Dr. H. J. Stoklosa
Central Rsch & Development Dept
E. I. du Pont de Nemours & Co.
Wilmington, Delaware 19898

Dr. F. Street
AEI Scientific Apparatus, Ltd.
Barton Dock Road
Urmston, Manchester M31 2LD
England

Dr. Robert M. Supnik
Massachusetts Computer Assoc.
26 Princess Street
Wakefield, Massachusetts 01880

Dr. H. G. J. Teisman
Netherlands Institute for
Dairy Research
Post Office Box 20
EDE, NETHERLANDS

Dr. Gareth Templeman
Rsch and Development Lab.
The Pillsbury Company
311 Second Street Southeast
Minneapolis, Minnesota 55414

Dr. Ernst Weber
Varian MAT
P.O. Box 144062
Bremen, West Germany

Dr. J. Wyatt
Code 6110
Naval Research Laboratory
Washington, D. C. 20375

7 APPENDICES

7.1 Appendix A
The Structures of All 4-Dimethyl Marine Sterols Reported to the Beginning of 1977.

Each sterol is given a unique number which is used in subsequent discussions in the text.

The molecular weight (M^+ and common trivial name are given for each sterol.

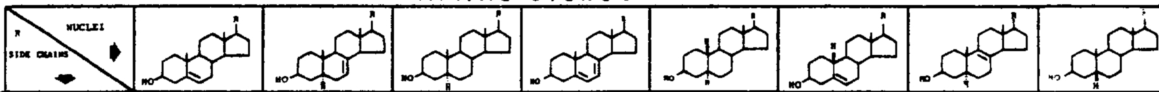
The nuclei all possess alternating trans-anti stereochemistry at the ring junctures, except the 5* stanols (farthest right hand column) which possess a cis-A,B ring fusion.

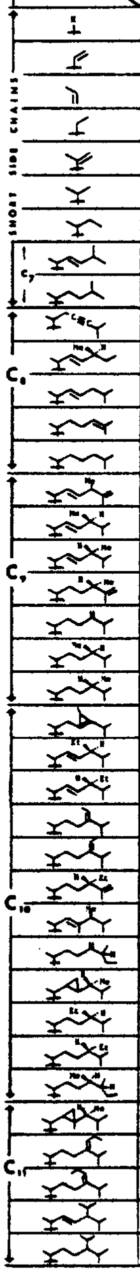
The number of carbon atoms in the side chains is indicated along the left hand border.

See p. 102a for Appendix I.

Appendix A.

