

## Supplementary Information

### **Chemometrics-based analysis of the phytochemical profile and antioxidant activity of *Salvia* species from Iran**

Atefeh Moshari-Nasirkandi<sup>1,†</sup>, Nunzia Iaccarino<sup>2,†</sup>, Francesca Romano<sup>2</sup>, Giulia Graziani<sup>2</sup>, Abolfazl Alirezalu<sup>1,\*</sup>, Hadi Alipour<sup>3</sup>, Jussara Amato<sup>2,\*</sup>

<sup>1</sup> *Department of Horticultural Sciences, Faculty of Agriculture, Urmia University, Urmia, Iran*

<sup>2</sup> *Department of Pharmacy, University of Naples Federico II, Naples, Italy*

<sup>3</sup> *Department of Plant Production and Genetics, Urmia University, Urmia, Iran*

† These authors contributed equally to this work

\*Corresponding authors

Jussara Amato – [orcid.org/0000-0001-6096-3544](https://orcid.org/0000-0001-6096-3544) – e-mail: [jussara.amato@unina.it](mailto:jussara.amato@unina.it)

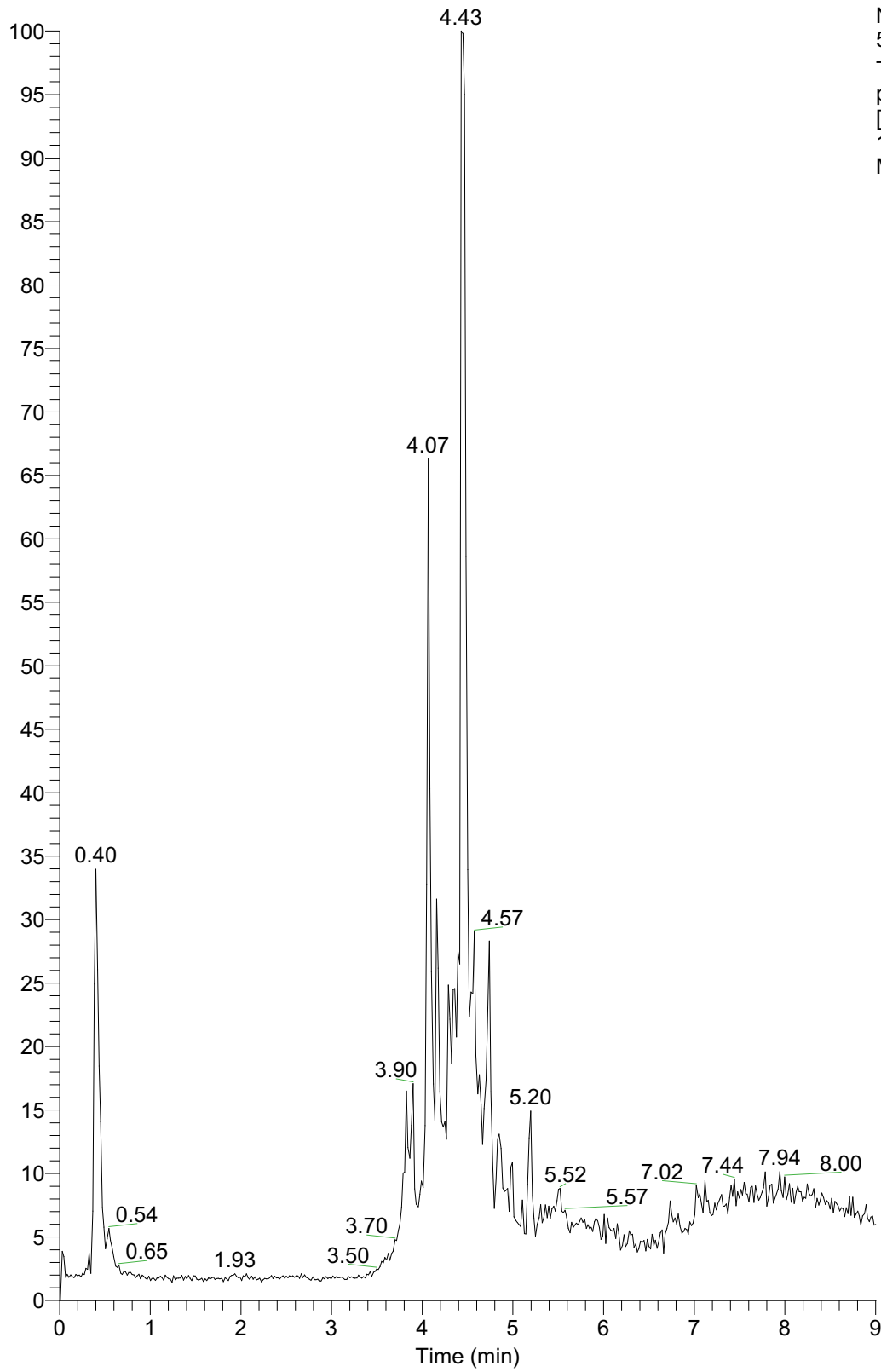
Abolfazl Alirezalu – [orcid.org/0000-0002-5882-8981](https://orcid.org/0000-0002-5882-8981) – e-mail: [a.alirezalu@urmia.ac.ir](mailto:a.alirezalu@urmia.ac.ir)

**Table S1.** Sampling locations of the 102 samples of *Salvia* studied.

Sample code	Species	Sampling Locations	Height	Longitude	Latitude
S1	<i>S. multicaulis</i>	Silvana	1629	44°23'04	39°02'40
S2	<i>S. limbata</i>	Talebin	1572	46°37'03	36°59'27
S3	<i>S. syriaca</i>	Shiban	1681	44°37'42	37°34'44
S4	<i>S. multicaulis</i>	Mavana	1630	44°57'11	38°00'46
S5	<i>S. verticillata</i>	Mavana	1630	44°17'15	39°01'57
S6	<i>S. nemorosa</i>	Silvana	1629	44°56'19	38°00'17
S7	<i>S. officinalis</i>	Urmia University	1366	46°11'34	36°23'43
S8	<i>S. officinalis</i>	Urmia University	1366	46°38'31	36°58'04
S9	<i>S. atropatana</i>	Kuh-e Sir daghi	1897	46°11'39	36°23'36
S10	<i>S. sclarea</i>	Urmia University	1366	45°17'14	36°29'36
S11	<i>S. syriaca</i>	Baruq	1355	46°12'38	36°36'42
S12	<i>S. multicaulis</i>	Aghbolagh	1832	46°38'31	36°58'04
S13	<i>S. nemorosa</i>	Aghbolagh	1832	45°07'18	37°17'57
S14	<i>S. limbata</i>	Aghbolagh	1832	46°38'30	36°58'10
S15	<i>S. multicaulis</i>	Hesarlu	1950	45°17'14	36°29'36
S16	<i>S. syriaca</i>	Shahindej-Tekab Rd	2207	45°17'14	36°29'36
S17	<i>S. nemorosa</i>	Urmia-Mahabad Rd	1318	45°43'24	36°52'45
S18	<i>S. syriaca</i>	Naghadeh-Piranshahr Rd	1395	45°19'2.5	36°55'58
S19	<i>S. atropatana</i>	Naghadeh-Piranshahr Rd	1395	45°19'2.5	36°55'58
S20	<i>S. bracteata</i>	Naghadeh-Piranshahr Rd	1395	45°19'2.5	36°55'58
S21	<i>S. nemorosa</i>	Miandoab	1298	46° 9'48	36°56'27
S22	<i>S. bracteata</i>	Piranshahr-Sardasht Rd	1456	45°17'17	36°29'31
S23	<i>S. nemorosa</i>	Piranshahr-Sardasht Rd	1456	45°17'17	36°29'31
S24	<i>S. limbata</i>	Bukan	1328	46°11'42	36°30'26
S25	<i>S. spinosa</i>	Bukan	1328	46°11'42	36°30'26
S26	<i>S. spinosa</i>	Saqqez	1520	46°15'36	36°17'33
S27	<i>S. syriaca</i>	Saqqez	1520	46°15'36	36°17'33
S28	<i>S. staminea</i>	Qahreman Kandi	2082	44°15'48	39°15'1.0
S29	<i>S. multicaulis</i>	Saqqez	1520	46°15'36	36°17'33
S30	<i>S. nemorosa</i>	Utmish	1414	46° 1'58	36°40'36
S31	<i>S. spinosa</i>	Mahabad-Miandoab Rd	1312	45°47'13	36°50'43
S32	<i>S. spinosa</i>	Qushchi	1362	44°59'59	37°57'28
S33	<i>S. syriaca</i>	Qushchi	1362	44°59'59	37°57'28
S34	<i>S. ceratophylla</i>	Qushchi	1362	44°59'59	37°57'28
S35	<i>S. atropatana</i>	Qushchi	1362	44°59'59	37°57'28
S36	<i>S. nemorosa</i>	Noshin Shahr	1316	45° 3'9.0	37°44'12
S37	<i>S. verticillata</i>	Qasemlu	1339	45° 9'13	37°21'5.7
S38	<i>S. nemorosa</i>	Qasemlu	1339	45° 9'13	37°21'5.7
S39	<i>S. limbata</i>	Qasemlu	1339	45° 9'13	37°21'5.7
S40	<i>S. syriaca</i>	Qasemlu	1339	45° 9'13	37°21'5.7
S41	<i>S. nemorosa</i>	Qasemlu	1339	45° 9'13	37°21'5.7
S42	<i>S. multicaulis</i>	Qasemlu	1339	45° 9'13	37°21'5.7
S43	<i>S. nemorosa</i>	Anhar Rd	1404	44°58'55	37°35'36
S44	<i>S. sclarea</i>	Marmisho	1746	44°38'14	37°35'2.5
S45	<i>S. macrochlamys</i>	Marmisho	1746	44°38'14	37°35'2.5
S46	<i>S. syriaca</i>	Marmisho	1746	44°38'14	37°35'2.5
S47	<i>S. verticillata</i>	Marmisho	1746	44°38'14	37°35'2.5
S48	<i>S. nemorosa</i>	Marmisho	1746	44°38'14	37°35'2.5
S49	<i>S. candidissima</i>	Marmisho	1746	44°38'14	37°35'2.5
S50	<i>S. limbata</i>	Marmisho	1746	44°38'14	37°35'2.5
S51	<i>S. syriaca</i>	Serow Rd	1346	44°58'40	37°40'1.2
S52	<i>S. limbata</i>	Serow Rd	1346	44°58'40	37°40'1.2
S53	<i>S. nemorosa</i>	Serow Rd	1346	44°58'40	37°40'1.2
S54	<i>S. verticillata</i>	Qurdik	2060	44°42'4.7	38°41'3.8
S55	<i>S. limbata</i>	Qurdik	2060	44°42'4.7	38°41'3.8
S56	<i>S. limbata</i>	Shahin Dej-Tekab Rd	2207	46°51'9.5	36°30'35
S57	<i>S. multicaulis</i>	Tekab	1732	47° 4'29	36°26'55
S58	<i>S. syriaca</i>	Takhte-Soleiman	1776	47° 6'16	36°24'42
S59	<i>S. nemorosa</i>	Khoy	1337	44°48'29	38°37'7.8

