

Full Isomer-Tables of Inositol-Oligomers up to Tetramers

Hans Dolhaine^a, Helmut Höning^{*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

(September 25th, 2002)

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 inositolts:

Inositol	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
D-chiro	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
L-chiro	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 I: Basic Substitutional Possibilities at all Nine Inositolts

Within the following tables, we will use the abbreviations given under "Abbr" in Table I. Small letters will be used for inositolts acting as substituents (ligands), while capital letters will be used for central (di- or tri-substituted) inositolts. 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 inositolts, "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 inositolts (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 I 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 inositolts: $\text{mono}_x * (\text{mono}_x + 1) / 2$. 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" inositolts, 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 inositolts the formula

logically is: mono_x * mono_y, x and y are indicating the respective inositol. 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 inositol, which have to be evaluated individually according to their number of enantiotopic monopositions and the number of monopositions located in the plane of symmetry (see ¹).

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

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 monopositions 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 **x-Y-x'**, where **x'** is still the same inositol as **x**, but with a different monoposition (e.g. *neo_1* and *neo_3*). For the former, the number of isomers is given by: $\text{mono}_x * \text{di-sy}$, while for the latter it is: $\text{mono}_x * \text{di-asy} * (\text{mono}_x - 1) / 2$. Within the tables, these terms again are combined to one sum. For trimers of the general form **x-Y-z** the number of isomers is: $\text{mono}_x * \text{di-asy} * \text{mono}_z$. 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-l** - pairs.

Linear Tetramers:

Here again one has to distinguish between two basic forms: Symmetrical cases of the general pattern: **x-Y-Y-x** or **x-X-X-x** and asymmetrical forms which are considered below. For symmetrical tetramers, the following formulas are applied: $\text{mono}_x * \text{di-asy} * (\text{mono}_x * \text{di-asy} + 1) / 2$ or $\text{mono}_x * \text{di-asx} * (\text{mono}_x * \text{di-asx} + 1) / 2$ respectively. For asymmetrical general patterns like **x-Y-Z-o**, the following formula is valid: $\text{mono}_x * \text{di-asy} * \text{di-asz} * \text{mono}_o$. 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-l** - 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 of this specific pairwise patterns have to be examined carefully for possible achiral *meso* forms.

1 <i>H</i>	iso	Ach	Tris																										
s,A,a	540	9	a,C,c	93	9	a,D,s	90	0	a,D,s	90	0	a,E,a	90	0	a,M,a	279	9	a,M,a	279	0	a,M,a	279	9	a,N,a	90	6	a,Y,a	90	9
s,A,c	180	0	a,C,c	30	0	a,D,s	90	0	a,D,s	90	0	a,E,c	90	0	a,M,c	90	0	a,M,c	90	0	a,M,c	90	0	a,S,c	90	0	a,Y,c	90	0
s,A,d	540	0	a,C,c	90	0	a,D,d	270	0	a,D,d	270	0	a,E,d	90	0	a,M,d	270	0	a,M,d	270	0	a,M,d	270	0	a,S,d	90	0	a,Y,d	90	0
s,A,e	180	0	a,C,c	90	0	a,D,d	240	0	a,D,d	240	0	a,E,f	90	0	a,M,f	240	0	a,M,f	240	0	a,M,f	240	0	a,S,f	90	0	a,Y,f	90	0
s,A,l	540	0	a,C,c	90	0	a,D,d	210	0	a,D,d	210	0	a,E,g	90	0	a,M,g	210	0	a,M,g	210	0	a,M,g	210	0	a,S,g	90	0	a,Y,g	90	0
s,A,m	540	0	a,C,m	90	0	a,D,m	270	0	a,D,m	270	0	a,E,m	90	0	a,M,m	270	0	a,M,m	270	0	a,M,m	270	0	a,S,m	90	0	a,Y,m	90	0
s,A,n	540	0	a,C,m	90	0	a,D,m	240	0	a,D,m	240	0	a,E,n	90	0	a,M,n	240	0	a,M,n	240	0	a,M,n	240	0	a,S,n	90	0	a,Y,n	90	0
s,A,o	180	0	a,C,m	90	0	a,D,m	210	0	a,D,m	210	0	a,E,o	90	0	a,M,o	210	0	a,M,o	210	0	a,M,o	210	0	a,S,o	90	0	a,Y,o	90	0
s,A,y	180	0	a,C,y	180	0	a,D,y	540	0	a,D,y	540	0	a,E,y	180	0	a,M,y	540	0	a,M,y	540	0	a,M,y	540	0	a,S,y	180	0	a,Y,y	180	0
s,A,z	15	1	a,C,z	15	1	a,D,z	90	0	a,D,z	90	0	a,E,z	15	1	a,M,z	90	0	a,M,z	90	0	a,M,z	90	0	a,S,z	15	1	a,Y,z	15	1
c,A,d	90	0	c,C,d	15	0	c,D,d	45	0	c,D,d	45	0	c,E,d	90	0	c,M,d	45	0	c,M,d	45	0	c,M,d	45	0	c,S,d	15	0	c,Y,d	90	0
c,A,e	180	0	c,C,e	30	2	c,D,e	90	0	c,D,e	90	0	c,E,e	180	4	c,M,e	90	0	c,M,e	90	2	c,M,e	90	0	c,S,e	30	2	c,Y,e	180	4
c,A,l	90	0	c,C,l	15	0	c,D,l	45	0	c,D,l	45	0	c,E,l	90	0	c,M,l	45	0	c,M,l	45	0	c,M,l	45	0	c,S,l	15	0	c,Y,l	90	0
c,A,m	90	0	c,C,m	15	1	c,D,m	45	0	c,D,m	45	0	c,E,m	90	2	c,L,m	45	0	c,M,m	45	1	c,M,m	45	1	c,S,m	15	1	c,Y,m	90	0
c,A,n	90	0	c,C,n	15	1	c,D,n	45	0	c,D,n	45	0	c,E,n	90	2	c,L,n	45	0	c,M,n	45	1	c,M,n	45	1	c,S,n	15	1	c,Y,n	90	2
c,A,s	30	0	c,C,s	5	1	c,D,s	15	0	c,D,s	15	0	c,E,s	30	2	c,L,s	15	0	c,M,s	15	1	c,M,s	15	1	c,S,s	5	1	c,Y,s	30	2
c,A,y	180	0	c,C,y	30	2	c,D,y	90	0	c,D,y	90	0	c,E,y	180	4	c,L,y	90	2	c,M,y	90	2	c,M,y	90	2	c,S,y	30	2	c,Y,y	180	4
d,A,d	135	0	d,C,d	24	0	d,D,d	72	0	d,D,d	72	0	d,E,d	135	0	d,L,d	72	0	d,M,d	72	0	d,M,d	72	0	d,N,d	27	0	d,V,d	135	0
d,A,e	540	0	d,C,e	90	0	d,D,e	270	0	d,D,e	270	0	d,E,e	540	0	d,L,e	270	0	d,M,e	270	0	d,M,e	270	0	d,N,e	90	0	d,Y,e	540	0
d,A,i	270	9	d,C,i	45	9	d,D,i	135	0	d,D,i	135	0	d,E,i	270	9	d,L,i	135	0	d,M,i	135	9	d,M,i	135	9	d,N,i	45	6	d,Y,i	270	9
d,A,m	270	0	d,C,m	45	0	d,D,m	135	0	d,D,m	135	0	d,E,m	270	0	d,L,m	135	0	d,M,m	135	0	d,M,m	135	0	d,N,m	45	0	d,Y,m	270	0
d,A,n	270	0	d,C,n	45	0	d,D,n	135	0	d,D,n	135	0	d,E,n	270	0	d,L,n	135	0	d,M,n	135	0	d,M,n	135	0	d,N,n	45	0	d,Y,n	270	0
d,A,s	90	0	d,C,s	15	2	d,D,s	45	0	d,D,s	45	0	d,E,s	90	0	d,L,s	45	0	d,M,s	45	0	d,M,s	45	0	d,S,s	15	0	d,Y,s	90	0
d,A,y	540	0	d,C,y	90	0	d,D,y	270	0	d,D,y	270	0	d,E,y	540	12	d,L,y	270	0	d,M,y	270	0	d,M,y	270	0	d,N,y	90	8	d,Y,y	540	12
c,A,c	540	12	c,C,c	93	12	c,D,c	270	0	c,D,c	270	0	c,E,c	540	12	c,L,c	270	0	c,M,c	270	0	c,M,c	270	0	c,S,c	90	12	c,Y,c	540	12
c,A,i	540	0	c,C,i	90	0	c,D,i	240	0	c,D,i	240	0	c,E,i	540	12	c,L,i	240	0	c,M,i	240	0	c,M,i	240	0	c,S,i	90	0	c,Y,i	540	0
c,A,m	540	0	c,C,m	90	2	c,D,m	270	0	c,D,m	270	0	c,E,m	540	4	c,L,m	270	0	c,M,m	270	2	c,M,m	270	2	c,S,m	90	2	c,Y,m	540	4
c,A,n	540	0	c,C,n	90	2	c,D,n	270	0	c,D,n	270	0	c,E,n	540	4	c,L,n	270	0	c,M,n	540	4	c,M,n	540	4	c,S,n	90	2	c,Y,n	540	4
c,A,s	180	0	c,C,s	30	2	c,D,s	90	0	c,D,s	90	0	c,E,s	180	4	c,L,s	90	0	c,M,s	90	2	c,M,s	90	2	c,S,s	90	2	c,Y,s	180	4
c,A,y	180	0	c,C,y	180	4	c,D,y	540	0	c,D,y	540	0	c,E,y	180	8	c,L,y	540	4	c,M,y	540	4	c,M,y	540	4	c,S,y	180	8	c,Y,y	180	8
j,A,m	270	0	j,C,m	45	0	j,D,m	135	0	j,D,m	135	0	j,E,m	270	0	j,L,m	135	0	j,M,m	135	0	j,M,m	135	0	j,N,m	270	0	j,Y,m	270	0
j,A,n	270	0	j,C,n	45	0	j,D,n	135	0	j,D,n	135	0	j,E,n	270	0	j,L,n	135	0	j,M,n	135	0	j,M,n	135	0	j,N,n	270	0	j,Y,n	270	0
j,A,s	90	0	j,C,s	15	0	j,D,s	45	0	j,D,s	45	0	j,E,s	90	0	j,L,s	45	0	j,M,s	45	0	j,M,s	45	0	j,S,s	90	0	j,Y,s	90	0
j,A,y	540	0	j,C,y	90	0	j,D,y	270	0	j,D,y	270	0	j,E,y	540	12	j,L,y	270	0	j,M,y	540	12	j,M,y	540	12	j,S,y	90	12	j,Y,y	540	12
j,A,z	540	0	j,C,z	90	0	j,D,z	270	0	j,D,z	270	0	j,E,z	540	12	j,L,z	270	0	j,M,z	540	12	j,M,z	540	12	j,S,z	90	12	j,Y,z	540	12
m,A,m	180	0	m,C,m	24	0	m,D,m	72	0	m,D,m	72	0	m,E,m	180	9	m,L,m	72	0	m,M,m	72	0	m,M,m	72	0	m,N,m	27	0	m,Y,m	180	9
m,A,n	180	0	m,C,n	24	0	m,D,n	72	0	m,D,n	72	0	m,E,n	180	9	m,L,n	72	0	m,M,n	72	0	m,M,n	72	0	m,N,n	27	0	m,Y,n	180	9
m,A,s	90	0	m,C,s	15	1	m,D,s	45	0	m,D,s	45	0	m,E,s	180	9	m,L,s	45	0	m,M,s	45	1	m,M,s	45	1	m,S,s	15	1	m,Y,s	90	1
m,A,y	540	0	m,C,y	90	0	m,D,y	270	0	m,D,y	270	0	m,E,y	540	4	m,L,y	270	0	m,M,y	270	2	m,M,y	270	2	m,S,y	90	2	m,Y,y	540	4
m,A,z	540	0	m,C,z	90	0	m,D,z	270	0	m,D,z	270	0	m,E,z	540	4	m,L,z	270	0	m,M,z	270	2	m,M,z	270	2	m,S,z	90	2	m,Y,z	540	4
m,A,x	180	0	m,C,x	30	2	m,D,x	90	0	m,D,x	90	0	m,E,x	180	9	m,L,x	90	0	m,M,x	180	9	m,M,x	180	9	m,N,x	27	0	m,Y,x	180	9
m,A,s	180	0	m,C,s	30	2	m,D,s	90	0	m,D,s	90	0	m,E,s	180	9	m,L,s	90	0	m,M,s	180	9	m,M,s	180	9	m,N,s	27	0	m,Y,s	180	9
m,A,y	540	0	m,C,y	93	6	m,D,y	279	0	m,D,y	279	0	m,E,y	540	12	m,L,y	279	0	m,M,y	279	12	m,M,y	279	12	m,S,y	93	8	m,Y,y	540	12

