

Supporting Information

Table of Content

	Page
Links to Thesis's	2
Mass Spectrometry	3
- (CN)Cbl MALDI, ESI	4
- (CN) ₂ Cby(OMe) ₇ MALDI, ESI	5
Elemental Analysis	6
References	6

1. Links to Thesis's.

Munk, W. Ph. D. Thesis, *ETH Zürich*, 1994.

http://www.library.ethz.ch/search/action/display.do?tabs=detailsTab&ct=display&fn=search&doc=ebi01_prod000971816&indx=1&recIds=ebi01_prod000971816&recIdxs=0&elementId=0&renderMode=poppedOut&displayMode=full&frbrVersion=&dscnt=0&fctN=facet_domain&frbg=&fctV=ETH+E-Collection&tab=default_tab&dstmp=1365510595010&srt=rank&mode=Basic&dum=true&fromLogin=true&backFromPreferences=true&v1%28freeText0%29=munk&cmslang=eng-GB&vid=DADS&prefLang=en_US

Kreppelt, F. Ph. D. Thesis, *ETH Zürich*, 1991.

http://www.library.ethz.ch/search/action/display.do?tabs=detailsTab&ct=display&fn=search&doc=ebi01_prod000626280&indx=2&recIds=ebi01_prod000626280&recIdxs=1&elementId=1&renderMode=poppedOut&displayMode=full&frbrVersion=&dscnt=1&v1%28134576197UI0%29=any&scp.scps=scope%3A%28ebi01_prod%29%2Cscope%3A%28EPICS%29%2Cscope%3A%28replay%29%2Cscope%3A%28retroseals%29%2Cscope%3A%28cmistar%29%2Cscope%3A%28%22ARCHIVDATENBANK%22%29&frbg=&tab=default_tab&dstmp=1365510643298&srt=rank&mode=Basic&dum=true&tb=t&v1%281UIStartWith0%29=contains&v1%28291561170UI1%29=all_items&v1%28freeText0%29=Kreppelt&vid=DADS

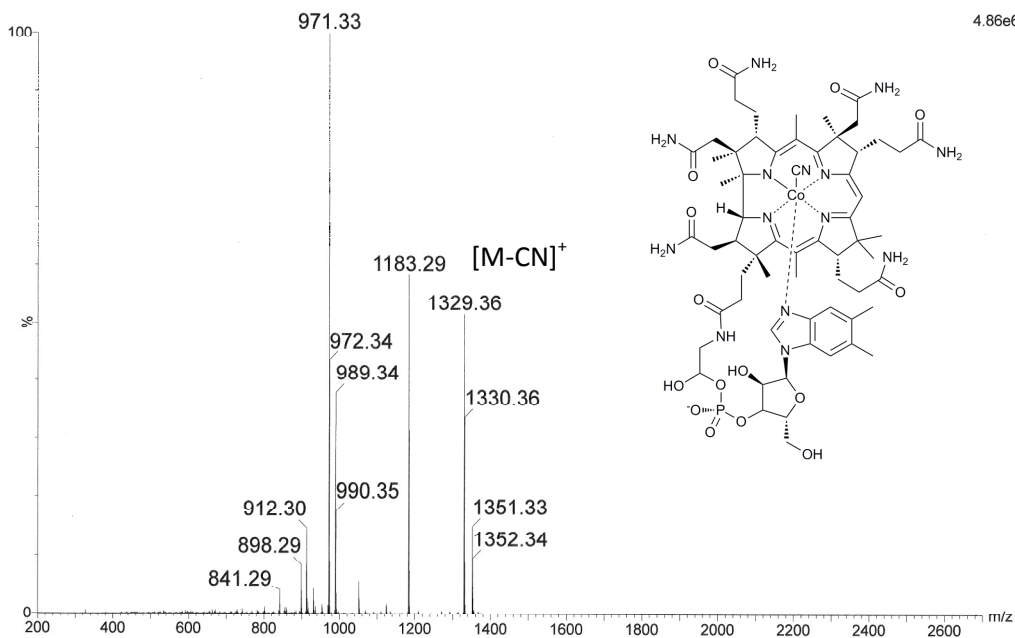
Caderas, C. Ph. D. Thesis, *ETH Zürich*, 1985.

