McLean Group Collision Cross Section Database
MALDI Generated Data

Biomolecular Class	Name (parent name if fragmented)	species	*m/z* (Da)	Ω (Å^2)	σ (# of measurements)
		Oligonucleotides[1]			
oligonucleotide	d2-G-H_2O (GACT)	$[M+H]^+$	492.1	129.2	0.3(6)
oligonucleotide	w2-G-H_2O (TCAG)	$[M+H]^+$	492.1	137.7	0.5(6)
oligonucleotide	w2-C-H_2O (TGAC)	$[M+H]^+$	492.6	135.5	0.4(6)
oligonucleotide	d2-C-H_2O or x2-T-H_2O (CAGT)	$[M+H]^+$	492.9	125.7	0.5(6)
oligonucleotide	a2 (TCGA)	$[M+H]^+$	514.1	134.3	0.5(6)
oligonucleotide	a2 (TCAG)	$[M+H]^+$	514.1	138.2	0.3(6)
oligonucleotide	a2 (TCG)	$[M+H]^+$	514.1	150.9	0.4(6)
oligonucleotide	a2-T (ACTG)	$[M+H]^+$	524.1	137.9	0.5(6)
oligonucleotide	z2 or a2 (GCAT)	$[M+H]^+$	539.1	141.6	0.4(6)
oligonucleotide	w2 (GCT)	$[M+H]^+$	610.1	154.9	0.6(6)
oligonucleotide	w2 (GTC)	$[M+H]^+$	612.1	145.5	0.4(6)
oligonucleotide	c2 (GCT)	$[M+H]^+$	618.1	163.1	0.5(6)
oligonucleotide	w2 (TGAC)	$[M+H]^+$	621.1	153.2	0.6(6)
oligonucleotide	w2 (TGCA)	$[M+H]^+$	621.1	156.7	0.3(6)
oligonucleotide	w2 (CGTA)	$[M+H]^+$	636.1	163.5	0.1(6)
oligonucleotide	w2 (GCTA)	$[M+H]^+$	636.1	165.1	0.4(6)
oligonucleotide	w2 (CGAT)	$[M+H]^+$	636.1	152	0.4(6)
oligonucleotide	w2 (GCAT)	$[M+H]^+$	636.1	153.7	0.2(6)
oligonucleotide	w2 (ACTG)	$[M+H]^+$	652.1	142.1	0.7(6)
oligonucleotide	w2 (CTG)	$[M+H]^+$	652.1	161.9	0.2(6)
oligonucleotide	w2 (TCAG)	$[M+H]^+$	661.1	158.4	0.2(6)
oligonucleotide	TGC-G (TGC)	$[M+H]^+$	710.2	171	1.3(6)
oligonucleotide	GTC-G (GTC)	$[M+H]^+$	710.2	172.5	0.2(6)
oligonucleotide	GCT-G (GCT)	$[M+H]^+$	710.2	176	0.9(6)
oligonucleotide	a3-G (ATGC)	$[M+H]^+$	716.2	171.7	0.3(6)
oligonucleotide	a3-C (TACG)	$[M+H]^+$	716.2	170.5	0.4(6)

