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**Brandt, SD, Elliott, SP, Kavanagh, PV, Dempster, NM, Meyer, MR, Maurer, HH and Nichols, DE**

**Analytical characterization of bioactive N-benzyl-substituted phenethylamines and 5-methoxytryptamines**

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### Article

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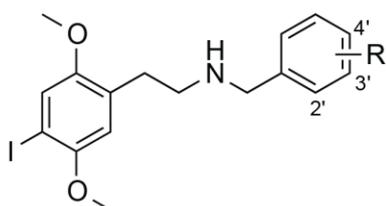
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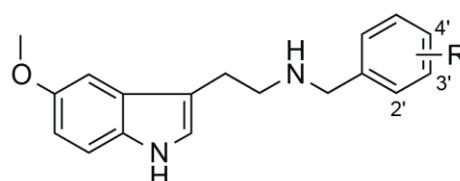
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## SUPPORTING INFORMATION

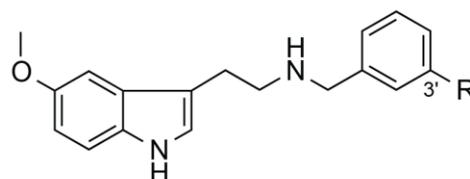
### Analytical characterization of bioactive *N*-benzyl-substituted phenethylamines and 5-methoxytryptamines



- (1a): R = 2'-OCH<sub>3</sub> (25I-NB2OMe) - **manuscript**  
(1b): R = 3'-OCH<sub>3</sub> (25I-NB3OMe) - **manuscript**  
(1c): R = 4'-OCH<sub>3</sub> (25I-NB4OMe) - **manuscript**  
(1d): R = 2'-Br (25I-NB2B) - suppl. information  
(1e): R = 3'-Br (25I-NB3B) - suppl. information  
(1f): R = 4'-Br (25I-NB4B) - suppl. information



- (2a): R = 2'-OCH<sub>3</sub> (5MT-NB2OMe) - **manuscript**  
(2b): R = 3'-OCH<sub>3</sub> (5MT-NB3OMe) - **manuscript**  
(2c): R = 4'-OCH<sub>3</sub> (5MT-NB4OMe) - **manuscript**  
(2d): R = 2'-Br (5MT-NB2B) - suppl. information  
(2e): R = 3'-Br (5MT-NB3B) - suppl. information  
(2f): R = 4'-Br (5MT-NB4B) - suppl. information



- (3a): R = CF<sub>3</sub> (5MT-NB3TFM) - suppl. information  
(3b): R = F (5MT-NB3F) - suppl. information  
(3c): R = CH<sub>3</sub> (5MT-NB3Me) - suppl. information  
(3d): R = Cl (5MT-NB3Cl) - suppl. information  
(3e): R = I (5MT-NB3I) - suppl. information  
(3f): R = SCH<sub>3</sub> (5MT-NB3SMe) - suppl. information

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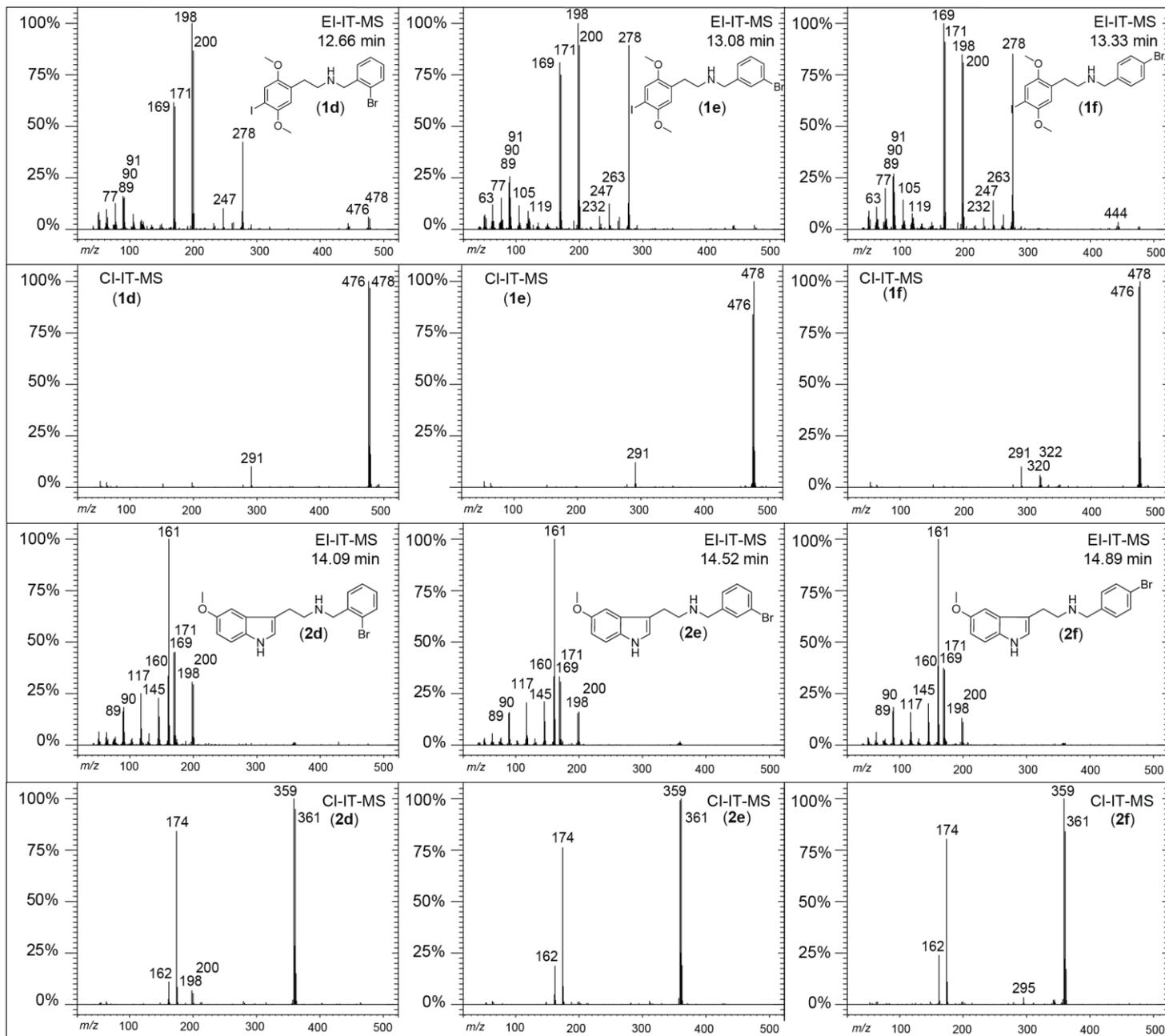
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**Page 22:** ATR-FT/IR spectra of *N*-(methoxybenzyl)-substituted 5-methoxytryptamines (**2a**)–(**2c**).

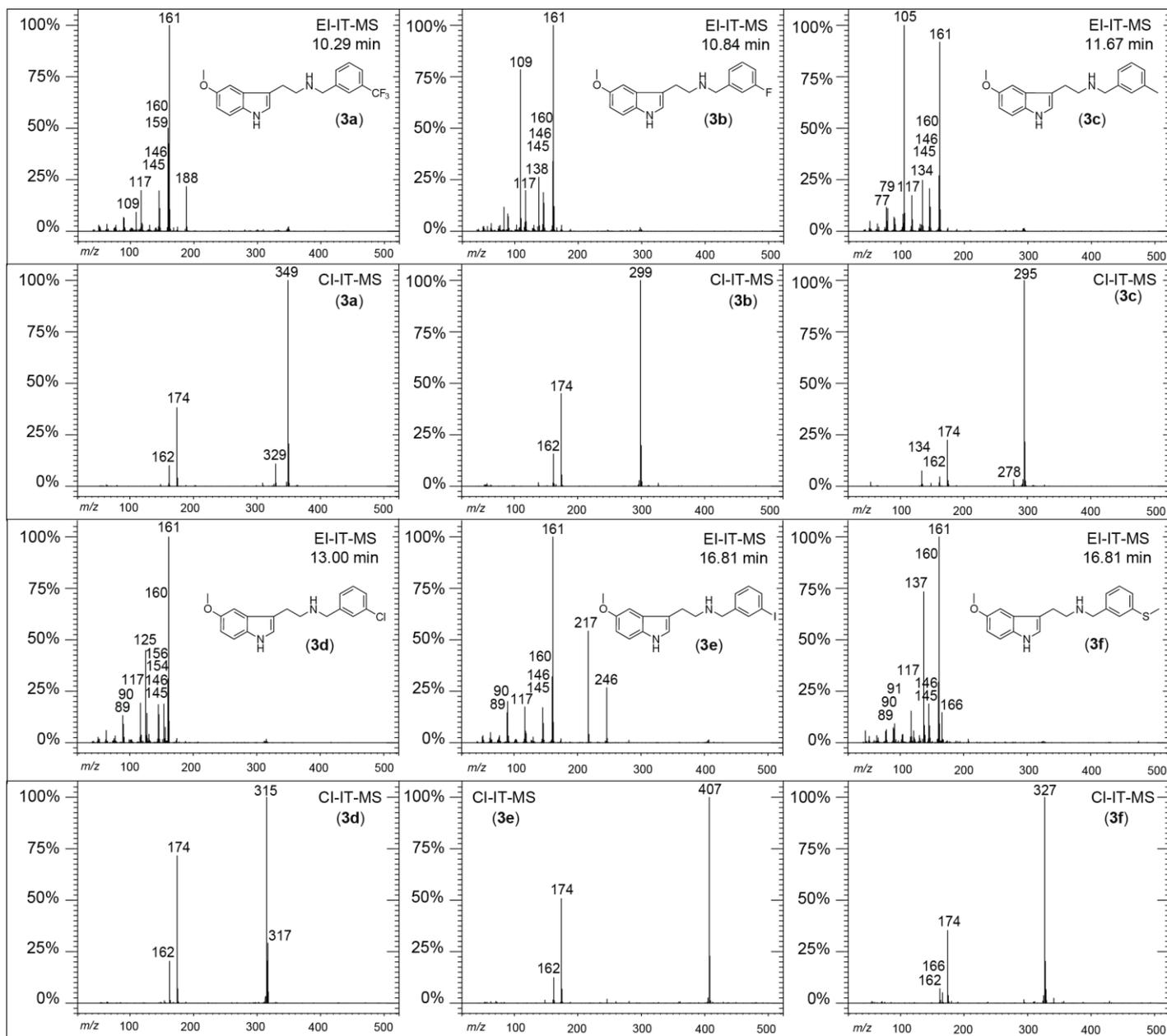
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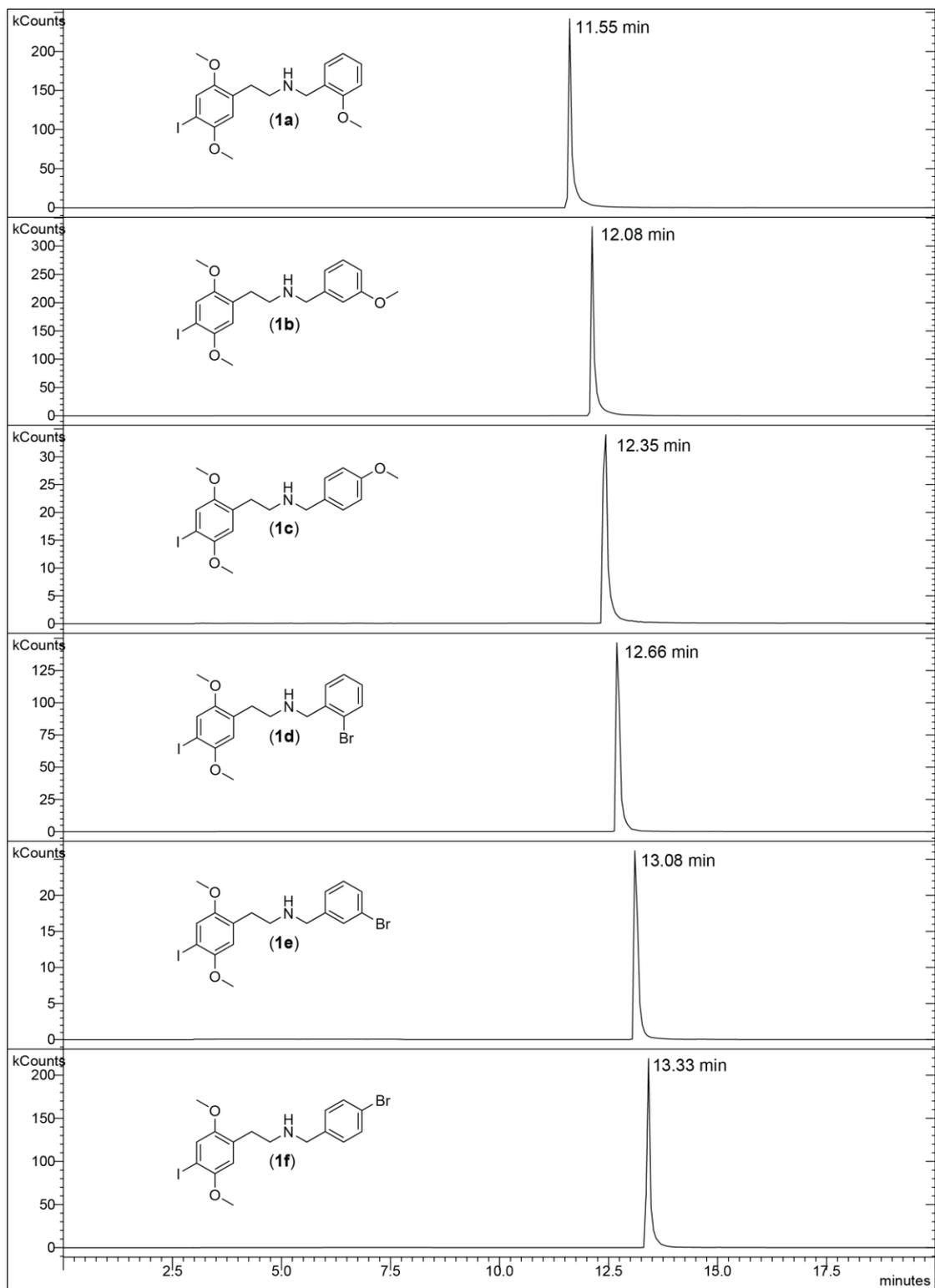
**Page 23:** ATR-FT/IR spectra of *N*-(methoxybenzyl)-substituted 5-methoxytryptamines (**3d**)–(**3f**).



