Supplementary Information (SI) for Journal of Materials Chemistry C.

Supporting Information - Structure Property Relationship of *p*-Alkoxy-Azobenzenes as Molecular Solar Thermal Phase Change Material Energy Storage Systems (MOST-PCM)

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1. General information

Chemicals were used as purchased from Sigma-Aldrich, Acros Organics, Alfa Aesar, TCIm Europe or BLD Pharm. Anhydrous solvents were purchased from Acros Organics. Technical grade solvents for workup and purification were distilled prior to use. Air and/or water-sensitive reactions were carried out under Schlenk-conditions or in a nitrogen-filled glovebox. Solids were dried under high vacuum (oil pump, ca 10^{-3} mbar) at room temperature (rt), 50 °C or 60 °C if necessary.

Flash column chromatography and column chromatography was carried out with Silica 60 M (0.04 – 0.063 mm) from Macherey Nagel GmbH & Co. KG. Thin layer chromatography was performed on Polygram® SIL G/UV254 from Macherey Nagel GmbH & Co. KG.

NMR spectra were measured on a Bruker Avance II 200 MHz, Avance II 400 MHz or Avance III 400 MHz HD spectrometer at rt, if not stated otherwise. Chemical shifts are reported in parts per million (ppm) relative to the solvent peak, coupling constants (J) are reported in Hertz (Hz). Deuterated solvents were obtained from Deutero GmbH (Kastellaun, Germany) or Euriso-Top GmbH.

Melting points were determined on a M5000 melting point meter from A.KRÜSS Optronic GmbH Germany. A heating rate of 1 °C min-1, a resolution of 0.1 °C and a measurement accuracy of ± 0.3 °C (25–200 °C) or ± 0,5 °C (200–400 °C) apply for this device

For all azobenzenes, the thermodynamically more stable (*E*)-isomer is reported if not stated otherwise. ESI-MS spectra were recorded on a Bruker Daltonics Micro TOF. Melting points were measured on a Krüss M5000 capillary melting point meter with a heating rate of 1 °C min^{-1}.

2. Synthesis

Synthesis of 4-Hydroxyazobenzene (2)

Aniline (30.0 mmol, 2.74 mL, 1.00 eq.) was added to an aqueous solution containing H_2O (60 mL) and 37% $HCl_{(aq)}$. (15 mL) to prepare an aniline solution, which was added dropwise into an aqueous solution containing $NaNO_2$ (39.0 mmol, 2.69 g, 1.30 eq.) in H_2O (15 mL) cooled in an ice water bath (0 °C) under strong stirring. After mixing, the resulting solution was stirred for 1 h at 0 °C to form a diazonium salt solution. Then, a separated aqueous solution containing phenol (30.0 mmol, 2.67 mL, 1.00 eq.) and NaOH (12.1 g, 300 mmol, 10.0 eq.) in H_2O (60 mL) was prepared, and the diazonium salt solution was added to the phenol solution slowly with cooling by an ice water bath. The color of the solution became dark during this process. After stirring at 0 °C for 1 h, the resulting solution was acidified by adding 20% $HCl_{(aq)}$ solution. Afterwards, the resulting solution was filtered by suction filtration to collect the dark solid which was washed by water, dissolved in acetone and reprecipitated by adding water slowly. Vacuum filtration afforded a brown powder as product with about 90% yield. The brown powder was further purified by column chromatography (silica, toluene / ethylacetate = 7 : 1) to obtain a brown solid (4.81 g, 81%).

^1H NMR (400 MHz, $CDCl_3$) δ 7.98 – 7.86 (m, 4H), 7.54 – 7.48 (m, 2H), 7.47 – 7.42 (m, 1H), 7.03 – 6.94 (m, 2H).

Analytical data corresponds to literature.[1]

Synthesis of *p*-OBu-Azobenzene (3a)

A mixture of 4-hydroxyazobenzene (404 mg, 2.04 mmol, 1.00 eq.) and K_2CO_3 (1.11 g, 8.02 mmol, 3.97 eq.) in acetone (100 mL) was dissolved in a 250 mL flask while stirring. To this solution the 1-bromobutane (0.87 mL, 8.13 mmol, 3.99 eq.) was added and stirred for 3 days at 70 °C. The solution turned yellow. After cooling the solution to rt, K_2CO_3 was removed by filtration, and the solvents were removed under *vacuo* to obtain the yellowish crude product. The product was purified by column chromatography (silica gel 50 g, toluene: cyclohexane = 1: 5) to obtain an orange solid (479 mg, 96%).

^1H-NMR (400 MHz, $CDCl_3$) δ = 7.99 – 7.92 (m, 2H), 7.93 – 7.84 (m, 2H), 7.54 – 7.47 (m, 2H), 7.47 – 7.40 (m, 1H), 7.04 – 6.98 (m, 2H), 4.06 (t, J = 6.5 Hz, 2H), 1.87 – 1.76 (m, 2H), 1.59 – 1.46 (m, 2H), 1.00 (t, J = 7.4 Hz, 3H).

Melting point: 64.3 °C

Analytical data corresponds to literature.[2]

Synthesis of *p*-OPen-Azobenzene (3b)

A mixture of 4-hydroxyazobenzene (402 mg, 2.03 mmol, 1.00 eq.) and K_2CO_3 (1.11 g, 8.06 mmol, 3.98 eq.) of in acetone (100 mL) were dissolved in a 250 mL flask while stirring. To this solution the 1-bromopentane (0.52 mL, 4.08 mmol, 2.01 eq.) was added and stirred for 3 days at 70 °C. The color of solution was changed to yellow. After cooling the solution to rt, K_2CO_3 was removed by filtration, and the solvents were removed under *vacuo* to obtain the yellowish crude product. The product was purified by column chromatography (silica gel 50 g, toluene / cyclohexane = 1 : 5) affording an orange solid (503 mg, 98%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 – 7.91 (m, 2H), 7.89 (dd, *J* = 7.4, 1.8 Hz, 2H), 7.50 (dd, *J* = 8.4, 6.6 Hz, 2H), 7.46 – 7.41 (m, 1H), 7.05 – 6.98 (m, 2H), 4.05 (t, *J* = 6.6 Hz, 2H), 1.89 – 1.78 (m, 2H), 1.52 – 1.36 (m, 4H), 0.95 (t, *J* = 7.0 Hz, 3H).

Melting point: 60.0 °C

Analytical data corresponds to literature.[3]

Synthesis of *p*-OHex-Azobenzene (3c)

A mixture of 4-hydroxyazobenzene (402 mg, 2.03 mmol, 1.00 eq.) and K_2CO_3 (1.21 g, 8.74 mmol, 4.31 eq.) in acetone (100 mL) was dissolved in a 250 mL flask while stirring. To this solution the 1-bromohexane (1.20 mL, 8.58 mmol, 4.23 eq.) was added and stirred for 3 days at 70 °C. The color of solution was changed to yellow. After cooling the solution to rt, K_2CO_3 was removed by filtration, and the solvents were removed under *vacuo* to obtain the yellowish crude product. The product was purified by column chromatography (silica gel 50 g, toluene / cyclohexane = 1 : 5) to obtain an orange solid (540 mg, 99%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 – 7.92 (m, 2H), 7.92 – 7.87 (m, 2H), 7.50 (dd, *J* = 8.4, 6.5 Hz, 2H), 7.47 – 7.40 (m, 1H), 7.07 – 6.97 (m, 2H), 4.05 (t, *J* = 6.6 Hz, 2H), 1.82 (dt, *J* = 14.7, 6.7 Hz, 2H), 1.49 (dtd, *J* = 14.9, 7.2, 4.5 Hz, 2H), 1.36 (h, *J* = 3.7 Hz, 4H), 0.98 – 0.88 (m, 3H).

Melting point: 57.3 °C

Analytical data corresponds to literature.[4]

Synthesis of *p*-OHep-Azobenzene (3d)

A mixture of 4-hydroxyazobenzene (403 mg, 2.03 mmol, 1.00 eq.) and K_2CO_3 (1.13 g, 8.14 mmol, 4.01 eq.) in acetone (100 mL) was dissolved in a 250 mL flask while stirring. To this solution the 1-bromohepane (1.30 mL, 8.19 mmol, 4.03 eq.) was added and stirred for 3 days at 70 °C. The color of solution was changed to yellow. After cooling the solution to rt, K_2CO_3 was removed by filtration, and the solvents were removed under *vacuo* to obtain the yellowish crude product. The product was purified by column chromatography (silica gel 50 g, toluene / cyclohexane = 1 : 4) to obtain an orange solid (491 mg, 86%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 – 7.90 (m, 2H), 7.90 – 7.84 (m, 2H), 7.56 – 7.47 (m, 2H), 7.47 – 7.38 (m, 1H), 7.05 – 6.96 (m, 2H), 4.04 (t, *J* = 6.6 Hz, 2H), 1.88 – 1.75 (m, 2H), 1.54 – 1.43 (m, 2H), 1.43 – 1.27 (m, 6H), 0.96 – 0.87 (m, 3H).^{13}C NMR (101 MHz, CDCl3) δ 161.99, 152.80, 146.90, 130.48, 129.18, 125.03, 122.68, 114.88, 68.55, 31.93, 29.35, 29.21, 26.13, 22.76, 14.24.

HRMS (ESI): m/z for $C_{19}H_{25}N_2O^+$; calcd 297.1962, found 297.1963

Melting point: 71.0 °C

Synthesis of *p*-OOct-Azobenzene (3e)

A mixture of 4-hydroxyazobenzene (408 mg, 2.06 mmol, 1.00 eq.) and K_2CO_3 (1.11 g, 8.00 mmol, 3.88 eq.) in acetone (100 mL) was dissolved in a 250 mL flask while stirring. To this solution the 1-bromooctane (1.40 mL, 8.05 mmol, 3.91 eq.) was added and stirred for 3 days at 70 °C. The color of solution was changed to yellow. After cooling the solution to rt, K_2CO_3 was removed by filtration, and the solvents were removed under *vacuo* to obtain the yellowish crude product. The product was purified by column chromatography (silica gel 50 g/ toluene: cyclohexane = 1 : 4) to obtain an orange solid (580 mg, 95%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 – 7.91 (m, 2H), 7.91 – 7.85 (m, 2H), 7.56 – 7.47 (m, 2H), 7.46 – 7.41 (m, 1H), 7.04 – 6.97 (m, 2H), 4.04 (t, *J* = 6.6 Hz, 2H), 1.88 – 1.77 (m, 3H), 1.54 – 1.43 (m, 2H), 1.43 – 1.22 (m, 8H), 0.94 – 0.85 (m, 3H).

Melting point: 72.1 °C

Analytical data corresponds to literature.[5]

Synthesis of *p*-ONon-Azobenzene (3f)

A mixture of 4-hydroxyazobenzene (399 mg, 2.01 mmol, 1.00 eq.) and K_2CO_3 (1.10 g, 7.92 mmol, 3.94 eq.) in acetone (100 mL) was dissolved in a 250 mL flask while stirring. To this solution the 1-bromononane (0.80 mL, 4.17 mmol, 2.07 eq.) was added and stirred for 3 days at 70 °C. The color of solution was changed to yellow. After cooling the solution to rt, K_2CO_3 was removed by filtration, and the solvents were removed under *vacuo* to obtain the yellowish crude product. The product was purified by column chromatography (silica gel 50 g/ toluene: cyclohexane = 1 : 4) to obtain an orange solid (609 mg, 98%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 – 7.92 (m, 2H), 7.92 – 7.86 (m, 2H), 7.55 – 7.47 (m, 2H), 7.47 – 7.40 (m, 1H), 7.05 – 6.97 (m, 2H), 4.05 (t, *J* = 6.6 Hz, 2H), 1.82 (dt, *J* = 14.6, 6.7 Hz, 2H), 1.54 – 1.43 (m, 2H), 1.41 – 1.23 (m, 10H), 0.93 – 0.84 (m, 3H). ^{13}C NMR (101 MHz, CDCl3) δ 162.00, 152.78, 146.88, 130.48, 129.18, 125.04, 122.68, 114.88, 68.56, 32.03, 29.68, 29.54, 29.41, 29.34, 26.16, 22.83, 14.27.

HRMS (ESI): m/z for $C_{21}H_{29}N_2O^+$; calcd 325.2275, found 325.2277

Melting point: 78.5 °C

Synthesis of *p*-ODec-Azobenzene (3g)

A mixture of 4-hydroxyazobenzene (400 mg, 2.02 mmol, 1.00 eq.) and K_2CO_3 (1.11 g, 8.05 mmol, 4.00 eq.) in acetone (100 mL) were dissolved in a 250 mL flask while stirring. To this solution the 1-bromodecane (1.10 mL, 5.32 mmol, 2.64 eq.) was added and stirred for 3 days at 70 °C. The color of solution changed to yellow. After cooling the solution to rt, K_2CO_3 was removed by filtration, and the solvents were removed under *vacuo* to obtain the yellowish crude product. The product was purified by column chromatography (silica gel 50 g/ toluene: cyclohexane = 1 : 4) to obtain an orange solid (617 mg, 95%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 – 7.90 (m, 2H), 7.91 – 7.84 (m, 2H), 7.54 – 7.47 (m, 2H), 7.47 – 7.40 (m, 1H), 7.05 – 6.96 (m, 2H), 4.04 (t, *J* = 6.6 Hz, 2H), 1.82 (dt, *J* = 14.6, 6.7 Hz, 2H), 1.55 – 1.43 (m, 2H), 1.43 – 1.20 (m, 13H), 0.93 – 0.84 (m, 3H).

Melting point: 63.0 °C

Analytical data corresponds to literature.[6]

Synthesis of *p*-OUndec-Azobenzene (3h)

A mixture of 4-hydroxyazobenzene (202 mg, 1.02 mmol, 1.00 eq.) and K_2CO_3 (601 mg, 4.35 mmol, 2.16 eq.) in acetone (100 mL) were dissolved in a 250 mL flask while stirring. To this solution the 1-bromoundecane (0.60 mL, 2.68 mmol, 1.33 eq.) was added and stirred for 3 days at 70 °C. The color of solution changed to yellow. After cooling the solution to rt, K_2CO_3 was removed by filtration, and the solvents were removed under *vacuo* to obtain the yellowish crude product. The product was purified by column chromatography (silica gel 50 g/ toluene: cyclohexane = 1 : 4) to obtain an orange solid (615 mg, 87%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 – 7.84 (m, 4H), 7.50 (dd, *J* = 8.2, 6.4 Hz, 2H), 7.47 – 7.39 (m, 1H), 7.00 (d, *J* = 8.5 Hz, 2H), 4.04 (t, *J* = 6.6 Hz, 2H), 1.92 – 1.76 (m, 2H), 1.54 – 1.42 (m, 2H), 1.42 – 1.22 (m, 15H), 0.93 – 0.85 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.92, 152.90, 146.97, 130.45, 129.17, 124.95, 122.71, 114.88, 68.54, 32.06, 29.88 – 29.63 (m), 29.51 (d, *J* = 4.5 Hz), 29.34, 26.16, 22.84, 14.27.

HRMS (ESI): m/z for $C_{23}H_{23}N_2O^+$; calcd 353.2588, found 353.2590

Melting point: 75.2 °C

Synthesis of *p*-ODodec-Azobenzene (3i)

A mixture of 4-hydroxyazobenzene (409 mg, 2.06 mmol, 1.00 eq.) and K_2CO_3 (1.14 g, 8.26 mmol, 4.11 eq.) in acetone (100 mL) were dissolved in a 250 mL flask while stirring. To this solution the 1-bromododecane (2.00 mL, 8.35 mmol, 4.15 eq.) was added and stirred for 3 days at 70 °C. The color of solution changed to yellow. After cooling the solution to rt, K_2CO_3 was removed by filtration, and the solvents were removed under *vacuo* to obtain the yellowish crude product. The product was purified by column chromatography (silica gel 50 g/ toluene: cyclohexane = 1 : 4) to obtain an orange solid (692 mg, 94%).

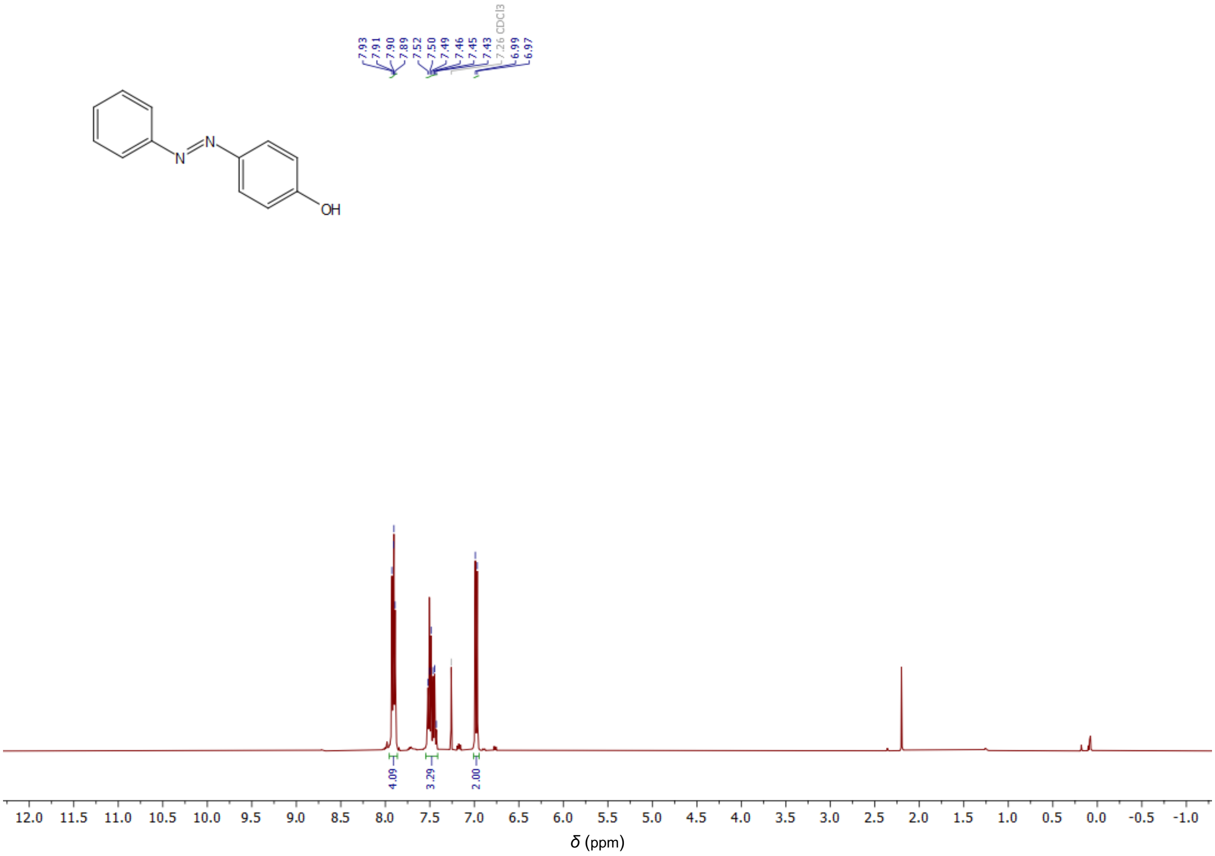
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 – 7.91 (m, 2H), 7.91 – 7.86 (m, 2H), 7.56 – 7.47 (m, 2H), 7.46 – 7.40 (m, 1H), 7.05 – 6.97 (m, 2H), 4.04 (t, *J* = 6.6 Hz, 2H), 1.82 (dt, *J* = 14.7, 6.7 Hz, 2H), 1.54 – 1.42 (m, 2H), 1.38 – 1.20 (m, 17H), 0.94 – 0.84 (m, 3H).