S60	<i>S. aethiopsis</i>	Dalamper	2784	44°48'20	37°10'46
S61	<i>S. limbata</i>	Takhte-Soleiman	1776	47° 6'16	36°24'42
S62	<i>S. sahendica</i>	Tabriz	2658	46°17'42	37°45'21
S63	<i>S. nemorosa</i>	Daryan	1676	45°38'31	38°12'54
S64	<i>S. verticillata</i>	Daryan	1676	45°38'31	38°12'54
S65	<i>S. aethiopsis</i>	Khoy	1337	44°48'29	38°37'7.8
S66	<i>S. spinosa</i>	Urmia-Tabriz Rd	1336	46° 2'25	37°57'53
S67	<i>S. multicaulis</i>	Urmia-Tabriz Rd	1336	46° 2'25	37°57'53
S68	<i>S. limbata</i>	Gareziaedin	1117	45° 2'15	38°54'58
S69	<i>S. syriaca</i>	Nokhtalu	1873	46°41'11	36°59'25
S70	<i>S. multicaulis</i>	Nokhtalu	1873	46°41'11	36°59'25
S71	<i>S. limbata</i>	Nokhtalu	1873	46°41'11	36°59'25
S72	<i>S. syriaca</i>	Daryan	1676	45°38'31	38°12'54
S73	<i>S. limbata</i>	Daryan	1676	45°38'31	38°12'54
S74	<i>S. ceratophylla</i>	Daryan	1676	45°38'31	38°12'54
S75	<i>S. spinosa</i>	Cheshmeh Kanan	1446	45°12'32	38°19'56
S76	<i>Salvia</i> sp.	Tupchi	1447	45°10'46	38°19'46
S77	<i>S. nemorosa</i>	Tasuj	1360	45°20'48	38°18'52
S78	<i>S. ceratophylla</i>	Miandoab-Bukan Rd	1325	46°12'17	36°37'35
S79	<i>S. syriaca</i>	Bukan-Mahabad Rd	1738	45°56'12	36°42'32
S80	<i>S. limbata</i>	Bukan-Mahabad Rd	1738	45°56'12	36°42'32
S81	<i>S. limbata</i>	Mahabad-Miandoab Rd	1312	45°47'13	36°50'43
S82	<i>S. poculata</i>	Qushchi	1362	44°59'59	37°57'28
S83	<i>S. hydrangea</i>	Qushchi	1362	44°59'59	37°57'28
S84	<i>S. syriaca</i>	Salmas-Khoy Rd	1177	44°56'15	38°28'18
S85	<i>S. ceratophylla</i>	Khalifatan	1524	44°52'31	37°34'42
S86	<i>S. limbata</i>	Chaldoran	1820	44°22'45	39° 4'22
S87	<i>S. multicaulis</i>	Khalifatan	1524	44°52'31	37°34'42
S88	<i>S. grossheimii</i>	Khaneqah Sorkh	1366	45° 2'3.3	37°45'9.5
S89	<i>S. multicaulis</i>	Khaneqah Sorkh	1366	45° 2'3.3	37°45'9.5
S90	<i>S. multicaulis</i>	Marmisho	1746	44°38'14	37°35'2.5
S91	<i>S. verticillata</i>	Marmisho	1746	44°38'14	37°35'2.5
S92	<i>S. syriaca</i>	Marmisho-Serow Rd	1365	44°55'57	37°40'20
S93	<i>S. multicaulis</i>	Marmisho-Serow Rd	1365	44°55'57	37°40'20
S94	<i>S. aethiopsis</i>	Marmisho-Serow Rd	1365	44°55'57	37°40'20
S95	<i>S. hydrangea</i>	Marmisho-Serow Rd	1365	44°55'57	37°40'20
S96	<i>S. macrochlamys</i>	Marmisho-Serow Rd	1365	44°55'57	37°40'20
S97	<i>S. ceratophylla</i>	Marmisho-Serow Rd	1365	44°55'57	37°40'20
S98	<i>S. atropatana</i>	Mishodagh	1900	45°37'51	38°16'37
S99	<i>S. sclarea</i>	Piranshahr-Sardasht Rd	1456	45°17'17	36°29'31
S100	<i>S. nemorosa</i>	Maku	1335	44°28'56	39°16'10
S101	<i>S. syriaca</i>	Oshnavieh-Piranshahr Rd	1436	45° 5'35	37° 0'31
S102	<i>S. multicaulis</i>	Oshnavieh-Piranshahr Rd	1436	45° 5'35	37° 0'31

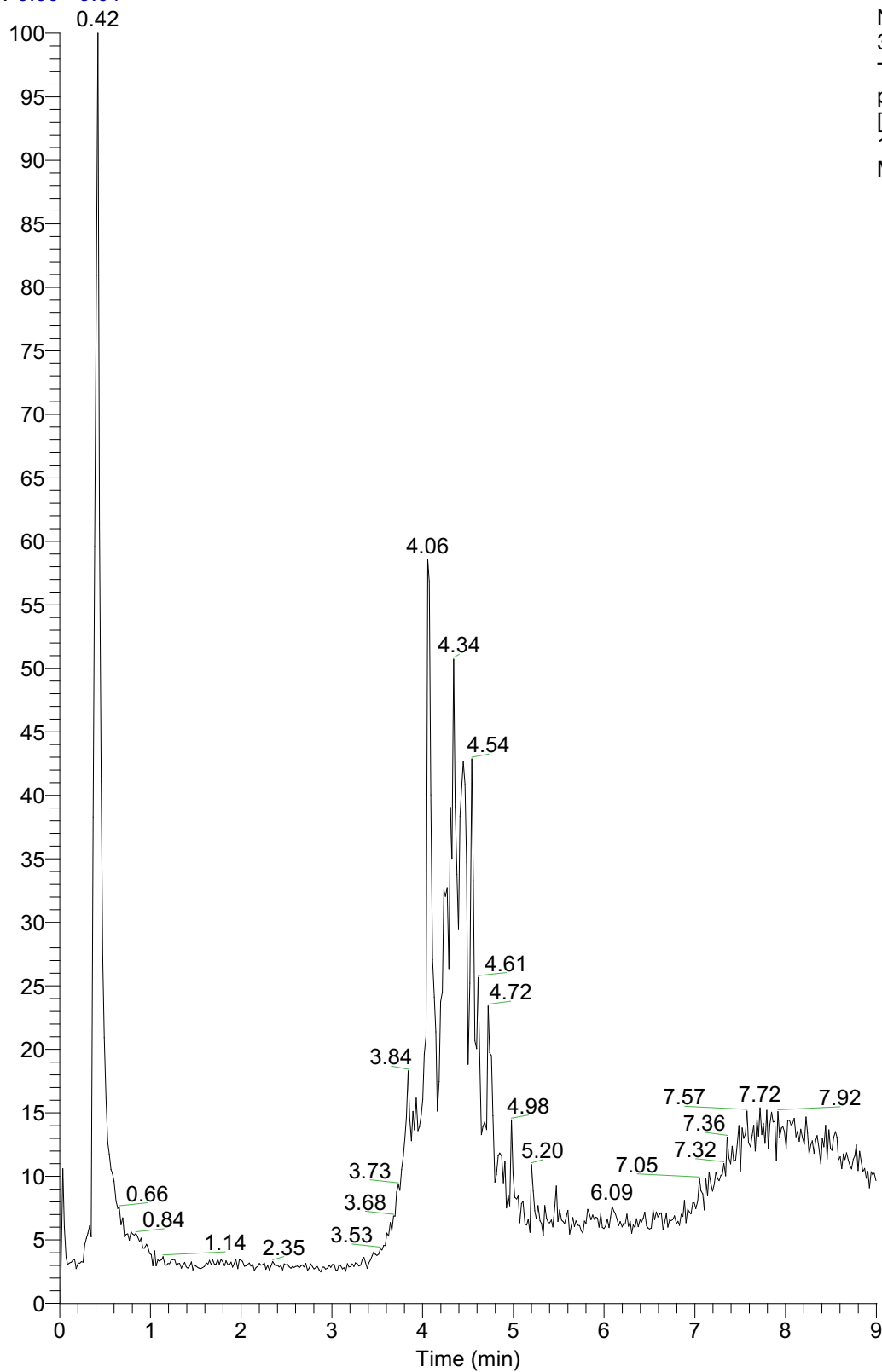
RT: 0.00 - 9.00



NL:  
5.25E9  
TIC F: FTMS -  
p ESI Full ms  
[100.0000-  
1200.0000]  
MS sample\_1

Figure S1: Representative chromatogram of an extract of *S. multicaulis* (sample S1).

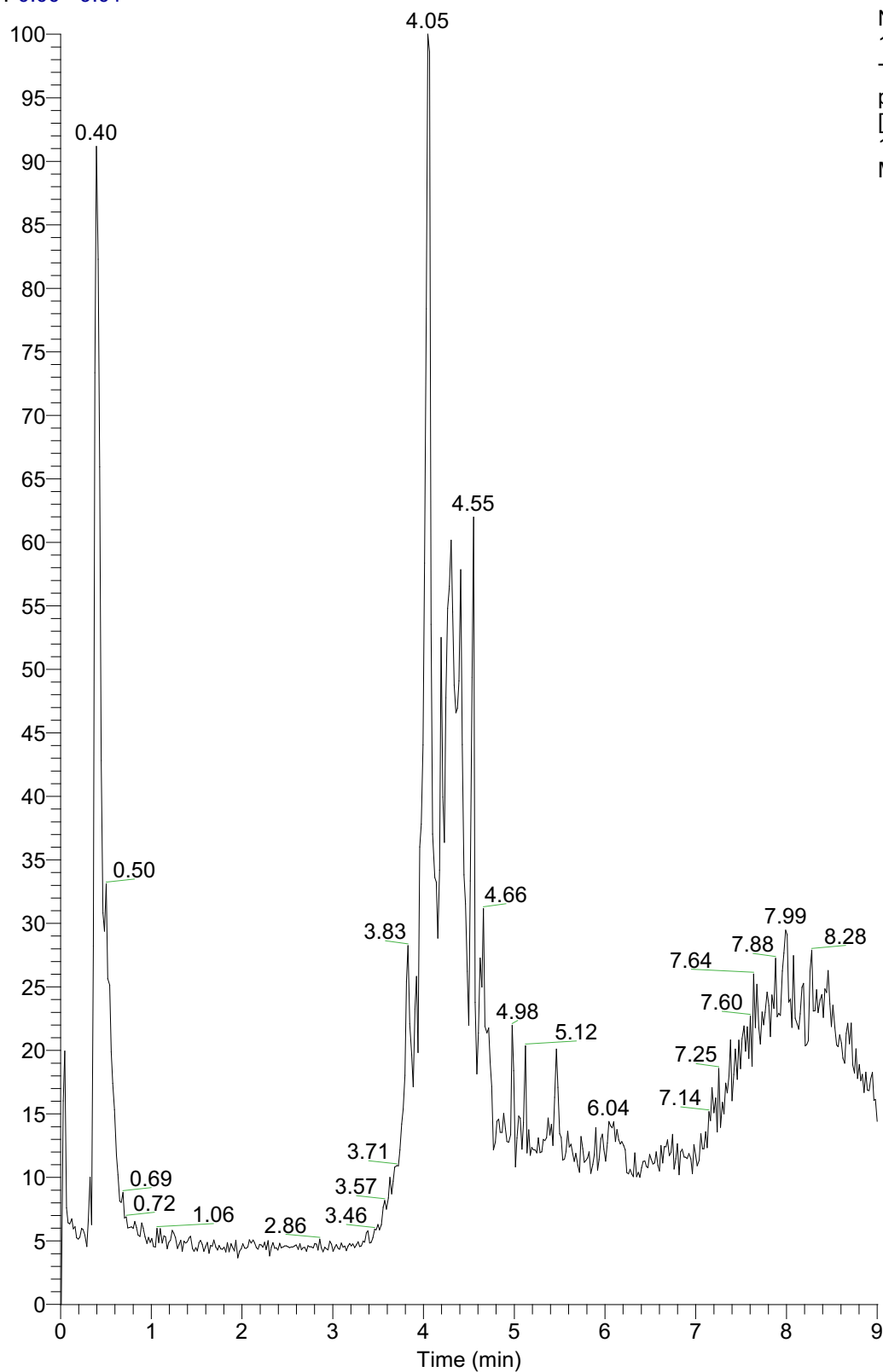
RT: 0.00 - 9.01



NL:  
3.17E9  
TIC F: FTMS -  
p ESI Full ms  
[100.0000-  
1200.0000]  
MS sample\_2

Figure S2: Representative chromatogram of an extract of *S. limbata* (sample S2).

