

Supplementary data

Eco-safe and highly efficient procedure for synthesis of 14-aryl-14H-dibenzo[a,j]xanthene derivatives promoted by acidic ionic liquids under solvent-free conditions

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Spectral data of products

14-Phenyl-14H-dibenzo[a,j]xanthene (3a)

White solid; FT-IR (KBr, cm⁻¹): 3074, 3020, 1591, 1403, 1253, 964, 827, 803, 744, 701, 609, 509; ¹HNMR (300 MHz, CDCl₃): δ 5.39 (1H, s, CH), 7.28-7.31 (d, 2H, *J* = 8.5 Hz, Ar-H), 6.68-6.74 (4H, m, Ar-H), 5.89-6.80 (11H, m, Ar-H); ¹³CNMR (75 MHz, CDCl₃): δ 38.03, 117.31, 118.01, 122.68, 124.23, 126.37, 126.78, 128.25, 128.47, 128.79, 128.85, 131.04, 131.44, 144.98, 148.7; MS (EI), *m/z*: 358 (M⁺), 282, 281, 252, 250, 179.

14-(2-chlorophenyl)-14H-dibenzo[a,j]xanthenes (3b)

White solid; FT-IR (KBr, cm⁻¹): 3057, 1591, 1514, 1431, 1238, 1031, 959, 829, 808, 744, 609, 520; ¹HNMR (300 MHz, CDCl₃): δ 5.69 (1H, s, CH), 5.81-5.82 (2H, d, Ar-H), 6.27-6.40 (5H, m, Ar-H), 6.50 (2H, d, Ar-H), 6.55-6.67 (4H, m, Ar-H), 7.63-7.66 (2H, *J* = 8.5, d, Ar-H); ¹³CNMR (75 MHz, CDCl₃): δ 34.63, 118.02, 118.11, 123.46, 124.44, 126.93, 127.87-127.94, 128.66, 129.08, 129.60, 130.13, 130.89, 131.76, 131.81, 143.57, 148.95; MS, *m/z*: 394, 392 (M⁺), 282, 281, 252, 250, 178, 177.

4-(4-Methoxyphenyl)-14H-dibenzo[a,j]xanthenes (3h)

Light brown solid; FT-IR (KBr, cm^{-1}): 3058, 2836, 1591, 1506, 1457, 1400, 1176, 1028, 961, 810, 746, 608, 509; ^1H NMR (300 MHz, CDCl_3): 2.49 (3H, s, OMe), 5.36 (1H, s, CH), 5.59-5.61 (2H, d, $J=8.66$ Hz, Ar-H), 6.32-6.45 (6H, m, Ar-H), 6.49-6.55 (2H, m, Ar-H), 6.69-6.76 (4H, m, Ar-H), 7.31-7.33 (2H, d, $J=8.48$, Ar-H); ^{13}C NMR (75 MHz, CDCl_3): 37.17, 55.05, 113.89, 117.58, 118.06, 122.77, 124.28, 126.81, 128.80, 128.87, 129.23, 131.13, 131.47, 137.45, 148.69, 157.89; MS, m/z : 388 (M^+), 282, 281, 252, 250, 194, 187.

14-(4-Bromophenyl)-14H-dibenzo[a,j]xanthenes (3i)

Pink solid; FT-IR (KBr, cm^{-1}): 33213062, 1590, 1512, 1400, 1237, 1009, 961, 805, 739, 704, 607, 516; ^1H NMR (300 MHz, CDCl_3): δ 5.34 (1H, s, CH), 6.16-6.48 (10H, m, Ar-H), 6.68-6.75 (4H, m, Ar-H), 7.19-7.22 (2H, m, $J = 7.8$, Ar-H). ^{13}C NMR (75 MHz, CDCl_3): δ 37.46, 116.65, 118.01, 120.21, 122.39, 124.37, 126.92, 128.91, 129.11, 129.88, 131.04, 131.24, 131.58, 143.98, 148.67; MS, m/z : 438, 436 (M^+), 282, 281, 252, 250, 179.

