

Modified Routes to the “Designer” Surfactant PQS

Supporting Information

Ralph Moser, Subir Ghorai, and Bruce H. Lipshutz*

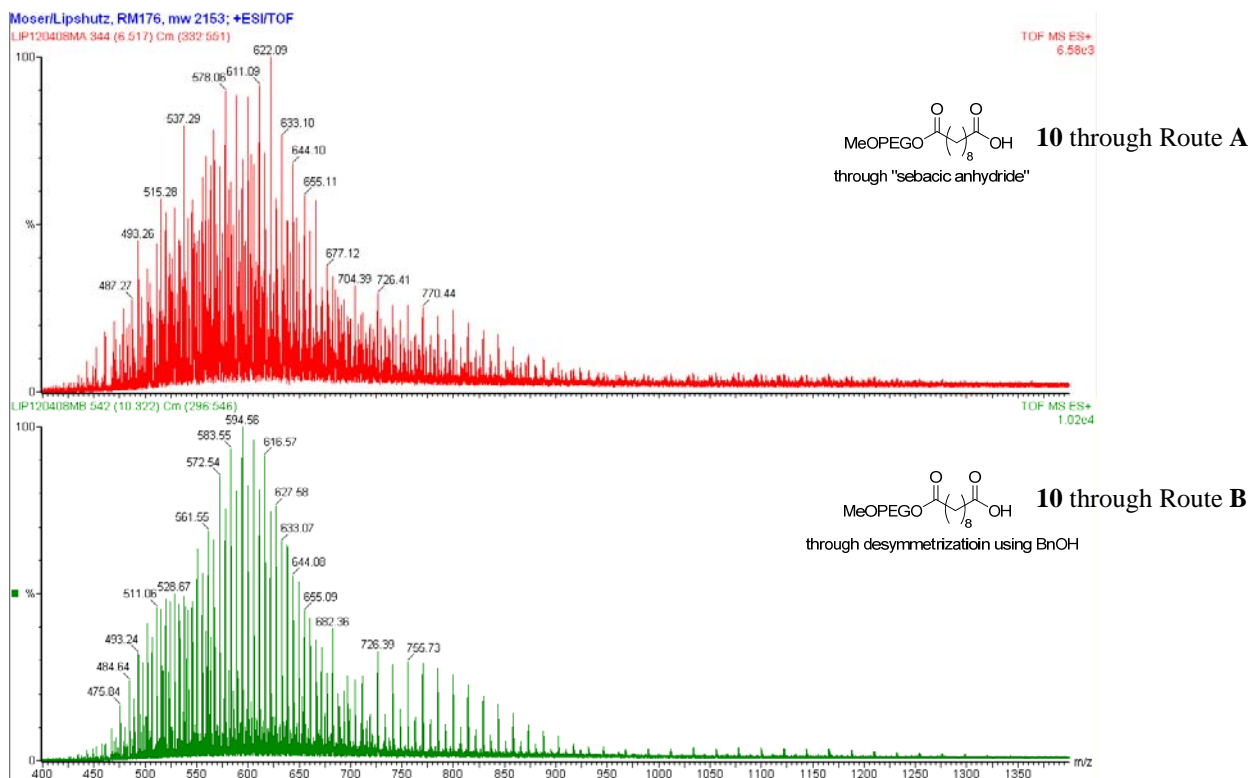
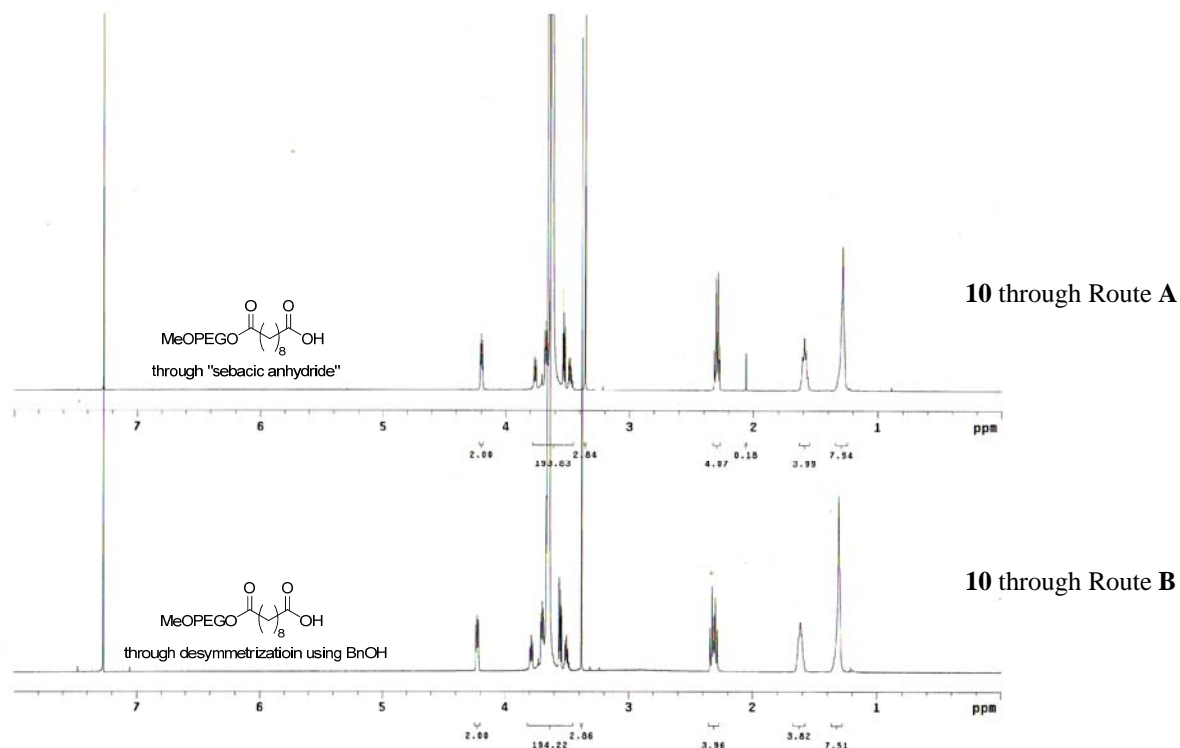
Department of Chemistry and Biochemistry
University of California, Santa Barbara, CA 93106
lipshutz@chem.uscb.edu

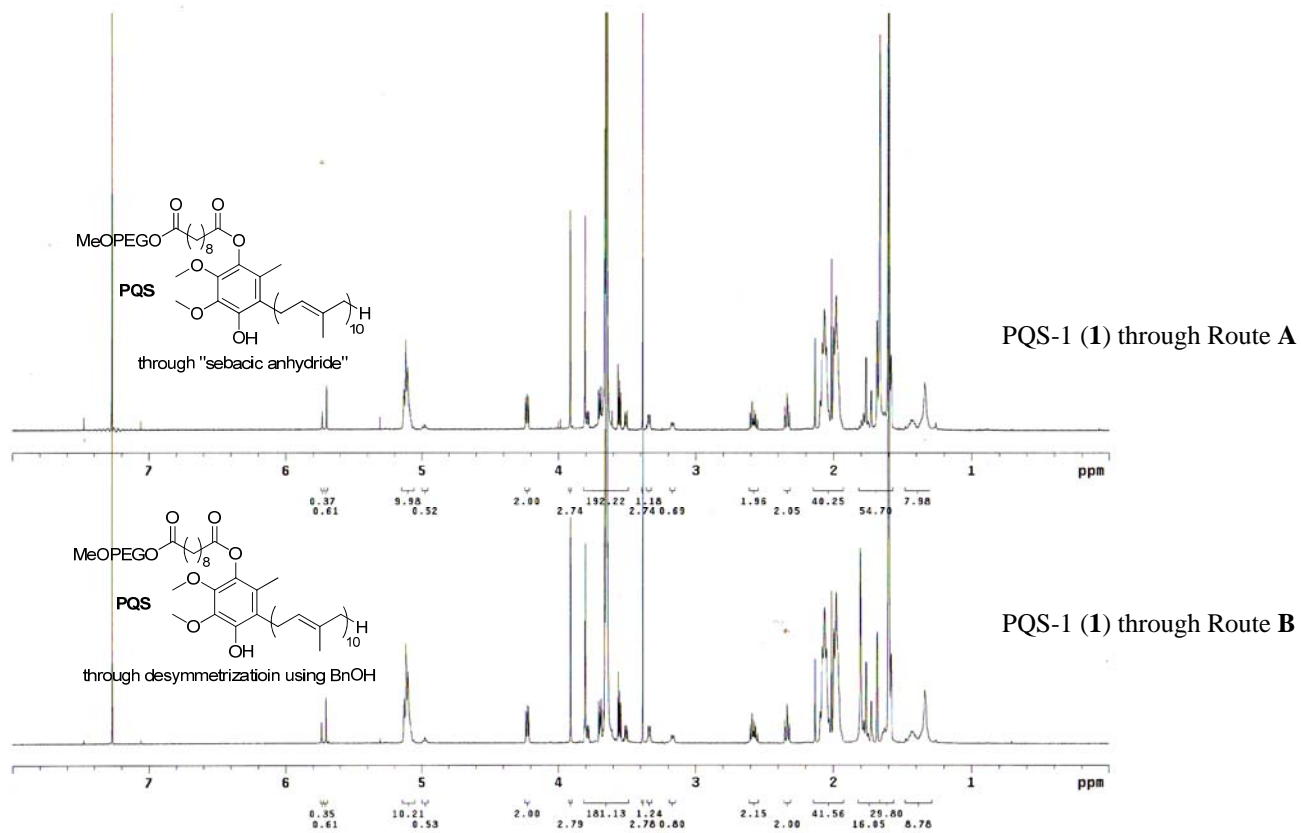
Table of Contents

I.	Spectral comparison of PQS-1 (1) obtained through Route A vs Route B	S2-S3
II.	Mass spectral data of PQS-3 (3)	S4-S9
III.	Spectral data (^1H and ^{13}C) of all new compounds	S10-S27

