

Full Isomer-Tables of Inositol-Oligomers up to Tetramers

Hans Dolhaine^a, Helmut Hönl^{*b}

^aBendgasse 20, D-41352 Korschenbroich-Glehn, Germany

^bInstitute for Organic Chemistry, Technical University Graz, Stremayrgasse 16, A-8010 Graz, Austria. email: helmut.hoenig@TUGraz.at

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Abstract

All possible combinations and stereoisomers of the known nine inositols in their dimers, trimers and tetramers have been calculated and are presented in tables. The respective achiral numbers are also given. Cumulative estimations of the number of possible linear pentamers, hexamers, heptamers, octamers and nonamers are included.

Introduction

In a recent contribution¹ we detailed the approaches and formulas for the number of tetramers of a selected subset of the known nine inositols, namely D- and L-*chiro*-, *muco*- and *neo*-inositols. For a preparative chemist however, there is probably the need to know in a detailed manner, how many stereoisomers are there to be expected for a linear tetramer made of two central *epi*- and two attached *scyllo*- inositols or for a branched tetramer made from a central *allo*- with two *neo*- and one *cis*-inositol attached ?

The respective basics are given in the preceding paper¹. Here we will just present the results in the form of comprehensive tables.

Calculations

The basis for all these estimations and procedures are the results from calculations with the MATHEMATICA - AddOn "ISOMERS"². For the sake of clarity, we will first again present the general substitutional possibilities at inositols:

<i>Inositol</i>	Abbr	mono	achir	di-s	achir	di-as	achir	AAA	achir	AAB	achir	ABC	achir
<i>allo</i>	a	6	0	15	3	30	0	20	0	60	0	120	0
<i>cis</i>	c	1	1	3	3	5	1	4	2	10	2	20	0
<i>D-chiro</i>	d	3	0	9	0	15	0	10	0	30	0	60	0
<i>epi</i>	e	6	2	15	3	30	2	20	4	60	4	120	0
<i>L-chiro</i>	l	3	0	9	0	15	0	10	0	30	0	60	0
<i>muco</i>	m	3	1	9	3	15	1	10	2	30	2	60	0
<i>neo</i>	n	3	1	9	3	15	1	10	2	30	2	60	0
<i>scyllo</i>	s	1	1	4	2	5	1	4	2	10	2	20	0
<i>myo</i>	y	6	2	15	3	30	2	20	4	60	4	120	0

Table 1: Basic Substitutional Possibilities at all Nine Inositols

Within the following tables, we will use the abbreviations given under "Abbr" in Table 1. Small letters will be used for inositols acting as substituents (ligands), while capital letters will be used for central (di- or tri-substituted) inositols. The substitutional possibilities are always given in the order: Sum of stereoisomers, achiral (*meso*-) forms thereof. Thus "mono" represents the monosubstitutional possibilities of the respective inositols, "achir" the achiral fraction thereof. With disubstitution, we have to distinguish between symmetrical ("di-s") and asymmetrical ("di-as") forms. Symmetrical in this context means structural symmetry (i.e. exactly position 1 at *muco* = *muco*_1), and not identity of inositols (i.e. just *muco*, regardless of the position at the latter, see discussion under dimers below). Similarly, there are three possibilities of trisubstitution presented in Table 1 by the acronyms AAA, AAB and ABC.

Dimers:

With the help of these numbers all possible dimers **x-y** can be calculated according to the following general formulas: Number of dimers of identical inositols: $\text{mono}_x * (\text{mono}_x + 1) / 2$. This sum results from a contribution of structurally symmetrical dimers, i.e. *muco*_1 & *muco*_1 (from those there exist exactly mono_x isomers) plus the fraction of structurally asymmetrical combinations of two "identical" inositols, i.e. *muco*_2 and *muco*_3. For the latter there are $\text{mono}_x * (\text{mono}_x - 1) / 2$ isomers. For dimers of different inositols the formula

logically is: $\text{mono}_x * \text{mono}_y$, x and y are indicating the respective inositols. The same formulas are valid for the achiral forms thereof, with the exception of the **d-l** - pair, which yields three *meso*-forms as well as all dimers of identical inositols, which have to be evaluated individually according to their number of enantiotopic monositions and the number of monositions located in the plane of symmetry (see¹).

