

A Bio-Guided Screening for Antioxidant, Anti-Inflammatory and Hypolipidemic Potential Supported by Non-Targeted Metabolomic Analysis of *Crepis* spp.

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Keywords: *Crepis*; Asteraceae; LC-MS; NMR; cichoric acid; phenolic acid; biological activity; mouse paw edema; antihyperlipidemic

Supplementary Materials

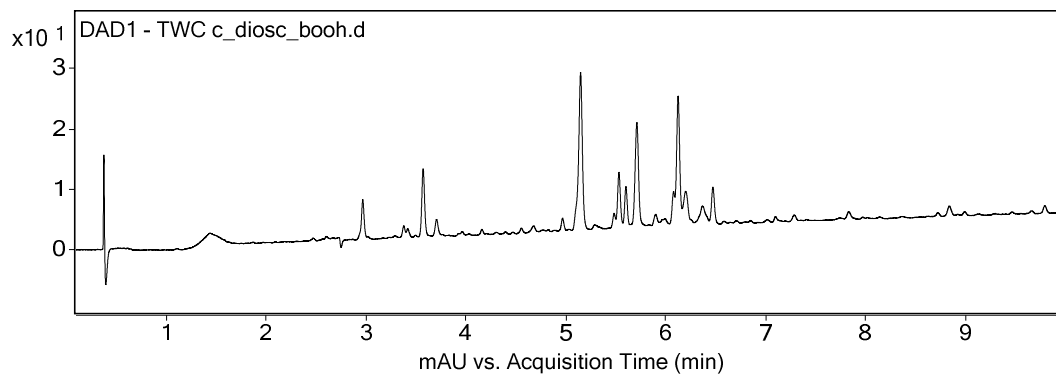
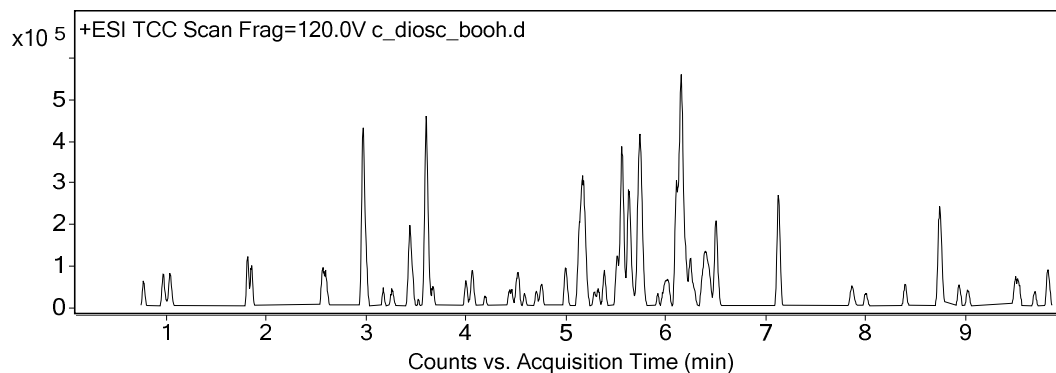
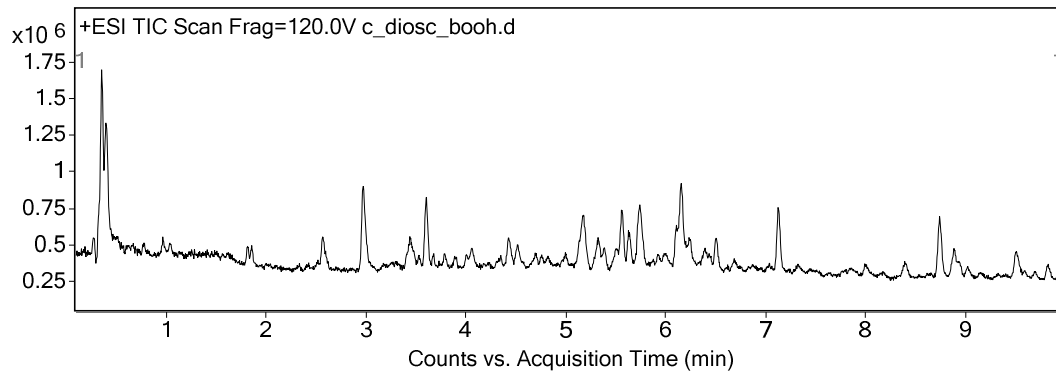
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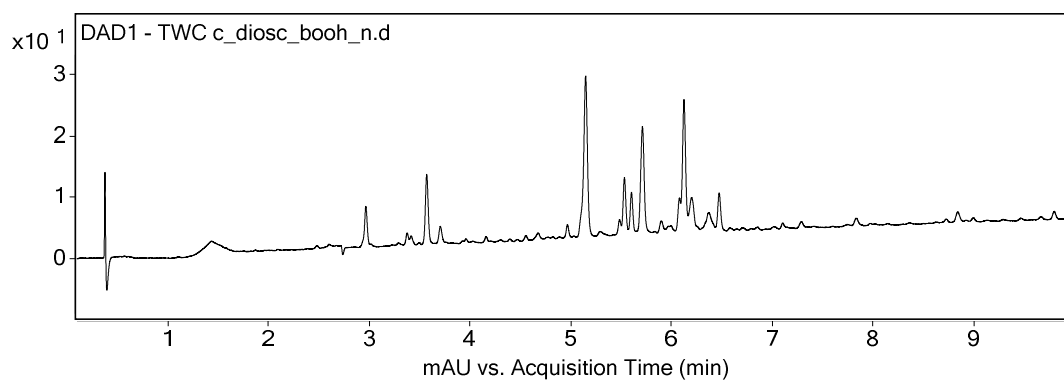
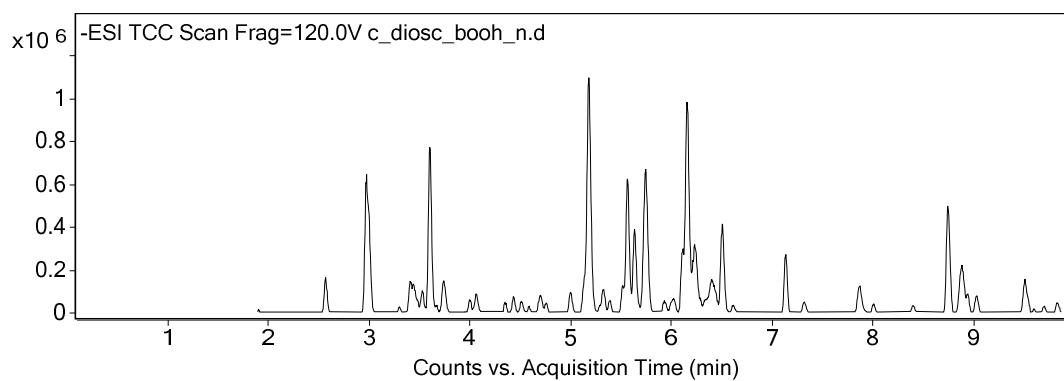
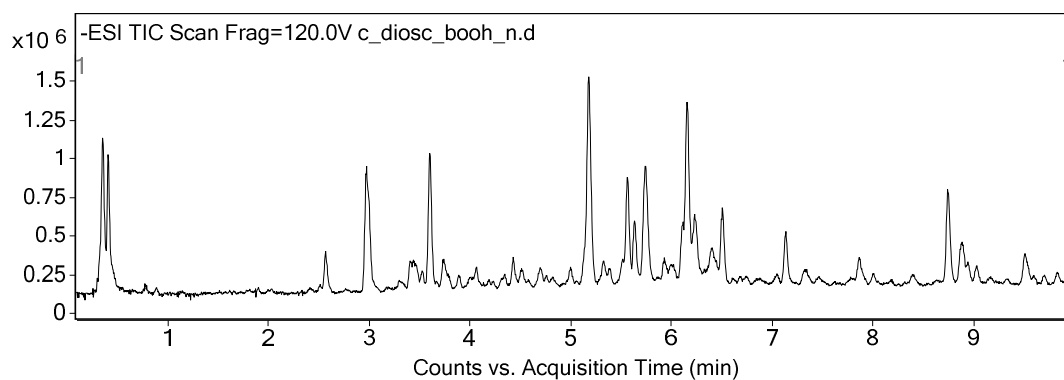
S1. LC-MS

S1.1 LC-ESI-MS of BuOH extract of *Crepis dioscoridis* in positive (A) and negative ion (B) modes.

A. LC-MS ESI+

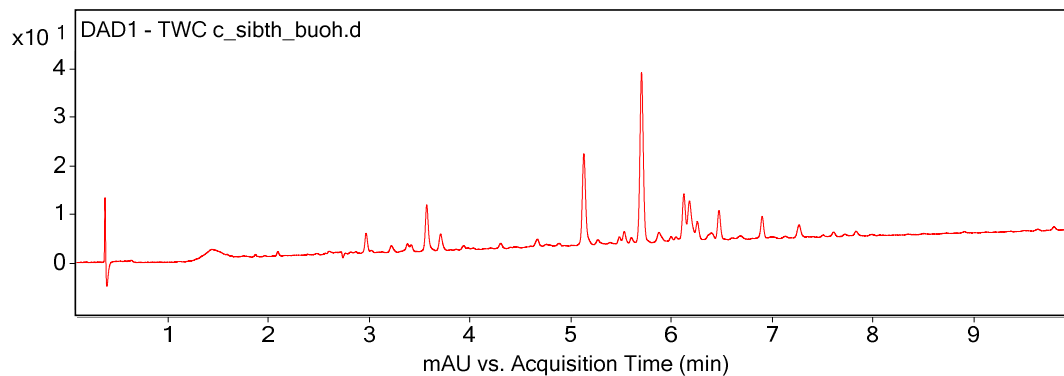
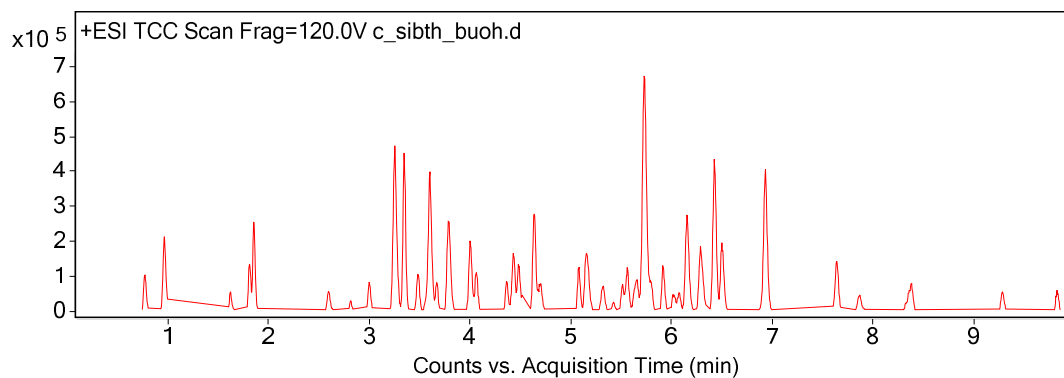
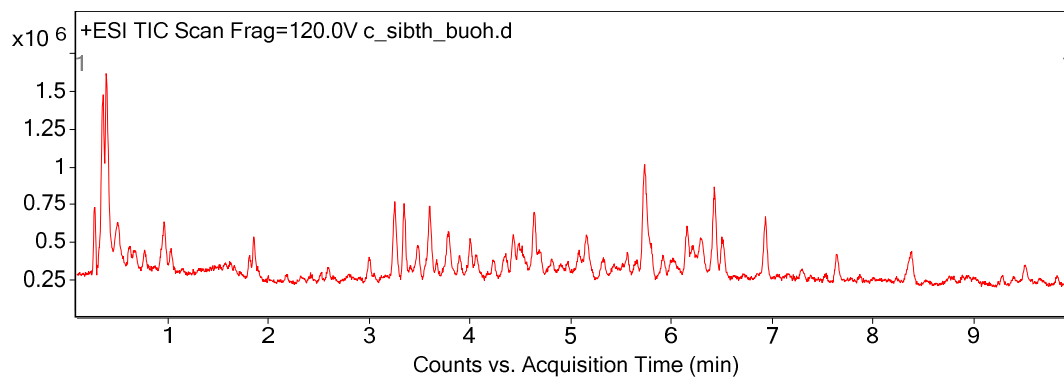


B. LC-MS ESI-

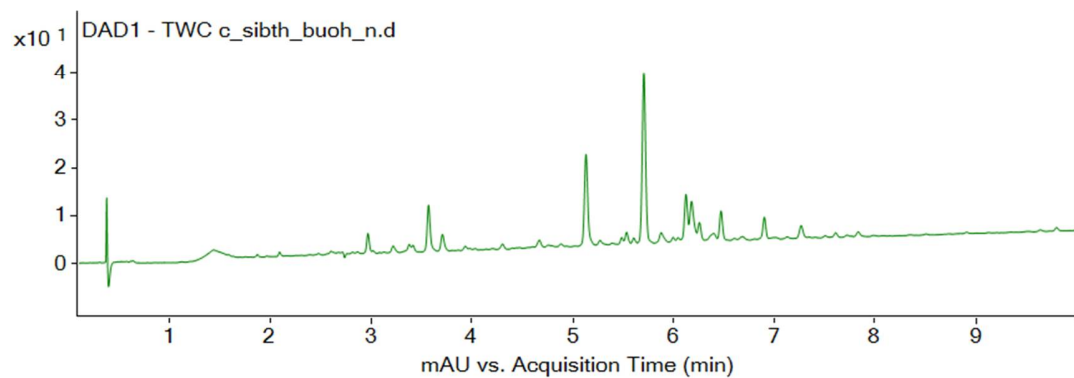
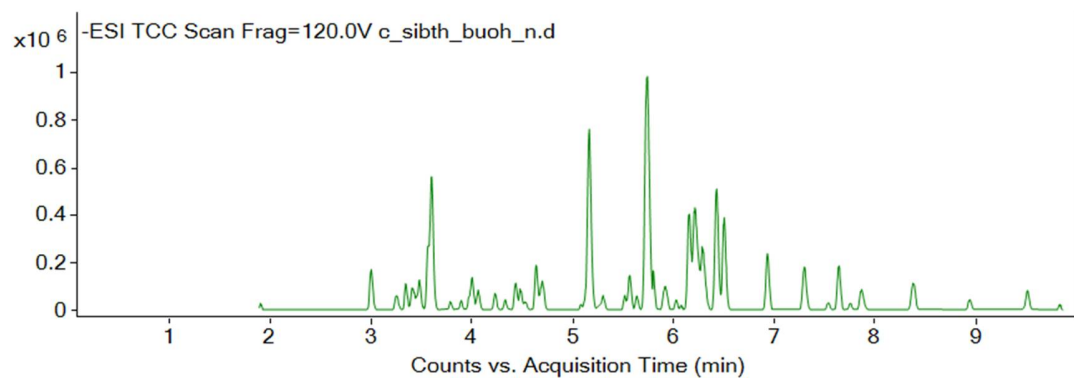
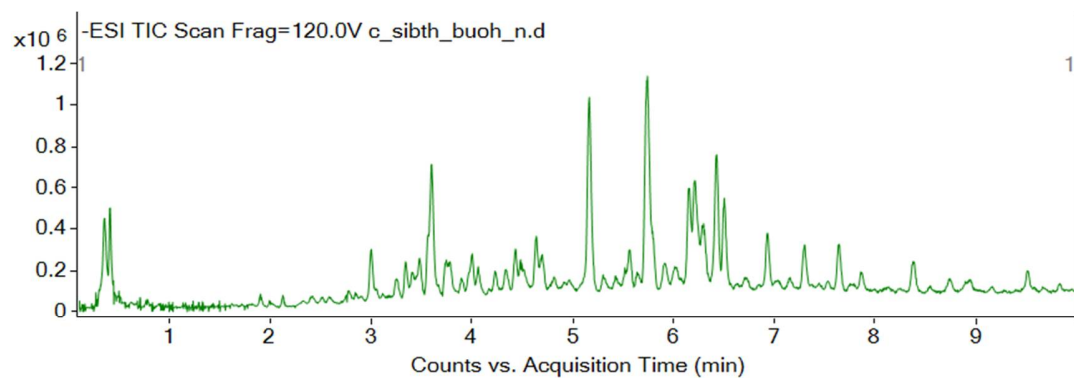


S1.2 LC-ESI-MS of BuOH extract of *Crepis sibthorpiana* in positive (A) and negative ion (B) modes.