Melting point: 70.5 °C

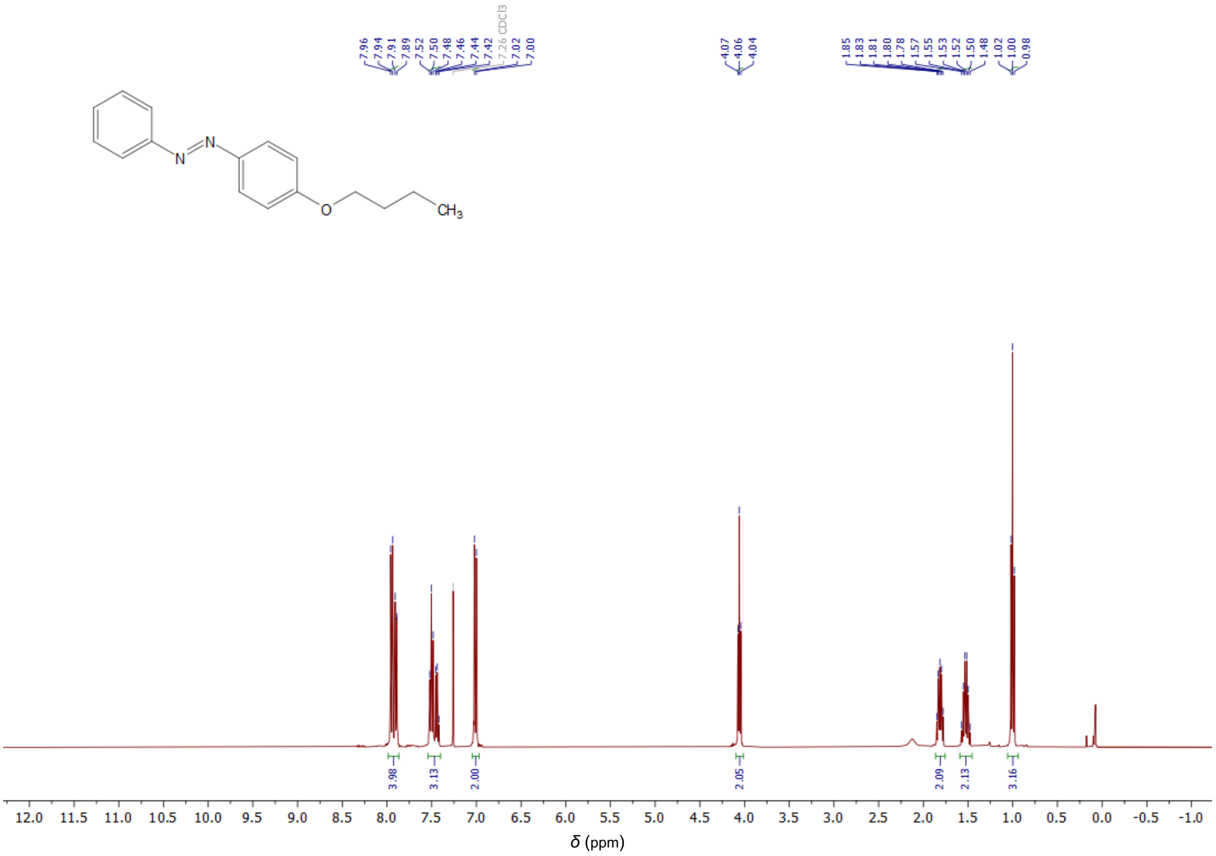
Analytical data corresponds to literature.[7]

3. NMR spectra

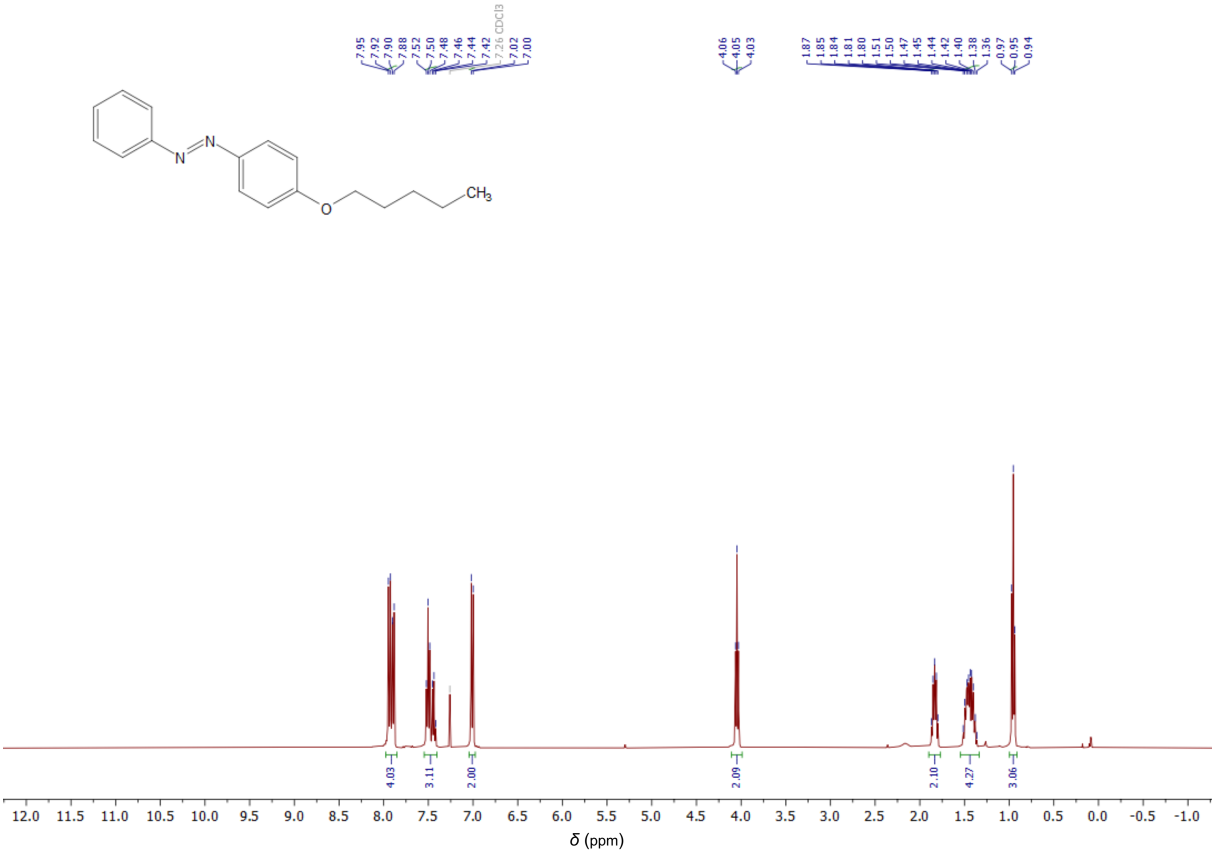
^{1}H-NMR of 4-Hydroxyazobenzene (2)



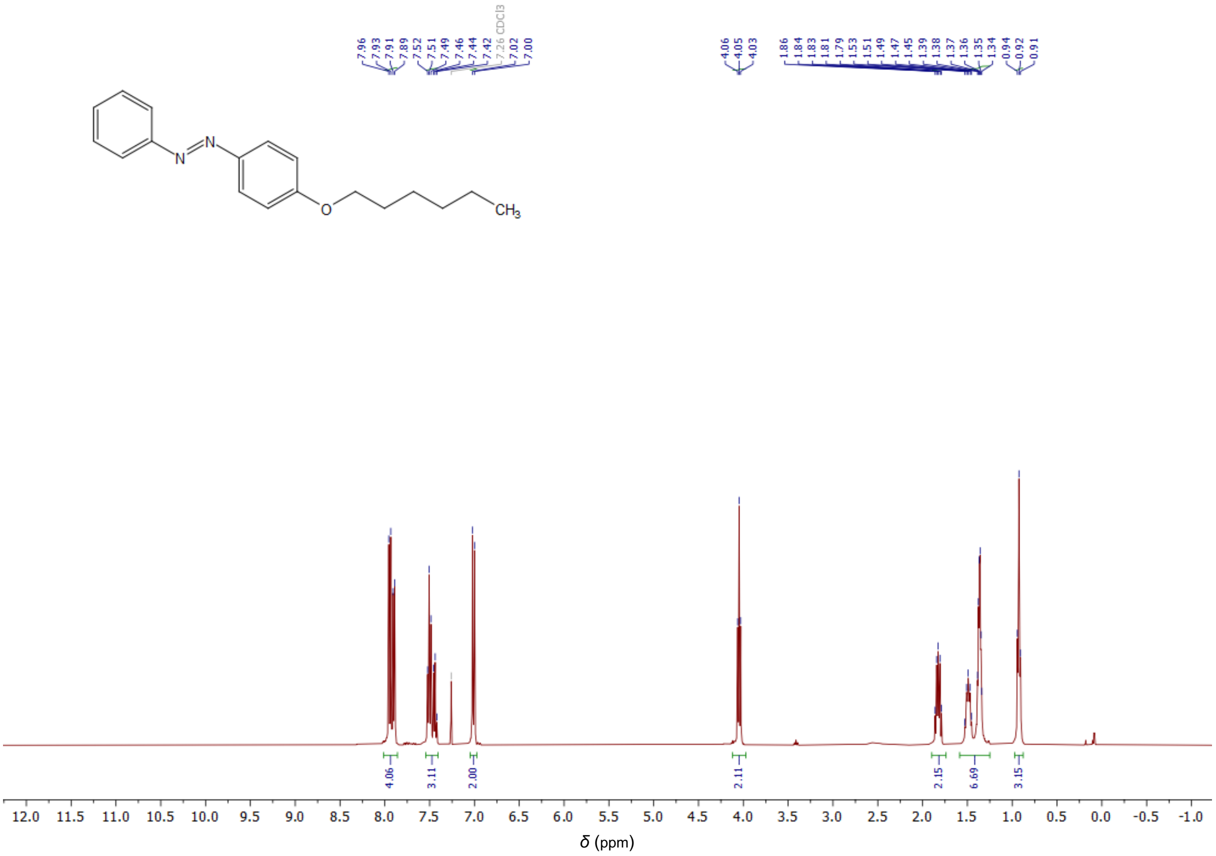
^{1}H-NMR of *p*-OBu-Azobenzene (3a)



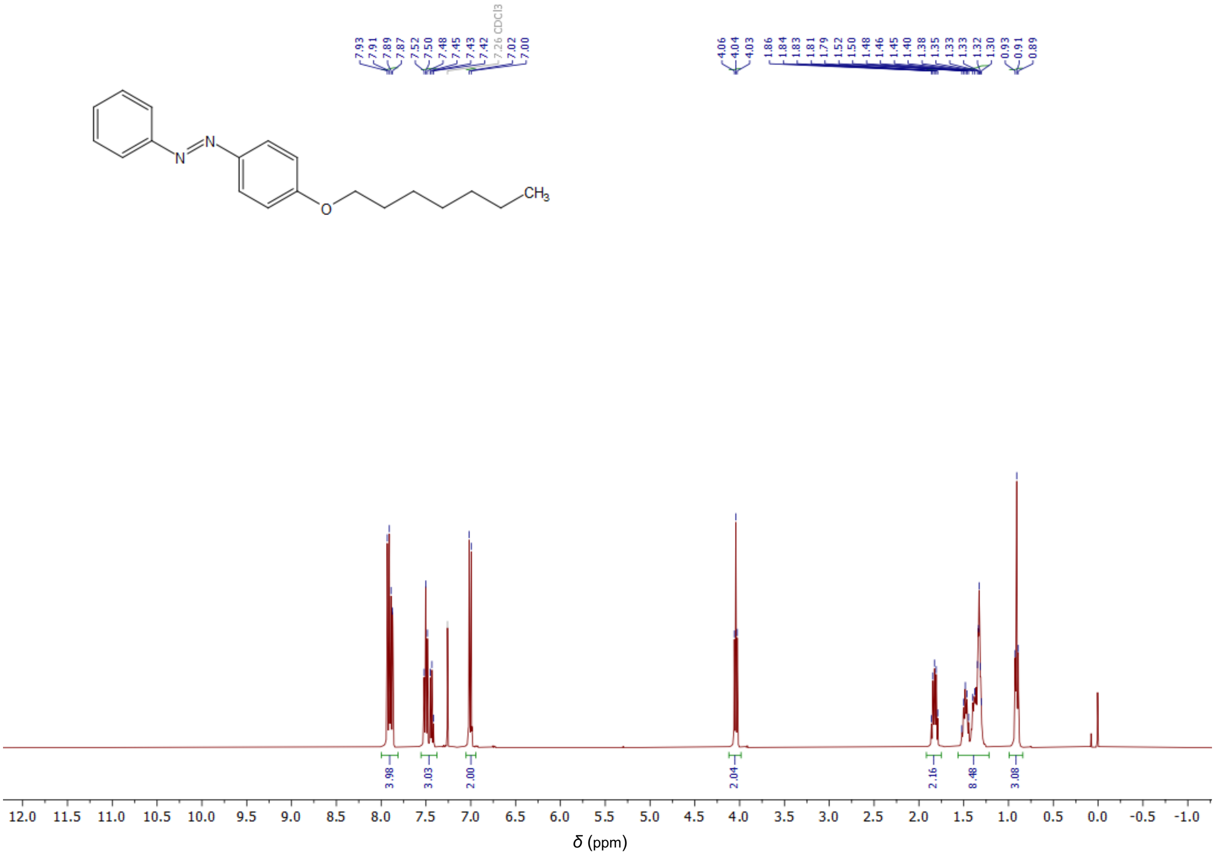
^{1}H-NMR of *p*-OPen-Azobenzene (3b)



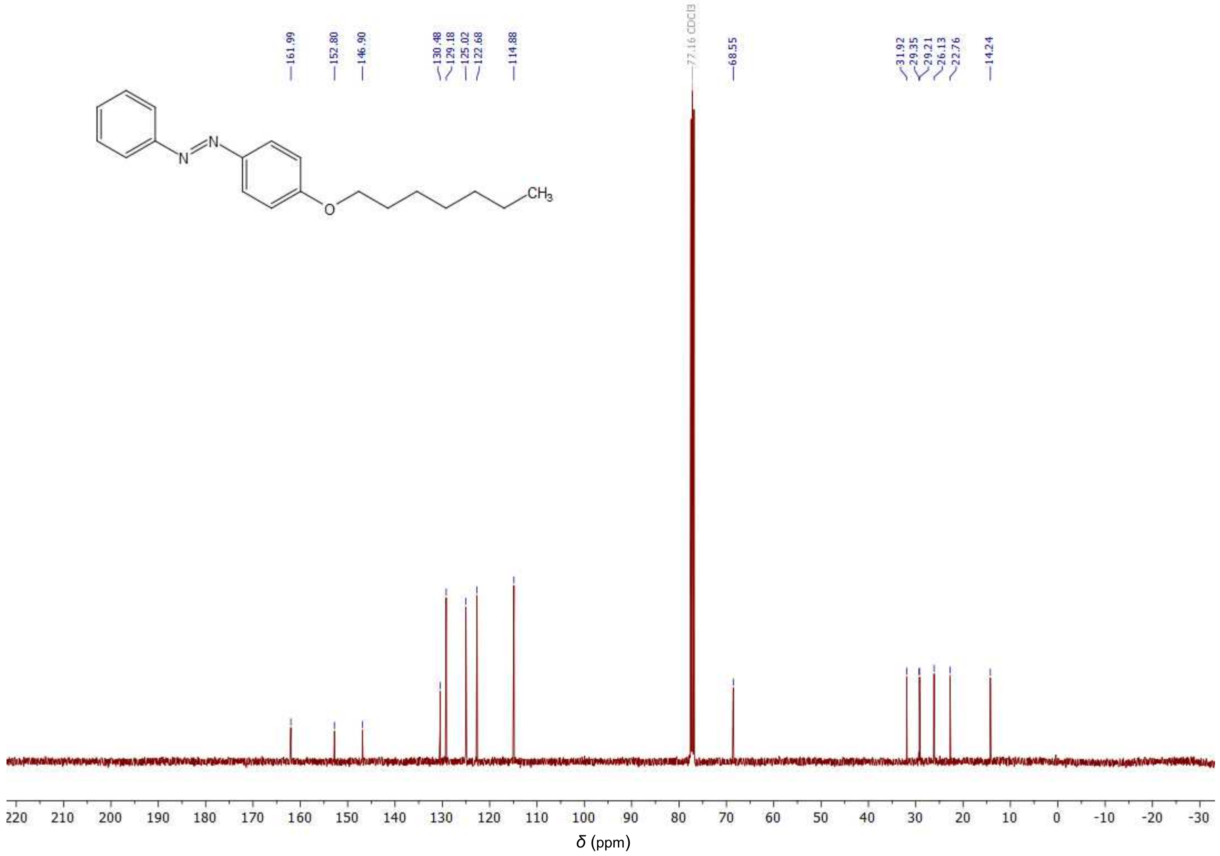
^{1}H-NMR of *p*-OHex-Azobenzene (3c)