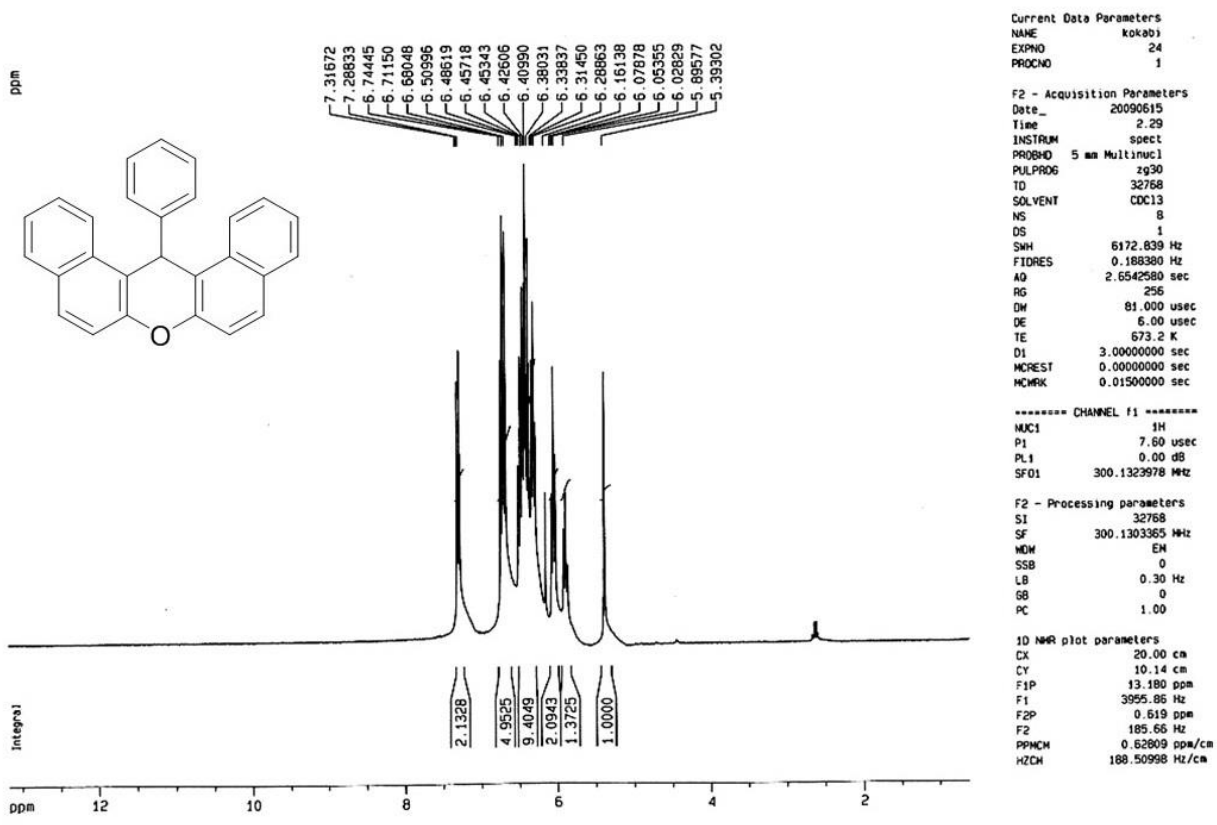
14-(4-fluorophenyl)-14H-dibenzo[a,j]xanthenes (3m)

Pink solid; FT-IR (KBr, cm^{-1}): 3068, 3034, 1591, 1500, 1235, 1211, 958, 812, 742, 607, 521, 486; ^1H NMR (300 MHz, CDCl_3): 5.38 (1H, s, CH), 5.69-5.72 (2H, d, $J=8.67$ Hz, Ar-H), 6.15-6.39 (6H, m, Ar-H), 6.46-6.51 (2H, m, Ar-H), 6.68-6.75 (4H, m, Ar-H), 7.22-7.25 (2H, d, $J=8.48$, Ar-H); ^{13}C NMR (75 MHz, CDCl_3): 37.18, 115.18, 115.47, 117.07, 118.03, 122.45, 124.33, 126.88, 128.89, 128.99, 129.56, 129.67, 131.04, 131.26, 140.80, 148.68; MS, m/z : 376 (M^+), 282, 281, 252, 250, 178.