MARINE STEROL NUCLEI





MARINE STEROL SIDE CHAINS

Side chains	Nucleus 1	Nucleus 2	Nucleus 3	Nucleus 4	Nucleus 5	Nucleus 6	Nucleus 7	Nucleus 8
SHORT SIDE CHAINS	274 **1**							
	300 **2**							
	300 **3**							
	302 **4**							
	314 **5**							
	316 GRYERIBOL **6**		318 **7**					
	330 **8**							
C_7	370 Δ^{22}-24-NOR-CHOLESTEROL **9**	370 ASTEROSTEROL **10**	372 **11**		358 **12**			
	24-NOR-CHOLESTEROL **13**							
C_8	382 **14**							
	384 OCCELASTEROL **15**	384 AMURESTEROL **16**	386 PATINOSTEROL **17**					
	384 Δ^{22}-CHOLESTEROL **18**	384 **19**	386 22,23-DEHYDRO-CHOLESTANOL **20**	382 **21**	372 **22**			
	384 DESMOSTEROL **23**	384 **24**						
	386 CHOLESTEROL **25**	386 LATHOSTEROL **26**	388 CHOLESTANOL **27**	384 7-DEHYDRO-CHOLESTEROL **28**	374 19-NOR-CHOLESTANOL **29**	372 19-NOR-CHOLESTEROL **30**	386 ZYMOSTENOL **31**	388 COPROSTANOL **32**
C_9		396 **33**						
	398 PINCSTEROL/CRINOSTEROL **34**	398 STELLASTEROL **35**	400 22,23-DEHYDRO-CAMPESTANOL **36**	396 **37**				
	398 BRASSICASTEROL **38**	398 5,6-DIHYDRO-ERGOSTEROL **39**	400 NEOSPONGOSTEROL **40**	396 ERGOSTEROL **41**	384 **42**			
	398 CODISTEROL **43**							
	398 CHALINASTEROL/OSTREASTEROL **44**	398 EPISTEROL **45**	400 24-METHYLENE-CHOLESTANOL **46**		386 **47**			
	400 CAMPESTEROL **48**	**49**	402 CAMPESTANOL **50**	398 7-DEHYDRO-CAMPESTEROL **51**				
	400 22,23-DIHYDRO-BRASSICASTEROL **52**	400 FUNGISTEROL **53**	402 ERGOSTANOL **54**	398 22,23-DIHYDRO-ERGOSTEROL **55**	388 **56**	386 **57**	400 **58**	
C_{10}	410 CALYSTEROL **59**							
	412 STIGMASTEROL **60**	412 (α)-SPINASTEROL/BITOBESTEROL **61**	414 **62**	410 CORBISTEROL **63**	400 **64**	398 **65**		
	412 PORIFERASTEROL **66**	412 CHONDRILLASTEROL **67**						
	412 FUCOSTEROL **68**	412 Δ^7-FUCOSTEROL **69**	414 FUCOSTANOL **70**					
	412 AVENASTEROL/28-ISOFUCOSTEROL **71**	412 Δ^7-AVENASTEROL **72**	414 28-ISOFUCOSTANOL **73**					
	412 CLEROSTEROL **74**							
	412 Δ^5-DEMETHYL-DINOSTEROL **75**				400 **76**			
	412 24,28-DIDEHYDRO-APLYSTEROL **77**							
	412 23-DEMETHYL-GORGOSTEROL **78**		414 23-DEMETHYL-GORGOSTANOL **79**					
	414 (β)-SITOSTEROL **80**	414 SCHOTTENOL **81**	416 STIGMASTANOL (β)-SITOSTANOL **82**	412 7-DEHYDRO-SITOSTEROL **83**	402 **84**		414 **85**	416 **86**
	414 CLIONASTEROL/γ-SITOSTEROL **87**	416 DIHYDROCHONDRILLASTEROL **88**		412 7-DEHYDRO-CLIONASTEROL **89**				
	416 APLYSTEROL **90**							
C_{11}	426 GORGOSTEROL **91**	428 ACANTHASTEROL **92**	428 GORGOSTANOL **93**					
	426 29-METHYL-28-ISOFUCOSTEROL **94**							
	426 29-METHYL-FUCOSTEROL **95**							
	426 Δ^{22}-24-ISOPROPYL CHOLESTEROL **96**							
	428 24-ISOPROPYL-CHOLESTEROL **97**							

7.2 Appendix B
Sources of Sterol Mass Spectra.

Sterol : names listed on the following two pages indicate spectra that were obtained from the old mass spectral files of Prof. Carl Djerassi. The spectra are divided into two groups: (1) sterols that are known to occur in marine sources, i.e. "4-demethyl marine sterol mass spectra" and (2) all other sterol mass spectra from those files grouped under "4-demethyl synthetic sterol mass spectra". The original CD number is given. These spectra were incorporated in the National Institutes of Health MSSS mass spectral data bank, which is available internationlly to researchers employing mass spectral identifications systems. See: S. R. Heller, Biomed. Mass., 1, 207 (1974).

All other mass spectra listed in Appendix 1 have been obtained by running mass spectra of authentic samples provided by researchers from around the world. The samples were either pure compounds or mixtures requiring subsequent purifications here. I would,therefore, like to join Professor Djerassi in thanking these researchers.

Dr. Aringer
(Karolinska Siukhuset, Stockholm)

Dr. J. T. Baker and Dr. R. J. Wells
(Roche Research Institute of Pharmacology,Australia)

Dr. M. Barbier
(Institut de Chimie des Substances Naturelles, France)

Dr. L. J. Goad
(University of Liverpool, England)

Dr. A. Kanazawa
(University of Kagoshima, Japan)

Dr. B. A. Knights
(University of Glasgow, Scotland)

Dr. M. Kobayashi
(Hokkaido University, Japan)

Dr. J. Mathieu
(Roussel-UCLAF Research Laboratories)

Dr. P. J. Scheuer
(University of Hawaii)

Dr. F. J. Schmitz
(University of Oklahoma)

Dr. R. H. Thomson
(University of Aberdeen)

Dr. A. J. Weinheimer
(University of Oklahoma)

I would also like to thank Willian A. Dow, Stanford University, for samples of aplysterol 90 and didehydroaplysterol 77 which he isolated from Verongia fistularis.