I. Spectral comparison of PQS-1 (1) obtained through Route A vs Route B

Spectral data:

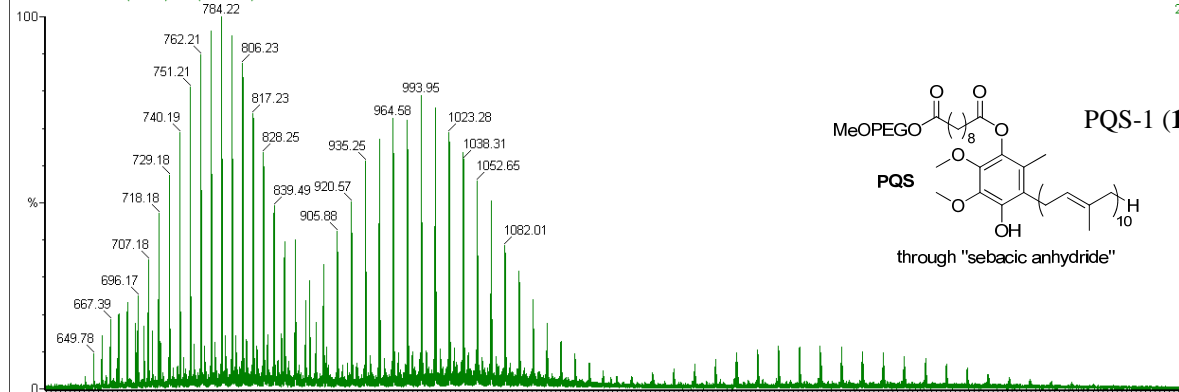




Moser/Lipshutz, RM180, mw 2999; +ESI/TOF

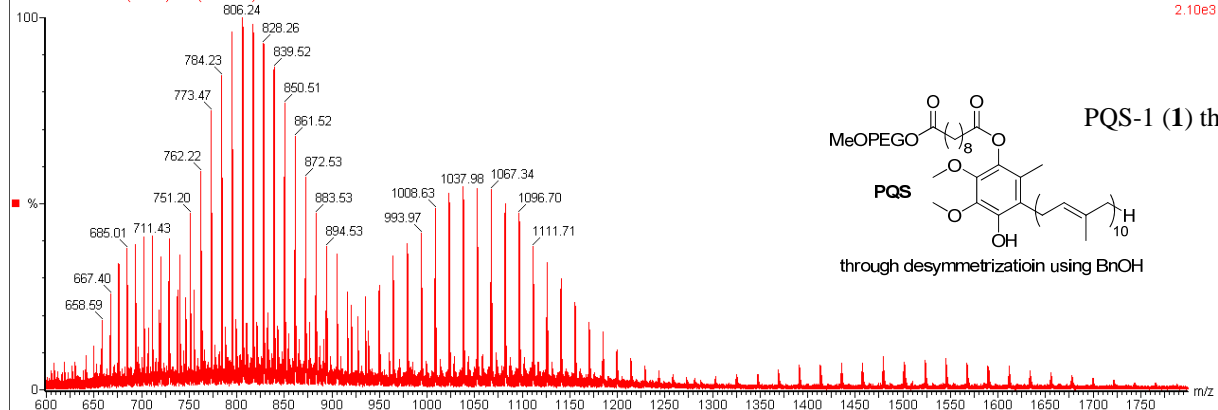
LIP121108MA 207 (3.919) Cm (207.323)

TOF MS ES+
2.38e3



LIP120408MD 397 (7.544) Cm (261.399)

TOF MS ES+
2.10e3

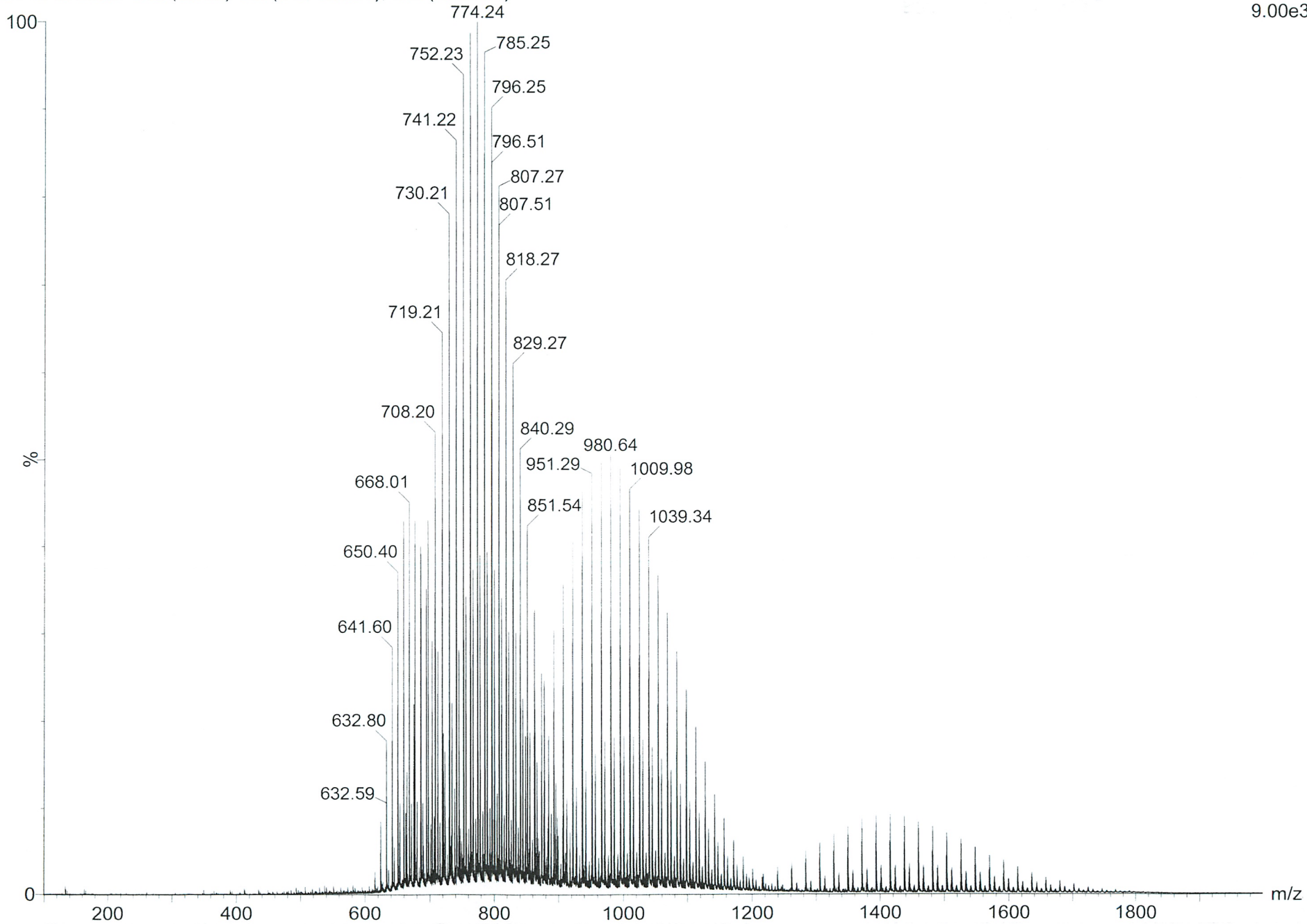


II. Mass spectral data of PQS-3 (3)

Ghosai/Lipshutz, SG/2/172B MW polymer +ESI/TOF

LIP071310MB 318 (6.052) Sm (SG, 3x4.00); Cm (270:320)