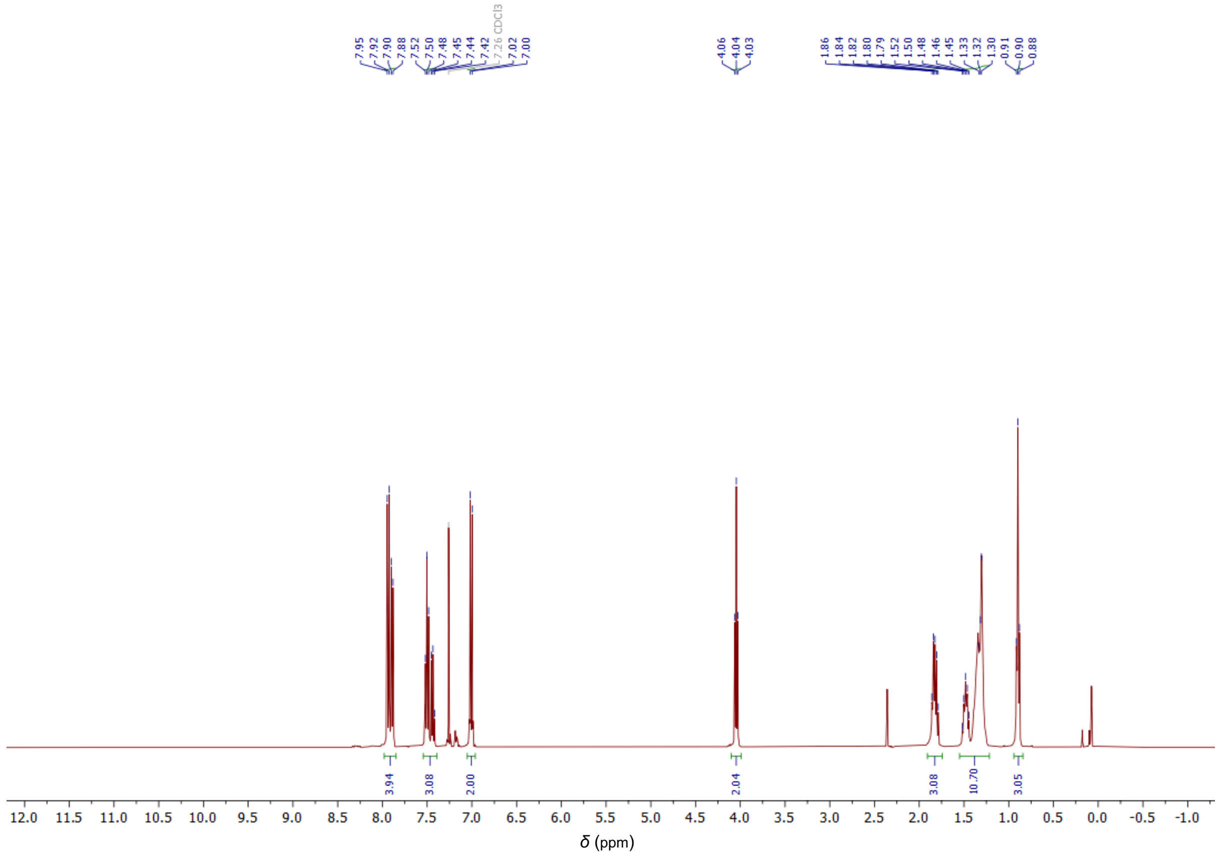
^{1}H-NMR of *p*-OHep-Azobenzene (3d)



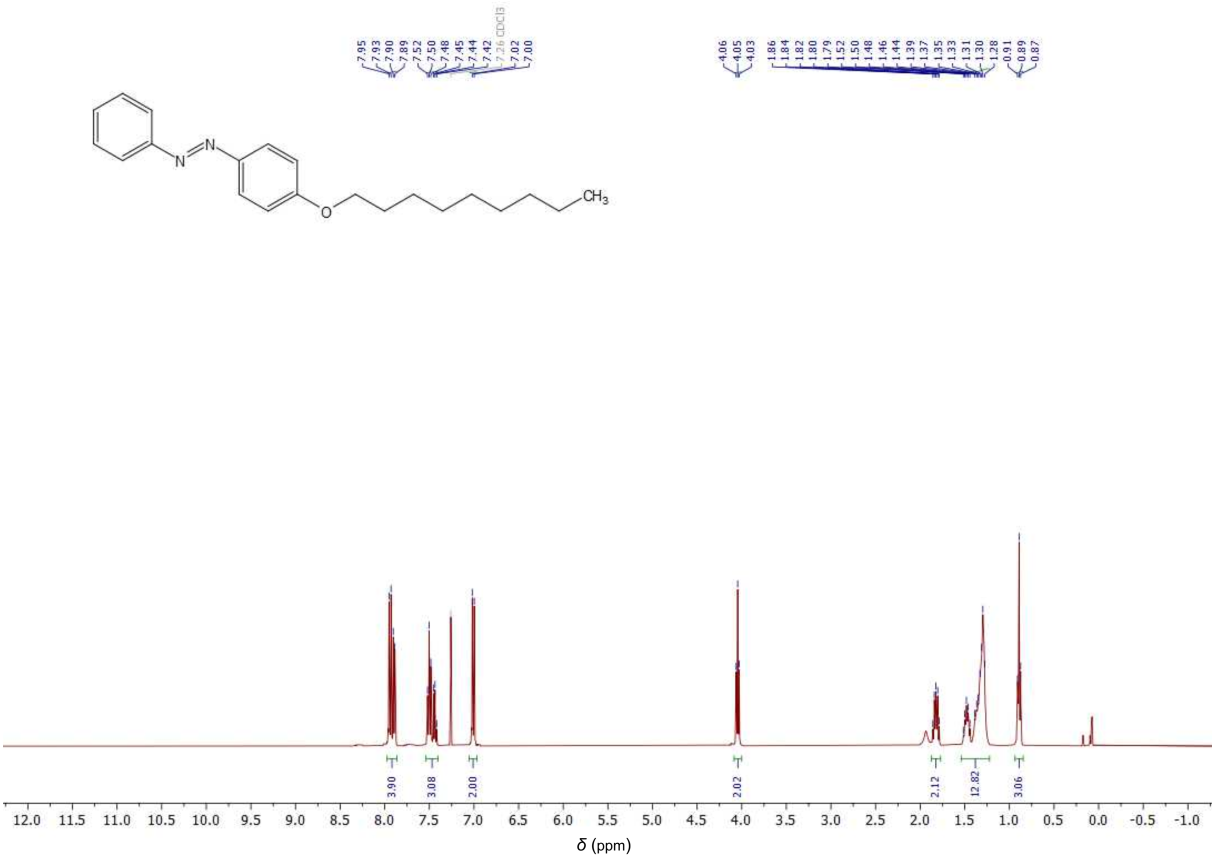
^{13}C-NMR of *p*-OHep-Azobenzene (3d)



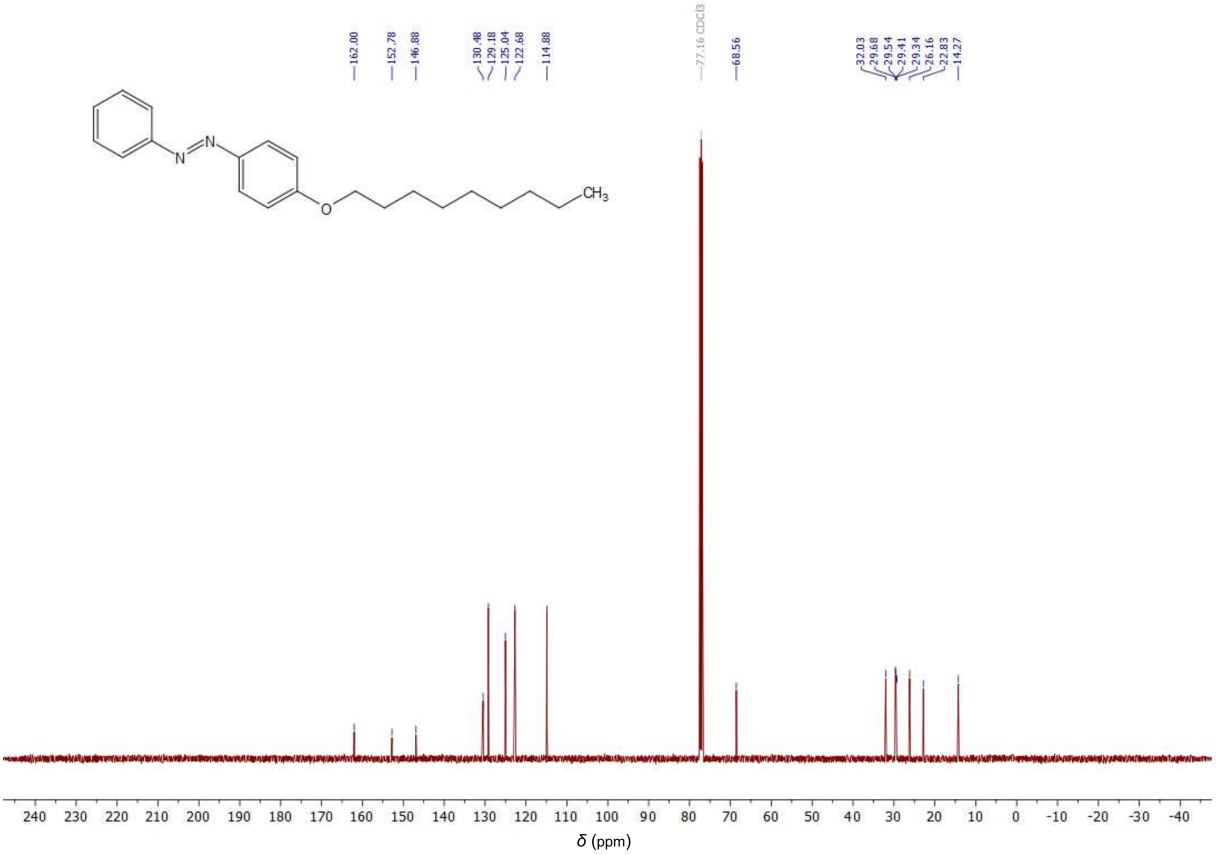
^{1}H-NMR of *p*-OOct-Azobenzene (3e)



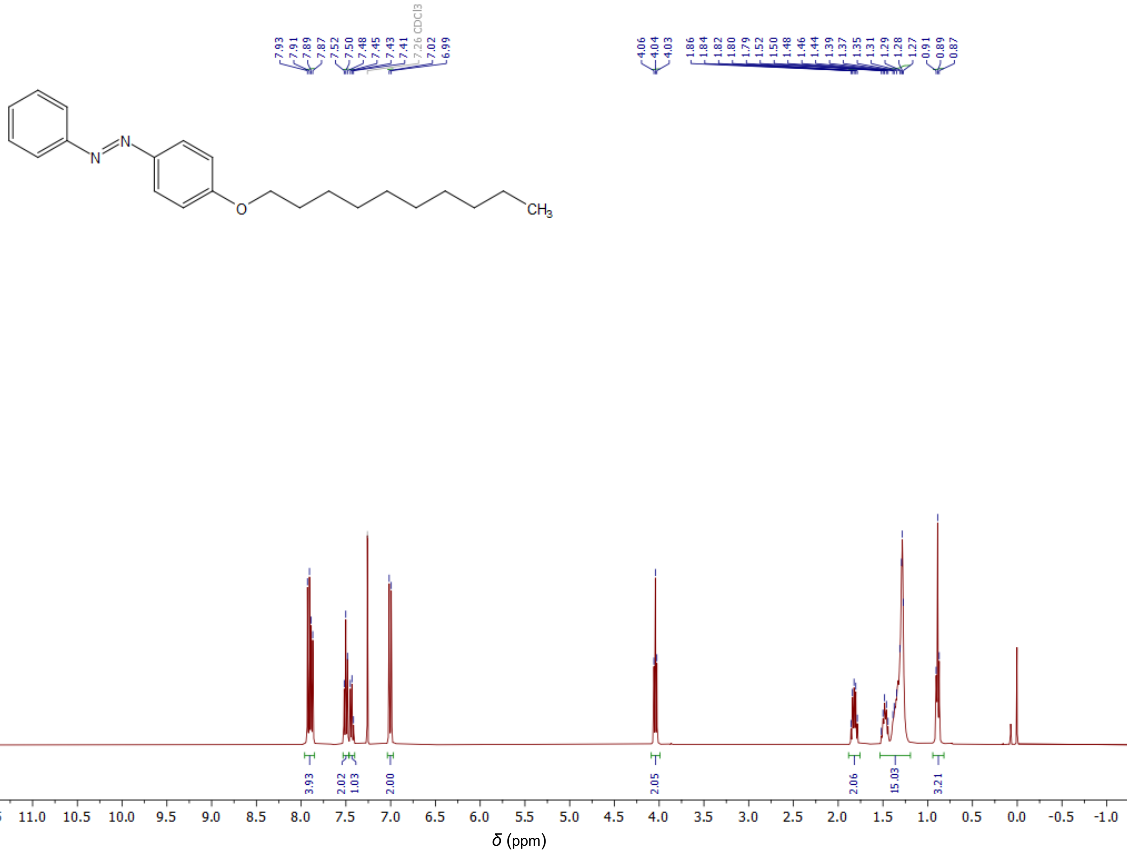
^{1}H-NMR of *p*-ONon-Azobenzene (3f)



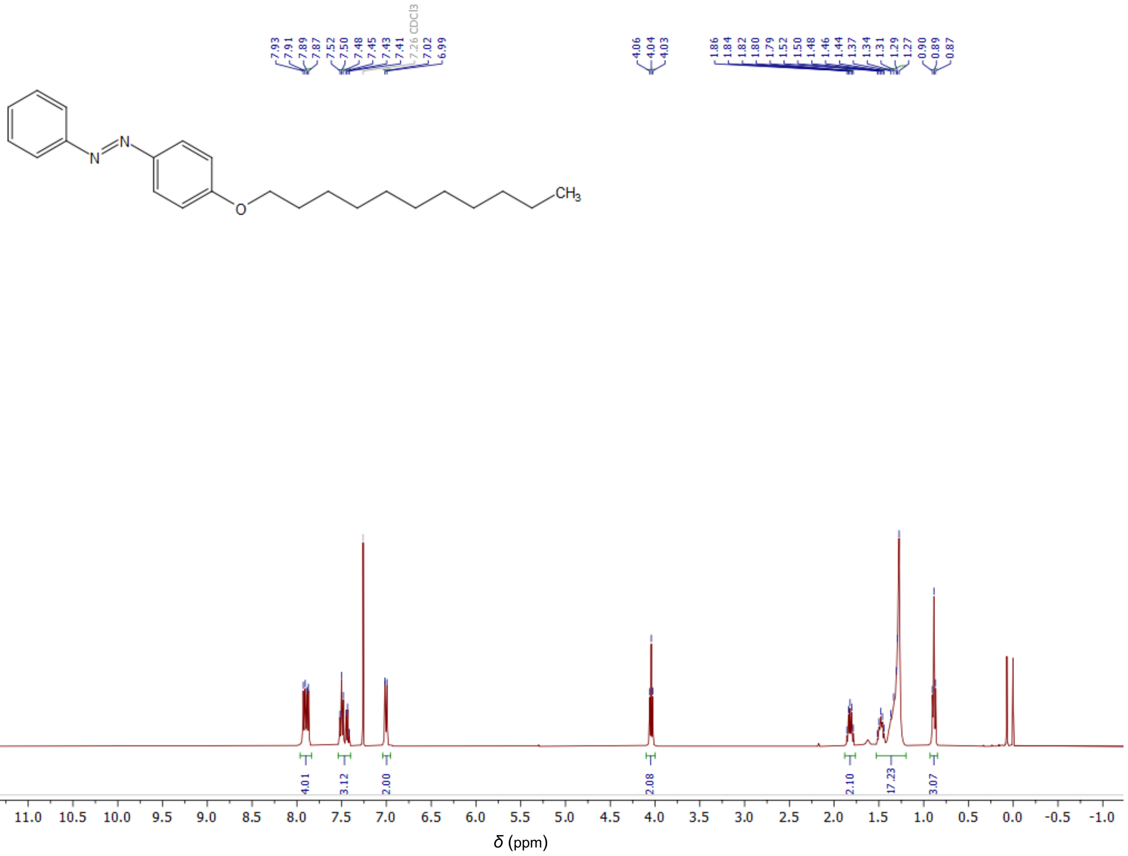
^{13}C-NMR of *p*-ONon-Azobenzene (3f)



