

**Fig. S7a**

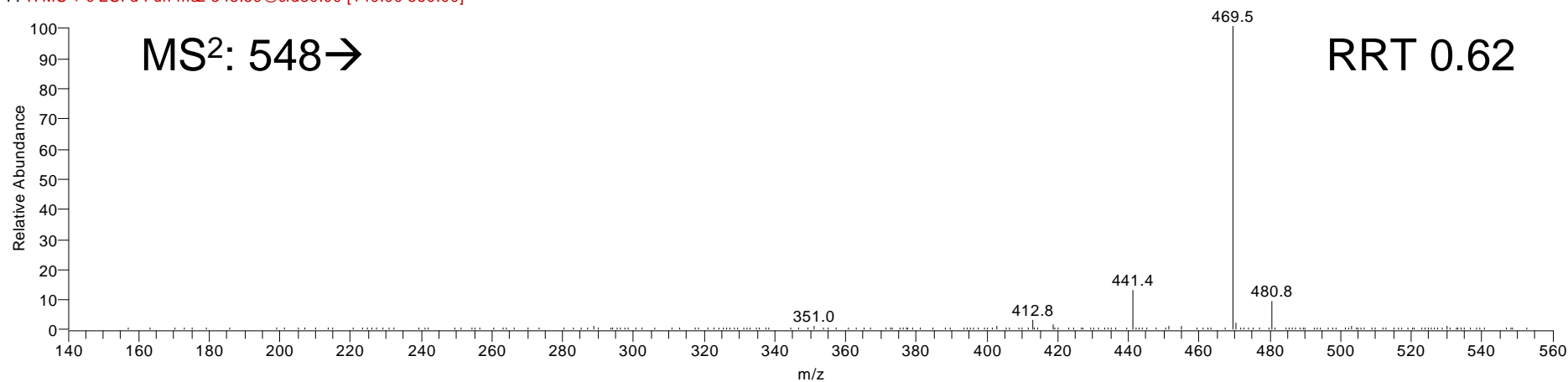
# CA<sup>4</sup>-3-one 3-GP

c:\documents and settings\...\sample\_33

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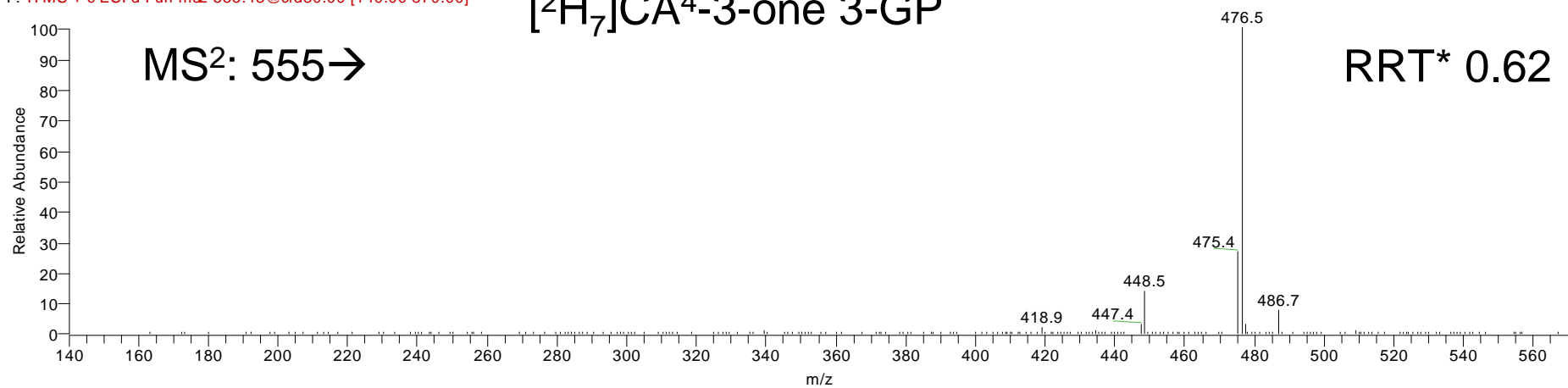
sample