Table III: All Linear Inositol Trimers, their Stereoisomer Numbers and Achiral meso-forms

Ter	Iso	Ac	Ter	Iso	Ac	Ter	Iso	Ac	Ter	Iso	Ac	Ter	Iso	Ac	Ter	Iso	Ac	Ter	Iso	Ac	Ter	Iso	Ac	Ter	Iso	Ac	Ter	Iso	Ac	Ter	Iso	Ac
AA	AC	AT	AD	AF	AL	AM	AN	AS	AV																							
a A A c 16290 45 s A C s 3400 0	a A D d 2000 0	s A L 16200 0	s A E a 2200 0	s A I a 16200 0	s A M a 16200 0	s A N a 16200 0	s A S a 16200 0	s A Y a 16200 0																								
a A A c 5400 0	a A C c 900 0	a A D c 2700 0	s A F c 3400 0	a A L c 2700 0	a A M c 2700 0	a A N c 2700 0	a A S c 2700 0	a A Y c 2700 0																								
s A A d 16200 0	s A C d 2700 0	s A D d 6200 0	s A F d 6200 0	s A L d 8100 0	s A M d 8100 0	s A N d 8100 0	s A S d 8100 0	s A Y d 8100 0																								
s A A e 32400 0	s A C e 5400 0	s A D e 6200 0	s A F e 7200 0	s A L e 7200 0	s A M e 7200 0	s A N e 7200 0	s A S e 7200 0	s A Y e 7200 0																								
a A A l 16200 0	s A C l 2700 0	a A D l 6200 0	s A F l 6200 0	s A L l 8100 0	s A M l 8100 0	s A N l 8100 0	s A S l 8100 0	s A Y l 8100 0																								
a A A m 16200 0	s A C m 2700 0	s A D m 6200 0	s A F m 6200 0	s A L m 8100 0	s A M m 8100 0	s A N m 8100 0	s A S m 8100 0	s A Y m 8100 0																								
a A A n 16200 0	s A C n 2700 0	s A D n 6200 0	s A F n 6200 0	s A L n 8100 0	s A M n 8100 0	s A N n 8100 0	s A S n 8100 0	s A Y n 8100 0																								
a A A s 5400 0	a A C s 900 0	a A D s 2700 0	s A F s 3400 0	s A L s 2700 0	s A M s 2700 0	s A N s 2700 0	s A S s 2700 0	s A Y s 2700 0																								
s A A y 32400 0	s A C y 5400 0	s A D y 2700 0	s A F y 6200 0	s A L y 16200 0	s A M y 16200 0	s A N y 16200 0	s A S y 16200 0	s A Y y 16200 0																								
c A A c 465 0	s A C c 150 0	a A D c 450 0	s A F c 900 0	s A L c 2700 0	s A M c 3500 0	s A N c 450 0	s A S c 1320 0	s A Y c 520 0																								
c A A d 450 0	s A C d 150 0	s A D d 2700 0	s A F d 6200 0	s A L d 16200 0	s A M d 2700 0	s A N d 2700 0	s A S d 450 0	s A Y d 2700 0																								
c A A e 5400 0	s A C e 900 0	s A D e 2700 0	s A F e 6200 0	s A L e 16200 0	s A M e 2700 0	s A N e 2700 0	s A S e 450 0	s A Y e 2700 0																								
c A A l 2700 0	s A C l 450 0	s A D l 2700 0	s A F l 6200 0	s A L l 16200 0	s A M l 2700 0	s A N l 2700 0	s A S l 450 0	s A Y l 2700 0																								
c A A m 2700 0	s A C m 450 0	s A D m 2700 0	s A F m 6200 0	s A L m 16200 0	s A M m 2700 0	s A N m 2700 0	s A S m 450 0	s A Y m 2700 0																								
c A A n 2700 0	s A C n 450 0	s A D n 2700 0	s A F n 6200 0	s A L n 16200 0	s A M n 2700 0	s A N n 2700 0	s A S n 450 0	s A Y n 2700 0																								
c A A s 5400 0	c A C s 150 0	a A D s 450 0	s A F s 900 0	s A L s 2700 0	s A M s 3500 0	s A N s 450 0	s A S s 150 0	s A Y s 520 0																								
c A A y 5400 0	c A C y 900 0	a A D y 2700 0	s A F y 6200 0	s A L y 16200 0	s A M y 16200 0	s A N y 16200 0	s A S y 16200 0	s A Y y 16200 0																								
d A A c 4095 0	d A C c 1350 0	d A D c 4050 0	s A F c 8100 0	s A L c 16200 0	d A M c 4050 0	d A N c 4050 0	d A S c 1350 0	d A Y c 520 0																								
d A A d 4050 0	d A C d 1350 0	d A D d 8100 0	s A F d 16200 0	d A L d 16200 0	d A M d 4050 0	d A N d 4050 0	d A S d 1350 0	d A Y d 520 0																								
d A A e 16200 0	d A C e 2700 0	d A D e 8100 0	d A F e 16200 0	d A L e 16200 0	d A M e 8100 0	d A N e 2700 0	d A S e 16200 0	d A Y e 8100 0																								
d A A l 8100 0	d A C l 450 0	d A D l 4050 0	d A F l 8100 0	d A L l 16200 0	d A M l 4050 0	d A N l 4050 0	d A S l 1350 0	d A Y l 520 0																								
d A A m 8100 0	d A C m 450 0	d A D m 4050 0	d A F m 8100 0	d A L m 16200 0	d A M m 4050 0	d A N m 4050 0	d A S m 1350 0	d A Y m 520 0																								
d A A n 8100 0	d A C n 450 0	d A D n 4050 0	d A F n 8100 0	d A L n 16200 0	d A M n 4050 0	d A N n 4050 0	d A S n 1350 0	d A Y n 520 0																								
d A A s 2700 0	d A C s 1350 0	d A D s 4050 0	d A F s 8100 0	d A L s 16200 0	d A M s 4050 0	d A N s 4050 0	d A S s 1350 0	d A Y s 520 0																								
d A A y 16200 0	d A C y 6200 0	d A D y 4050 0	s A F y 8100 0	d A L y 16200 0	d A M y 4050 0	d A N y 4050 0	d A S y 1350 0	d A Y y 520 0																								
e A A c 2700 0	s A C c 2700 0	a A D c 8100 0	s A F c 16200 0	s A L c 2700 0	s A M c 8100 0	s A N c 16200 0	s A S c 2700 0	s A Y c 8100 0																								
e A A d 2700 0	s A C d 8100 0	a A D d 16200 0	s A F d 2700 0	s A L d 8100 0	s A M d 16200 0	s A N d 2700 0	s A S d 8100 0	s A Y d 16200 0																								
e A A e 16200 0	s A C e 2700 0	s A D e 8100 0	s A F e 16200 0	s A L e 2700 0	s A M e 8100 0	s A N e 16200 0	s A S e 2700 0	s A Y e 8100 0																								
e A A l 8100 0	s A C l 8100 0	s A D l 8100 0	s A F l 16200 0	s A L l 2700 0	s A M l 8100 0	s A N l 16200 0	s A S l 2700 0	s A Y l 8100 0																								
e A A m 8100 0	s A C m 8100 0	s A D m 8100 0	s A F m 16200 0	s A L m 2700 0	s A M m 8100 0	s A N m 16200 0	s A S m 2700 0	s A Y m 8100 0																								
e A A n 8100 0	s A C n 8100 0	s A D n 8100 0	s A F n 16200 0	s A L n 2700 0	s A M n 8100 0	s A N n 16200 0	s A S n 2700 0	s A Y n 8100 0																								