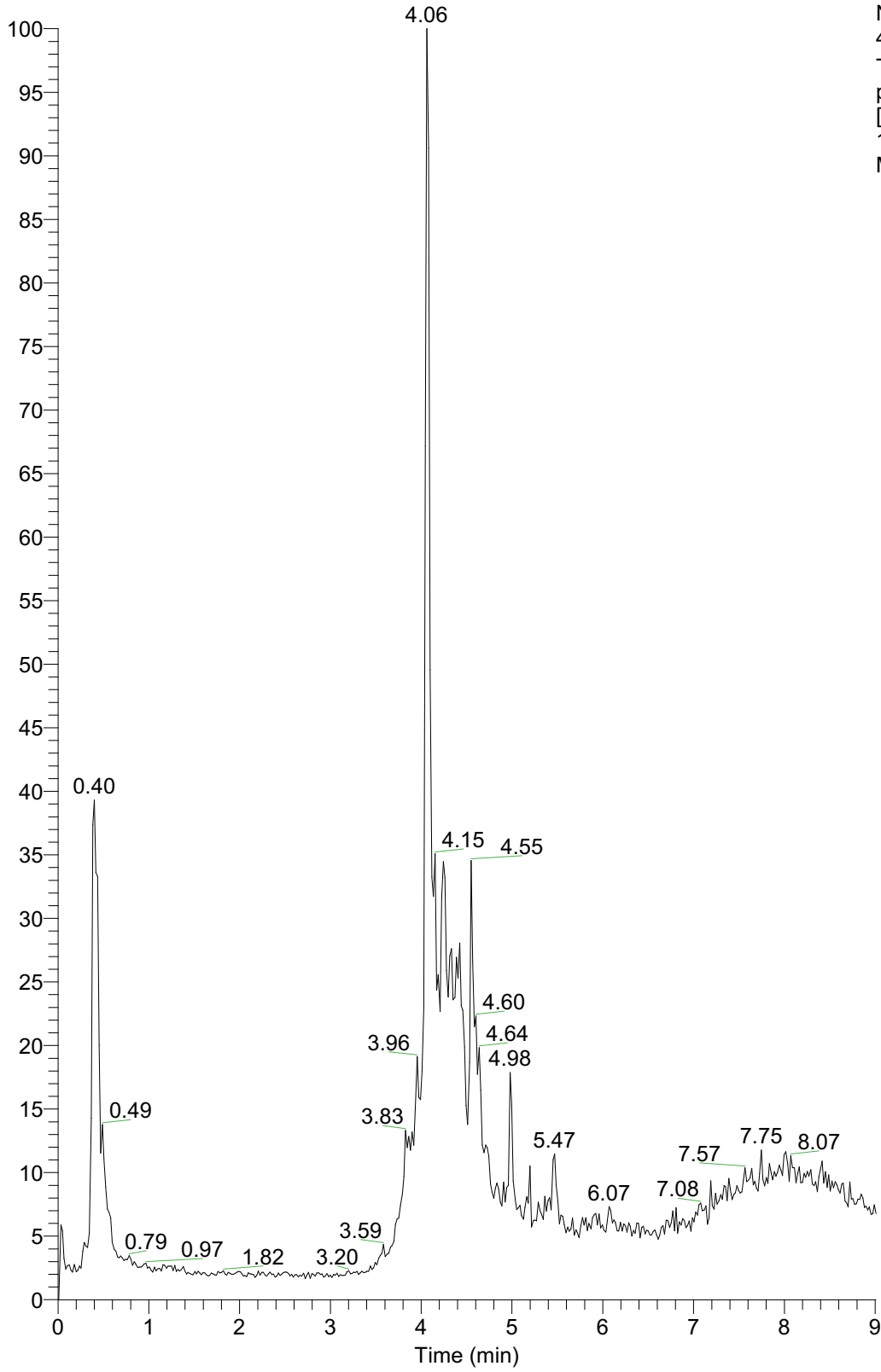
RT: 0.00 - 9.01



NL:  
1.77E9  
TIC F: FTMS -  
p ESI Full ms  
[100.0000-  
1200.0000]  
MS sample\_3

**Figure S3:** Representative chromatogram of an extract of *S. syriaca* (sample S3).

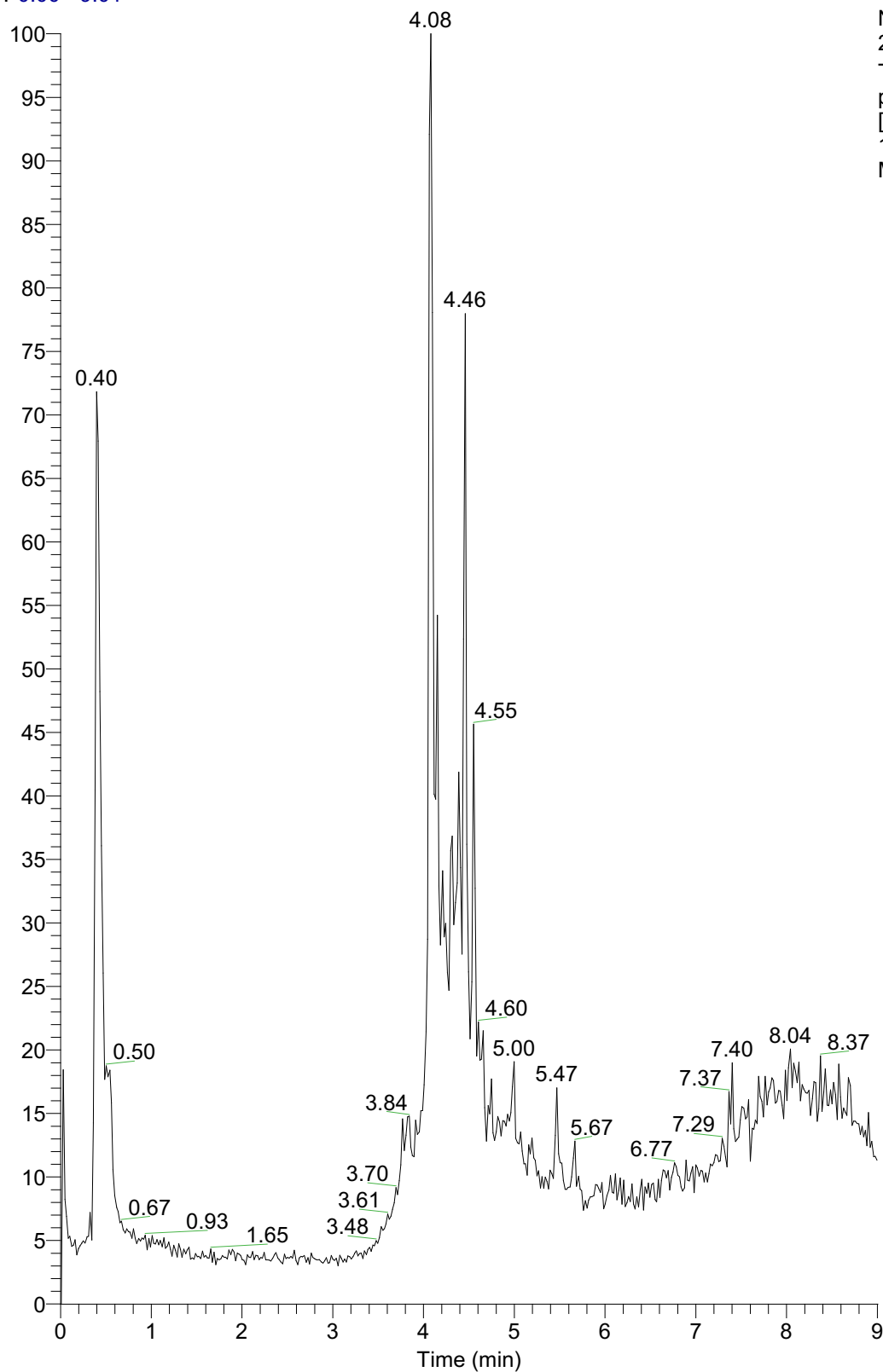
RT: 0.00 - 9.01



NL:  
4.09E9  
TIC F: FTMS -  
p ESI Full ms  
[100.0000-  
1200.0000]  
MS sample\_5

Figure S4: Representative chromatogram of an extract of *S. verticillata* (sample S5).

RT: 0.00 - 9.01

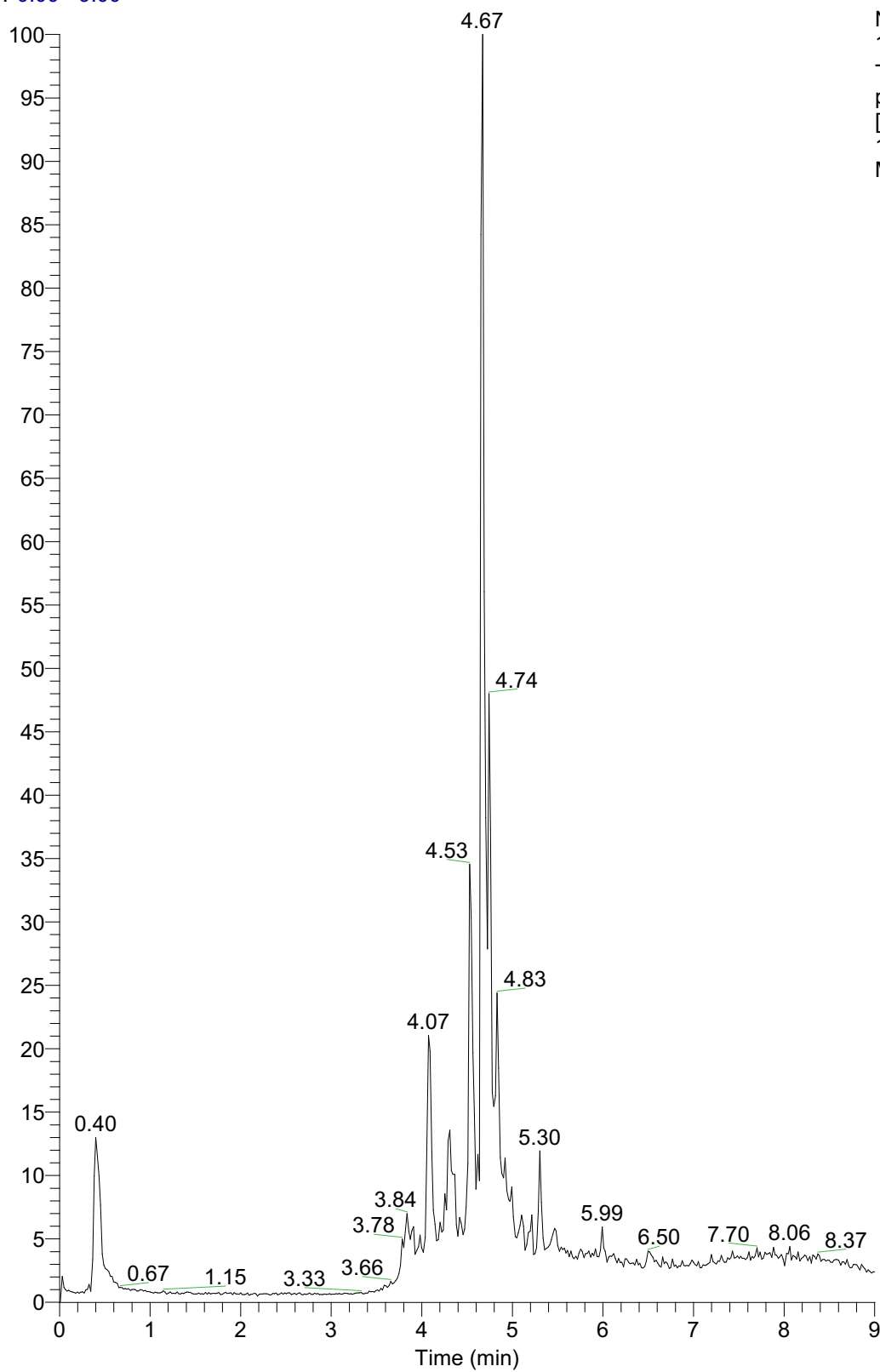


NL:  
2.20E9  
TIC F: FTMS -  
p ESI Full ms  
[100.0000-  
1200.0000]  
MS sample\_6

Figure S5: Representative chromatogram of an extract of *S. nemorosa* (sample S6).