Dimer		Number of Isomers	Achirals
x	y		
a	a	21	3
a	c	6	0
a	d	18	0
a	e	36	0
a	l	18	0
a	m	18	0
a	n	18	0
a	s	6	0
a	y	36	0
c	c	1	1
c	d	3	0
c	e	6	2
c	l	3	0
c	m	3	1
c	n	3	1
c	s	1	1
c	y	6	2
d	d	6	0
d	e	18	0
d	l	9	3
d	m	9	0
d	n	9	0
d	s	3	0
d	y	18	0

Dimer		Number of Isomers	Achirals
x	y		
e	e	21	4
e	l	18	0
e	m	18	2
e	n	18	2
e	s	6	2
e	y	36	4
l	l	6	0
l	m	9	0
l	n	9	0
l	s	3	0
l	y	18	0
m	m	6	2
m	n	9	1
m	s	3	1
m	y	18	2
n	n	6	2
n	s	3	1
n	y	18	2
s	s	1	1
s	y	6	2
y	y	21	4
Sum			
45	528	46	

Table II: Number of Inositol Dimers and Achiral *meso* Forms thereof

As can be seen from Table II, there are 45 general types of inositol dimers, yielding 528 stereoisomers and 46 achiral *meso* forms in total. The overall sum of dimers can also be generated by taking the general formula $[n * (n + 1) / 2]$ with n = the sum of all monositions possible (32).

Trimers:

For inositol trimers the following considerations are valid: Trimers of the general form **x-Y-x** have to be split into the really symmetrical forms **x-Y-x** (x being the same monosubstitutional

position, e.g. *muco_1*) and $\mathbf{x-Y-x'}$, where $\mathbf{x'}$ is still the same inositol as \mathbf{x} , but with a different monoposition (e.g. *neo_1* and *neo_3*). For the former, the number of isomers is given by: $\text{mono}_x * \text{di-s}_y$, while for the latter it is: $\text{mono}_x * \text{di-as}_y * (\text{mono}_x - 1) / 2$. Within the tables, these terms again are combined to one sum. For trimers of the general form $\mathbf{x-Y-z}$ the number of isomers is: $\text{mono}_x * \text{di-as}_y * \text{mono}_z$. The results are summarized in *Table III*. As can be seen from this compilation, there are 405 general trimers which yield 82,176 isomers, 630 thereof are achiral. The achiral isomers again have to be evaluated individually by carefully examining the symmetrical isomers as well as those with **d-I** - pairs.

Linear Tetramers:

Here again one has to distinguish between two basic forms: Symmetrical cases of the general pattern: $\mathbf{x-Y-Y-x}$ or $\mathbf{x-X-X-x}$ and asymmetrical forms which are considered below. For symmetrical tetramers, the following formulas are applied: $\text{mono}_x * \text{di-as}_y * (\text{mono}_x * \text{di-as}_y + 1) / 2$ or $\text{mono}_x * \text{di-as}_x * (\text{mono}_x * \text{di-as}_x + 1) / 2$ respectively. For asymmetrical general patterns like $\mathbf{x-Y-Z-o}$, the following formula is valid: $\text{mono}_x * \text{di-as}_y * \text{di-as}_z * \text{mono}_o$. The results are summarized in *Table IV*. From this table we learn, that there are 3,321 general patterns of linear inositol tetramers, yielding 13,109,760 stereoisomers, of which we estimate 3,377 to be achiral. The cumulative number of isomers can also be obtained by taking the sum of monosubstitutional possibilities at the nine inositols (32) times the sum of the asymmetrical disubstitutional possibilities at those (160) and taking the half matrix including the diagonal of this product (5,120): $5,120 * 5,121 / 2 = 13,109,760$. For the achiral forms thereof, no general formula can be given because some of the central dimers to which two ligands (inositols) are attached are *meso* forms built from a pair of enantiomers (in the case of D- and L-*chiro*-inositols) or a pair of enantiotopic mono-positions at some inositols with a plane of symmetry (symmetrical dimers of *allo*-, *epi*-, *muco*-, *neo*- and *myo*-inositols) as indicated already within the discussion of the dimers. To such dimers, besides the "normal" achiral positions of inositols again there can be attached either a **d-I** - pair or a pair of interrelated enantiotopic monopositions of identical inositols to yield achiral *meso* forms. So, tetramers containing **D-L** or symmetrical central dimers as well as attached ligands **D** of this specific pairwise patterns have to be examined carefully for possible achiral *meso* forms.