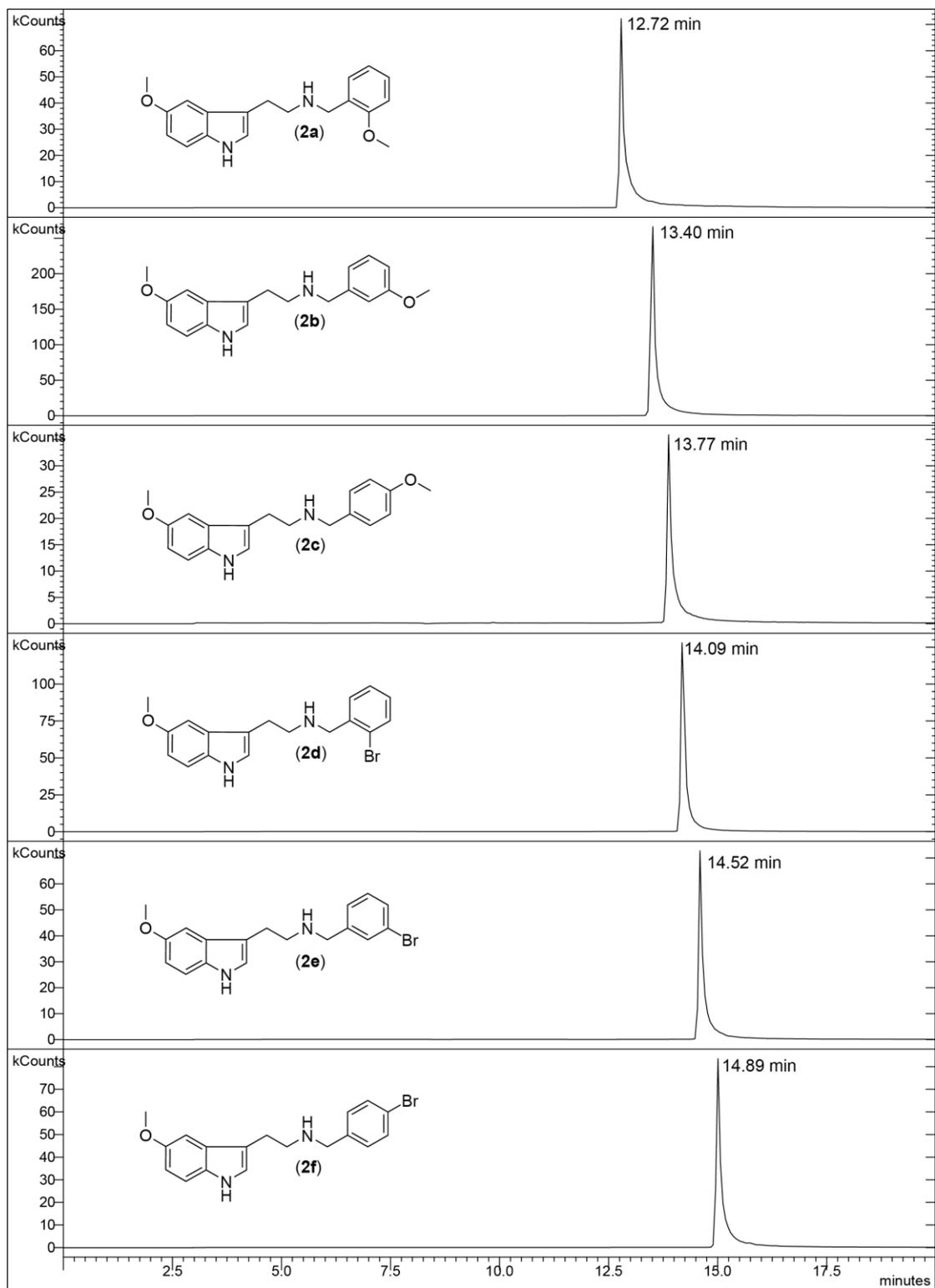
GC/MS retention times, EI- and CI ion trap mass spectra



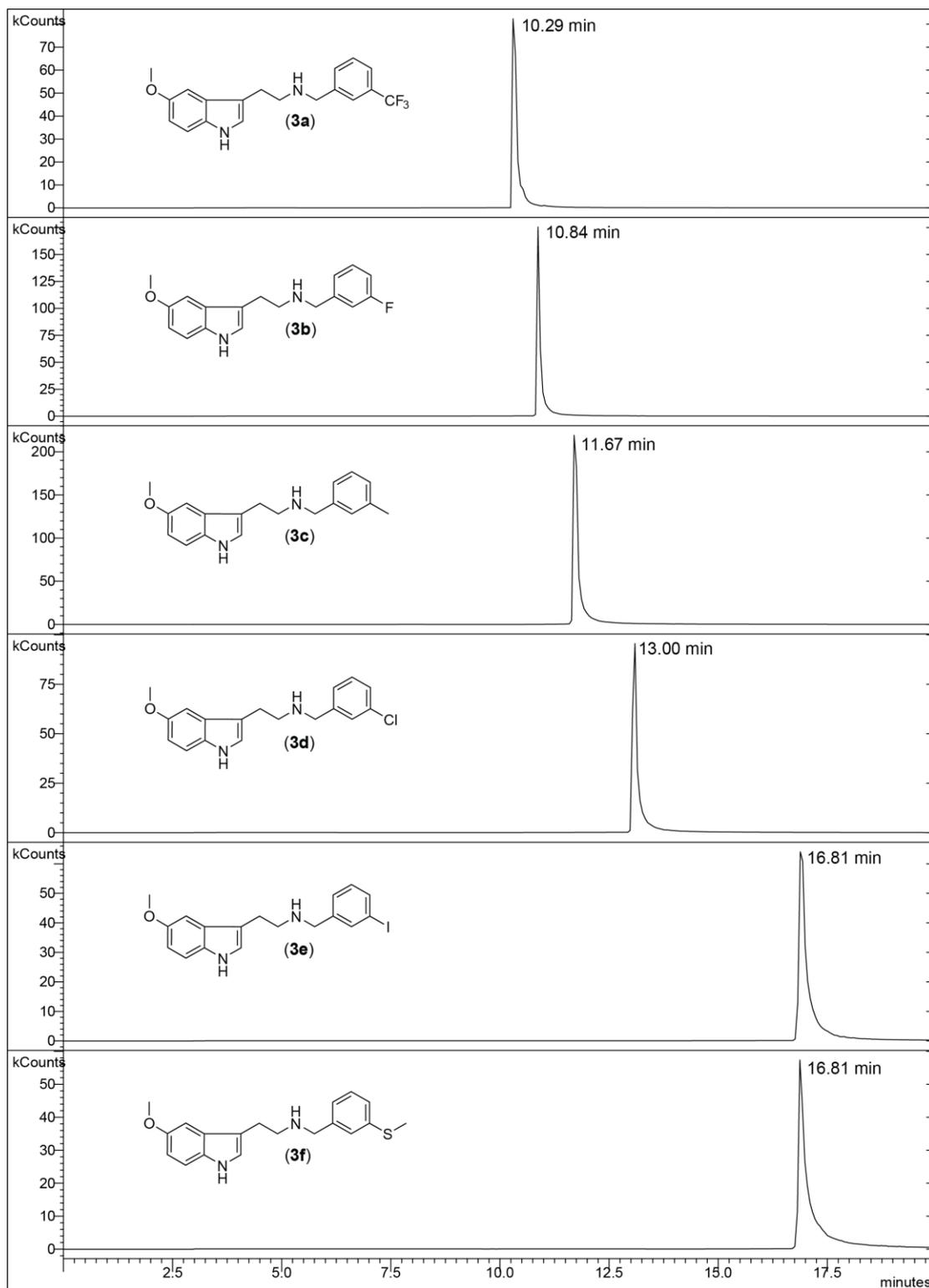
GC/MS retention times, EI- and CI ion trap mass spectra



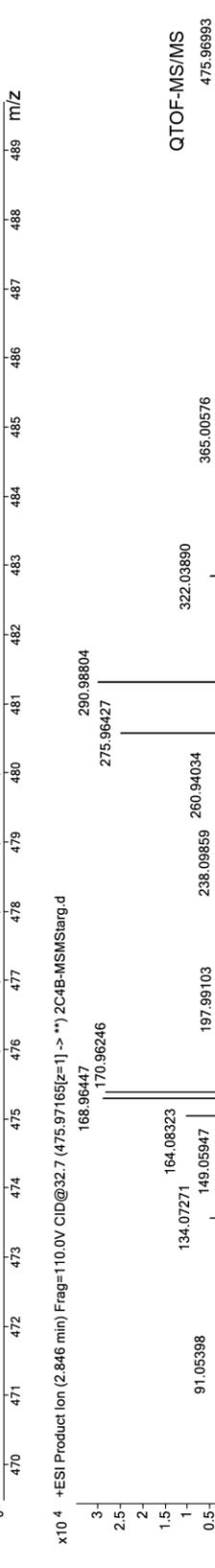
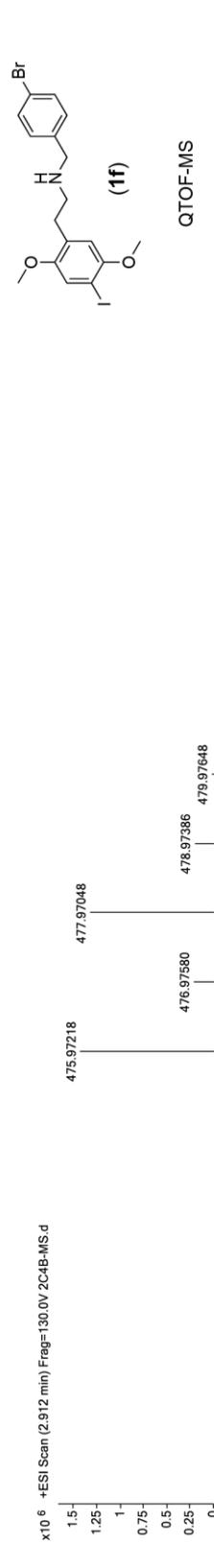
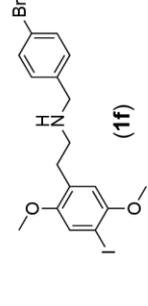
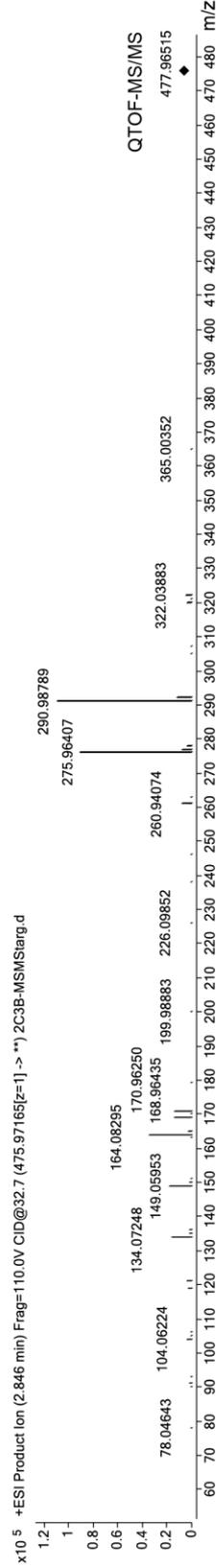
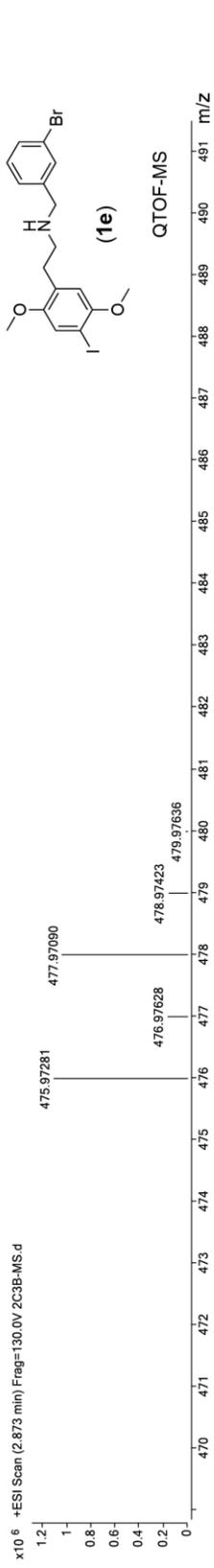
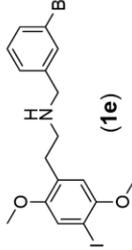
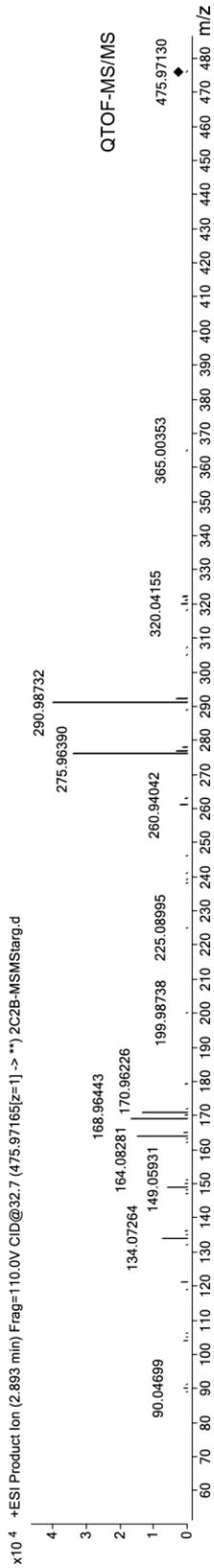
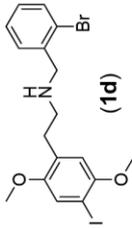
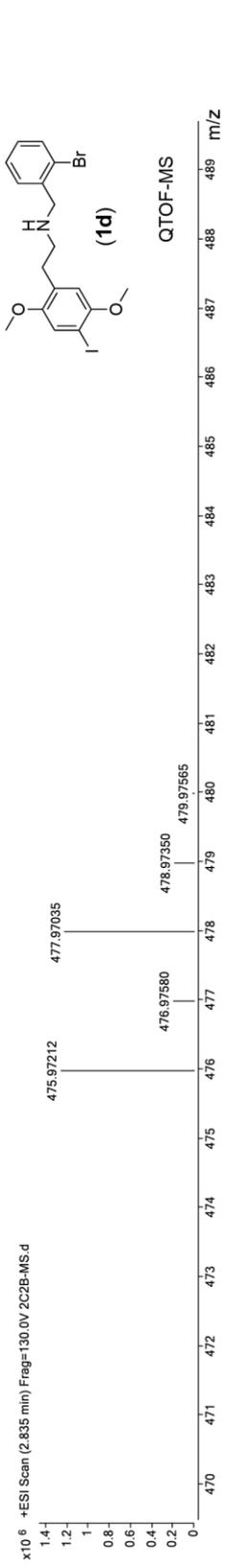
GC/MS chromatograms