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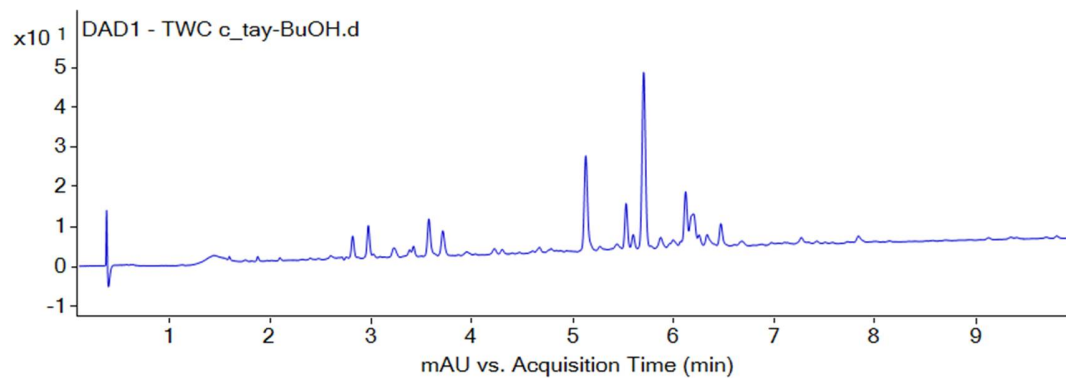
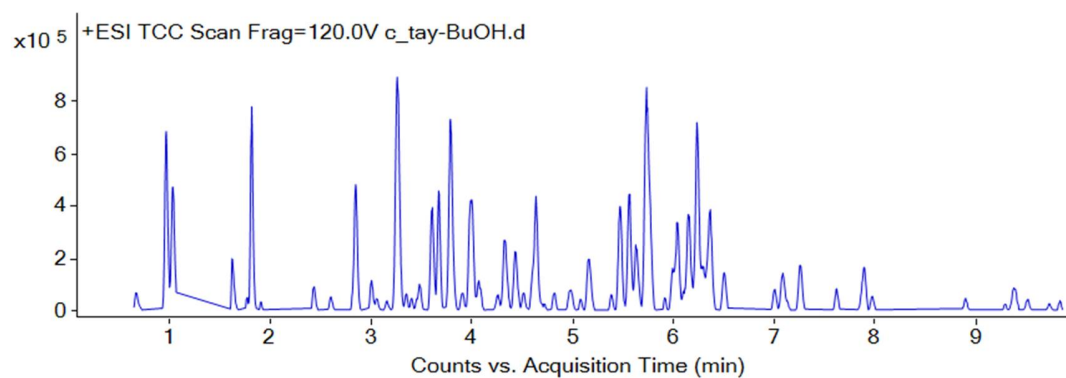
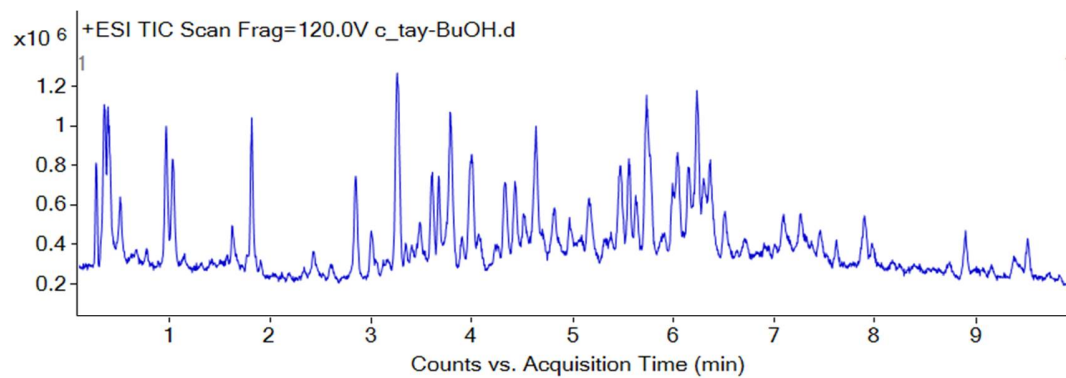


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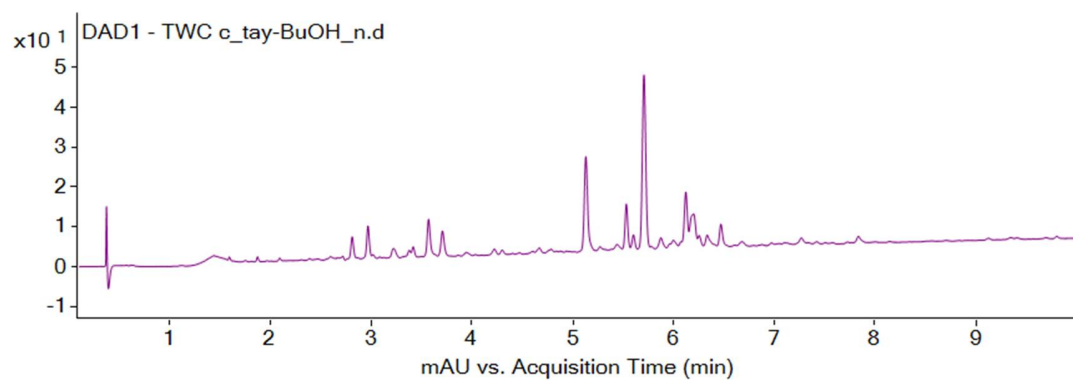
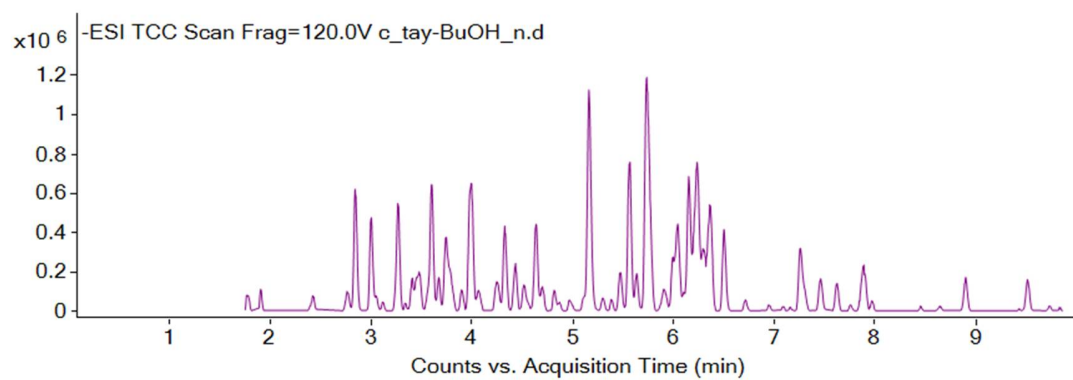
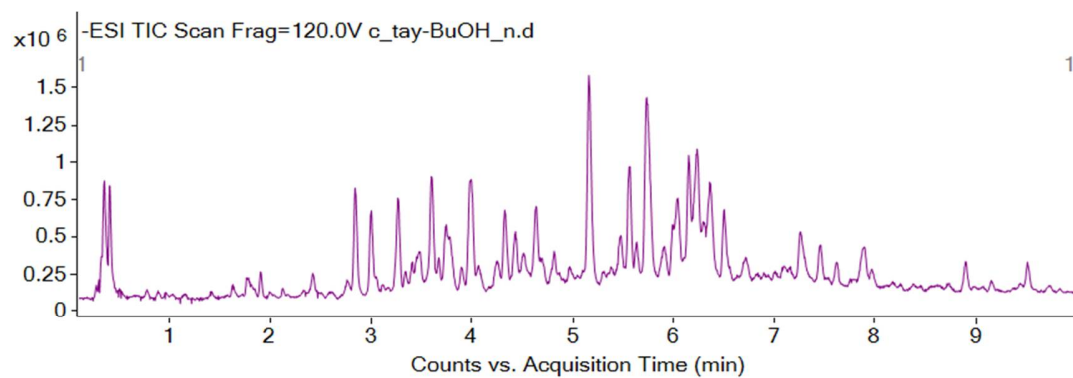


S1.3 LC-ESI-MS of BuOH extract of *Crepis heldreichiana* in positive (A) and negative ion (B) modes.

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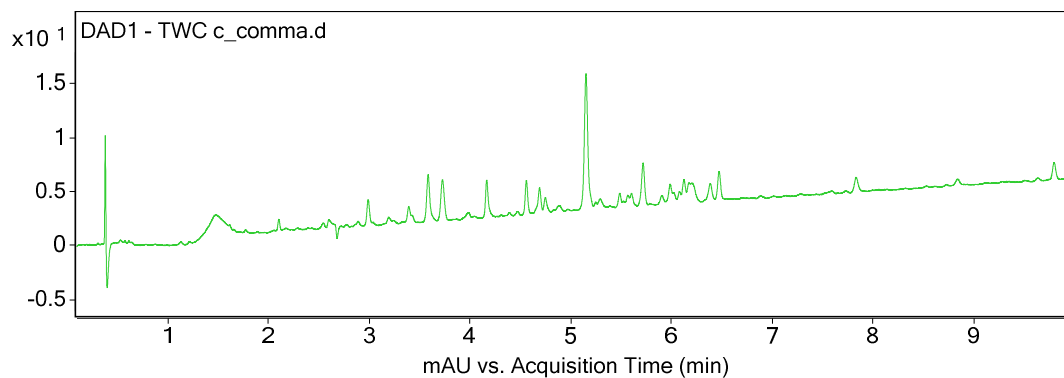
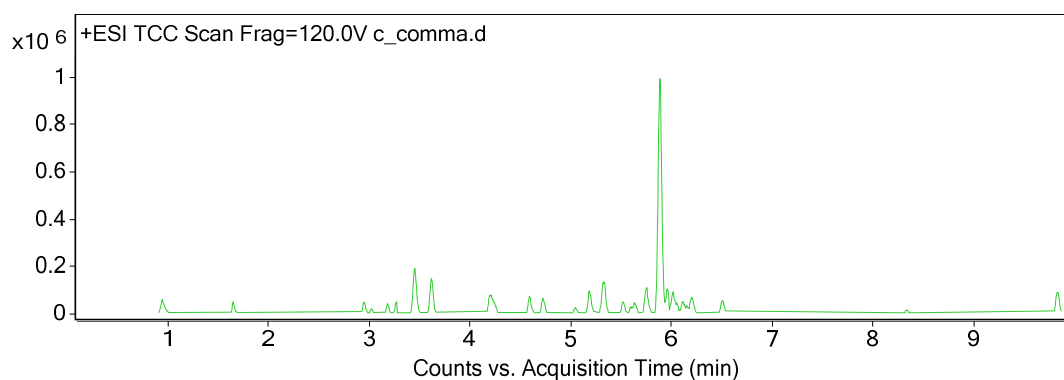
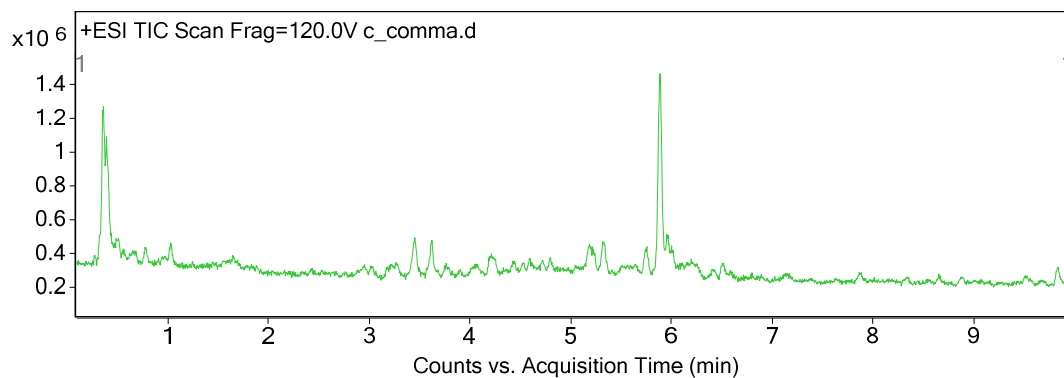


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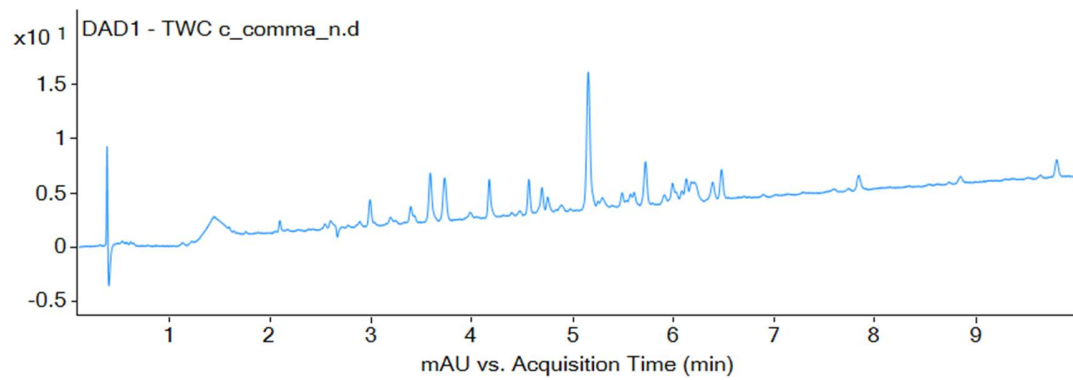
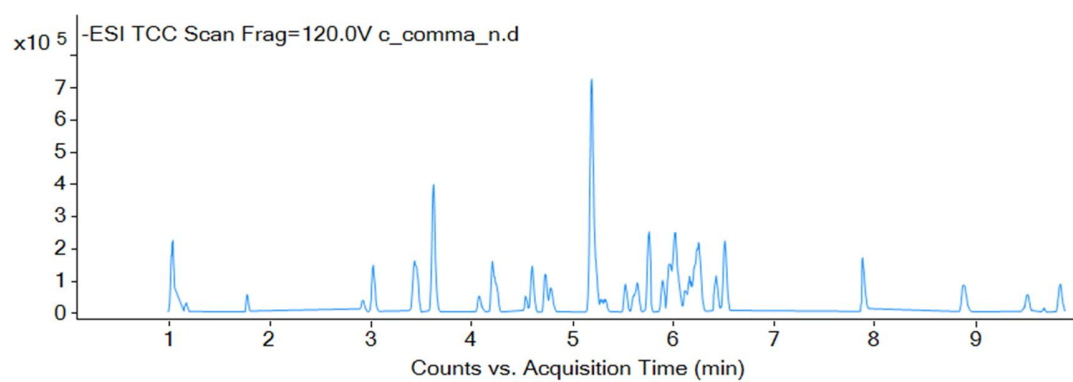
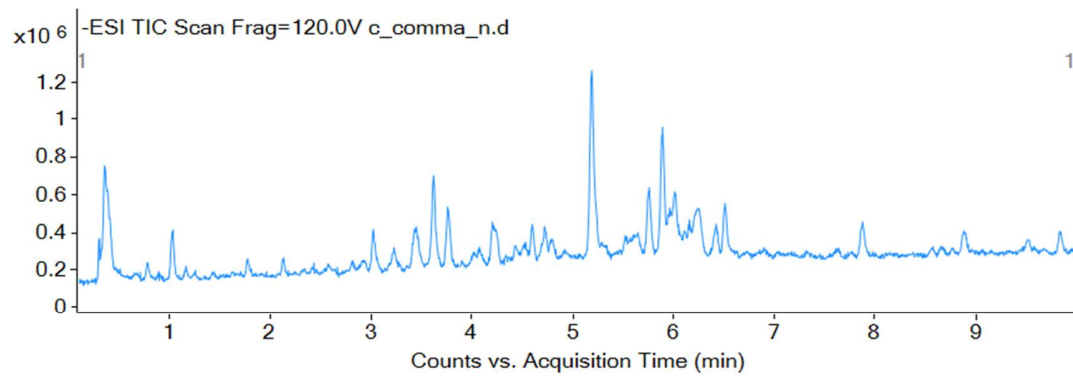


S1.4 LC-ESI-MS of BuOH extract of *Crepis commutata* in positive (A) and negative ion (B) modes.

