

Supplementary Information
for
**Photoresponsive Peptoid Oligomers
Bearing Azobenzene Side Chains**

Neel H. Shah and Kent Kirshenbaum*

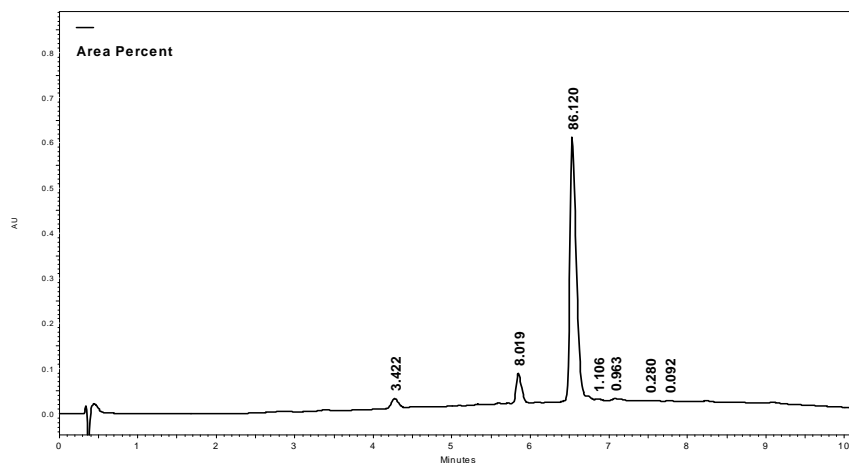
Department of Chemistry, New York University, 100 Washington Square East, New York, NY 10003-6688, USA. E-mail: kent@nyu.edu; Fax: +1 212 260 7905; Tel: +1 212 998 8487

TABLE OF CONTENTS:

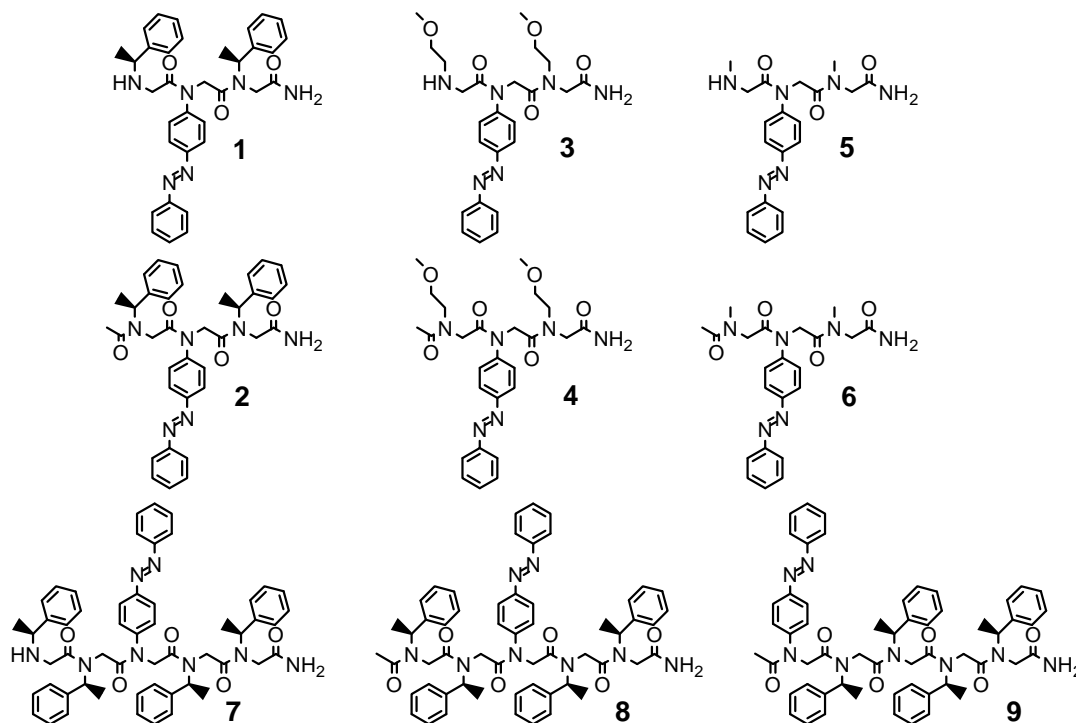
Synthesis of peptoid oligomers	S2
Structures of peptoid oligomers	S2-S3
Characterization of peptoid oligomers	S3-S7
Characterization of 14	S7
Photoisomerization of 1	S8
Calculation of rate constants for thermal back-isomerization	S8-S9