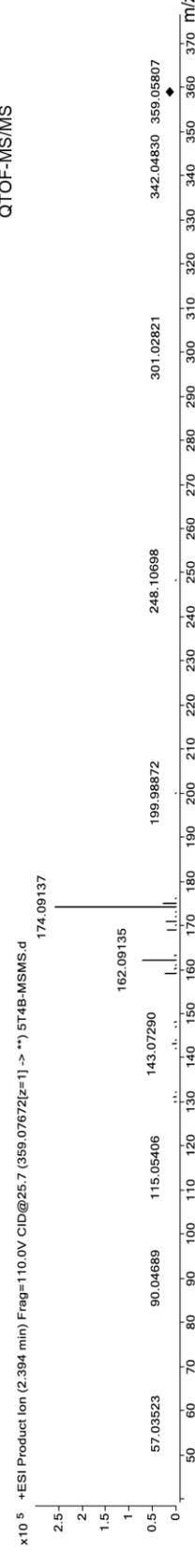
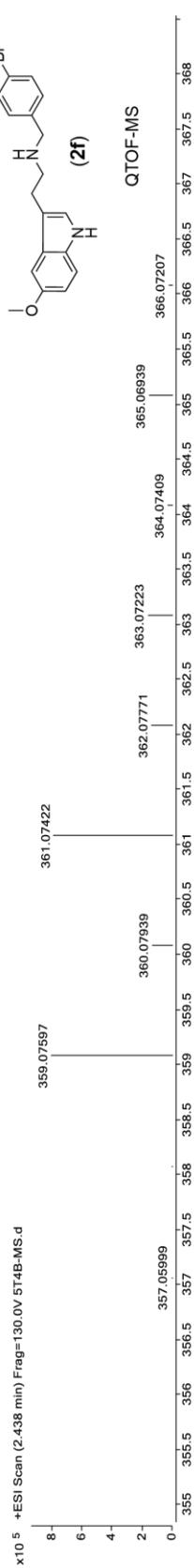
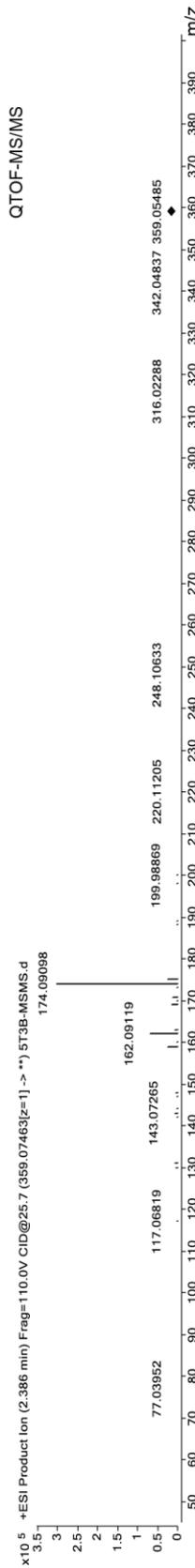
GC/MS chromatograms



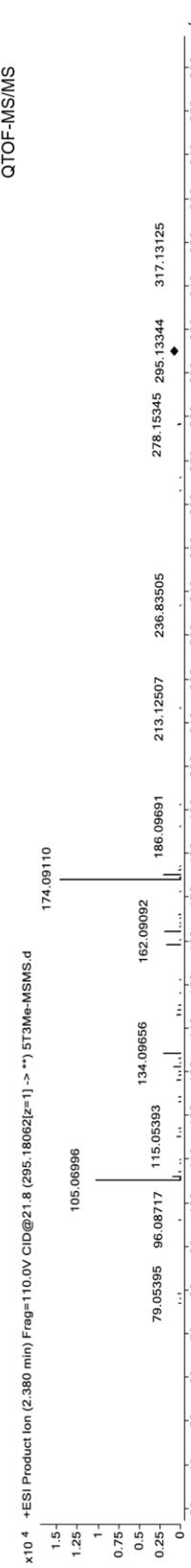
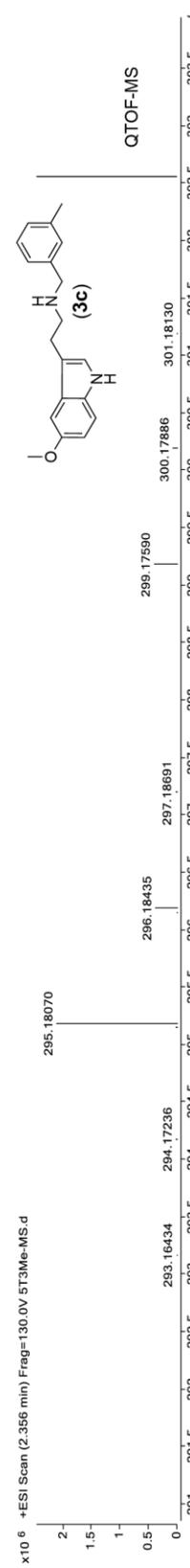
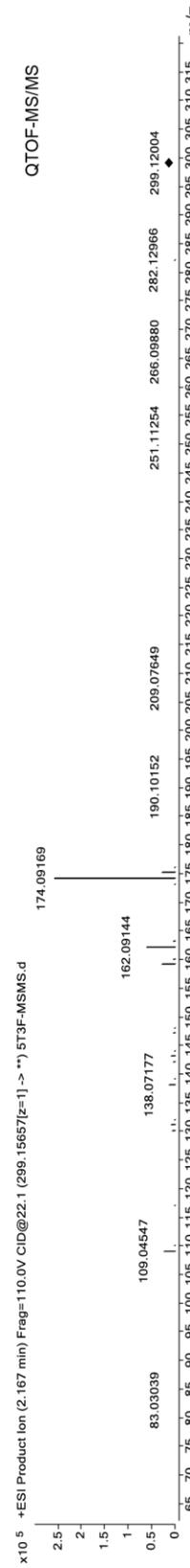
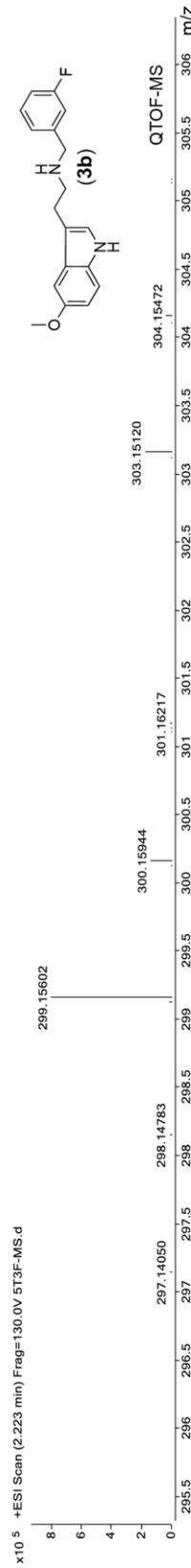
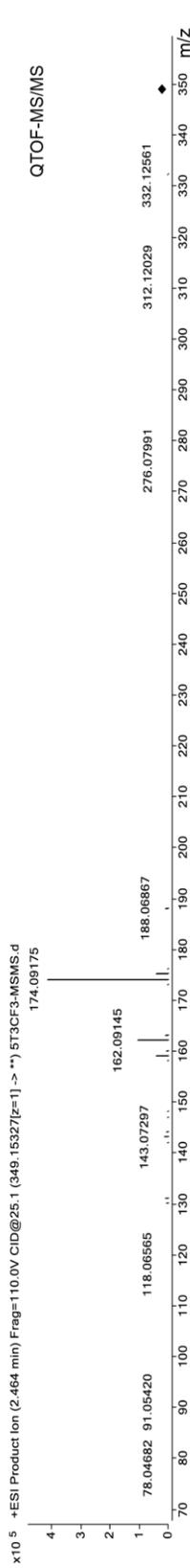
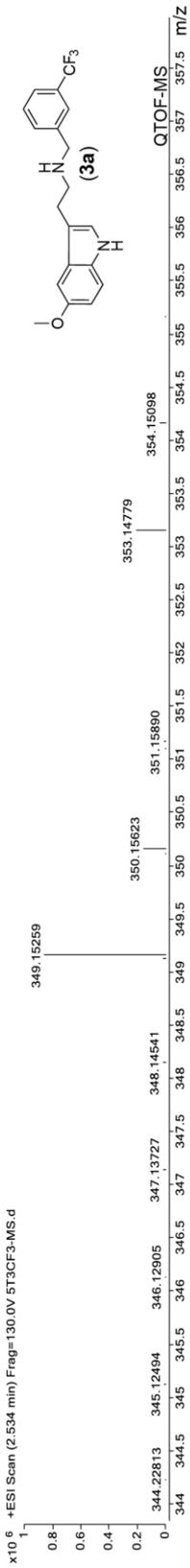
GC/MS chromatograms



