

'Replacement of Dichloromethane within Chromatographic Separations: A Guide to Alternative Solvents'

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Supporting Information

1. General

1.1. Reagents

All compounds (with the exception of **83**, **94**, and **95**) and solvents were obtained from commercial suppliers and were used as supplied and without further purification. Compounds **83,94** and **95** were gratefully received from Professor Colin J. Suckling at the University of Strathclyde.

1.2. Equipment Specifications

Thin layer chromatography was carried out using Macherey-Nagel Polygram SIL G/UV₂₅₄ 0.2mm silica gel, pre-coated polyester-backed TLC plates of dimension 40 x 80 mm. These were developed in CAMAG TLC tanks of dimension H: 130 mm, W: 130 mm, L: 56 mm, with a fully-fitting metal lid. Eluent mixtures were made using standard measuring cylinders.

2. Experimental Procedures

TLC plate baseline was drawn at 15 mm from one of the 40 mm edges of the plate and the eluent was allowed to run to a distance of approx. 5 mm from the top edge of the plate. Sample solutions were spotted with a capillary to give a spot of approx. 3 mm. 5-12 compounds were developed on each plate with each plate run separately and in triplicate. Plates were analysed under 254 nm UV light and R_f values were measured in millimetres.

3. Experimental Data

3.1 Compound Library – PCA Contributors

Physicochemical parameters were computed using KNIME version 2.6.0 (build July 31st, 2012).¹ Briefly, an sdf file representing the compound library was generated from ChemDraw. This was loaded into KNIME and a workflow subsequently generated using the Chemistry Development Kit (CDK) community node to calculate PSA, HBA, HBD, MW, and rotatable bonds. XLogP was determined separately and combined with the other descriptors. SMILES descriptors of each compound were also generated using the ChemAxon conversion tools in KNIME. Principal component analysis (PCA) was performed using the mining node in KNIME, projecting the space defined by the physicochemical descriptors into two dimensions. Finally, the dataset was converted into either an sdf file for viewing in ChemDraw for Excel or an xls file for visualisation in Spotfire. The outputs from the KNIME PCA are given below:

