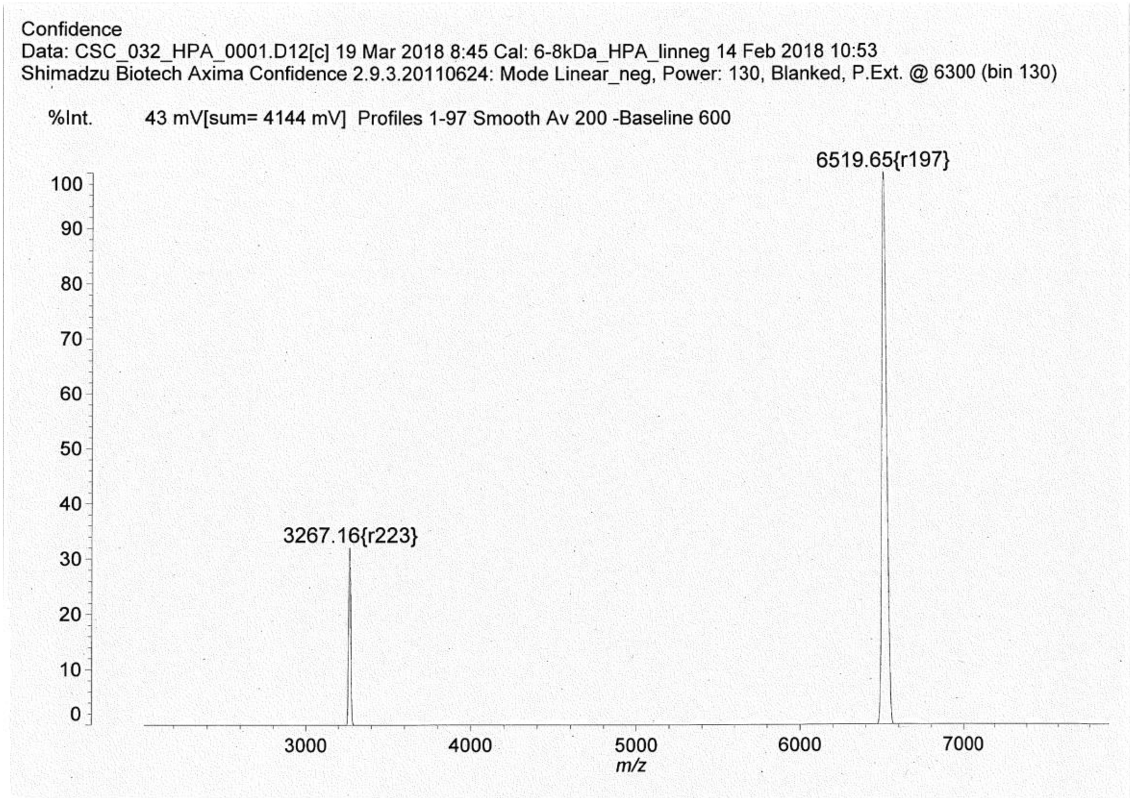
DNA9:


DNA9
RT = 18.3 min
Intensity [a. u.]
Retention Time RT [min]
3000
2000
1000
0
0
10
20
30
40

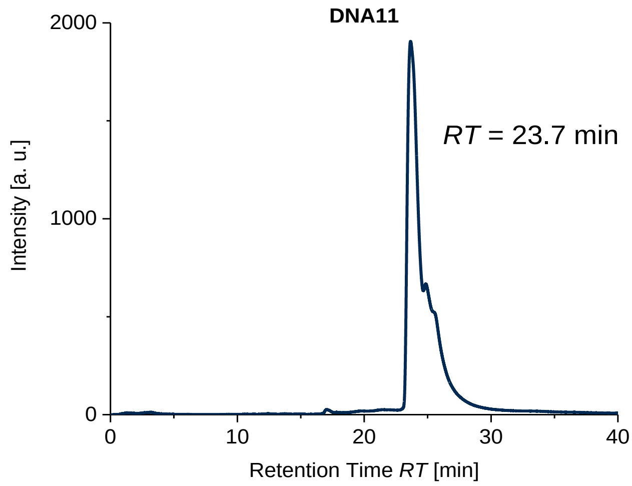

Confidence
Data: CSC_031_HPA_0001.D11[c] 19 Mar 2018 8:44 Cal: 6-8kDa_HPA_linneg 14 Feb 2018 10:53
Shimadzu Biotech Axima Confidence 2.9.3.20110624: Mode Linear_neg, Power: 130, Blanked, P.Ext. @ 6300 (bin 130)
%Int.
48 mV[sum= 4822 mV] Profiles 1-100 Smooth Av 30 -Baseline 100
3258.36{r729}
6501.67{r465}
m/z

