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Aptamer Design

Aptamers, short DNA/RNA sequences, have strong and specific binding properties through molecular recognition and are promising tools in studying molecular biology with recognized therapeutic and diagnostic clinical applications. In the past, aptamers are only selected by the technique of Systematic Evolution of Ligands by EXponential enrichment (SELEX).

MDT Canada Inc. employs validated Entropic Fragment Based Approach (EFBA) proprietary technology, which applies maximum entropy-based information processing approach to utilize information of energy and structure to design aptamers.

		Aptamer	Antibody
Why aptamers?	Method	in vitro selection	Biological systems based selection
 Aptamers are potential replacements of antibodies Aptamers have several advantages over antibodies as promising 	Targets	Any proteins, small molecules or entire organisms	Difficult targeting toxins or non-immunogenic targets
	Binding affinity and specificity	High	High
	Modifications	Wide variety of chemical modifications and can be labeled easily	Limited modifications of molecules and difficult for labeling
tools in therapeutic and	Activity	Uniform activity	Varies from batch to batch
diagnostic clinical applications	Immunogenicity	Not yet been found	Significant

$C_{\text{omparison between our technology and conventional approach}$				
	EFBA	SELEX		
Methodology	Design based on purposes	<i>in vitro</i> selection and can not be designed to bind to specific regions of targets		
Target	Structures to be provided	Any targets		
Time required	14-mer sequences/week	Days to months		



An example of success: Structure snapshot of Thrombin-EFBA (pink) and SELEX aptamer (yellow) at 5 ns in molecular dynamic simulation [Chem Biol & Drug Design 78, 1 (2011)].

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Page 1

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Aptamer Design

We offer a few services using our proprietary technology. All services require only information of target structures. Furthermore, clients can either choose blind design (binding pockets are uncertain) or orientated design (binding pockets are suggested).

Service	What do you get?
Basic 1	For targets and its crystal structures are known, service includes sequences of top four candidates and basic <i>in silico</i> validation report.
Basic 2	For targets are known only, service includes homology modeling of target structures, sequences of top four candidates and basic <i>in silico</i> validation report.
Basic 3	Including either Basic 1 or 2, we also ship aptamers with the quantity you want to you. Shipment cost is included.
Complete 1	For targets and its crystal structures are known, service includes sequences of top four candidates and complete (i) <i>in silico</i> or/and (ii) <i>in vitro</i> validation report
Complete 2	For targets are known only, service includes homology modeling of target structures, sequences of top four candidates with complete (i) <i>in silico</i> or/and (ii) <i>in vitro</i> validation report
Complete 3	Including either Complete 1 or 2, we also ship aptamers with the quantity you need. Shipment cost is included.

Why MDT Canada Inc.?

We have a unique platform combining theoretical, computational and experimental expertise and techniques to provide services and fulfil your needs through consultations.

Please send all of your inquiries to <u>contact@mdtcanada.ca</u>

We will be happy to set up a meeting with you to discuss your needs. A quotation will be made considering services you choose.

When you can design why select!