http://www.library.ethz.ch/search/action/display.do?tabs=detailsTab&ct=display&fn=search&doc=ebi01_prod000346933&indx=1&recIds=ebi01_prod000346933&recIdxs=0&elementId=0&renderMode=poppedOut&displayMode=full&frbrVersion=&fctN=facet_domain&dscnt=0&v1%28134576197UI0%29=any&scp.scps=scope%3A%28ebi01_prod%29%2Cscope%3A%28EPICS%29%2Cscope%3A%28replay%29%2Cscope%3A%28retroseals%29%2Cscope%3A%28cmistar%29%2Cscope%3A%28%22ARCHIVDATENBANK%22%29&fctV=ETH+E-Collection&frbg=&tab=default_tab&dstmp=1365510683678&srt=rank&mode=Basic&dum=true&tb=t&v1%281UIStartWith0%29=contains&v1%28291561170UI1%29=all_items&v1%28freeText0%29=Caderas&vid=DADS

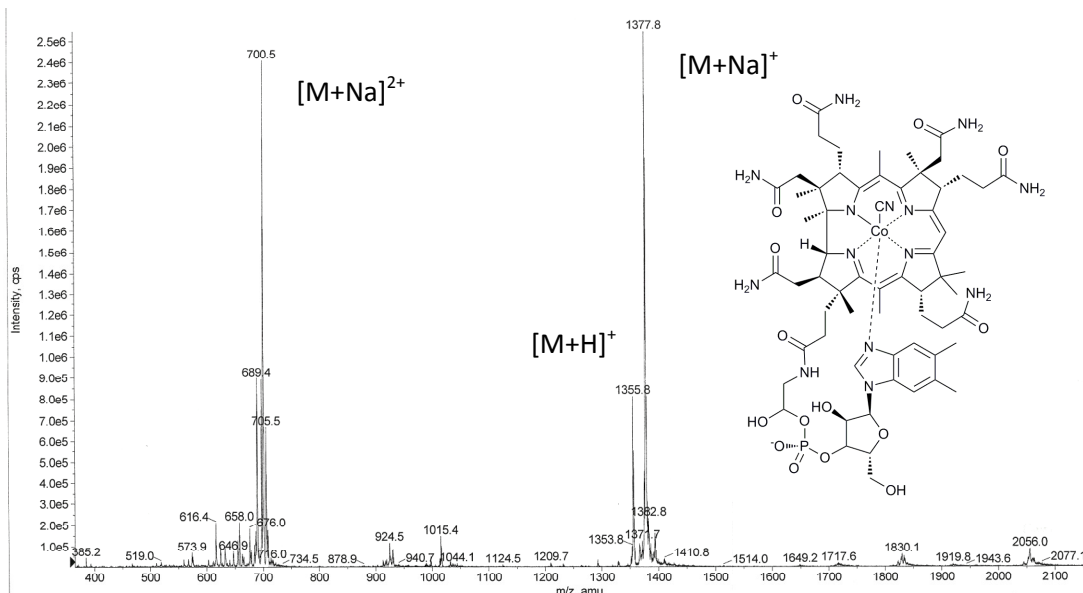
2. Mass Spectrometry: In our experience, ESI is the most suitable ionization technique for mass spectrometry experiments for most of the vitamin B₁₂ derivatives, in which mono-charged signals for [M-CN]⁺ or [M+Na]⁺ cations are usually obtained.¹ However, due to the size of the compound MALDI is also commonly used. Examples of MS spectra for (CN)Cbl and (CN)₂Cby(OMe)₇ are shown below.