Tetr		Iso		AC		Tetr		Iso		AC		Tetr		Iso		AC			
s.L.A.c	8100	0	s.L.C.c	450	0	s.L.D	1350	0	s.L.E	2700	0	s.L.F	8100	0	s.L.H	1350	0		
s.L.A.d	2700	0	s.L.C.d	1350	0	s.L.D.d	4050	0	s.L.E.d	8100	0	s.L.F.d	2700	0	s.L.H.d	4050	0	s.L.M	1350
s.L.A.e	16200	0	s.L.C.e	2700	0	s.L.D.e	16200	0	s.L.E.e	8100	0	s.L.F.e	16200	0	s.L.H.e	16200	0	s.L.M.e	2700
s.L.A.i	8100	0	s.L.C.i	1350	0	s.L.D.i	8100	0	s.L.E.i	8100	0	s.L.F.i	8100	0	s.L.H.i	1350	0	s.L.M.i	8100
s.L.A.m	8100	0	s.L.C.m	1350	0	s.L.D.m	8100	0	s.L.E.m	8100	0	s.L.F.m	8100	0	s.L.H.m	1350	0	s.L.M.m	8100
s.L.A.s	8100	0	s.L.C.s	450	0	s.L.D.s	1350	0	s.L.E.s	2700	0	s.L.F.s	8100	0	s.L.H.s	1350	0	s.L.M.s	2700
s.L.A.y	16200	0	s.L.C.y	2700	0	s.L.D.y	16200	0	s.L.E.y	16200	0	s.L.F.y	16200	0	s.L.H.y	16200	0	s.L.M.y	2700
s.L.A.e	1700	0	s.L.C.e	225	0	s.L.D.e	675	0	s.L.E.e	1500	0	s.L.F.e	450	0	s.L.H.e	675	0	s.L.M.e	1500
s.L.A.i	1350	0	s.L.C.i	225	0	s.L.D.i	675	0	s.L.E.i	1350	0	s.L.F.i	450	0	s.L.H.i	675	0	s.L.M.i	1350
s.L.A.m	1350	0	s.L.C.m	225	0	s.L.D.m	675	0	s.L.E.m	1350	0	s.L.F.m	450	0	s.L.H.m	675	0	s.L.M.m	1350
s.L.A.n	1350	0	s.L.C.n	225	0	s.L.D.n	675	0	s.L.E.n	1350	0	s.L.F.n	450	0	s.L.H.n	675	0	s.L.M.n	1350
s.L.A.s	450	0	s.L.C.s	75	0	s.L.D.s	225	0	s.L.E.s	450	0	s.L.F.s	135	0	s.L.H.s	225	0	s.L.M.s	450
s.L.A.y	2700	0	s.L.C.y	450	0	s.L.D.y	1350	0	s.L.E.y	2700	0	s.L.F.y	810	0	s.L.H.y	1350	0	s.L.M.y	450
d.L.A.e	8100	0	d.L.C.e	4050	0	d.L.D.e	4050	0	d.L.E.e	8100	0	d.L.F.e	8100	0	d.L.H.e	4050	0	d.L.M.e	8100
d.L.A.i	4050	0	d.L.C.i	1350	0	d.L.D.i	2025	0	d.L.E.i	4050	0	d.L.F.i	4050	0	d.L.H.i	1350	0	d.L.M.i	4050
d.L.A.m	4050	0	d.L.C.m	1350	0	d.L.D.m	2025	0	d.L.E.m	4050	0	d.L.F.m	4050	0	d.L.H.m	1350	0	d.L.M.m	4050
d.L.A.n	4050	0	d.L.C.n	1350	0	d.L.D.n	2025	0	d.L.E.n	4050	0	d.L.F.n	4050	0	d.L.H.n	1350	0	d.L.M.n	4050