4-DEMETHYL SYNTHETIC STEROL MASS SPECTRA FROM THE FILES OF CARL DJERASSI JAN. 7, 1976 (ALL SPECTRA RECORDED AT 70EV)

	SB#	CAT#	CD#	MW	MS	FORMULA	STEROL
1		401	05203	276	CEC-103	C19H320	5ALPHA-ANDROSTAN-3BETA-OL
2		→ 99	16309	300	AEI-MS9	C21H320	(17(20)Z)-PREGNA-5,17(20)-DIEN-3BETA-OL
3		→221	99999	302	MAT-CH4	C21H340	PREG-5-EN-3BETA-OL
4		219	09576	316	AEI-MS9	C22H340	23,24-DINOR-CHOL-20-EN-3BETA-OL
5		---	11111	328	U	C23H340	24-NOR-CHOLA-5,22-DIEN-3BETA-OL
6		5673	20636	342	U	C24H380	(22E)-CHOLA-5,22-DIEN-3BETA-OL
7		5672	20637	342	U	C24H380	(22Z)-CHOLA-5,22-DIEN-3BETA-OL
8		78	18697	346	AEI-MS9	C24H420	5BETA-CHOLAN-3BETA-OL
9		76	18713	346	U	C24H420	5BETA-CHOLAN-3ALPHA-OL
10		5671	20641	356	U	C25H400	(22Z)-26,27-DINOR-CHOLESTA-5,22-DIEN-3BETA-OL
11		5670	20639	356	U	C25H400	(22E)-26,27-DINOR-CHOLESTA-5,22-DIEN-3BETA-OL
12		5669	20659	370	U	C26H420	(22Z)-24-NOR-CHOLESTA-5,22-DIEN-3BETA-OL
13		5345	99690	370	U	C26H420	24-NOR-CHOLESTA-5,25-DIEN-3BETA-OL
14		5344	99691	370	U	C26H420	24-NOR-CHOLESTA-5,23-DIEN-3BETA-OL
15		4691	18661	382	MAT-CH4	C27H420	CHOLESTA-5,20(21),24-TRIEN-3BETA-OL
16		4692	18659	382	MAT-CH4	C27H420	(17(20)E)-CHOLESTA-5,17(20),24-TRIEN-3BETA-OL
17		5667	20525	384	U	C27H440	(22Z)-27-NOR-24-METHYLCHOLESTA-5,22-DIEN-3BETA-OL
18		4693	18803	384	MAT-CH4	C27H440	(20(22)E)-CHOLESTA-5,20(22)-DIEN-3BETA-OL
19		4698	18723	384	U	C27H440	CHOLESTA-5,20(21)-DIEN-3BETA-OL
20		3299	99812	386	U	C27H460	CHOLEST-8(14)-EN-3BETA-OL
21		231	06032	398	CEC-103	C28H460	24-METHYLCHOLESTA-5,24(25)-DIEN-3BETA-OL
22		234	09180	400	MAT-CH4	C28H480	24-METHYLCHOLEST-8(14)-EN-3BETA-OL
23		3518	19479	410	U	C29H460	22,23-METHYLENE-24-METHYLCHOLESTA-5,24(28)-DIEN-3β-O
24		4785	19338	412	MAT-CH4	C29H480	(22E)-24-DIMETHYLCHOLESTA-5,22-DIEN-3BETA-OL

SB# = SAMPLE BOX NUMBER
CAT# = TABLET CATALOG NUMBER
CD# = CARL DJERASSI MASS SPECTRUM NUMBER
MW = MOLECULAR WEIGHT
MS = MASS SPECTROMETER

"→" indicates that spectrum has subsequently been moved to the marine file.