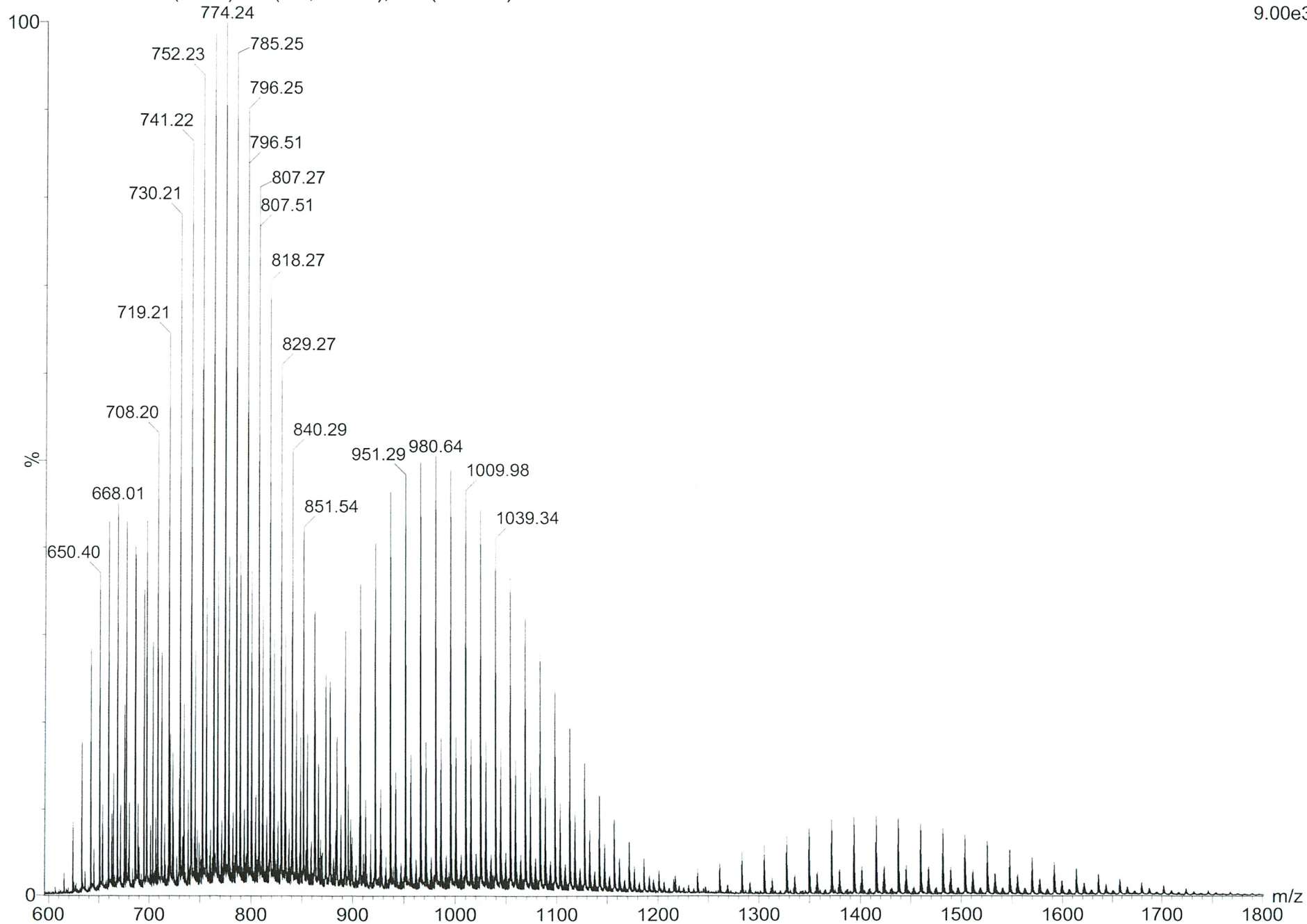
TOF MS ES+
9.00e3



Ghosai/Lipshutz, SG/2/172B MW polymer +ESI/TOF

LIP071310MB 318 (6.052) Sm (SG, 3x4.00); Cm (270:320)

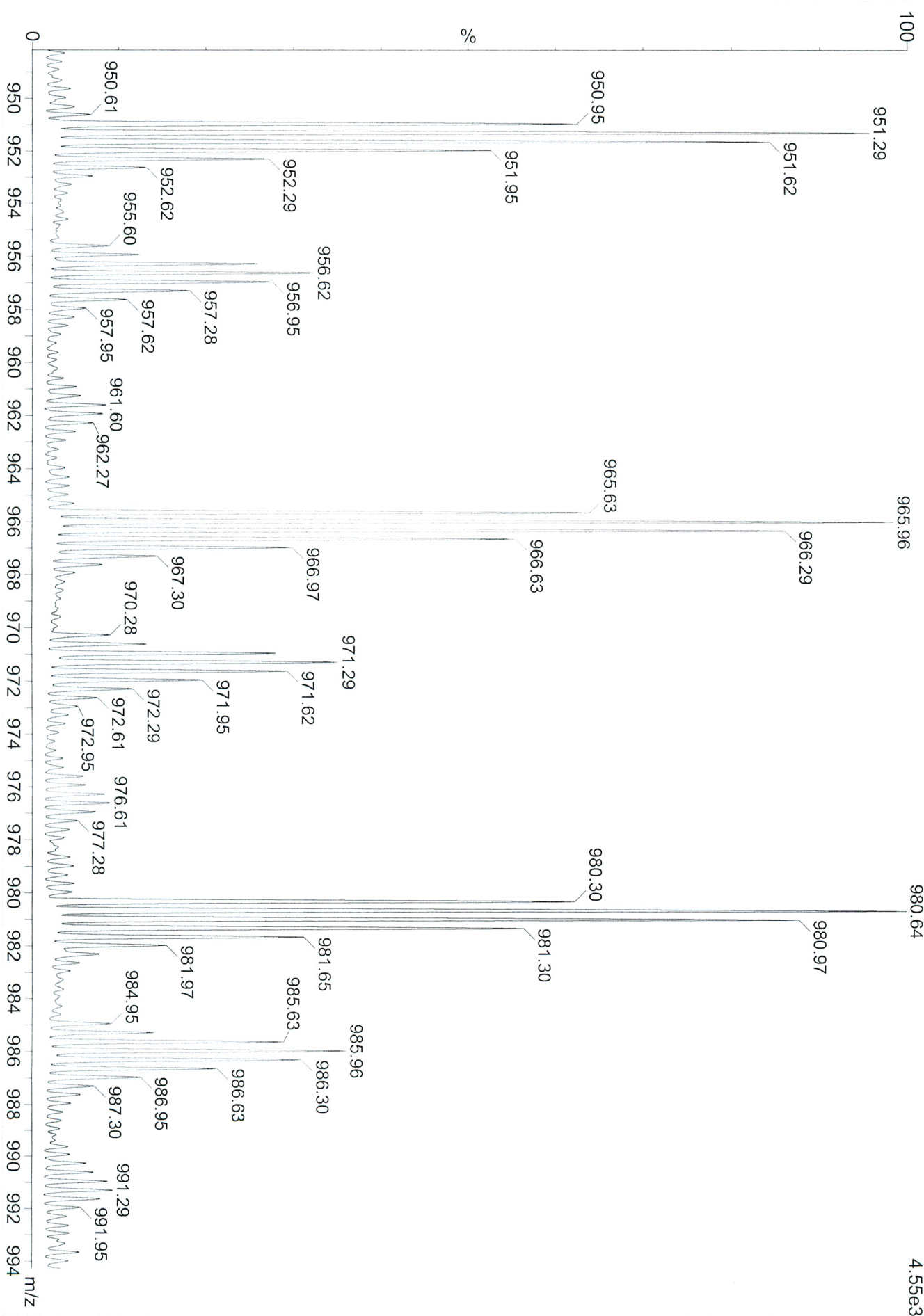
TOF MS ES+
9.00e3



Ghosai/Lipshutz, SG/2/172B MW polymer +ESI/TOF

LIP071310MB 318 (6.052) Sm (SG, 3x4.00); Cm (270:320)

TOF MS ES+
4.55e3



Ghosai/Lipshutz, SG/2/172B MW polymer +ESI/TOF

LIP071310MB 318 (6.052) Sm (SG, 3x4.00); Cm (270:320)

100
1393.43

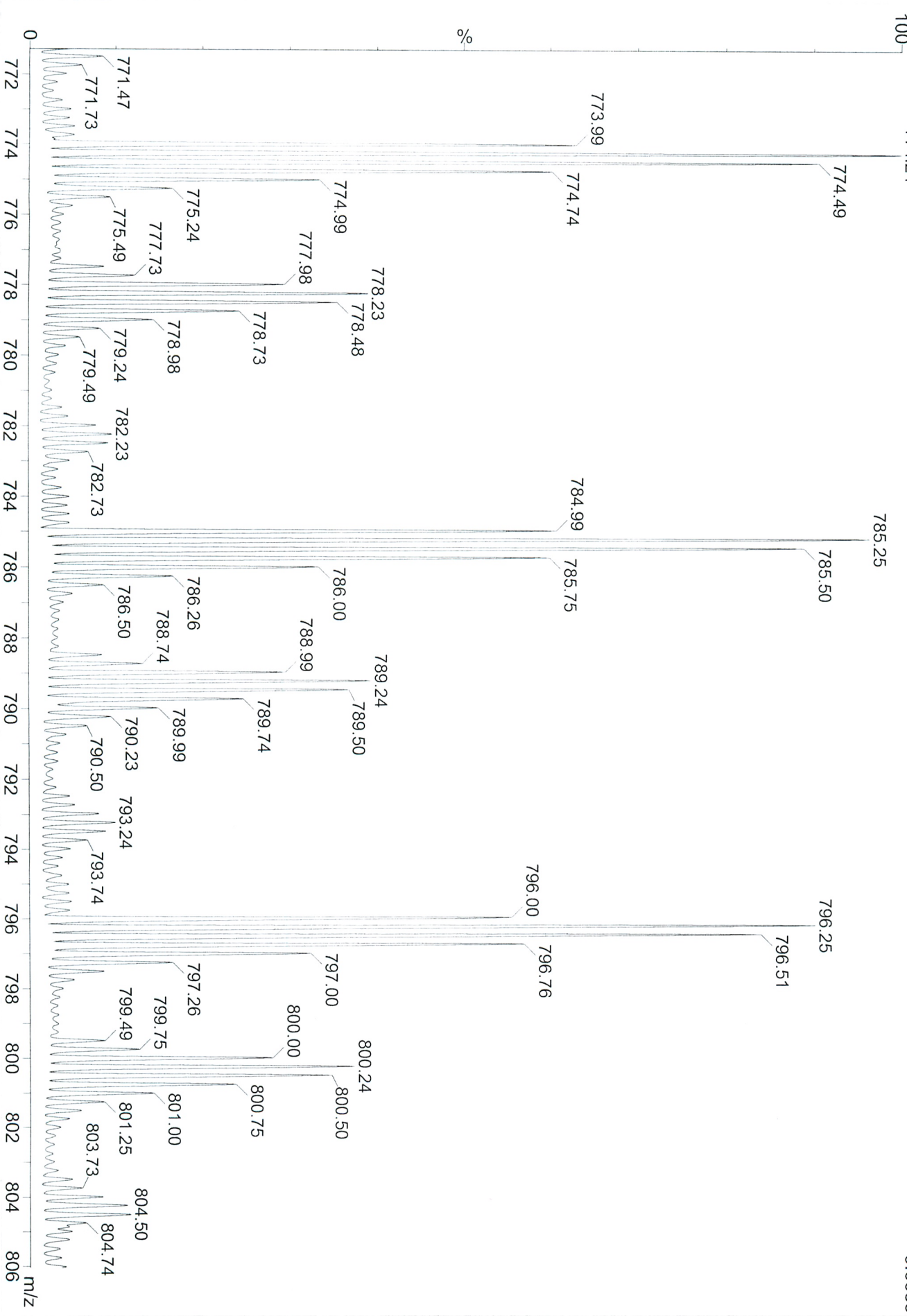
TOF MS ES+
835



Ghosai/Lipshutz, SG/2/172B MW polymer +ESI/TOF

LIP071310MB 318 (6.052) Sm (SG, 3x4.00); Cm (270:320)