e A A s 2700 0	s A C s 8100 0	s A D s 8100 0	s A F s 16200 0	s A L s 2700 0	s A M s 8100 0	s A N s 16200 0	s A S s 2700 0	s A Y s 8100 0																								
e A A y 16200 0	s A C y 8100 0	s A D y 8100 0	s A F y 16200 0	s A L y 2700 0	s A M y 8100 0	s A N y 16200 0	s A S y 2700 0	s A Y y 8100 0																								
f A A c 4095 0	s A C c 1350 0	s A D c 4050 0	s A F c 8100 0	s A L c 16200 0	f A M c 4050 0	f A N c 4050 0	f A S c 1350 0	f A Y c 520 0																								
f A A d 4050 0	s A C d 1350 0	s A D d 4050 0	s A F d 8100 0	s A L d 16200 0	f A M d 4050 0	f A N d 4050 0	f A S d 1350 0	f A Y d 520 0																								
f A A e 8100 0	s A C e 1350 0	s A D e 4050 0	s A F e 8100 0	s A L e 16200 0	f A M e 4050 0	f A N e 4050 0	f A S e 1350 0	f A Y e 520 0																								
f A A l 8100 0	s A C l 1350 0	s A D l 4050 0	s A F l 8100 0	s A L l 16200 0	f A M l 4050 0	f A N l 4050 0	f A S l 1350 0	f A Y l 520 0																								
f A A m 8100 0	s A C m 1350 0	s A D m 4050 0	s A F m 8100 0	s A L m 16200 0	f A M m 4050 0	f A N m 4050 0	f A S m 1350 0	f A Y m 520 0																								
f A A n 8100 0	s A C n 1350 0	s A D n 4050 0	s A F n 8100 0	s A L n 16200 0	f A M n 4050 0	f A N n 4050 0	f A S n 1350 0	f A Y n 520 0																								
f A A s 2700 0	s A C s 1350 0	s A D s 4050 0	s A F s 8100 0	s A L s 16200 0	f A M s 4050 0	f A N s 4050 0	f A S s 1350 0	f A Y s 520 0																								
f A A y 16200 0	s A C y 1350 0	s A D y 4050 0	s A F y 8100 0	s A L y 16200 0	f A M y 4050 0	f A N y 4050 0	f A S y 1350 0	f A Y y 520 0																								
g A A c 4095 0	s A C c 1350 0	s A D c 4050 0	s A F c 8100 0	s A L c 16200 0	g A M c 4050 0	g A N c 4050 0	g A S c 1350 0	g A Y c 520 0																								
g A A d 4050 0	s A C d 1350 0	s A D d 4050 0	s A F d 8100 0	s A L d 16200 0	g A M d 4050 0	g A N d 4050 0	g A S d 1350 0	g A Y d 520 0																								
g A A e 8100 0	s A C e 1350 0	s A D e 4050 0	s A F e 8100 0	s A L e 16200 0	g A M e 4050 0	g A N e 4050 0	g A S e 1350 0	g A Y e 520 0																								
g A A l 8100 0	s A C l 1350 0	s A D l 4050 0	s A F l 8100 0	s A L l 16200 0	g A M l 4050 0	g A N l 4050 0	g A S l 1350 0	g A Y l 520 0																								
g A A m 8100 0	s A C m 1350 0	s A D m 4050 0	s A F m 8100 0	s A L m 16200 0	g A M m 4050 0	g A N m 4050 0	g A S m 1350 0	g A Y m 520 0																								
g A A n 8100 0	s A C n 1350 0	s A D n 4050 0	s A F n 8100 0	s A L n 16200 0	g A M n 4050 0	g A N n 4050 0	g A S n 1350 0	g A Y n 520 0																								
g A A s 2700 0	s A C s 1350 0	s A D s 4050 0	s A F s 8100 0	s A L s 16200 0	g A M s 4050 0	g A N s 4050 0	g A S s 1350 0	g A Y s 520 0																								
g A A y 16200 0	s A C y 1350 0	s A D y 4050 0	s A F y 8100 0	s A L y 16200 0	g A M y 4050 0	g A N y 4050 0	g A S y 1350 0	g A Y y 520 0																								
h A A c 2700 0	s A C c 2700 0	s A D c 8100 0	s A F c 16200 0	s A L c 2700 0	h A M c 2700 0	h A N c 8100 0	h A S c 16200 0	h A Y c 8100 0																								
h A A d 2700 0	s A C d 8100 0	s A D d 16200 0	s A F d 2700 0	s A L d 8100 0	h A M d 2700 0	h A N d 16200 0	h A S d 8100 0	h A Y d 2700 0																								
h A A e 16200 0	s A C e 2700 0	s A D e 8100 0	s A F e 16200 0	s A L e 2700 0	h A M e 2700 0	h A N e 8100 0	h A S e 16200 0	h A Y e 2700 0																								
h A A l 8100 0	s A C l 2700 0	s A D l 8100 0	s A F l 16200 0	s A L l 2700 0	h A M l 2700 0	h A N l 8100 0	h A S l 16200 0	h A Y l 2700 0																								
h A A m 8100 0	s A C m 2700 0	s A D m 8100 0	s A F m 16200 0	s A L m 2700 0	h A M m 2700 0	h A N m 8100 0	h A S m 16200 0	h A Y m 2700 0																								
h A A n 8100 0	s A C n 2700 0	s A D n 8100 0	s A F n 16200 0	s A L n 2700 0	h A M n 2700 0	h A N n 8100 0	h A S n 16200 0	h A Y n 2700 0																								
h A A s 16200 0	s A C s 2700 0	s A D s 8100 0	s A F s 16200 0	s A L s 2700 0	h A M s 2700 0	h A N s 8100 0	h A S s 16200 0	h A Y s 2700 0																								
h A A y 16200 0	s A C y 2700 0	s A D y 8100 0	s A F y 16200 0	s A L y 2700 0	h A M y 2700 0	h A N y 8100 0	h A S y 16200 0	h A Y y 2700 0																								
i A A c 465 0	s A C c 15 0	s A D c 450 0	s A F c 90 0	s A L c 270 0	i A M c 450 0	i A N c 90 0	i A S c 270 0	i A Y c 90 0																								
i A A d 465 0	s A C d 15 0	s A D d 270 0	s A F d 90 0	s A L d 810 0	i A M d 450 0	i A N d 90 0	i A S d 270 0	i A Y d 90 0																								
i A A e 465 0	s A C e 15 0	s A D e 270 0	s A F e 90 0	s A L e 810 0	i A M e 450 0	i A N e 90 0	i A S e 270 0	i A Y e 90 0																								
i A A l 465 0	s A C l 15 0	s A D l 270 0	s A F l 90 0	s A L l 810 0	i A M l 450 0	i A N l 90 0	i A S l 270 0	i A Y l 90 0																								
i A A m 465 0	s A C m 15 0	s A D m 270 0	s A F m 90 0	s A L m 810 0	i A M m 450 0	i A N m 90 0	i A S m 270 0	i A Y m 90 0																								
i A A n 465 0	s A C n 15 0	s A D n 270 0	s A F n 90 0	s A L n 810 0	i A M n 450 0	i A N n 90 0	i A S n 270 0	i A Y n 90 0																								
i A A s 465 0	s A C s 15 0	s A D s 270 0	s A F s 90 0	s A L s 810 0	i A M s 450 0	i A N s 90 0	i A S s 270 0	i A Y s 90 0																								
i A A y 465 0	s A C y 15 0	s A D y 270 0	s A F y 90 0	s A L y 810 0	i A M y 450 0	i A N y 90 0	i A S y 270 0	i A Y y 90 0																								