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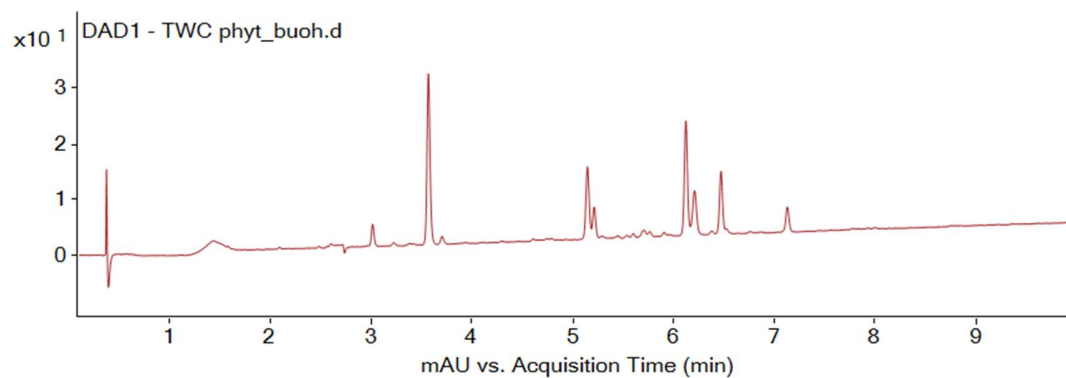
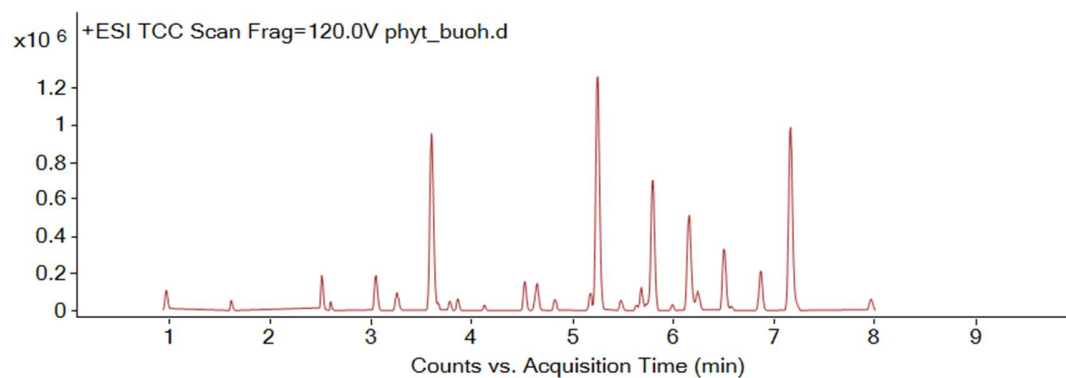
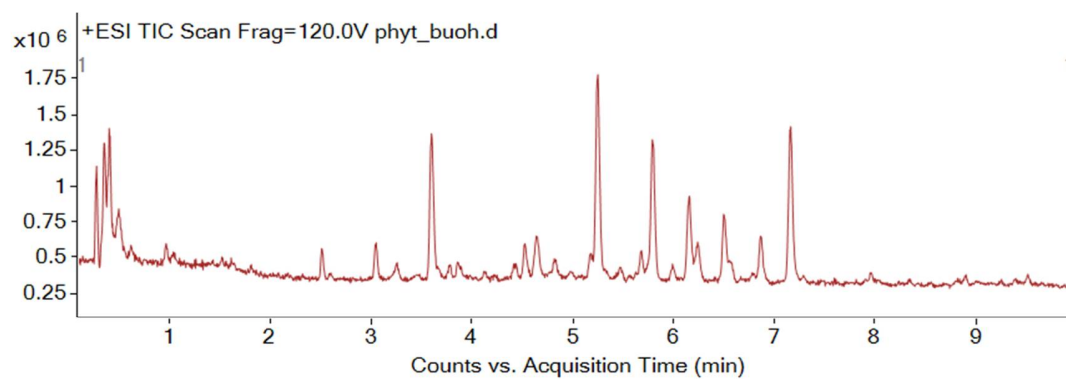


B. LC-MS ESI-

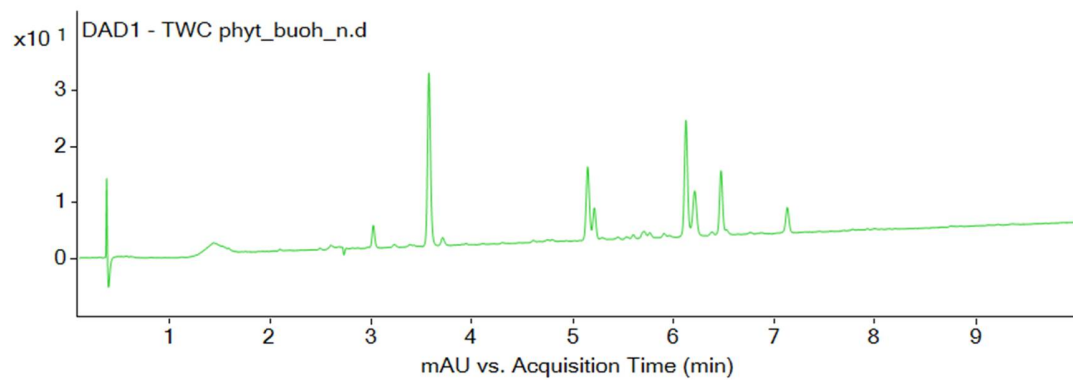
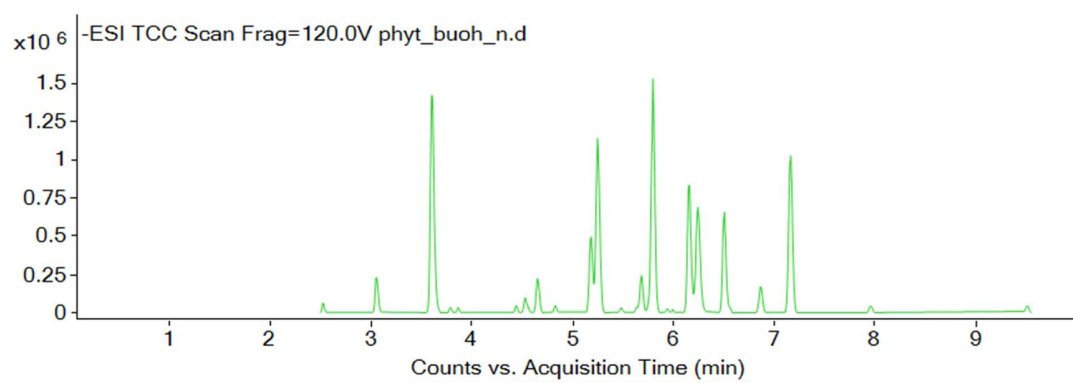
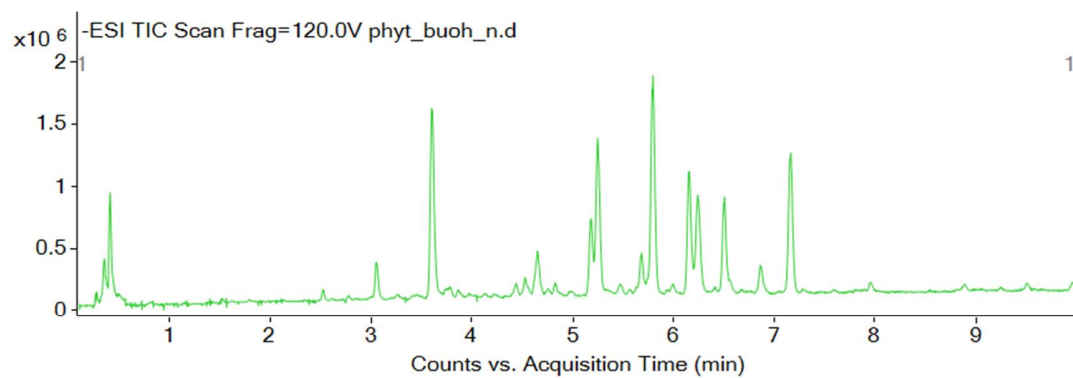


S1.5 LC-ESI-MS of BuOH extract of *Phytosia crocifolia* in positive (A) and negative ion (B) modes.

A. LC-MS ESI+

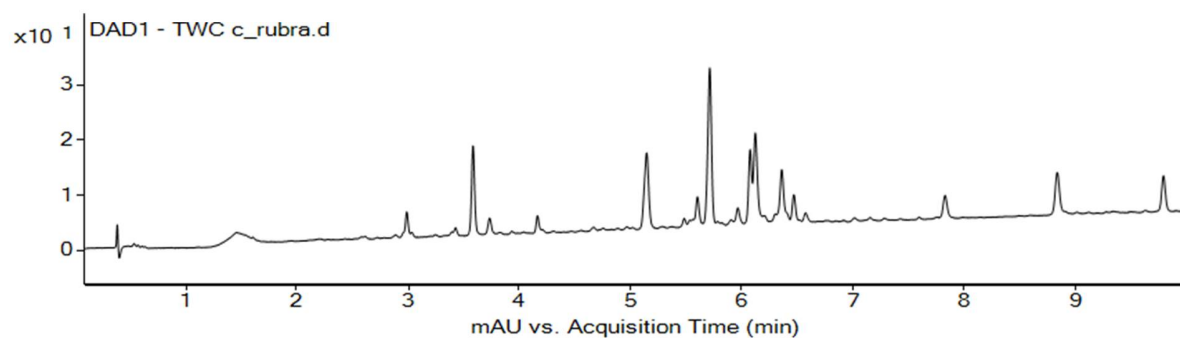
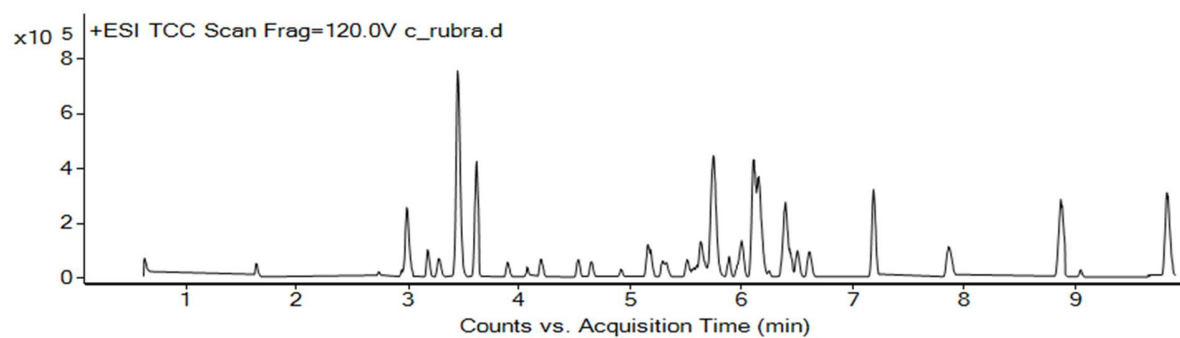
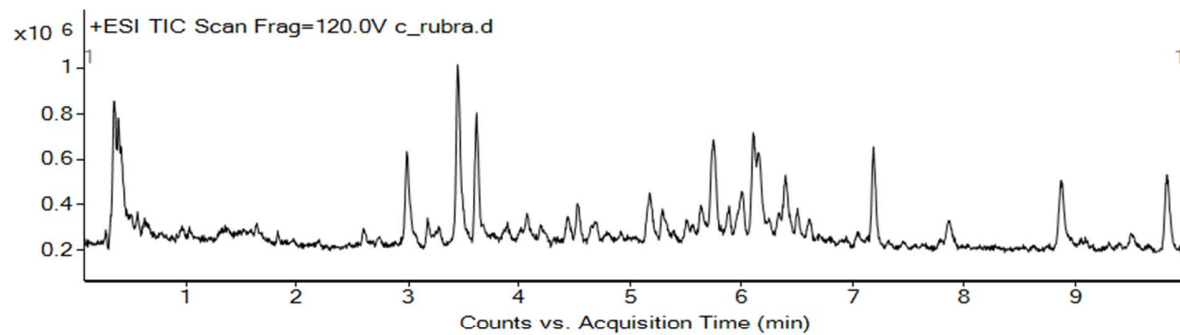


B. LC-MS ESI-

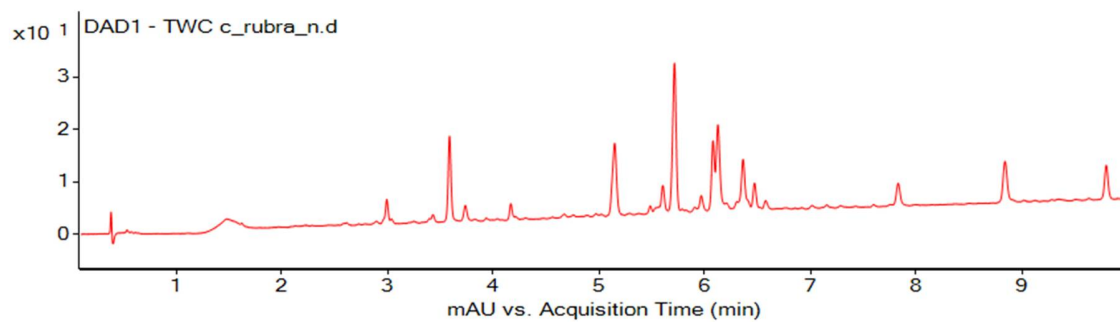
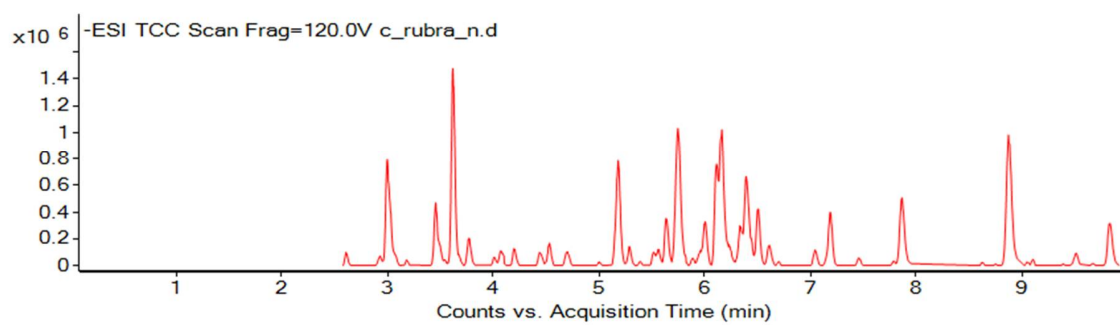
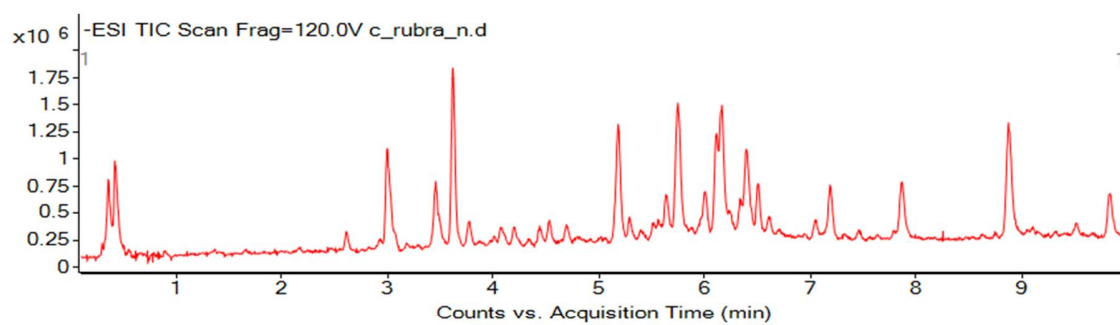


S1.6 LC-ESI-MS of BuOH extract of *Crepis rubra* in positive (A) and negative ion (B) modes.

A. LC-MS ESI+

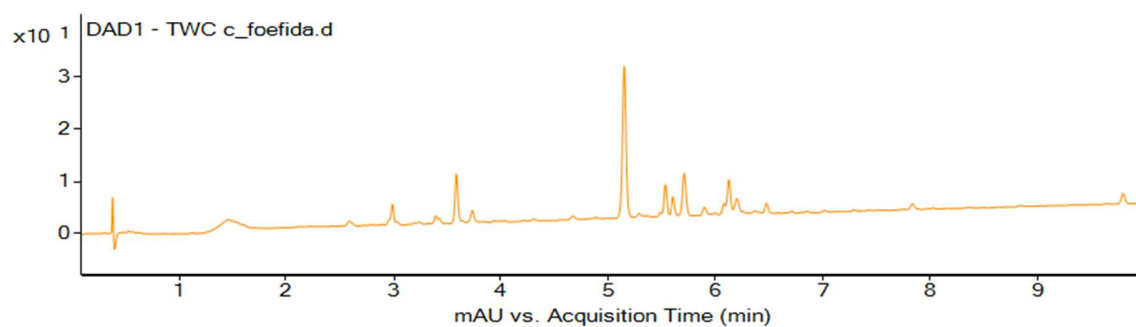
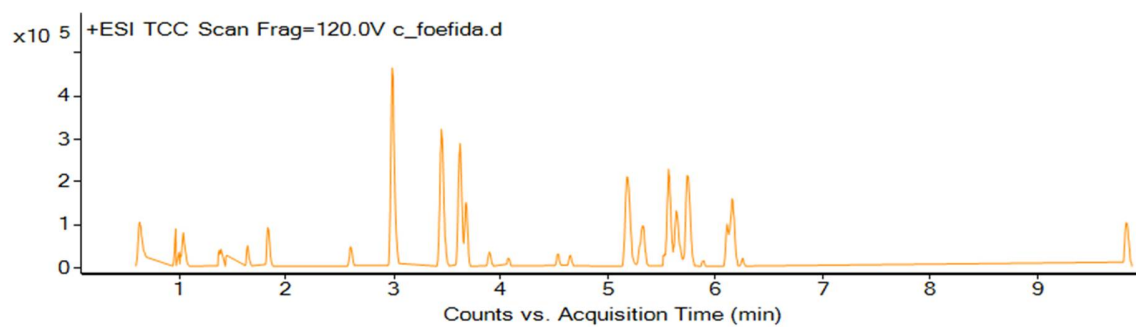
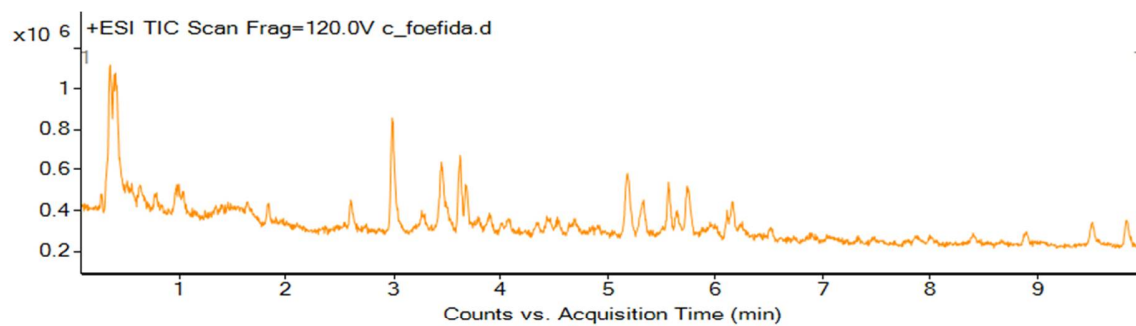