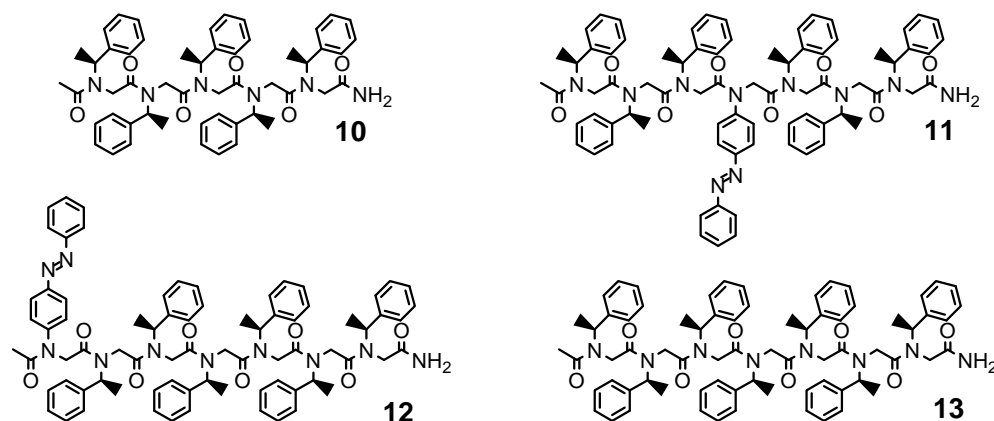
Synthesis of peptoid oligomers

A representative RP-HPLC analytical chromatograph of crude peptoid **1** is shown below. The dominant peak corresponds to the *trans*-azobenzene isomer, and the second-largest peak corresponds to the *cis*-azobenzene isomer.



Structures of peptoid oligomers





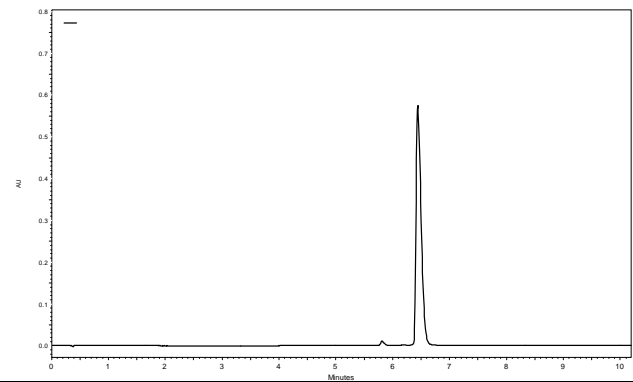
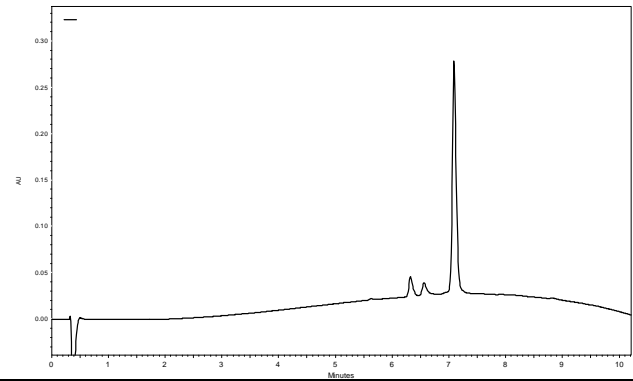
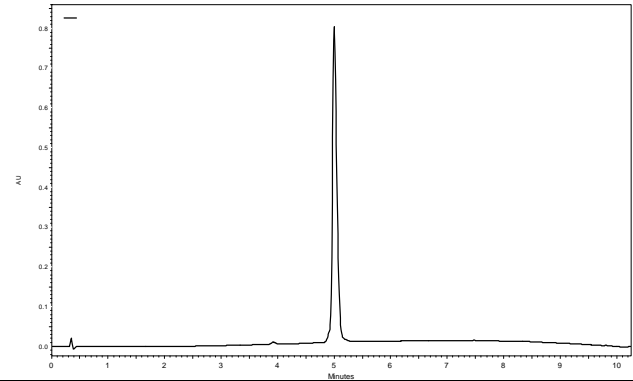
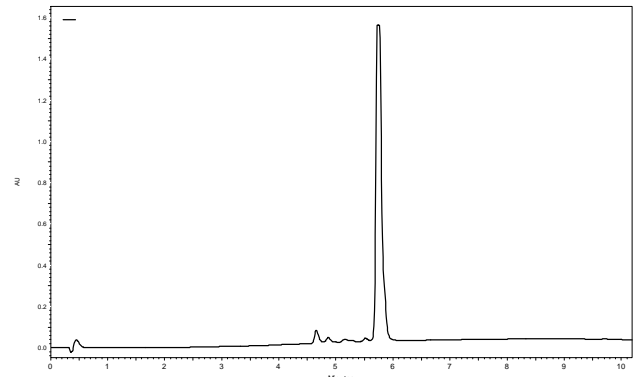
Characterization of peptoid oligomers