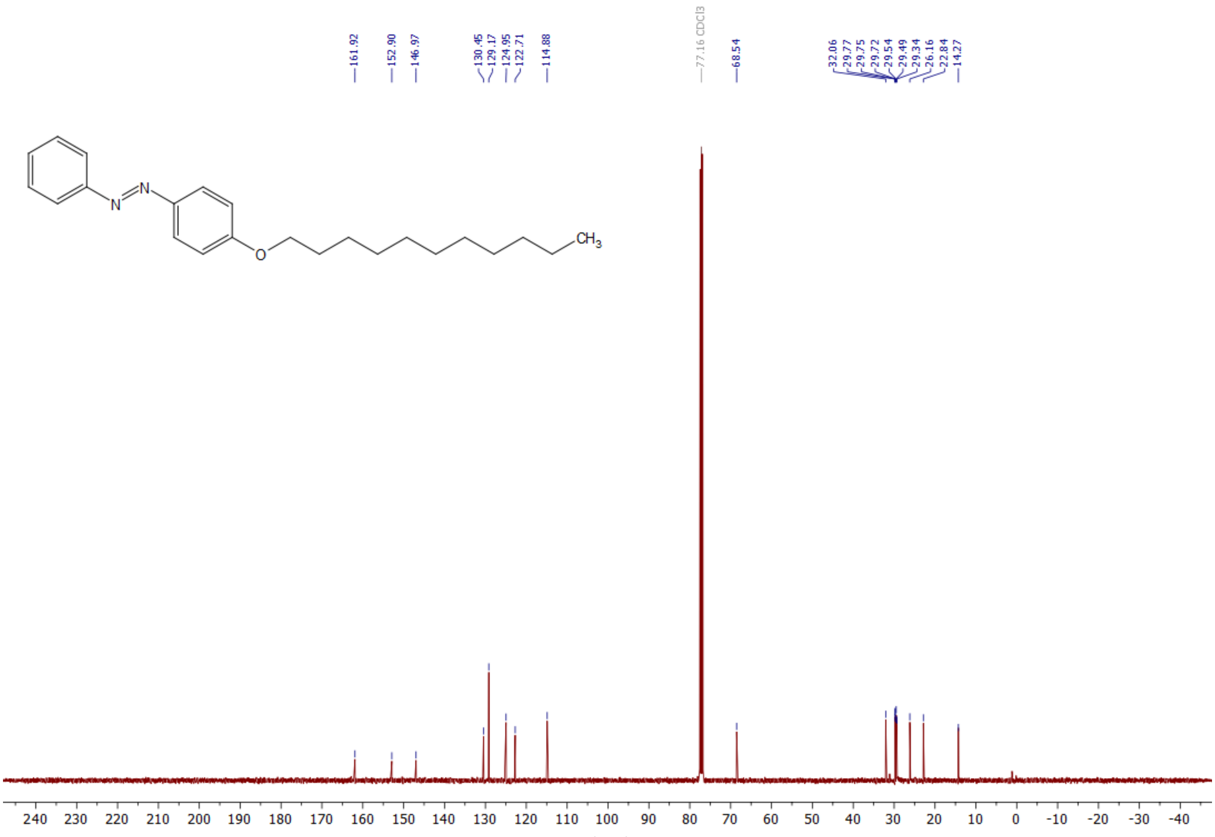
^{1}H-NMR of *p*-ODec-Azobenzene (3g)



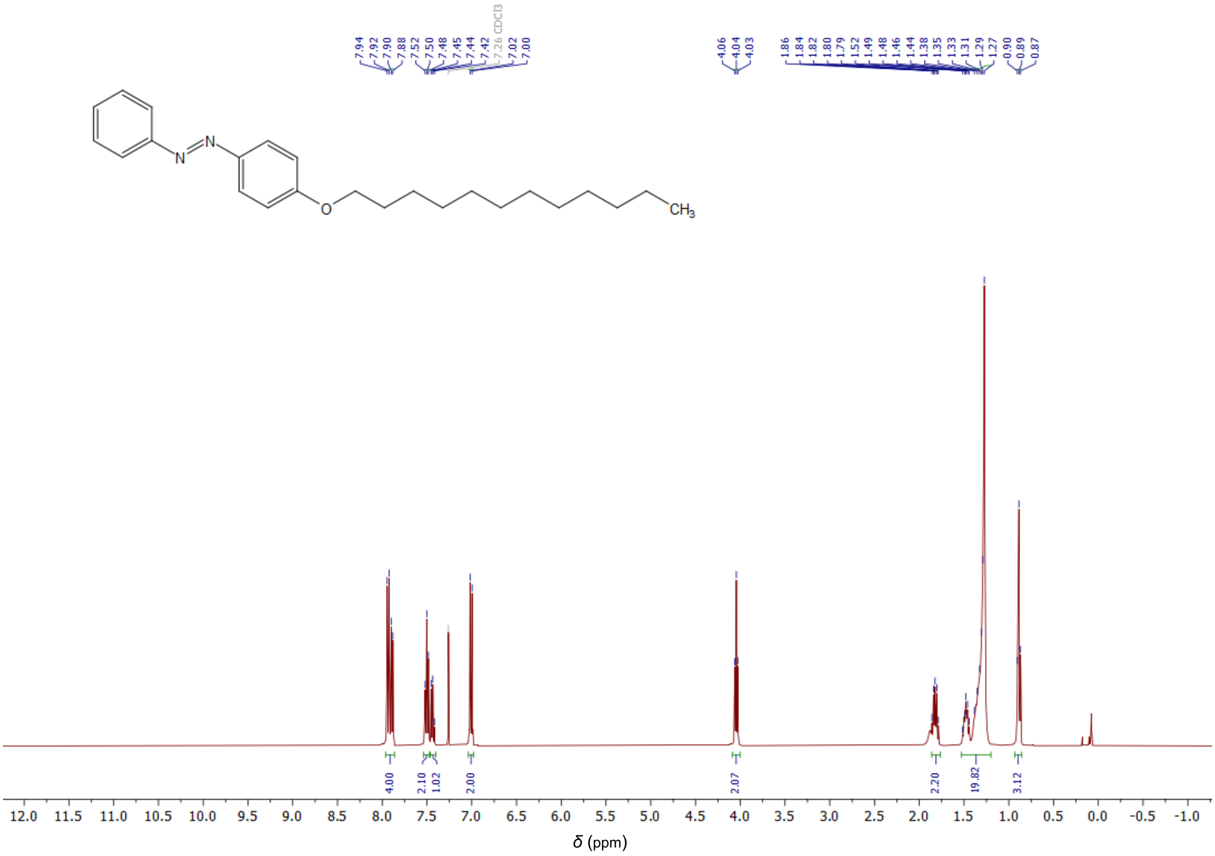
^{1}H-NMR of *p*-OUndec-Azobenzene (3h)



^{12}C-NMR of *p*-OUndec-Azobenzene (3h)



^{1}H-NMR of *p*-ODodec-Azobenzene (3i)



4. Melting Points

Table S1: Threefold determination of melting points for each *p*-alkoxy-ABs.

Compound	1. T_m [°C]	2. T_m [°C]	3. T_m [°C]	⌀ T_m [°C]
p-OMe-AB	55.0	54.9	55.0	55.0
p-OBu-AB	64.4	64.3	64.3	64.3
p-OPen-AB	59.9	60.0	60.1	60.0
p-OHex-AB	57.3	57.3	57.2	57.3
p-OHep-AB	71.1	70.8	71.1	71.0
p-OOct-AB	72.2	72.0	72.2	72.1
p-ONon-AB	78.4	78.6	78.4	78.5
p-ODec-AB	63.0	63.1	63.0	63.0
p-OUndec-AB	75.2	75.1	75.4	75.2
p-Dodec-AB	70.6	70.4	70.4	70.5

5. Irradiation experiments

NMR tubes or UV-Vis samples were irradiated in a custom in-house built box using high power LEDs by Thorlabs powered with T-Cube™ LED Driver with Trigger Mode with max. 1200 mA. After the specified irradiation times, the samples were immediately placed and measured in the corresponding spectrometer. The neat compounds were irradiated on a glass slide with a standard size according to DIN ISO 8037/1. For the use of thin films, the compounds were thermally melted between two glass plates, which allowed a better observation of the photoliquefaction.

Table S2: LEDs used for all irradiation experiments with their specifications.

λ_{max} / nm	$\Delta\lambda$FWHM / nm	Luminous Flux / mW	Product name
265	11	3036	M265L5
300	20	2275	M300L4
325	12	3120	M325L5
365	9	3850	M365L3
385	11	3700	M385L3
405	12.5	3400	M405L4
530	35	3600	M530L4
660	20	3120	M660L4

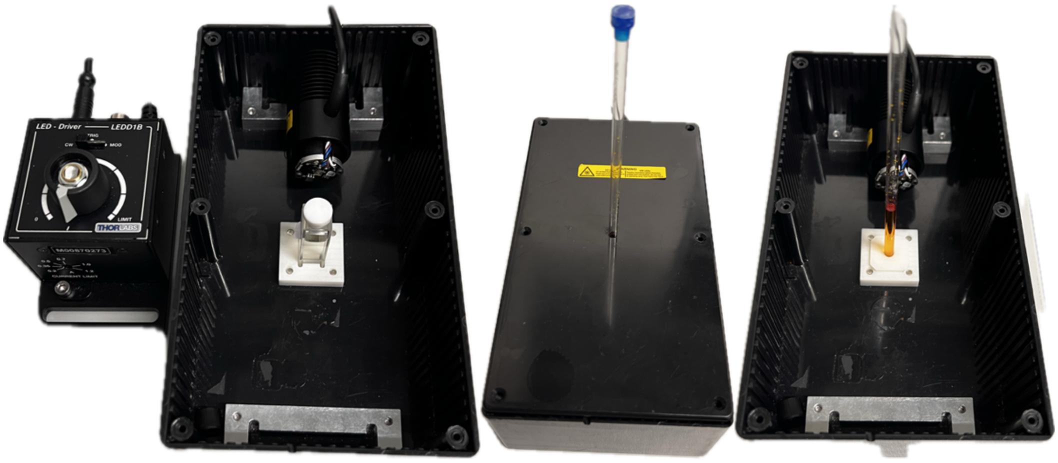


Figure S1: In-house build LED irradiation box for UV-Vis cuvettes and NMR tubes.

For the irradiation experiments of the neat compounds, the respective *p*-alkoxy-AB were placed on a glass slide as a thin layer and irradiated with an LED at a variable distance. For the preparation of the thin layers each compound was grinded to obtain an even distributed particle size. To obtain an even and thin layer the fine powders were placed between two glass slides which were pressed together. The exact thickness of the layer and particle size were not determined for the irradiation experiments.

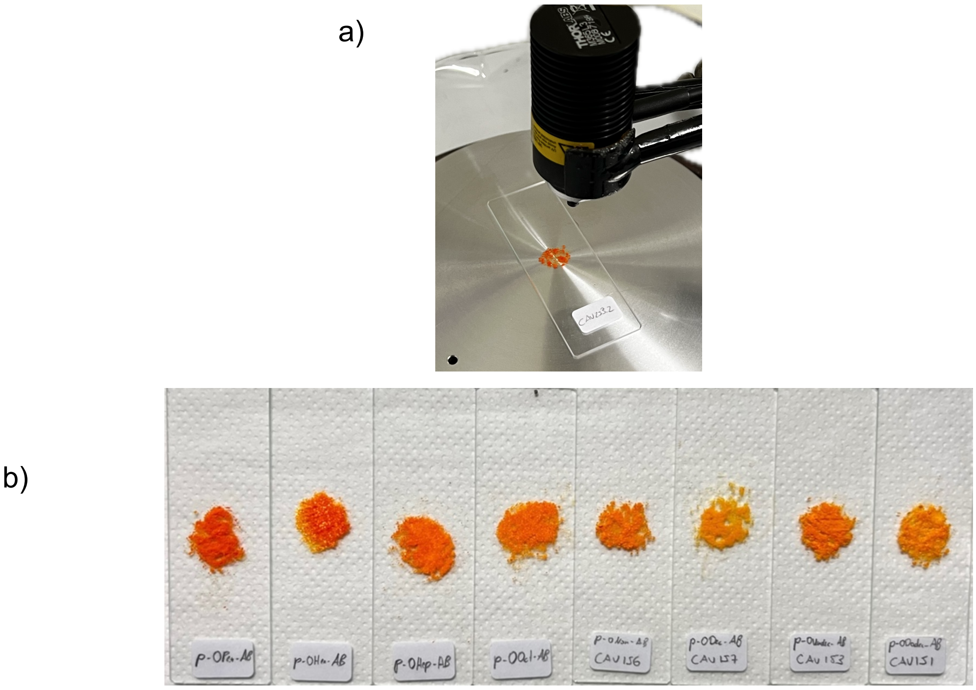


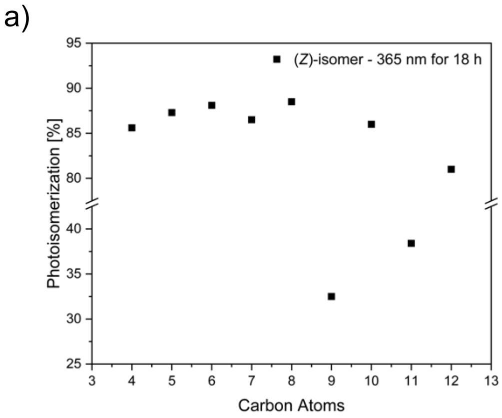
Figure S2: a) Irradiation of neat compounds on glass slides with 365 nm with 3850 mW on temperature-controlled aluminum block with a distance of about 15 cm and b) prepared samples for irradiation experiments.

To assess the photoliquefaction of the neat compounds, the respective *p*-alkoxy-AB were applied as thin layer of powder on a slide and then irradiated at room temperature for approx.

18 h at a wavelength of 365 nm. To exclude thermal effects, the LEDs were placed at a distance of approx. 15 cm above the sample. To determine the degree of photoisomerization, the content of the (*E*)- and (*Z*)-isomers was determined by ^{1}H-NMR spectroscopy. For the irradiation experiments at different ambient temperatures the compounds were thermally melted between two glass plates. The compound was placed on a glass slide and heated until it melted. A second glass plate was then placed on top of the melted compound. The capillary action was used to produce thin and uniform thin films (see Figure S3 a). The thin films were placed on a temperature-controlled aluminum block and then irradiated with 365 nm at a distance of approx. 15 cm. For irradiation at temperatures below room temperature an additional nitrogen stream was used to prevent condensation of water. The thin films were irradiated overnight. By using thin films, successful photoliquefication could be better evaluated. The thickness of the thin films and the composition after irradiation was not determined.

Table S3: Determination of composition of *p*-alkoxy-ABs after irradiation of the solid compound with 365 nm for 18 h at rt *via* ^{1}H-NMR spectroscopy.

Compound	Signal 1 (*E*)-isomer	Signal 1 (*Z*)-isomer	(*Z*)-isomer / %	Signal 2 (*E*)-isomer	Signal 2 (*Z*)-isomer	(*Z*)-isomer / %	Mean (*Z*)-isomer / %
OBu	0.33	2.00	85.8	0.34	1.99	85.4	85.6
OPen	0.32	2.00	86.2	0.25	1.91	88.4	87.3
OHex	0.28	2.00	87.7	0.26	1.98	88.4	88.1
OHep	0.32	2.00	86.2	0.30	1.97	86.8	86.5
OOct	0.26	2.00	88.5	0.26	2.01	88.5	88.5
ONon	2.00	0.95	32.2	2.00	0.98	32.9	**32.5**
ODec	0.35	2.00	85.1	0.30	1.98	86.8	86.0
OUndec	3.25	2.00	38.1	3.21	2.03	38.7	**38.4**
ODodec	0.47	2.00	81.0	0.47	2.01	81.0	81.0



b)

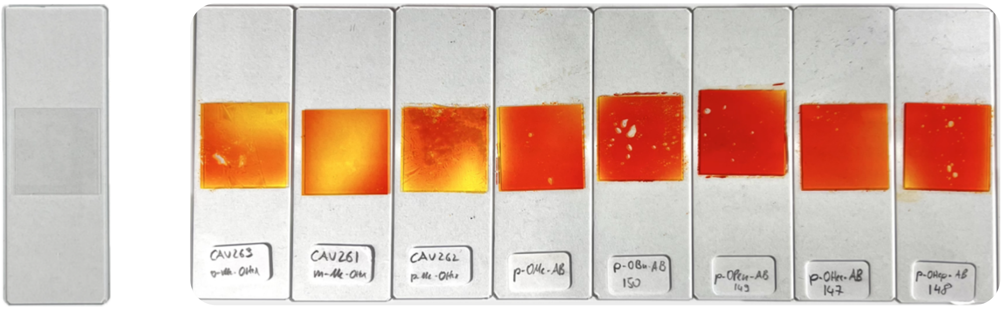
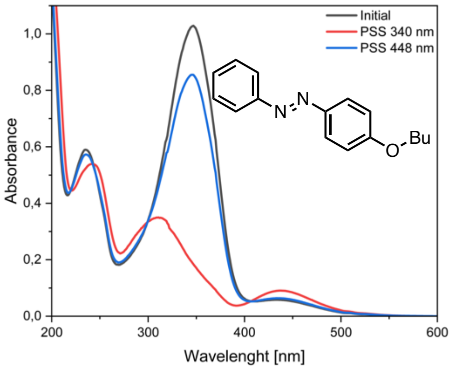
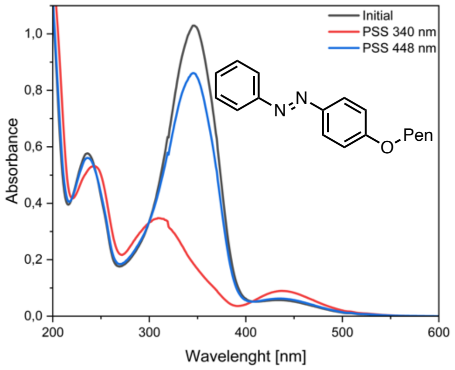


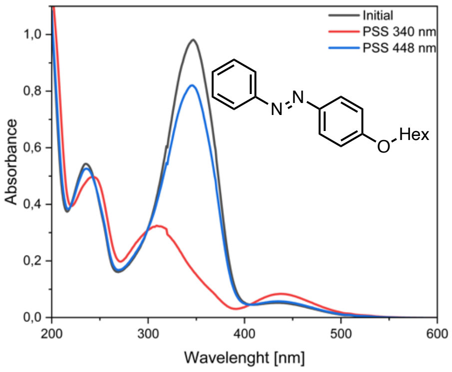
Figure S3: a) Content of (*Z*)-isomer after irradiation with 365 nm with 3850 mW for 18 h at rt on temperature-controlled aluminum block with a distance of about 15 cm and b) testing photoliquefication of neat compounds between two glass slides after photoliquefication.