B. LC-MS ESI-

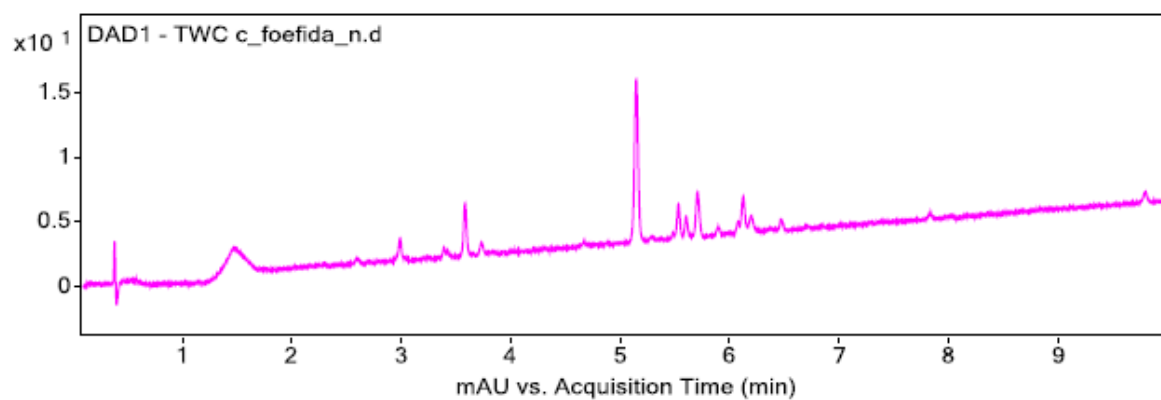
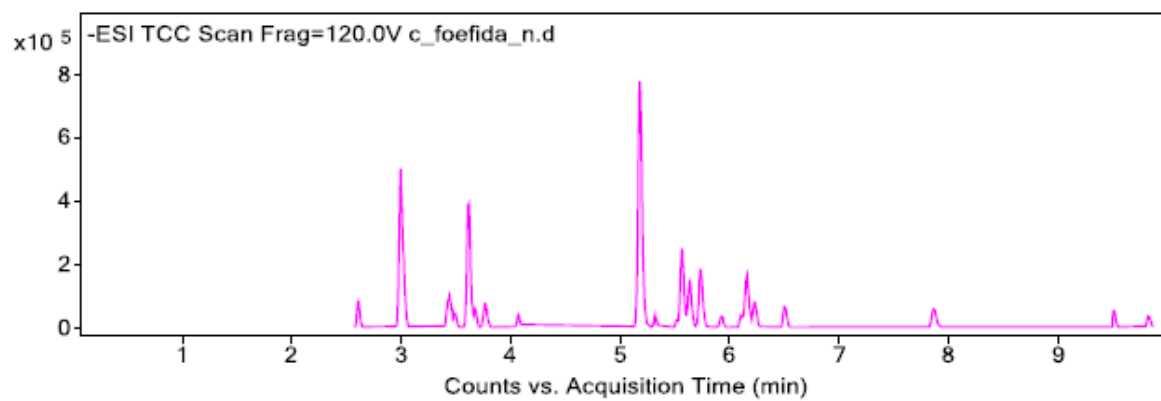
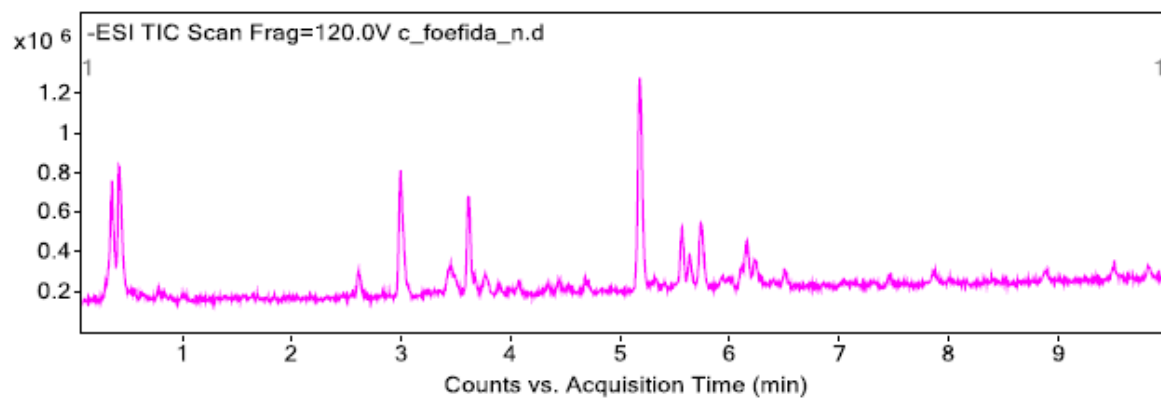


S1.7 LC-ESI-MS of BuOH extract of *Crepis foetida* in positive (A) and negative ion (B) modes.

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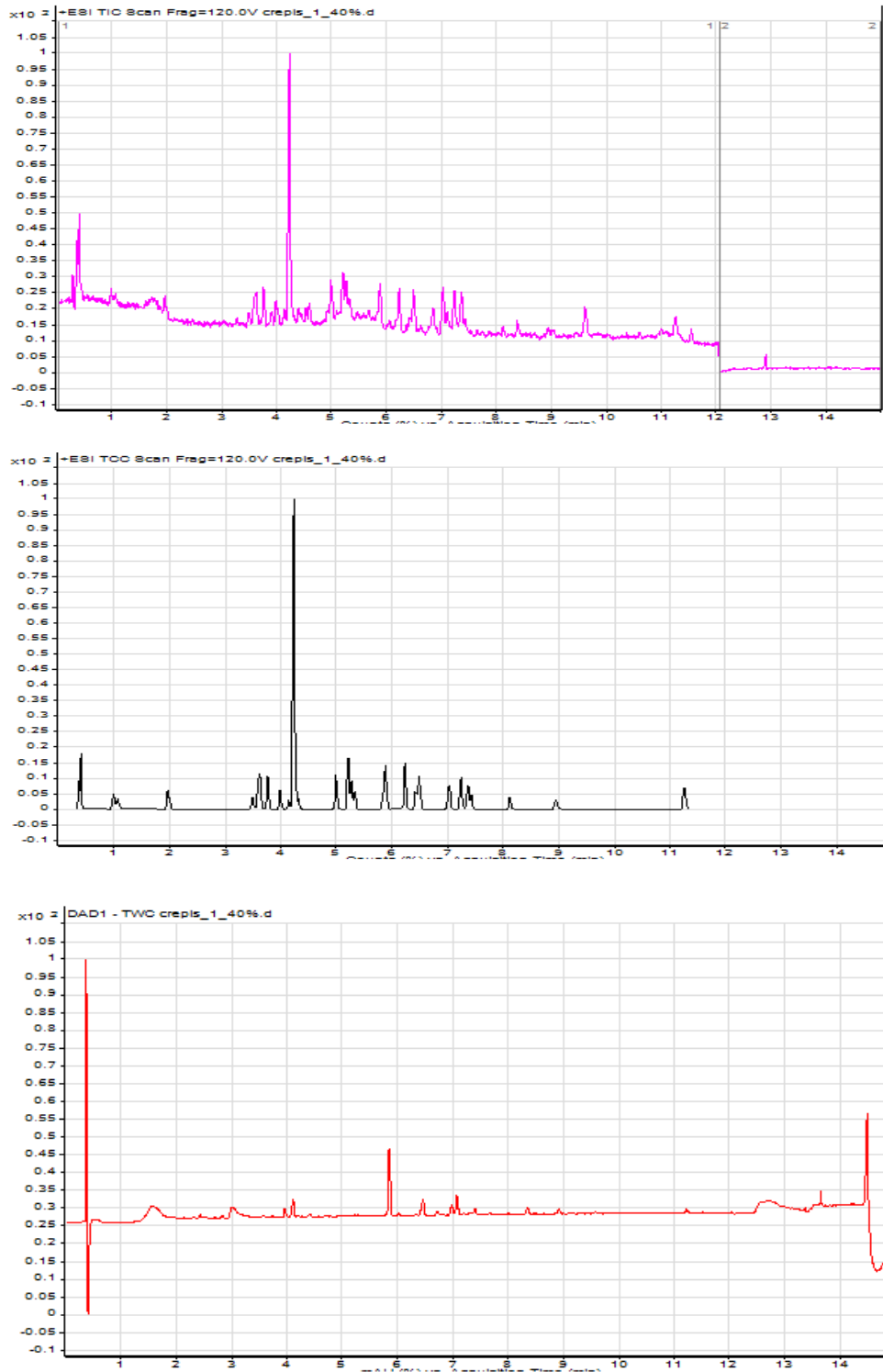


B. LC-MS ESI-

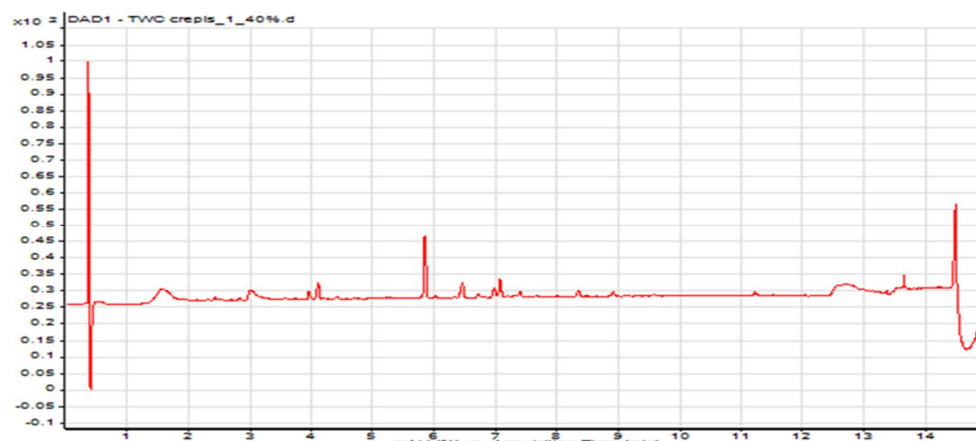
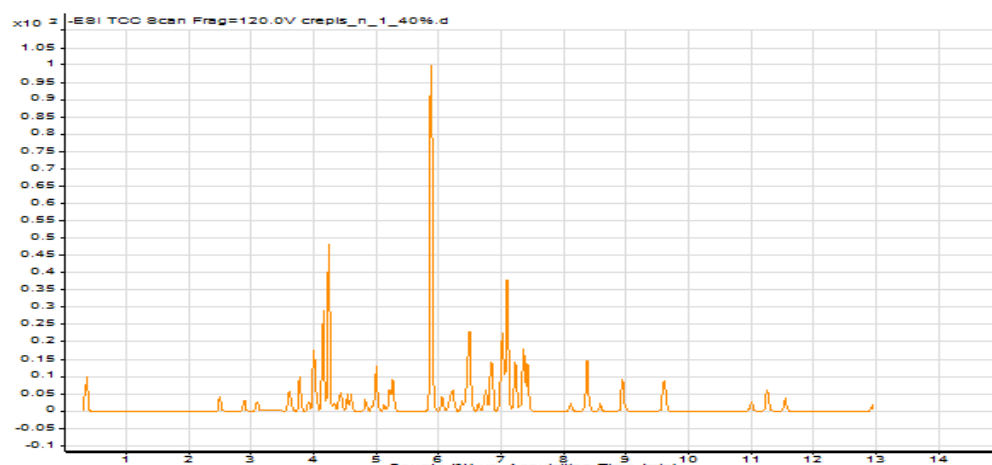
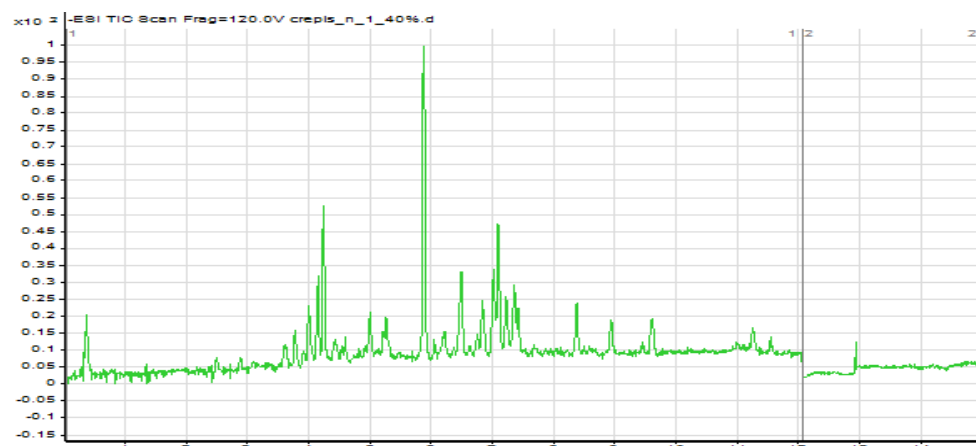


S1.8 LC-ESI-MS of BuOH extract of *Crepis incana* in positive (A) and negative ion (B) modes.

A. LC-MS ESI+



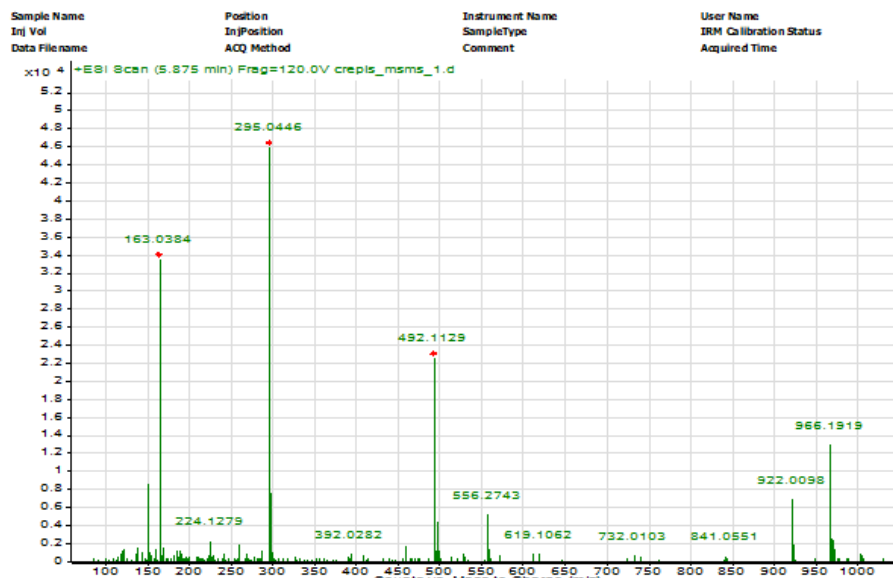
B. LC-MS ESI-



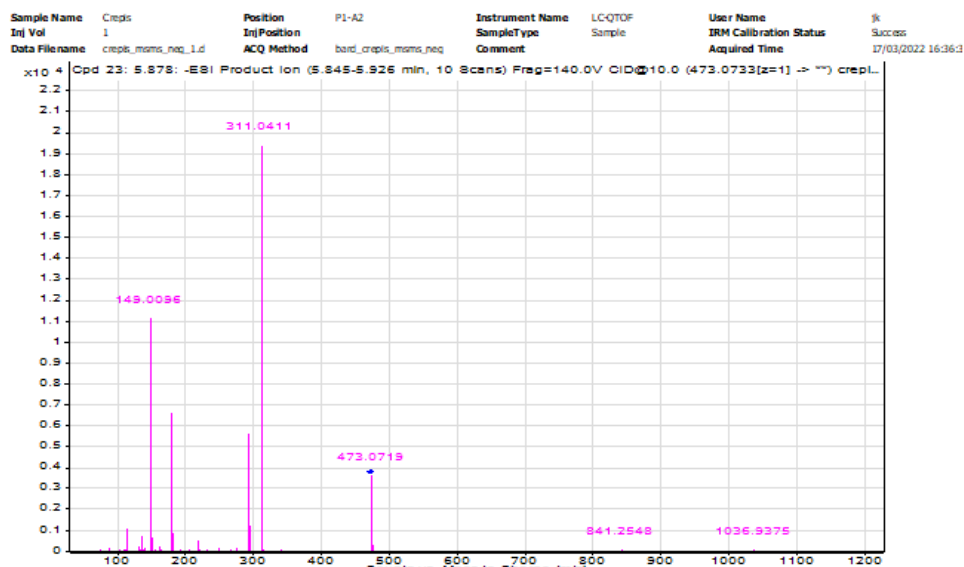
S.2 MS-MS spectrum of selected compounds in positive (A) and/or negative (B) ion mode

S.2.1 MS-MS spectrum of cichoric acid

A.

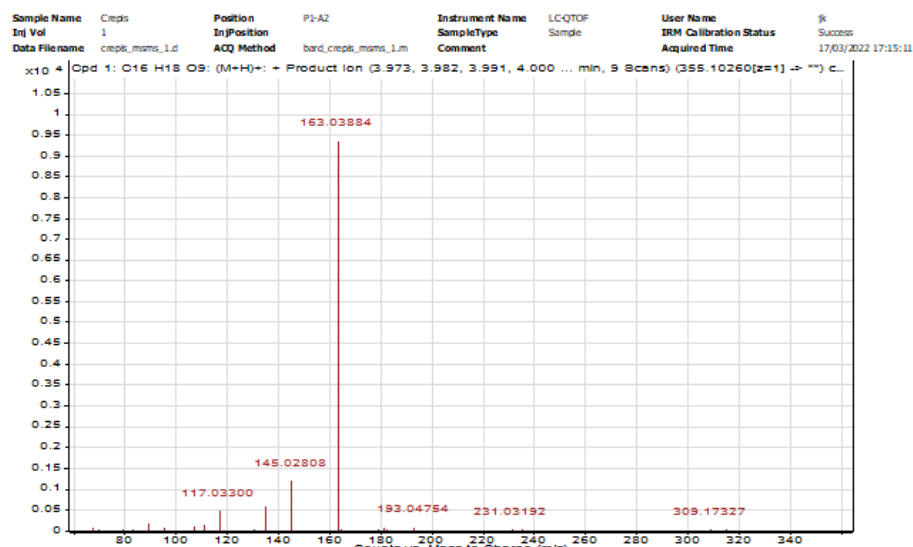


B.