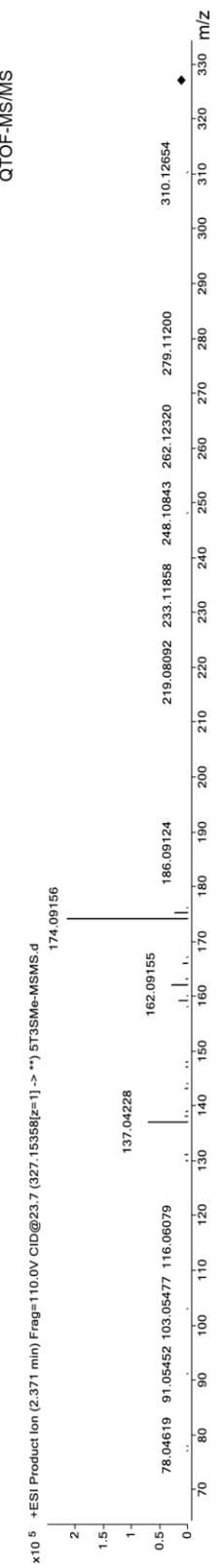
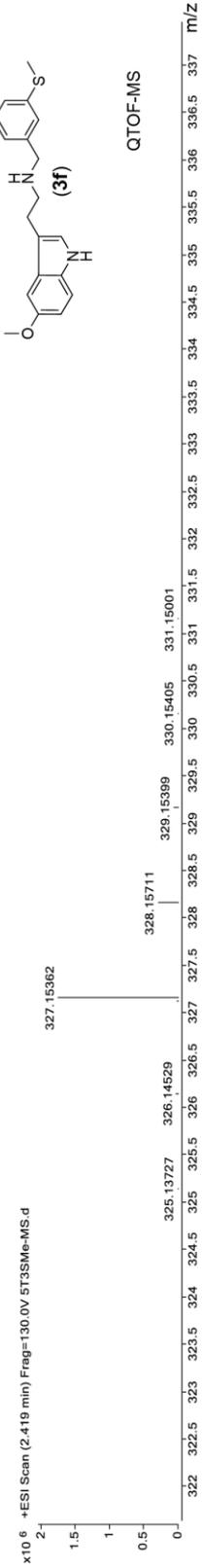
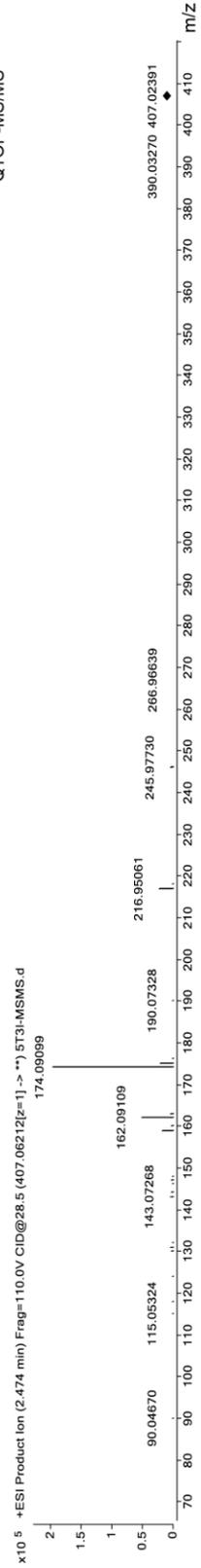
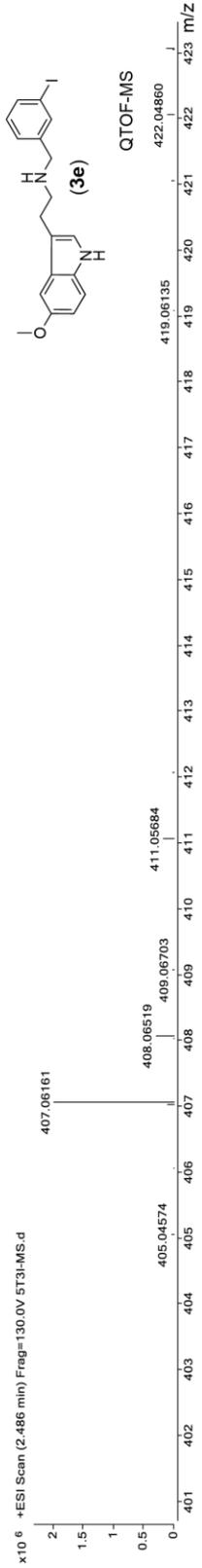
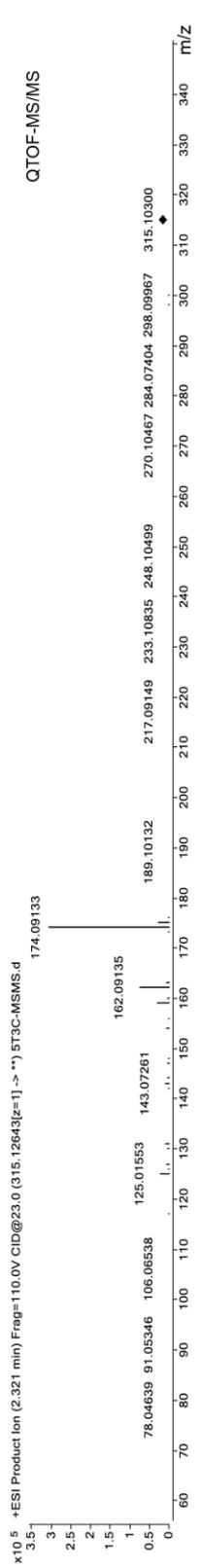
QTOF-MS and QTOF-MS/MS



QTOF-MS and QTOF-MS/MS

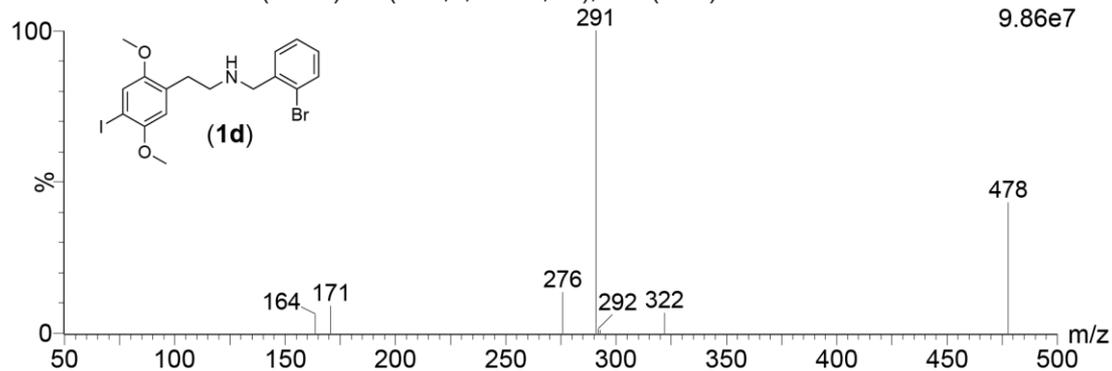


QTOF-MS and QTOF-MS/MS

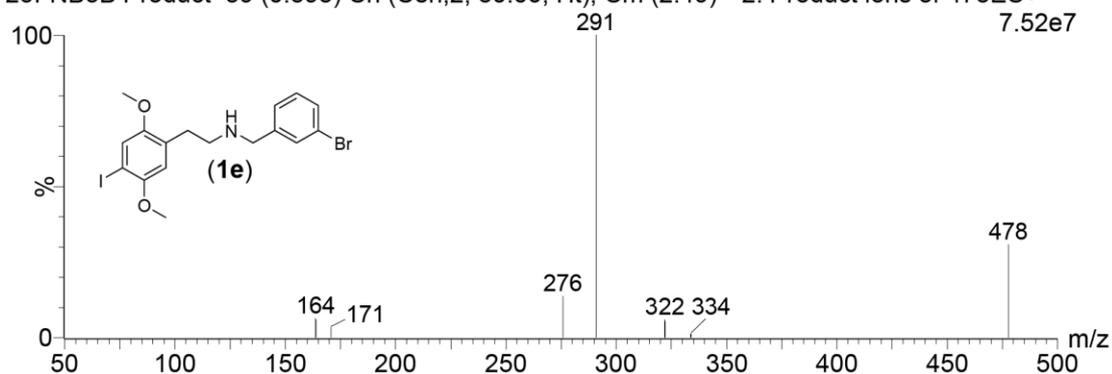


QTOF-MS and QTOF-MS/MS

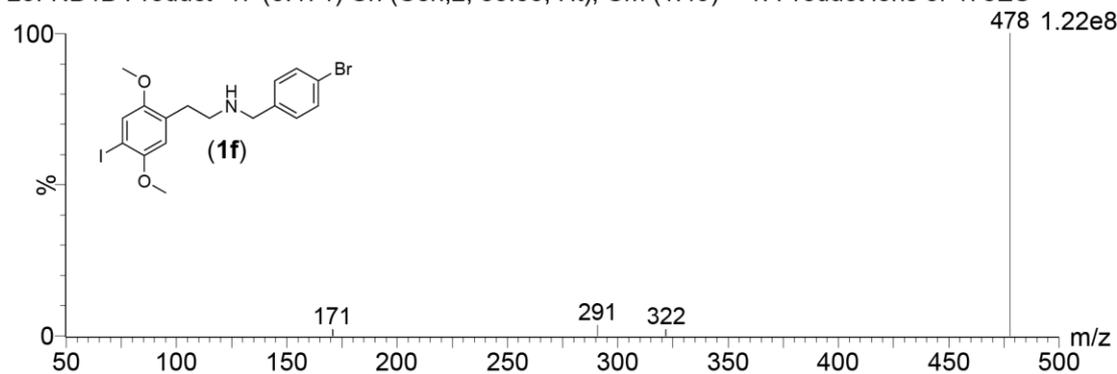
25I-NB2B Product 12 (0.626) Cn (Cen,2, 80.00, Ht); Cm (1:50) 2: Product ions of 478ES+ 9.86e7



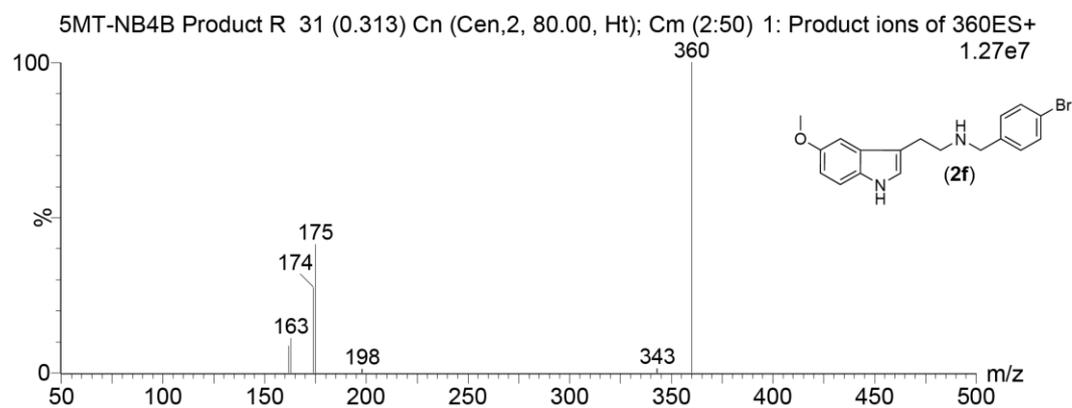
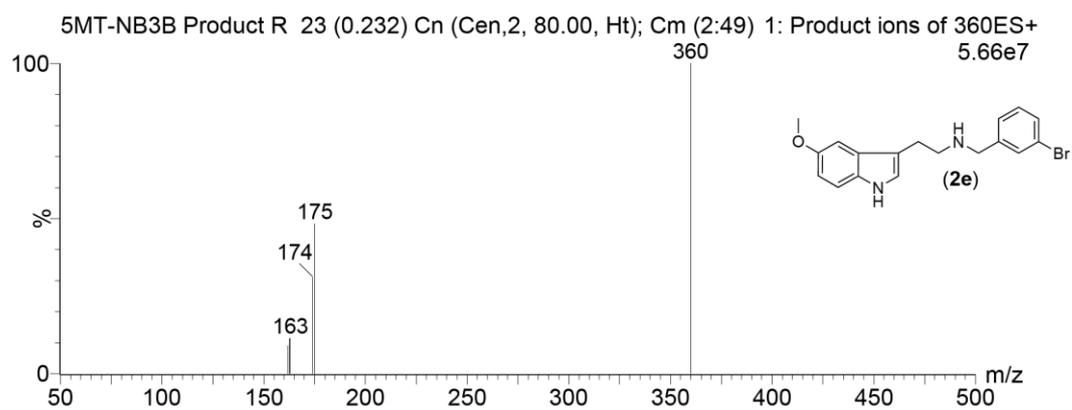
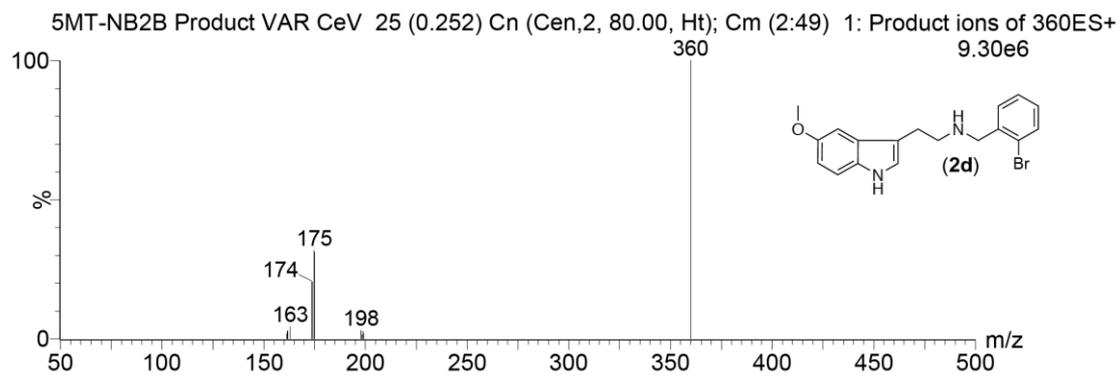
25I-NB3B Product 39 (0.898) Cn (Cen,2, 80.00, Ht); Cm (2:49) 2: Product ions of 478ES+ 7.52e7



25I-NB4B Product 47 (0.474) Cn (Cen,2, 80.00, Ht); Cm (1:49) 1: Product ions of 478ES+ 1.22e8