| ID | H-Bond Acceptors | H-Bond Donors | Rotatable Bonds | Polar Surface Area | Molecular Weight | XLogP | PCA Dimension 0 | PCA Dimension 1 |
|----|------------------|---------------|-----------------|--------------------|------------------|--------|-----------------|-----------------|
| 1 | 3 | 1 | 4 | 97.69 | 278.0361 | 1.011 | 74.91781 | -29.0673 |
| 2 | 3 | 1 | 5 | 106.92 | 308.0467 | 1.04 | 106.1604 | -32.2516 |
| 3 | 3 | 1 | 4 | 54.55 | 301.0384 | 1.674 | 89.06115 | 17.71563 |
| 4 | 5 | 1 | 3 | 94.84 | 215.0252 | -0.705 | 12.58009 | -38.6676 |
| 5 | 5 | 2 | 2 | 105.84 | 201.0096 | -1.237 | 0.969585 | -52.215 |
| 6 | 3 | 1 | 1 | 68.54 | 157.0197 | -0.559 | -49.4841 | -24.1668 |
| 7 | 2 | 0 | 2 | 42.52 | 168.0245 | 0.861 | -43.7654 | 3.557009 |
| 8 | 2 | 1 | 2 | 62.6 | 168.0245 | 1.257 | -39.8427 | -16.1315 |
| 9 | 2 | 1 | 1 | 37.3 | 172.0524 | 2.124 | -40.8389 | 9.467885 |
| 10 | 2 | 1 | 1 | 37.3 | 199.9473 | 1.313 | -13.4896 | 14.89742 |
| 11 | 3 | 2 | 2 | 57.53 | 152.0473 | -0.16 | -56.4871 | -14.3587 |
| 12 | 3 | 1 | 4 | 63.6 | 180.0423 | 0.263 | -27.8251 | -14.8124 |
| 13 | 4 | 2 | 4 | 66.4 | 205.0739 | 1.255 | -2.71173 | -12.691 |
| 14 | 4 | 2 | 1 | 76.21 | 138.0429 | -1 | -66.5804 | -35.4434 |
| 15 | 3 | 1 | 2 | 78.43 | 171.0354 | 0.055 | -33.7943 | -31.1085 |
| 16 | 4 | 1 | 1 | 63.08 | 124.0273 | -1.365 | -82.8906 | -25.302 |
| 17 | 4 | 2 | 1 | 65.98 | 162.0429 | 1.358 | -45.0319 | -20.6797 |
| 18 | 2 | 2 | 1 | 40.46 | 122.0539 | 0.007 | -89.2549 | -3.45817 |
| 19 | 2 | 2 | 1 | 40.46 | 140.0445 | -0.088 | -71.6142 | 0.052959 |
| 20 | 2 | 3 | 1 | 60.69 | 138.0488 | -0.285 | -69.6218 | -20.1853 |
| 21 | 2 | 2 | 1 | 40.46 | 136.0696 | 0.399 | -75.5098 | -0.71259 |
| 22 | 2 | 2 | 1 | 40.46 | 189.976 | 0.95 | -22.6483 | 9.826381 |
| 23 | 2 | 2 | 1 | 40.46 | 199.9644 | 0.549 | -12.8557 | 11.76814 |
| 24 | 3 | 1 | 2 | 42.09 | 125.0477 | 0.768 | -72.2142 | -1.71477 |
| 25 | 3 | 1 | 4 | 42.09 | 203.0946 | 1.549 | -9.41078 | 10.79695 |
| 26 | 2 | 0 | 3 | 54.54 | 156.0245 | 1.443 | -53.1705 | -10.5532 |
| 27 | 3 | 0 | 6 | 59.32 | 331.1208 | 2.922 | 119.5201 | 18.96171 |
| 28 | 1 | 0 | 1 | 17.07 | 174.1045 | 2.315 | -42.7896 | 29.74251 |
| 29 | 2 | 1 | 1 | 32.86 | 109.0528 | 0.709 | -103.487 | 1.485354 |
| 30 | 2 | 0 | 2 | 20.31 | 149.0841 | 0.964 | -66.6697 | 21.62599 |
| 31 | 4 | 1 | 3 | 59.3 | 203.0582 | 0.723 | -6.09414 | -6.1191 |
| 32 | 3 | 1 | 3 | 46.17 | 163.0633 | 0.009 | -47.8898 | -1.0523 |
| 33 | 0 | 1 | 1 | 29.46 | 124.0524 | 0.975 | -89.4677 | 7.803321 |
| 34 | 1 | 1 | 2 | 20.23 | 208.0888 | 2.075 | -8.83151 | 33.25765 |
| 35 | 2 | 2 | 1 | 36.02 | 147.0684 | 0.622 | -65.5897 | 5.791296 |
| 36 | 1 | 1 | 0 | 33.12 | 109.0528 | 0.059 | -103.467 | 1.242031 |
| 37 | 2 | 2 | 2 | 66.76 | 318.0892 | 1.613 | 108.1235 | 9.0852 |
| 38 | 1 | 1 | 0 | 20.23 | 134.0732 | 0.855 | -81.4436 | 18.77748 |
| 39 | 2 | 1 | 2 | 37.3 | 136.0524 | 0.207 | -76.1333 | 2.395522 |
| 40 | 1 | 1 | 3 | 63.37 | 167.0582 | 0.335 | -40.643 | -17.0697 |
| 41 | 4 | 1 | 0 | 75.59 | 120.0436 | -1.749 | -84.3729 | -38.3478 |
| 42 | 2 | 2 | 0 | 52.04 | 108.0687 | -0.168 | -100.725 | -17.541 |
| 43 | 2 | 2 | 0 | 27.82 | 172.1 | 0.746 | -42.658 | 18.71828 |
| 44 | 1 | 1 | 1 | 26.02 | 161.0452 | 1.204 | -53.8501 | 18.37794 |
| 45 | 3 | 2 | 0 | 64.93 | 109.064 | -1.025 | -97.2248 | -30.023 |
| 46 | 3 | 2 | 0 | 54.7 | 133.064 | 0.693 | -75.6791 | -15.2733 |
| 47 | 1 | 1 | 2 | 35.25 | 137.0841 | 0.344 | -75.5345 | 4.634473 |
| 48 | 3 | 2 | 1 | 69.11 | 136.0637 | -0.231 | -69.9163 | -28.8296 |
| 49 | 3 | 1 | 1 | 55.98 | 170.0247 | -0.109 | -39.1798 | -9.30868 |
| 50 | 3 | 1 | 1 | 55.98 | 199.9585 | -0.483 | -9.82917 | -3.47139 |
| 51 | 2 | 1 | 1 | 15.27 | 162.1157 | 1.085 | -54.8844 | 29.09367 |
| 52 | 2 | 0 | 5 | 38.77 | 389.0627 | 2.582 | 172.2981 | 50.43355 |
| 53 | 3 | 1 | 3 | 38.33 | 237.1165 | 0.741 | 23.19855 | 21.10798 |
| 54 | 1 | 1 | 0 | 44.48 | 137.0477 | 0.731 | -73.7972 | -4.40897 |
| 55 | 2 | 1 | 1 | 35.25 | 195.1059 | 0.465 | -18.6405 | 15.94237 |
| 56 | 2 | 2 | 3 | 51.04 | 190.1106 | 0.687 | -20.4245 | -0.52173 |
| 57 | 1 | 1 | 0 | 21.26 | 189.1154 | 1.219 | -27.2683 | 28.52476 |
| 58 | 4 | 1 | 1 | 41.57 | 250.1118 | 0.765 | 36.55778 | 20.44598 |
| 59 | 1 | 1 | 0 | 12.03 | 133.0891 | 0.717 | -84.0087 | 26.61815 |
| 60 | 3 | 1 | 1 | 74.17 | 203.0695 | 1.483 | -3.22185 | -20.6466 |
| 61 | 1 | 0 | 0 | 12.89 | 143.0735 | 1.055 | -74.0531 | 27.75166 |
| 62 | 1 | 0 | 0 | 41.13 | 127.0456 | 0.854 | -84.262 | -3.05742 |
| 63 | 2 | 0 | 0 | 25.78 | 94.0531 | -0.717 | -119.601 | 5.482544 |
| 64 | 2 | 1 | 0 | 28.68 | 195.9636 | 1.514 | -19.091 | 22.57156 |
| 65 | 4 | 1 | 1 | 54.46 | 146.0592 | 0.509 | -62.9599 | -12.5111 |
| 66 | 2 | 0 | 2 | 17.82 | 158.0844 | 1.358 | -58.3282 | 25.83239 |
| 67 | 2 | 1 | 0 | 67.48 | 150.0252 | 1.149 | -56.5701 | -24.4307 |
| 68 | 2 | 1 | 0 | 32.86 | 135.0684 | 0.658 | -77.9915 | 6.564798 |
| 69 | 2 | 1 | 0 | 28.68 | 195.9636 | 1.938 | -19.0891 | 22.58086 |
| 70 | 4 | 0 | 0 | 40.62 | 217.9691 | 0.162 | 4.833005 | 15.10623 |
| 71 | 2 | 1 | 0 | 28.68 | 195.9636 | 1.266 | -19.0921 | 22.56612 |
| 72 | 2 | 0 | 1 | 33.45 | 211.0633 | 1 | -1.37058 | 21.24126 |
| 73 | 4 | 2 | 1 | 44.37 | 217.1215 | 0.203 | 4.756267 | 11.22822 |