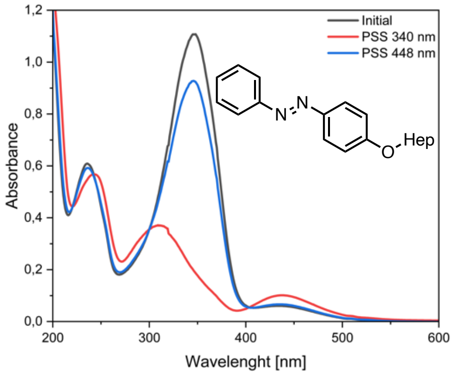
6. UV-Vis spectroscopy

The UV-Vis absorption spectra in solution were recorded using a SPECORD® 200 PLUS UV-Vis spectrophotometer equipped with two automatic eightfold cell changers and a Peltier thermostat system for temperature control manufactured by Analytik Jena. The spectrophotometer system was operated by the software Aspect UV from Analytik Jena. The samples were measured in QS High Precision Cells made of Quartz Suprasil® by Hellma Analytics with a light path of 10 mm. The sample volume was 3 mL and the sample concentration 5 x 10^{-5} M. As solvent UV-Vis grated acetonitrile and water was used from VWR chemicals was used.









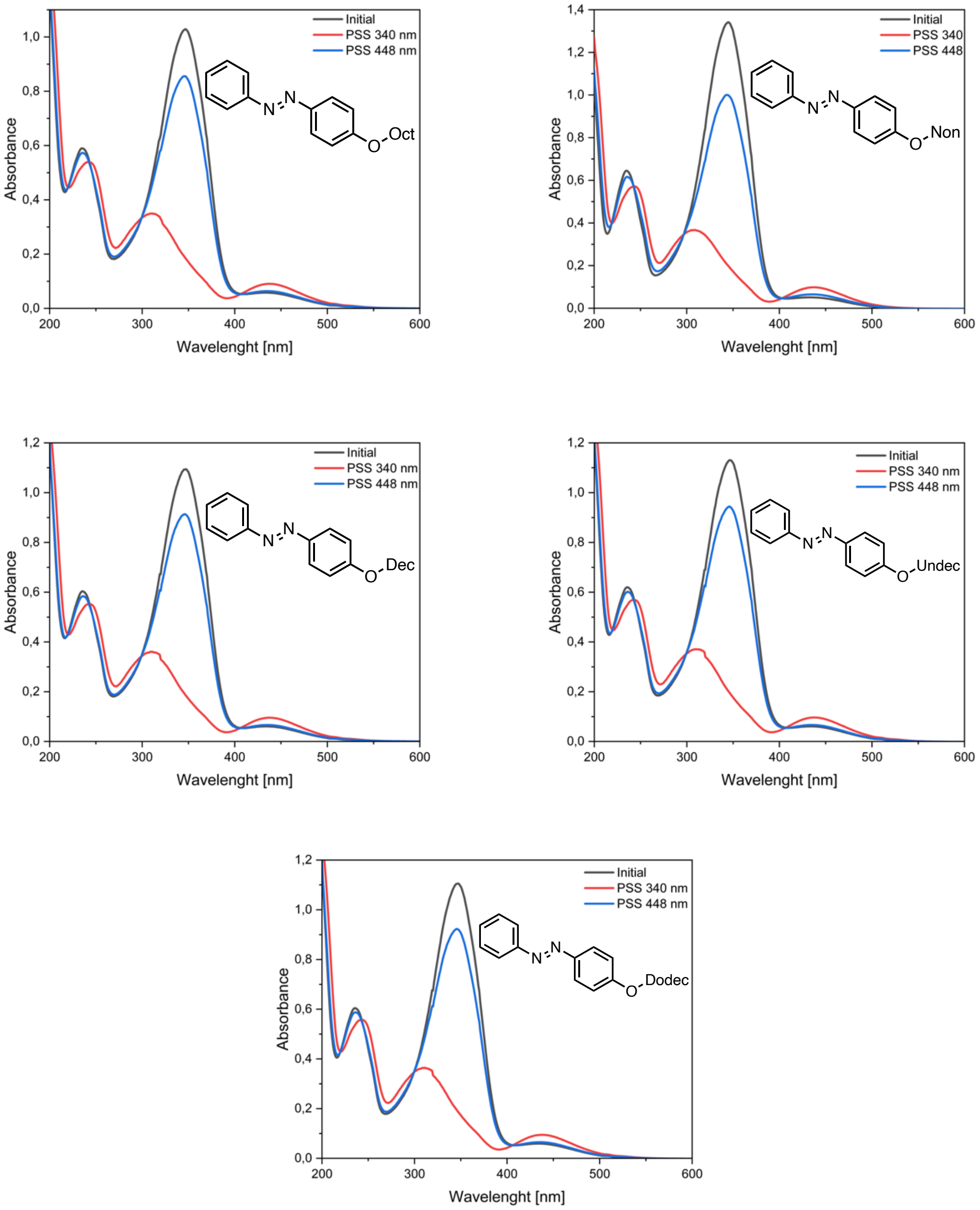


Figure S4: a) UV-Vis absorption spectra of *p*-alkoxy-AB in ACN.

UV-Vis absorption spectra of the neat compounds were conducted with thin films. The samples were measured in between two QS High Precision Rectangular Windows made of Quartz Suprasil® by Hellma Analytics with a thickness of 1.25 mm, which were places in a cell holder for demountable Hellma® High Precision rectangular Cell Type 106. Approx. 5 mg of the sample was heated to the melting point on the glass slides using a hotplate. The second glass plate was then placed on top to create a thin film. Gentle pressure was applied to the two glass plates to produce a uniform and consistent thin film. After the sample had cooled down, the two glass plates were inserted into the cuvette holder. The sample was then irradiated with 365 nm and then 448 nm at short intervals. Absorption spectra were measured between the time intervals. This process was repeated until no further change in the absorption spectrum was detected.

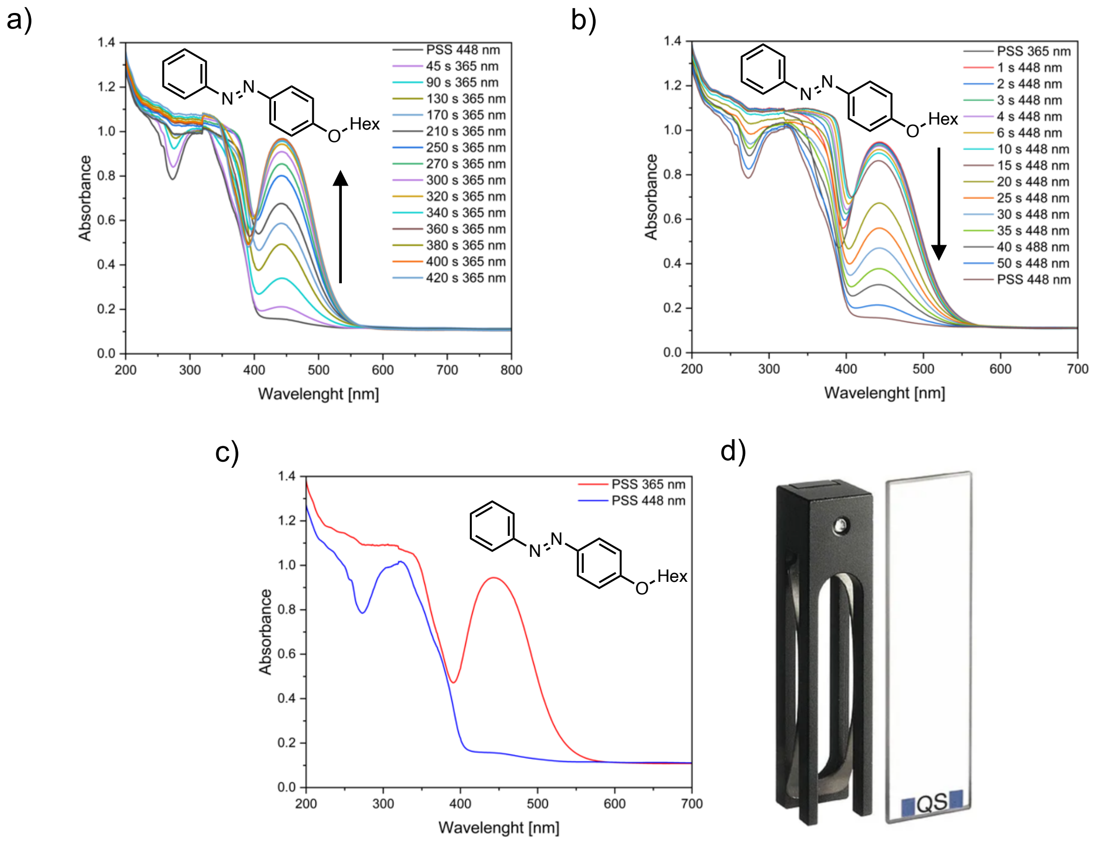


Figure S5: UV-Vis Absorption spectra of a thin film of *p*-OHex-AB for a) photoliquefication with 365 nm and b) back switching with 448 nm and c) the corresponding PSS and d) Used rectangular Window and a cell holder.

7. Half-life in solution *via* UV-Vis spectroscopy

All samples were irradiated at the corresponding wavelengths for 5-10 min prior to the kinetic measurements. UV-Vis absorption spectra were recorded from 200 – 600 nm with a scan speed of 20 nm/s. The thermal isomerization was monitored in 30 min intervals at 25 °C for 40 h. All compounds were measured three-fold at concentrations of $3 \cdot 10^{-5}$ mol/L in acetonitrile. For data analysis, Origin Pro 2023 by Origin Lab Corporation was used. The absorbances *A* at the absorption maxima of 346 nm were plotted against the time *t* elapsed after the start of the measurements. Rate constants *k* and half-lives $t_{1/2}$ were determined after fitting the data with an Exponential Decay Function (ExpDec1, Origin) according to the literature.

$$y = y_0 + A_1 \cdot e^{-x/t_1}$$

Equation S1: Exponential Decay 1 function of Origin.

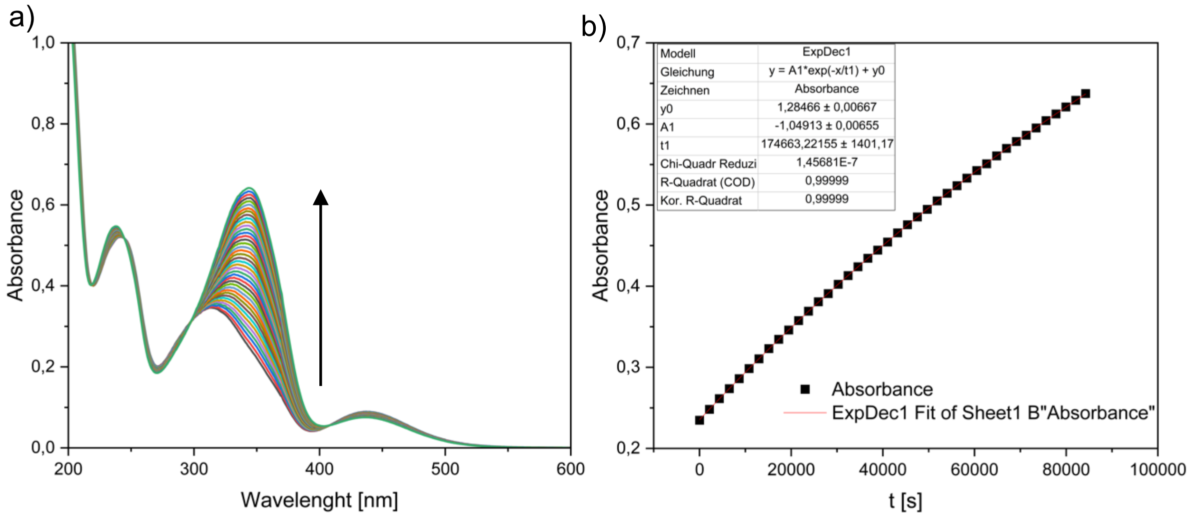
The exponential time constant t_1 was obtained by fitting the change in absorbance at 346 nm vs. time. The time constant t_1 was further used to calculate the rate constant k by Equation S2 and the half-life $t_{1/2}$ by Equation S3.

$$k = 1 / t_1$$

Equation S2: Calculation of rate constant *k*.

$$t_{1/2} = \ln 2 \cdot t_1$$

Equation S3: Calculation of half-life $t_{1/2}$.



Modell	ExpDec1
Gleichung	y = A1*exp(-x/t1) + y0
Zeichnen	Absorbance
y0	1,28466 ± 0,00667
A1	-1,04913 ± 0,00655
t1	174663,22155 ± 1401,17
Chi-Quadr Reduzi	1,45681E-7
R-Quadrat (COD)	0,99999
Kor. R-Quadrat	0,99999

Figure S6: a) Example of UV-Vis absorption spectra during thermal relaxation at 25 °C in ACN and b) change of the absorption maxima at 346 nm.

Table S4: Kinetic constants at 25 °C for *p*-alkoxy-ABs in ACN 3 x 10^{-5} M.

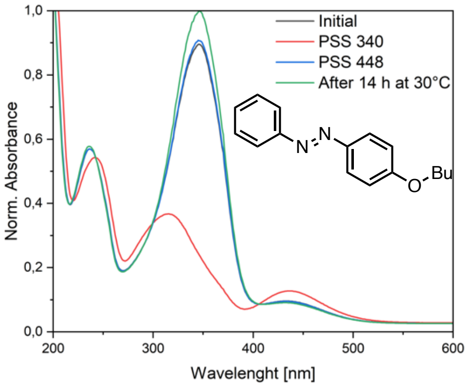
Compound	1. k / 10^{-6} s^{-1}	2. k / 10^{-6} s^{-1}	3. k / 10^{-6} s^{-1}	⌀k / 10^{-6} s^{-1}	σ k / 10^{-6} s^{-1}
OBu	3.58	3.04	3.24	3.29	2.2
OPen	3.95	3.89	4.09	3.98	0.8
OHex	3.22	3.14	3.10	3.15	0.5
OHep	3.49	3.75	3.91	3.71	1.7
OOct	3.12	3.11	3.18	3.14	0.3
ONon	3.44	3.32	3.45	3.40	0.6
ODec	3.22	3.11	3.13	3.15	0.5
OUndec	3.44	3.24	3.38	3.35	0.8
ODodec	3.52	2.99	3.43	3.31	2.3

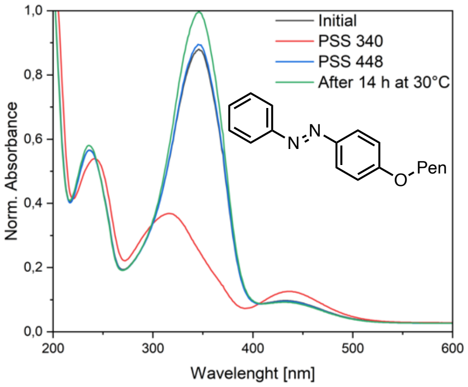
Table S5: Half-lives at 25 °C for *p*-alkoxy-ABs in ACN 3 x 10^{-5} M.

Compound	1. $t_{1/2}$ / h	2. $t_{1/2}$ / h	3. $t_{1/2}$ / h	$\varnothing$ $t_{1/2}$ / h	σ $t_{1/2}$ / h
OBu	53.83	63.34	59.43	58.9	3.9
OPen	48.69	49.45	47.11	48.4	1.0
OHex	59.72	61.42	62.12	61.1	1.0
OHep	55.24	51.41	49.26	52.0	2.5
OOct	61.74	61.90	60.46	61.4	0.6
ONon	55.99	58.07	55.89	56.7	1.0
ODec	59.81	61.96	61.52	61.1	0.9
OUndec	55.93	59.49	57.04	57.5	1.5
ODodec	54.75	64.42	56.17	58.5	4.3

8. Determination of PSS in solution and neat *via* HPLC

The PSS isomer concentrations were determined with a Shimadzu LCMS-2020 system using a 150 x 4 mm Eurospher 100^{-5} C18 column with acetonitrile/water (90:10) as isocratic eluent (1.5 mL/min). Detection was carried out using a Shimadzu SPD-M20A diode array detector at the previously determined isosbestic wavelengths. Therefore, a UV-Vis absorption spectra was measured each compound in acetonitrile (see Figure S4) and acetonitrile/water (90:10) (see Figure S7). The change from pure acetonitrile to acetonitrile/water (90:10) in the separation had only a negligible effect on the isosbestic wavelengths.