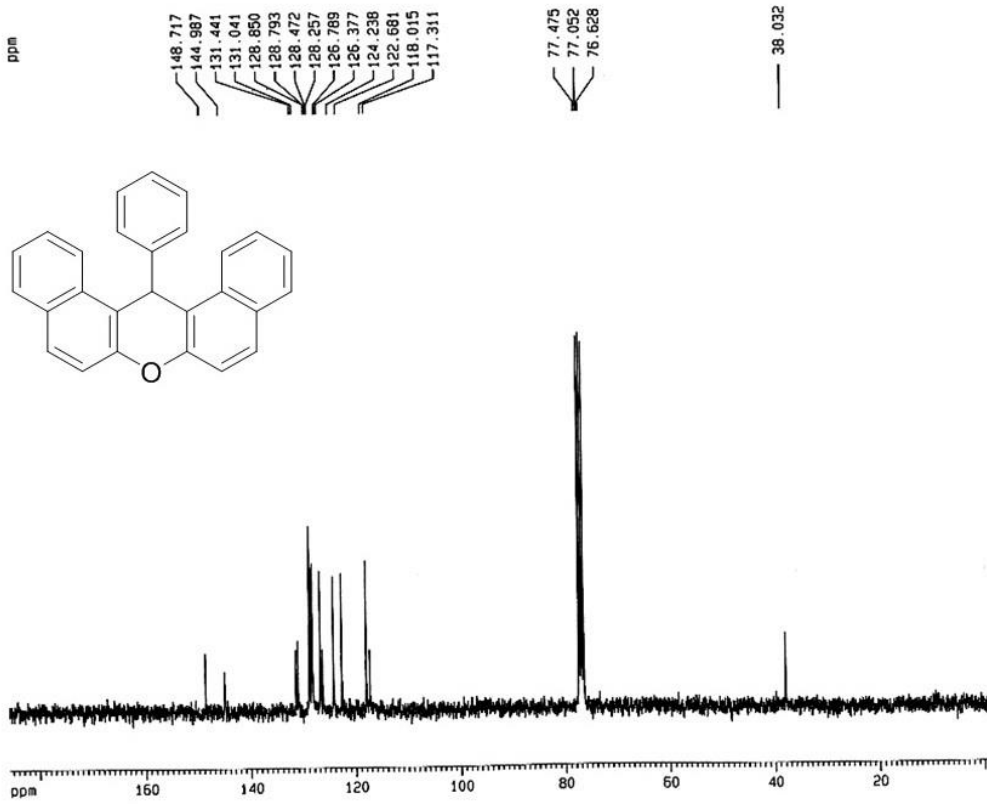
14-(4-Nitrophenyl)-14H-dibenzo[a,j]xanthenes (3p)

Yellow solid; FT-IR (KBr, cm^{-1}): 3070, 3037, 1590, 1509, 1338, 1236, 1105, 826, 806, 741, 605, 513, 440; ^1H NMR (300 MHz, CDCl_3): δ 5.44 (1H, s, CH), 6.33-6.57 (8H, m, Ar-H), 6.71-6.76 (4H, m, Ar-H), 6.85-6.89 (2H, d, Ar-H), 7.15-7.18 (2H, $J = 8.3$, Ar-H); ^{13}C NMR (75 MHz, CDCl_3): δ 37.88, 115.75, 118.06, 122.04, 123.86, 124.58, 127.19, 128.96, 129.06, 129.59, 131.07, 146.27, 148.75, 152.01; MS, m/z : 403 (M^+), 282, 281, 252, 250, 178, 141.