Sample\_502673\_2\_12 #827 RT: 8.09 AV: 1 NL: 7.49E3  
F: ITMS + c ESI d Full ms2 548.39@cid30.00 [140.00-560.00]



sample\_33 #791 RT: 7.79 AV: 1 NL: 1.13E4  
F: ITMS + c ESI d Full ms2 555.43@cid30.00 [140.00-570.00]

## [<sup>2</sup>H<sub>7</sub>]CA<sup>4</sup>-3-one 3-GP



**Fig. S7b****CA<sup>4</sup>-3-one 3-GP**

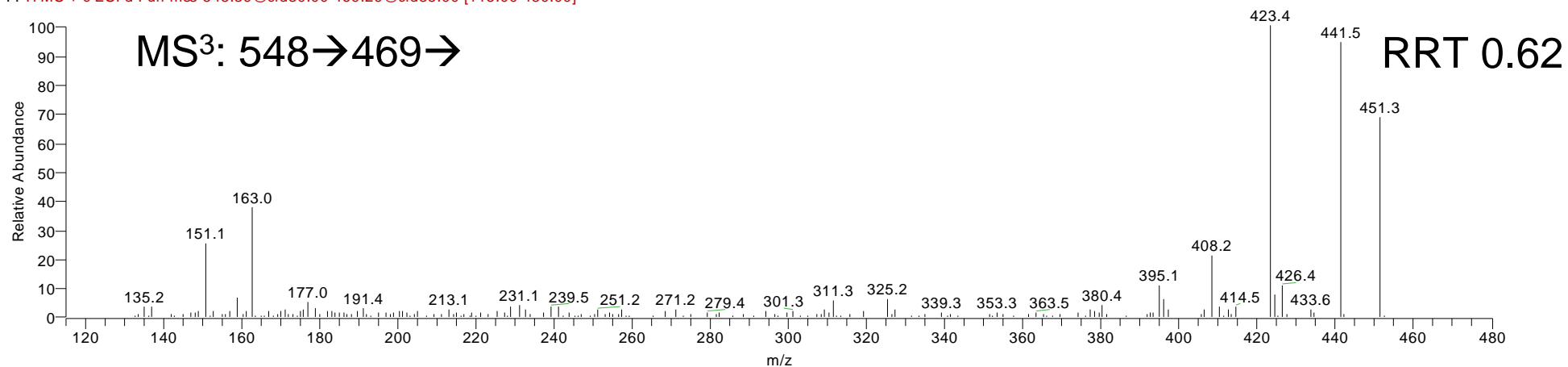
c:\documents and settings\...\sample\_33

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sample

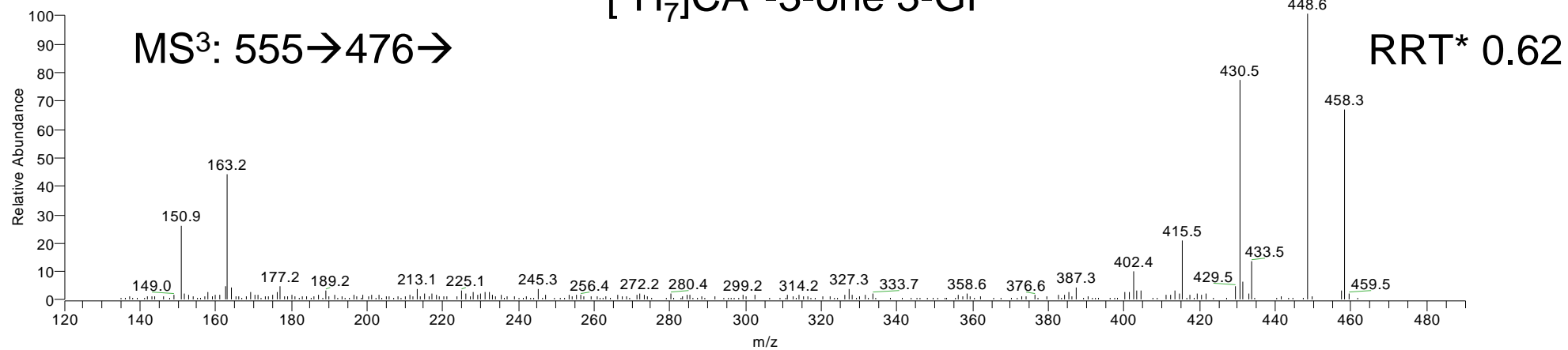
Sample\_502673\_2\_12 #828 RT: 8.10 AV: 1 NL: 4.33E2