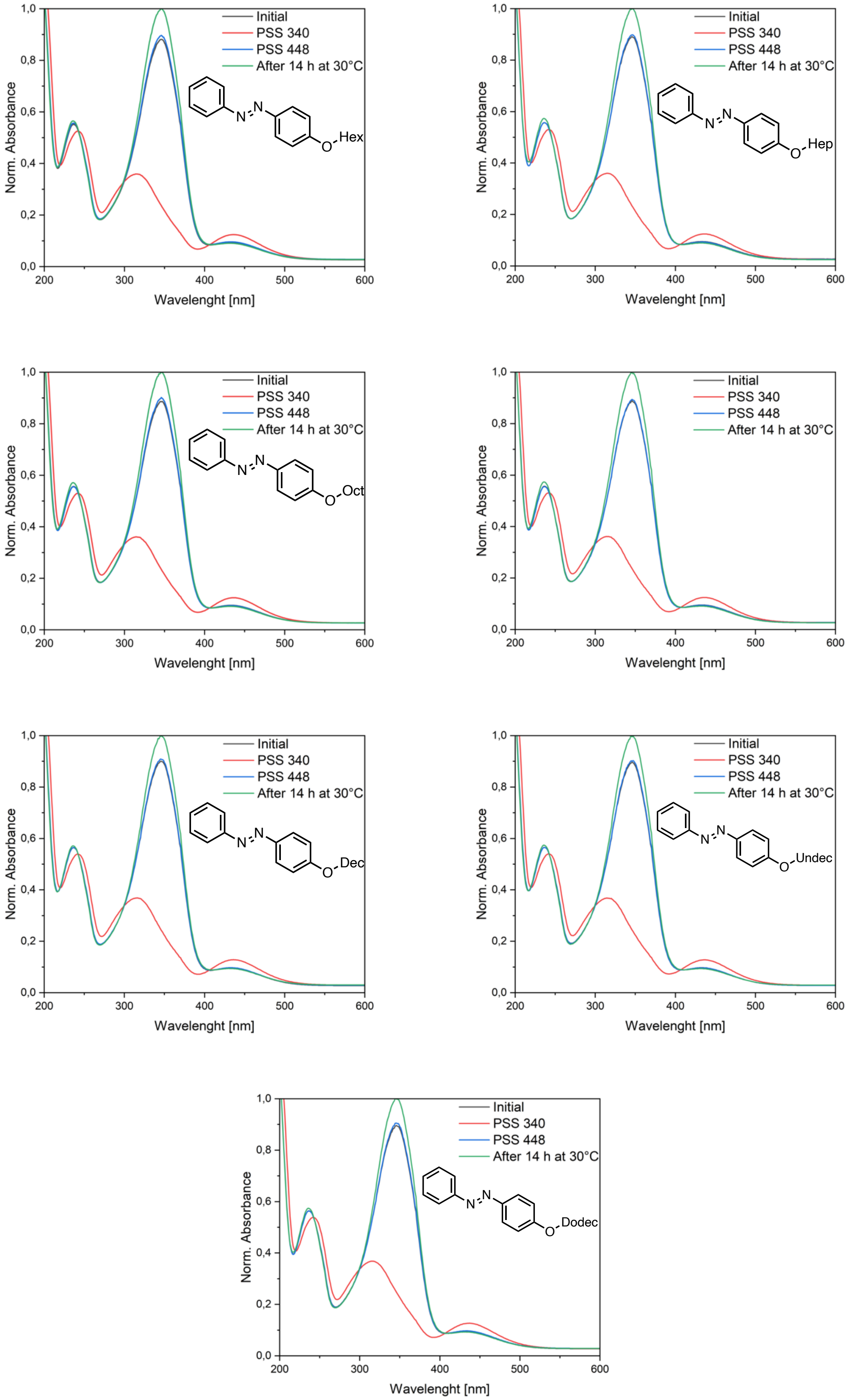


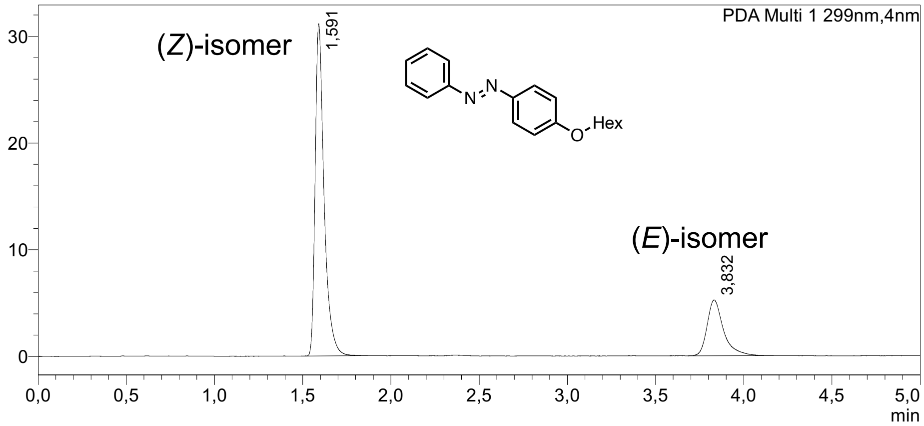
Figure S7: UV-Vis Absorption spectra of corresponding *p*-alkoxy-ABs in ACN:H_2O (90:10) with a concentration of 5 x 10^{-5} M.

Table S6: Isosbestic points of *p*-alkoxy-ABs in ACN:H_2O (90:10) for determination of the composition of (*E*)- and (*Z*)-isomers *via* HPLC.

Compound	Isosbestic point / nm
p-OBu-AB	299
p-OPen-AB	299
p-OHex-AB	299
p-OHep-AB	299
p-OOct-AB	299
p-ONon-AB	299
p-OUndec-AB	300
p-ODodec-AB	300

By integration of the signals of the respective isomers in the PSS for 340 nm and 448 nm in the chromatogram at the wavelength of the isosbestic point, the composition of the isomers was determined. The samples were dissolved in 2 mL glass vials in acetonitrile with a concentration of $5 \cdot 10^{-4}$ mol/L, from which aliquots of 10 µL were injected for analysis. For all determined isomer ratios, an error of ±1% is assumed. Each dissolved sample was irradiated with 340 nm or 448 nm for 5 - 10 min.

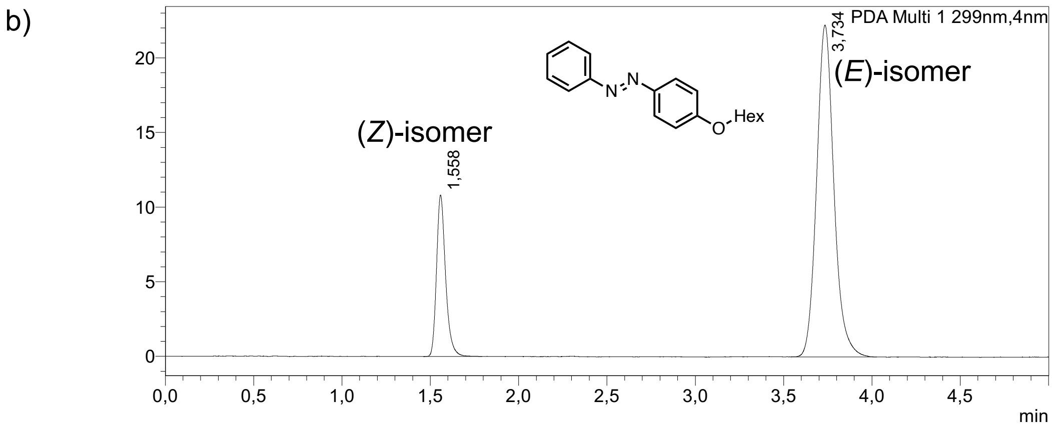
a)



Peak Table

PDA Ch1 299nm

Peak#	Ret. Time	Area	Height	Conc.
1	1,591	109622	30596	76,364
2	3,832	33931	5211	23,636
Total		143553	35807	



Peak Table

PDA Ch1 299nm

Peak#	Ret. Time	Area	Height	Conc.
1	1,558	38700	10605	20,385
2	3,734	151147	22117	79,615
Total		189847	32722	

Figure S8: Example of chromatograms of the PSSs of *p*-OHex-AB, detected at the isosbestic wavelength of 299 nm a) after irradiation with 340 nm for 5 min and b) after irradiation with 448 nm for 5 min.

Table S7: Threefold determination of the PSS at 340 nm and 448 nm in ACN *via* HPLC.

		PSS_{340} / %		PSS_{448} / %	
		(*E*)-Isomer	(*Z*)-Isomer	(*E*)-Isomer	(*Z*)-Isomer
p-OBu-AB	Run 1	23.6	76.4	79.6	20.4
	Run 2	22.9	77.1	79.6	20.4
	Run 3	22.7	77.3	79.6	20.4
	Mean	23.1	76.9	79.6	20.4
	Δ	0.4	0.4	0	0
p-OPen-AB	Run 1	23.2	76.8	79.6	20.4
	Run 2	22.9	77.1	79.6	20.4
	Run 3	22.7	77.3	79.8	20.2
	Mean	22.9	77.1	79.7	20.3
	Δ	0.3	0.2	0.1	0.1
p-OHex-AB	Run 1	23.6	76.4	79.8	20.2
	Run 2	26.2	73.8	79.6	20.4
	Run 3	22.4	77.6	79.8	20.2
	Mean	24.1	75.9	79.7	20.3
	Δ	1.9	1.6	0.1	0.1
p-OHept-AB	Run 1	26.7	73.3	80.2	19.8
	Run 2	25.3	74.7	80.1	19.9
	Run 3	24.5	75.5	80.2	19.8
	Mean	25.5	74.5	80.2	19.8

	Δ	1.1	0.9	0.0	0.0
p-Oct-AB	Run 1	25.2	74.5	80.5	19.5
	Run 2	25.4	74.6	80.6	19.4
	Run 3	25.1	74.9	80.4	19.6
	Mean	25.3	74.7	80.5	19.5
	Δ	0.2	0.21	0.1	0.1
p-ONon-AB	Run 1	25.9	74.1	81.0	19.0
	Run 2	27.1	72.9	80.8	19.2
	Run 3	26.1	73.9	80.8	19.2
	Mean	26.4	73.6	80.9	19.1
	Δ	0.6	0.6	0.1	0.1
p-ODec-AB	Run 1	25.4	74.4	80.2	19.8
	Run 2	27.3	72.7	79.9	20.1
	Run 3	29.0	71.0	80.1	19.9
	Mean	27.3	72.7	80.1	19.9
	Δ	1.7	1.4	0.1	0.1
p-OUndec-AB	Run 1	27.0	73.0	81.1	18.9
	Run 2	26.8	73.2	80.8	19.2
	Run 3	27.2	72.8	81.3	18.7
	Mean	27.0	73.0	81.0	19.0
	Δ	0.2	0.2	0.2	0.2
p-ODodec-AB	Run 1	28.8	71.2	82.5	17.5
	Run 2	25.6	74.4	81.8	18.2
	Run 3	25.6	74.4	81.1	18.9
	Mean	26.7	73.3	81.8	18.2
	Δ	1.8	1.5	0.6	0.6

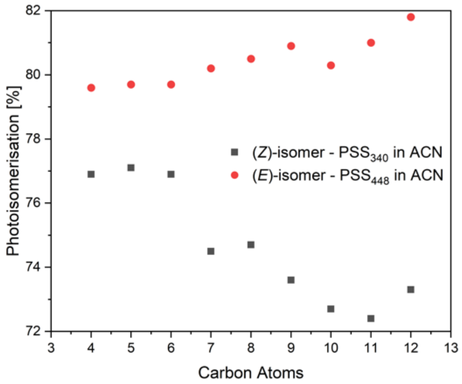


Figure S9: Content of (*E*)- and (*Z*)-Isomer at the PSS for 365 nm and 448 nm in ACN.

To determine the composition of the isomers at PSS$_{365}$ of the neat compounds, the solid *p*-alkoxy-AB was placed as a fine powder as a thin layer on a glass slide according to the procedure for the preparation of thin layers of the compounds on a glass slide explained in section 5. Irradiation experiments (see Figure S2a). Each compound was irradiated with a LED at 365 nm with a distance of approx. 10 cm at rt. The samples were irradiated until they fully turned into the liquid phase. Irradiation was continued until no further changes in composition could be detected *via* HPLC.

Table S8: Determination of the PSS at 365 nm of neat *p*-alkoxy-AB´s *via* HPLC.

Compound	(*Z*)-isomer / %
p-OBu-AB	91.6
p-OPen-AB	92.8
p-OHex-AB	93.3
p-OHep-AB	93.3
p-OOct-AB	93.8
p-ONon-AB	92.7
p-ODec-AB	94.5
p-OUndec-AB	93.5
p-ODodec-AB	94.4

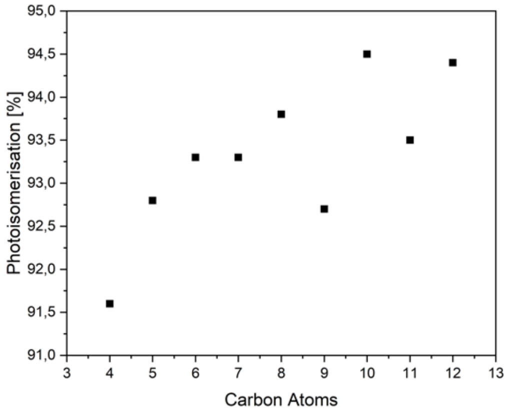


Figure S10: Content of (*Z*)-Isomer at the PSS_{365} after irradiation of neat *p*-alkoxy-AB with 365 nm with 3850 mW at rt on temperature-controlled aluminum black with a distance of about 10 cm.

9. Neat half-life *via* HPLC and UV-Vis spectroscopy

To determine the thermal half-life of the neat *p*-alkoxy-ABs, a thin powder layer of the respective compound was placed on a glass slide according to the procedure for the preparation of thin layers of the compounds on a glass slide explained in section 5. Irradiation experiments (see Figure S2 a). Each compound was irradiated overnight at a wavelength of 365 nm with a distance of about 10 cm at room temperature. Each compound was irradiated until no further changes in the composition of (*E*)- and (*Z*)-isomers was measured *via* HPCL. In an interval of 1 h aliquots of the respective compounds were taken with a spatula and dissolved in about 0.5 mL ACN in a 2 mL vial. The isomer composition was determined by HPLC. The measurements were taken over a period of 11 h at room temperature.

Figure S11: Irradiation setup for irradiation with 365 nm with 3850 mW at rt on temperature-controlled aluminum block with a distance of about 10 cm and neat samples before irradiation for kinetic measurements.

Table S9: Content of the (*Z*)-isomer during thermal relaxation at rt of neat *p*-OBu-AB.

Time / min	(*Z*)-Isomer / %	Time / min	(*Z*)-Isomer / %	Time / min	(*Z*)-Isomer / %
0	91.58	300	82.81	600	74.89
60	89.95	360	81.27	660	72.62
120	87.94	420	79.25	3020	34.92
180	86.39	480	77.38	3378	32.73
240	84.64	540	75.92	4585	24.37

Table S10: Content of the (*Z*)-isomer during thermal relaxation at rt of neat *p*-OPen-AB.

Time / min	(*Z*)-Isomer / %	Time / min	(*Z*)-Isomer / %	Time / min	(*Z*)-Isomer / %
0	92.44	360	81.95	1320	52.60
60	90.97	420	79.94	1440	57.60
120	88.89	480	78.26	3015	36.45
180	86.79	540	76.71	3373	34.57
240	85.21	600	75.33	4586	24.34
300	83.35	660	73.40		

Table S11: Content of the (*Z*)-isomer during thermal relaxation at rt of neat *p*-OHex-AB.

Time / min	(*Z*)-Isomer / %	Time / min	(*Z*)-Isomer / %	Time / min	(*Z*)-Isomer / %
0	93.21	360	81.60	1320	57.70
60	91.37	420	80.04	1440	51.00
120	89.13	480	78.89	3028	40.61
180	87.62	540	77.54	3369	35.92
240	85.67	600	75.71	4580	22.81
300	84.02	660	73.79		

Table S12: Content of the (*Z*)-isomer during thermal relaxation at rt of neat *p*-OHep-AB.

Time / min	(*Z*)-Isomer / %	Time / min	(*Z*)-Isomer / %	Time / min	(*Z*)-Isomer / %
0	93.93	360	82.86	3000	41.27
60	91.90	420	81.94	3365	29.57
120	90.00	480	80.32	4576	28.67
180	88.26	540	76.74		
240	86.34	600	74.99		
300	84.65	660	75.13		

Table S13: Content of the (*Z*)-isomer during thermal relaxation at rt of neat *p*-OOct-AB.

Time / min	(*Z*)-Isomer / %	Time / min	(*Z*)-Isomer / %	Time / min	(*Z*)-Isomer / %
0	94.01	360	82.18	660	69.90
60	91.99	420	80.49	1320	63.10
120	89.91	480	80.28	3004	29.40
180	88.10	490	79,10	3364	35.64
240	86.35	540	76.56	4576	28.19
300	84.79	600	69.00		

Table S14: Content of the (*Z*)-isomer during thermal relaxation at rt of neat *p*-ODec-AB.

Time / min	(*Z*)-Isomer / %	Time / min	(*Z*)-Isomer / %	Time / min	(*Z*)-Isomer / %
0	94.21	300	84.36	600	74.38
60	92.39	360	82.73	660	72.76
120	89.96	420	77.67	3008	40.08
180	88.39	480	77.31	3363	35.41
240	86.48	540	77.84	4580	32.48

The change of the concentration of the (*Z*)-isomers were plotted against the time t elapsed after the start of the measurements. Rate constants k and half-lives $t_{1/2}$ were determined after fitting the data with an Exponential Decay Function (ExpDec1, Origin). For data analysis, Origin Pro 2023 by Origin Lab Corporation was used. The exponential time constant t_1 was obtained by fitting the change in the concentration of the (*Z*)-isomers vs. time. The time constant t_1 was further used to calculate the rate constant k by Equation S2 and the half-life $t_{1/2}$ by Equation S3. For *p*-ONon-AB, *p*-Undec-AB and *p*-Dodec-AB non neat kinetic investigation was made do to decomposition.