¹H NMR (300 MHz, CDCl₃) spectrum of 14-Phenyl-14H-dibenzo[a,j]xanthene



¹³C NMR (75 MHz, CDCl₃) spectrum of 14-Phenyl-14H-dibenzo[a,j]xanthene



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Current Data Parameters
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PROCNO       1

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PULPROG     zgpg30
ID          32768
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DS          2
SWH         17985.611 Hz
FIDRES     0.548877 Hz
AQ         0.9110004 sec
RG         6502
DM         27.800 usec
DE         6.00 usec
TE         673.2 K
D1         3.0000000 sec
d11        0.0300000 sec
ICREST     0.0000000 sec
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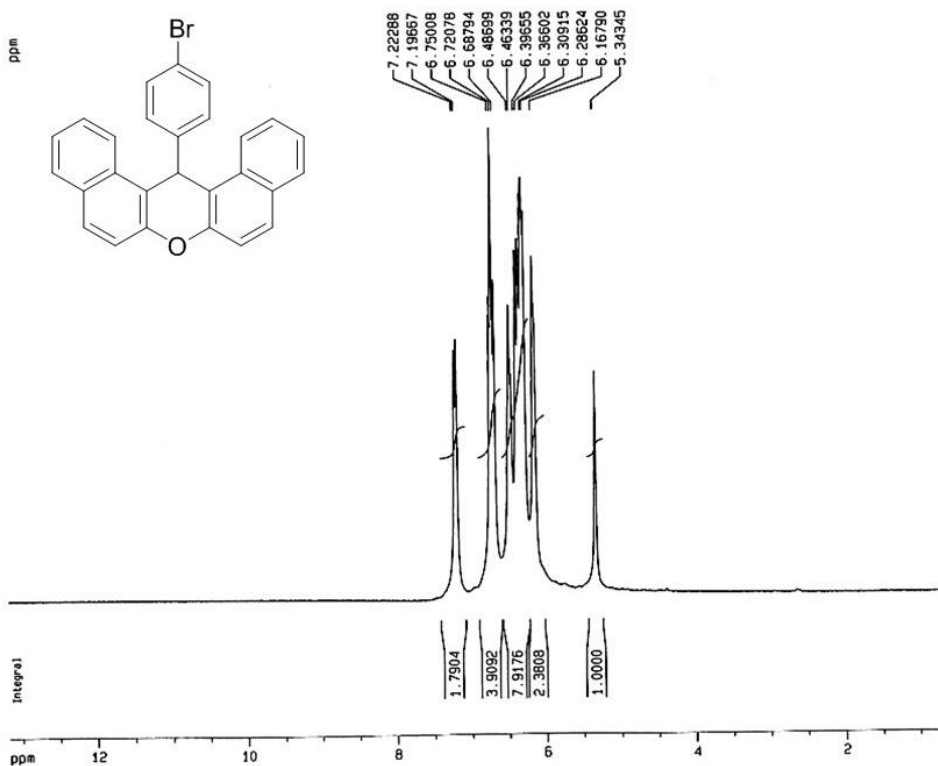
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NUC2        1H
PCPD2      80.00 usec
PL2         0.00 dB
PL12       21.00 dB
PL13       21.00 dB
SFO2      300.1312005 MHz

F2 - Processing parameters
SI          32768
SF         75.4677490 MHz
WDW         EM
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LB         2.00 Hz
GB         0
PC         1.40

1D NMR plot parameters
CX         20.00 cm
CY         9.00 cm
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F1         14016.73 Hz
F2P        -1.002 ppm
F2         -75.65 Hz
PPHQA      9.33659 ppm/cm
HZCHA      704.61920 Hz/cm
    
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¹H NMR (300 MHz, CDCl₃) spectrum of 14-(4-Bromophenyl)-14H-dibenzo[a,j]xanthenes



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Current Data Parameters
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PROCNO       1