oligonucleotide	a3-G (TAGC)	$[M+H]^+$	716.2	173.7	0.3(6)
oligonucleotide	a3-C (ATCG)	$[M+H]^+$	716.2	172.2	0.1(6)
oligonucleotide	CGT-C (CGT)	$[M+H]^+$	750.2	170.9	0.3(6)
oligonucleotide	TCG-C (TCG)	$[M+H]^+$	750.2	182.9	1.0(6)
oligonucleotide	CTG-C (CTG)	$[M+H]^+$	750.2	176.3	1.3(6)
oligonucleotide	x3-G or w3-G-H_2O (CATG)	$[M+H]^+$	796.1	179.8	0.4(6)
oligonucleotide	x3-G or w3-G-H_2O (CTAG)	$[M+H]^+$	796.1	181.6	0.8(6)
oligonucleotide	c3-G or x3-C (GATC)	$[M+H]^+$	796.1	181.8	0.3(6)
oligonucleotide	c3-G (GTAC)	$[M+H]^+$	796.1	179.2	0.3(6)
oligonucleotide	w3-C (GACT)	$[M+H]^+$	814.1	156.1	0.4(6)
oligonucleotide	w3-G or d3-C (CATG)	$[M+H]^+$	814.1	179.5	0.7(6)
oligonucleotide	w3-G or d3-C (CTAG)	$[M+H]^+$	814.1	186.4	1.3(6)
oligonucleotide	d3-G or w3-C (GATC)	$[M+H]^+$	814.1	182	0.3(6)
oligonucleotide	d3-G or w3-C (GTAC)	$[M+H]^+$	814.1	183.1	0.3(6)
oligonucleotide	w3-G (CTGA)	$[M+H]^+$	814.1	170.4	0.8(6)
oligonucleotide	w3-C (GCAT)	$[M+H]^+$	814.1	180.3	0.4(6)
oligonucleotide	w3-C (GTCA)	$[M+H]^+$	814.1	172.1	0.8(6)
oligonucleotide	w3-G (CAGT)	$[M+H]^+$	814.3	172	0.7(6)
oligonucleotide	CGT	$[M+H]^+$	861.2	187.6	0.6(6)
oligonucleotide	TCG	$[M+H]^+$	861.2	186.1	0.4(6)
oligonucleotide	TGC	$[M+H]^+$	861.2	190.2	0.3(6)
oligonucleotide	GTC	$[M+H]^+$	861.2	187.2	0.1(6)
oligonucleotide	GCT	$[M+H]^+$	861.2	198.3	0.1(6)
oligonucleotide	CTG	$[M+H]^+$	861.2	190.5	0.2(6)
oligonucleotide	w3 (GCTA)	$[M+H]^+$	925.2	187.8	0.1(6)
oligonucleotide	w3 (GACT)	$[M+H]^+$	925.2	191.4	0.3(6)
oligonucleotide	w3 (GATC)	$[M+H]^+$	925.2	193.8	0.2(6)
oligonucleotide	w3 (GTAC)	$[M+H]^+$	925.2	197.3	0.1(6)
oligonucleotide	w3 (GCAT)	$[M+H]^+$	925.2	200.6	0.5(6)
oligonucleotide	w3 (GTCA)	$[M+H]^+$	925.2	202.3	0.2(6)
oligonucleotide	w3 (CAGT)	$[M+H]^+$	965.2	197.9	0.5(6)
oligonucleotide	w3 (CGTA)	$[M+H]^+$	965.2	193	0.6(6)