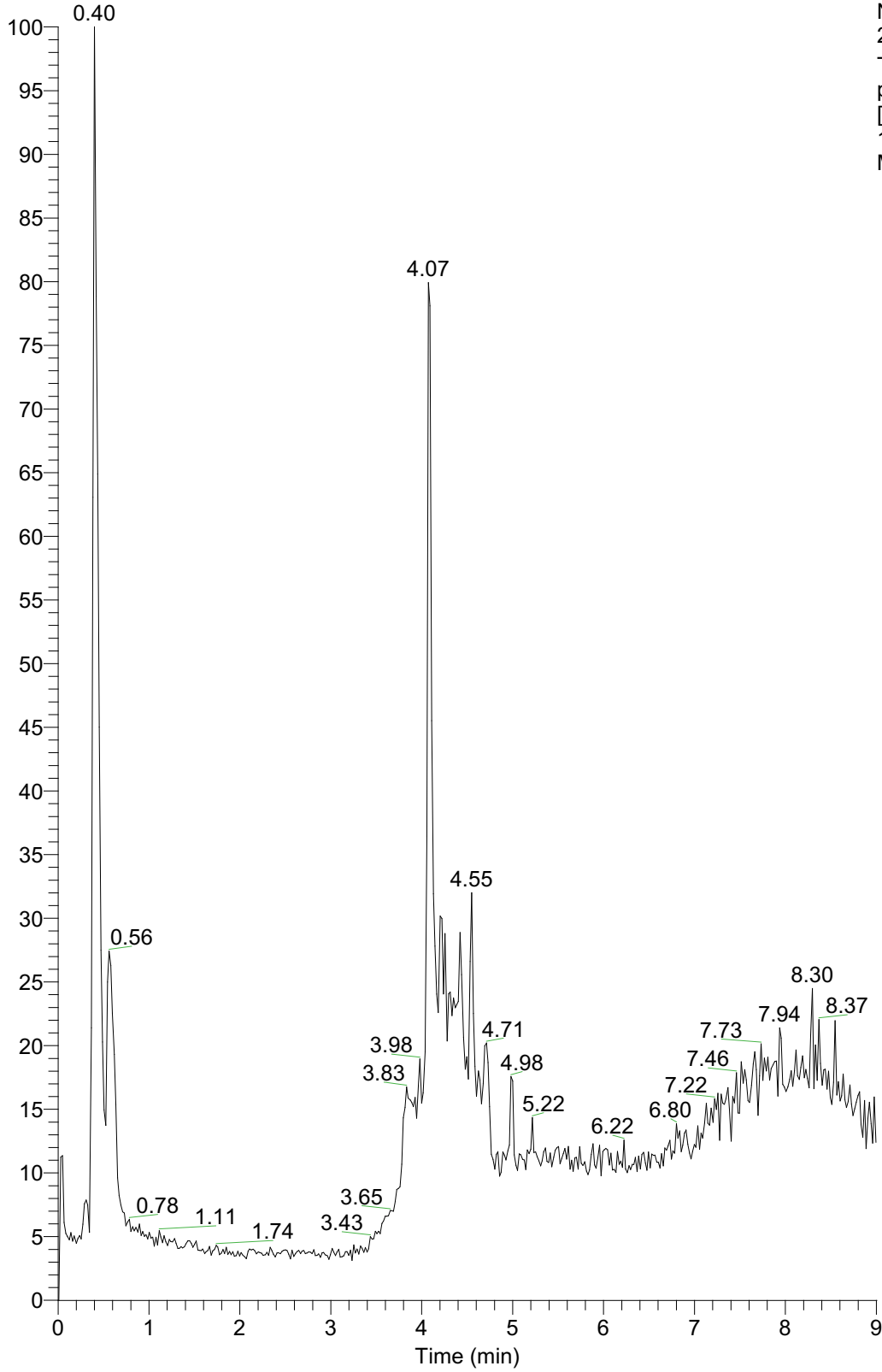
RT: 0.00 - 9.00



NL:  
1.17E10  
TIC F: FTMS -  
p ESI Full ms  
[100.0000-  
1200.0000]  
MS sample\_7

Figure S6: Representative chromatogram of an extract of *S. officinalis* (sample S7).

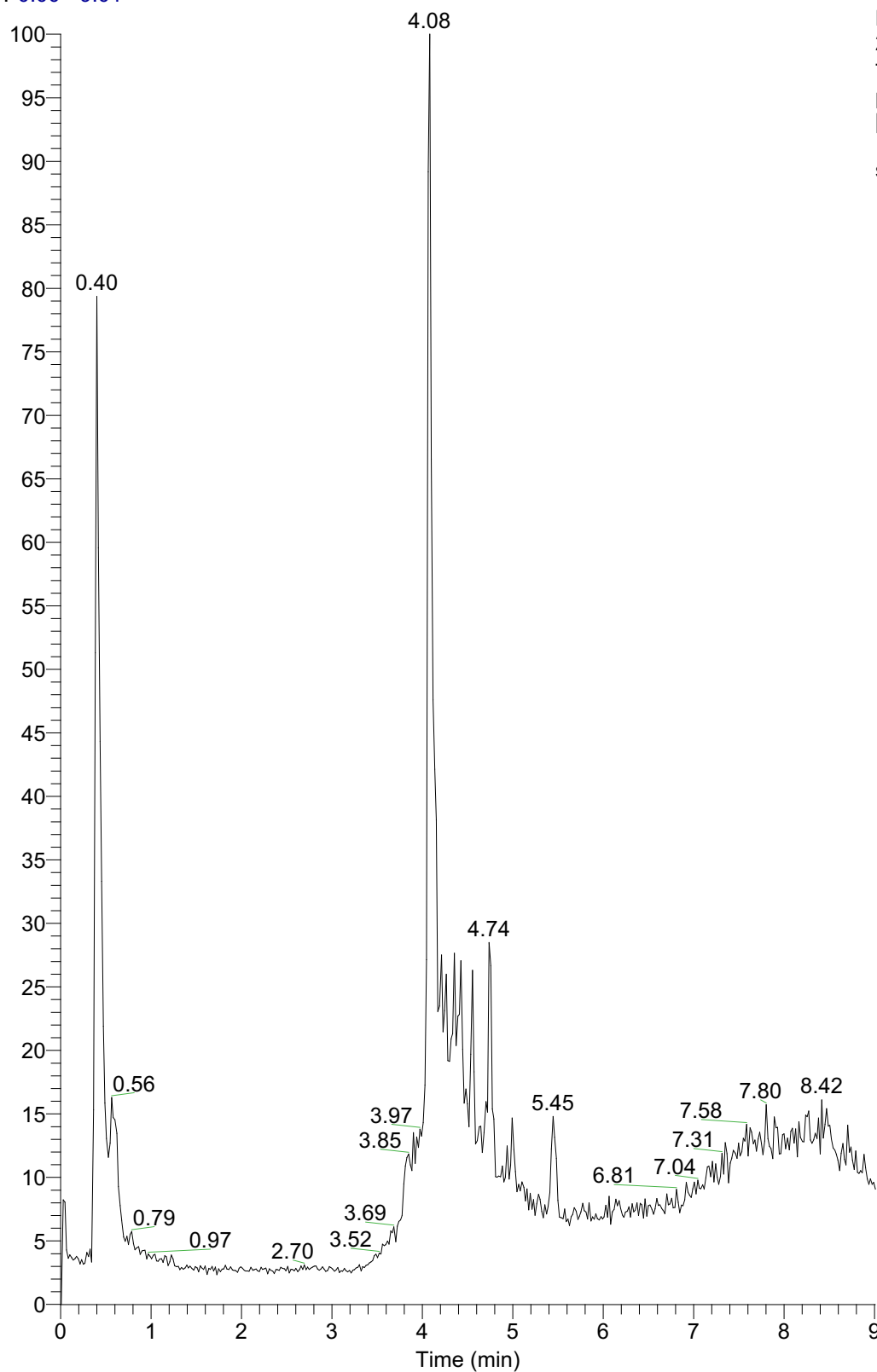
RT: 0.00 - 9.01



NL:  
2.08E9  
TIC F: FTMS -  
p ESI Full ms  
[100.0000-  
1200.0000]  
MS sample\_9

Figure S7: Representative chromatogram of a *S. atropatana* extract (sample S9).

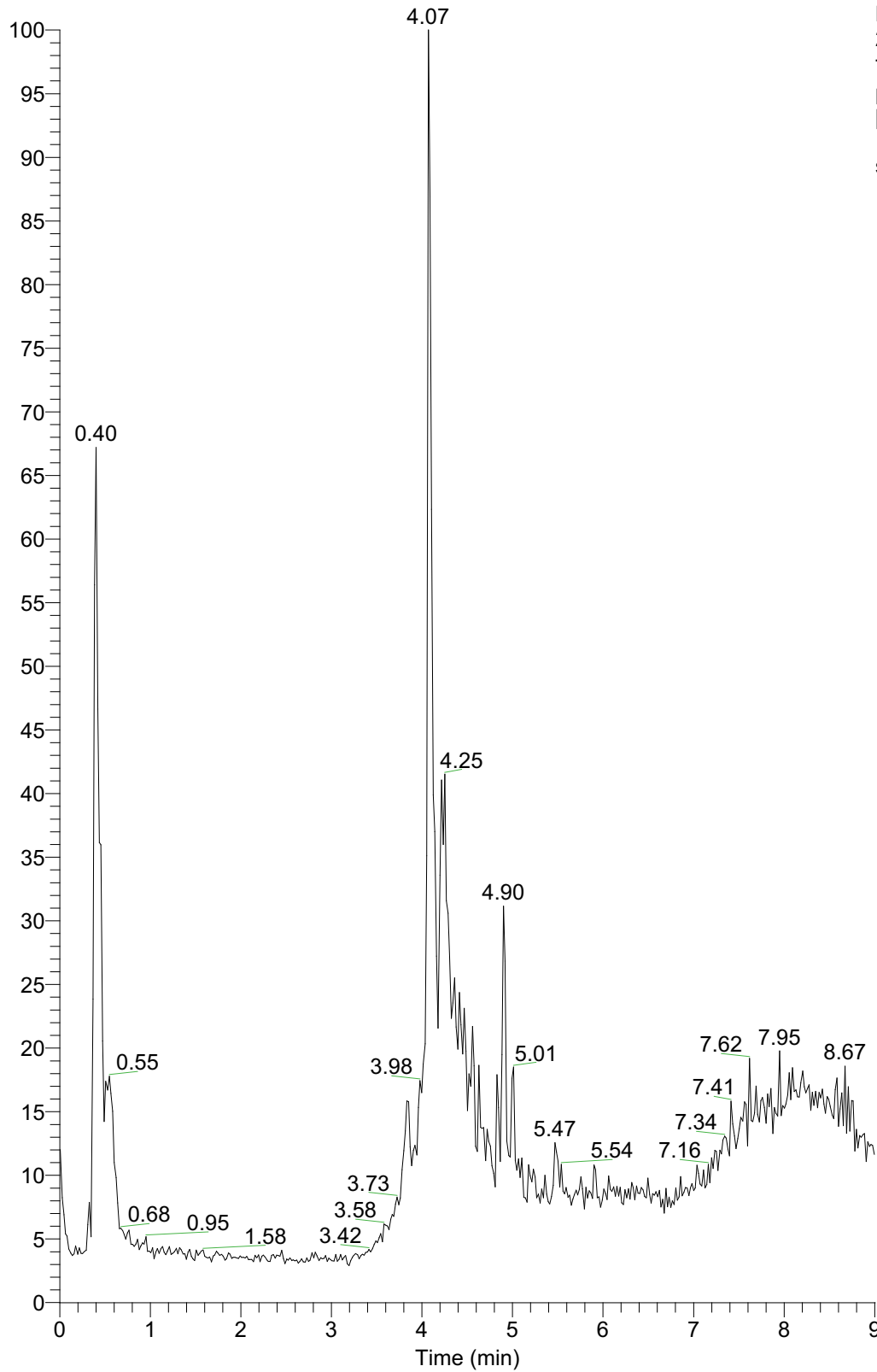
RT: 0.00 - 9.01



NL:  
2.76E9  
TIC F: FTMS -  
p ESI Full ms  
[100.0000-  
1200.0000] MS  
sample\_10

Figure S8: Representative chromatogram of a *S. sclarea* extract (sample S10).