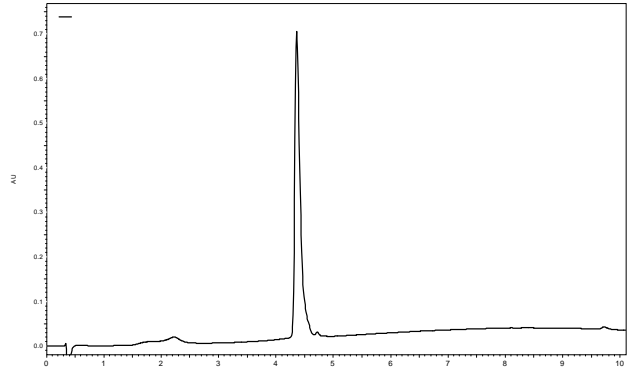
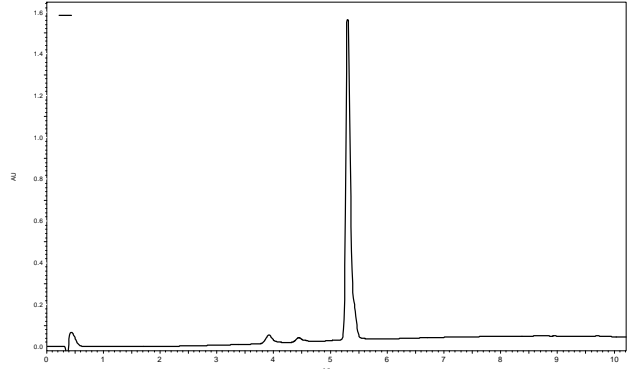
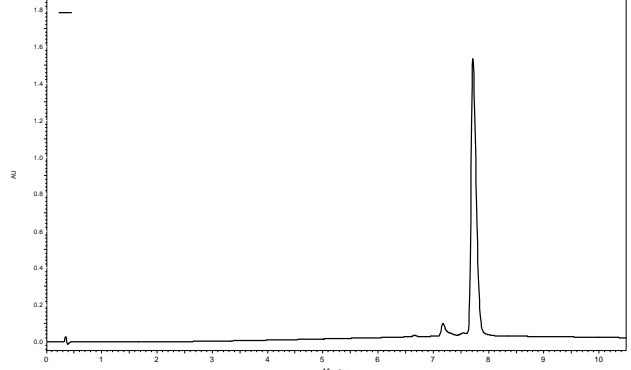
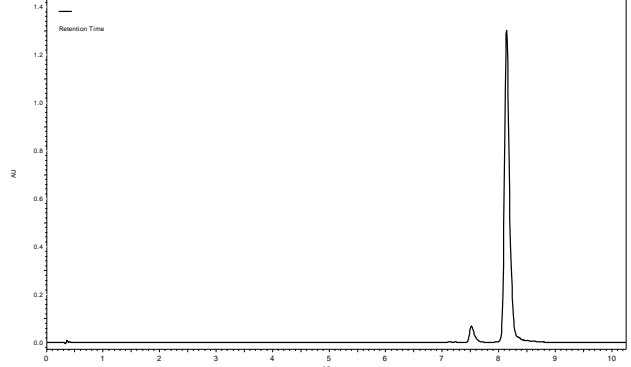
1. Liquid Chromatography/Mass Spectrometry of purified oligomers:

