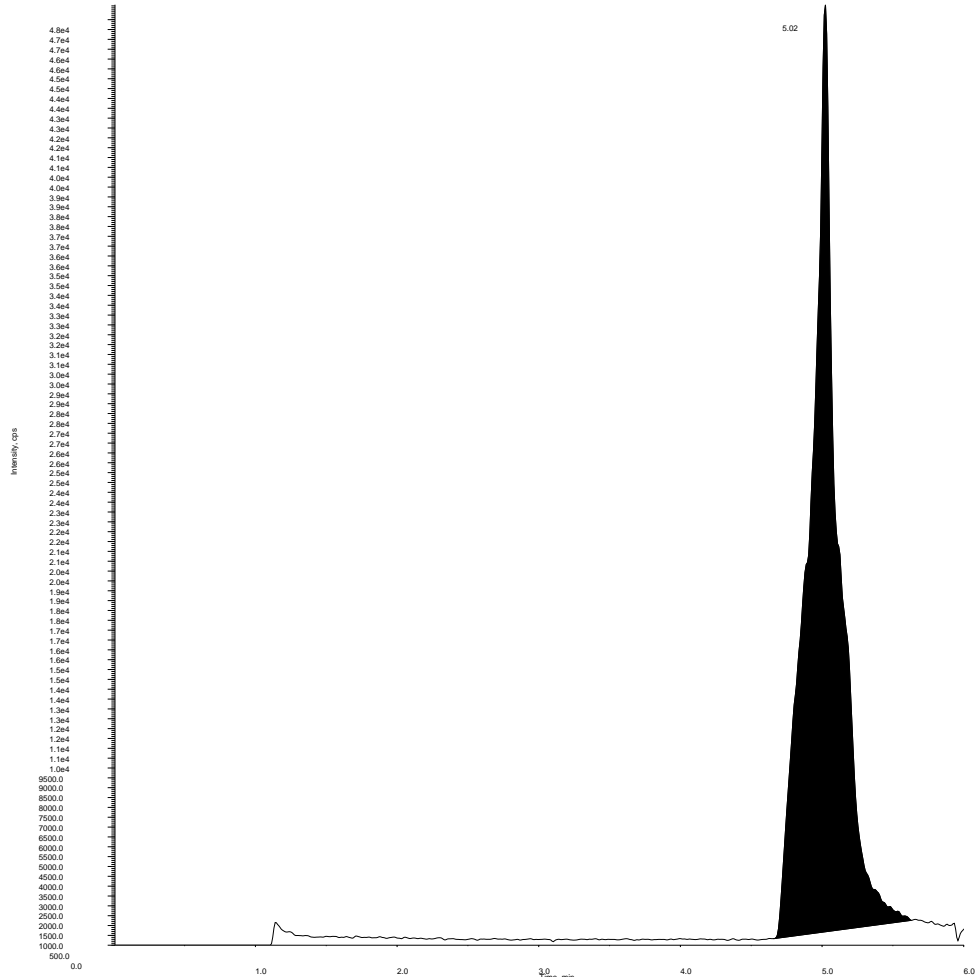


Figure S1. Effect of TFA on retention of isoniazid. LC condition: A= 10mM NH4FA, B=MeCN, flow rate, 0.4mL/min, Isocratic mode. Column, Hypersil Silica (50x2.1 mm, 3um, Thermo-Fisher).

Sample Name: STD0000 Sample ID: File: 011608 Cal.wif
 Peak Name: Isoniazid Annotation: 138.000*121.000 Da
 Comment:
 Sample Index: 25
 Sample Type: Standard
 Concentration: 5000 ng/mL
 Calculated Conc: 5000 ng/mL
 Acq. Date: 1/16/2009
 Acq. Time: 8:25:41 PM
 Modified: Yes
 Proc. Algorithm: Analyt. Classic
 Smoothing Factor: 15.01 cps
 Noise Threshold: 50.94 cps
 Area Threshold: 2.0
 Sep. Width: 0.01
 Sep. Peak Ratio: 1.00
 Sep. Adj. Ratio: 1.00
 Sep. Val. Ratio: 1.00
 Exp. Width: 31.0 sec
 Exp. Relative ST: No
 Int. Type: Base To Base
 Retention Time: 4.98 min
 Area: 6.48e05 counts
 Height: 4.73e04 cps
 Peak Time: 4.98 min
 End Time: 4.98 min