4-DEMETHYL MARINE STEROL MASS SPECTRA FROM THE FILES OF CARL DJERASSI JAN, 7, 1976 (ALL SPECTRA RECORDED AT 70EV)

	SB#	CAT#	CD #	MW	MS	FORMULA	STEROL
1	A-2	5668	20660	370	U	C26H420	24-NOR-CHOLESTA-5,22-DIEN-3BETA-OL
2	A-1	5339	18380	372	AEI-MS9	C26H440	24-NOR-CHOLEST-5-EN-3BETA-OL
3	E-2	4739	99754	372	U	C26H440	→(22E)-19-NOR-5ALPHA,10BETA-CHOLEST-22-EN-3BETA-OL
4	A-15	100	16746	384	AEI-MS9	C27H440	CHOLESTA-5,7-DIEN-3BETA-OL
5	A-8	237	05570	384	MAT-CH4	C27H440	CHOLESTA-5,24-DIEN-3BETA-OL
6	B-2	103	16793	384	AEI-MS9	C27H440	➧5ALPHA-CHOLESTA-7,9(11)-DIEN-3BETA-OL
7	A-5	4732	17657	386	U	C27H460	CHOLEST-5-EN-3BETA-OL
8	A-11	101	16778	386	AEI-MS9	C27H460	5ALPHA-CHOLEST-7-EN-3BETA-OL
9	A-18	2509	18633	388	U	C27H480	5ALPHA-CHOLESTAN-3BETA-OL
10	A-18	406	05557	388	CEC-103	C27H480	5ALPHA-CHOLESTAN-3BETA-OL
11	B-5	4748	20063	398	AEI-MS9	C28H460	(22E)-24-METHYLCHOLESTA-5,22-DIEN-3BETA-OL
12	B-5	2455	15214	398	U	C28H460	(22E)-24-METHYLCHOLESTA-5,22-DIEN-3BETA-OL
13	B-10	232	06060	398	MAT-CH4	C28H460	24-METHLYCHOLESTA-5,24(28)-DIEN-3BETA-OL
14	B-13	233	09125	398	MAT-CH4	C28H460	(22E)-24-METHYL-5ALPHA-CHOLESTA-7,22-DIEN-3BETA-OL
15	C-7	3503	15281	412	AEI-MS9	C29H480	(22E)-24-ETHYLCHOLESTA-5,22-DIEN-3BETA-OL
16	C-7	2454	14916	412	U	C29H480	(22E)-24-ETHYLCHOLESTA-5,22-DIEN-3BETA-OL
17	C-20	236	06052	412	MAT-CH4	C29H480	(22E)-24-ETHYL-5ALPHA-CHOLESTA-7,22-DIEN-3BETA-OL
18	C-9	2438	12489	412	U	C29H480	(24E)-STIGMASTA-5,24(28)-DIEN-3BETA-OL
19	C-9	3406	11257	412	AEI-MS9	C29H480	(24E)-STIGMASTA-5,24(28)-DIEN-3BETA-OL
20	C-9	4742	99752	412	U	C29H480	(24E)-STIGMASTA-5,24(28)-DIEN-3BETA-OL
21	C-9	238	06237	412	AEI-MS9	C29H480	(24E)-STIGMASTA-5,24(28)-DIEN-3β-ol
22	D-9	4738	18100	416	U	C29H520	24-ETHYL-5ALPHA-CHOLESTAN-3BETA-OL
23	D-14	2450	13915	426	AEI-MS9	C30H500	GORGOSTEROL
24	D-14	4733	17659	426	U	C30H500	GORGOSTEROL
25	D-12	4740	19975	426	U	C30H500	(24Z)-24-PROPYLIDENECHOLEST-5-EN-3BETA-OL

SB# = SAMPLE BOX NUMBER
CAT# = TABLET CATALOG NUMBER
CD# = CARL DJERASSI MASS SPECTRUM NUMBER
MW = MOLECULAR WEIGHT
MS = MASS SPECTROMETER

➧ indicates spectrum has been moved to the synthetic file

"→" indicates spectrum has subsequently been deleted because of poor quality.

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The undersigned agrees to accept responsibility for the scientific and technical conduct of the project and for provision of required progress reports if a grant is awarded as the result of this application.

1/26/78
Date

Principal Investigator or
Program Director