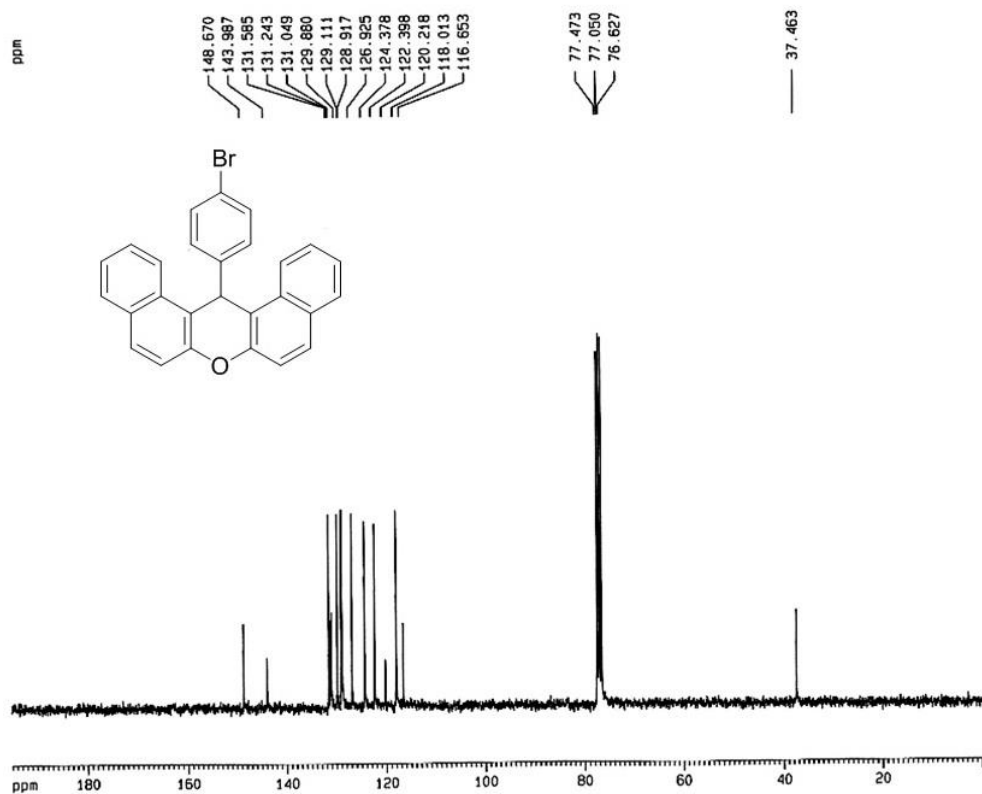
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TD           32768
SOLVENT      CDCl3
NS           1
DS           1
SMB         6172.830 Hz
FIDRES      0.188380 Hz
AQ          2.6542580 sec
RG          256
DM          81.000 usec
DE          6.00 usec
TE          673.2 K
D1          3.00000000 sec
MCREST      0.00000000 sec
MCMARK      0.01500000 sec

***** CHANNEL f1 *****
NUC1         1H
P1           7.60 usec
PL1          0.00 dB
SFO1        300.1323978 MHz

F2 - Processing parameters
SI           32768
SF          300.1303365 MHz
WDW          EM
SSB          0
LB           0.30 Hz
GB           0
PC           1.00

1D NMR plot parameters
CX           20.00 cm
CY           10.14 cm
F1P         13.180 ppm
F1          3955.86 Hz
F2P         0.619 ppm
F2          185.56 Hz
PPHMCN      0.62809 ppm/cm
HZCM        188.50998 Hz/cm
    
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¹³C NMR (75 MHz, CDCl₃) spectrum of 14-(4-Bromophenyl)-14H-dibenzo[a,j]xanthenes



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Current Data Parameters
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EXPNO    19
PROCNO   1

F2 - Acquisition Parameters
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AQ         0.9110004 sec
RG         6502
DW         27.800 usec
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dCREST    0.0000000 sec
dCMR8K    0.0150000 sec