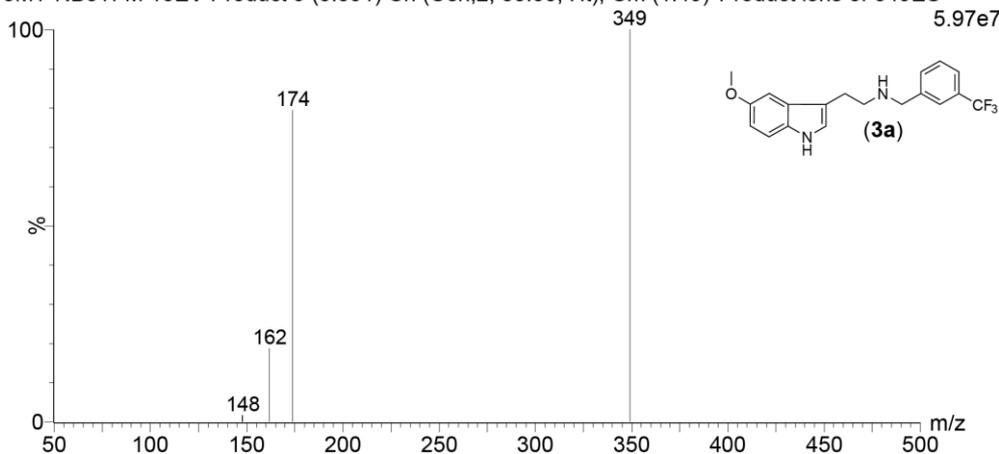


ESI-QqQ-MS/MS

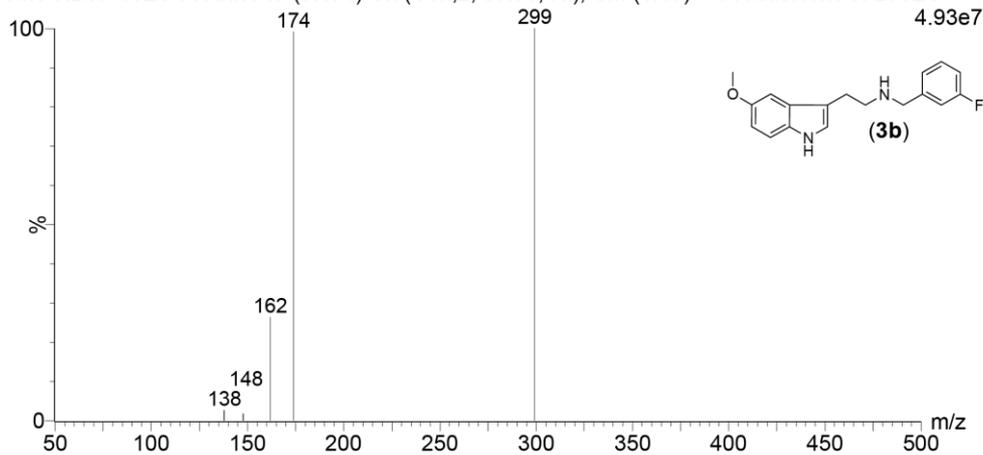


ESI-QqQ-MS/MS

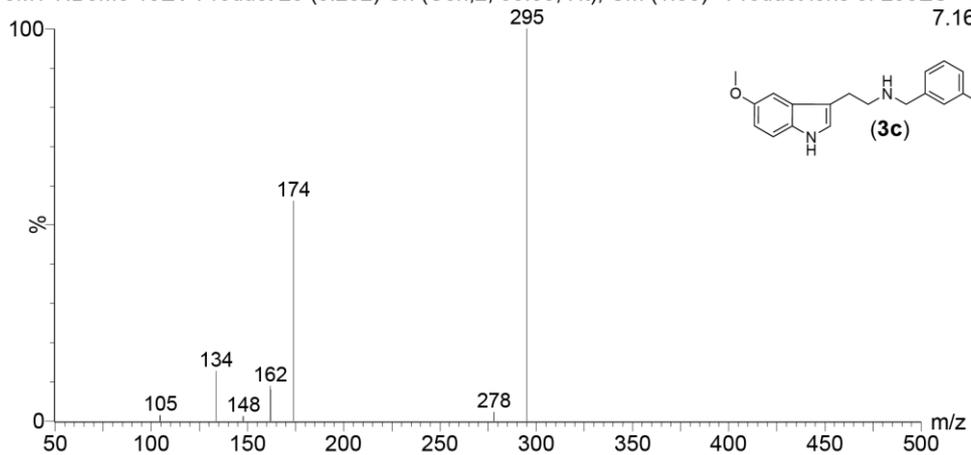
5MT-NB3TFM 10EV Product 9 (0.091) Cn (Cen,2, 80.00, Ht); Cm (1:49) Product ions of 349ES+ 5.97e7



5MT-NB3F 10EV Product 47 (0.474) Cn (Cen,2, 80.00, Ht); Cm (1:49) Product ions of 299ES+ 4.93e7

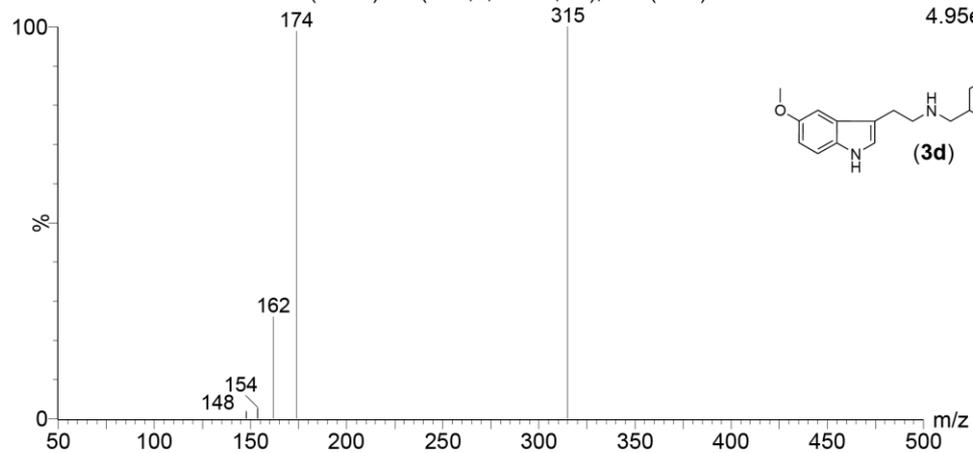


5MT-NB3Me 10EV Product 23 (0.232) Cn (Cen,2, 80.00, Ht); Cm (1:50) Product ions of 295ES+ 7.16e7

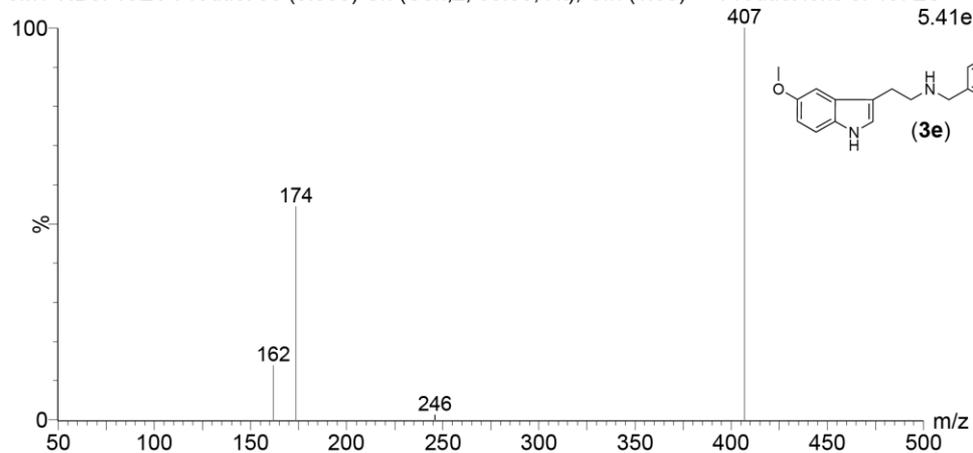


ESI-QqQ-MS/MS

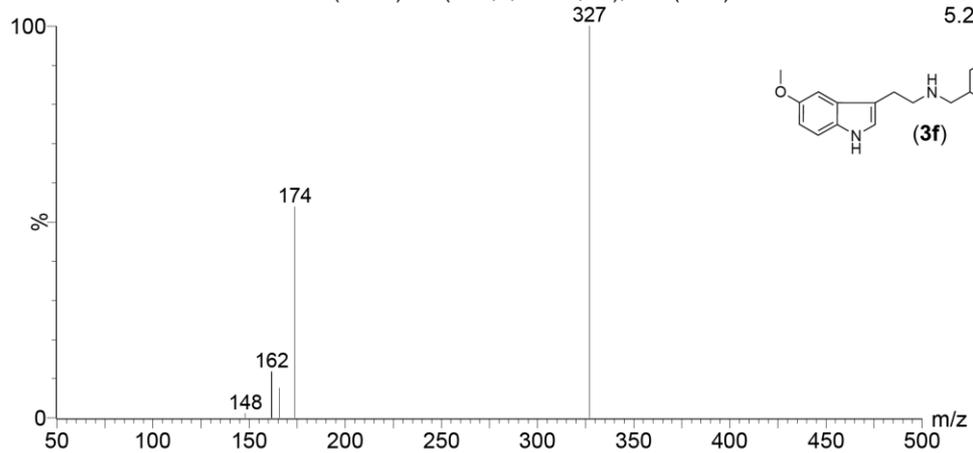
5MT-NB3Cl 10EV Product 44 (0.444) Cn (Cen,2, 80.00, Ht); Cm (1:49) Product ions of 315ES+ 4.95e7



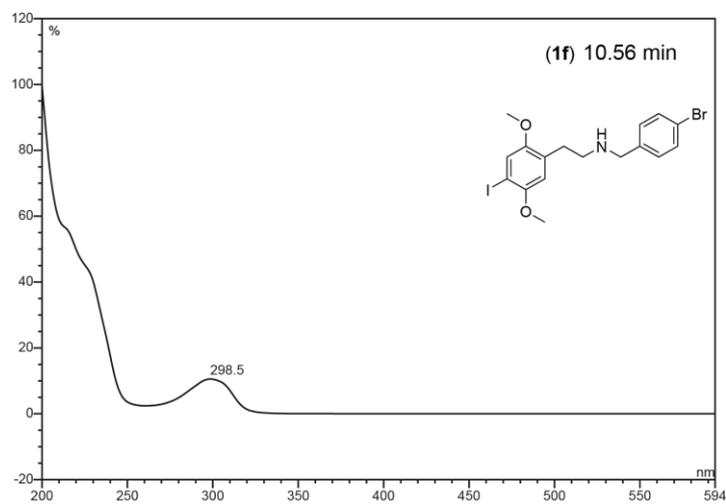
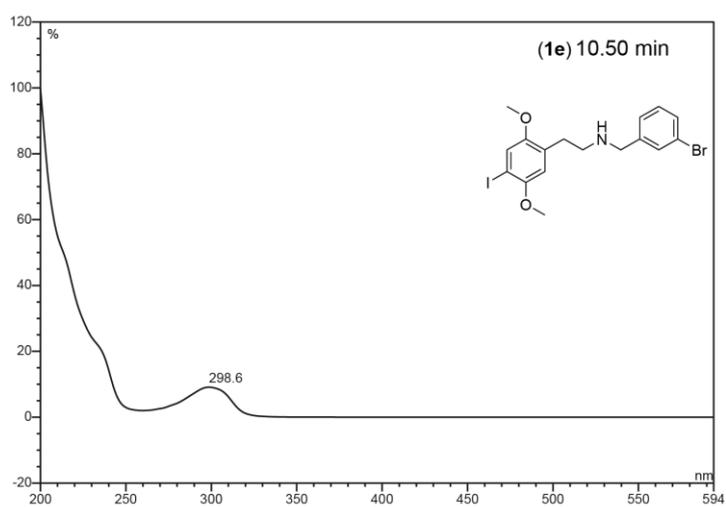
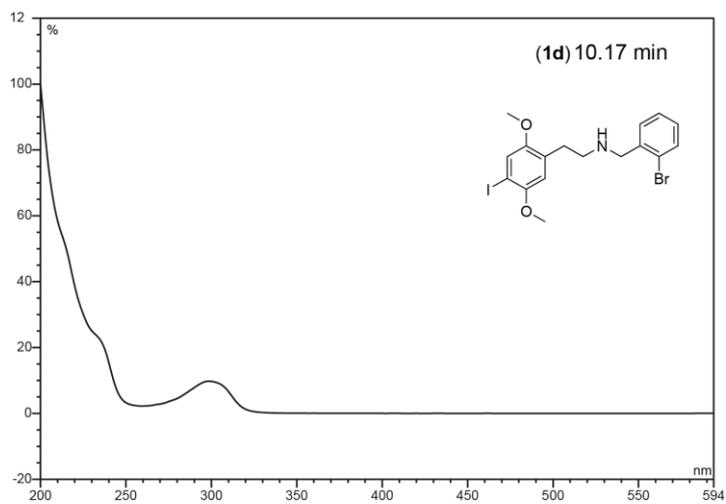
5MT-NB3I 10EV Product 36 (0.363) Cn (Cen,2, 80.00, Ht); Cm (1:50) Product ions of 407ES+ 5.41e7