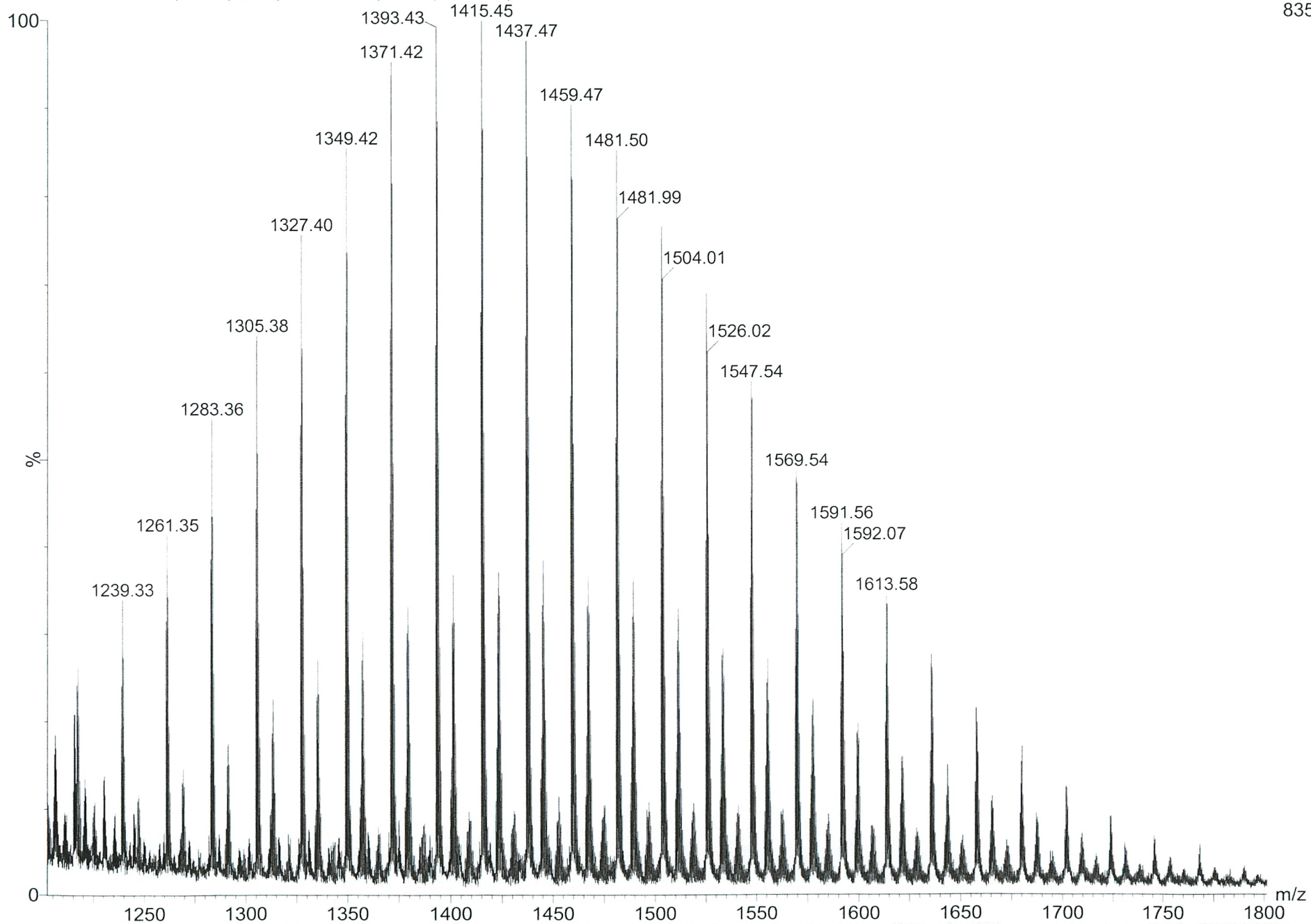
TOF MS ES+
9.00e3



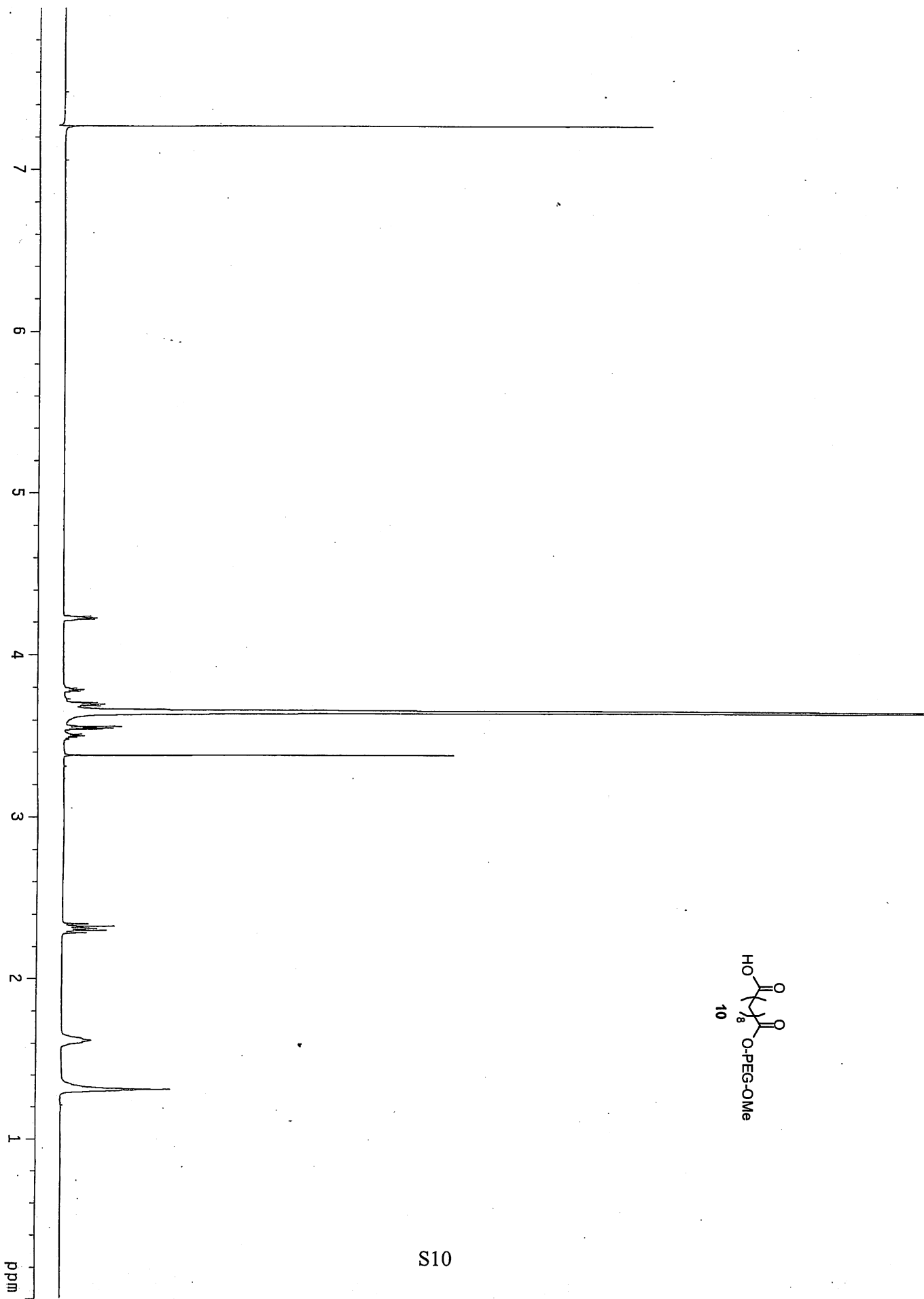
Ghosai/Lipshutz, SG/2/172B MW polymer +ESI/TOF