| | | | | | | | | |
|----|----|---|----|--------|----------|--------|----------|----------|
| 74 | 2 | 0 | 1 | 20.31 | 221.0841 | 2.278 | 5.897956 | 36.10313 |
| 75 | 6 | 2 | 0 | 83.98 | 214.0491 | -1.086 | 9.476699 | -28.268 |
| 76 | 5 | 1 | 2 | 54.56 | 340.1787 | 1.464 | 127.4398 | 25.29394 |
| 77 | 5 | 2 | 2 | 65.56 | 354.1943 | 1.694 | 143.334 | 17.23703 |
| 78 | 2 | 2 | 3 | 32.26 | 165.1154 | 0.77 | -48.597 | 13.00308 |
| 79 | 5 | 2 | 1 | 90.71 | 255.0079 | 1.329 | 50.96415 | -26.7866 |
| 80 | 3 | 1 | 3 | 36.36 | 294.1732 | 0.987 | 78.76354 | 34.18602 |
| 81 | 4 | 1 | 2 | 71.97 | 204.0203 | 1.461 | -2.69069 | -18.3312 |
| 82 | 4 | 1 | 0 | 66.91 | 229.9917 | 0.967 | 21.75779 | -8.31122 |
| 83 | 7 | 2 | 6 | 102.74 | 262.1542 | -1.064 | 60.40762 | -37.2848 |
| 84 | 3 | 1 | 1 | 36.86 | 313.0982 | 1.951 | 97.39345 | 37.41327 |
| 85 | 5 | 1 | 3 | 54.7 | 354.1943 | 2.163 | 141.2281 | 27.90885 |
| 86 | 2 | 4 | 0 | 133.52 | 302.0063 | 1.366 | 105.3533 | -59.5224 |
| 87 | 3 | 1 | 1 | 69.81 | 201.0361 | 1.618 | -6.06564 | -16.768 |
| 88 | 4 | 2 | 5 | 105.51 | 290.1379 | -0.545 | 88.33515 | -34.4465 |
| 89 | 4 | 1 | 6 | 87.08 | 369.0759 | 0.667 | 162.1603 | -0.92485 |
| 90 | 1 | 2 | 2 | 75.99 | 284.0685 | 1.364 | 76.54959 | -6.58358 |
| 91 | 2 | 3 | 2 | 77.76 | 180.0423 | 0.888 | -25.0948 | -28.6875 |
| 92 | 3 | 1 | 1 | 46.33 | 236.095 | 0.792 | 23.72843 | 13.07017 |
| 93 | 12 | 6 | 5 | 220.15 | 822.4051 | 3.238 | 632.764 | -43.048 |
| 94 | 11 | 3 | 13 | 122.52 | 631.2907 | 2.156 | 426.4049 | 15.36433 |
| 95 | 10 | 3 | 14 | 118.86 | 610.2904 | 2.76 | 405.1023 | 14.88867 |