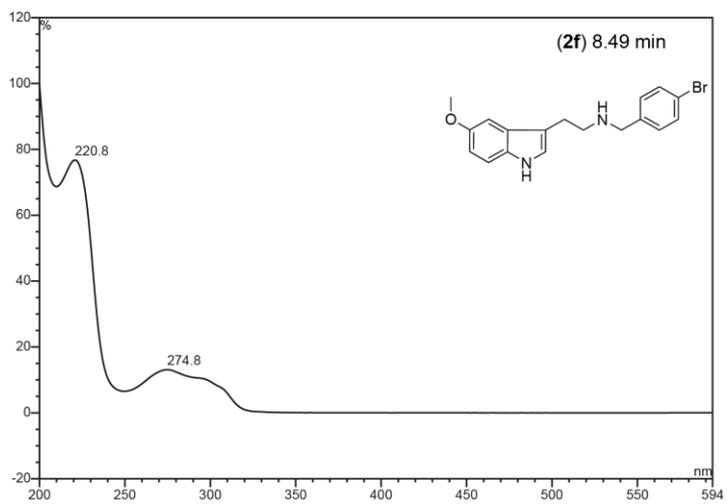
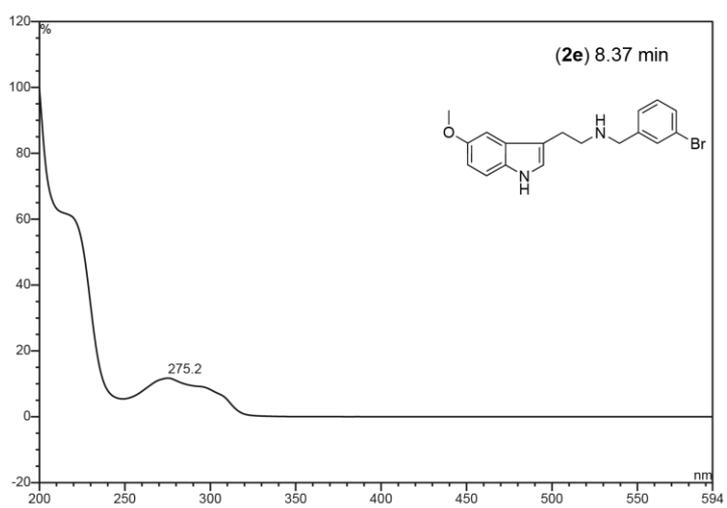
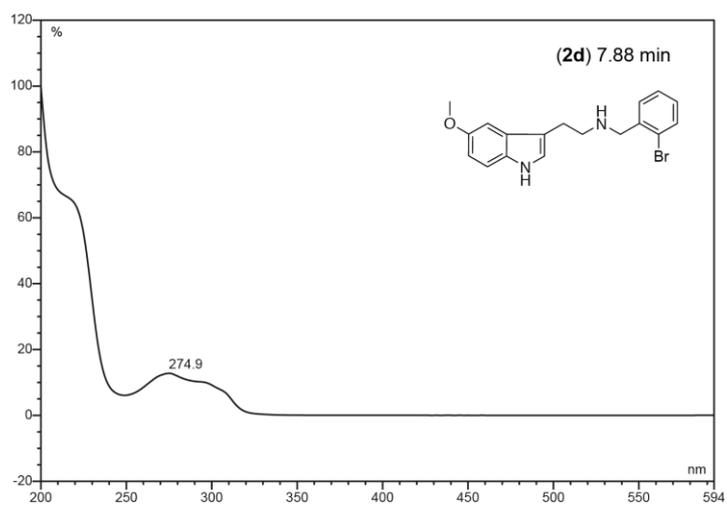
5MT-NB3SMe 10EV Product 36 (0.363) Cn (Cen,2, 80.00, Ht); Cm (1:48) Product ions of 327ES+ 5.21e7



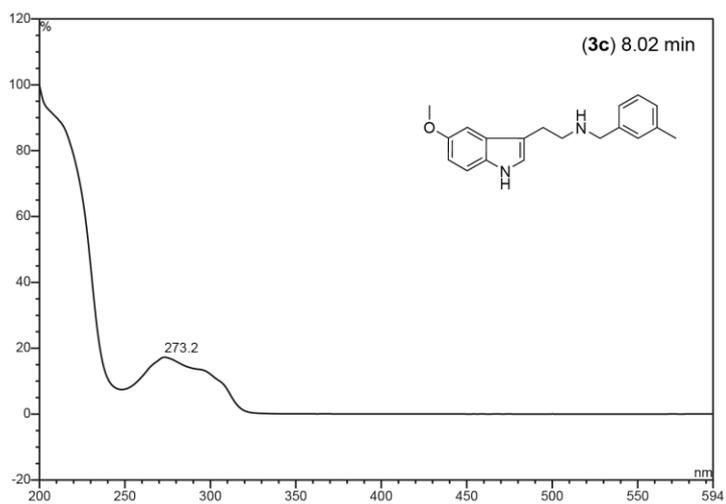
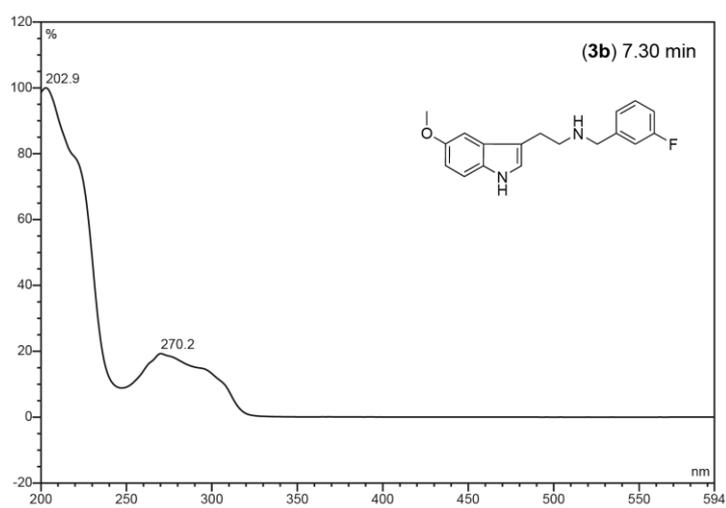
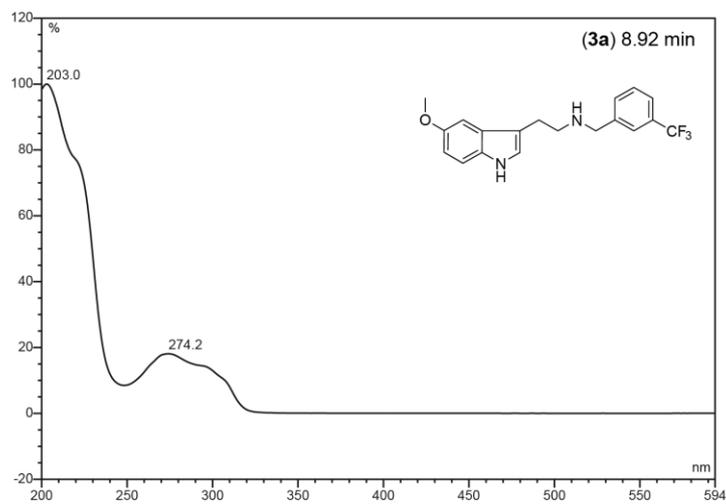
ESI-QqQ-MS/MS



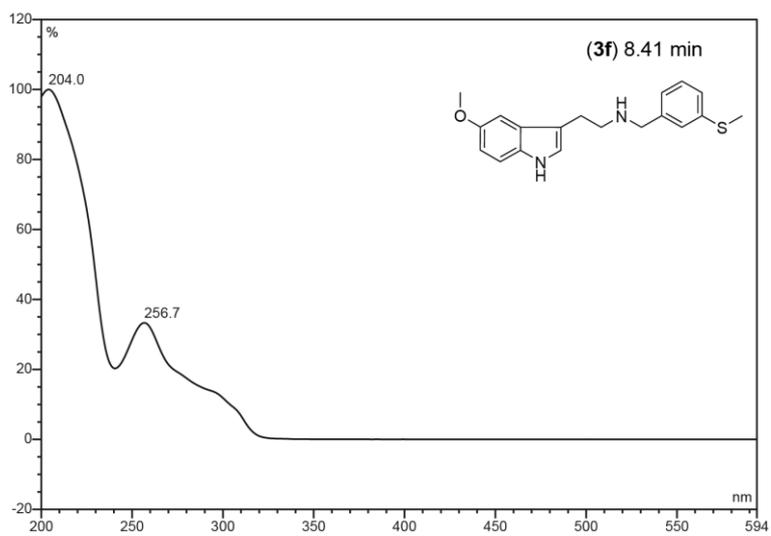
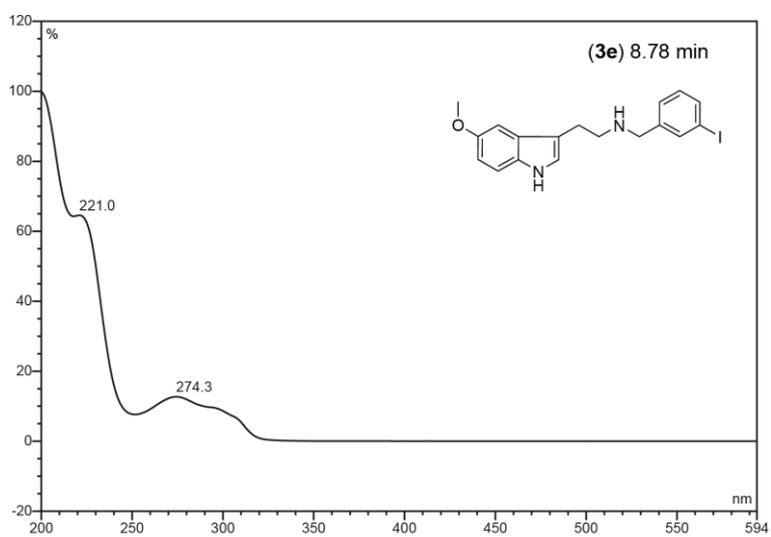
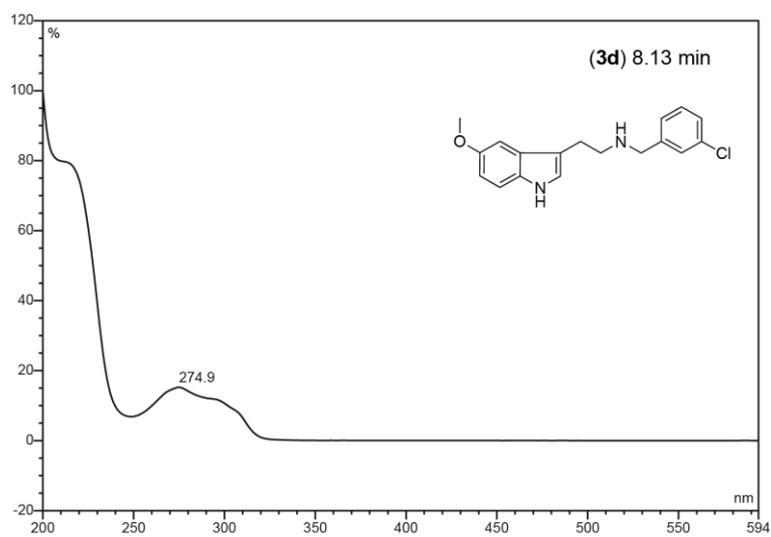
LC/UV retention times and diode array full scan spectra



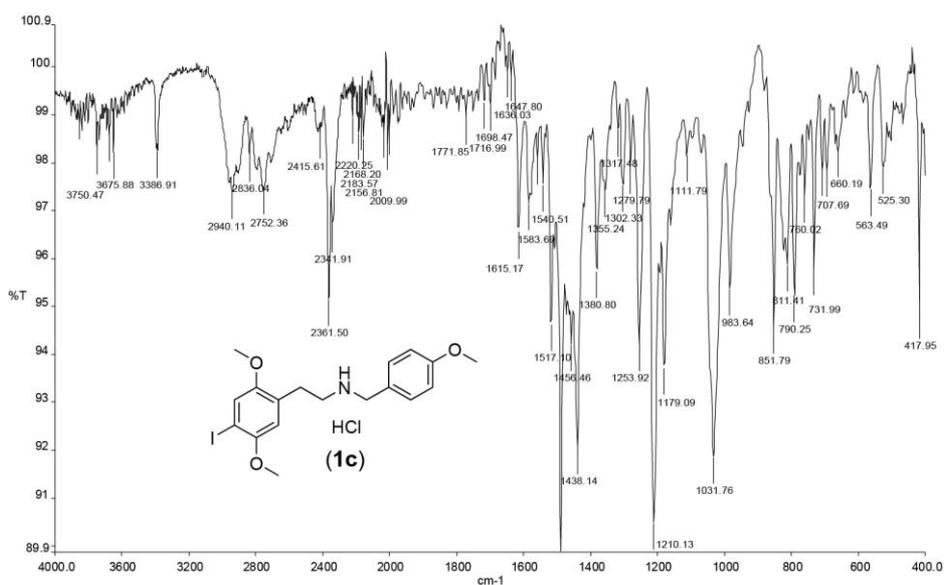
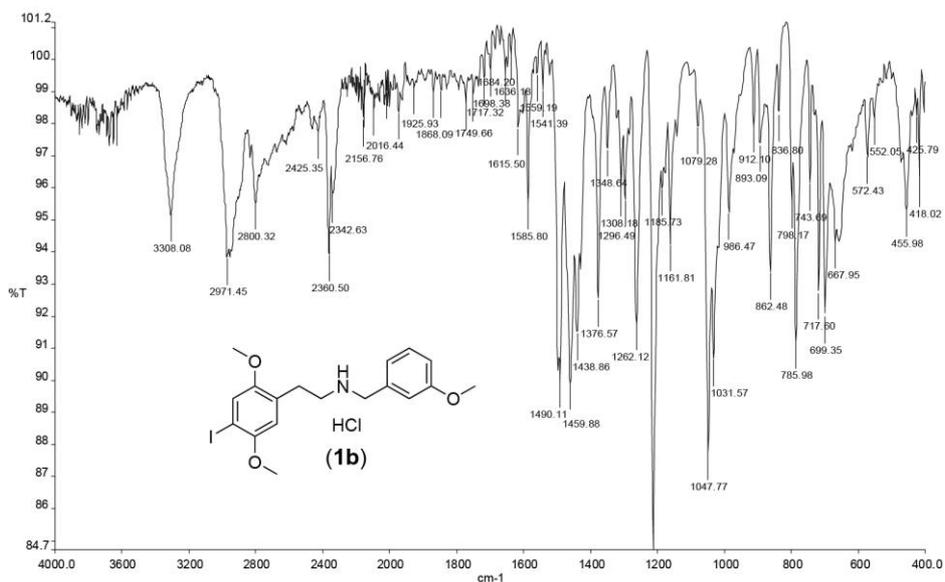
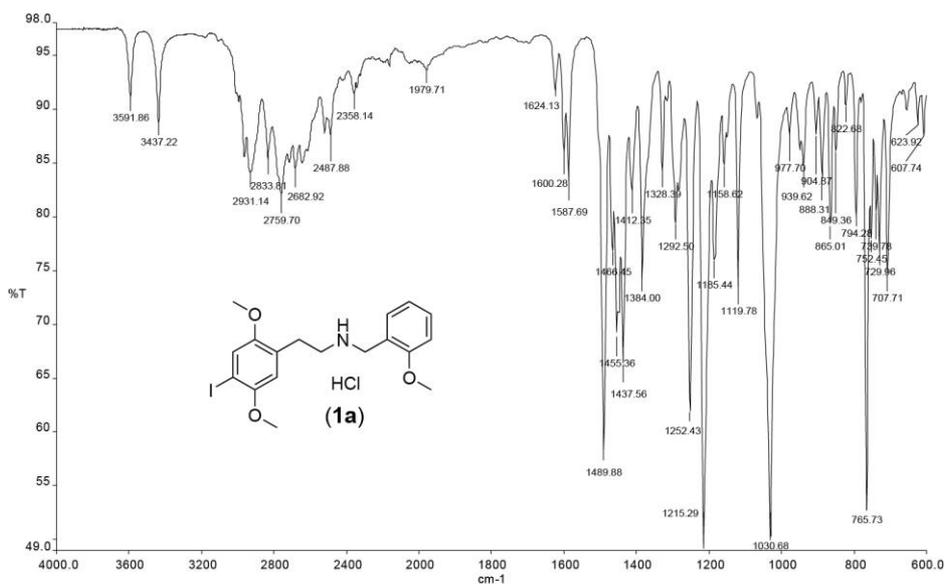
LC/UV retention times and diode array full scan spectra