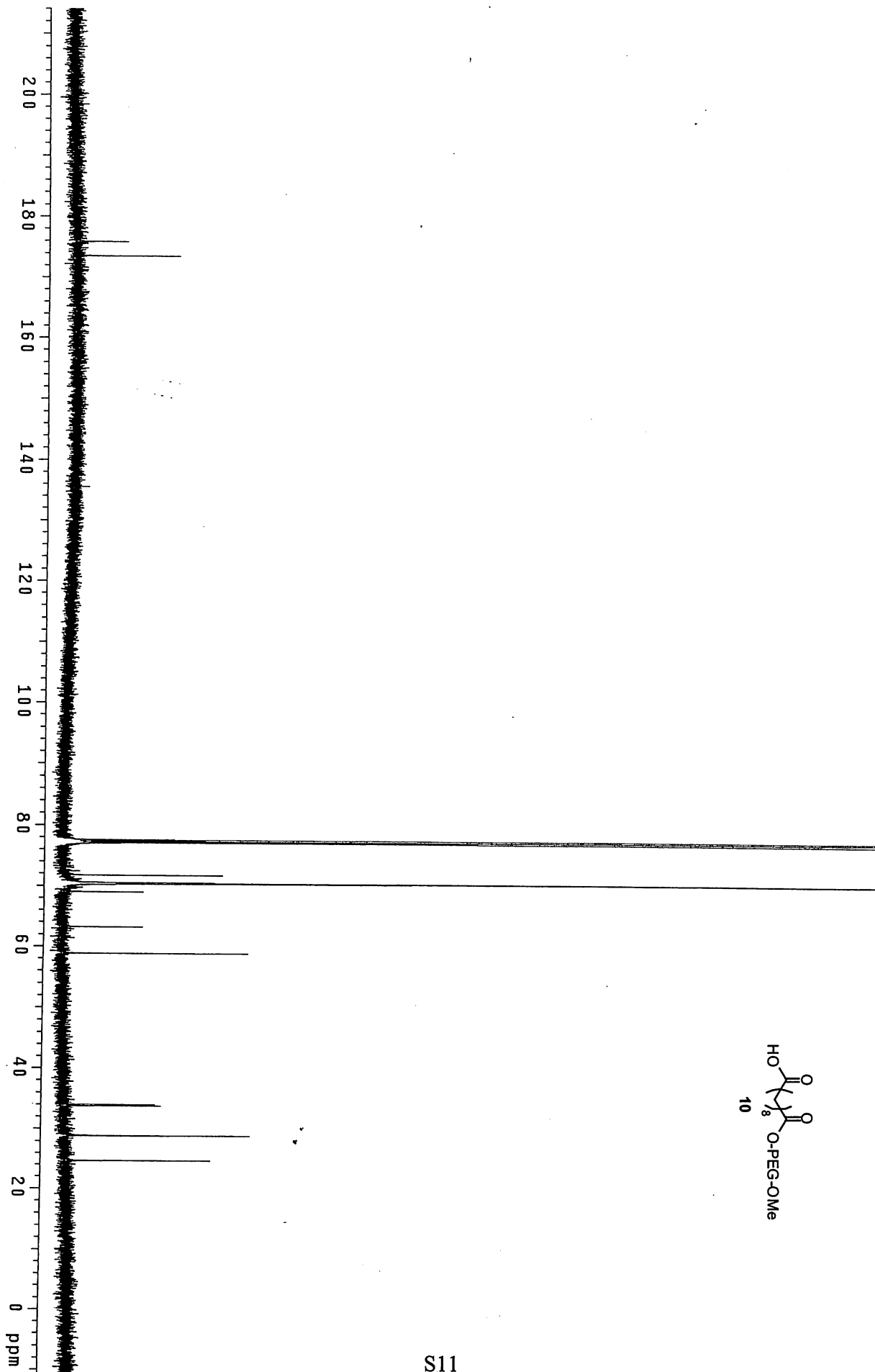
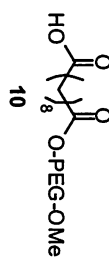
LIP071310MB 318 (6.052) Sm (SG, 3x4.00); Cm (270:320)

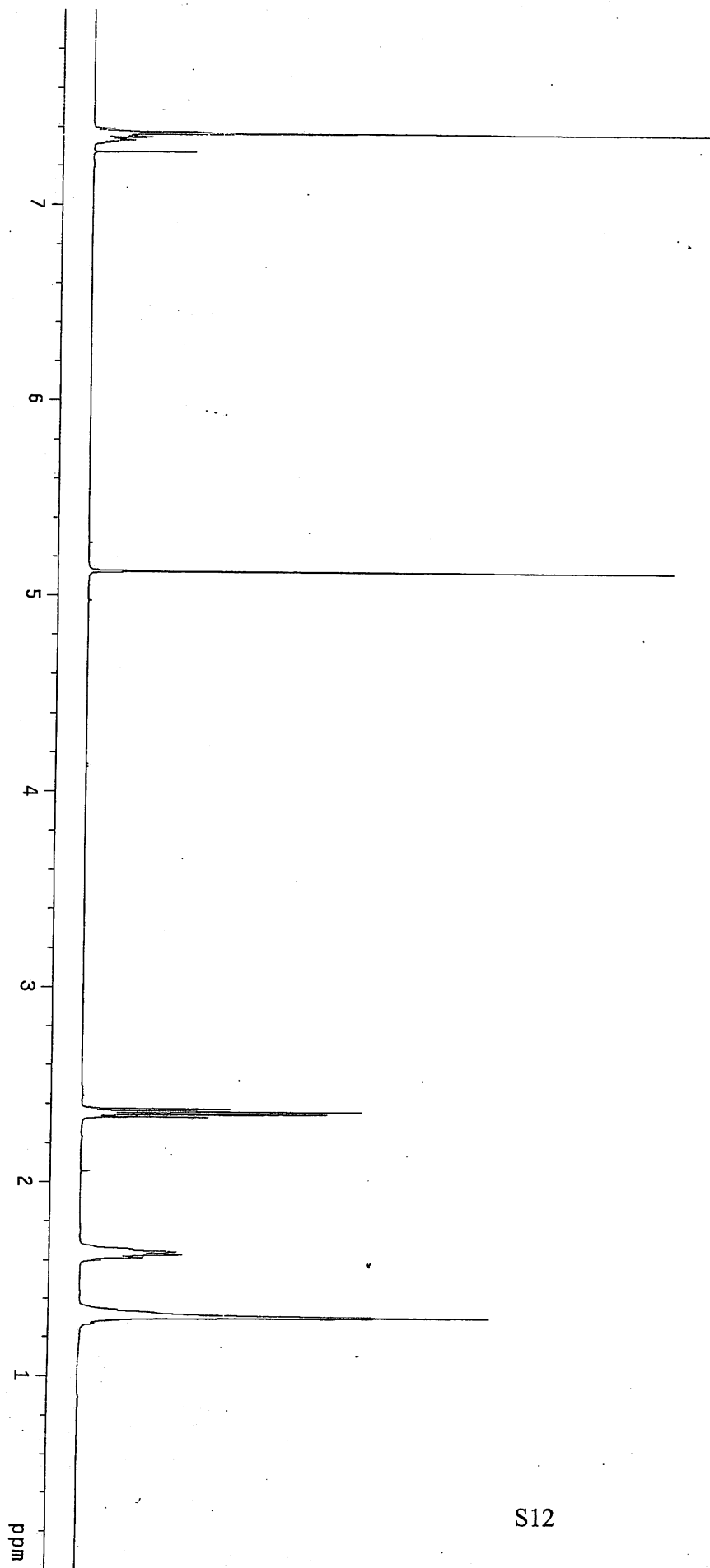
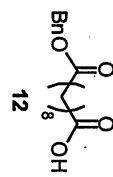
TOF MS ES+
835



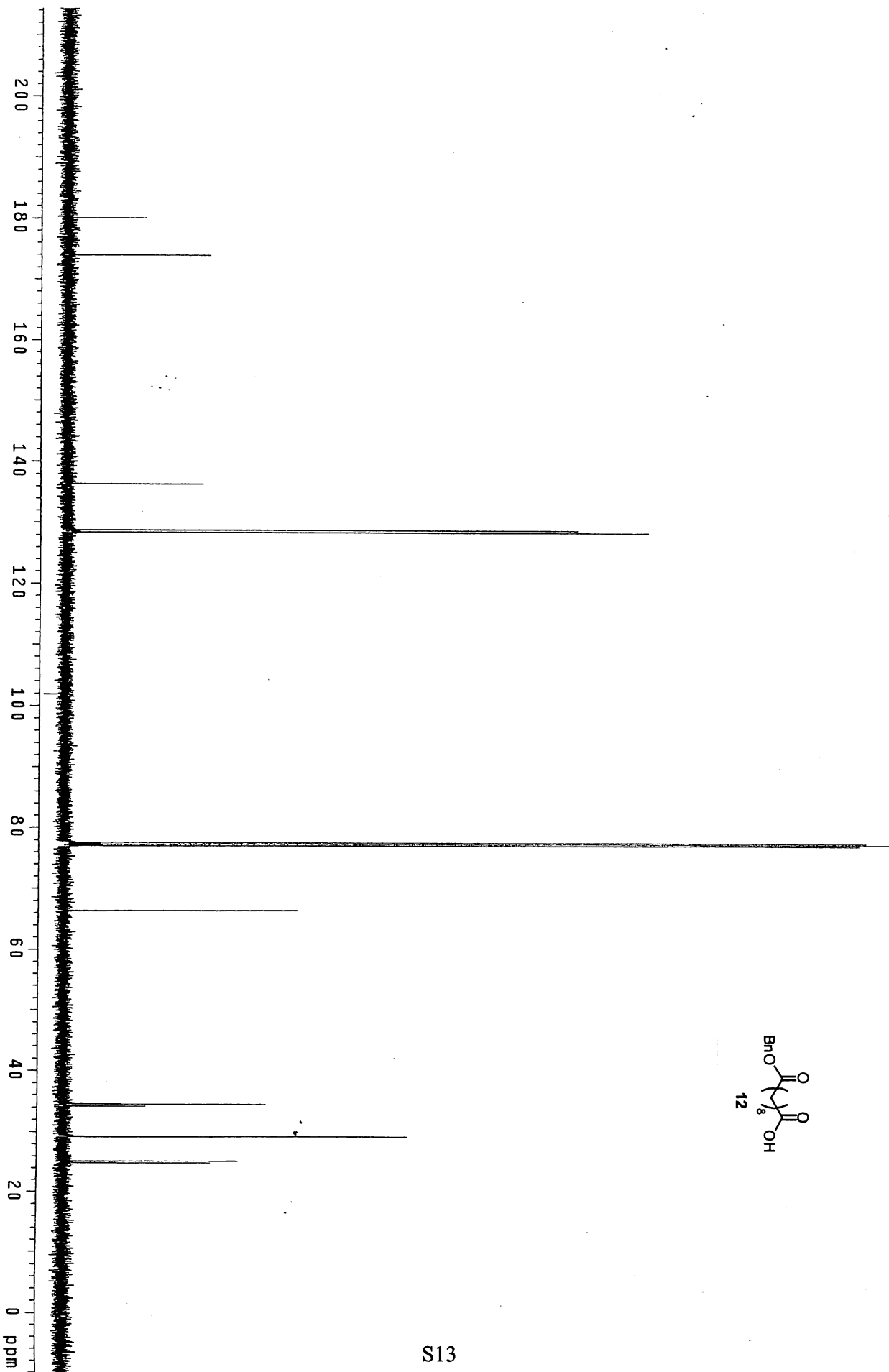
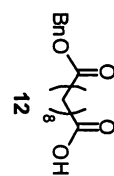
III. Spectral data (^1H and ^{13}C) of all new compounds