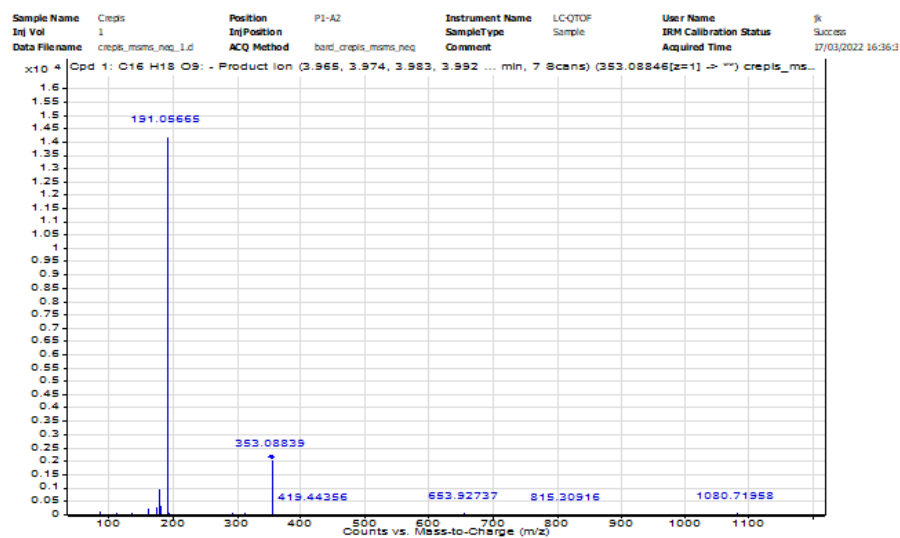


S.2.2 MS-MS spectrum of chlorogenic acid isomer

A.

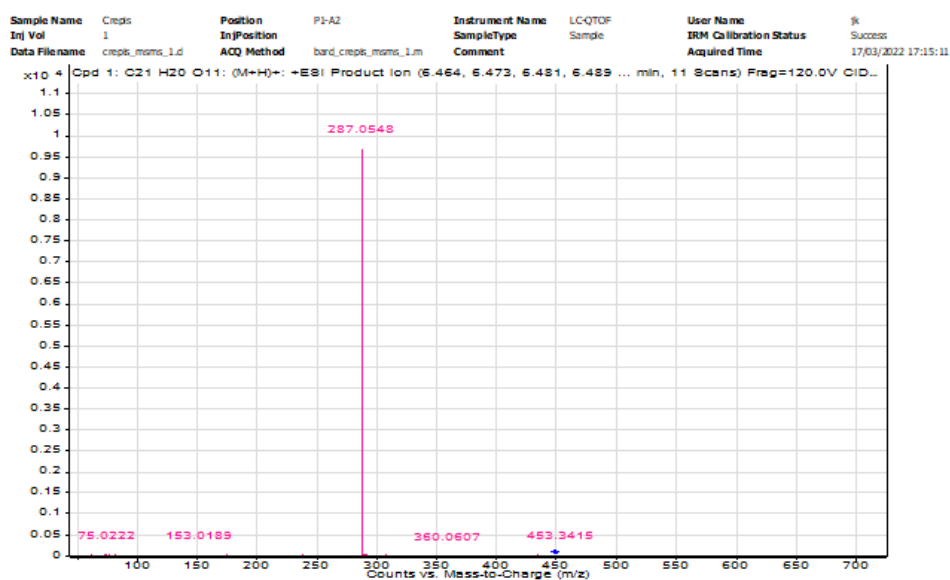


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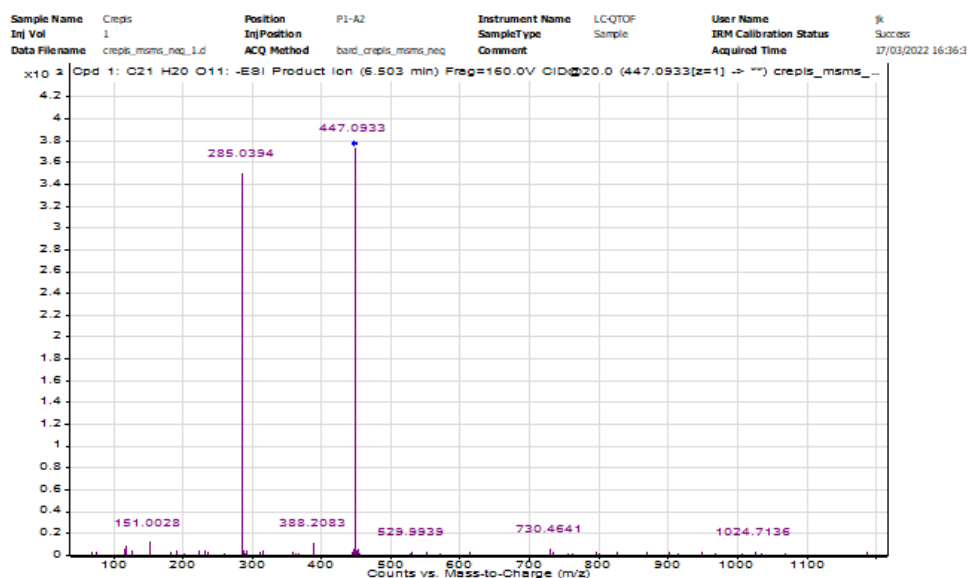


S.2.3 MS-MS spectrum of luteolin 7-glucoside (Cynaroside)

A.

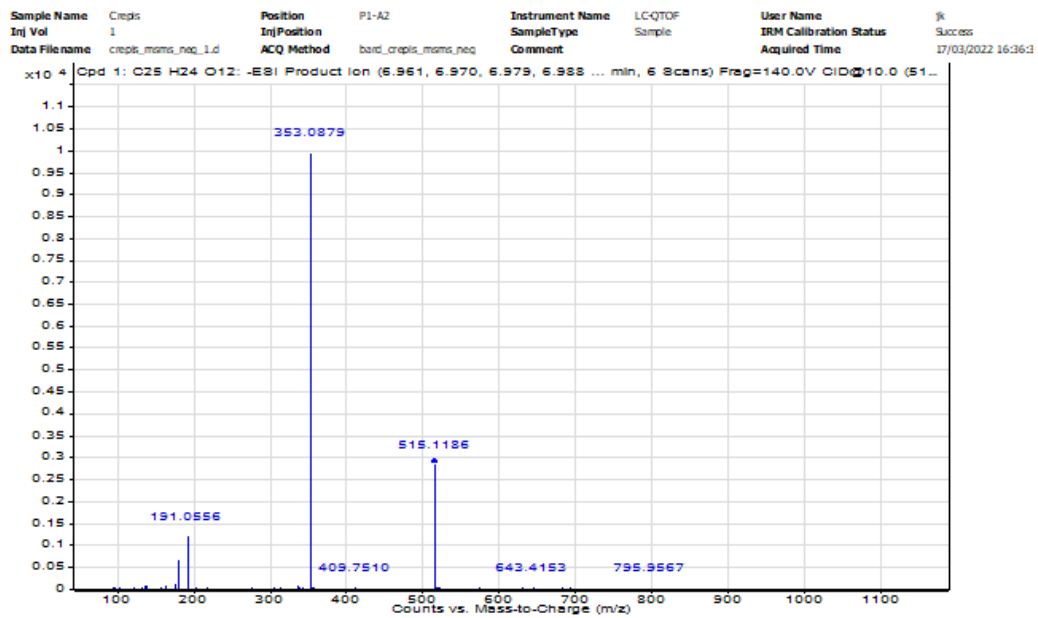


B.



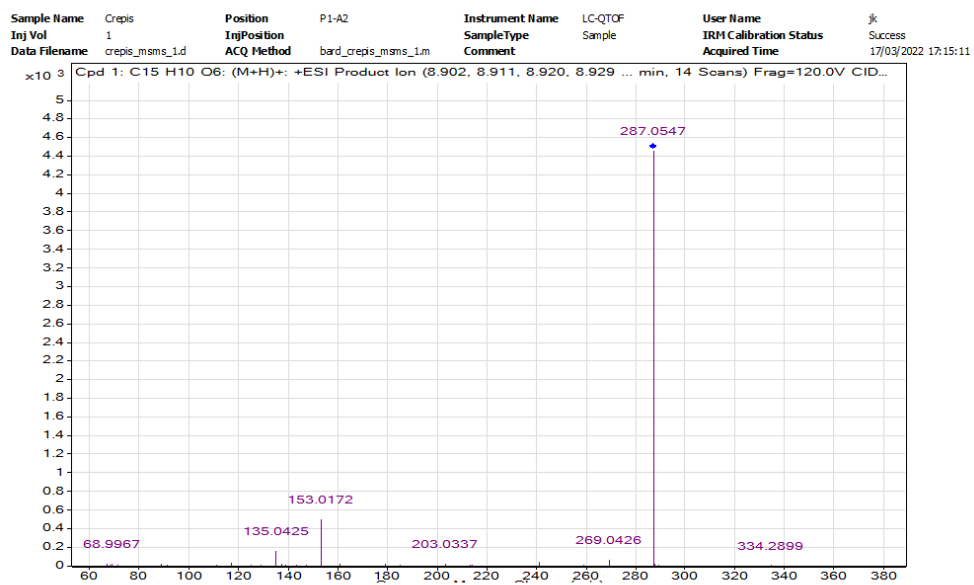
S.2.4 MS-MS spectrum of Di-caffeoylquinic acid isomer

B.

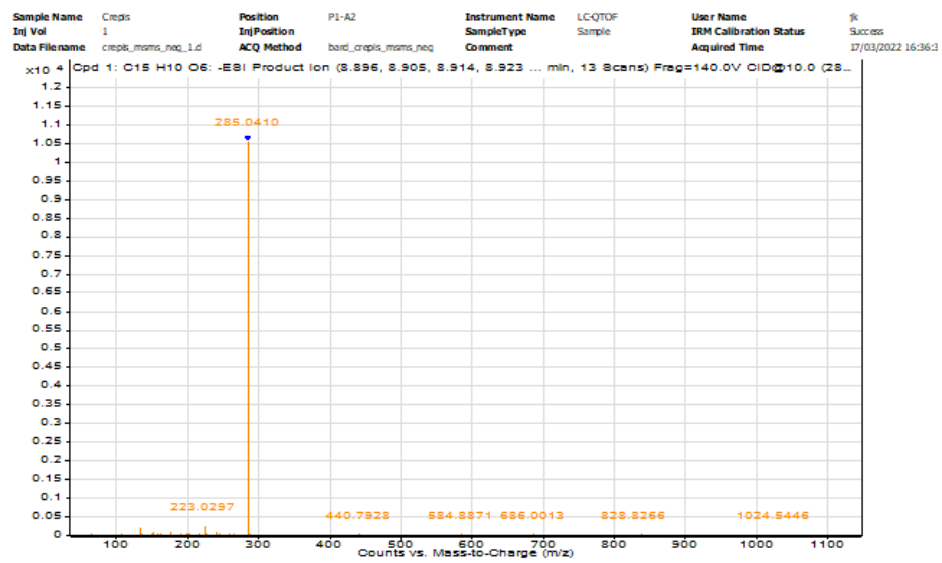


S.2.5 MS-MS spectrum of luteolin

A.

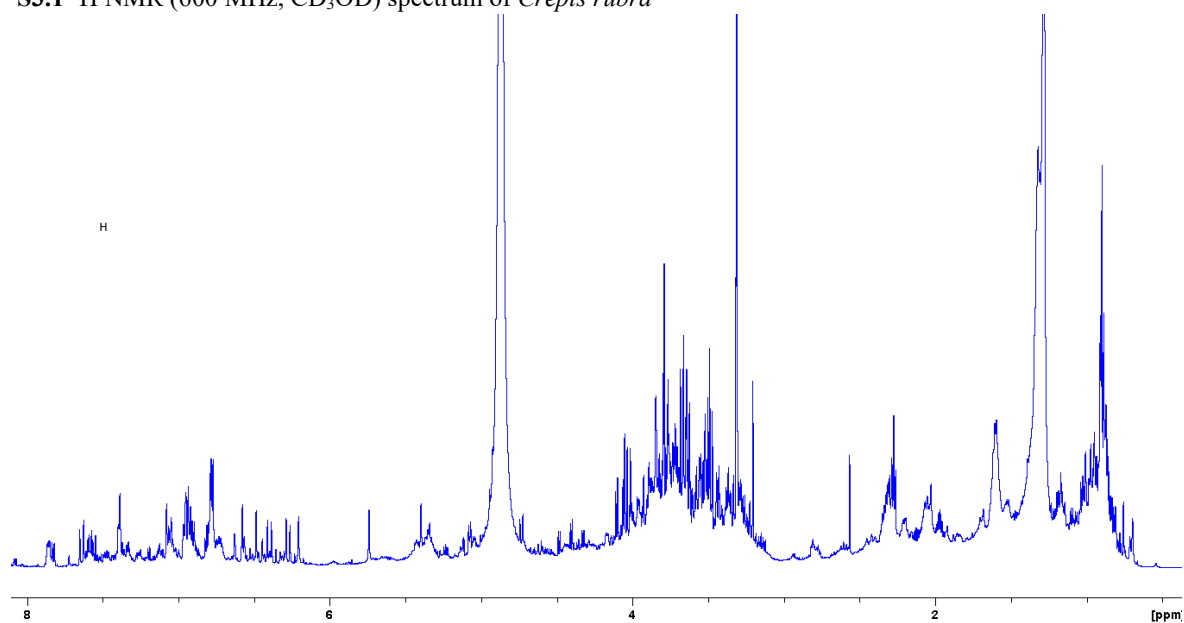


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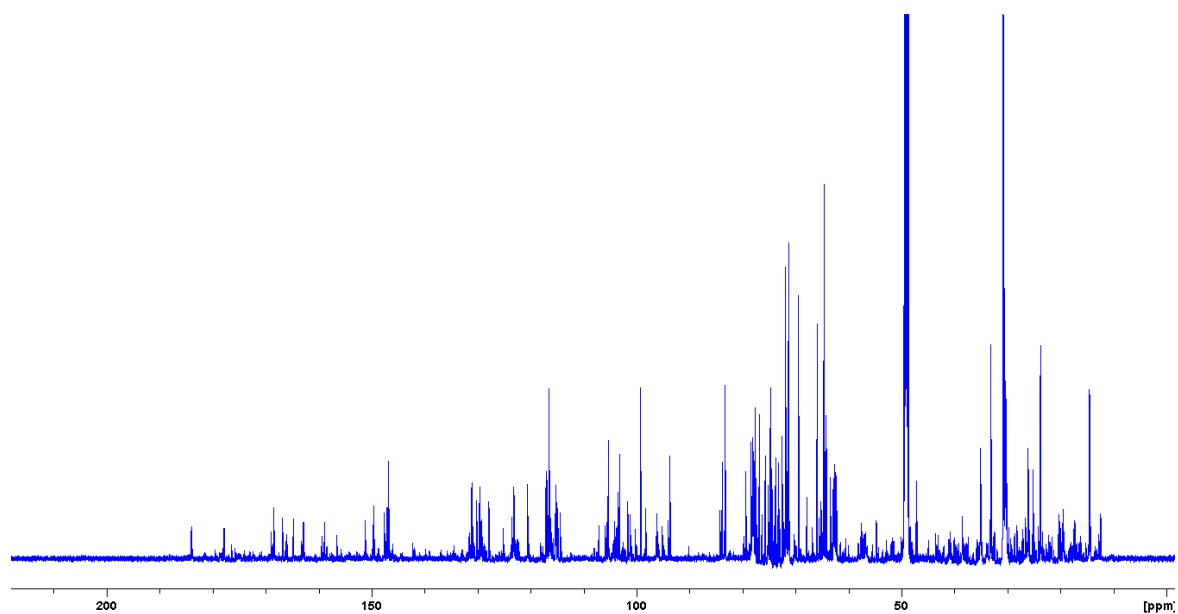