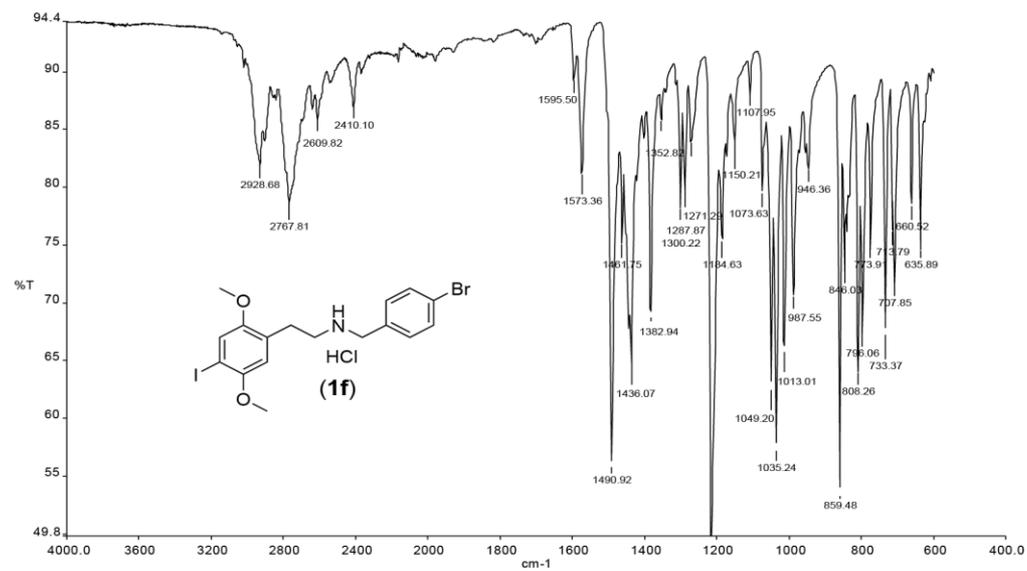
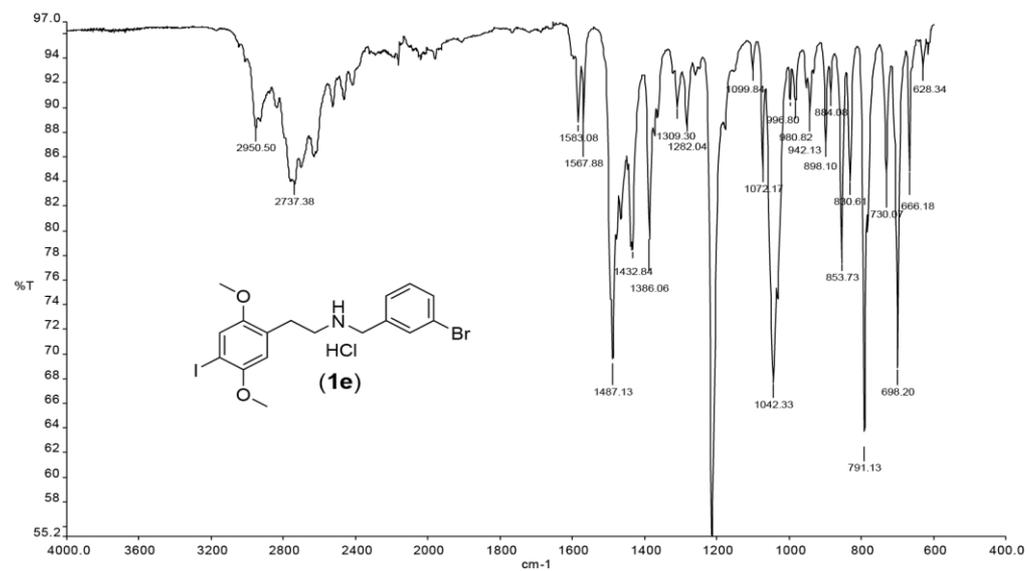
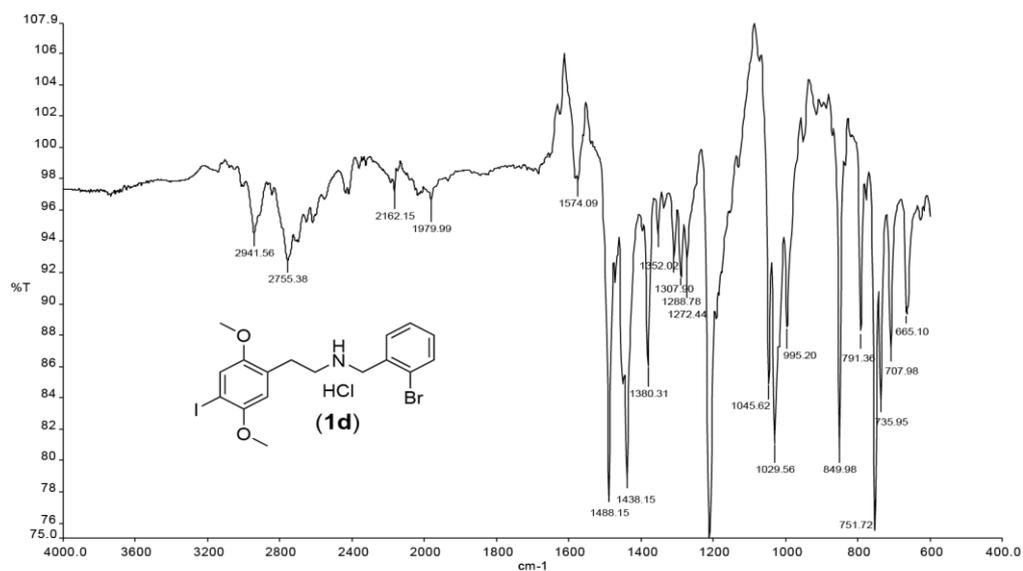
LC/UV retention times and diode array full scan spectra



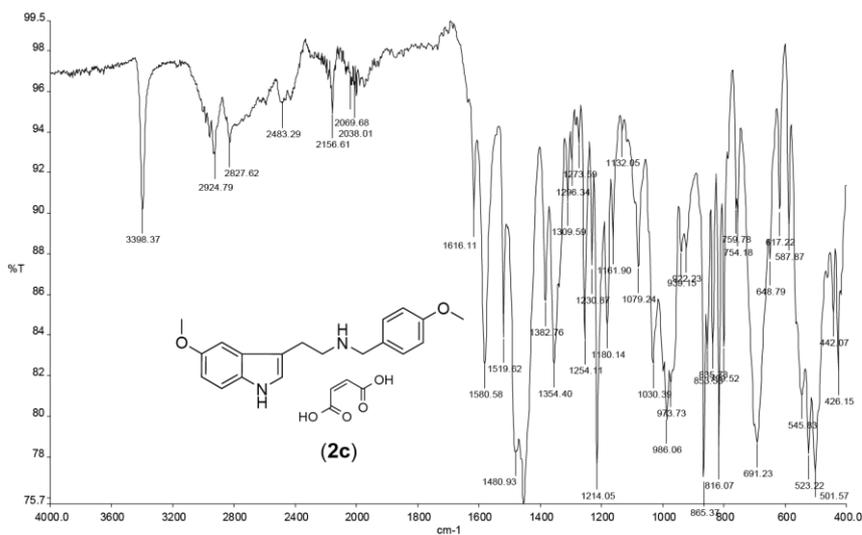
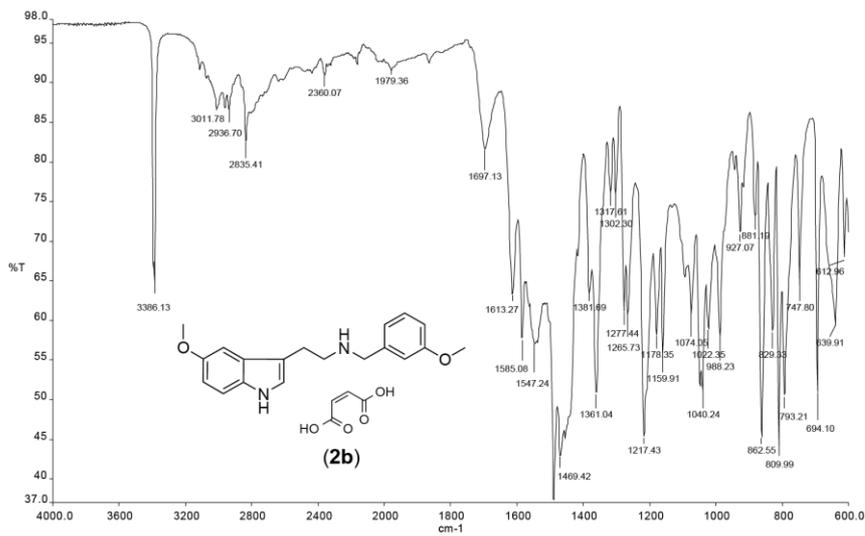
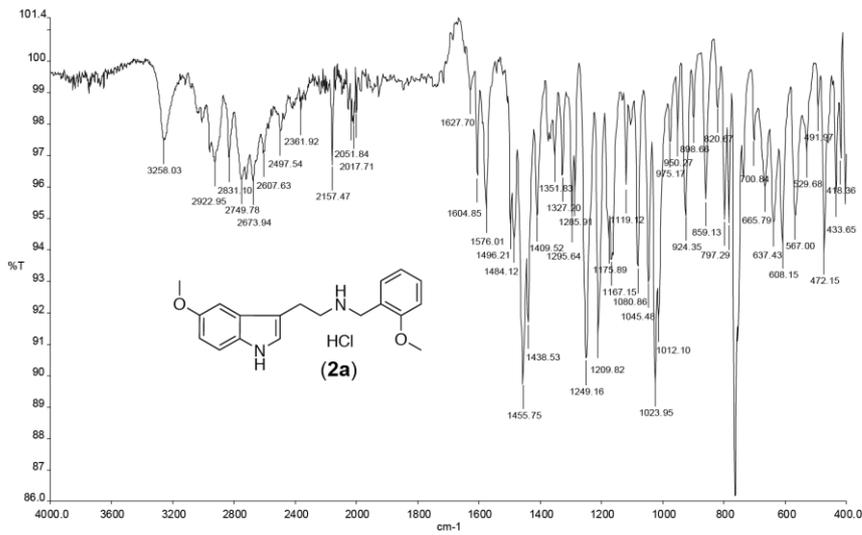
LC/UV retention times and diode array full scan spectra