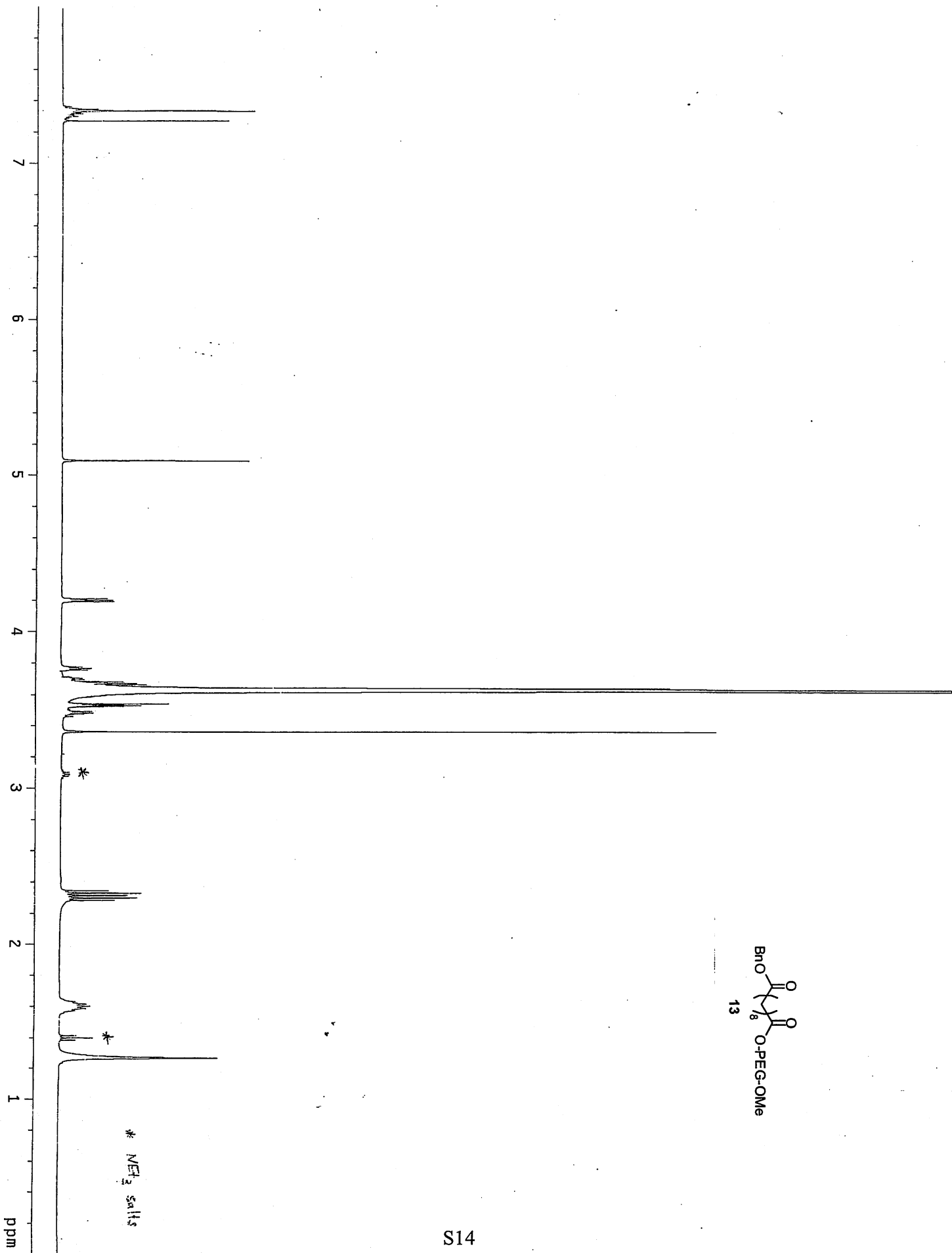
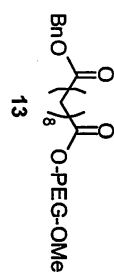


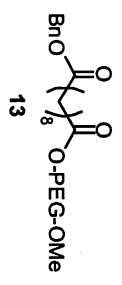
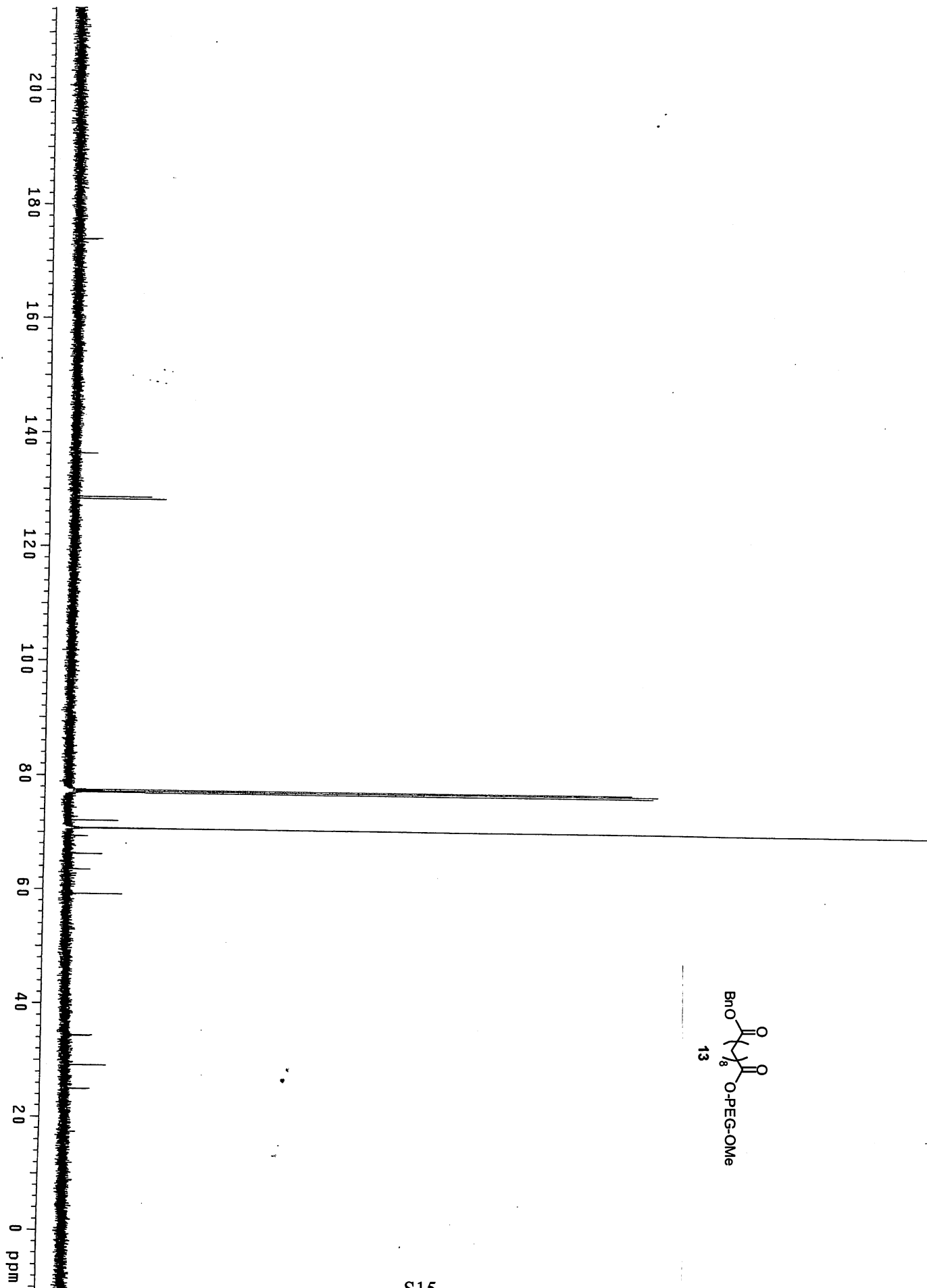