Sample Name: STD0000 Sample ID: File: 011608 noTFA.wif
 Peak Name: Isoniazid Annotation: 138.000*121.000 Da
 Comment:
 Sample Index: 25
 Sample Type: Unknown
 Concentration: N/A
 Calculated Conc: No Intercept
 Acq. Date: 1/17/09 AM
 Acq. Time:
 Modified: Yes
 Proc. Algorithm: Analyt. Classic
 Smoothing Factor: 150.00 cps
 Noise Threshold: 30.00 cps
 Area Threshold: 1
 Sep. Width: 0.20
 Sep. Peak Ratio: 0.00
 Sep. Adj. Ratio: 0.00
 Sep. Val. Ratio: 0.00
 Exp. Width: 31.0 sec
 Exp. Relative ST: No
 Int. Type: Base To Base
 Retention Time: 2.10 min
 Area: 4.39e+05 counts
 Height: 2.39e+05 cps
 Peak Time: 2.10 min
 End Time: 2.10 min

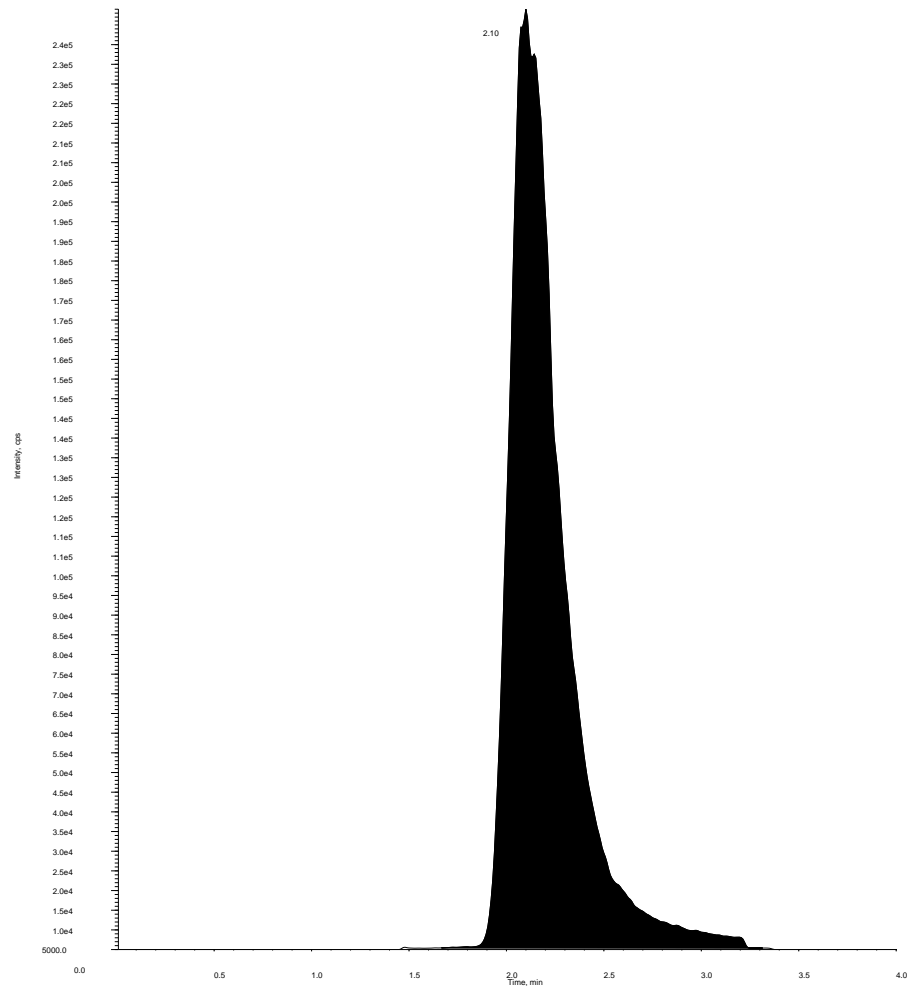
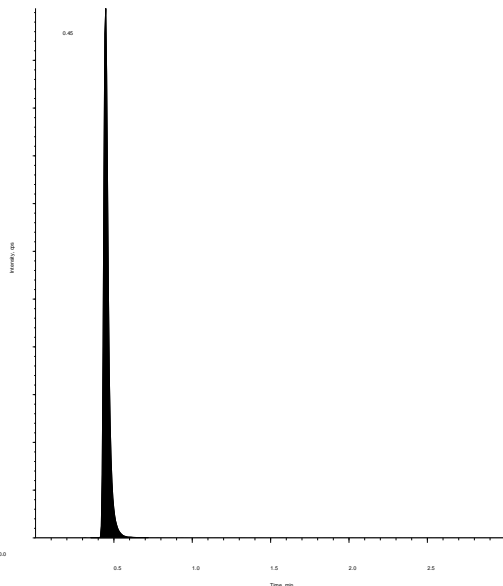
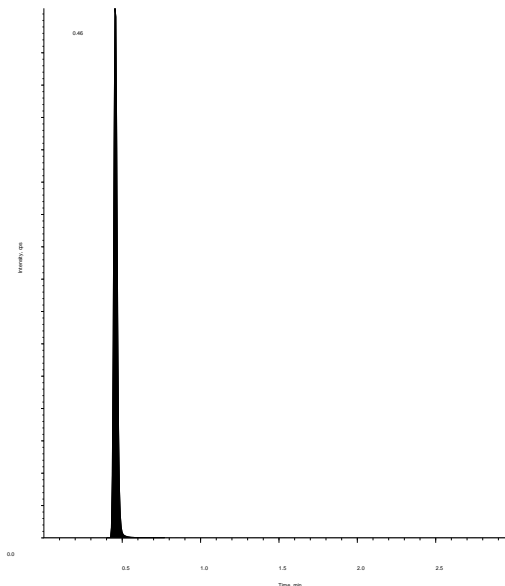