3.2 Thin Layer Chromatography Data for Compound Library

3.2.1 MeOH/CH₂Cl₂ R_f Data

| Compound 1 | | | | | |
|----------------|-------|-------|-------|---------|----------------|
| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
| 2% | 0.3 | 0.3 | 0.42 | 0.34 | 0.0400 |
| 5% | 0.74 | 0.62 | 0.63 | 0.66 | 0.0384 |
| 10% | 0.74 | 0.7 | 0.71 | 0.72 | 0.0120 |
| 20% | 0.87 | 0.89 | 0.91 | 0.89 | 0.0115 |
| 25% | 1 | 1 | 1 | 1.00 | 0.0000 |

| Compound 2 | | | | | |
|----------------|-------|-------|-------|---------|----------------|
| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
| 2% | 0.19 | 0.19 | 0.28 | 0.22 | 0.0400 |
| 5% | 0.49 | 0.5 | 0.48 | 0.49 | 0.0058 |
| 10% | 0.68 | 0.66 | 0.67 | 0.67 | 0.0058 |
| 20% | 0.85 | 0.88 | 0.9 | 0.88 | 0.0145 |
| 25% | 1 | 1 | 1 | 1.00 | 0.0000 |

| Compound 3 | | | | | |
|----------------|-------|-------|-------|---------|----------------|
| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
| 2% | 0.44 | 0.42 | 0.56 | 0.47 | 0.0300 |
| 5% | 0.68 | 0.74 | 0.73 | 0.72 | 0.0186 |
| 10% | | 0.83 | 0.83 | 0.83 | 0.0000 |
| 20% | 0.86 | 0.9 | 0.94 | 0.90 | 0.0231 |
| 25% | 1 | 1 | 1 | 1.00 | 0.0000 |