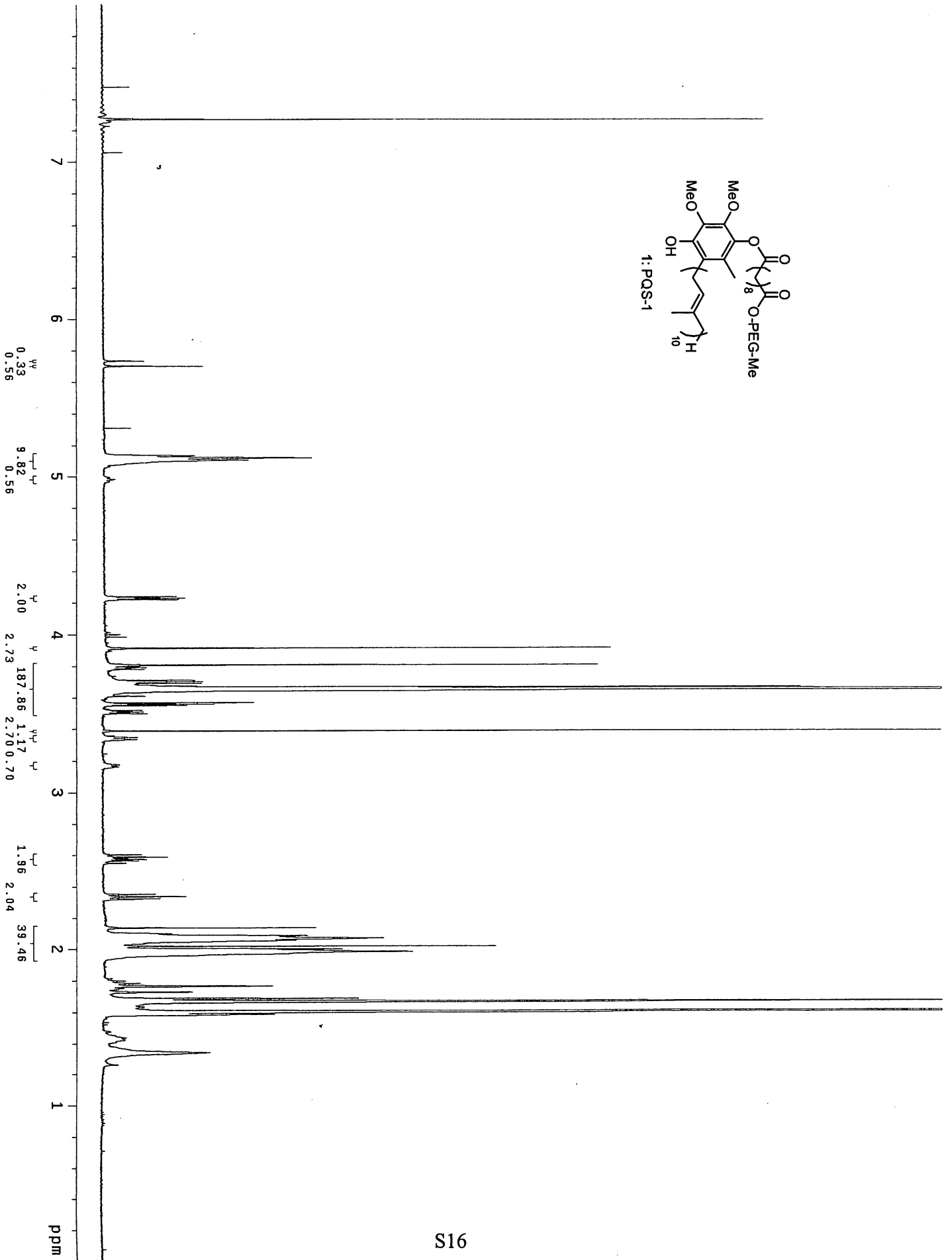
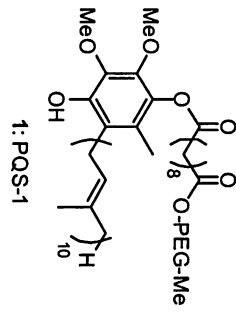


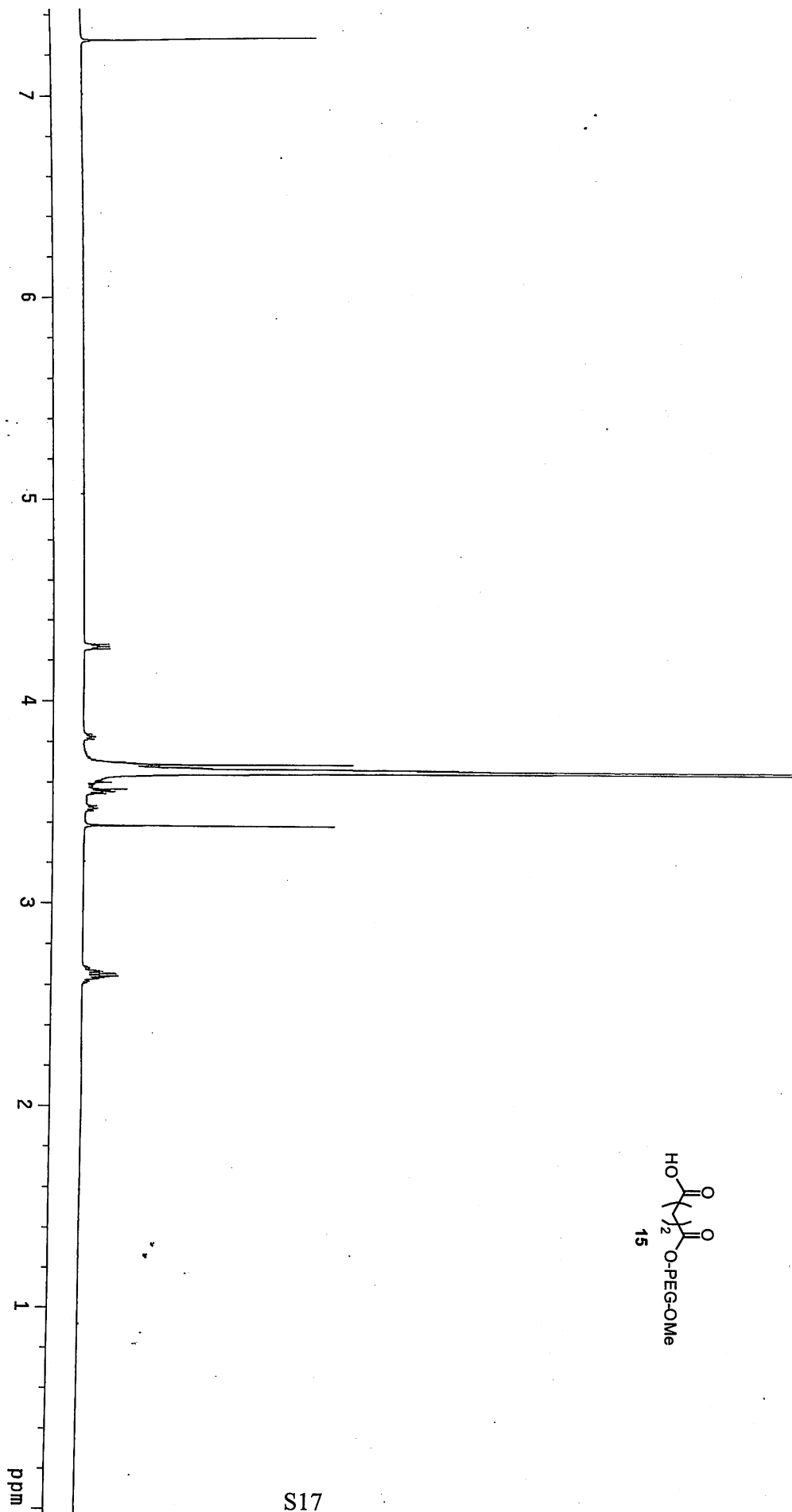
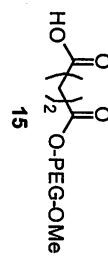
S12

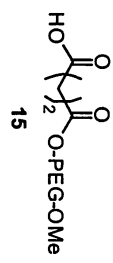
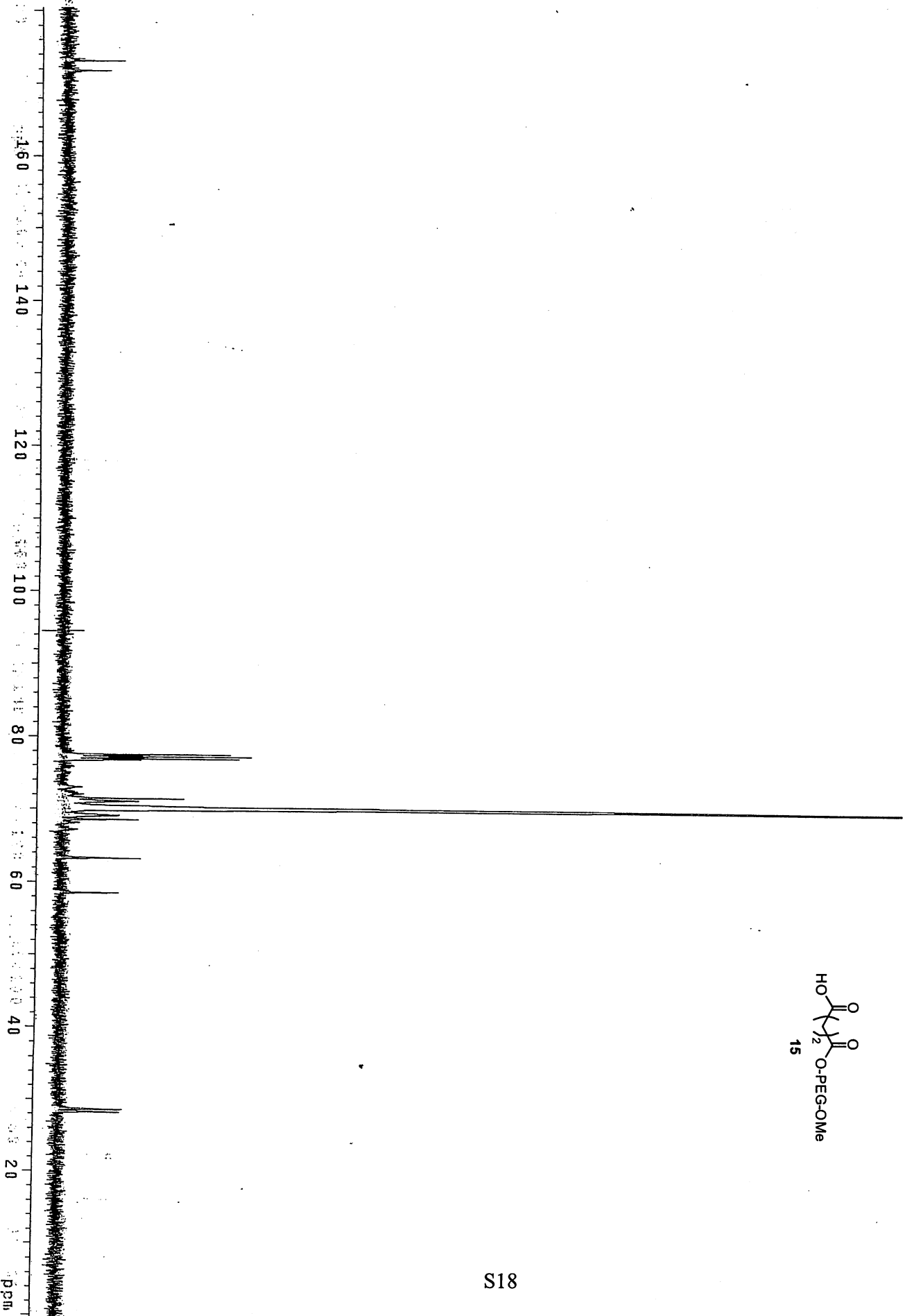