S3. NMR data

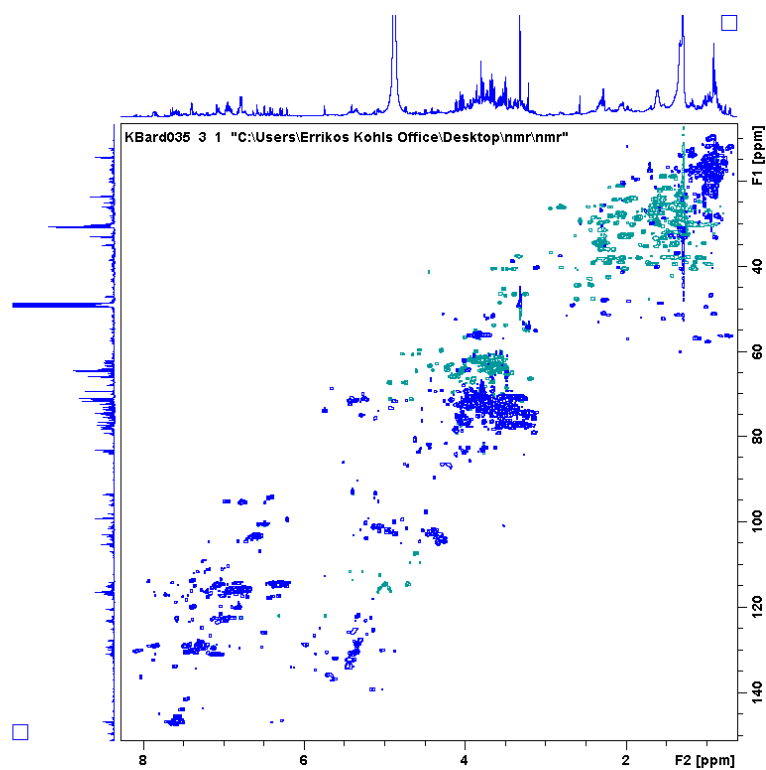
S3.1 ^1H NMR (600 MHz, CD_3OD) spectrum of *Crepis rubra*



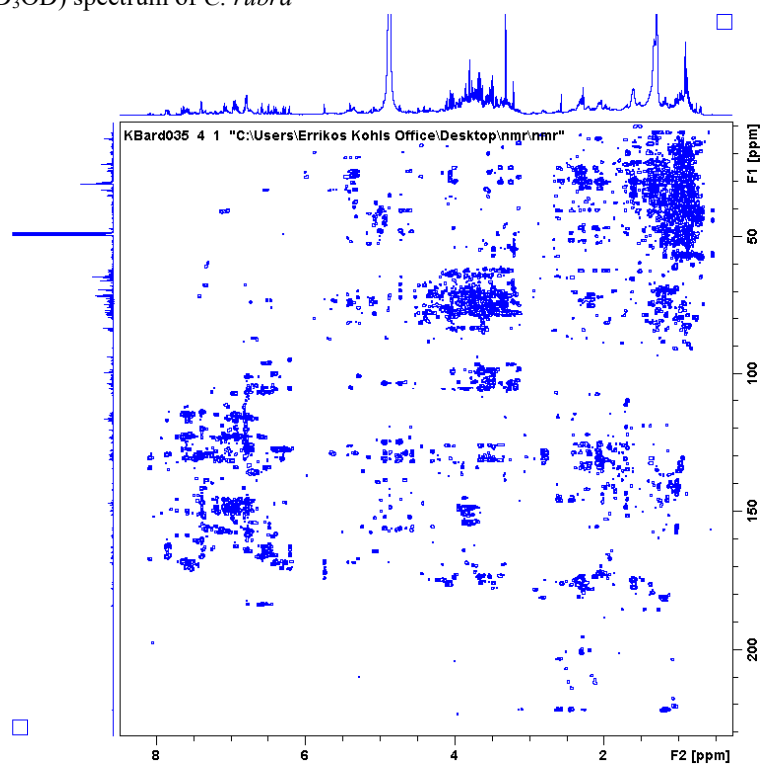
S3.2 ^{13}C NMR (150 MHz, CD_3OD) spectrum of *C. rubra*



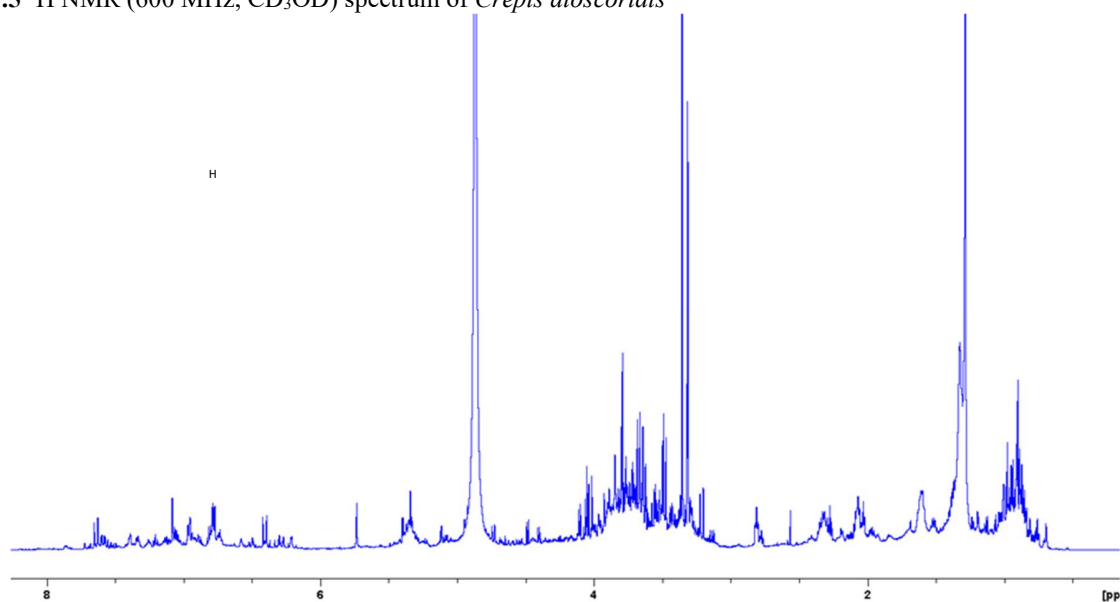
S3.3 HSQC (CD₃OD) spectrum of *C. rubra*



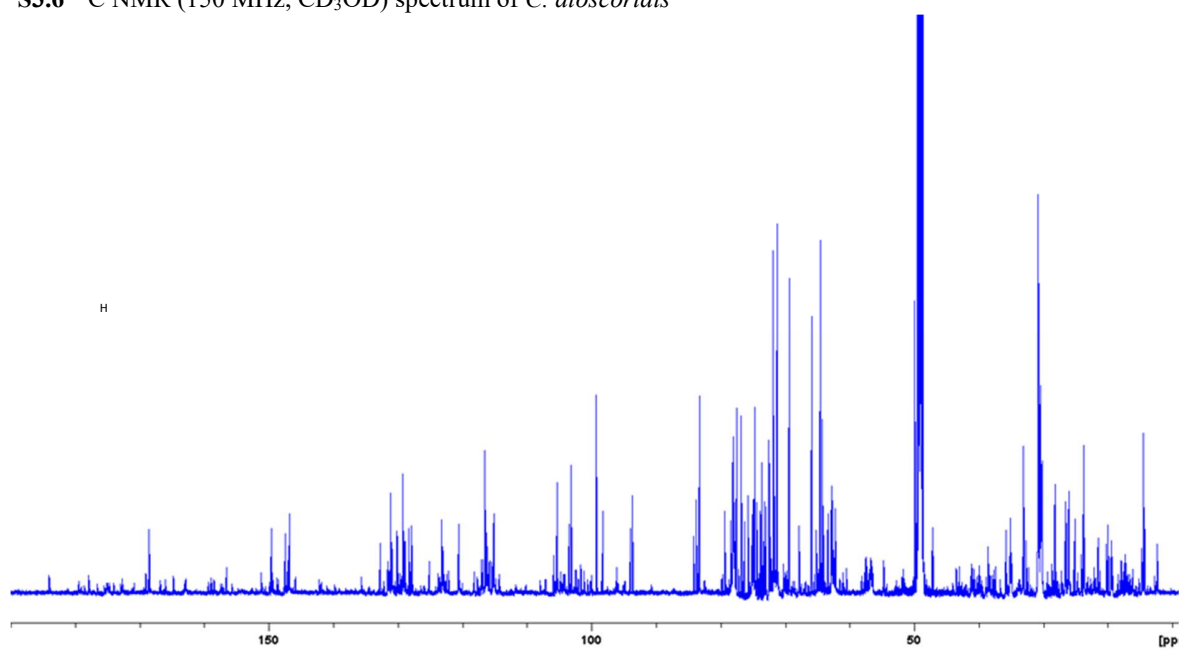
S3.4 HMBC (CD₃OD) spectrum of *C. rubra*



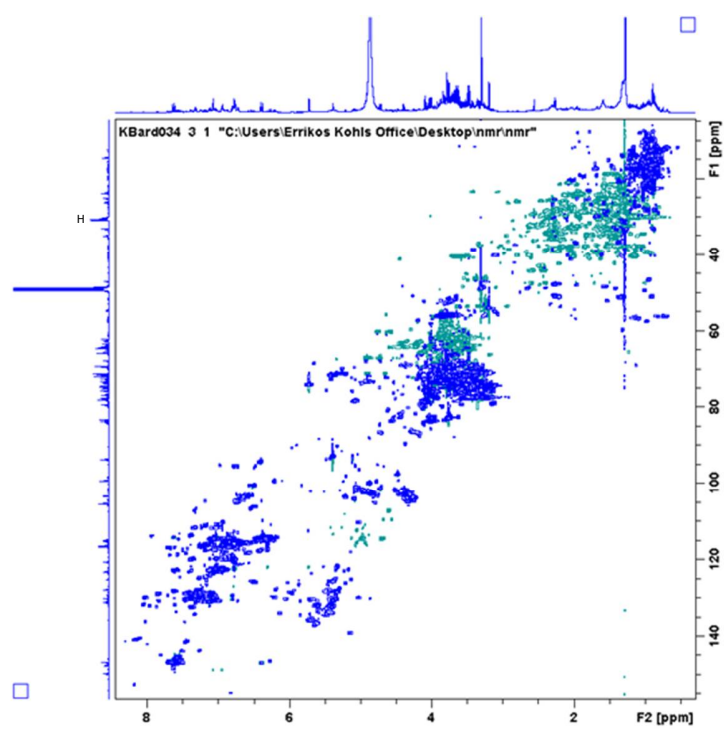
S3.5 ¹H NMR (600 MHz, CD₃OD) spectrum of *Crepis dioscoridis*



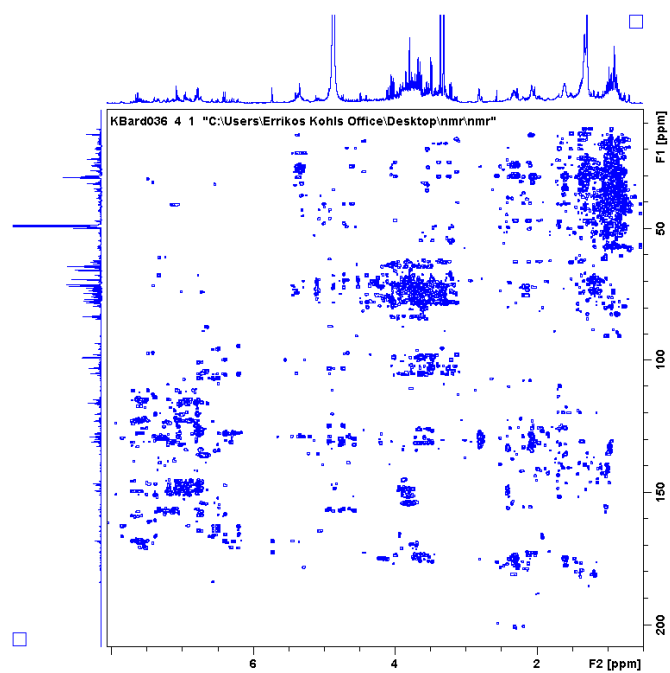
S3.6 ^{13}C NMR (150 MHz, CD_3OD) spectrum of *C. dioscoridis*



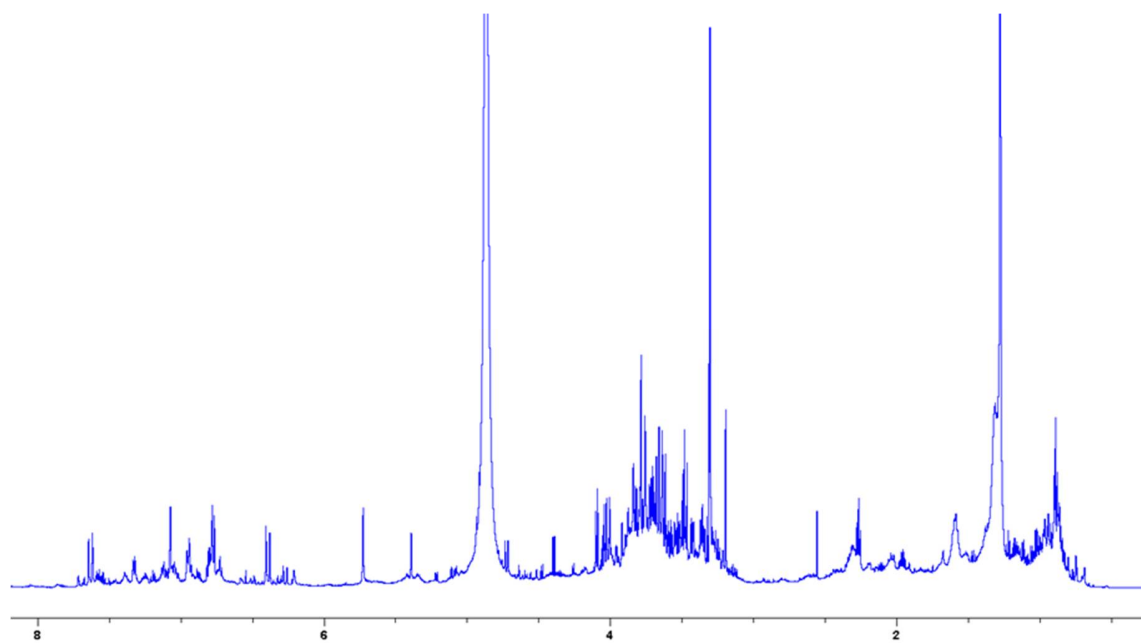
S3.7 HSQC (CD_3OD) spectrum of *C. dioscoridis*



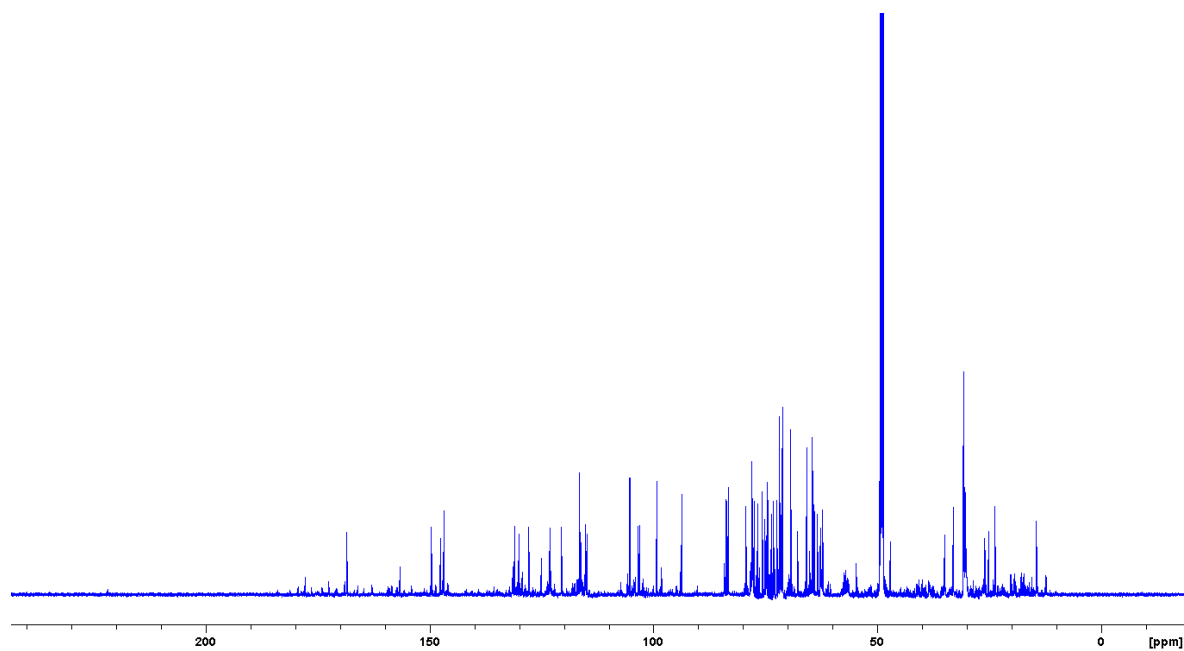
S3.8 HMBC (CD₃OD) spectrum of *C. dioscoridis*



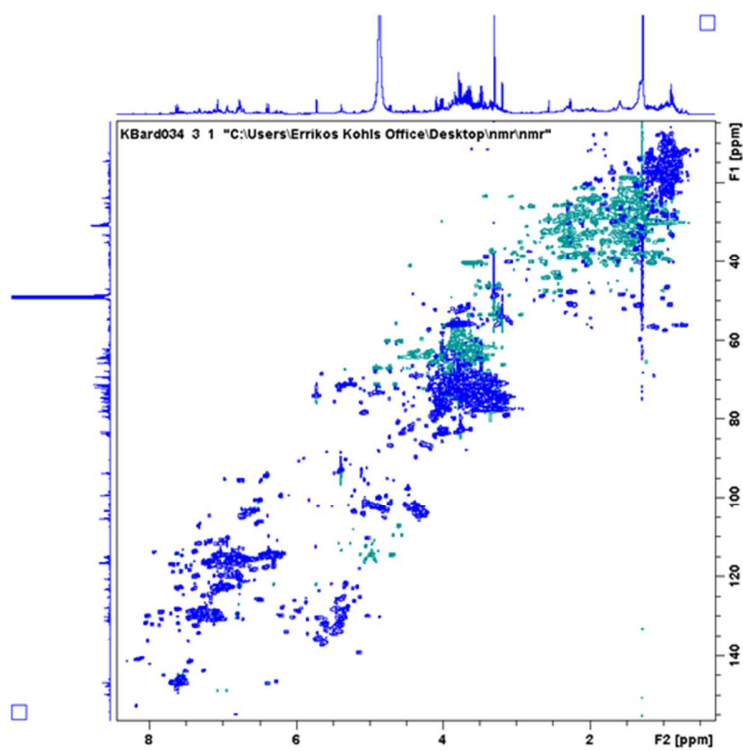
S3.9 ¹H NMR (600 MHz, CD₃OD) spectrum of *Crepis foetida*