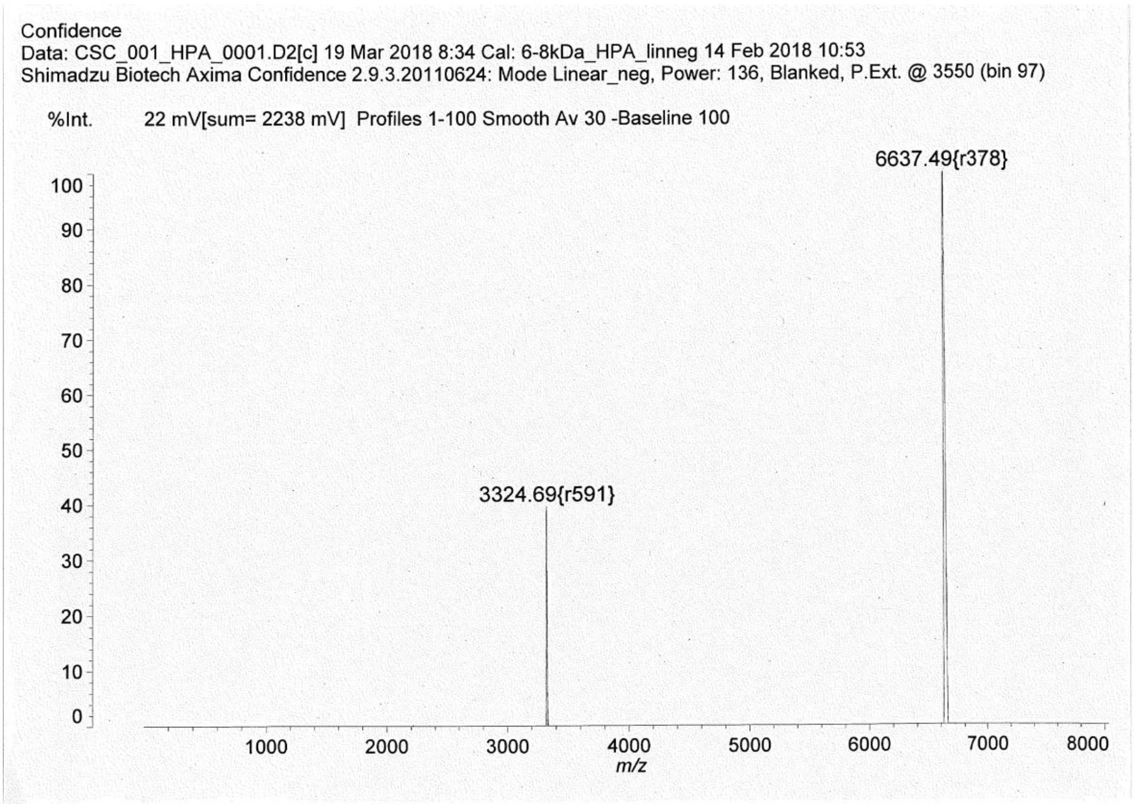
DNA10:


DNA10
Intensity [a. u.]
1000
0
RT = 18.5 min
0
10
20
30
40
Retention Time RT [min]

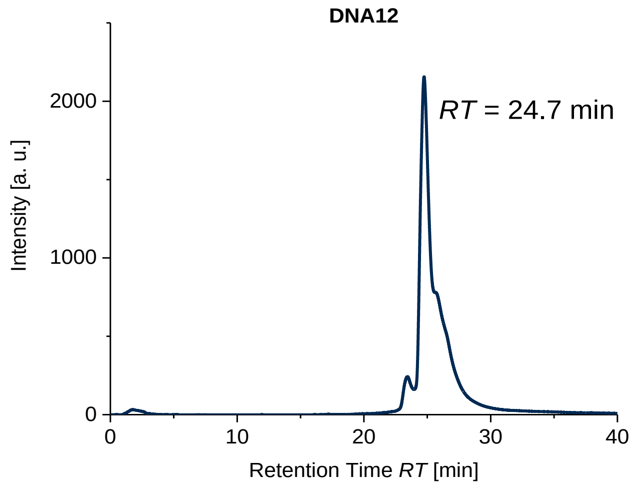

Confidence
Data: CSC_032_HPA_0001.D12[c] 19 Mar 2018 8:45 Cal: 6-8kDa_HPA_linneg 14 Feb 2018 10:53
Shimadzu Biotech Axima Confidence 2.9.3.20110624: Mode Linear_neg, Power: 130, Blanked, P.Ext. @ 6300 (bin 130)
%Int.
43 mV[sum= 4144 mV] Profiles 1-97 Smooth Av 200 -Baseline 600
6519.65{r197}
3267.16{r223}
100
90
80
70
60
50
40
30
20
10
0
3000
4000
5000
6000
7000
m/z