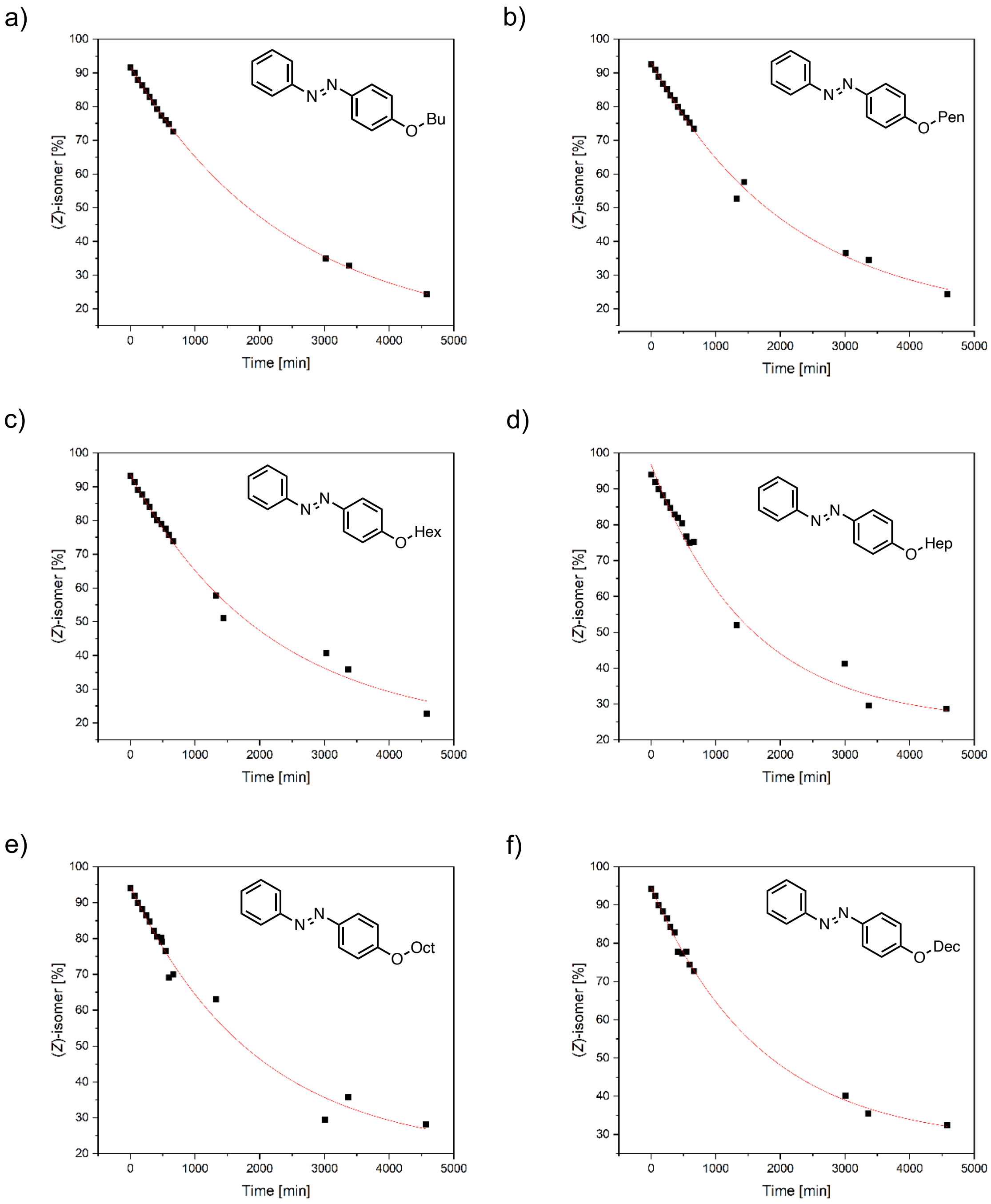


Figure S12: Thermal half-lives of neat *p*-alkoxy-AB at rt.

Table 15: Thermal half-lives of neat *p*-alkoxy-AB´s at rt.

Compound	*k* / 10^{-4} s^{-1}	σ *k* / 10^{-5} s^{-1}	$t_{1/2}$ / h	σ $t_{1/2}$ / h
p-OBu-AB	4.11	1.0	28.1	0.7
p-OPen-AB	4.68	4.4	24.7	2.3
p-OHex-AB	4.68	5,8	24.7	3.1
p-OHep-AB	6.59	10.1	17.5	2.7
p-OOct-AB	5.17	8.4	22.3	3.6
p-ODec-AB	5.95	3.8	19.4	1.2

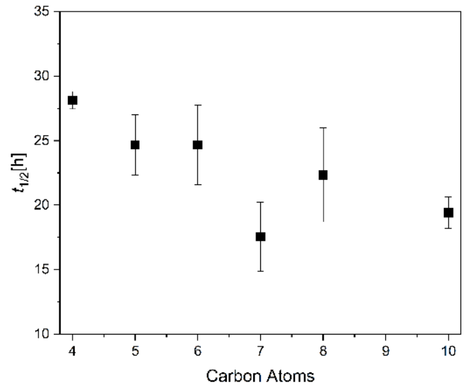


Figure S13: Thermal half-lives of neat *p*-alkoxy-AB at rt.

The change in the absorption spectrum of the neat compound during thermal relaxation was monitored by thin layer UV-Vis spectroscopy as described in section 6. UV-Vis spectroscopy. Therefore, *p*-OHex-AB was used as an example. The thin film was irradiated with 365 nm until the photostationary state was reached. The thermal isomerization was monitored in 60 min intervals at 25 °C for 40 h. The process of thermal isomerization is divided into two separate processes.

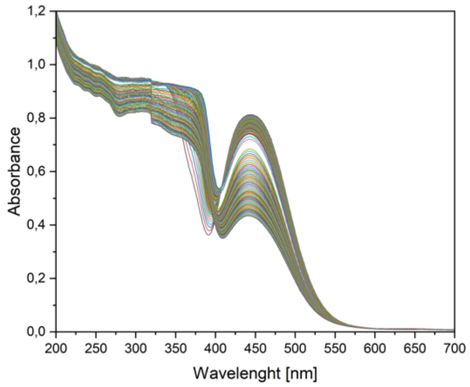


Figure S14: UV-Vis absorption spectra of thermal isomerization of neat thin film of *p*-OHex-AB at rt after irradiation with 365 nm.

The process of thermal isomerization was divided into two individual processes to demonstrate the change in the absorption spectrum. The first process is the thermal isomerization in the liquid phase, which is characterized by the presence of an isosbestic point. The second process involves a phase transition from liquid to solid, which causes the unusual changes in the absorption spectrum. To clarify the change in absorption at a wavelength of 365 nm and 448 nm, the change in absorption at these wavelengths is graphically represented by the change in time.

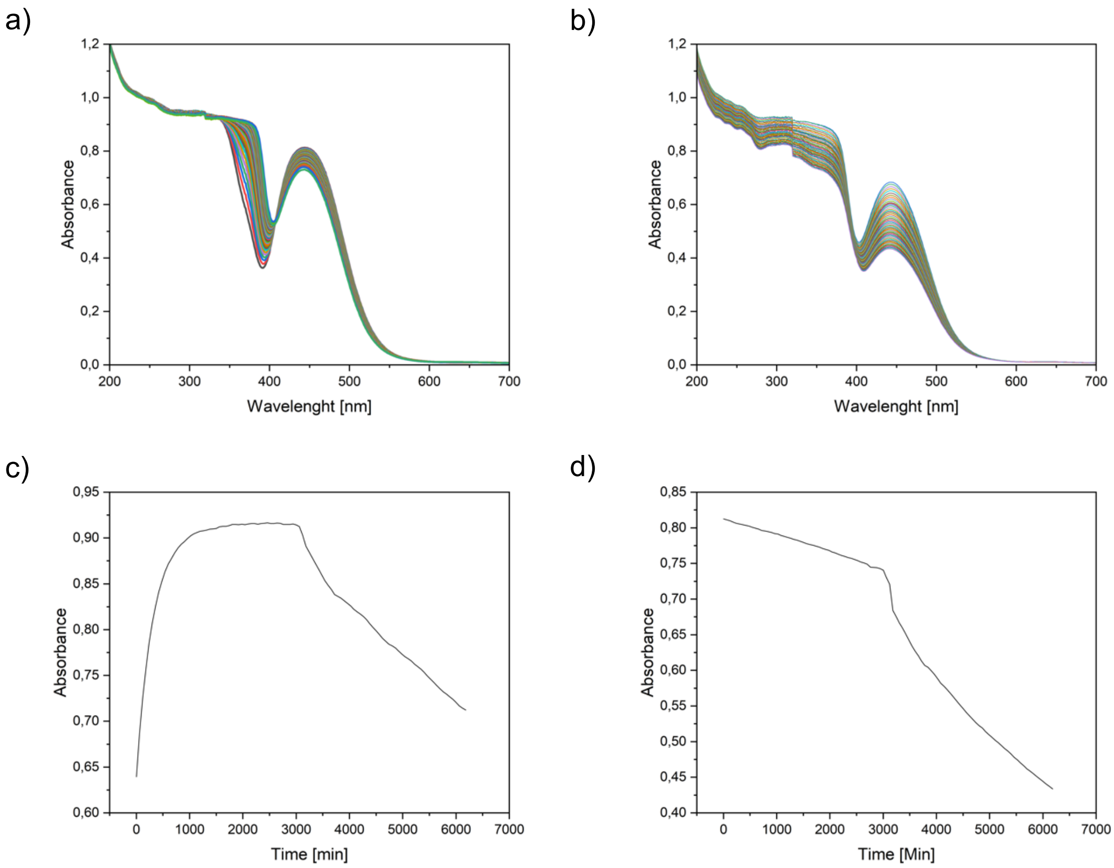


Figure S15: Thermal isomerization of neat *p*-OHex-AB in a) liquid phase and b) phase transition to solid state. Change of the absorbance at c) 365 nm and d) 444 nm.

10. Photoliquefication *via* HPLC and PXRD

To evaluate the effectiveness of the photoisomerization *p*-OHex-AB was irradiated as an example as a thin powder layer on a glass slide according to the procedure for the preparation of thin layers of the compounds on a glass slide explained in section 5. Irradiation experiments (see Figure S2 a). The compound was irradiated with 365 nm and a distance of 10 cm or 5 cm at rt. The change in isomer composition was determined using HPLC. For this purpose, an aliquot of the irradiated sample was taken at different time intervals and dissolved in ACN in a 2 ml vial. It should be noted that during irradiation at the phase transition from the solid to the liquid phase, errors can occur when taking an aliquot, as the sample composition is not fully homogeneous during the photoliquefication process.

Table S16: Determination of the (*E*)-isomer content during irradiation of neat *p*-OHex-AB with 365 nm with a distance of the LED of 10 cm at rt detected *via* HPLC.

Time / min	(*E*)-Isomer / %	Time / min	(*E*)-Isomer / %	Time / min	(*E*)-Isomer / %
0	100	23	96.3	88	83.4
1	100	28	97.0	109	77.8
3	99.8	33	94.0	129	72.2
8	99.1	43	92.8	169	43.2
13	98.5	53	91.2	209	21.6
18	97.5	68	86.8		

Table S17: Determination of the (*E*)-isomer content during irradiation of neat *p*-OHex-AB with 365 nm with a distance of the LED of 5 cm at rt detected *via* HPLC.

Time / min	(*E*)-Isomer / %	Time / min	(*E*)-Isomer / %	Time / min	(*E*)-Isomer / %
0	100	40	86.6	80	71.5
5	99.3	45	83.1	85	69.0
10	95.3	50	85.6	90	66.1
15	94.6	55	83.0	95	48.8
20	92.3	60	80.1	100	45.6
25	93.1	65	78.2	105	53.9
30	86.1	70	79.8	110	24.2
35	92.0	75	65.4	115	11.4

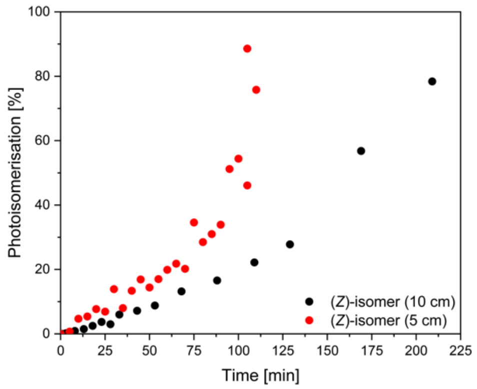


Figure S16: Change of (*Z*)-isomer content during irradiation with 365 nm of neat *p*-OHex-AB at rt with a distance of the LED of 5 cm (red) and 10 cm (black).

Powder XRD measurement was performed with the *p*-OHex-AB as an example to monitor the decreasing crystallinity during the phase transition from solid to liquid due to irradiation with a wavelength of 365 nm. A thin layer of powder was irradiated at a distance of 15 cm from the LED at room temperature over a period of 90 min (see figure S17).

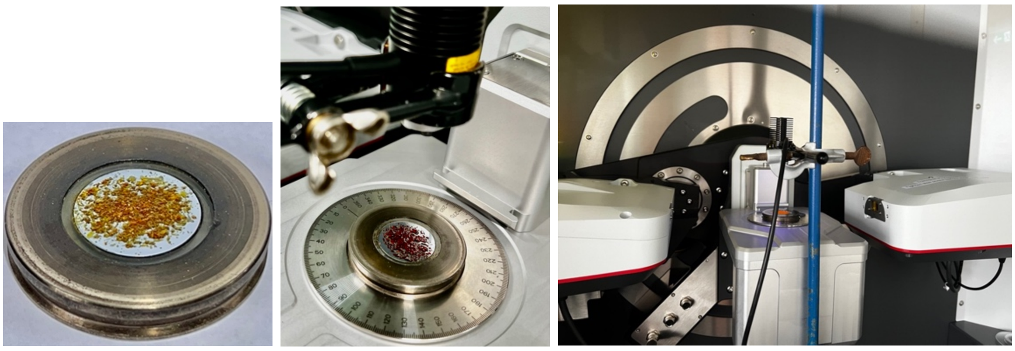


Figure S17: Setup for powder XRD irradiation experiments.

The photoliquefication was monitored in 1 min intervals at rt for 90 min.

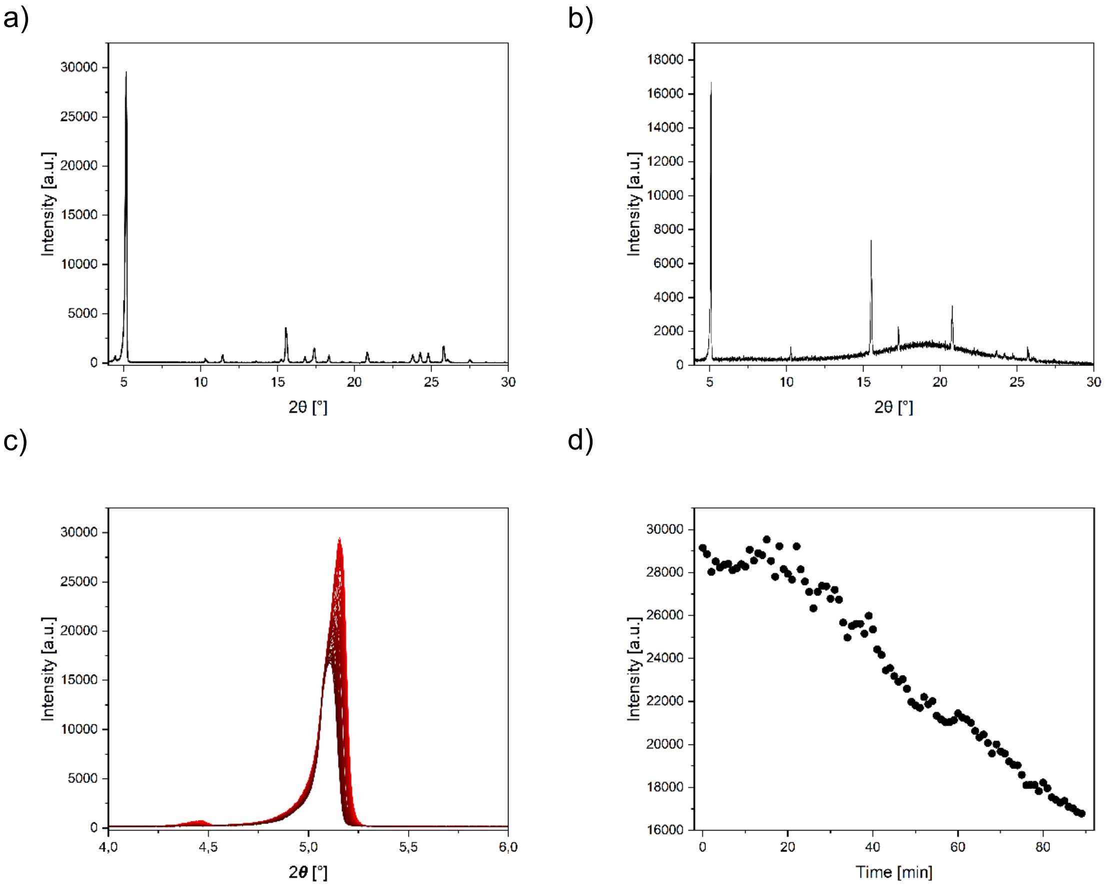
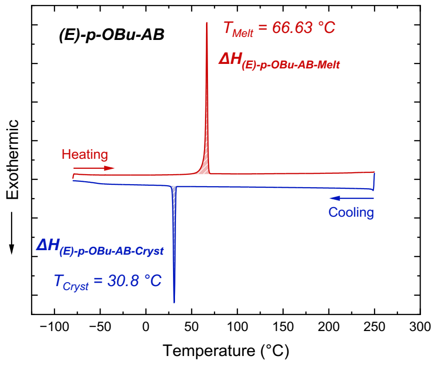
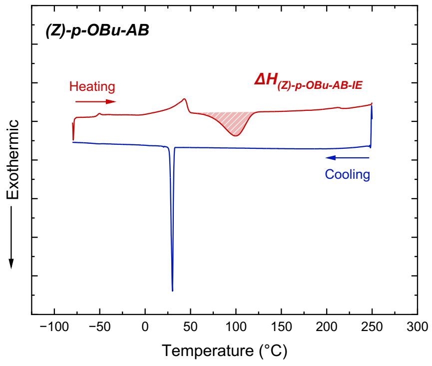


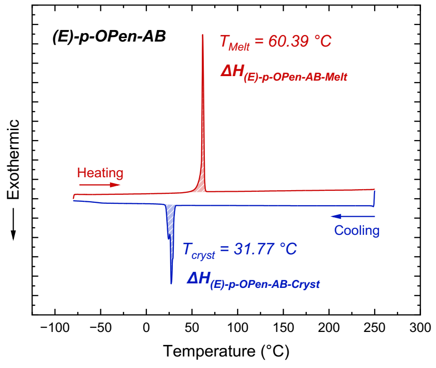
Figure S18: PXRD a) before irradiation and b) after 90 min 365 nm. c) Changes in the PXRD spectrum over 90 min at 365 nm in a range of 4 - 6° 2θ. d) Plotting the decrease in maximum intensity against time.