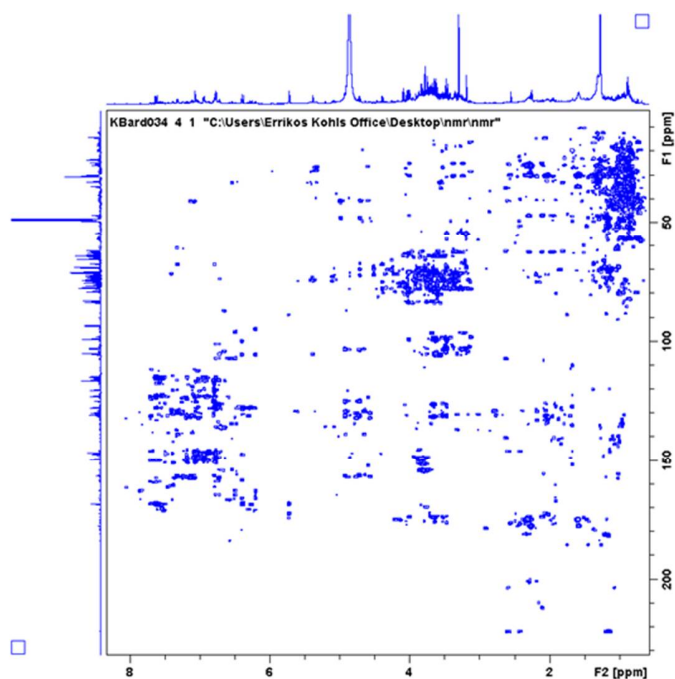
S3.10 ^{13}C (150 MHz, CD_3OD) spectrum of *C. foetida*



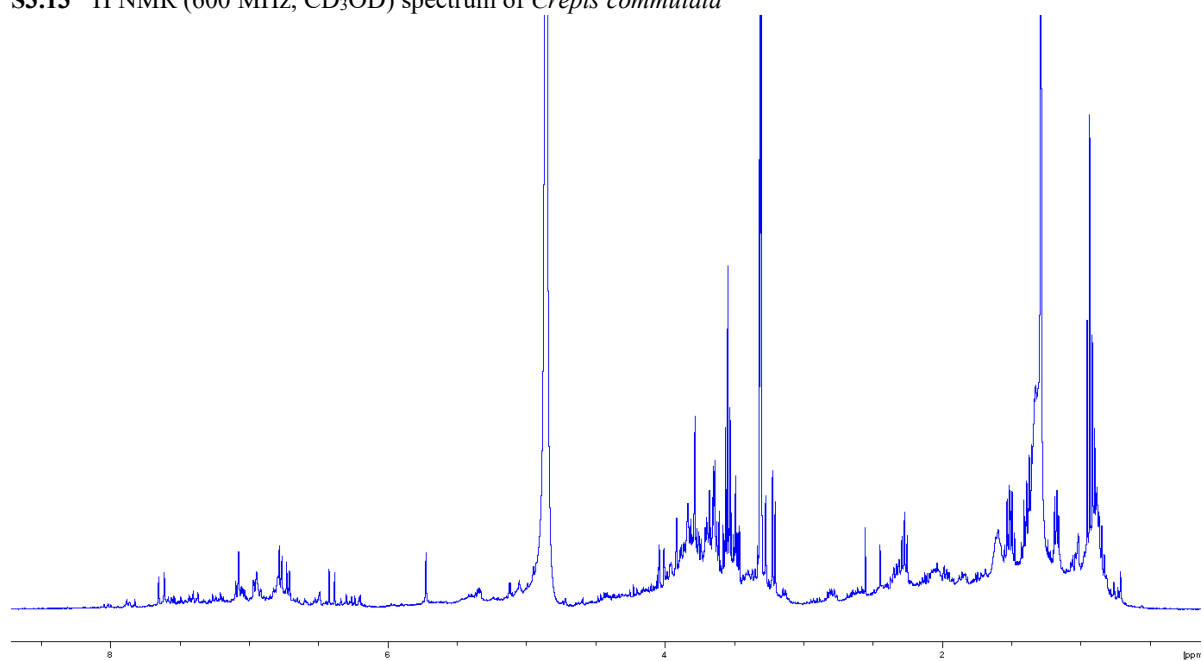
S3.11 HSQC (CD_3OD) spectrum of *C. foetida*



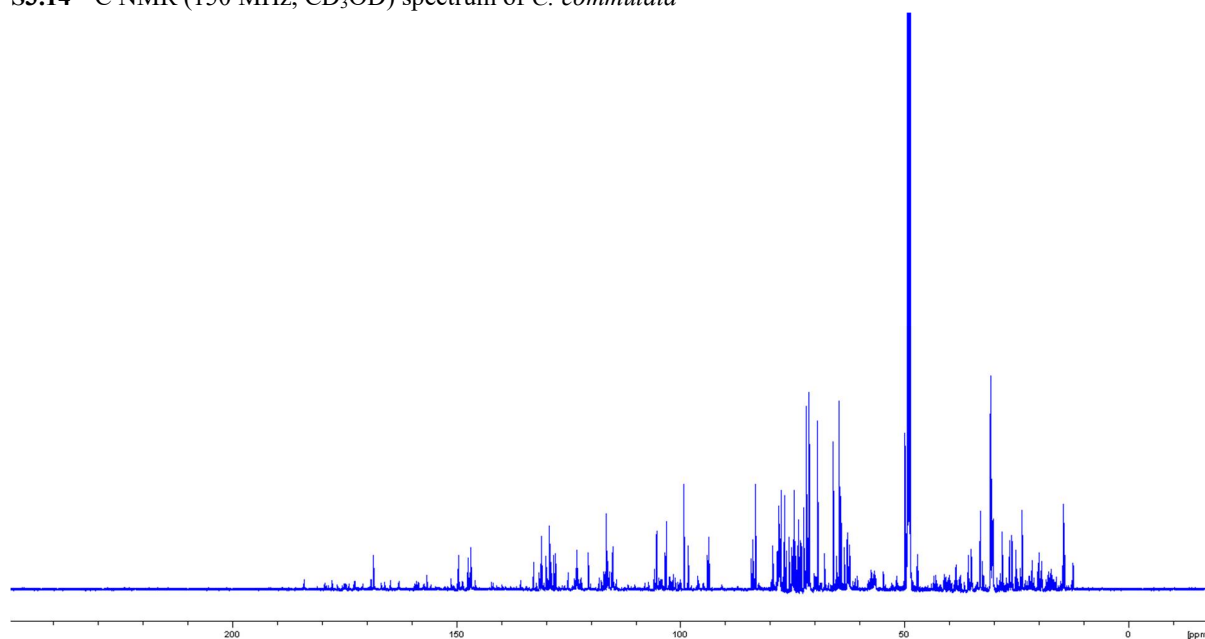
S3.12. HMBC (CD₃OD) spectrum of *C. foetida*



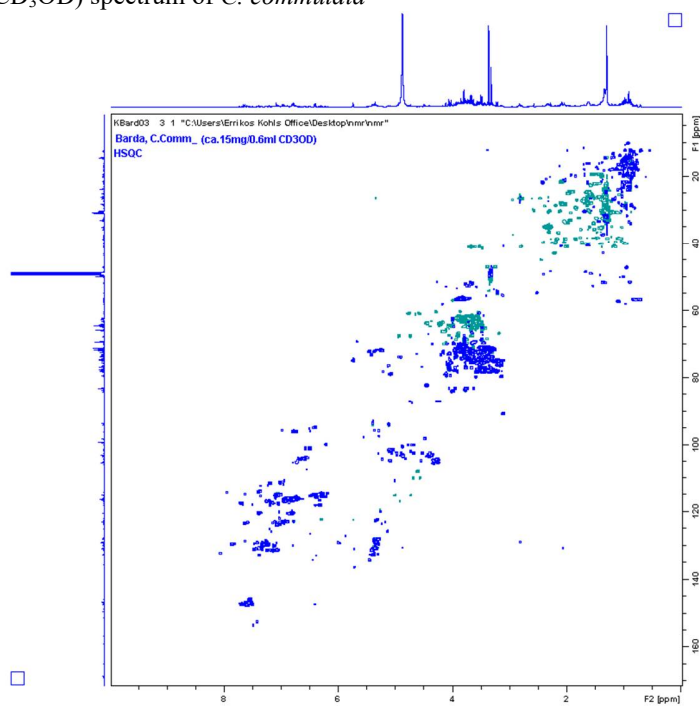
S3.13 ¹H NMR (600 MHz, CD₃OD) spectrum of *Crepis commutata*



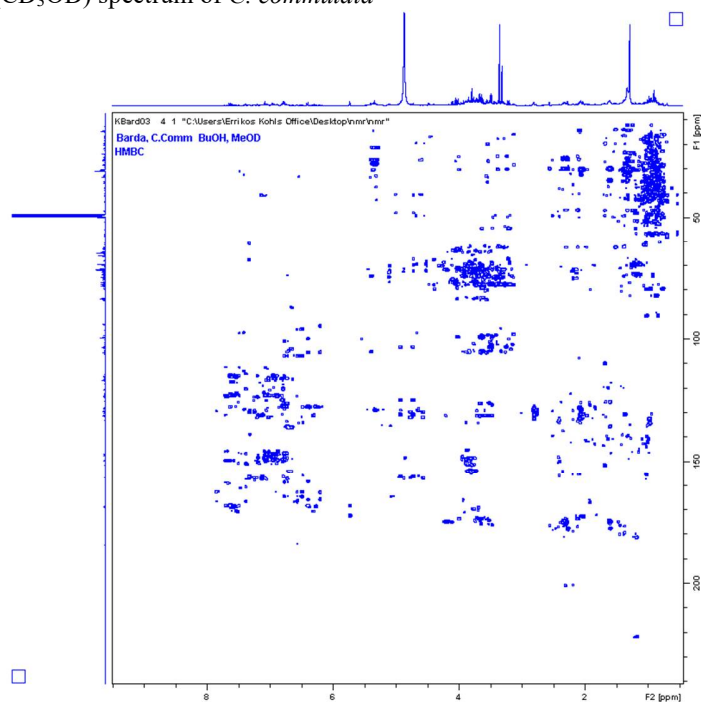
S3.14 ^{13}C NMR (150 MHz, CD_3OD) spectrum of *C. commutata*



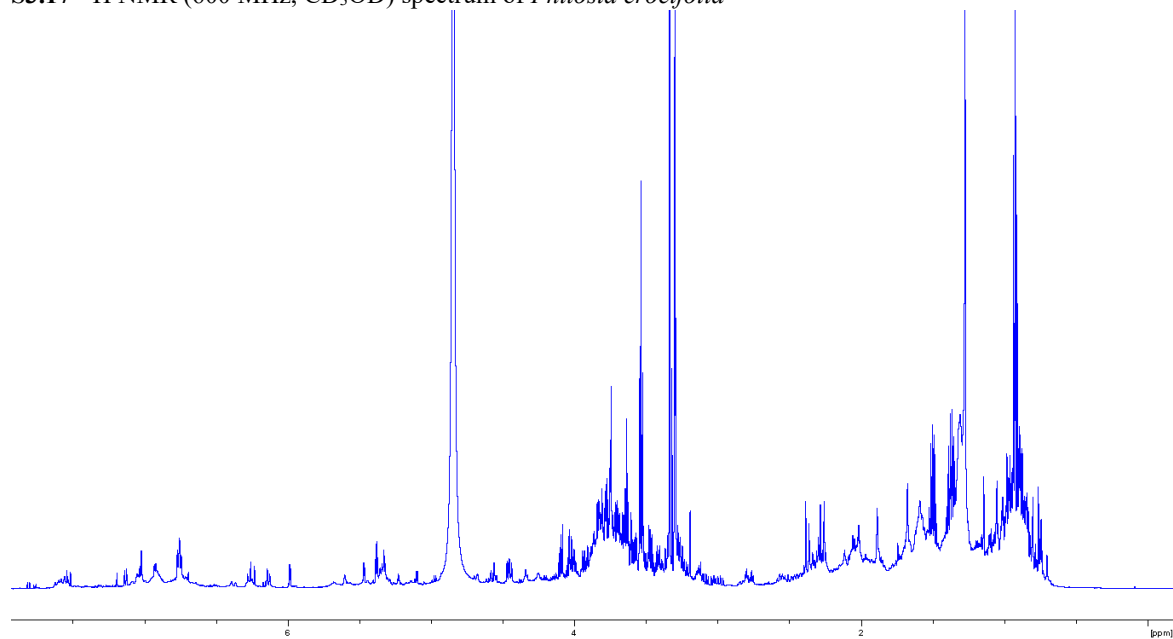
S3.15 HSQC (CD_3OD) spectrum of *C. commutata*



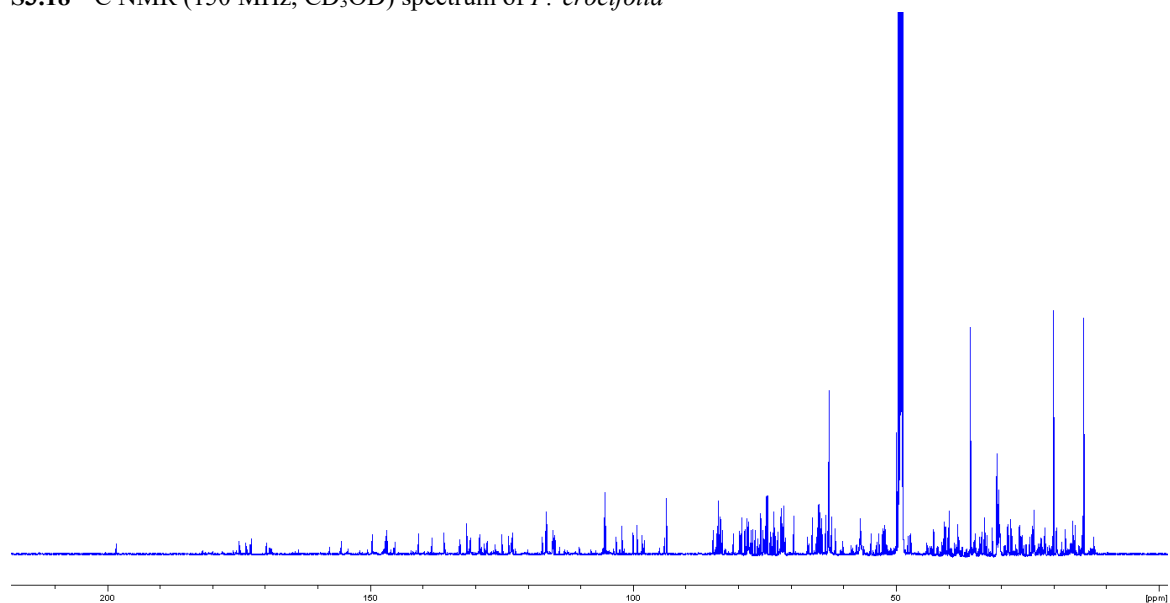
S3.16 HMBC (CD₃OD) spectrum of *C. commutata*



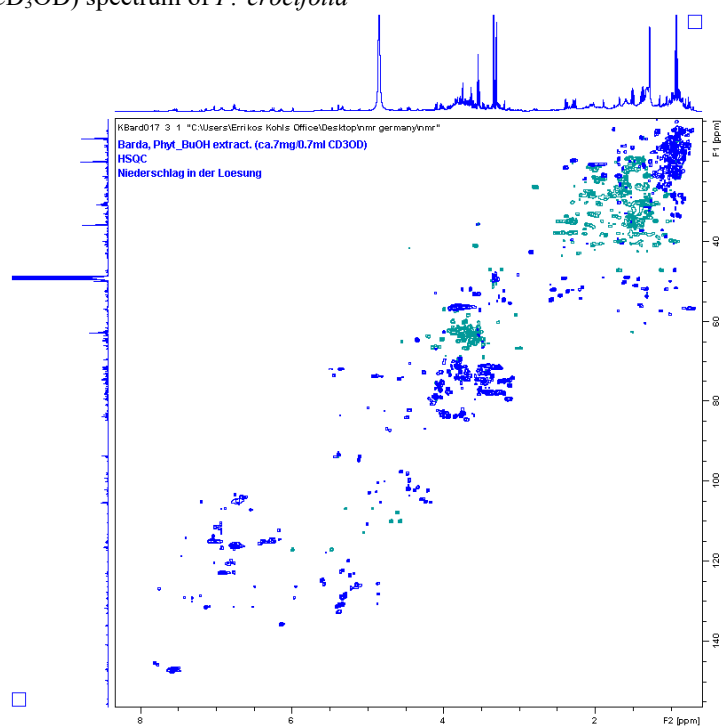
S3.17 ¹H NMR (600 MHz, CD₃OD) spectrum of *Phitosia crocifolia*