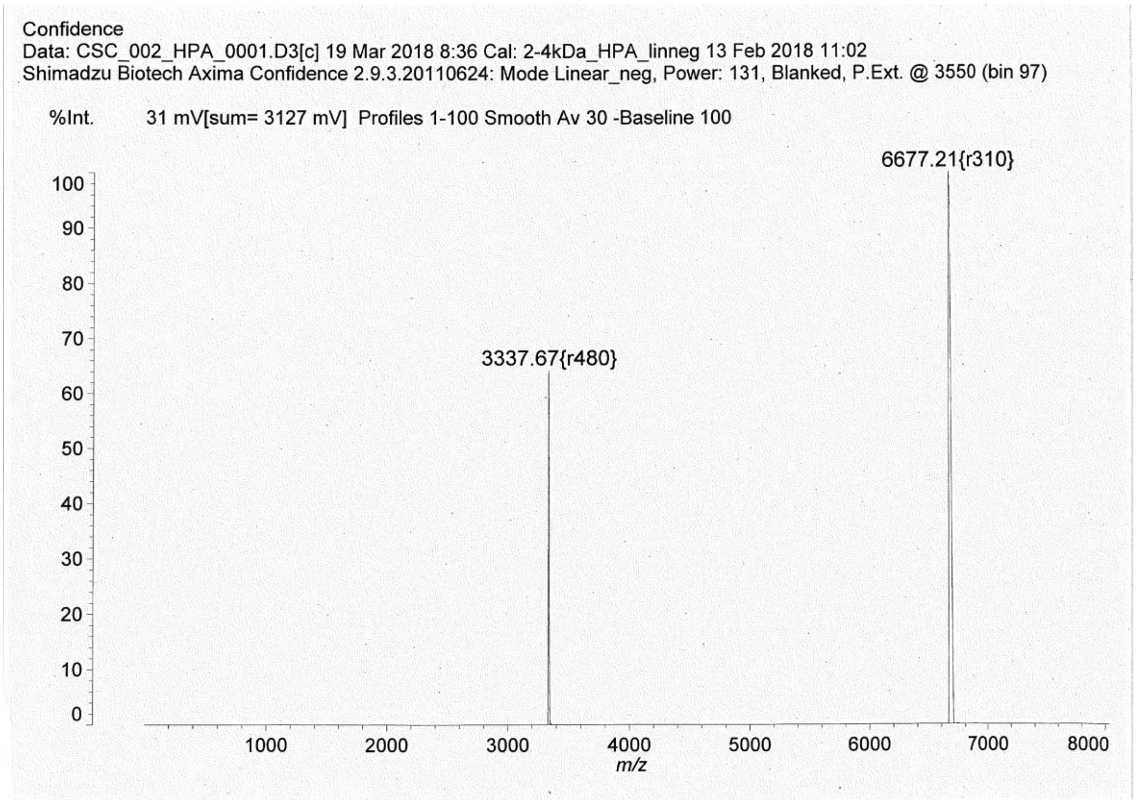
DNA11:


DNA11
RT = 23.7 min
Intensity [a. u.]
2000
1000
0
0
10
20
30
40
Retention Time RT [min]


Confidence
Data: CSC_001_HPA_0001.D2[c] 19 Mar 2018 8:34 Cal: 6-8kDa_HPA_linneg 14 Feb 2018 10:53
Shimadzu Biotech Axima Confidence 2.9.3.20110624: Mode Linear_neg, Power: 136, Blanked, P.Ext. @ 3550 (bin 97)
%Int.
22 mV[sum= 2238 mV] Profiles 1-100 Smooth Av 30 -Baseline 100
6637.49{r378}
3324.69{r591}
100
90
80
70
60
50
40
30
20
10
0
1000
2000
3000
4000
5000
6000
7000
8000
m/z

DNA12:


DNA12
RT = 24.7 min
Intensity [a. u.]
2000
1000
0
0
10
20
30
40
Retention Time RT [min]


Confidence
Data: CSC_002_HPA_0001.D3[c] 19 Mar 2018 8:36 Cal: 2-4kDa_HPA_linneg 13 Feb 2018 11:02
Shimadzu Biotech Axima Confidence 2.9.3.20110624: Mode Linear_neg, Power: 131, Blanked, P.Ext. @ 3550 (bin 97)
%Int.
31 mV[sum= 3127 mV] Profiles 1-100 Smooth Av 30 -Baseline 100
6677.21{r310}
3337.67{r480}
100
90
80
70
60
50
40
30
20
10
0
1000
2000
3000
4000
5000
6000
7000
8000
m/z

16. References

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