Figure S2. Optimization of TCA concentration. LC condition: A=0.14% TFA, 10mM NH4FA, B= MeCN. Flow rate, 0.6 mL/min, gradient: B% (time), 3 (0min)--3 (0.1min)--30 (2.6 min)--90(2.61min)--90(3.00min)--3(3.01min)--3(3.5min).

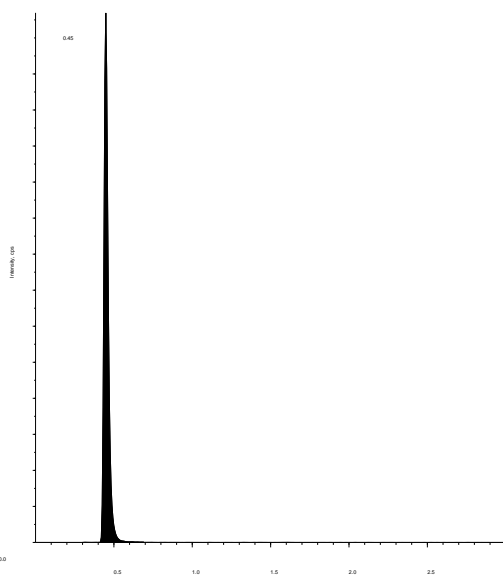
Sample Name: "04TBM_H0N7CA" Sample ID: " File "D:\10\22TBM_optmrc.vwf"
 Peak Name: "TBM2" Mass(es): "468.10024.000 Da"
 Comment: " Annotation: "
 Sample Index: 9
 Sample Type: Unknown
 Concentration: N/A
 Calculated Conc: No Intervept
 Acq. Date: 10/22/2012
 Acq. Time: 2:41:13 PM
 MultiFind: Yes
 Proc. Algorithm: Analyst Classic
 Washing Factor: 4
 Noise Threshold: 5.27 cps
 Area Threshold: 26.37 cps
 Min. Abund: 2
 Rep. Width: 0.20
 Rep. Weight: 0.01
 Exp. Peak Ratio: 5.00
 Exp. Adj. Ratio: 4.00
 Exp. Val. Ratio: 3.00
 RT Window: 30.0 sec
 Expected RT: 0.448 min
 Use Relative RT: No
 Int. Type: Valley
 Retention Time: 0.447 min
 Area: 1.18e+05 counts
 Weight: 5.27e+00 cps
 Start Time: 0.362 min
 End Time: 0.730 min