(CN)Cbl MALDI

Matrix: α -cyano-4-hydroxycinnamic acid

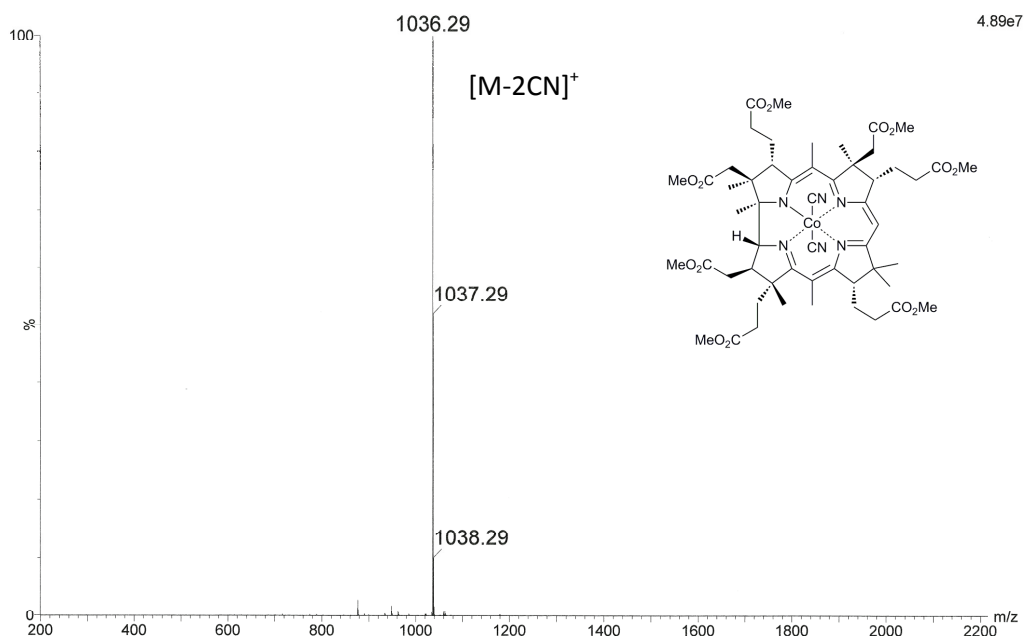


(CN)Cbl ESI

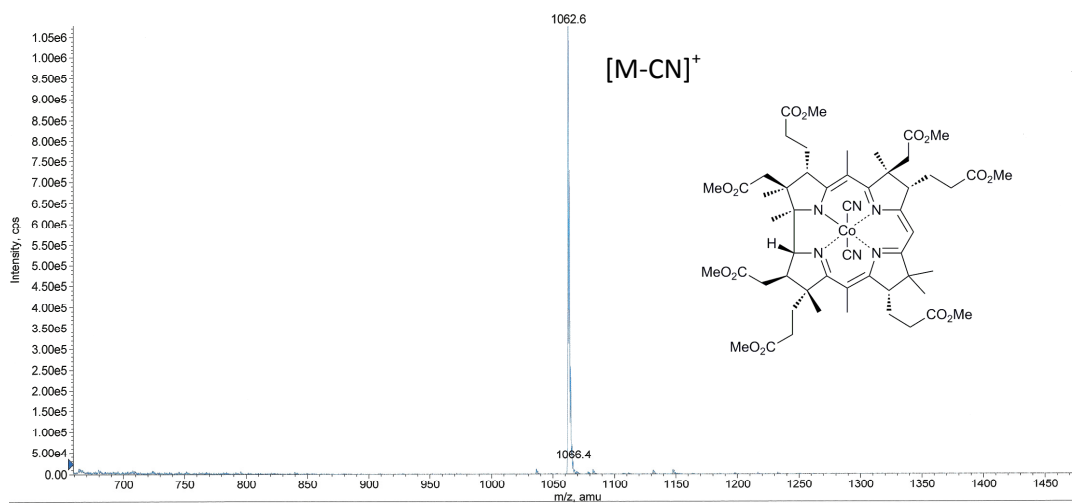


(CN)₂Cby(OMe)₇ MALDI

Matrix: α -cyano-4-hydroxycinnamic acid



(CN)₂Cby(OMe)₇ ESI



3. Elemental Analysis

It is common for many analogues to coordinate water molecules, which must be included in the calculated values for elemental analysis.

4. References

ⁱ Świder, P. Ph. D. Thesis, *Institute of Organic Chemistry PAS*, 2012.