d.L.A.s	1350	0	d.L.C.s	225	0	d.L.D.s	675	0	d.L.E.s	1350	0	d.L.F.s	405	0	d.L.H.s	675	0	d.L.M.s	1350
d.L.A.y	8100	0	d.L.C.y	4050	0	d.L.D.y	4050	0	d.L.E.y	8100	0	d.L.F.y	8100	0	d.L.H.y	4050	0	d.L.M.y	8100
s.L.A.m	8100	0	s.L.C.m	1350	0	s.L.D.m	8100	0	s.L.E.m	8100	0	s.L.F.m	8100	0	s.L.H.m	1350	0	s.L.M.m	8100
s.L.A.n	8100	0	s.L.C.n	1350	0	s.L.D.n	8100	0	s.L.E.n	8100	0	s.L.F.n	8100	0	s.L.H.n	1350	0	s.L.M.n	8100
s.L.A.s	2700	0	s.L.C.s	450	0	s.L.D.s	1350	0	s.L.E.s	2700	0	s.L.F.s	8100	0	s.L.H.s	1350	0	s.L.M.s	2700
s.L.A.y	16200	0	s.L.C.y	2700	0	s.L.D.y	16200	0	s.L.E.y	16200	0	s.L.F.y	16200	0	s.L.H.y	16200	0	s.L.M.y	2700
s.L.A.m	4050	0	s.L.C.m	675	0	s.L.D.m	2025	0	s.L.E.m	4050	0	s.L.F.m	4050	0	s.L.H.m	675	0	s.L.M.m	4050
s.L.A.n	4050	0	s.L.C.n	675	0	s.L.D.n	2025	0	s.L.E.n	4050	0	s.L.F.n	4050	0	s.L.H.n	675	0	s.L.M.n	4050
s.L.A.s	1350	0	s.L.C.s	225	0	s.L.D.s	675	0	s.L.E.s	1350	0	s.L.F.s	405	0	s.L.H.s	675	0	s.L.M.s	1350
s.L.A.y	8100	0	s.L.C.y	4050	0	s.L.D.y	4050	0	s.L.E.y	8100	0	s.L.F.y	8100	0	s.L.H.y	4050	0	s.L.M.y	8100
m.L.A.n	4050	0	m.L.C.n	675	0	m.L.D.n	2025	0	m.L.E.n	4050	0	m.L.F.n	4050	0	m.L.H.n	675	0	m.L.M.n	4050
m.L.A.s	1350	0	m.L.C.s	225	0	m.L.D.s	675	0	m.L.E.s	1350	0	m.L.F.s	405	0	m.L.H.s	675	0	m.L.M.s	1350
m.L.A.y	8100	0	m.L.C.y	4050	0	m.L.D.y	4050	0	m.L.E.y	8100	0	m.L.F.y	8100	0	m.L.H.y	4050	0	m.L.M.y	8100
n.L.A.s	1350	0	n.L.C.s	225	0	n.L.D.s	675	0	n.L.E.s	1350	0	n.L.F.s	405	0	n.L.H.s	675	0	n.L.M.s	1350
n.L.A.y	8100	0	n.L.C.y	4050	0	n.L.D.y	4050	0	n.L.E.y	8100	0	n.L.F.y	8100	0	n.L.H.y	4050	0	n.L.M.y	8100
s.L.A.y	2700	0	s.L.C.y	450	0	s.L.D.y	1350	0	s.L.E.y	2700	0	s.L.F.y	8100	0	s.L.H.y	1350	0	s.L.M.y	2700
y.L.A.y	2700	0	y.L.C.y	4095	0	y.L.D.y	4095	0	y.L.E.y	2700	0	y.L.F.y	8100	0	y.L.H.y	4095	0	y.L.M.y	2700
y.L.A.y	2700	0	y.L.C.y	4095	0	y.L.D.y	4095	0	y.L.E.y	2700	0	y.L.F.y	8100	0	y.L.H.y	4095	0	y.L.M.y	2700