Nspe = (S)-N-(1-phenylethyl)glycine, *Nazb* = N-(p-phenylazo-phenyl)glycine, *Nme* = N-(2-methoxy-ethyl)glycine, *Sar* = N-(methyl)glycine or sarcosine

Compound	Sequence	Formula	Calc. m/z	Obs. m/z	Ion
1	<i>Nspe-Nazb-Nspe</i>	$C_{34}H_{36}N_6O_3$	576.28	577.3	$M+H^+$
				599.3	$M+Na^+$
2	<i>Ac-Nspe-Nazb-Nspe</i>	$C_{36}H_{38}N_6O_4$	618.30	619.1	$M+H^+$
				641.1	$M+Na^+$
3	<i>Nme-Nazb-Nme</i>	$C_{24}H_{32}N_6O_5$	484.24	485.2	$M+H^+$
				507.2	$M+Na^+$
4	<i>Ac-Nme-Nazb-Nme</i>	$C_{26}H_{34}N_6O_6$	526.25	427.0	$M+H^+$
				549.0	$M+Na^+$
5	<i>Sar-Nazb-Sar</i>	$C_{20}H_{24}N_6O_3$	396.19	397.0	$M+H^+$
				399.0	$M+Na^+$
6	<i>Ac-Sar-Nazb-Sar</i>	$C_{22}H_{26}N_6O_4$	438.20	439.0	$M+H^+$
				461.0	$M+Na^+$
7	$(Nspe)_2-Nazb-(Nspe)_2$	$C_{54}H_{58}N_8O_5$	898.45	899.4	$M+H^+$
				921.4	$M+Na^+$
8	<i>Ac-(Nspe)₂-Nazb-(Nspe)₂</i>	$C_{56}H_{60}N_8O_6$	940.46	941.4	$M+H^+$
				963.4	$M+Na^+$
9	<i>Ac-Nazb-(Nspe)₄</i>	$C_{56}H_{60}N_8O_6$	940.46	941.4	$M+H^+$
				963.4	$M+Na^+$
10	<i>Ac-(Nspe)₅</i>	$C_{52}H_{60}N_6O_6$	864.46	865.4	$M+H^+$
				887.4	$M+Na^+$
11	<i>Ac-(Nspe)₃-Nazb-(Nspe)₃</i>	$C_{76}H_{82}N_{10}O_8$	1262.63	1263.7	$M+H^+$
				1285.8	$M+Na^+$
12	<i>Ac-Nazb-(Nspe)₆</i>	$C_{76}H_{82}N_{10}O_8$	1262.63	1263.7	$M+H^+$
				1285.7	$M+Na^+$
13	<i>Ac-(Nspe)₇</i>	$C_{72}H_{82}N_8O_8$	1186.63	1187.6	$M+H^+$
				1209.7	$M+Na^+$

2. Analytical Reverse Phase High Performance Liquid Chromatography of purified oligomers (5-95% acetonitrile in water, 10 minutes, 214 nm):

Compound	RP-HPLC Chromatograph	Retention Time
1		6.442 min
2		7.092 min
3		5.000 min
4		5.742 min

5		4.358 min
6		5.308 min
7		7.717 min
8		8.142 min