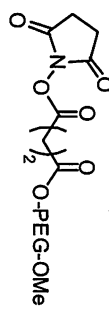




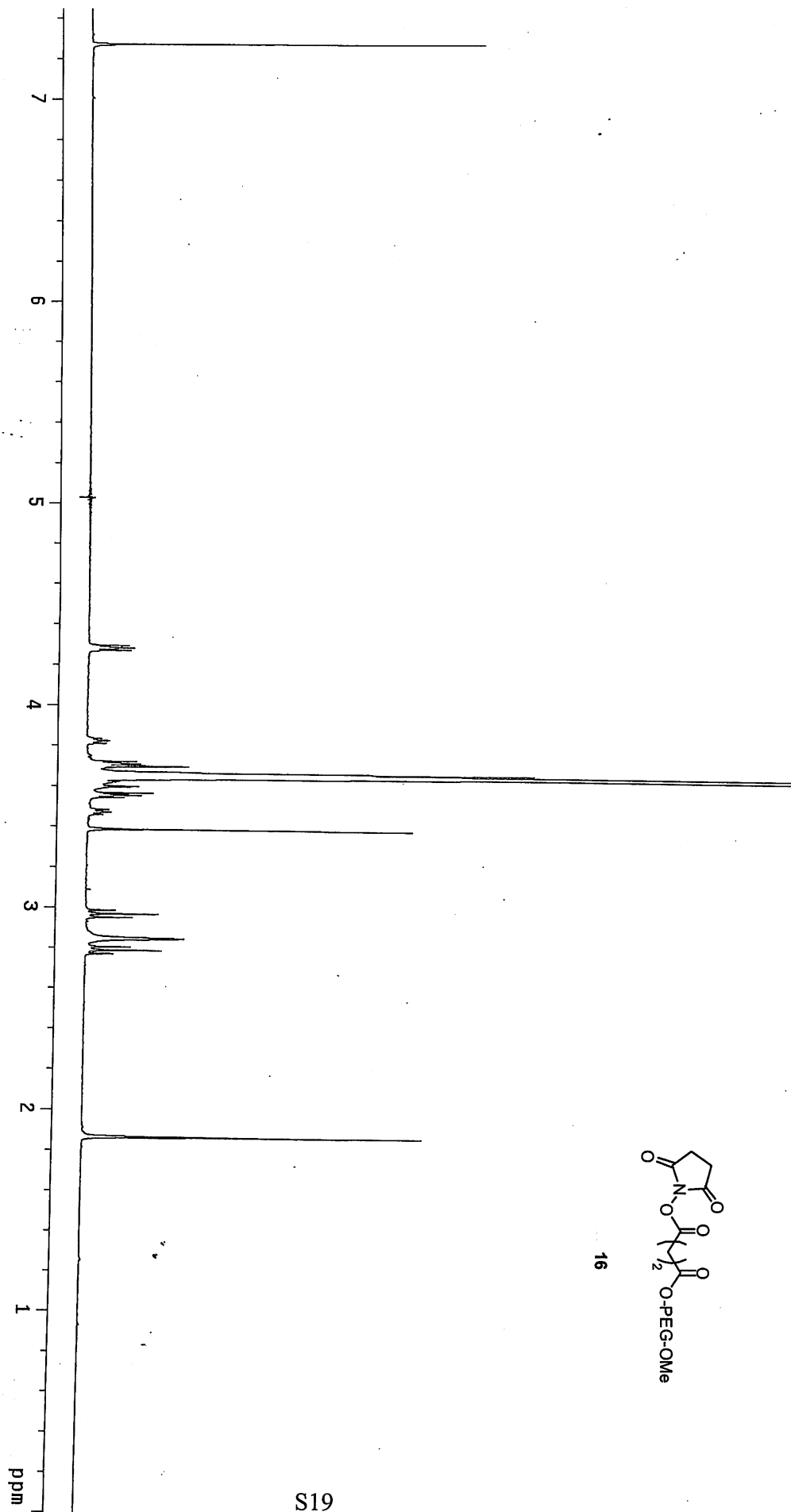




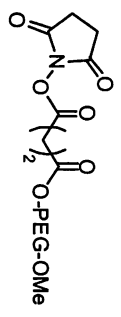
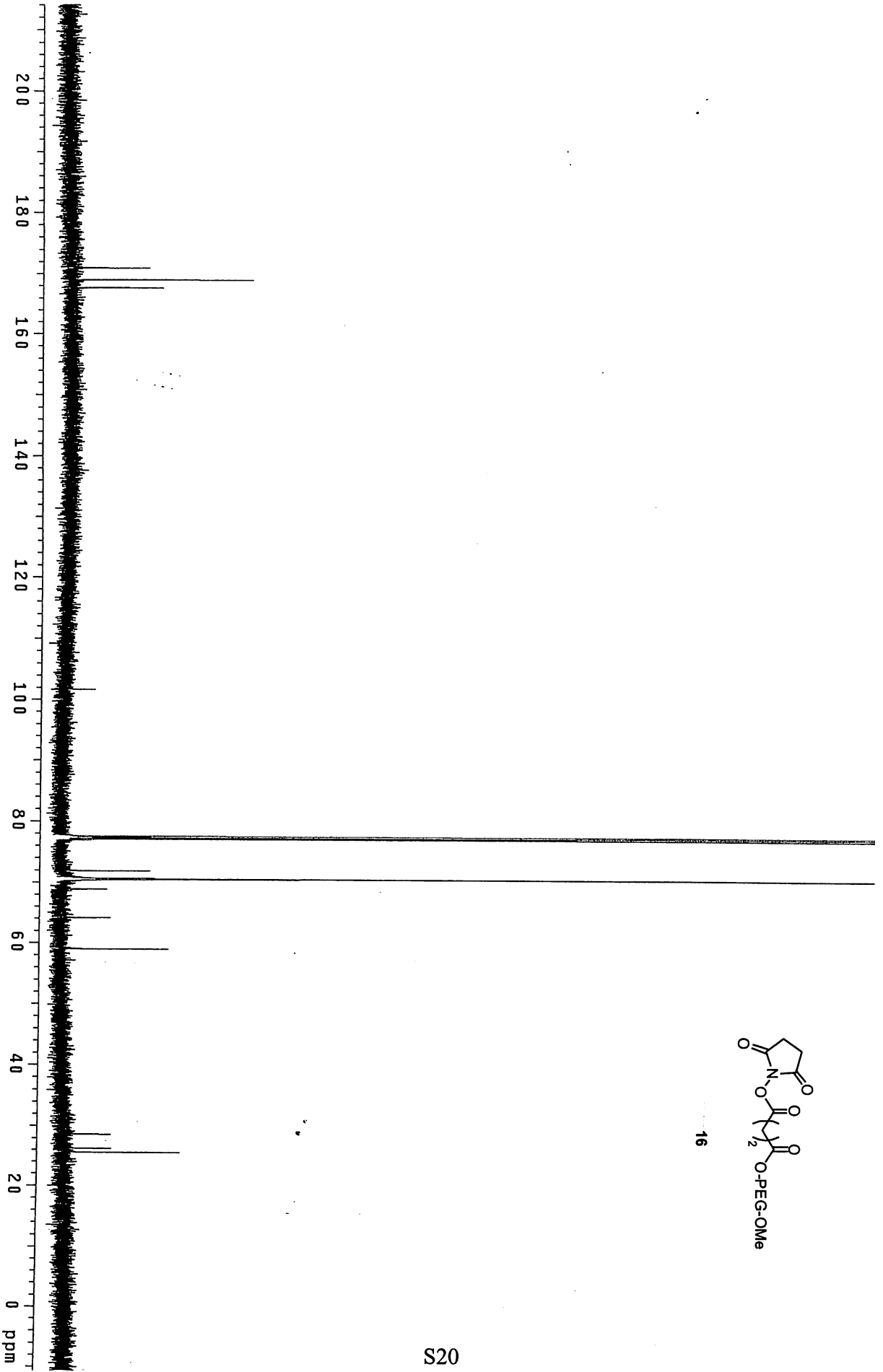




16



S19



16