F: ITMS + c ESI d Full ms3 548.39@cid30.00 469.29@cid35.00 [115.00-480.00]



sample\_33 #792 RT: 7.80 AV: 1 NL: 8.78E2

F: ITMS + c ESI d Full ms3 555.43@cid30.00 476.41@cid35.00 [120.00-490.00]

**[<sup>2</sup>H<sub>7</sub>]CA<sup>4</sup>-3-one 3-GP**

**Fig. S7c**

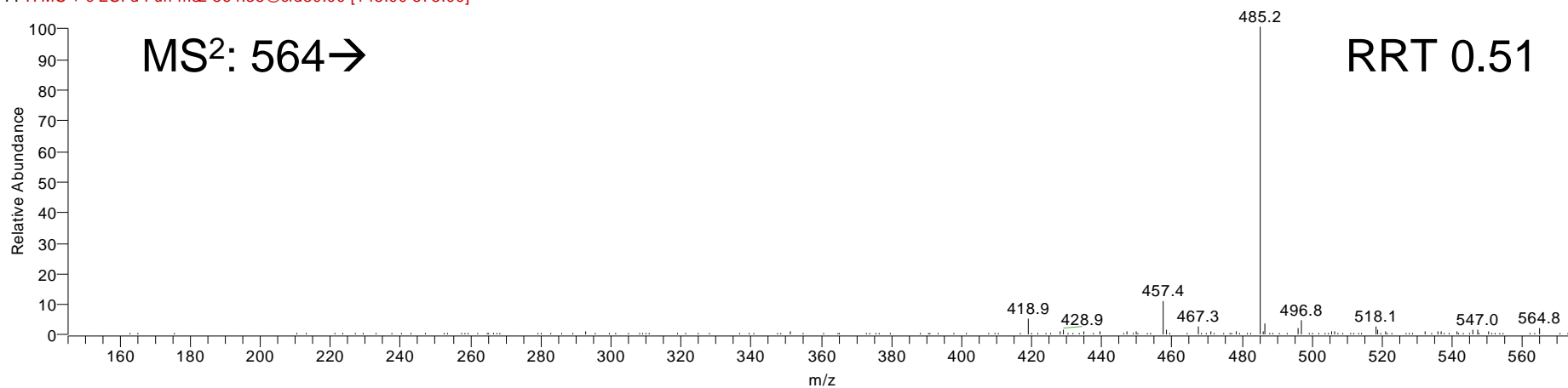
**CA<sup>4</sup>-7 $\alpha$ -ol-3-one 3-GP**