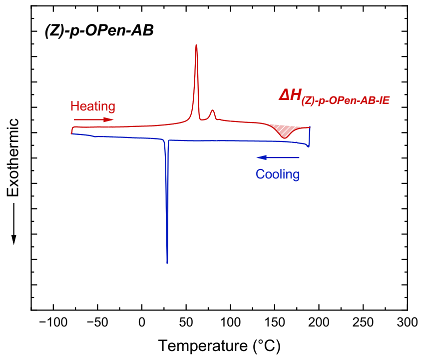
11. DSC measurements

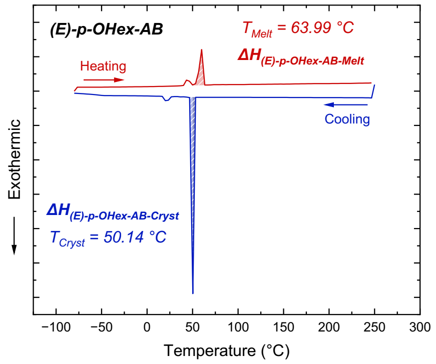
To measure the energy storage capacity of a *p*-alkoxy-Azobenzenes, DSC curves were scanned on a DSC3+ STAR^e system (METTER TOLEDO) at a heating rate of 10 °C/min under N_2 atmosphere. Approximately 5–8 mg of the sample was weighed and dissolved in 3 mL of acetonitrile (ACN). The solution was irradiated for 24 hours. The photoisomerization was detected *via* UV-Vis spectroscopy. Irradiation of the solution was continued until no further change in the UV-Vis spectra was observed. Once complete conversion was confirmed, the solvent was evaporated under continued irradiation at room temperature, and the remaining oil was weighed and transferred into a differential scanning calorimetry (DSC) pan. DSC analysis was then conducted on the known mass of the sample.

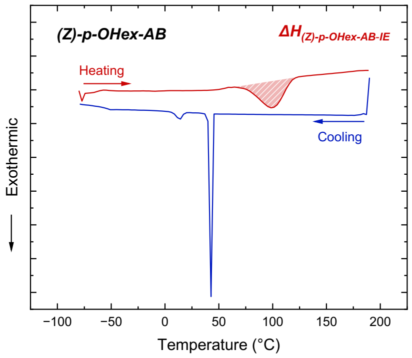


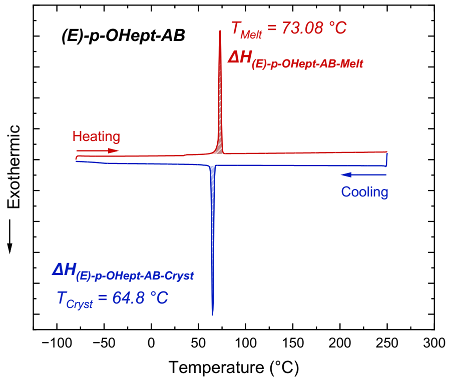


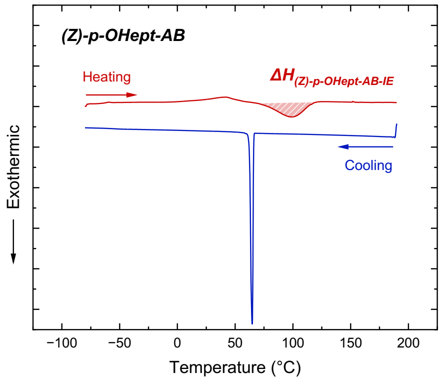


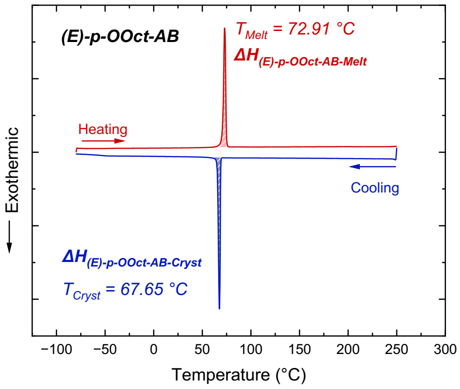


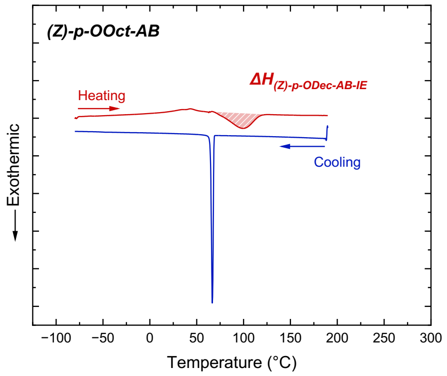

(E)-p-OHex-AB
T_{Melt} = 63.99 °C
$\Delta H_{(E)-p-OHex-AB-Melt}$
Heating
Cooling
Exothermic
$\Delta H_{(E)-p-OHex-AB-Cryst}$
T_{Cryst} = 50.14 °C
−100 −50 0 50 100 150 200 250 300
Temperature (°C)

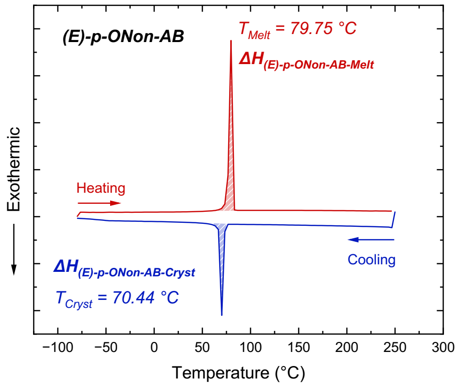

(Z)-p-OHex-AB
$\Delta H_{(Z)-p-OHex-AB-IE}$
Heating
Cooling
Exothermic
−100 −50 0 50 100 150 200
Temperature (°C)

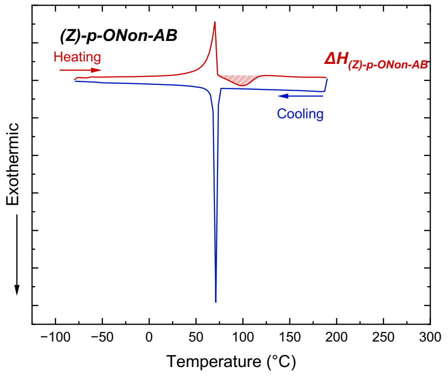

(E)-p-OHept-AB
T_{Melt} = 73.08 °C
$\Delta H_{(E)-p-OHept-AB-Melt}$
Heating
Cooling
Exothermic
$\Delta H_{(E)-p-OHept-AB-Cryst}$
T_{Cryst} = 64.8 °C
−100 −50 0 50 100 150 200 250 300
Temperature (°C)


(Z)-p-OHept-AB
Heating
$\Delta H_{(Z)-p-OHept-AB-IE}$
Cooling
Exothermic
−100 −50 0 50 100 150 200
Temperature (°C)


(E)-p-OOct-AB
T_{Melt} = 72.91 °C
$\Delta H_{(E)-p-OOct-AB-Melt}$
Heating
Cooling
Exothermic
$\Delta H_{(E)-p-OOct-AB-Cryst}$
T_{Cryst} = 67.65 °C
−100 −50 0 50 100 150 200 250 300
Temperature (°C)


(Z)-p-OOct-AB
$\Delta H_{(Z)-p-ODec-AB-IE}$
Heating
Cooling
Exothermic
−100 −50 0 50 100 150 200 250 300
Temperature (°C)


(E)-p-ONon-AB
T_{Melt} = 79.75 °C
$\Delta H_{(E)-p-ONon-AB-Melt}$
Heating
Exothermic
$\Delta H_{(E)-p-ONon-AB-Cryst}$
T_{Cryst} = 70.44 °C
Cooling
−100 −50 0 50 100 150 200 250 300
Temperature (°C)


(Z)-p-ONon-AB
Heating
$\Delta H_{(Z)-p-ONon-AB}$
Cooling
Exothermic
−100 −50 0 50 100 150 200 250 300
Temperature (°C)

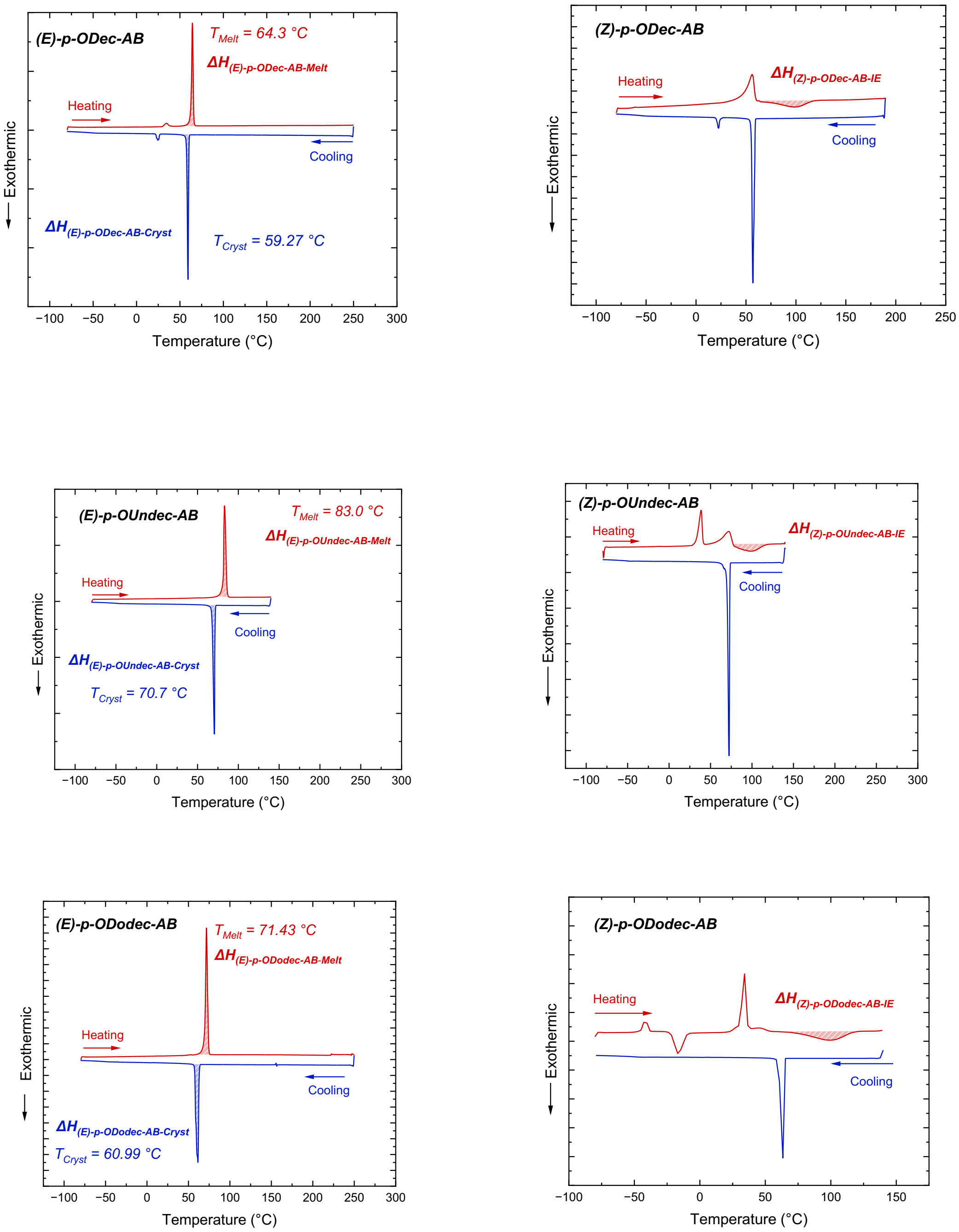


Figure S19: DSC measurements of neat *p*-alkoxy-AB.

The isomerization enthalpy was measured for PSS_{340} in ACN. The previous determined composition at PSS_{340} in ACN was used to calculate the potential energies for a conversion of 100% as well as for the measured PSS composition in the solid state PSS_{365}.

$$\Delta H_{\text{iso.;PSS}_{365}} = \Delta H_{\text{iso.;PSS}_{340}} \cdot \frac{[(Z)_{\text{PSS}_{365}}]}{[(Z)_{\text{PSS}_{340}}]}$$

Equation S4: Calculation of $\Delta H_{\text{iso.}}$ at PSS_{365}.

$$\Delta H_{\text{iso.;100\%}} = \Delta H_{\text{iso.;PSS}_{340}} \cdot \frac{100\%}{[(Z)_{\text{PSS}_{340}}]}$$

Equation S5: Calculation of $\Delta H_{\text{iso.}}$ for 100% photoconversion.

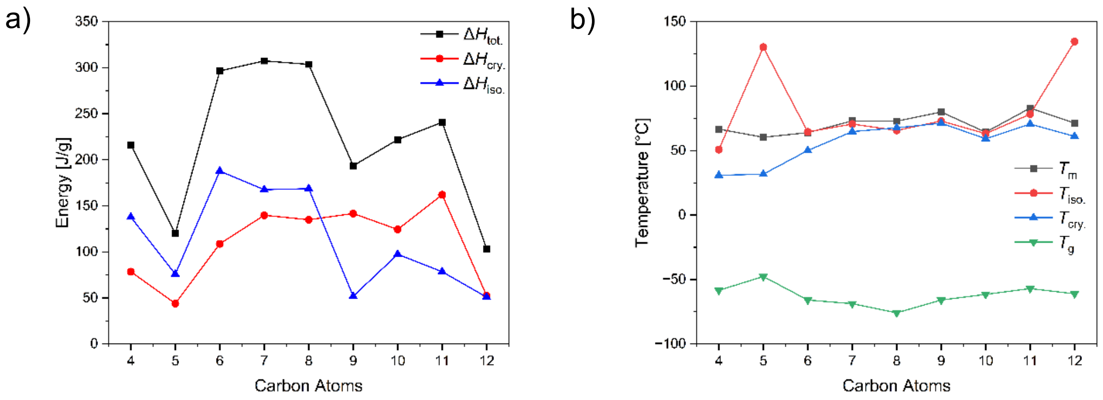


Figure S20: a) measured $\Delta H_{\text{cry.}}$ and $\Delta H_{\text{iso.}}$ and $\Delta H_{\text{tot.}}$ calculated for 100% conversion b) Melting (T_m), crystallization (T_c), glass (T_g) and isomerization (T_i) Temperatures for *p*-alkoxy-AB measured *via* DSC.

Table S18: ΔH_{iso} measured at the PSS_{340} and calculated for PSS_{365} and for 100% conversion.

Compound	(Z) [%] at PSS_{340}	$\Delta H_{\text{iso.}}$ [J/g] at PSS_{340}	(Z) [%] at PSS_{365}	$\Delta H_{\text{iso.}}$ [J/g] at PSS_{365}	$\Delta H_{\text{iso.}}$ [J/g] for 100%
p-OBu-AB	76.9	105.97	91.6	126.23	137.80
p-OPen-AB	77.1	58.46	92.8	70.36	75.82
p-OHex-AB	76.9	144.38	93.3	175.17	187.75
p-OHep-AB	74.5	124.80	93.3	156.29	167.52
p-OOct-AB	74.7	125.97	93.8	158.18	168.63
p-ONon-AB	73.6	38.19	92.7	48.10	51.89
p-ODec-AB	72.7	70.87	94.5	92.12	97.48
p-OUndec-AB	73.0	57.37	93.5	73.48	78.59
p-ODodec-AB	73.3	37.38	94.4	48.14	51.00

Table S19: Measured ΔH_{tot} at the PSS_{340} and calculated at PSS_{365} and for 100% conversion.

Compound	$\Delta H_{\text{cry.}}$ [j/g]	$\Delta H_{\text{tot.}}$ [j/g] at PSS_{340}	$\Delta H_{\text{tot.}}$ [j/g] at PSS_{365}	$\Delta H_{\text{tot.}}$ [j/g] for 100%
p-OBu-AB	78.49	184.46	204.72	216.29
p-OPen-AB	44.06	102.52	114.42	119.88
p-OHex-AB	108.80	253.18	283.97	296.55
p-OHep-AB	139.90	264.7	296.19	307.42

p-OOct-AB	135.01	260.98	293.19	303.64
p-ONon-AB	141.70	179.89	189.80	193.59
p-ODec-AB	124.46	195.33	216.58	221.94
p-OUndec-AB	162.15	219.52	235.63	240.74
p-ODodec-AB	52.45	89.83	100.59	103.45

Table S20: Melting (T_m), crystallization (T_c), glass (T_g) and isomerization (T_i) Temperatures for *p*-alkoxy-AB measured *via* DSC.

Compound	(*E*)-isomer		(*Z*)-isomer	
	T_m [°C]	T_c [°C]	T_g [°C]	T_i [°C]
p-OBu-AB	66.63	30.80	-58.33	50.82
p-OPen-AB	60.39	31.77	-47.66	130.32
p-OHex-AB	63.99	50.14	-65.83	64.49
p-OHep-AB	73.08	64.80	-68.66	70.66
p-OOct-AB	72.91	67.65	-75.83	65.65
p-ONon-AB	80.00	71.27	-65.83	72.99
p-ODec-AB	64.30	59.27	-61.51	63.13
p-OUndec-AB	83.01	70.65	-56.98	78.32
p-ODodec-AB	71.43	60.99	-61.04	134.66

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