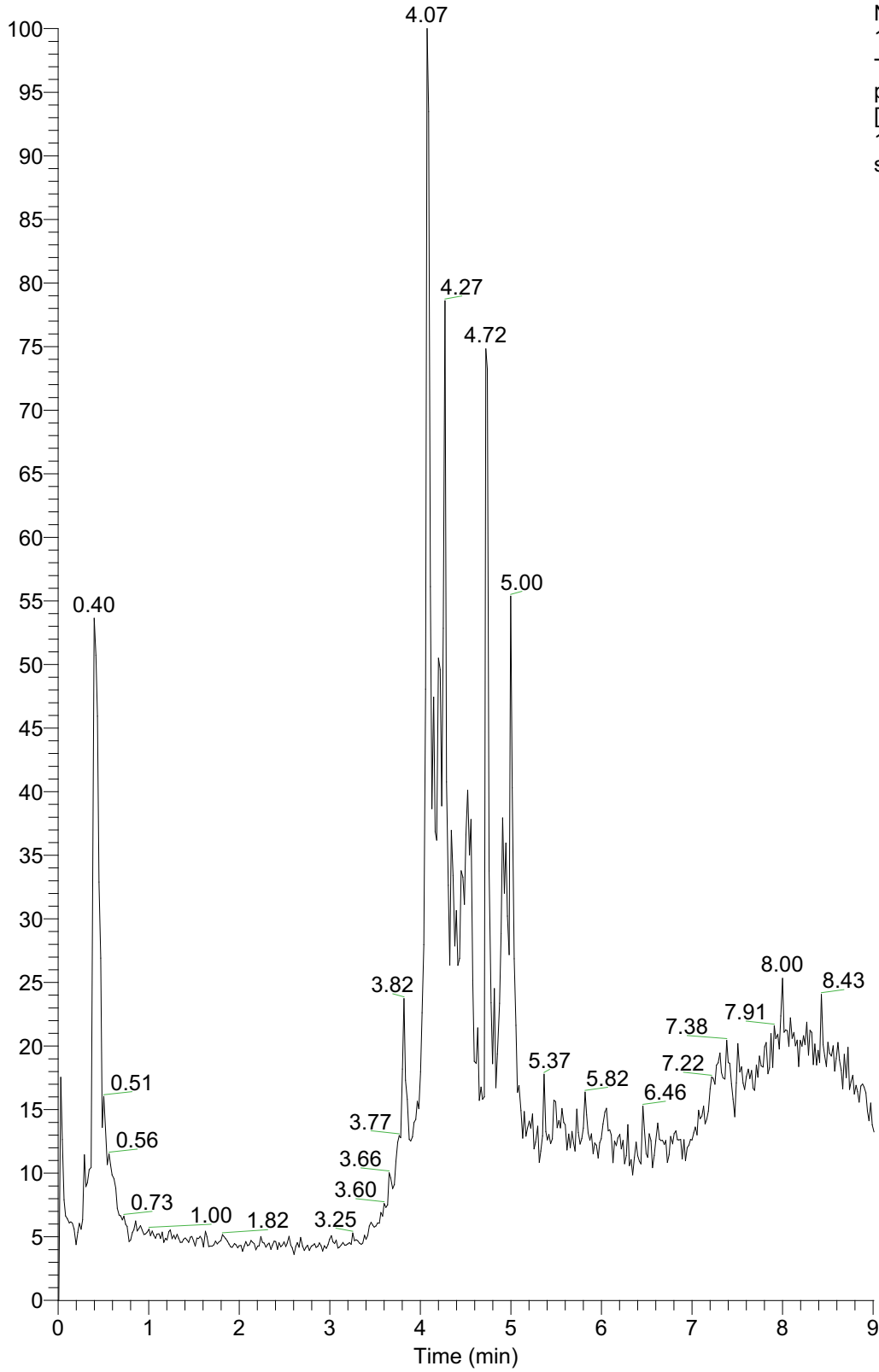
RT: 0.00 - 9.01



NL:  
2.18E9  
TIC F: FTMS -  
p ESI Full ms  
[100.0000-  
1200.0000] MS  
sample\_20

**Figure S9:** Representative chromatogram of an extract of *S. bracteata* (sample S20).

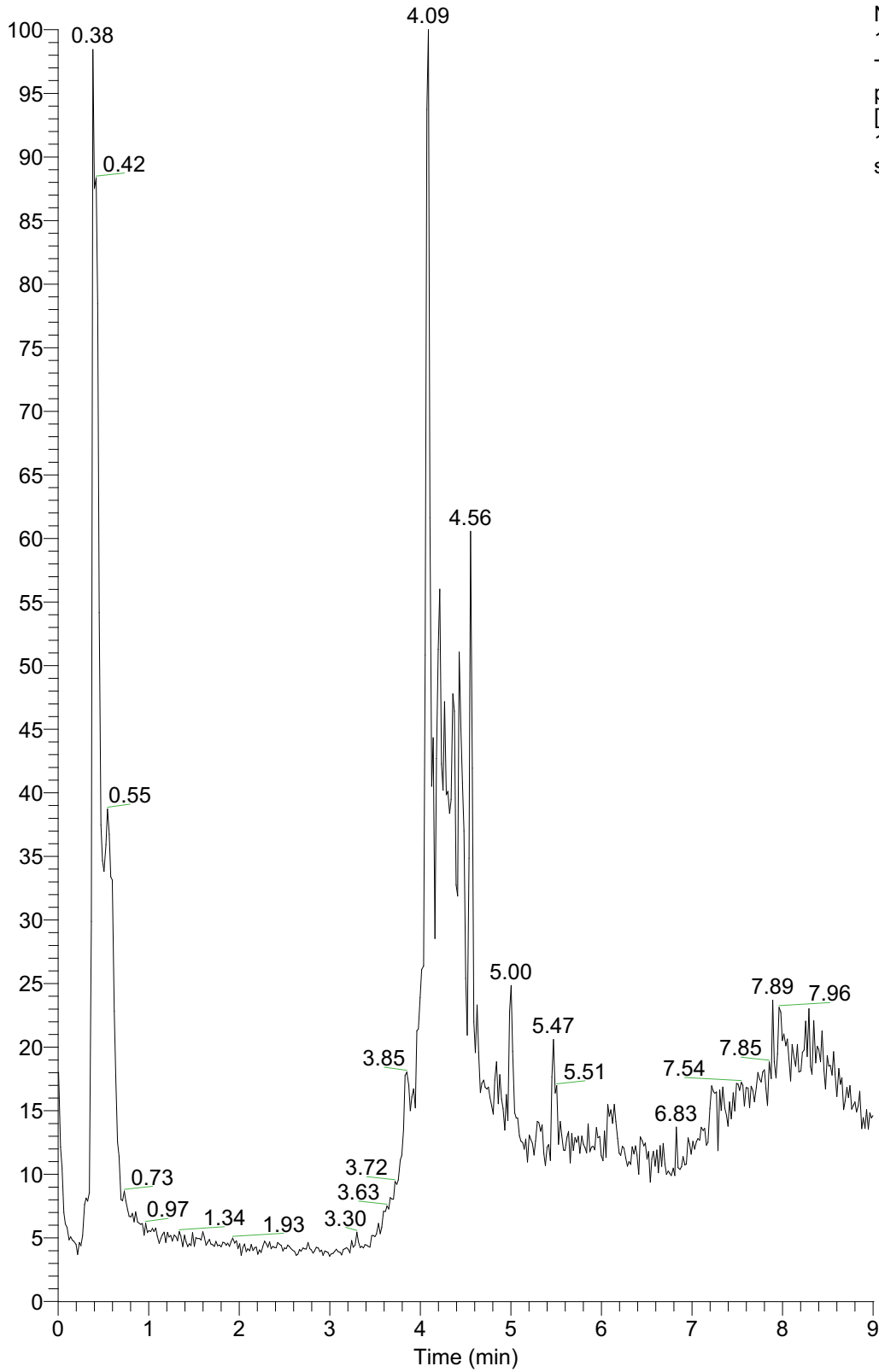
RT: 0.00 - 9.01



NL:  
1.62E9  
TIC F: FTMS -  
p ESI Full ms  
[100.0000-  
1200.0000] MS  
sample\_25

Figure S10: Representative chromatogram of an extract of *S. spinosa* (sample S25).

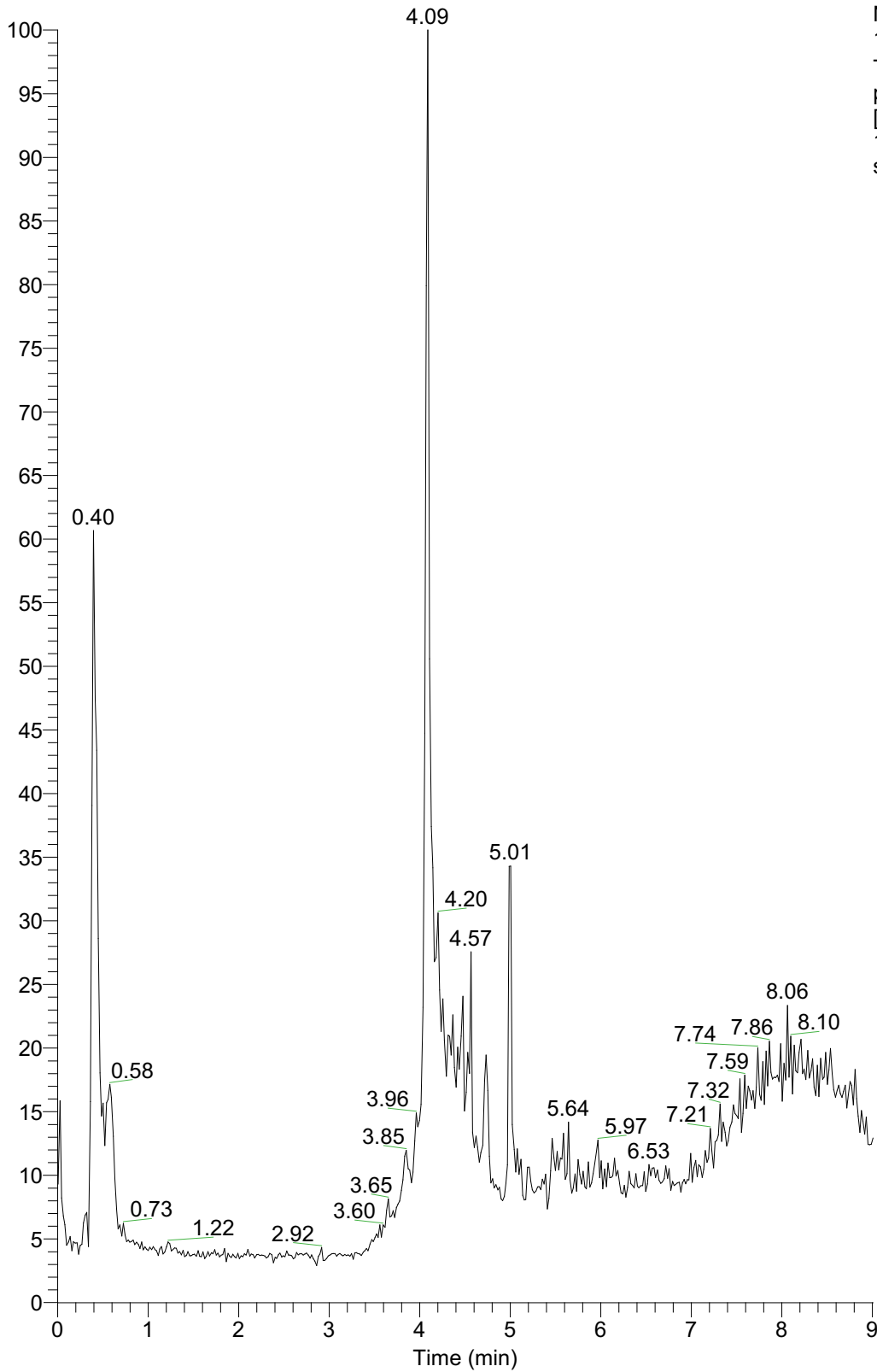
RT: 0.00 - 9.01



NL:  
1.79E9  
TIC F: FTMS -  
p ESI Full ms  
[100.0000-  
1200.0000] MS  
sample\_28

Figure S11: Representative chromatogram of a *S. staminea* extract (sample S28).