| Compound 4 | | | | | |
|----------------|-------|-------|-------|---------|----------------|
| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
| 2% | 0.39 | 0.38 | 0.45 | 0.41 | 0.0219 |
| 5% | 0.64 | 0.68 | 0.71 | 0.68 | 0.0203 |
| 10% | 0.85 | 0.76 | 0.77 | 0.79 | 0.0285 |
| 20% | 0.87 | 0.88 | 0.87 | 0.87 | 0.0033 |
| 25% | 0.97 | 0.97 | 0.97 | 0.97 | 0.0000 |

| Compound 5 | | | | | |
|----------------|-------|-------|-------|---------|----------------|
| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
| 2% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 5% | 0.04 | 0.04 | 0.04 | 0.04 | 0.0000 |
| 10% | 0.2 | 0.19 | 0.16 | 0.18 | 0.0120 |
| 20% | 0.5 | 0.52 | 0.44 | 0.49 | 0.0240 |
| 25% | 0.52 | 0.53 | 0.56 | 0.54 | 0.0120 |

| Compound 6 | | | | | |
|----------------|-------|-------|-------|---------|----------------|
| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
| 2% | 0.2 | 0.19 | 0.26 | 0.22 | 0.0219 |
| 5% | 0.38 | 0.37 | 0.38 | 0.38 | 0.0033 |
| 10% | 0.57 | 0.53 | 0.51 | 0.54 | 0.0176 |
| 20% | 0.8 | 0.82 | 0.81 | 0.81 | 0.0058 |
| 25% | 0.92 | 0.97 | 1 | 0.96 | 0.0233 |

Compound 7

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.57 | 0.54 | 0.53 | 0.55 | 0.0120 |
| 5% | 0.7 | 0.7 | 0.71 | 0.70 | 0.0033 |
| 10% | 0.78 | 0.79 | 0.79 | 0.79 | 0.0033 |
| 20% | 0.84 | 0.85 | 0.83 | 0.84 | 0.0058 |
| 25% | 0.9 | 0.88 | 0.88 | 0.89 | 0.0067 |

Compound 8

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.17 | 0.15 | 0.14 | 0.15 | 0.0437 |
| 5% | 0.3 | 0.35 | 0.33 | 0.33 | 0.0145 |
| 10% | 0.53 | 0.58 | 0.56 | 0.56 | 0.0145 |
| 20% | 0.88 | 0.87 | 0.89 | 0.88 | 0.0058 |
| 25% | 0.89 | 0.92 | 0.9 | 0.90 | 0.0088 |

Compound 9

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.17 | 0.17 | 0.24 | 0.19 | 0.0233 |
| 5% | 0.4 | 0.41 | 0.36 | 0.39 | 0.0153 |
| 10% | 0.64 | 0.56 | 0.57 | 0.59 | 0.0252 |
| 20% | 0.82 | 0.83 | 0.82 | 0.82 | 0.0033 |
| 25% | 0.95 | 0.96 | 0.94 | 0.95 | 0.0058 |

Compound 10

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.12 | 0.1 | 0.08 | 0.10 | 0.0115 |
| 5% | 0.25 | 0.24 | 0.22 | 0.24 | 0.0088 |
| 10% | 0.36 | 0.34 | 0.32 | 0.34 | 0.0115 |
| 20% | 0.71 | 0.65 | 0.54 | 0.63 | 0.0498 |
| 25% | 0.75 | 0.79 | 0.83 | 0.79 | 0.0231 |

Compound 11

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 5% | 0.08 | 0.15 | 0.1 | 0.11 | 0.0208 |
| 10% | 0.25 | 0.28 | 0.35 | 0.29 | 0.0296 |
| 20% | 0.45 | 0.44 | 0.43 | 0.44 | 0.0058 |
| 25% | 0.77 | 0.72 | 0.7 | 0.73 | 0.0208 |