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

Ter	Iso	Ac	Ter	Iso	Ac	Ter	Iso	Ac	Ter	Iso	Ac	Ter	Iso	Ac	Ter	Iso	Ac	Ter	Iso	Ac		
L	A	C	L	A	C	L	A	C	L	A	C	L	A	C	L	A	C	L	A	C		
a	L	c	2700	0	a	L	c	450	0	a	L	c	1550	0	a	L	c	2700	0	a	L	c
a	L	d	8100	0	a	L	c	1350	0	a	L	d	4050	0	a	L	c	1350	0	a	L	s
a	L	e	16200	0	a	L	c	2700	0	a	L	d	8100	0	a	L	e	16200	0	a	L	d
a	L	f	8100	0	a	L	c	1350	0	a	L	d	4050	0	a	L	e	16200	0	a	L	e
a	L	m	8100	+	a	L	c	1350	0	a	L	d	4050	0	a	L	m	8100	+	a	L	m
a	L	n	8100	+	a	L	c	1350	0	a	L	d	4050	0	a	L	m	8100	+	a	L	m
a	L	s	2700	+	a	L	c	450	0	a	L	d	1350	0	a	L	s	2700	+	a	L	s
a	L	y	16200	0	a	L	c	2700	0	a	L	d	8100	0	a	L	y	16200	0	a	L	y
c	L	a	1350	0	c	L	c	225	0	c	L	d	675	0	c	L	e	1350	0	c	L	d
c	L	b	2700	0	c	L	c	450	0	c	L	d	1350	0	c	L	e	1350	0	c	L	d
c	L	i	1350	0	c	L	c	225	0	c	L	d	675	0	c	L	e	1350	0	c	L	e
c	L	m	1350	0	c	L	c	450	0	c	L	d	1350	0	c	L	e	1350	0	c	L	e
c	L	n	1350	0	c	L	c	225	0	c	L	d	675	0	c	L	e	1350	0	c	L	e
c	L	s	1350	0	c	L	c	450	0	c	L	d	1350	0	c	L	e	1350	0	c	L	e
c	L	y	1350	0	c	L	c	225	0	c	L	d	675	0	c	L	e	1350	0	c	L	e
d	L	a	4050	0	d	L	c	1350	0	d	L	d	4050	0	d	L	e	1350	0	d	L	d
d	L	m	4050	0	d	L	c	675	0	d	L	d	2025	45	d	L	e	2025	0	d	L	e
d	L	s	4050	0	d	L	c	225	0	d	L	d	4050	0	d	L	e	2025	0	d	L	e
d	L	y	4050	0	d	L	c	675	0	d	L	d	2025	45	d	L	e	2025	0	d	L	e
d	L	s	225	0	d	L	c	225	0	d	L	d	675	0	d	L	e	1350	0	d	L	e
d	L	y	225	0	d	L	c	225	0	d	L	d	675	0	d	L	e	1350	0	d	L	e
d	L	a	450	0	d	L	c	1350	0	d	L	d	4050	0	d	L	e	1350	0	d	L	e
d	L	m	450	0	d	L	c	675	0	d	L	d	2025	45	d	L	e	2025	0	d	L	e
d	L	s	450	0	d	L	c	225	0	d	L	d	675	0	d	L	e	1350	0	d	L	e
d	L	y	450	0	d	L	c	675	0	d	L	d	2025	45	d	L	e	2025	0	d	L	e
d	L	s	1350	0	d	L	c	225	0	d	L	d	675	0	d	L	e	1350	0	d	L	e
d	L	y	1350	0	d	L	c	675	0	d	L	d	2025	45	d	L	e	2025	0	d	L	e
d	L	a	1350	0	d	L	c	225	0	d	L	d	675	0	d	L	e	1350	0	d	L	e
d	L	m	1350	0	d	L	c	675	0	d	L	d	2025	45	d	L	e	1350	0	d	L	e
d	L	s	1350	0	d	L	c	225	0	d	L	d	675	0	d	L	e	1350	0	d	L	e
d	L	y	1350	0	d	L	c	675	0	d	L	d	2025	45	d	L	e	1350	0	d	L	e
d	L	a	4050	0	d	L	c	1350	0	d	L	d	4050	0	d	L	e	1350	0	d	L	e
d	L	m	4050	0	d	L	c	675	0	d	L	d	2025	45	d	L	e	1350	0	d	L	e
d	L	s	4050	0	d	L	c	225	0	d	L	d	675	0	d	L	e	1350	0	d	L	e
d	L	y	4050	0	d	L	c	675	0	d	L	d	2025	45	d	L	e	1350	0	d	L	e
d	L	a	1350	0	d	L	c	225	0	d	L	d	675	0	d	L	e	1350	0	d	L	e
d	L	m	1350	0	d	L	c	675	0	d	L	d	2025	45	d	L	e	1350	0	d	L	e
d	L	s	1350	0	d	L	c	225	0	d	L	d	675	0	d	L	e	1350	0	d	L	e
d	L	y	1350	0	d	L	c	675	0	d	L	d	2025	45	d	L	e	1350	0	d	L	e
d	L	a	450	0	d	L	c	1350	0	d	L	d	4050	0	d	L	e	1350	0	d	L	e
d	L	m	450	0	d	L	c	675	0	d	L	d	2025	45	d	L	e	1350	0	d	L	e
d	L	s	450	0	d	L	c	225	0	d	L	d	675	0	d	L	e	1350	0	d	L	e
d	L	y	450	0	d	L	c	675	0	d	L	d	2025	45	d	L	e	1350	0	d	L	e
d	L	a	1350	0	d	L	c	225	0	d	L	d	675	0	d	L	e	1350	0	d	L	e
d	L	m	1350	0	d	L	c	675	0	d	L	d	2025	45	d	L	e	1350	0	d	L	e
d	L	s	1350	0	d	L	c	225	0	d	L	d	675	0	d	L	e	1350	0	d	L	e
d	L	y	1350	0	d	L	c	675	0	d	L	d	2025	45	d	L	e	1350	0	d	L	e
d	L	a	8100	0	d	L	c	1350	0	d	L	d	4050	0	d	L	e	1350	0	d	L	e
d	L	m	8100	0	d	L	c	675	0	d	L	d	2025	45	d	L	e	1350	0	d	L	e
d	L	s	8100	0	d	L	c	225	0	d	L	d	675	0	d	L	e	1350	0	d	L	e
d	L	y	8100	0	d	L	c	675	0	d	L	d	2025	45	d	L	e	1350	0	d	L	e
d	L	a	2700	0	d	L	c	1350	0	d	L	d	4050	0	d	L	e	1350	0	d	L	e
d	L	m	2700	0	d	L	c	675	0	d	L	d	2025	45	d	L	e	1350	0	d	L	e
d	L	s	2700	0	d	L	c	225	0	d	L	d	675	0	d	L	e	1350	0	d	L	e
d	L	y	2700	0	d	L	c	675	0	d	L	d	2025	45	d	L	e	1350	0	d	L	e

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

Ter.	Iso.	Ac.	Igr.	Iso.	Ac.	Ter.	Iso.	Ac.	Ter.	Iso.	Ac.	Ter.	Iso.	Ac.	Ter.	Iso.	Ac.	Ter.	Iso.	Ac.	Ter.	Iso.	Ac.	Ter.	Iso.	Ac.	Ter.	Iso.	Ac.										
Ma	Ma	Ma	Ma	Ma	Ma	Ma	Ma	Ma	Ma	Ma	Ma	Ma	Ma	Ma	Ma	Ma	Ma	Ma	Ma	Ma	Ma	Ma	Ma	Ma	Ma	Ma	Ma	Ma	Ma	Ma	Ma								
a	Ma	s	2700	0	a	Mc	c	450	0	a	Md	c	1350	0	a	Md	c	2700	0	a	Md	c	4050	24	a	Md	c	8100	0	a	Md	c	2700	0					
a	Ma	d	8100	0	a	Mc	d	1350	0	a	Md	d	4050	0	a	Mc	d	8100	0	a	Mc	d	4050	0	a	Mc	d	1350	0	a	Mc	d	4050	0					
a	Ma	c	16200	0	a	Mc	e	2700	0	a	Md	e	8100	0	a	Md	e	16200	0	a	Md	e	8100	0	a	Md	e	16200	0	a	Md	e	16200	0					
a	Ma	i	8100	0	a	Mc	i	1350	0	a	Md	i	4050	0	a	Mc	i	8100	0	a	Mc	i	4050	0	a	Mc	i	8100	0	a	Mc	i	8100	0					
a	Ma	m	8100	0	a	Mc	m	1350	0	a	Md	m	4050	0	a	Mc	m	8100	0	a	Mc	m	4050	0	a	Mc	m	8100	0	a	Mc	m	8100	0					
a	Ma	n	8100	0	a	Mc	n	1350	0	a	Md	n	4050	0	a	Mc	n	8100	0	a	Mc	n	4050	0	a	Mc	n	8100	0	a	Mc	n	8100	0					
a	Ma	s	2700	0	a	Mc	s	450	0	a	Md	s	1350	0	a	Md	s	2700	0	a	Md	s	4050	0	a	Md	s	1350	0	a	Md	s	8100	0					
a	Ma	y	16200	0	a	Mc	y	2700	0	a	Md	y	8100	0	a	Md	y	16200	0	a	Md	y	8100	0	a	Md	y	16200	0	a	Md	y	8100	0					
c	Ma	d	1350	0	c	Mc	d	225	0	c	Md	d	675	0	c	Md	d	675	0	c	Md	d	675	0	c	Md	d	675	0	c	Md	d	675	0					
c	Ma	i	1350	0	c	Mc	i	450	0	c	Md	i	1350	0	c	Md	i	1350	0	c	Md	i	1350	0	c	Md	i	1350	0	c	Md	i	1350	0					
c	Ma	m	1350	0	c	Mc	m	225	0	c	Md	m	675	0	c	Md	m	675	0	c	Md	m	675	0	c	Md	m	675	0	c	Md	m	675	0					
c	Ma	n	1350	0	c	Mc	n	450	0	c	Md	n	1350	0	c	Md	n	1350	0	c	Md	n	1350	0	c	Md	n	1350	0	c	Md	n	1350	0					
c	Ma	s	1350	0	c	Mc	s	75	0	c	Md	s	225	0	c	Md	s	225	0	c	Md	s	225	0	c	Md	s	225	0	c	Md	s	225	0					
c	Ma	y	2700	0	c	Mc	y	1350	0	c	Md	y	225	0	c	Md	y	225	0	c	Md	y	225	0	c	Md	y	225	0	c	Md	y	225	0					
j	Ma	c	8100	0	j	Mc	c	1350	0	j	Md	c	4050	0	j	Md	c	8100	0	j	Md	c	4050	0	j	Md	c	8100	0	j	Md	c	4050	0					
j	Ma	i	4050	0	j	Mc	i	1350	0	j	Md	i	4050	0	j	Md	i	8100	0	j	Md	i	4050	0	j	Md	i	8100	0	j	Md	i	4050	0					
j	Ma	m	4050	0	j	Mc	m	675	0	j	Md	m	225	0	j	Md	m	225	0	j	Md	m	225	0	j	Md	m	225	0	j	Md	m	225	0					
j	Ma	n	4050	0	j	Mc	n	1350	0	j	Md	n	4050	0	j	Md	n	8100	0	j	Md	n	4050	0	j	Md	n	8100	0	j	Md	n	4050	0					
j	Ma	s	16200	0	j	Mc	s	675	0	j	Md	s	225	0	j	Md	s	225	0	j	Md	s	225	0	j	Md	s	225	0	j	Md	s	225	0					
j	Ma	y	8100	0	j	Mc	y	1350	0	j	Md	y	225	0	j	Md	y	225	0	j	Md	y	225	0	j	Md	y	225	0	j	Md	y	225	0					
l	Ma	m	8100	0	l	Mc	m	1350	0	l	Md	m	4050	0	l	Md	m	8100	0	l	Md	m	4050	0	l	Md	m	8100	0	l	Md	m	4050	0					
l	Ma	n	8100	0	l	Mc	n	675	0	l	Md	n	225	0	l	Md	n	225	0	l	Md	n	225	0	l	Md	n	225	0	l	Md	n	225	0					
l	Ma	s	8100	0	l	Mc	s	675	0	l	Md	s	225	0	l	Md	s	225	0	l	Md	s	225	0	l	Md	s	225	0	l	Md	s	225	0					
l	Ma	y	8100	0	l	Mc	y	1350	0	l	Md	y	225	0	l	Md	y	225	0	l	Md	y	225	0	l	Md	y	225	0	l	Md	y	225	0					
m	Ma	n	4050	0	m	Mc	n	675	1	m	Md	n	2025	0	m	Md	n	4050	2	m	Md	n	1025	1	m	Md	n	675	1	m	Md	n	2025	0					
m	Ma	s	1350	0	m	Mc	s	225	1	m	Md	s	675	0	m	Md	s	1350	0	m	Md	s	675	1	m	Md	s	1350	0	m	Md	s	675	1					
m	Ma	y	8100	0	m	Mc	y	1350	0	m	Md	y	4050	0	m	Md	y	8100	0	m	Md	y	4050	0	m	Md	y	8100	0	m	Md	y	4050	0					
n	Ma	s	1350	0	n	Mc	s	225	1	n	Md	s	675	0	n	Md	s	1350	2	n	Md	s	675	1	n	Md	s	1350	2	n	Md	s	675	1					
n	Ma	y	8100	0	n	Mc	y	1350	0	n	Md	y	4050	0	n	Md	y	8100	0	n	Md	y	4050	0	n	Md	y	8100	0	n	Md	y	4050	0					
s	Ma	y	2700	0	s	Mc	y	450	2	s	Md	y	1350	0	s	Md	y	2700	4	s	Md	y	1350	0	s	Md	y	450	2	s	Md	y	1350	0	s	Md	y	450	2