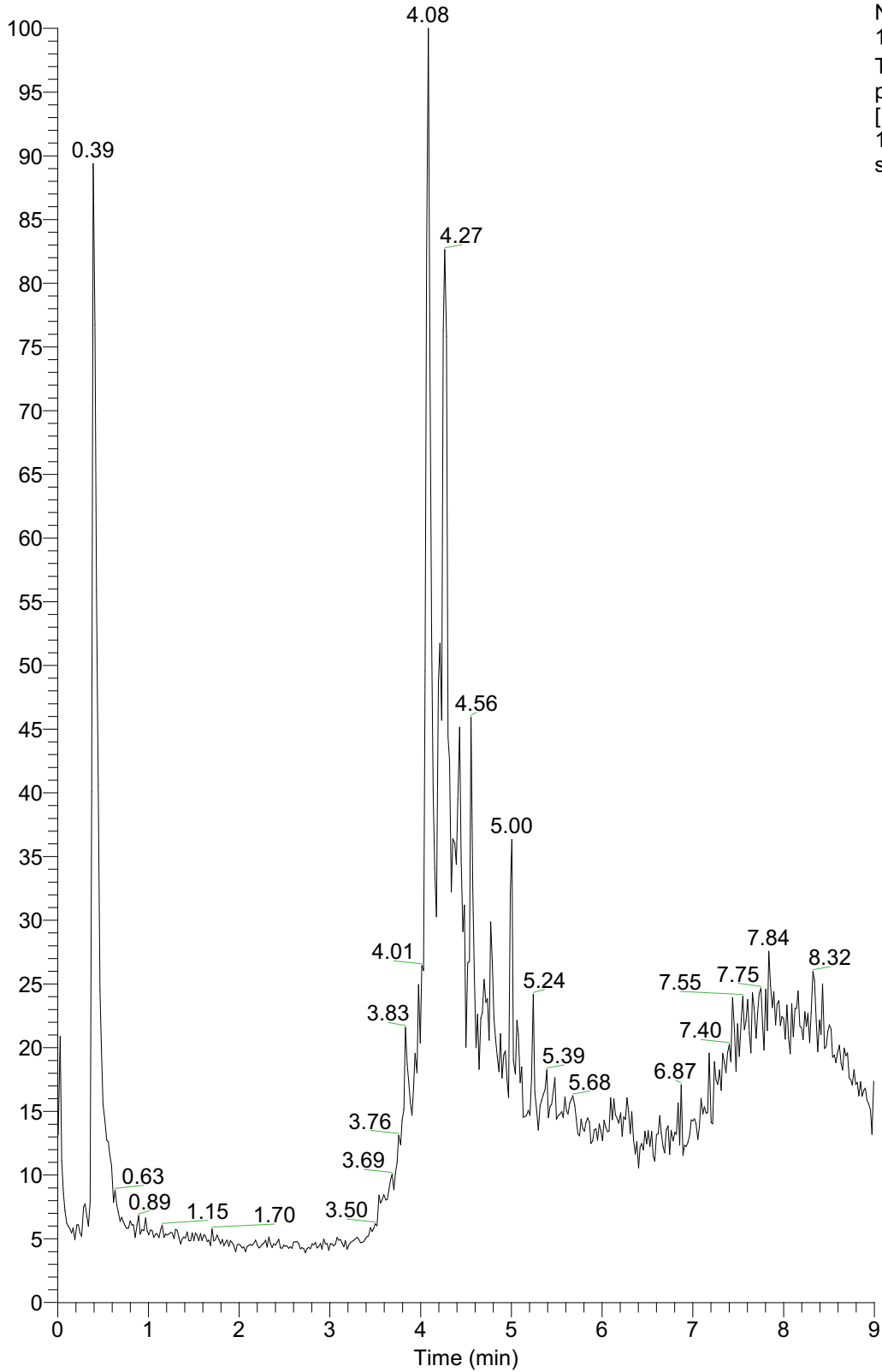
RT: 0.00 - 9.01



NL:  
1.81E9  
TIC F: FTMS -  
p ESI Full ms  
[100.0000-  
1200.0000] MS  
sample\_34

Figure S12: Representative chromatogram of a *S. ceratophylla* extract (sample S34).

RT: 0.00 - 9.00

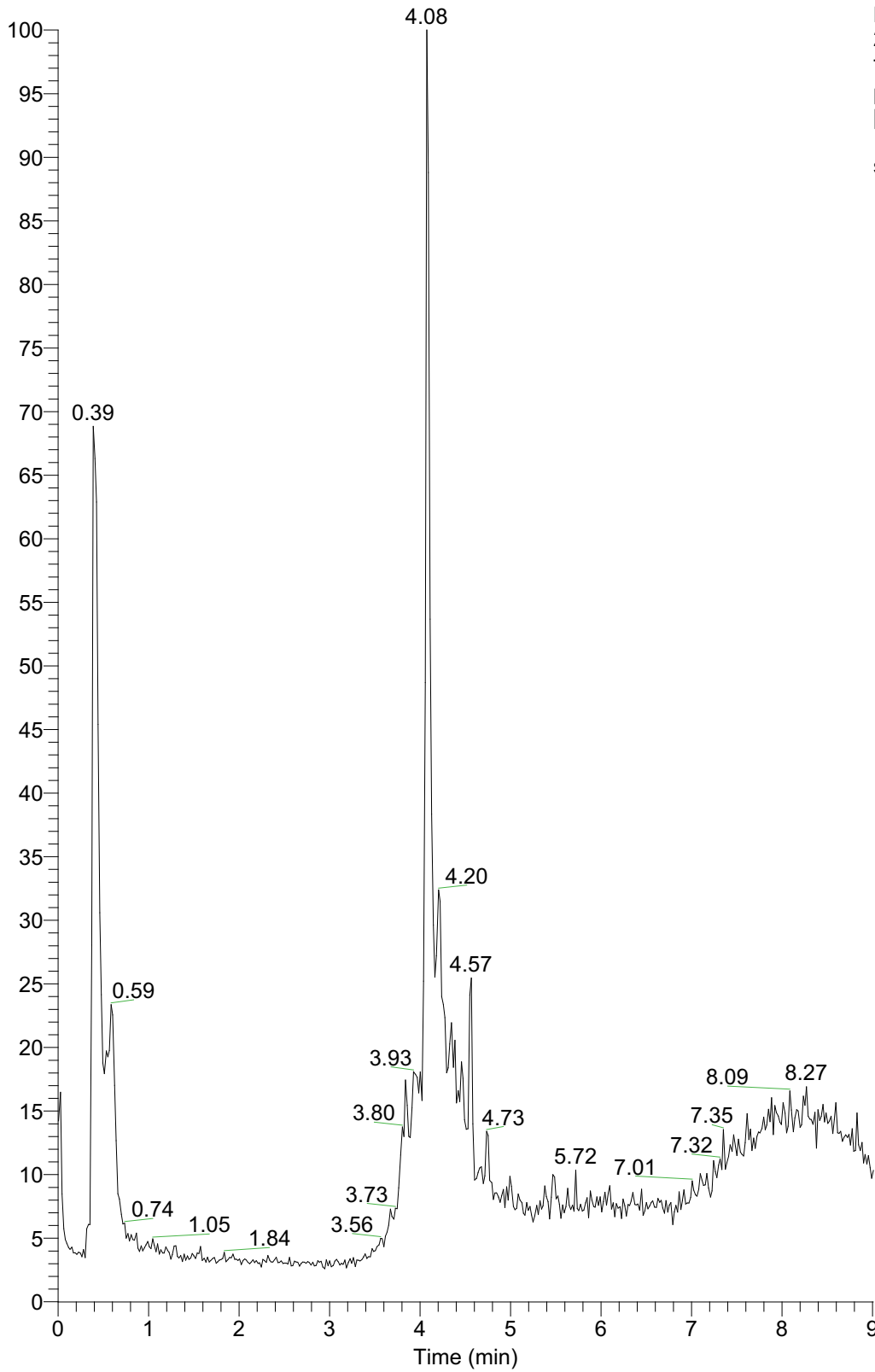


NL:  
1.54E9  
TIC F: FTMS -  
p ESI Full ms  
[100.0000-  
1200.0000] MS  
sample\_45

Figure S13: Representative chromatogram of an extract of *S. macrochlamys* (sample S45).



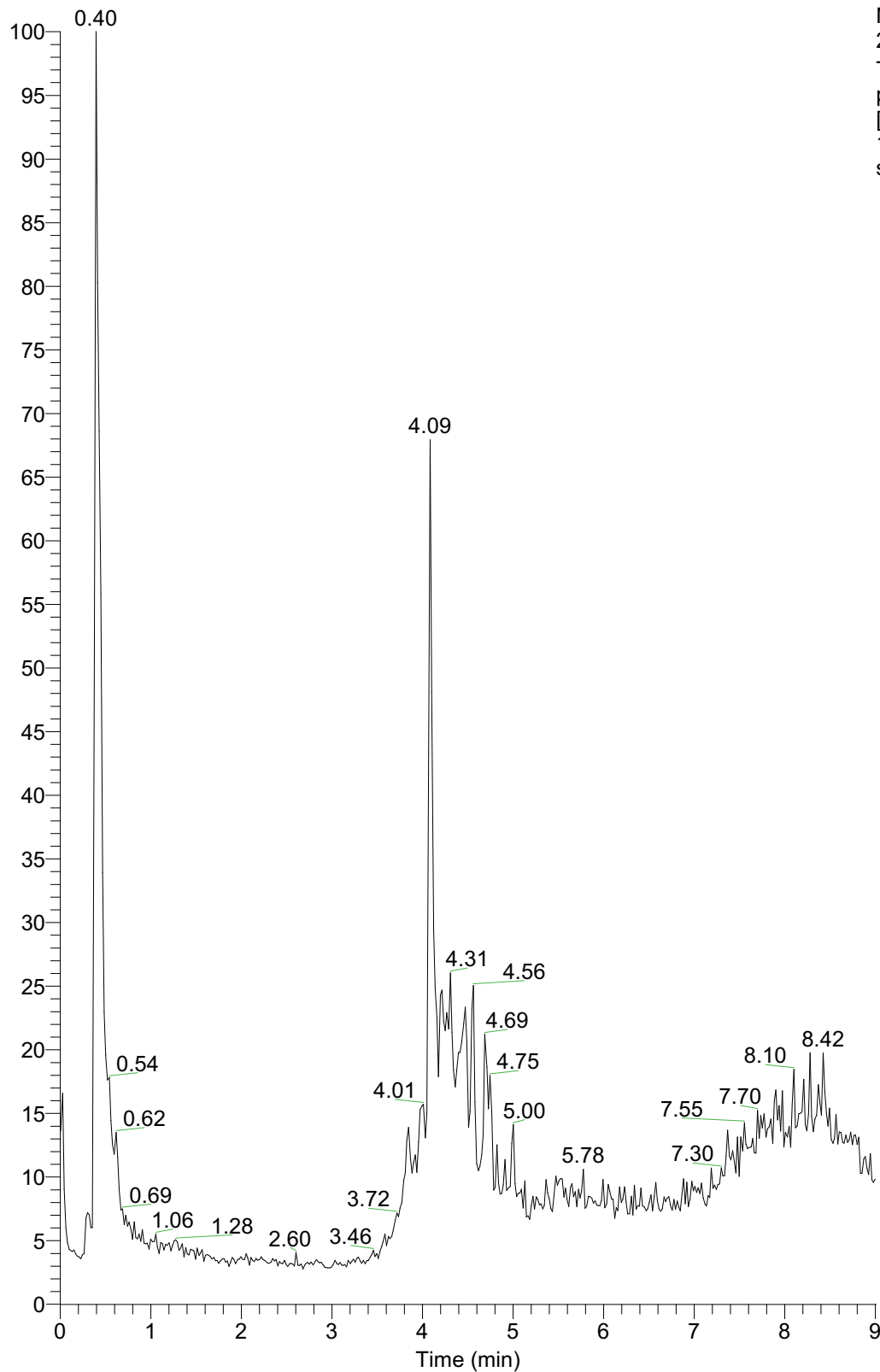
RT: 0.00 - 9.01



NL:  
2.32E9  
TIC F: FTMS -  
p ESI Full ms  
[100.0000-  
1200.0000] MS  
sample\_49

Figure S14: Representative chromatogram of an extract of *S. candidissima* (sample S49).