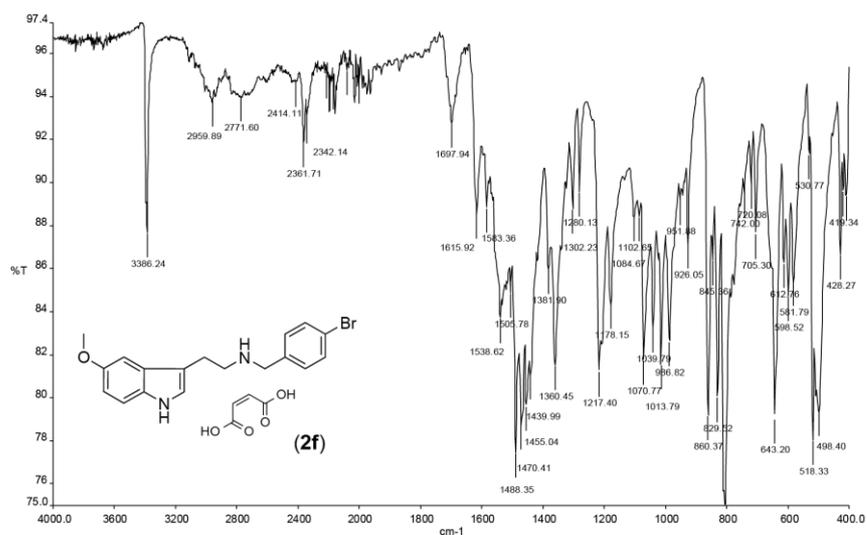
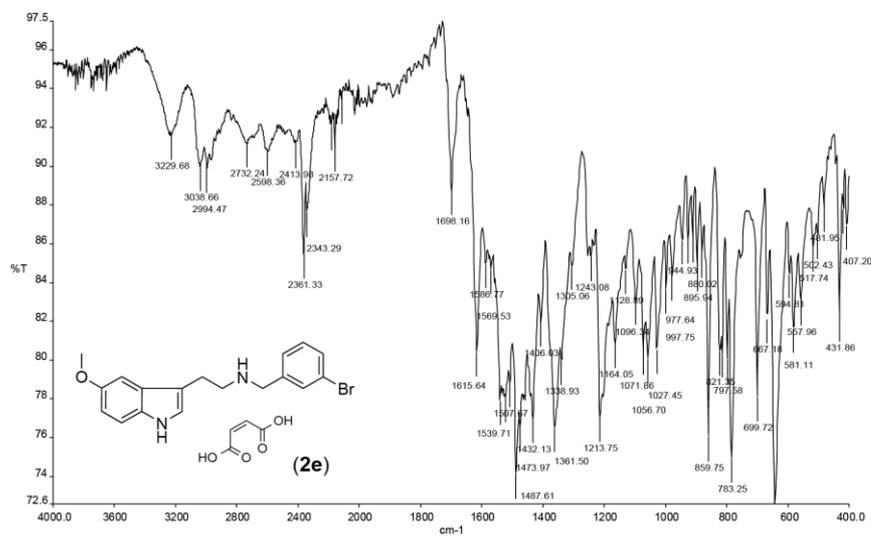
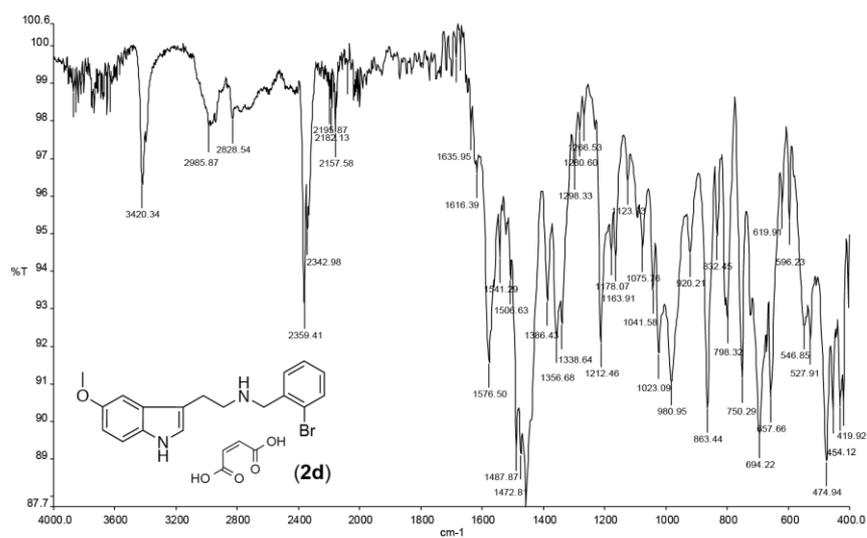
ATR-FTIR spectra



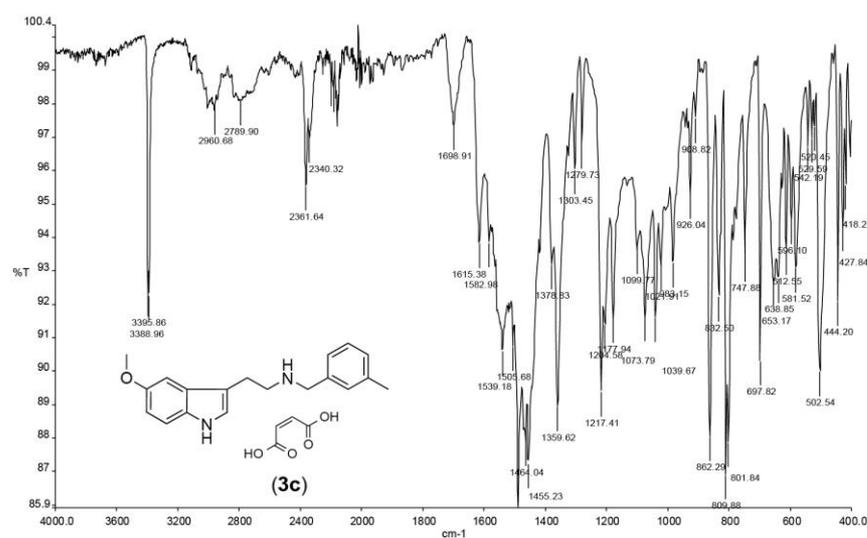
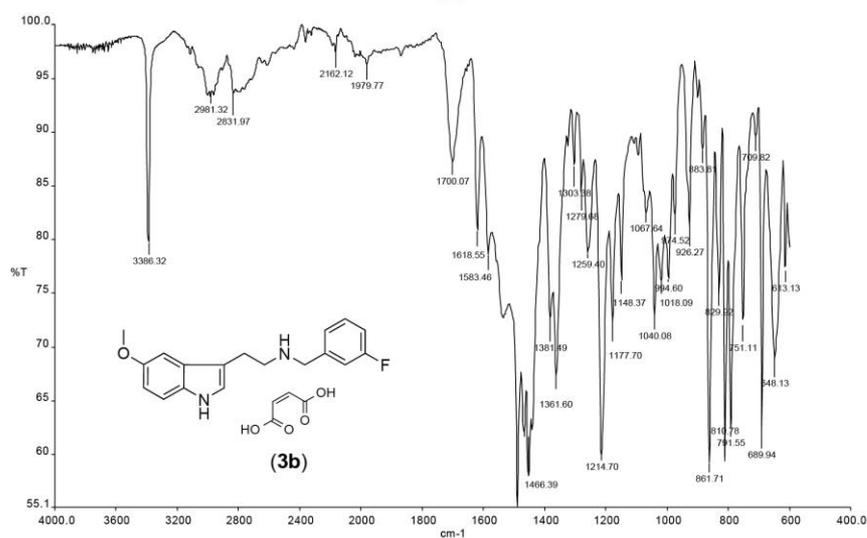
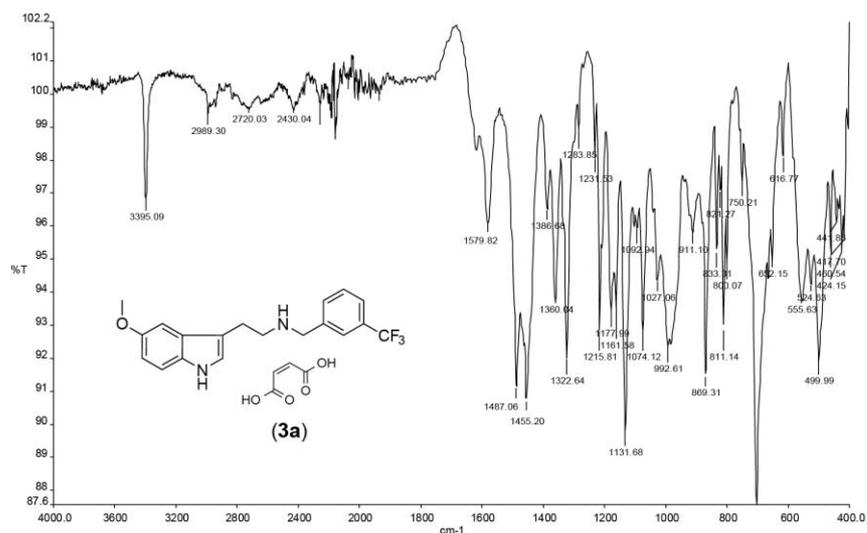
ATR-FTIR spectra



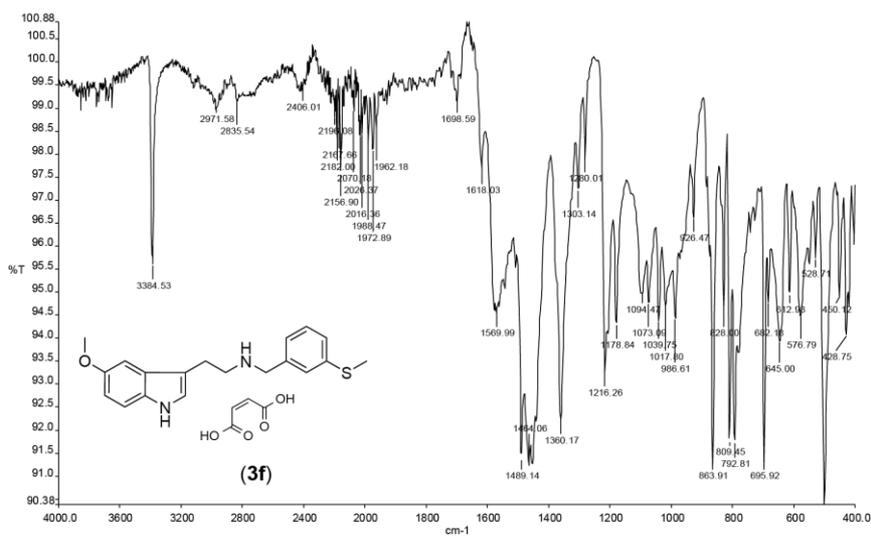
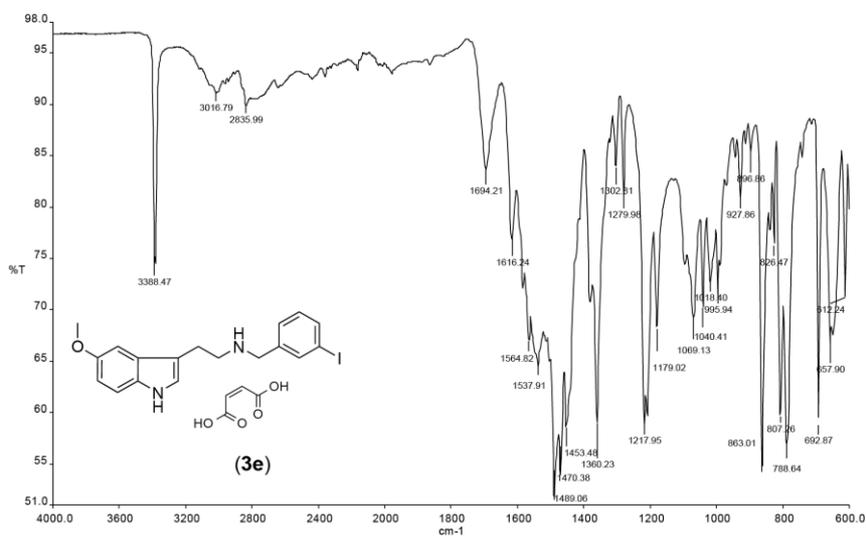
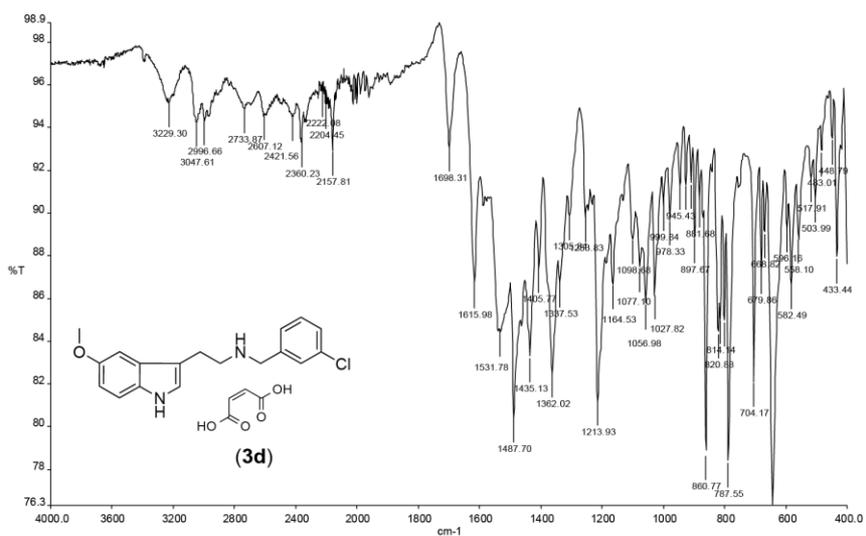
ATR-FTIR spectra



ATR-FTIR spectra



ATR-FTIR spectra



ATR-FTIR spectra