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

Ter	In	Ax	Ten	Sc	No	Ax	Ter	In	Ax	Ter	No	Ax	Ter	In	Ax	Si	SM	Ter	In	No	Ax	Ter	In	Ax											
s SA s	900	0	a S C c	150	0	a S D m	450	0	a S L s	450	0	a S M c	450	0	a S N d	450	0	a S M n	450	0	a S S d	450	0	a S S n	450	0	a S A d	465	9	a S V	5400	0			
s SA d	2700	0	a S C d	450	0	a S D d	1350	0	a S E d	2700	0	a S L d	1350	0	a S M d	1350	0	a S N d	1350	0	a S M d	1350	0	a S S d	1350	0	a S A d	1450	0	a S V	5400	0			
s SA c	5400	0	a S C c	900	0	a S D m	2700	0	a S E d	5400	0	a S L s	2700	0	a S M e	5400	0	a S N e	2700	0	a S M e	5400	0	a S S d	450	0	a S S e	900	0	a S A c	2700	0	a S V	5400	0
s SA l	2700	0	a S C l	450	0	a S D d	1350	0	a S E l	2700	0	a S L l	1350	0	a S M l	1350	0	a S N l	1350	0	a S M l	1350	0	a S S l	1350	0	a S A l	2700	0	a S V	5400	0			
s SA m	2700	0	a S C m	450	0	a S D m	1350	0	a S E m	2700	0	a S L m	1350	0	a S M m	1350	0	a S N m	1350	0	a S M m	1350	0	a S S m	1350	0	a S A m	2700	0	a S V	5400	0			
s SA n	2700	0	a S C n	450	0	a S D n	1350	0	a S E n	2700	0	a S L n	1350	0	a S M n	1350	0	a S N n	1350	0	a S M n	1350	0	a S S n	1350	0	a S A n	2700	0	a S V	5400	0			
s SA x	900	0	a S C x	150	0	a S D x	450	0	a S E x	900	0	a S L s	450	0	a S M x	900	0	a S N x	2700	0	a S M x	900	0	a S S x	450	0	a S A x	2700	0	a S V	5400	0			
s SA y	5400	0	a S C y	900	0	a S D y	2700	0	a S E y	5400	0	a S L y	2700	0	a S M y	2700	0	a S N y	2700	0	a S M y	2700	0	a S S y	2700	0	a S A y	5400	0	a S V	5400	0			
s SA d	450	0	a S C d	75	0	a S D d	225	0	a S E d	450	0	a S L d	225	0	a S M d	225	0	a S N d	225	0	a S M d	450	0	a S S d	150	0	a S A d	450	0	a S V	450	0			
s SA x	900	0	a S C x	150	0	a S D x	225	0	a S E x	900	0	a S L x	150	0	a S M x	450	0	a S N x	150	0	a S M x	450	0	a S S x	150	0	a S A x	900	0	a S V	900	0			
s SA l	450	0	a S C l	75	0	a S D l	225	0	a S E l	450	0	a S L l	225	0	a S M l	225	0	a S N l	225	0	a S M l	225	0	a S S l	75	0	a S A l	450	0	a S V	450	0			
s SA m	450	0	a S C m	75	0	a S D m	225	0	a S E m	450	0	a S L m	225	0	a S M m	225	0	a S N m	225	0	a S M m	225	0	a S S m	75	0	a S A m	450	0	a S V	450	0			
s SA n	450	0	a S C n	75	0	a S D n	225	0	a S E n	450	0	a S L n	225	0	a S M n	225	0	a S N n	225	0	a S M n	225	0	a S S n	75	0	a S A n	450	0	a S V	450	0			
s SA z	90	0	a S C z	25	0	a S D z	75	0	a S E z	90	0	a S L z	75	0	a S M z	75	0	a S N z	75	0	a S M z	75	0	a S S z	15	0	a S A z	90	0	a S V	90	0			
s SA z	900	0	a S C z	150	0	a S D z	225	0	a S E z	900	0	a S L z	150	0	a S M z	450	0	a S N z	150	0	a S M z	450	0	a S S z	150	0	a S A z	900	0	a S V	900	0			
d SA e	2700	0	d S C e	450	0	d S D e	1350	0	d S E e	2700	0	d S L e	1350	0	d S M e	1350	0	d S N e	1350	0	d S M e	1350	0	d S S e	1350	0	d S A e	2700	0	d S V	2700	0			
d SA i	1350	0	d S C i	450	0	d S D i	1350	0	d S E i	1350	0	d S L i	675	0	d S M i	675	0	d S N i	675	0	d S M i	675	0	d S S i	675	0	d S A i	1350	0	d S V	1350	0			
d SA m	1350	0	d S C m	225	0	d S D m	675	0	d S E m	1350	0	d S L m	675	0	d S M m	675	0	d S N m	675	0	d S M m	675	0	d S S m	675	0	d S A m	1350	0	d S V	1350	0			
d SA n	1350	0	d S C n	1350	0	d S D n	675	0	d S E n	1350	0	d S L n	675	0	d S M n	675	0	d S N n	675	0	d S M n	675	0	d S S n	675	0	d S A n	1350	0	d S V	1350	0			
d SA x	450	0	d S C s	75	0	d S D s	225	0	d S E s	450	0	d S L s	225	0	d S M s	225	0	d S N s	225	0	d S M s	225	0	d S S s	75	0	d S A x	450	0	d S V	450	0			
d SA y	2700	0	d S C y	450	0	d S D y	1350	0	d S E y	2700	0	d S L y	1350	0	d S M y	1350	0	d S N y	1350	0	d S M y	1350	0	d S S y	1350	0	d S A y	2700	0	d S V	2700	0			
c SA l	2700	0	c S C l	450	0	c S D l	1350	0	c S E l	2700	0	c S L l	1350	0	c S M l	1350	0	c S N l	1350	0	c S M l	1350	0	c S S l	1350	0	c S A l	2700	0	c S V	2700	0			
c SA m	2700	0	c S C m	225	0	c S D m	675	0	c S E m	1350	0	c S L m	1350	0	c S M m	1350	0	c S N m	1350	0	c S M m	1350	0	c S S m	1350	0	c S A m	2700	0	c S V	2700	0			
c SA n	2700	0	c S C n	1350	0	c S D n	675	0	c S E n	1350	0	c S L n	675	0	c S M n	675	0	c S N n	675	0	c S M n	675	0	c S S n	675	0	c S A n	2700	0	c S V	2700	0			
e SA l	2700	0	e S C l	450	0	e S D l	1350	0	e S E l	2700	0	e S L l	1350	0	e S M l	1350	0	e S N l	1350	0	e S M l	1350	0	e S S l	1350	0	e S A l	2700	0	e S V	2700	0			
e SA m	2700	0	e S C m	225	0	e S D m	675	0	e S E m	1350	0	e S L m	1350	0	e S M m	1350	0	e S N m	1350	0	e S M m	1350	0	e S S m	1350	0	e S A m	2700	0	e S V	2700	0			
e SA n	2700	0	e S C n	1350	0	e S D n	675	0	e S E n	1350	0	e S L n	675	0	e S M n	675	0	e S N n	675	0	e S M n	675	0	e S S n	675	0	e S A n	2700	0	e S V	2700	0			
e SA x	900	0	e S C x	150	0	e S D x	225	0	e S E x	450	0	e S L x	900	0	e S M x	450	0	e S N x	900	0	e S M x	450	0	e S S x	900	0	e S A x	900	0	e S V	900	0			
e SA y	900	0	e S C y	900	0	e S D y	2700	0	e S E y	900	0	e S L y	2700	0	e S M y	2700	0	e S N y	2700	0	e S M y	2700	0	e S S y	2700	0	e S A y	900	0	e S V	900	0			
i SA m	1350	0	i S C m	225	0	i S D m	675	0	i S E m	1350	0	i S L m	675	0	i S M m	675	0	i S N m	675	0	i S M m	675	0	i S S m	675	0	i S A m	1350	0	i S V	1350	0			
i SA n	1350	0	i S C n	225	0	i S D n	675	0	i S E n	1350	0	i S L n	675	0	i S M n	675	0	i S N n	675	0	i S M n	675	0	i S S n	675	0	i S A n	1350	0	i S V	1350	0			
i SA y	2700	0	i S C y	450	0	i S D y	1350	0	i S E y	2700	0	i S L y	1350	0	i S M y	1350	0	i S N y	1350	0	i S M y	1350	0	i S S y	1350	0	i S A y	2700	0	i S V	2700	0			
m SA m	1350	0	m S C m	225	0	m S D m	675	0	m S E m	1350	0	m S L m	675	0	m S M m	675	0	m S N m	675	0	m S M m	675	0	m S S m	675	0	m S A m	1350	0	m S V	1350	0			
m SA n	1350	0	m S C n	225	0	m S D n	675	0	m S E n	1350	0	m S L n	675	0	m S M n	675	0	m S N n	675	0	m S M n	675	0	m S S n	675	0	m S A n	1350	0	m S V	1350	0			
m SA x	450	0	m S C x	75	0	m S D x	225	0	m S E x	450	0	m S L x	75	0	m S M x	225	0	m S N x	75	0	m S M x	225	0	m S S x	75	0	m S A x	450	0	m S V	450	0			
m SA y	2700	0	m S C y	450	0	m S D y	1350	0	m S E y	2700	0	m S L y	1350	0	m S M y	1350	0	m S N y	1350	0	m S M y	1350	0	m S S y	1350	0	m S A y	2700	0	m S V	2700	0			
n SA s	450	0	n S C s	75	0	n S D s	225	0	n S E s	450	0	n S L s	75	0	n S M s	225	0	n S N s	75	0	n S M s	225	0	n S S s	75	0	n S A s	450	0	n S V	450	0			
n SA x	2700	0	n S C x	450	0	n S D x	1350	0	n S E x	2700	0	n S L x	1350	0	n S M x	1350	0	n S N x	1350	0	n S M x	1350	0	n S S x	1350	0	n S A x	2700	0	n S V	2700	0			
y SA x	900	0	y S C y	150	0	y S D y	450	0	y S E y	900	0	y S L y	450	0	y S M y	900	0	y S N y	450	0	y S M y	900	0	y S S y	450	0	y S A x	900	0	y S V	900	0			