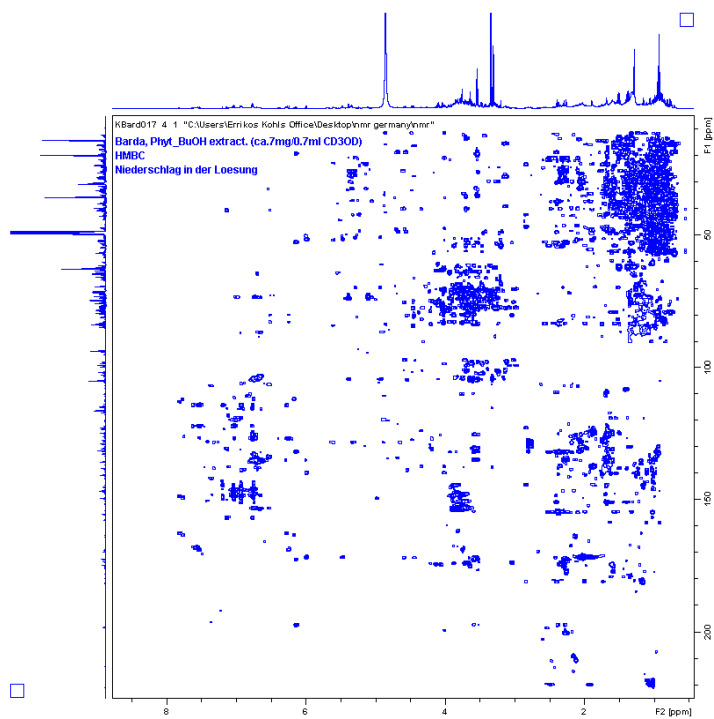
S3.18 ^{13}C NMR (150 MHz, CD_3OD) spectrum of *P. crocifolia*



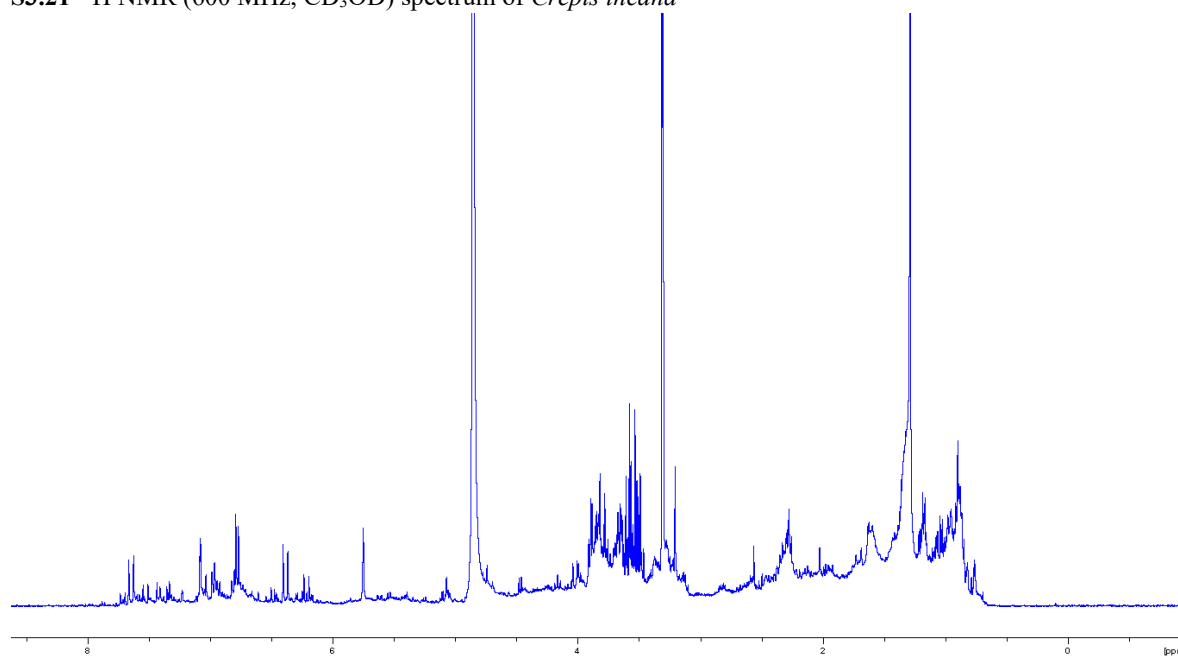
S3.19 HSQC (CD_3OD) spectrum of *P. crocifolia*



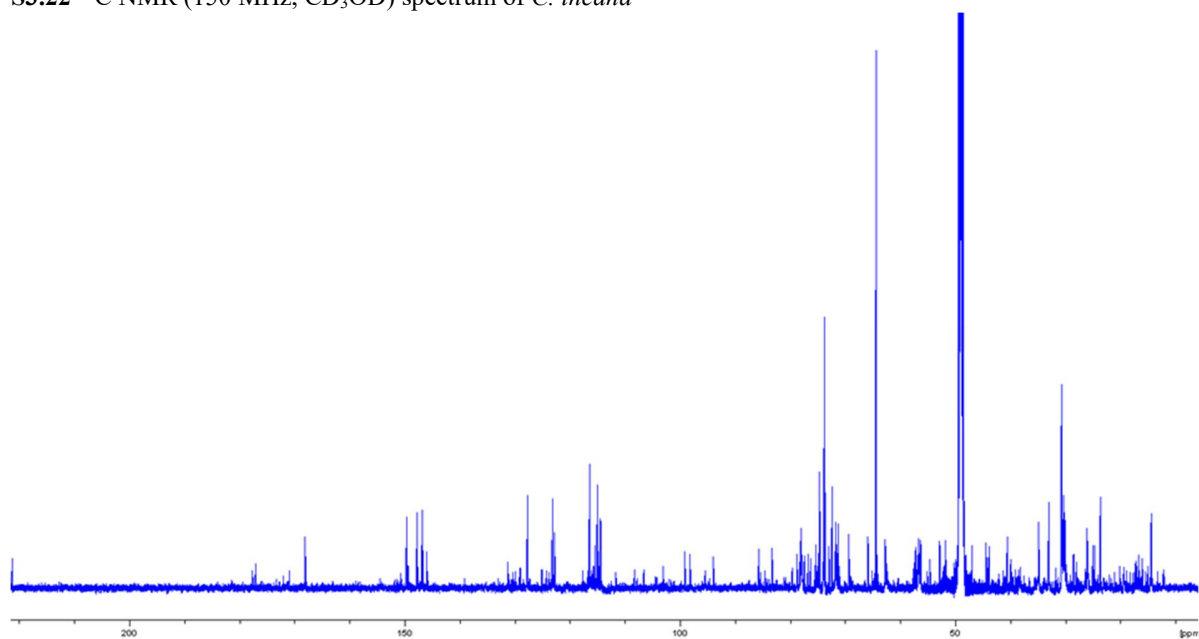
S3.20 HMBC (CD_3OD) spectrum of *P. crocifolia*



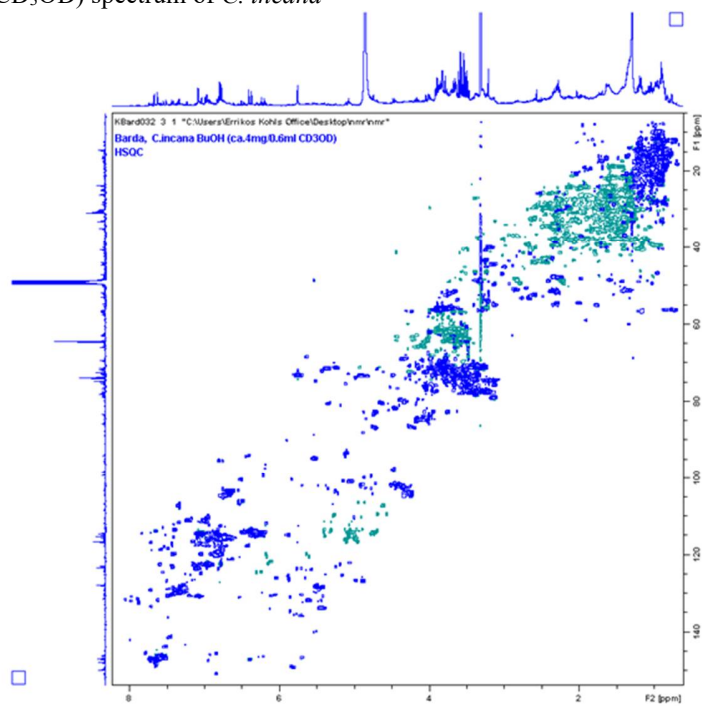
S3.21 ^1H NMR (600 MHz, CD_3OD) spectrum of *Crepis incana*



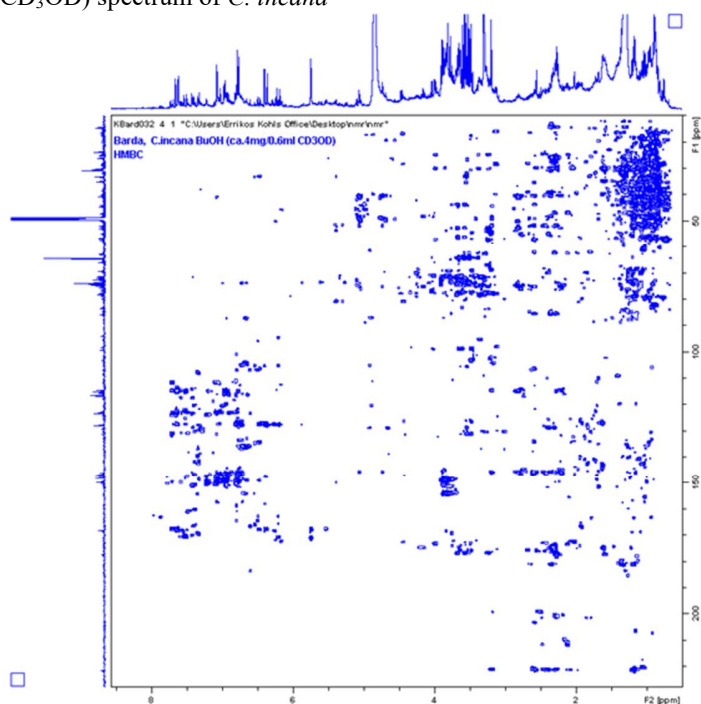
S3.22 ^{13}C NMR (150 MHz, CD_3OD) spectrum of *C. incana*



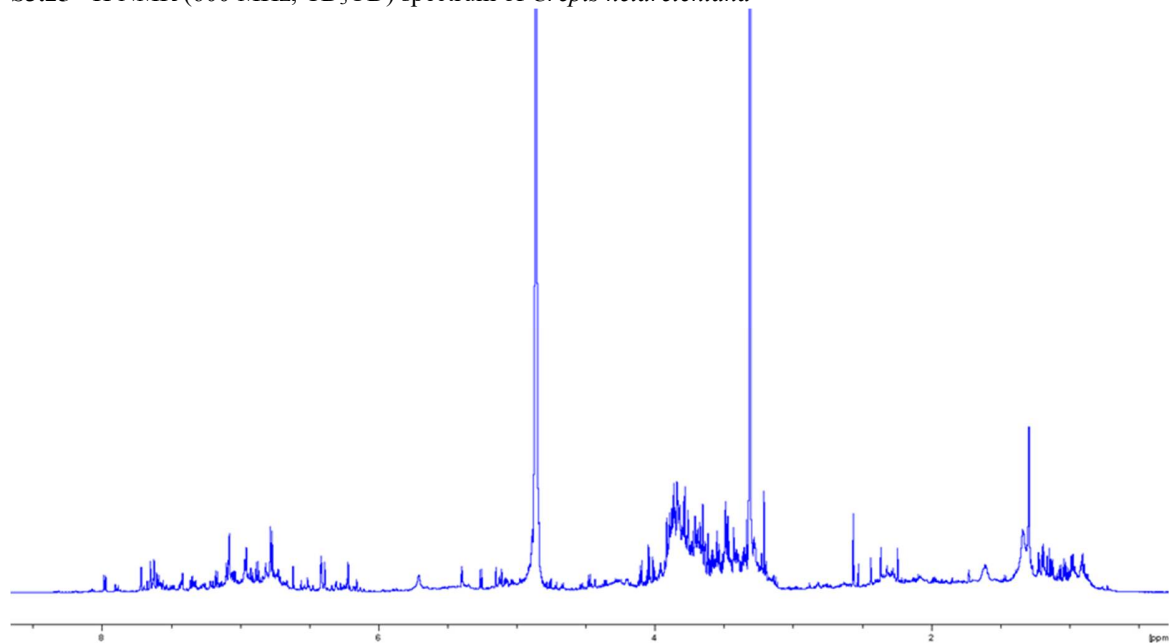
S3.23 HSQC (CD_3OD) spectrum of *C. incana*



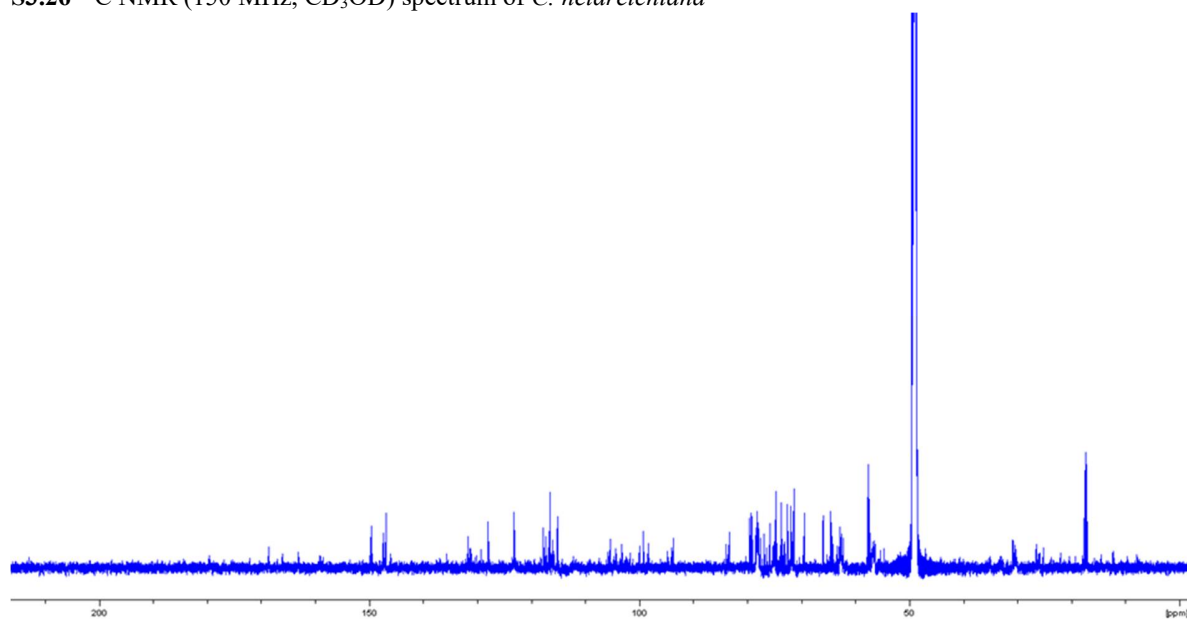
S3.24 HMBC (CD₃OD) spectrum of *C. incana*



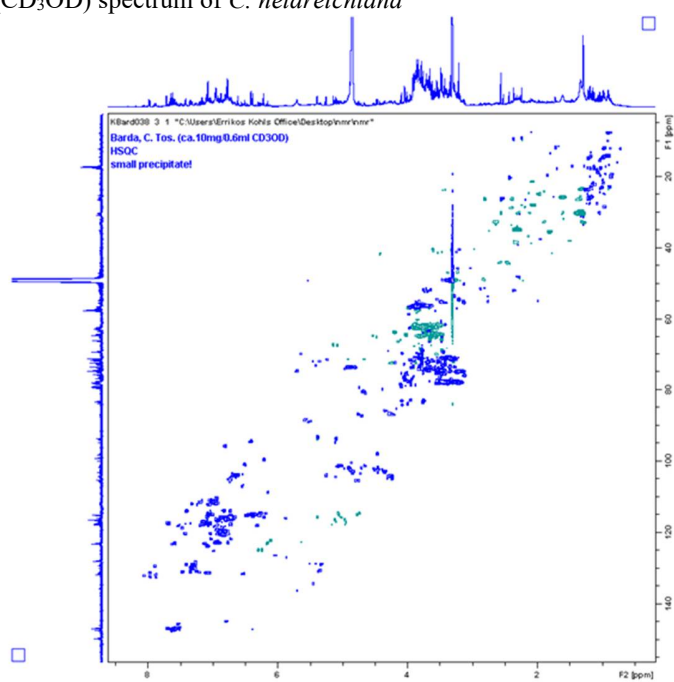
S3.25 ¹H NMR (600 MHz, CD₃OD) spectrum of *Crepis heldreichiana*



S3.26 ^{13}C NMR (150 MHz, CD_3OD) spectrum of *C. heldreichiana*



S3.27 HSQC (CD_3OD) spectrum of *C. heldreichiana*



S3.28 HMBC (CD₃OD) spectrum of *C. heldreichiana*