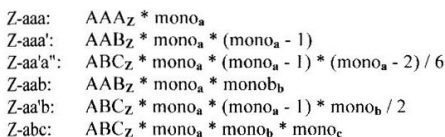
Table IV: All Linear Inostol Tetramers, their Stereoisomer Numbers and Achiral meso-forms

Tetr	iso	Ac	Tetr	iso	Ac	Tetr	iso	Ac	Tetr	iso	Ac	Tetr	iso	Ac	Tetr	iso	Ac													
a	N	a	NC	450	0	n	N	d	1350	0	n	N	a	4095	24	a	N	a	2700	0	a	N	a	16200	0					
a	N	a	d	8100	0	a	N	d	1350	0	a	N	d	4050	0	a	N	c	450	0	a	N	c	2700	0					
a	N	a	e	16200	0	a	N	e	8100	0	a	N	e	16200	0	a	N	s	d	1350	0	a	N	s	8100	0				
a	N	a	f	8100	0	a	N	f	1350	0	a	N	f	4050	0	a	N	s	e	2700	0	a	N	s	e	16200	0			
a	N	m	8100	0	a	N	m	1350	0	a	N	m	4050	0	a	N	m	1350	0	a	N	m	4050	0	a	N	m	16200	0	
a	N	a	g	2700	0	a	N	g	4050	0	a	N	g	1350	0	a	N	s	1350	0	a	N	s	450	0	a	N	s	2700	0
a	N	a	y	16200	0	a	N	y	8100	0	a	N	y	16200	0	a	N	s	y	2700	0	a	N	s	y	16200	0			
c	N	a	d	1350	0	c	N	d	675	0	c	N	d	675	0	c	N	s	e	75	1	c	N	s	e	450	2			
c	N	a	f	2700	4	c	N	f	1350	4	c	N	f	1350	2	c	N	s	e	450	2	c	N	s	e	2700	4			
c	N	a	g	1350	0	c	N	g	1350	0	c	N	g	675	0	c	N	s	e	225	1	c	N	s	e	1350	0			
c	N	m	1350	0	c	N	m	225	1	c	N	m	675	1	c	N	m	675	1	c	N	m	225	1	c	N	m	1350	0	
c	N	a	h	1350	0	c	N	h	450	2	c	N	h	450	2	c	N	s	e	75	1	c	N	s	e	450	2			
c	N	a	y	2700	0	c	N	y	1350	0	c	N	y	1350	0	c	N	s	e	y	2700	4	c	N	s	e	y	2700	4	
d	N	a	e	8100	0	d	N	e	8100	0	d	N	e	4050	0	d	N	s	e	1350	0	d	N	s	e	8100	0			
d	N	a	f	4050	0	d	N	f	4050	0	d	N	f	2025	0	d	N	s	e	675	0	d	N	s	e	4050	0			
d	N	a	g	4050	0	d	N	g	2025	0	d	N	g	2025	0	d	N	s	e	675	0	d	N	s	e	4050	0			
d	N	a	h	1350	0	d	N	h	675	0	d	N	h	675	0	d	N	s	e	225	0	d	N	s	e	1350	0			
d	N	a	y	8100	0	d	N	y	1350	0	d	N	y	4050	0	d	N	s	e	y	2700	4	d	N	s	e	y	16200	8	
e	N	a	f	8100	0	e	N	f	8100	0	e	N	f	4050	0	e	N	s	e	1350	0	e	N	s	e	8100	0			
e	N	a	g	8100	0	e	N	g	8100	4	e	N	g	4050	2	e	N	s	e	1350	2	e	N	s	e	8100	4			
e	N	a	h	8100	0	e	N	h	8100	4	e	N	h	4050	2	e	N	s	e	1350	2	e	N	s	e	8100	4			
e	N	a	y	2700	0	e	N	y	1350	0	e	N	y	1350	0	e	N	s	e	y	2700	4	e	N	s	e	y	2700	4	
f	N	a	g	4050	0	f	N	g	2025	0	f	N	g	2025	0	f	N	s	e	675	0	f	N	s	e	4050	0			
f	N	a	h	1350	0	f	N	h	675	0	f	N	h	675	0	f	N	s	e	225	0	f	N	s	e	1350	0			
f	N	a	y	8100	0	f	N	y	1350	0	f	N	y	4050	0	f	N	s	e	y	2700	4	f	N	s	e	y	16200	8	
m	N	a	g	4050	0	m	N	g	4050	2	m	N	g	2025	1	m	N	s	e	675	1	m	N	s	e	4050	2			
m	N	a	h	1350	0	m	N	h	1350	2	m	N	h	675	1	m	N	s	e	225	1	m	N	s	e	1350	2			
m	N	a	y	8100	0	m	N	y	1350	2	m	N	y	4050	2	m	N	s	e	y	2700	4	m	N	s	e	y	16200	8	
n	N	a	g	1350	0	n	N	g	675	0	n	N	g	675	0	n	N	s	e	225	0	n	N	s	e	1350	0			
n	N	a	h	8100	0	n	N	h	8100	4	n	N	h	4050	2	n	N	s	e	1350	2	n	N	s	e	8100	4			
n	N	a	y	2700	0	n	N	y	1350	2	n	N	y	4050	2	n	N	s	e	y	2700	4	n	N	s	e	y	16200	8	
s	N	a	g	2700	0	s	N	g	450	2	s	N	g	450	2	s	N	s	e	75	1	s	N	s	e	450	2			
s	N	a	h	16200	0	s	N	h	8100	4	s	N	h	8100	4	s	N	s	e	75	1	s	N	s	e	16200	8			
s	N	a	y	2700	0	s	N	y	1350	4	s	N	y	1350	4	s	N	s	e	y	2700	4	s	N	s	e	y	16200	8	

Table IV. All Linear Inositol Tetramers, their Stereoisomer Numbers and Achiral meso-forms

Branched Tetramers:

Here again, careful distinctions according to the substitutional patterns are necessary:



The results are summarized in *Table V*. From this compilation we learn, that there are 1,485 general branched types of tetramers with 3,495,296 stereoisomers. The latter sum of the number of inositol isomers can also be derived from the general formulas for trisubstituted inositols¹ ($n =$ the sum of monopositions of all inositols = 32) as shown below in *Table VI*.

<i>Central Inositol</i>	<i>Isomers</i>	<i>Achirals</i>	<i>Isomers</i>	<i>Achirals (Theory)</i>	<i>Achirals (incl. meso forms)</i>
A	$20 n^3$	0	655,360	0	0
C, S (2)	$2n * (5 n^2 + 1) / 3$	$2 n^2$	109,248	128	352
D, L (2)	$10 n^3$	0	327,680	0	0
E, Y (2)	$20 n^3$	$4 n^2$	655,360	256	704
M, N (2)	$10 n^3$	$2 n^2$	327,680	128	352
Sum			3,495,296	1,024	2,816

Table VI: General Formulas at Trisubstituted Inositols and Resulting Branched Tetramers

As can be seen from *Table V*, in addition to the achiral forms estimated by the general formula given above, there are quite some other achiral *meso* forms possible which have to be evaluated manually. The exact number - as we estimate - is 2,816. The main contribution to these additional achiral isomers again stems from symmetrical structures.