Table IV: All Linear Isohost Tetramers, their Stereoseomer Numbers and Achiral meso-forms

Ter	Iso	Ac	Ter	Iso	Ac	Ter	Iso	Ac	Ter	Iso	Ac	Ter	Iso	Ac	Ter	Iso	Ac	Ter	Iso	Ac	Ter	Iso	Ac	Ter	Iso	Ac	Ter	Iso	Ac		
Y\A	Y\A	Y\A	Y\A	Y\A	Y\A	Y\A	Y\A	Y\A	Y\A	Y\A	Y\A	Y\A	Y\A	Y\A	Y\A	Y\A	Y\A	Y\A	Y\A	Y\A	Y\A	Y\A	Y\A	Y\A	Y\A	Y\A	Y\A	Y\A	Y\A	Y\A	
a	Y,A,c	5400	0	a	Y,C,c	900	0	a	Y,D,c	2700	0	a	Y,E,c	5400	0	a	Y,L,c	2700	0	a	Y,M,c	2700	0	a	Y,N,c	2700	0	a	Y,S,c	900	0
a	Y,A,d	16200	0	a	Y,C,d	2700	0	a	Y,D,d	8100	0	a	Y,E,d	16200	0	a	Y,L,d	8100	0	a	Y,M,d	8100	0	a	Y,N,d	8100	0	a	Y,S,d	2700	0
a	Y,A,e	32400	0	a	Y,C,e	5400	0	a	Y,D,e	16200	0	a	Y,E,e	32400	0	a	Y,L,e	16200	0	a	Y,M,e	16200	0	a	Y,N,e	16200	0	a	Y,S,e	5400	0
a	Y,A,f	16200	0	a	Y,C,f	2700	0	a	Y,D,f	8100	0	a	Y,E,f	16200	0	a	Y,L,f	8100	0	a	Y,M,f	8100	0	a	Y,N,f	8100	0	a	Y,S,f	2700	0
a	Y,A,m	16200	0	a	Y,C,m	2700	0	a	Y,D,m	8100	0	a	Y,E,m	16200	0	a	Y,L,m	8100	0	a	Y,M,m	8100	0	a	Y,N,m	8100	0	a	Y,S,m	2700	0
a	Y,A,n	16200	0	a	Y,C,n	2700	0	a	Y,D,n	8100	0	a	Y,E,n	16200	0	a	Y,L,n	8100	0	a	Y,M,n	8100	0	a	Y,N,n	8100	0	a	Y,S,n	2700	0
a	Y,A,s	5400	0	a	Y,C,s	900	0	a	Y,D,s	2700	0	a	Y,E,s	5400	0	a	Y,L,s	2700	0	a	Y,M,s	2700	0	a	Y,N,s	2700	0	a	Y,S,s	900	0
a	Y,A,y	32400	0	a	Y,C,y	5400	0	a	Y,D,y	16200	0	a	Y,E,y	32400	0	a	Y,L,y	16200	0	a	Y,M,y	16200	0	a	Y,N,y	16200	0	a	Y,S,y	5400	0
c	Y,A,d	2700	0	c	Y,C,d	1350	0	c	Y,D,d	2700	0	c	Y,E,d	1350	0	c	Y,L,d	2700	0	c	Y,M,d	1350	0	c	Y,N,d	1350	0	c	Y,S,d	450	0
c	Y,A,e	5400	0	c	Y,C,e	900	4	c	Y,D,e	1350	0	c	Y,E,e	5400	8	c	Y,L,e	2700	4	c	Y,M,e	2700	4	c	Y,N,e	2700	4	c	Y,S,e	900	4
c	Y,A,l	2700	0	c	Y,C,l	1350	0	c	Y,D,l	2700	0	c	Y,E,l	1350	0	c	Y,L,l	2700	0	c	Y,M,l	1350	0	c	Y,N,l	1350	0	c	Y,S,l	450	0
c	Y,A,m	2700	0	c	Y,C,m	450	2	c	Y,D,m	1350	0	c	Y,E,m	2700	0	c	Y,L,m	1350	0	c	Y,M,m	1350	2	c	Y,N,m	1350	2	c	Y,S,m	450	2
c	Y,A,n	2700	0	c	Y,C,n	450	2	c	Y,D,n	1350	0	c	Y,E,n	2700	0	c	Y,L,n	1350	0	c	Y,M,n	1350	2	c	Y,N,n	1350	2	c	Y,S,n	450	2
c	Y,A,s	900	0	c	Y,C,s	150	2	c	Y,D,s	450	0	c	Y,E,s	900	4	c	Y,L,s	2700	4	c	Y,M,s	2700	4	c	Y,N,s	2700	4	c	Y,S,s	900	3
c	Y,A,y	900	0	c	Y,C,y	150	4	c	Y,D,y	2700	0	c	Y,E,y	5400	8	c	Y,L,y	2700	4	c	Y,M,y	2700	4	c	Y,N,y	2700	4	c	Y,S,y	900	4
d	Y,A,c	16200	0	d	Y,C,c	2700	0	d	Y,D,c	8100	0	d	Y,E,c	16200	0	d	Y,L,c	8100	0	d	Y,M,c	8100	0	d	Y,N,c	8100	0	d	Y,S,c	2700	0
d	Y,A,i	16200	0	d	Y,C,i	1350	0	d	Y,D,i	4050	0	d	Y,E,i	16200	0	d	Y,L,i	4050	0	d	Y,M,i	4050	0	d	Y,N,i	4050	0	d	Y,S,i	1350	0
d	Y,A,m	8100	0	d	Y,C,m	1350	0	d	Y,D,m	4050	0	d	Y,E,m	8100	0	d	Y,L,m	4050	0	d	Y,M,m	4050	0	d	Y,N,m	4050	0	d	Y,S,m	1350	0
d	Y,A,n	8100	0	d	Y,C,n	450	0	d	Y,D,n	1350	0	d	Y,E,n	8100	0	d	Y,L,n	1350	0	d	Y,M,n	4050	0	d	Y,N,n	8100	0	d	Y,S,n	1350	0
d	Y,A,y	16200	0	d	Y,C,y	2700	0	d	Y,D,y	8100	0	d	Y,E,y	16200	0	d	Y,L,y	8100	0	d	Y,M,y	8100	0	d	Y,N,y	1350	0	d	Y,S,y	2700	0
e	Y,A,i	16200	0	e	Y,C,i	2700	0	e	Y,D,i	8100	0	e	Y,E,i	16200	0	e	Y,L,i	8100	0	e	Y,M,i	8100	0	e	Y,N,i	8100	0	e	Y,S,i	2700	0
e	Y,A,m	16200	0	e	Y,C,m	2700	4	e	Y,D,m	8100	0	e	Y,E,m	16200	8	e	Y,L,m	8100	0	e	Y,M,m	8100	4	e	Y,N,m	2700	4	e	Y,S,m	16200	0
e	Y,A,n	16200	0	e	Y,C,n	2700	4	e	Y,D,n	8100	0	e	Y,E,n	16200	8	e	Y,L,n	8100	0	e	Y,M,n	8100	4	e	Y,N,n	2700	4	e	Y,S,n	16200	0
e	Y,A,y	5400	0	e	Y,C,y	900	4	e	Y,D,y	1350	0	e	Y,E,y	5400	8	e	Y,L,y	2700	4	e	Y,M,y	2700	4	e	Y,N,y	2700	4	e	Y,S,y	900	4
e	Y,A,y	32400	0	e	Y,C,y	5400	8	e	Y,D,y	16200	0	e	Y,E,y	32400	16	e	Y,L,y	16200	0	e	Y,M,y	16200	8	e	Y,N,y	16200	8	e	Y,S,y	5400	12
i	Y,A,m	8100	0	i	Y,C,m	1350	0	i	Y,D,m	4050	0	i	Y,E,m	8100	0	i	Y,L,m	4050	0	i	Y,M,m	8100	0	i	Y,N,m	4050	0	i	Y,S,m	1350	0
i	Y,A,n	8100	0	i	Y,C,n	1350	0	i	Y,D,n	4050	0	i	Y,E,n	8100	0	i	Y,L,n	4050	0	i	Y,M,n	8100	0	i	Y,N,n	4050	0	i	Y,S,n	1350	0
i	Y,A,y	2700	0	i	Y,C,y	1350	0	i	Y,D,y	8100	0	i	Y,E,y	2700	0	i	Y,L,y	8100	0	i	Y,M,y	8100	0	i	Y,N,y	8100	0	i	Y,S,y	2700	0
i	Y,A,y	16200	0	i	Y,C,y	1350	0	i	Y,D,y	8100	0	i	Y,E,y	16200	0	i	Y,L,y	8100	0	i	Y,M,y	8100	0	i	Y,N,y	8100	0	i	Y,S,y	16200	0
m	Y,A,n	8100	0	m	Y,C,n	1350	2	m	Y,D,n	4050	0	m	Y,E,n	8100	4	m	Y,L,n	4050	0	m	Y,M,n	4050	2	m	Y,N,n	1350	2	m	Y,S,n	450	3
m	Y,A,s	2700	0	m	Y,C,s	450	2	m	Y,D,s	1350	0	m	Y,E,s	2700	4	m	Y,L,s	1350	0	m	Y,M,s	1350	0	m	Y,N,s	8100	4	m	Y,S,s	2700	3
n	Y,A,s	2700	0	n	Y,C,s	450	2	n	Y,D,s	1350	0	n	Y,E,s	2700	4	n	Y,L,s	1350	0	n	Y,M,s	1350	2	n	Y,N,s	8100	4	n	Y,S,s	2700	3
n	Y,A,y	16200	0	n	Y,C,y	2700	4	n	Y,D,y	8100	0	n	Y,E,y	16200	8	n	Y,L,y	8100	0	n	Y,M,y	8100	4	n	Y,N,y	2700	4	n	Y,S,y	16200	6
s	Y,A,y	5400	0	s	Y,C,y	900	4	s	Y,D,y	2700	0	s	Y,E,y	5400	8	s	Y,L,y	2700	4	s	Y,M,y	2700	4	s	Y,N,y	2700	4	s	Y,S,y	900	6

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:

Z-aaa:	$AAA_Z * \text{mono}_a$
Z-aaa':	$AAB_Z * \text{mono}_a * (\text{mono}_a - 1)$
Z-aa'a":	$ABC_Z * \text{mono}_a * (\text{mono}_a - 1) * (\text{mono}_a - 2) / 6$
Z-aab:	$AAB_Z * \text{mono}_a * \text{monob}_b$
Z-aa'b:	$ABC_Z * \text{mono}_a * (\text{mono}_a - 1) * \text{mono}_b / 2$
Z-abc:	$ABC_Z * \text{mono}_a * \text{mono}_b * \text{mono}_c$

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.