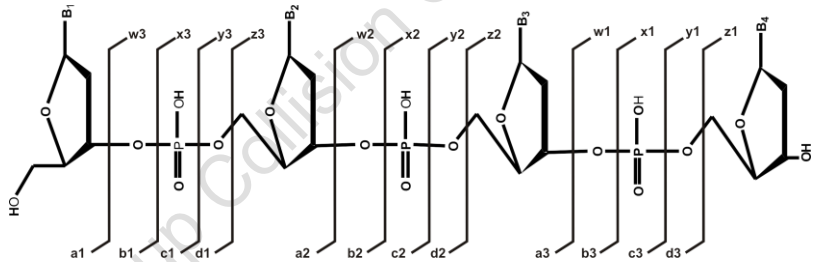
oligonucleotide	W3 (ACTG)	$[M+H]^+$	965.2	199.1	0.3(6)
oligonucleotide	w3 (CTAG)	$[M+H]^+$	965.2	191.2	0.5(6)
oligonucleotide	w3 (CGAT)	$[M+H]^+$	965.2	200.5	0.3(6)
oligonucleotide	w3 (CTGA)	$[M+H]^+$	965.2	202.6	0.3(6)
oligonucleotide	GACT-G (GACT)	$[M+H]^+$	1023.2	211.9	0.4(6)
oligonucleotide	GCTA-G (GCTA)	$[M+H]^+$	1023.2	209.2	0.8(6)
oligonucleotide	GATC-G (GATC)	$[M+H]^+$	1023.2	212.5	0.4(6)
oligonucleotide	GTAC-G (GTAC)	$[M+H]^+$	1023.2	211.4	0.5(6)
oligonucleotide	GCAT-G (GCAT)	$[M+H]^+$	1023.2	215	0.6(6)
oligonucleotide	GTCA-G (GTCA)	$[M+H]^+$	1023.2	216.3	0.7(6)
oligonucleotide	ATGC-C (ATGC)	$[M+H]^+$	1063.2	213.2	0.6(6)
oligonucleotide	CAGT-C (CAGT)	$[M+H]^+$	1063.2	214.4	0.8(6)
oligonucleotide	CGTA-C (CGTA)	$[M+H]^+$	1063.2	215.7	0.8(6)
oligonucleotide	CGAT-C (CGAT)	$[M+H]^+$	1063.2	216.3	0.7(6)
oligonucleotide	CGTA	$[M+H]^+$	1174.2	234	0.5(6)
oligonucleotide	ACGT	$[M+H]^+$	1174.3	219.3	0.3(6)
oligonucleotide	AGTC	$[M+H]^+$	1174.3	214.3	0.4(6)
oligonucleotide	ATGC	$[M+H]^+$	1174.3	232.3	0.3(6)
oligonucleotide	CAGT	$[M+H]^+$	1174.3	220.7	0.5(6)
oligonucleotide	GCTA	$[M+H]^+$	1174.3	223.1	0.7(6)
oligonucleotide	TACG	$[M+H]^+$	1174.3	231.9	0.5(6)
oligonucleotide	GACT	$[M+H]^+$	1174.3	228.6	0.2(6)
oligonucleotide	GCTA	$[M+H]^+$	1174.3	223.3	0.6(6)
oligonucleotide	TCGA	$[M+H]^+$	1174.3	217.2	0.5(6)
oligonucleotide	ACTG	$[M+H]^+$	1174.3	227.4	0.4(6)
oligonucleotide	CATG	$[M+H]^+$	1174.3	216.7	0.4(6)
oligonucleotide	CTAG	$[M+H]^+$	1174.3	231.6	0.3(6)
oligonucleotide	GATC	$[M+H]^+$	1174.3	210.7	0.4(6)
oligonucleotide	GTAC	$[M+H]^+$	1174.3	224.1	0.3(6)
oligonucleotide	TAGC	$[M+H]^+$	1174.3	220.3	0.4(6)
oligonucleotide	TGAC	$[M+H]^+$	1174.3	224.3	0.4(6)
oligonucleotide	AGCT	$[M+H]^+$	1174.3	232.4	0.5(6)
oligonucleotide	ATCG	$[M+H]^+$	1174.3	226.2	0.6(6)

oligonucleotide	CGAT	$[M+H]^+$	1174.3	215.4	0.4(6)
oligonucleotide	CTGA	$[M+H]^+$	1174.3	231.4	0.4(6)
oligonucleotide	GCAT	$[M+H]^+$	1174.3	229.1	0.5(6)
oligonucleotide	TCAG	$[M+H]^+$	1174.3	233	0.1(6)
oligonucleotide	TGCA	$[M+H]^+$	1174.3	230	0.3(6)

Footnotes on table nomenclature:

1. Oligonucleotide nomenclature:

G - Guanine
A - Adenine
C - Cytosine
T – Thymine



Scheme S1. Oligonucleotide fragmentation is specified in McLucky nomenclature (McLuckey SA, Habibi-Goudarzi S. (1993) J. Am. Chem. Soc. 115: 12085-12095). In this table, tentative fragment ion assignments are given by the predominant fragmentation channels observed previously.