Year	1850	1852	1854	1856	1858	1860	1862	1864	1866	1868	1870	1872	1874	1876	1878	1880	1882	1884	1886	1888	1890	1892	1894	1896	1898	1900	1902	1904	1906	1908	1910	1912	1914	1916	1918	1920	1922	1924	1926	1928	1930	1932	1934	1936	1938	1940	1942	1944	1946	1948	1950	1952	1954	1956	1958	1960	1962	1964	1966	1968	1970	1972	1974	1976	1978	1980	1982	1984	1986	1988	1990	1992	1994	1996	1998	2000																								
C	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58	59	60	61	62	63	64	65	66	67	68	69	70	71	72	73	74	75	76	77	78	79	80	81	82	83	84	85	86	87	88	89	90	91	92	93	94	95	96	97	98	99	100
C	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58	59	60	61	62	63	64	65	66	67	68	69	70	71	72	73	74	75	76	77	78	79	80	81	82	83	84	85	86	87	88	89	90	91	92	93	94	95	96	97	98	99	100	
C	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58	59	60	61	62	63	64	65	66	67	68	69	70	71	72	73	74	75	76	77	78	79	80	81	82	83	84	85	86	87	88	89	90	91	92	93	94	95	96	97	98	99	100		
C	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58	59	60	61	62	63	64	65	66	67	68	69	70	71	72	73	74	75	76	77	78	79	80	81	82	83	84	85	86	87	88	89	90	91	92	93	94	95	96	97	98	99	100			
C	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58	59	60	61	62	63	64	65	66	67	68	69	70	71	72	73	74	75	76	77	78	79	80	81	82	83	84	85	86	87	88	89	90	91	92	93	94	95	96	97	98	99	100				
C	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58	59	60	61	62	63	64	65	66	67	68	69	70	71	72	73	74	75	76	77	78	79	80	81	82	83	84	85	86	87	88	89	90	91	92	93	94	95	96	97	98	99	100					

Table V. All Branched Inositol Tetramers, their Stereoisomer Numbers and Achiral meso-forms



Tetr	iso	Ac	Tetr	iso	Ac	Tetr	iso	Ac	Tetr	iso	Ac	Tetr	iso	Ac	Tetr	iso	Ac
N. r. r. r. r.	2160	0															
N. r. r. r. d.	3240	0															
N. r. r. d. r.	6480	12															
N. r. r. d. d.	12960	0															
N. r. d. r. r.	3240	0															
N. r. d. r. d.	6480	0															
N. r. d. d. r.	12960	0															
N. r. d. d. d.	25920	0															
N. d. r. r. r.	1080	6															
N. d. r. r. d.	180	0															
N. d. r. d. r.	1080	0															
N. d. r. d. d.	2160	0															
N. d. d. r. r.	1080	0															
N. d. d. r. d.	2160	0															
N. d. d. d. r.	4320	0															
N. d. d. d. d.	8640	0															
N. r. r. r. r.	6480	0															
N. r. r. r. d.	10800	0															
N. r. r. d. r.	16200	12															
N. r. r. d. d.	32400	0															
N. r. d. r. r.	8100	0															
N. r. d. r. d.	16200	0															
N. r. d. d. r.	32400	0															
N. r. d. d. d.	64800	0															
N. d. r. r. r.	10800	6															
N. d. r. r. d.	21600	0															
N. d. r. d. r.	43200	0															
N. d. r. d. d.	86400	0															
N. d. d. r. r.	10800	0															
N. d. d. r. d.	21600	0															
N. d. d. d. r.	43200	0															
N. d. d. d. d.	86400	0															
N. r. r. r. r.	6480	0															
N. r. r. r. d.	10800	0															
N. r. r. d. r.	16200	12															
N. r. r. d. d.	32400	0															
N. r. d. r. r.	8100	0															
N. r. d. r. d.	16200	0															
N. r. d. d. r.	32400	0															
N. r. d. d. d.	64800	0															
N. d. r. r. r.	10800	6															
N. d. r. r. d.	21600	0															
N. d. r. d. r.	43200	0															
N. d. r. d. d.	86400	0															
N. d. d. r. r.	10800	0															
N. d. d. r. d.	21600	0															
N. d. d. d. r.	43200	0															
N. d. d. d. d.	86400	0															
N. r. r. r. r.	6480	0															
N. r. r. r. d.	10800	0															
N. r. r. d. r.	16200	12															
N. r. r. d. d.	32400	0															
N. r. d. r. r.	8100	0															
N. r. d. r. d.	16200	0															
N. r. d. d. r.	32400	0															
N. r. d. d. d.	64800	0															
N. d. r. r. r.	10800	6															
N. d. r. r. d.	21600	0															
N. d. r. d. r.	43200	0															
N. d. r. d. d.	86400	0															
N. d. d. r. r.	10800	0															
N. d. d. r. d.	21600	0															
N. d. d. d. r.	43200	0															
N. d. d. d. d.	86400	0															
N. r. r. r. r.	6480	0															
N. r. r. r. d.	10800	0															
N. r. r. d. r.	16200	12															
N. r. r. d. d.	32400	0															
N. r. d. r. r.	8100	0															
N. r. d. r. d.	16200	0															
N. r. d. d. r.	32400	0															
N. r. d. d. d.	64800	0															
N. d. r. r. r.	10800	6															
N. d. r. r. d.	21600	0															
N. d. r. d. r.	43200	0															
N. d. r. d. d.	86400	0															
N. d. d. r. r.	10800	0															
N. d. d. r. d.	21600	0															
N. d. d. d. r.	43200	0															
N. d. d. d. d.	86400	0															

N

Table V: All Branched Inositol Tetramers, their Stereoisomer Numbers and Achiral meso-forms

Higher Linear Oligomers:

From ISOMERS² we can derive the number of isomers for higher linear oligomers in the form of a model: Take a chain with 9 differently colored beads. Then the following number of possible arrangements are summarized in *Table VII*: Case (a) lists the possible combinations with all 9 beads of different color, case (b) allows for all possible combinations including multiple occurrences of each colored bead.