四

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

Tet-	Iso-	Ac-	Tet-	Iso-	Ac-	Tet-	Iso-	Ac-	Tet-	Iso-	Ac-	Tet-	Iso-	Ac-	
E	E	E	4320	0											
E	E	E	2150	12											
E	E	E	6360	0											
E	E	E	6389	12											
E	E	E	5485	12											
E	E	E	1195	12											
E	E	E	1258	0											
E	E	E	1349	0											
E	E	E	260	0	E	E	E	20	4						
E	E	E	2160	0	F	E	E	180	0						
E	E	E	3420	0	F	E	E	160	0						
E	E	E	2150	0	F	E	E	140	0						
E	E	E	2150	0	F	E	E	120	0						
E	E	E	2150	0	F	E	E	100	0						
E	E	E	2150	0	F	E	E	80	0						
E	E	E	2150	0	F	E	E	60	4						
E	E	E	250	0	E	E	E	60	8						
E	E	E	4320	0	E	E	E	360	8						
E	E	E	3240	0	E	E	E	340	8						
E	E	E	12560	0	E	E	E	2160	0						
E	E	E	12560	0	E	E	E	1960	0						
E	E	E	12560	0	E	E	E	1760	0						
E	E	E	12560	0	E	E	E	1560	0						
E	E	E	12560	0	E	E	E	1360	0						
E	E	E	12560	0	E	E	E	1160	0						
E	E	E	6380	0	F	E	E	1080	0						
E	E	E	2160	0	F	E	E	980	0						
E	E	E	2160	0	F	E	E	880	0						
E	E	E	2160	0	F	E	E	780	0						
E	E	E	2160	0	F	E	E	680	0						
E	E	E	2160	0	F	E	E	580	0						
E	E	E	2160	0	F	E	E	480	0						
E	E	E	2160	0	F	E	E	380	0						
E	E	E	2160	0	F	E	E	280	0						
E	E	E	2160	0	F	E	E	180	0						
E	E	E	2160	0	F	E	E	80	0						
E	E	E	2160	0	F	E	E	40	0						
E	E	E	2160	0	F	E	E	10	0						
E	E	E	2160	0	F	E	E	0	0						
E	E	E	2160	0	F	E	E	240	0	F	E	E	4320	32	
E	E	E	2160	0	F	E	E	2340	0	F	E	E	4380	0	
E	E	E	2160	0	F	E	E	2300	0	F	E	E	4480	0	
E	E	E	2160	0	F	E	E	2260	0	F	E	E	4580	0	
E	E	E	2160	0	F	E	E	2220	0	F	E	E	4680	0	
E	E	E	2160	0	F	E	E	2180	0	F	E	E	4780	0	
E	E	E	2160	0	F	E	E	2140	0	F	E	E	4880	0	
E	E	E	2160	0	F	E	E	2100	0	F	E	E	4980	0	
E	E	E	2160	0	F	E	E	2060	0	F	E	E	5080	0	
E	E	E	2160	0	F	E	E	2020	0	F	E	E	5180	0	
E	E	E	2160	0	F	E	E	1980	0	F	E	E	5280	0	
E	E	E	2160	0	F	E	E	1940	0	F	E	E	5380	0	
E	E	E	2160	0	F	E	E	1900	0	F	E	E	5480	0	
E	E	E	2160	0	F	E	E	1860	0	F	E	E	5580	0	
E	E	E	2160	0	F	E	E	1820	0	F	E	E	5680	0	
E	E	E	2160	0	F	E	E	1780	0	F	E	E	5780	0	
E	E	E	2160	0	F	E	E	1740	0	F	E	E	5880	0	
E	E	E	2160	0	F	E	E	1700	0	F	E	E	5980	0	
E	E	E	2160	0	F	E	E	1660	0	F	E	E	6080	0	
E	E	E	2160	0	F	E	E	1620	0	F	E	E	6180	0	
E	E	E	2160	0	F	E	E	1580	0	F	E	E	6280	0	
E	E	E	2160	0	F	E	E	1540	0	F	E	E	6380	0	
E	E	E	2160	0	F	E	E	1500	0	F	E	E	6480	0	
E	E	E	2160	0	F	E	E	1460	0	F	E	E	6580	0	
E	E	E	2160	0	F	E	E	1420	0	F	E	E	6680	0	
E	E	E	2160	0	F	E	E	1380	0	F	E	E	6780	0	
E	E	E	2160	0	F	E	E	1340	0	F	E	E	6880	0	
E	E	E	2160	0	F	E	E	1300	0	F	E	E	6980	0	
E	E	E	2160	0	F	E	E	1260	0	F	E	E	7080	0	
E	E	E	2160	0	F	E	E	1220	0	F	E	E	7180	0	
E	E	E	2160	0	F	E	E	1180	0	F	E	E	7280	0	
E	E	E	2160	0	F	E	E	1140	0	F	E	E	7380	0	
E	E	E	2160	0	F	E	E	1100	0	F	E	E	7480	0	
E	E	E	2160	0	F	E	E	1060	0	F	E	E	7580	0	
E	E	E	2160	0	F	E	E	1020	0	F	E	E	7680	0	
E	E	E	2160	0	F	E	E	980	0	F	E	E	7780	0	
E	E	E	2160	0	F	E	E	940	0	F	E	E	7880	0	
E	E	E	2160	0	F	E	E	900	0	F	E	E	7980	0	
E	E	E	2160	0	F	E	E	860	4	F	E	E	8080	4	
E	E	E	2160	0	F	E	E	820	0	F	E	E	8180	0	
E	E	E	2160	0	F	E	E	780	0	F	E	E	8280	0	
E	E	E	2160	0	F	E	E	740	0	F	E	E	8380	0	
E	E	E	2160	0	F	E	E	700	0	F	E	E	8480	0	
E	E	E	2160	0	F	E	E	660	0	F	E	E	8580	0	
E	E	E	2160	0	F	E	E	620	0	F	E	E	8680	0	
E	E	E	2160	0	F	E	E	580	0	F	E	E	8780	0	
E	E	E	2160	0	F	E	E	540	0	F	E	E	8880	0	
E	E	E	2160	0	F	E	E	500	0	F	E	E	8980	0	
E	E	E	2160	0	F	E	E	460	4	F	E	E	9080	4	
E	E	E	2160	0	F	E	E	420	0	F	E	E	9180	0	
E	E	E	2160	0	F	E	E	380	0	F	E	E	9280	0	
E	E	E	2160	0	F	E	E	340	0	F	E	E	9380	0	
E	E	E	2160	0	F	E	E	300	0	F	E	E	9480	0	
E	E	E	2160	0	F	E	E	260	0	F	E	E	9580	0	
E	E	E	2160	0	F	E	E	220	0	F	E	E	9680	0	
E	E	E	2160	0	F	E	E	180	0	F	E	E	9780	0	
E	E	E	2160	0	F	E	E	140	0	F	E	E	9880	0	
E	E	E	2160	0	F	E	E	100	0	F	E	E	9980	0	
E	E	E	2160	0	F	E	E	60	4	F	E	E	10080	4	
E	E	E	2160	0	F	E	E	20	4	F	E	E	10180	4	
E	E	E	2160	0	F	E	E	80	0	F	E	E	10280	0	
E	E	E	2160	0	F	E	E	40	0	F	E	E	10380	0	
E	E	E	2160	0	F	E	E	0	0	F	E	E	10480	0	
E	E	E	2160	0	F	E	E	240	0	F	E	E	10580	0	
E	E	E	2160	0	F	E	E	200	0	F	E	E	10680	0	
E	E	E	2160	0	F	E	E	160	0	F	E	E	10780	0	
E	E	E	2160	0	F	E	E	120	0	F	E	E	10880	0	
E	E	E	2160	0	F	E	E	80	0	F	E	E	10980	0	
E	E	E	2160	0	F	E	E	40	0	F	E	E	11080	0	
E	E	E	2160	0	F	E	E	0	0	F	E	E	11180	0	
E	E	E	2160	0	F	E	E	240	0	F	E	E	11280	0	
E	E	E	2160	0	F	E	E	200	0	F	E	E	11380	0	
E	E	E	2160	0	F	E	E	160	0	F	E	E	11480	0	
E	E	E	2160	0	F	E	E	120	0	F	E	E	11580	0	
E	E	E	2160	0	F	E	E	80	0	F	E	E	11680	0	
E	E	E	2160	0	F	E	E	40	0	F	E	E	11780	0	
E	E	E	2160	0	F	E	E	0	0	F	E	E	11880	0	
E	E	E	2160	0	F	E	E	240	0	F	E	E	11980	0	
E	E	E	2160	0	F	E	E	200	0	F	E	E	12080	0	
E	E	E	2160	0	F	E	E	160	0	F	E	E	12180	0	
E	E	E	2160	0	F	E	E	120	0	F	E	E	12280	0	
E	E	E	2160	0	F	E	E	80	0	F	E	E	12380	0	
E	E	E	2160	0	F	E	E	40	0	F	E	E	12480	0	
E	E	E	2160	0	F	E	E	0	0	F	E	E	12580	0	