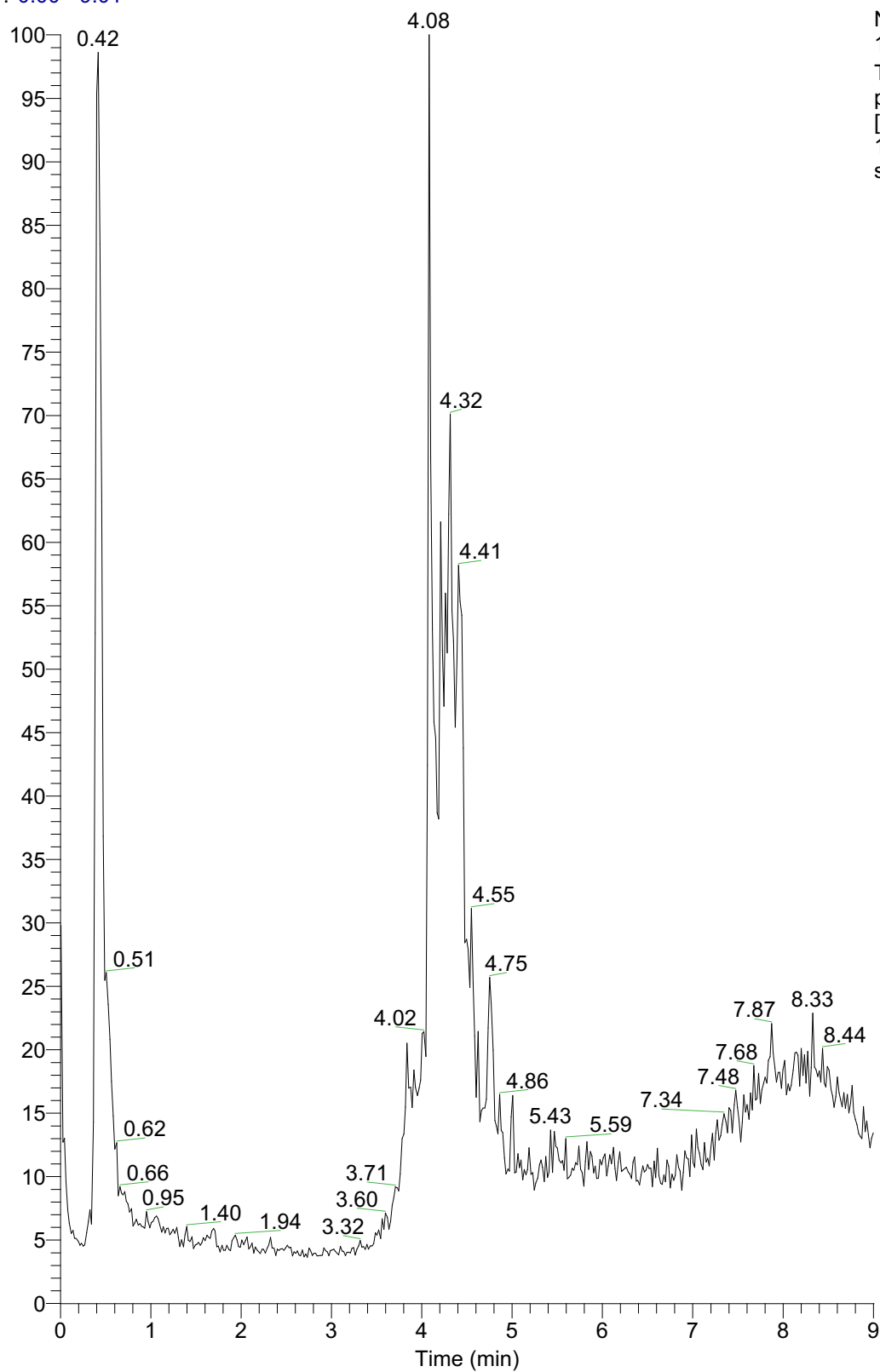
RT: 0.00 - 9.01



NL:  
2.35E9  
TIC F: FTMS -  
p ESI Full ms  
[100.0000-  
1200.0000] MS  
sample\_60

**Figure S15:** Representative chromatogram of a *S. aethiopsis* extract (sample S60).

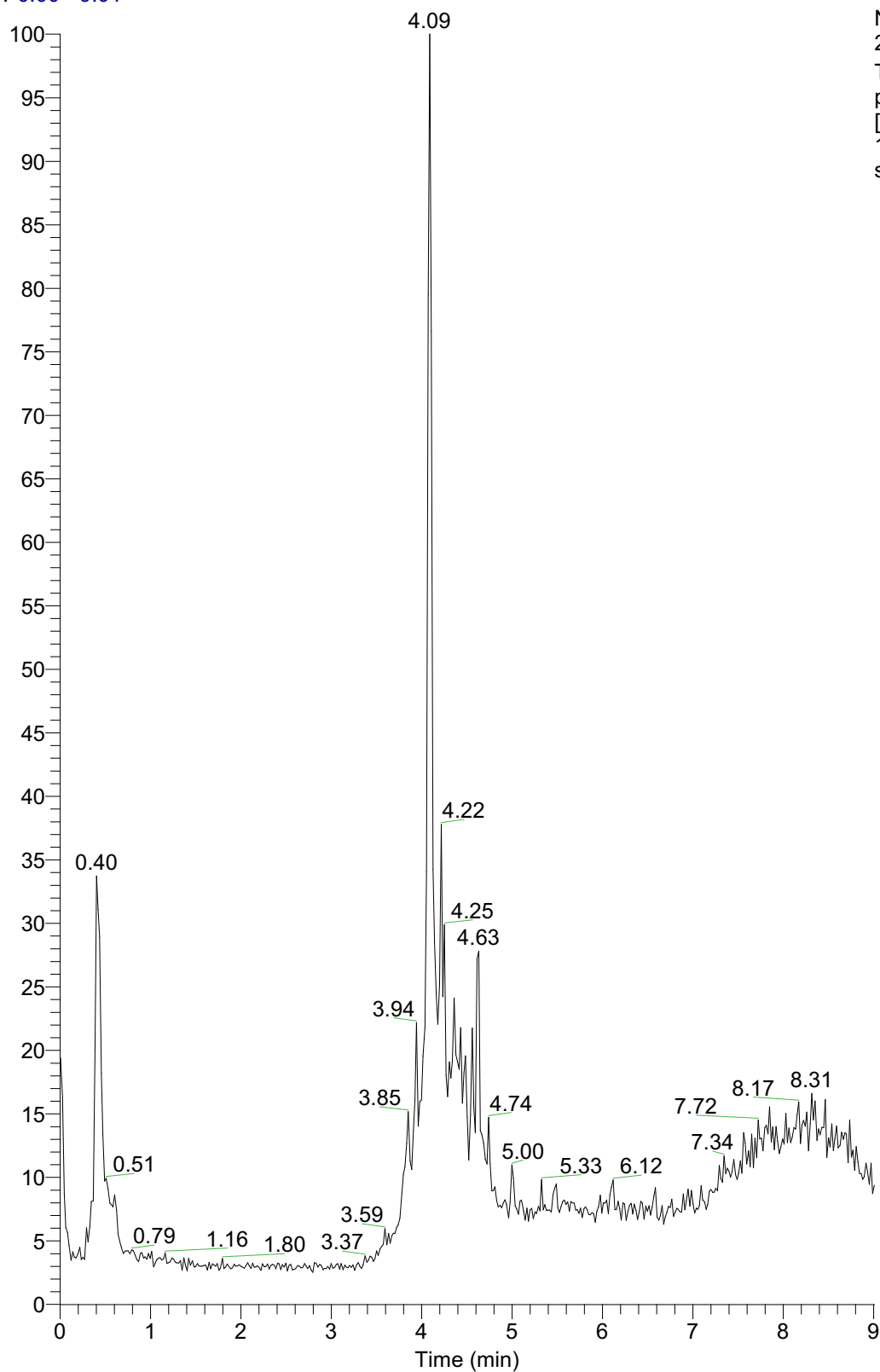
RT: 0.00 - 9.01



NL:  
1.91E9  
TIC F: FTMS -  
p ESI Full ms  
[100.0000-  
1200.0000] MS  
sample\_62

Figure S16: Representative chromatogram of an extract of *S. sahendica* (sample S62).

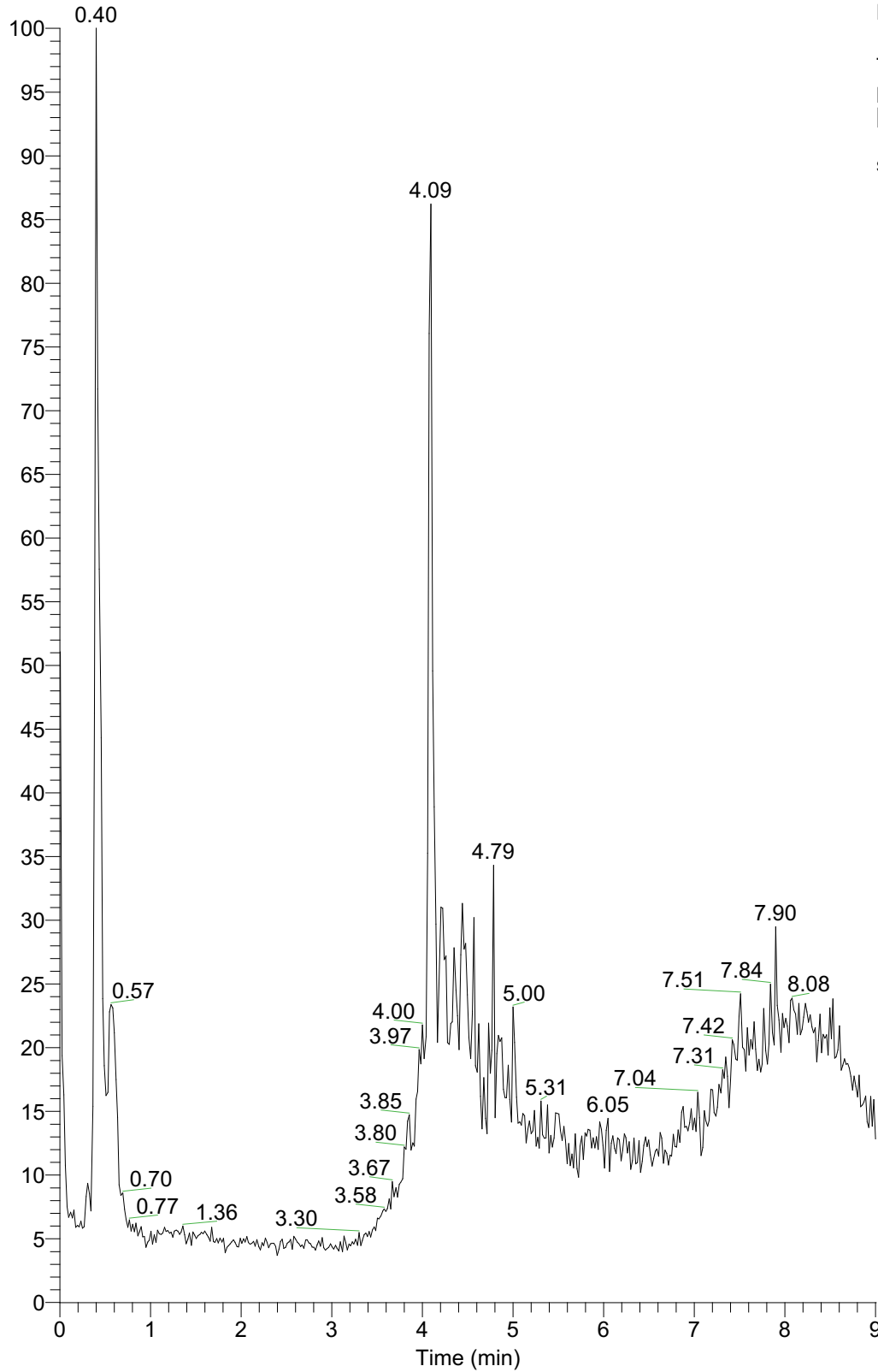
RT: 0.00 - 9.01



NL:  
2.33E9  
TIC F: FTMS -  
p ESI Full ms  
[100.0000-  
1200.0000] MS  
sample\_76

Figure S17: Representative chromatogram of an extract of *Salvia. sp* (sample S76).