<i>Linear Oligomer</i>	<i>General Isomers (a)</i>	<i>General Isomers (b)</i>
Dimer	36	45
Trimer	252	405
Tetramer	1,512	3,321
Pentamer	7,560	29,889
Hexamer	30,240	266,085
Heptamer	90,720	2,394,765
Octamer	181,440	21,526,641
Nonamer	181,440	193,739,769

Table VII: Numbers of General Oligomers with 9 Elements

Now we replace the colored beads by the nine different inositols with their multifunctional binding possibilities outlined in *Table I*. As can be seen from this table, the relation of monopositions (*mono*) to asymmetrical disubstitutions (*di-as*) for all inositols is always 1 : 5. We use the asymmetrical disubstitutional possibilities, since regardless of the oligomer, the inner inositols are all substituted in this way, because we use different inositols to fill the patterns. Again from *Table I* we can gather, that the 9 inositols can be classified according to their *mono*- and *di-as*-possibilities (in round brackets) into three principle groups [in square brackets]: *cis* and *scyllo* (1 / 5) [X]; **D-chiro**, **L-chiro**, **muco** and **neo** (3 / 15) [Y] and **allo**, **epi** and **myo** (6 / 30) [Z]. Within the following compilation (*Table VIII*) we will use these abbreviations (X, Y and Z) and their **count** of members within the group (2, 4 and 3) to derive the **count** of all possible patterns. Let us take e.g. pattern XYZZZ of the pentamers: The count for this specific pattern can be derived by the product of the individual counts: count of X(= 2) times count of Y(= 4) times count of ZZZ(= 1) equals 8. A general formula for this would be (n_x , n_y and n_z being the respective numbers of the three types of inositols):

$$\text{Pattern_count}(n_x, n_y, n_z) = \binom{2}{n_x} \binom{4}{n_y} \binom{3}{n_z}.$$

The figure given under **isomers/count** is then derived by a simple product of all *di-as* – possibilities divided by 25 for the two outer inositols, because their *mono*-possibilities are 5 times less each: $X(=5) * Y(=15) * Z(=30) * Z(=30) * Z(=30) / 25 = 81,000$. In a general way this would amount to: $\text{Isomers/count} = 5^{n_x} * 15^{n_y} * 30^{n_z} / 25$. The product of **count** times **isomers/count** (given in the column “**product**”) thus represents the amount of individual patterns with the respective inositols filled into the general patterns. The sum of these products for each oligomer then has to be multiplied by the possible combinations to yield the final number of inositol stereoisomers for each oligomer given under “**TOTAL**”. The figure given under **combinations** represents the number of combinations of *n* different elements within a “*n*-mer” (e.g. *n* = five for a pentamer results in 60 combinations). In general terms this is exactly $n! / 2$. The factor 1 / 2 stems from the twofold symmetry of such linear oligomers. The product of the sum of counts for the general isomers times the combinations thus represents the figures given in *Table VII* for the general isomers (a) thereof (e.g. $84 * 3 = 252$ for trimers). In the way outlined above the following *Table VIII* has been derived, from which the summary in the subsequent *Table IX* has been extracted.

general								
inositol	type (mono / di-as)	count	type	count	type	count	type	count
c, s	X (1 / 5)	2	XX	1	YY	6	YYY	4
d, l, m, n	Y (3 / 15)	4	XY	8	YZ	12	ZZZ	1
a, e, y	Z (6 / 30)	3	XZ	6	ZZ	3	YYYY	1
	sum	9						
linear dimers (AB)								
pattern	count	isomers/count	product	combinations	TOTAL			
XX	1	1	1					
XY	8	3	24					
XZ	6	6	36					
YY	6	9	54					
YZ	12	18	216					
ZZ	3	36	108					
gen. isomers	sum	36	439	1				439
linear trimers (ABC)								
pattern	count	isomers/count	product	combinations	TOTAL			
XXY	4	15	60					
XXZ	3	30	90					
XYY	12	45	540					
XYZ	24	90	2,160					
XZZ	6	180	1,080					
YYY	4	135	540					
YYZ	18	270	4,860					
YZZ	12	540	6,480					
ZZZ	1	1,080	1,080					
gen. isomers	sum	84	16,890	3				50,670