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

L

Tetr	Iso	Ac	Tetr	Iso	Ac	Tetr	Iso	Ac	Tetr	Iso	Ac	Tetr	Iso	Ac	Tetr	Iso	Ac	Tetr	Iso	Ac
l, s, s, l	2160	0																		
l, s, m, l	1060	0																		
l, s, m, m	6480	0																		
l, s, m, m	5420	0																		
l, s, m, m	5460	0																		
l, s, m, m	5480	0																		
l, s, c, s	180	0	l, s, c, e	10	0															
l, s, c, d	1080	0	l, s, c, d	90	0															
l, s, d, m	2160	0	l, s, d, e	180	0															
l, s, d, m	1060	0	l, s, d, e	90	0															
l, s, d, m	6480	0	l, s, d, e	50	0															
l, s, d, m	350	0	l, s, d, e	30	0															
l, s, e, s	2160	0	l, s, e, s	180	0															
l, s, e, s	1080	0	l, s, e, s	90	0															
l, s, e, s	5420	0	l, s, e, s	50	0															
l, s, e, s	5460	0	l, s, e, s	40	0															
l, s, e, s	5480	0	l, s, e, s	30	0															
l, s, e, m	2160	0	l, s, e, m	180	0															
l, s, e, m	1080	0	l, s, e, m	90	0															
l, s, e, m	5420	0	l, s, e, m	50	0															
l, s, e, m	5460	0	l, s, e, m	40	0															
l, s, e, m	5480	0	l, s, e, m	30	0															
l, s, d, m	2160	0	l, s, d, m	180	0															
l, s, d, m	1080	0	l, s, d, m	90	0															
l, s, d, m	5420	0	l, s, d, m	50	0															
l, s, d, m	5460	0	l, s, d, m	40	0															
l, s, d, m	5480	0	l, s, d, m	30	0															
l, s, d, m	2160	0	l, s, d, e	180	0															
l, s, d, m	1080	0	l, s, d, e	90	0															
l, s, d, m	5420	0	l, s, d, e	50	0															
l, s, d, m	5460	0	l, s, d, e	40	0															
l, s, d, m	5480	0	l, s, d, e	30	0															
l, s, d, m	2160	0	l, s, e, m	180	0															
l, s, d, m	1080	0	l, s, e, m	90	0															
l, s, d, m	5420	0	l, s, e, m	50	0															
l, s, d, m	5460	0	l, s, e, m	40	0															
l, s, d, m	5480	0	l, s, e, m	30	0															
l, s, e, m	2160	0	l, s, e, m	180	0															
l, s, e, m	1080	0	l, s, e, m	90	0															
l, s, e, m	5420	0	l, s, e, m	50	0															
l, s, e, m	5460	0	l, s, e, m	40	0															
l, s, e, m	5480	0	l, s, e, m	30	0															
l, s, e, m	2160	0	l, s, e, y	180	0															
l, s, e, m	1080	0	l, s, e, y	90	0															
l, s, e, m	5420	0	l, s, e, y	50	0															
l, s, e, m	5460	0	l, s, e, y	40	0															
l, s, e, m	5480	0	l, s, e, y	30	0															
l, s, e, s	2160	0	l, s, e, s	180	0															
l, s, e, s	1080	0	l, s, e, s	90	0															
l, s, e, s	5420	0	l, s, e, s	50	0															
l, s, e, s	5460	0	l, s, e, s	40	0															
l, s, e, s	5480	0	l, s, e, s	30	0															

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

	Tetr	Iso	An	Tetr	Iso	An	Tetr	Iso	An	Tetr	Iso	An	Tetr	Iso	An	Tetr	Iso	An	Tetr	Iso	An
S	#	c	724	0	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
S	#	d	360	0	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
S	#	e	1080	0	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
S	#	m	1080	6	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
S	#	a	150	6	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
S	#	b	2150	12	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
S	#	c	60	0	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
S	#	d	360	0	S	c	c	4	2	-	-	-	-	-	-	-	-	-	-	-	-
S	#	e	720	0	S	c	c	4	2	-	-	-	-	-	-	-	-	-	-	-	-
S	#	m	360	0	S	c	c	4	2	-	-	-	-	-	-	-	-	-	-	-	-
S	#	a	360	0	S	c	m	21	2	-	-	-	-	-	-	-	-	-	-	-	-
S	#	b	130	0	S	c	m	21	2	-	-	-	-	-	-	-	-	-	-	-	-
S	#	c	72	0	S	c	m	21	2	-	-	-	-	-	-	-	-	-	-	-	-
S	#	d	540	0	S	c	d	90	3	S	d	d	92	0	-	-	-	-	-	-	-
S	#	e	2160	0	S	c	d	180	0	S	d	d	240	0	-	-	-	-	-	-	-
S	#	m	1080	0	S	c	d	180	0	S	d	d	270	0	-	-	-	-	-	-	-
S	#	a	1080	0	S	c	d	180	0	S	d	d	360	0	-	-	-	-	-	-	-
S	#	b	1080	0	S	c	d	180	0	S	d	d	720	0	-	-	-	-	-	-	-
S	#	c	540	0	S	c	d	60	0	S	d	d	96	0	-	-	-	-	-	-	-
S	#	d	2160	0	S	c	d	160	0	S	d	d	540	0	-	-	-	-	-	-	-
S	#	e	2160	0	S	c	e	360	0	S	d	e	1080	12	S	e	e	724	16	-	-
S	#	m	2160	0	S	c	e	360	0	S	d	e	1080	0	S	e	e	1080	0	-	-
S	#	a	1080	0	S	c	e	360	0	S	d	e	1080	0	S	e	e	1080	0	-	-
S	#	b	1080	0	S	c	e	360	0	S	d	e	1080	0	S	e	e	1080	0	-	-
S	#	c	720	0	S	c	e	360	0	S	d	e	1080	0	S	e	e	1080	0	-	-
S	#	d	2160	0	S	c	e	720	0	S	d	e	2160	0	S	e	e	2160	0	-	-
S	#	e	1080	0	S	c	e	1080	0	S	d	e	2160	0	S	e	e	2160	0	-	-
S	#	m	1080	0	S	c	e	1080	0	S	d	e	720	0	S	e	e	720	0	-	-
S	#	a	1080	0	S	c	e	1080	0	S	d	e	540	0	S	e	e	540	0	-	-
S	#	b	2160	0	S	c	e	1080	0	S	d	e	540	0	S	e	e	540	0	-	-
S	#	c	540	0	S	c	e	1080	0	S	d	e	1080	0	S	e	e	1080	0	-	-
S	#	d	2160	0	S	c	e	540	0	S	d	e	1080	0	S	e	e	1080	0	-	-
S	#	e	720	0	S	c	e	540	0	S	d	e	1080	0	S	e	e	1080	0	-	-
S	#	m	720	0	S	c	e	540	0	S	d	e	2160	0	S	e	e	2160	0	-	-
S	#	a	1080	0	S	c	e	540	0	S	d	e	1080	0	S	e	e	1080	0	-	-
S	#	b	2160	0	S	c	e	540	0	S	d	e	1080	0	S	e	e	1080	0	-	-
S	#	c	2160	0	S	c	e	540	0	S	d	e	2160	0	S	e	e	2160	0	-	-
S	#	d	720	0	S	c	e	2160	0	S	d	e	2160	0	S	e	e	2160	0	-	-
S	#	e	720	0	S	c	e	2160	0	S	d	e	720	0	S	e	e	720	0	-	-
S	#	m	2160	0	S	c	e	720	0	S	d	e	720	0	S	e	e	720	0	-	-

Table 4: All Branched insular Tetramers, their Stereocustomer Numbers and Achiral meforms.

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 inositolts 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 inositolts is always 1 : 5. We use the asymmetrical disubstitutional possibilities, since regardless of the oligomer, the inner inositolts are all substituted in this way, because we use different inositolts to fill the patterns. Again from *Table I* we can gather, that the 9 inositolts 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 inositolts):

$$\text{Pattern_count } (n_X, n_Y, n_Z) = \binom{2}{n_X} \binom{4}{n_Y} \binom{3}{n_Z}.$$

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 inositol, 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: 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 inositol 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	1	
XY	8	3	24		
XZ	6	6	36		
YY	6	9	54		
YZ	12	18	216		
ZZ	3	36	108		
gen. isomers	36		439	1	439
sum					

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	84		16,890	3	50,670
sum					

linear tetramers (ABCD)

pattern	count	isomers/count	product	combinations	TOTAL
XXYY	6	225	1,350		
XXYZ	12	450	5,400		
XXZ	3	900	2,700		
XXXX	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		
XXYYZ	18	6,750	121,500		
XXYZZ	12	13,500	162,000		
XXZZZ	1	27,000	27,000		
XYYYY	2	10,125	20,250		
XYYYZ	24	20,250	486,000		
XYYZZ	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		
XXYYYZ	12	101,250	1,215,000		
XXYYZZ	18	202,500	3,645,000		
XXYZZZ	4	405,000	1,620,000		
XYYYYY	6	303,750	1,822,500		
XYYYZZ	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
XXXXXXXX	3	1,518,750	4,556,250		
XXYYYYZ	12	3,037,500	36,450,000		
XXYYZZZ	6	6,075,000	36,450,000		
XXYYZZZ	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 (ABCDEFGHI)					
	pattern	count	isomers/count	product	combinations
	XXYYYYZZ	3	45,562,500	136,687,500	
	XXYYYZZZ	4	91,125,000	364,500,000	
	XYYYYYZZ	2	273,375,000	546,750,000	
gen. isomers	sum	9		1,047,937,500	20,160

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

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

<i>Linear Oligomer</i>	<i>Inositol Stereoisomers (a)</i>	<i>Inositol Stereoisomers (b)</i>
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., Höning, H., On the Number of Some Inositol - Tetramers. *MATCH* **2002**, submitted.
- [2] (a) Dolhaine, H.; Höning, H.; van Almsick, M. Sample Applications of an Algorithm for the Calculation of the Number of Isomers With more Than One Type of Achiral Substituent. *MATCH* **1999**, 39, 21-37.
(b) van Almsick, M.; Dolhaine, H.; Höning, H. Efficient Algorithms to Enumerate Isomers and Diamutamers With More Than One Type of Substituent. *J. Chem. Inf. Comput. Sci.* **2000**, 40, 956-966.
(c) van Almsick, M.; Dolhaine, H.; Höning, H. Isomer- and Diamutamer-Enumeration with MATHEMATICA. *MATCH* **2001**, 43, 143-157.
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 web-page: <http://www.cis.TUGraz.at/orgc/institut/softnew.htm>