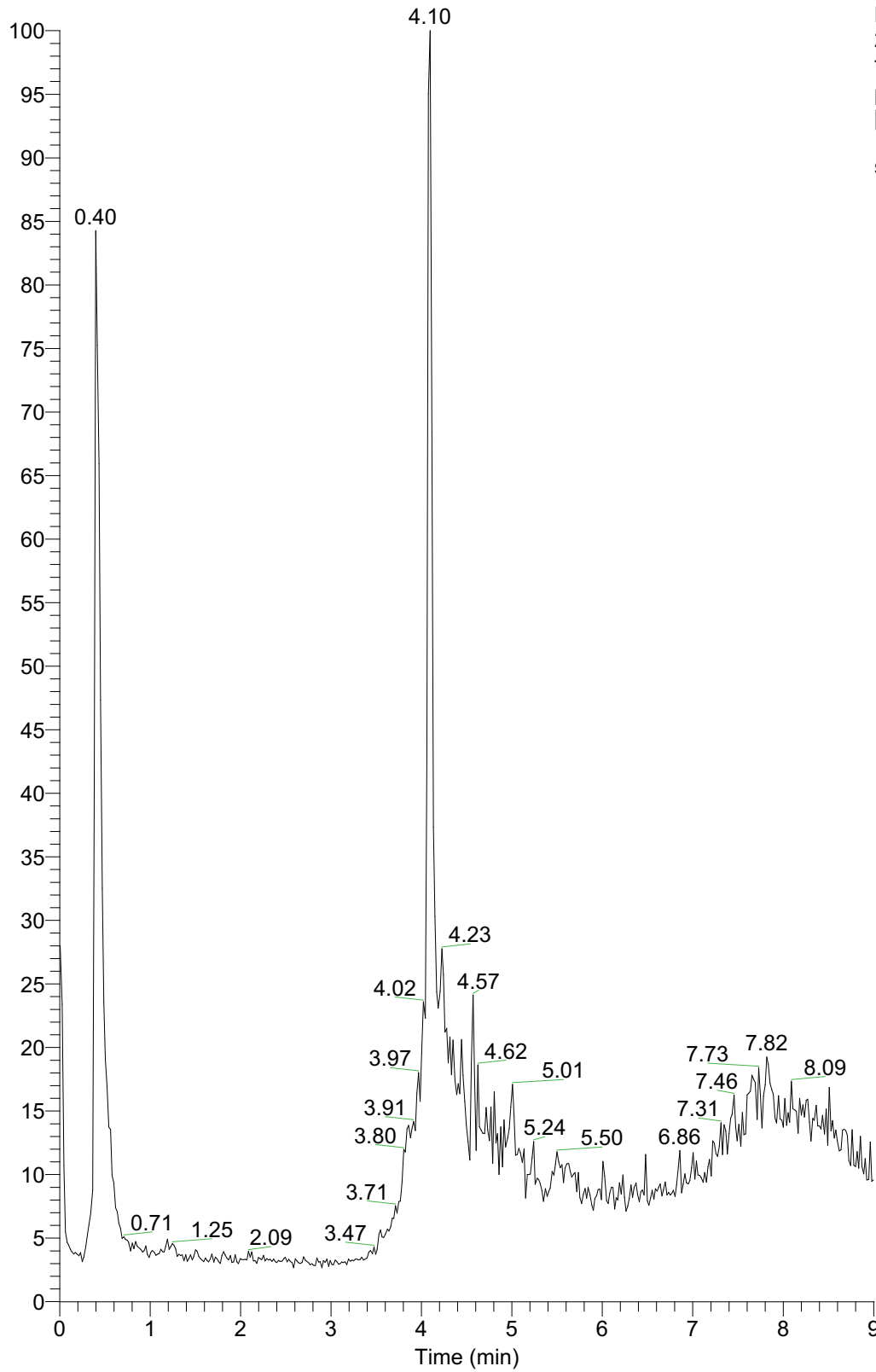
RT: 0.00 - 9.01



NL:  
1.48E9  
TIC F: FTMS -  
p ESI Full ms  
[100.0000-  
1200.0000] MS  
sample\_82

Figure S18: Representative chromatogram of an extract of *S. poculata* (sample S82).

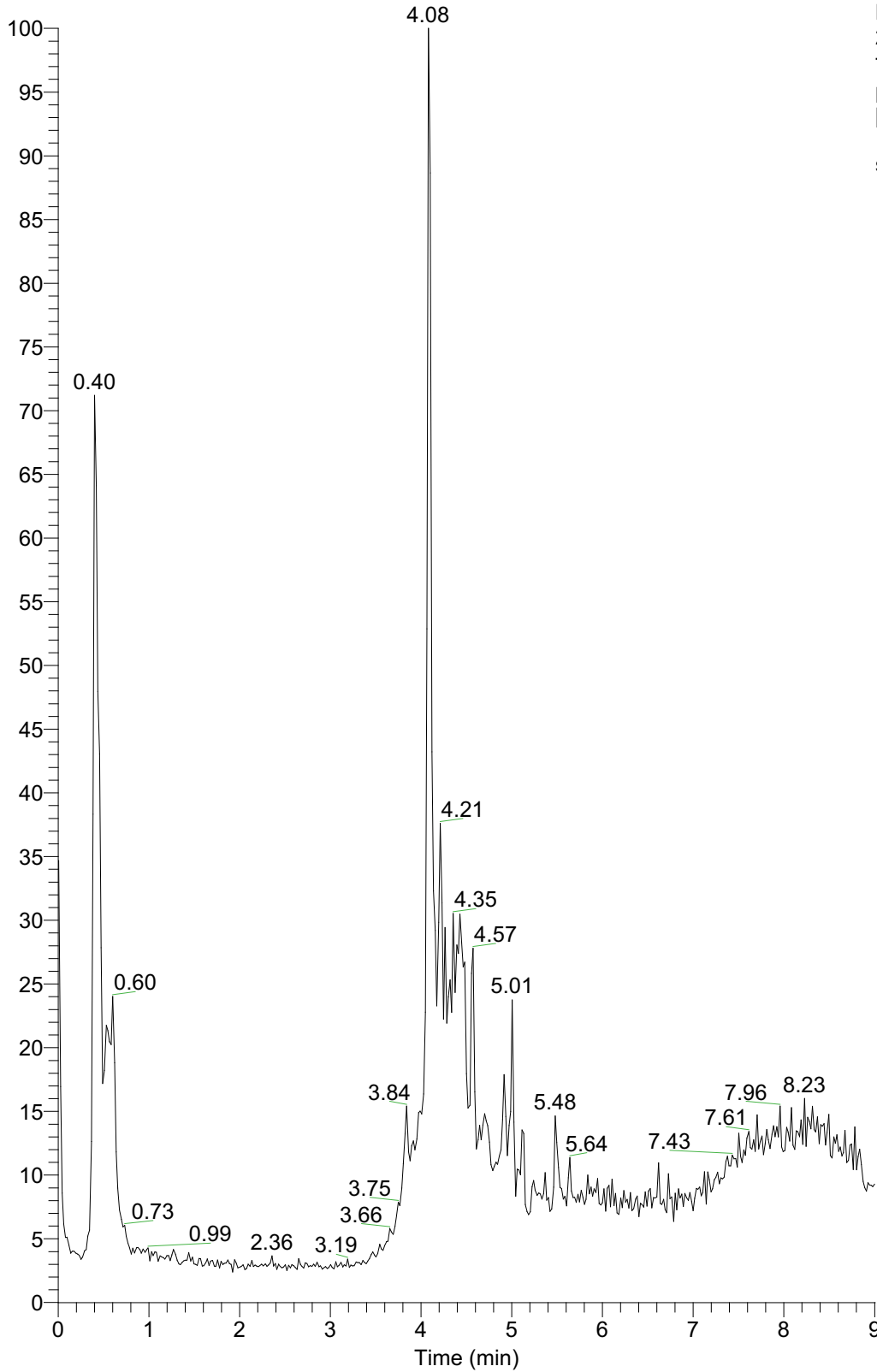
RT: 0.00 - 9.01



NL:  
2.21E9  
TIC F: FTMS -  
p ESI Full ms  
[100.0000-  
1200.0000] MS  
sample\_83

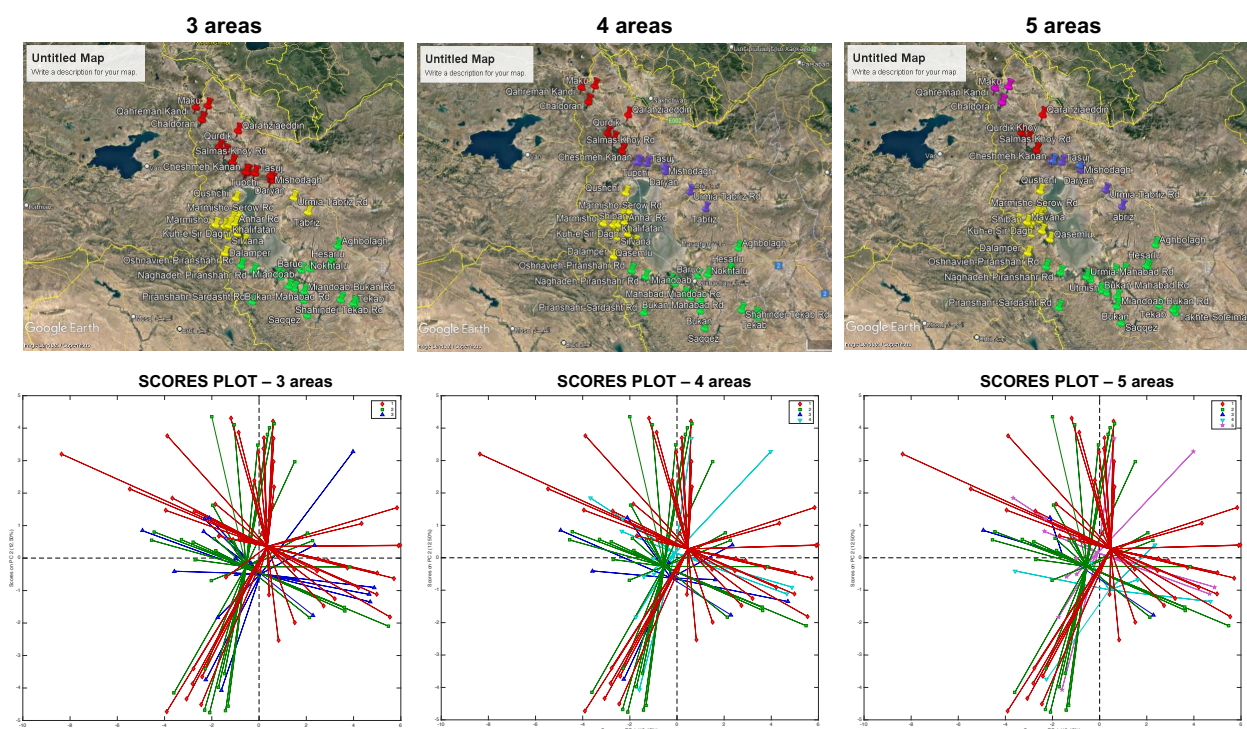
Figure S19: Representative chromatogram of an extract of *S. hydrangea* (sample S83).

RT: 0.00 - 9.01



NL:  
2.35E9  
TIC F: FTMS -  
p ESI Full ms  
[100.0000-  
1200.0000] MS  
sample\_88

**Figure S20:** Representative chromatogram of an extract of *S. grossheimii* (sample S88).



**Figure S21:** (Top) Satellite image of West Azerbaijan Province showing 3, 4 or 5 distinct collection areas where *Salvia* samples were picked. (Bottom) PCA scores plot coloured by collection areas obtained from the data of the 10 colorimetric determinations (TPC, TFC, TTC, AAC, FRAP, DPPH, Ca, Cb, Cxc, and  $\beta$ -carotene) and 40 chemical compounds identified for the 102 *Salvia* extracts. No significant separation was observed. Keys (left satellite image): 1<sup>st</sup> collection area, red; 2<sup>nd</sup> collection area, yellow; 3<sup>rd</sup> collection area, green. Keys (middle satellite image): 1<sup>st</sup> collection area, red; 2<sup>nd</sup> collection area, purple; 3<sup>rd</sup> collection area, yellow; 4<sup>th</sup> collection area, green. Keys (right satellite image): 1<sup>st</sup> collection area, red; 2<sup>nd</sup> collection area, purple; 3<sup>rd</sup> collection area, yellow; 4<sup>th</sup> collection area, green; 5<sup>th</sup> collection area, pink. Keys (left PCA scores plot): 1<sup>st</sup> collection area, red; 2<sup>nd</sup> collection area, green; 3<sup>rd</sup> collection area, blue. Keys (middle PCA scores plot): 1<sup>st</sup> collection area, red; 2<sup>nd</sup> collection area, green; 3<sup>rd</sup> collection area, blue; 4<sup>th</sup> collection area, light blue. Keys (right PCA scores plot): 1<sup>st</sup> collection area, red; 2<sup>nd</sup> collection area, green; 3<sup>rd</sup> collection area, blue; 4<sup>th</sup> collection area, light blue; 5<sup>th</sup> collection area, pink.