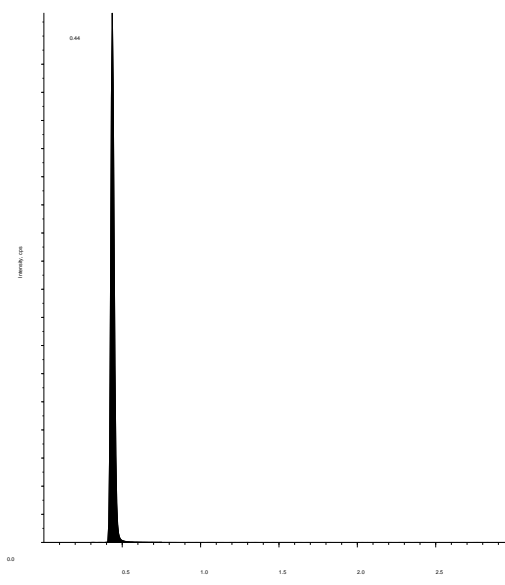
Sample Name: "04TBM_H0N7CA" Sample ID: " File "D:\10\22TBM_optmrc.vwf"
 Peak Name: "TBM2" Mass(es): "468.10024.000 Da"
 Comment: " Annotation: "
 Sample Index: 13
 Sample Type: Unknown
 Concentration: N/A
 Calculated Conc: No Intervept
 Acq. Date: 10/22/2012
 Acq. Time: 2:43:10 PM
 MultiFind: Yes
 Proc. Algorithm: Analyst Classic
 Washing Factor: 4
 Noise Threshold: 5.27 cps
 Area Threshold: 26.37 cps
 Min. Abund: 2
 Rep. Width: 0.20
 Rep. Weight: 0.01
 Exp. Peak Ratio: 5.00
 Exp. Adj. Ratio: 4.00
 Exp. Val. Ratio: 3.00
 RT Window: 30.0 sec
 Expected RT: 0.454 min
 Use Relative RT: No
 Int. Type: Valley
 Retention Time: 0.454 min
 Area: 1.18e+05 counts
 Weight: 5.27e+00 cps
 Start Time: 0.403 min
 End Time: 0.771 min



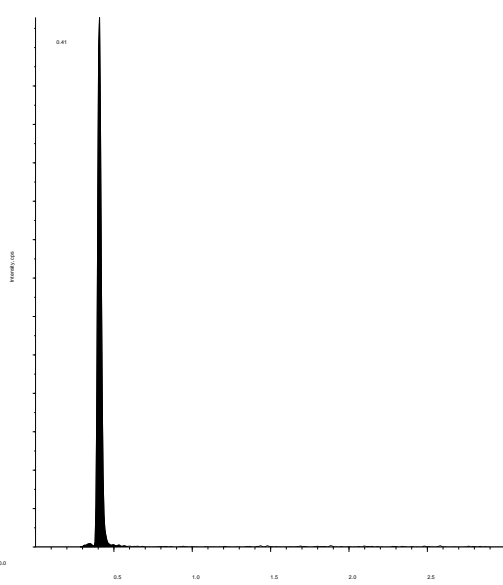
Sample Name: "04TBM_H0N7CA" Sample ID: " File "D:\10\22TBM_optmrc.vwf"
 Peak Name: "TBM2" Mass(es): "468.10024.000 Da"
 Comment: " Annotation: "
 Sample Index: 14
 Sample Type: Unknown
 Concentration: N/A
 Calculated Conc: No Intervept
 Acq. Date: 10/22/2012
 Acq. Time: 2:50:15 PM
 MultiFind: Yes
 Proc. Algorithm: Analyst Classic
 Washing Factor: 4
 Noise Threshold: 5.27 cps
 Area Threshold: 26.37 cps
 Min. Abund: 2
 Rep. Width: 0.20
 Rep. Weight: 0.01
 Exp. Peak Ratio: 5.00
 Exp. Adj. Ratio: 4.00
 Exp. Val. Ratio: 3.00
 RT Window: 30.0 sec
 Expected RT: 0.448 min
 Use Relative RT: No
 Int. Type: Valley
 Retention Time: 0.448 min
 Area: 5.54e+05 counts
 Weight: 2.46e+00 cps
 Start Time: 0.433 min
 End Time: 0.492 min