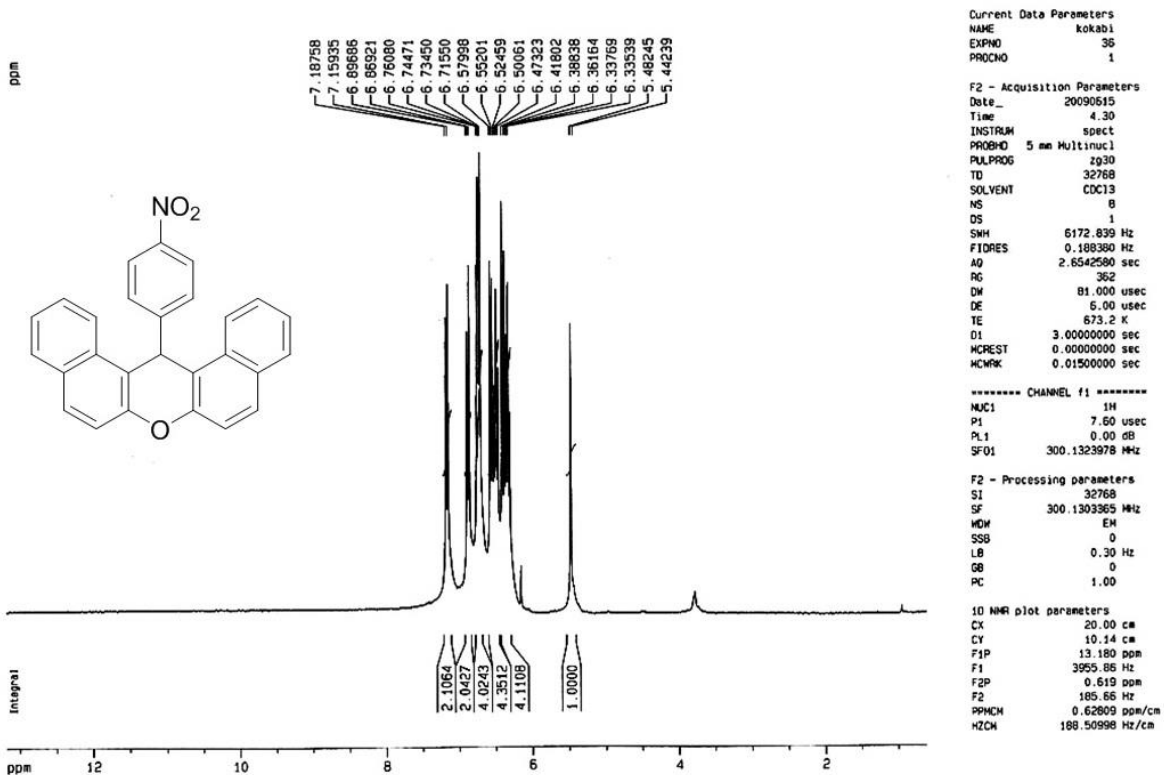
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***** CHANNEL f2 *****
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NUC2       1H
PCPD2     80.00 usec
PL2        0.00 dB
PL12       21.00 dB
PL13       21.00 dB
SF02     300.1312005 MHz

F2 - Processing parameters
SI         32768
SF         75.4577490 MHz
WDW        EM
SSB         0
LB          2.00 Hz
GB          0
PC          1.40

1D NMR plot parameters
CX         20.00 cm
CY          8.00 cm
F1P        195.177 ppm
F1         14729.50 Hz
F2P        -1.002 ppm
F2          -75.65 Hz
PPNCH      9.60898 ppm/cm
HZCN       740.26154 Hz/cm
    
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¹H NMR (300 MHz, CDCl₃) spectrum of 14-(4-Nitrophenyl)-14H-dibenzo[a,j]xanthenes



¹³C NMR (75 MHz, CDCl₃) spectrum of 14-(4-Nitrophenyl)-14H-dibenzo[a,j]xanthenes