linear tetramers (ABCD)						
	pattern	count	isomers/count	product	combinations	TOTAL
	XXYY	6	225	1,350		
	XXYZ	12	450	5,400		
	XXZZ	3	900	2,700		
	XYYY	8	675	5,400		
	XYYZ	36	1,350	48,600		
	XYZZ	24	2,700	64,800		
	XZZZ	2	5,400	10,800		
	YYYY	1	2,025	2,025		
	YYYZ	12	4,050	48,600		
	YYZZ	18	8,100	145,800		
	YZZZ	4	16,200	64,800		
gen. isomers	sum	126		400,275	12	4,803,300

linear pentamers (ABCDE)						
	pattern	count	isomers/count	product	combinations	TOTAL
	XXXXY	4	3,375	13,500		
	XXXXZ	18	6,750	121,500		
	XXYZZ	12	13,500	162,000		
	XXZZZ	1	27,000	27,000		
	XXYYY	2	10,125	20,250		
	XXYYZ	24	20,250	486,000		
	XXYZZ	36	40,500	1,458,000		
	XYZZZ	8	81,000	648,000		
	YYYYZ	3	60,750	182,250		
	YYYZZ	12	121,500	1,458,000		
	YYZZZ	6	243,000	1,458,000		
gen. isomers	sum	126		6,034,500	60	362,070,000

linear hexamers (ABCDEF)						
	pattern	count	isomers/count	product	combinations	TOTAL
	XXXXYY	1	50,625	50,625		
	XXXXYZ	12	101,250	1,215,000		
	XXXXZZ	18	202,500	3,645,000		
	XXYYZZ	4	405,000	1,620,000		
	XXYYYZ	6	303,750	1,822,500		
	XXYYZZ	24	607,500	14,580,000		
	XYZZZZ	12	1,215,000	14,580,000		
	YYYYZZ	3	1,822,500	5,467,500		
	YYZZZZ	4	3,645,000	14,580,000		
gen. isomers	sum	84		57,560,625	360	20,721,825,000

linear heptamers (ABCDEFG)						
	pattern	count	isomers/count	product	combinations	TOTAL
	XXXXYYZ	3	1,518,750	4,556,250		
	XXXXYZZ	12	3,037,500	36,450,000		
	XXYYZZZ	6	6,075,000	36,450,000		
	XXYYYZZ	6	9,112,500	54,675,000		
	XXYYZZZ	8	18,225,000	145,800,000		
	YYYYZZZ	1	54,675,000	54,675,000		
gen. isomers	sum	36		332,606,250	2,520	838,167,750,000

linear octamers (ABCDEFGH)						
	pattern	count	isomers/count	product	combinations	TOTAL
	XXYYYYZZ	3	45,562,500	136,687,500		
	XXYYYYZZ	4	91,125,000	364,500,000		
	XYYYYZZZ	2	273,375,000	546,750,000		
gen. isomers	sum	9		1,047,937,500	20,160	21,126,420,000,000

linear nonamers (ABCDEFGHI)						
	pattern	count	isomers/count	product	combinations	TOTAL
	XXYYYYZZZ	1	1,366,875,000	1,366,875,000		
gen. isomers	sum	1		1,366,875,000	181,440	248,005,800,000,000

Table VIII: Calculation of Higher Oligomers and their Inositol Isomer Numbers

Linear Oligomer	Inositol Stereoisomers (a)	Inositol Stereoisomers (b)
Dimer	439	528
Trimer	50,670	82,176
Tetramer	4,803,300	13,109,760
Pentamer	362,070,000	§
Hexamer	20,721,825,000	§
Heptamer	838,167,750,000	§
Octamer	21,126,420,000,000	§
Nonamer	248,005,800,000,000	§

Table IX: Summary of Numbers of Oligomers including Stereoisomers with all nine Inositols

Within Table IX, (a) and (b) have the same meaning as in Table VII: Column (a) lists the total number of stereoisomers for the case of all nine inositols within the oligomer being different (taken from Table VIII), while column (b) lists the figures for all combinations including multiple occurrence as far as calculated in this paper. The estimation of patterns and numbers for inositol oligomers (b) higher than tetramers (§) lies well beyond our present computational possibilities.

Summary and Conclusion

With these comprehensive tables we hope to have contributed concrete help to all chemists looking for numbers of inositol oligomers including all stereoisomers of a general or a specific form. The generation of the achiral *meso* forms thereof via an automated way is still a theoretical as well as practical task well ahead.

References and Notes

- [1] Dolhaine, H.; Hönig, H., On the Number of Some Inositol - Tetramers. *MATCH* **2002**, submitted.
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The MATHEMATICA - AddOn "Isomers.m" together with some help browser files is available free of charge (for academics only) by registration at the bottom of the webpage: <http://www.cis.TUGraz.at/orgc/institut/softnew.htm>