Sample Name: "04TBM_H0N7CA" Sample ID: " File "D:\10\22TBM_optmrc.vwf"
 Peak Name: "TBM2" Mass(es): "468.10024.000 Da"
 Comment: " Annotation: "
 Sample Index: 17
 Sample Type: Unknown
 Concentration: N/A
 Calculated Conc: No Intervept
 Acq. Date: 10/22/2012
 Acq. Time: 2:52:43 PM
 MultiFind: Yes
 Proc. Algorithm: Analyst Classic
 Washing Factor: 4
 Noise Threshold: 5.27 cps
 Area Threshold: 26.37 cps
 Min. Abund: 2
 Rep. Width: 0.20
 Rep. Weight: 0.01
 Exp. Peak Ratio: 5.00
 Exp. Adj. Ratio: 4.00
 Exp. Val. Ratio: 3.00
 RT Window: 30.0 sec
 Expected RT: 0.437 min
 Use Relative RT: No
 Int. Type: Valley
 Retention Time: 0.437 min
 Area: 5.97e+05 counts
 Weight: 3.70e+00 cps
 Start Time: 0.394 min
 End Time: 0.754 min



Sample Name: "04TBM_H0N7CA" Sample ID: " File "D:\10\22TBM_optmrc.vwf"
 Peak Name: "TBM2" Mass(es): "468.10024.000 Da"
 Comment: " Annotation: "
 Sample Index: 20
 Sample Type: Unknown
 Concentration: N/A
 Calculated Conc: No Intervept
 Acq. Date: 10/22/2012
 Acq. Time: 2:54:15 PM
 MultiFind: No
 Proc. Algorithm: Analyst Classic
 Washing Factor: 4
 Noise Threshold: 5.27 cps
 Area Threshold: 26.37 cps
 Min. Abund: 2
 Rep. Width: 0.20
 Rep. Weight: 0.01
 Exp. Peak Ratio: 5.00
 Exp. Adj. Ratio: 4.00
 Exp. Val. Ratio: 3.00
 RT Window: 30.0 sec
 Expected RT: 0.244 min
 Use Relative RT: No
 Int. Type: Mass To Mass
 Retention Time: 0.437 min
 Area: 2.33e+04 counts
 Weight: 1.38e+04 cps
 Start Time: 0.244 min
 End Time: 0.444 min



Sample Name: "04TBM_H0N7CA" Sample ID: " File "D:\10\22TBM_optmrc.vwf"
 Peak Name: "TBM2" Mass(es): "468.10024.000 Da"
 Comment: " Annotation: "
 Sample Index: 21
 Sample Type: Unknown
 Concentration: N/A
 Calculated Conc: No Intervept
 Acq. Date: 10/22/2012
 Acq. Time: 2:58:10 PM
 MultiFind: No
 Proc. Algorithm: Analyst Classic
 Washing Factor: 4
 Noise Threshold: 5.27 cps
 Area Threshold: 26.37 cps
 Min. Abund: 2
 Rep. Width: 0.20
 Rep. Weight: 0.01
 Exp. Peak Ratio: 5.00
 Exp. Adj. Ratio: 4.00
 Exp. Val. Ratio: 3.00
 RT Window: 30.0 sec
 Expected RT: 0.244 min
 Use Relative RT: No
 Int. Type: Mass To Mass
 Retention Time: 0.333 min
 Area: 5.83e+04 counts
 Weight: 2.33e+04 cps
 Start Time: 0.244 min
 End Time: 0.444 min