Sample\_502673\_2\_11\_x2

27/07/2007 15:46:16

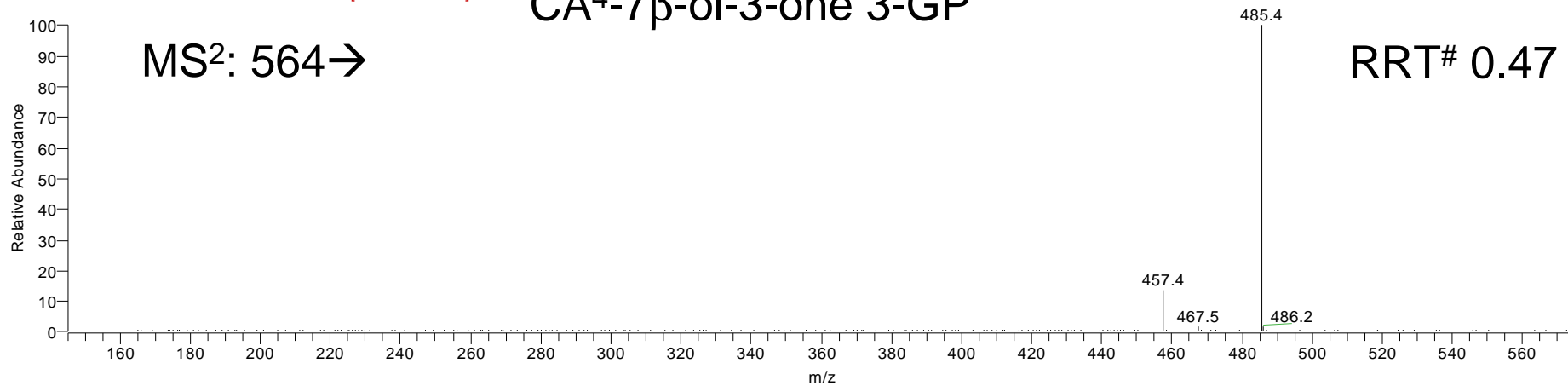
sample

Sample\_502673\_2\_11\_x2 #658 RT: 6.53 AV: 1 NL: 2.14E3  
F: ITMS + c ESI d Full ms2 564.38@cid30.00 [145.00-575.00]



sample\_37 #584 RT: 5.83 AV: 1 NL: 1.16E5  
F: ITMS + c ESI d Full ms2 564.38@cid30.00 [145.00-575.00]

**CA<sup>4</sup>-7 $\beta$ -ol-3-one 3-GP**



**Fig. S7d****CA<sup>4</sup>-7 $\alpha$ -ol-3-one 3-GP**

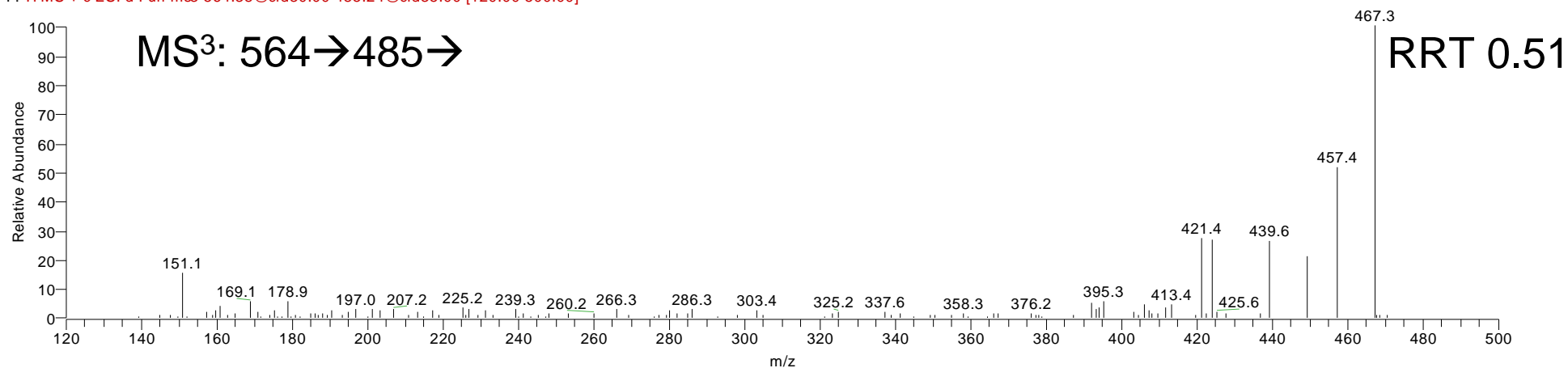
Sample\_502673\_2\_11\_x2

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sample

Sample\_502673\_2\_11\_x2 #659 RT: 6.53 AV: 1 NL: 2.08E2

F: ITMS + c ESI d Full ms3 564.38@cid30.00 485.24@cid35.00 [120.00-500.00]



sample\_37 #585 RT: 5.83 AV: 1 NL: 1.24E4

F: ITMS + c ESI d Full ms3 564.38@cid30.00 485.20@cid35.00 [120.00-500.00]

**CA<sup>4</sup>-7 $\beta$ -ol-3-one 3-GP**