Compound 12

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 5% | 0.03 | 0.04 | 0.03 | 0.03 | 0.0033 |
| 10% | 0.23 | 0.2 | 0.23 | 0.22 | 0.0100 |
| 20% | 0.45 | 0.53 | 0.45 | 0.48 | 0.0267 |
| 25% | 0.76 | 0.71 | 0.73 | 0.73 | 0.0145 |

Compound 13

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.01 | 0.02 | 0.01 | 0.01 | 0.0033 |
| 5% | 0.03 | 0.05 | 0.01 | 0.03 | 0.0115 |
| 10% | 0.12 | 0.15 | 0.11 | 0.13 | 0.0120 |
| 20% | 0.47 | 0.6 | 0.48 | 0.52 | 0.0418 |
| 25% | 0.82 | 0.82 | 0.79 | 0.81 | 0.0100 |

Compound 14

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 5% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 10% | 0 | 0.01 | 0.02 | 0.01 | 0.0058 |
| 20% | 0.05 | 0.05 | 0.04 | 0.05 | 0.0033 |
| 25% | 0.06 | 0.09 | 0.07 | 0.07 | 0.0088 |

Compound 15

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 5% | 0.14 | 0.14 | 0.09 | 0.12 | 0.0167 |
| 10% | 0.44 | 0.44 | 0.4 | 0.43 | 0.0133 |
| 20% | 0.63 | 0.61 | 0.63 | 0.62 | 0.0067 |
| 25% | 0.78 | 0.74 | 0.7 | 0.74 | 0.0231 |

Compound 16

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 5% | 0.06 | 0.06 | 0.03 | 0.05 | 0.0100 |
| 10% | 0.09 | 0.09 | 0.13 | 0.10 | 0.0133 |
| 20% | 0.18 | 0.14 | 0.16 | 0.16 | 0.0115 |
| 25% | 0.23 | 0.22 | 0.27 | 0.24 | 0.0153 |

Compound 17

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 5% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 10% | 0.11 | 0.1 | 0.14 | 0.12 | 0.0120 |
| 20% | 0.2 | 0.29 | 0.25 | 0.25 | 0.0260 |
| 25% | 0.3 | 0.24 | 0.33 | 0.29 | 0.0265 |

Compound 18

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.25 | 0.19 | 0.2 | 0.21 | 0.0186 |
| 5% | 0.39 | 0.37 | 0.43 | 0.40 | 0.0176 |
| 10% | 0.55 | 0.5 | 0.55 | 0.53 | 0.0167 |
| 20% | 0.74 | 0.69 | 0.72 | 0.72 | 0.0145 |
| 25% | 0.78 | 0.81 | 0.83 | 0.81 | 0.0145 |

Compound 19

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.45 | 0.43 | 0.48 | 0.45 | 0.0145 |
| 5% | 0.6 | 0.62 | 0.55 | 0.59 | 0.0208 |
| 10% | 0.7 | 0.65 | 0.69 | 0.68 | 0.0153 |
| 20% | 0.82 | 0.81 | 0.8 | 0.81 | 0.0058 |
| 25% | 0.85 | 0.9 | 0.88 | 0.88 | 0.0145 |

Compound 20

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 5% | 0.08 | 0.08 | 0.08 | 0.08 | 0.0000 |
| 10% | 0.26 | 0.28 | 0.27 | 0.27 | 0.0058 |
| 20% | 0.68 | 0.55 | 0.58 | 0.60 | 0.0393 |
| 25% | 0.7 | 0.76 | 0.74 | 0.73 | 0.0176 |

Compound 21

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.25 | 0.24 | 0.26 | 0.25 | 0.0058 |
| 5% | 0.41 | 0.43 | 0.43 | 0.42 | 0.0067 |
| 10% | 0.55 | 0.59 | 0.55 | 0.56 | 0.0133 |
| 20% | 0.72 | 0.75 | 0.73 | 0.73 | 0.0088 |
| 25% | 0.83 | 0.85 | 0.81 | 0.83 | 0.0115 |

Compound 22

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.24 | 0.25 | 0.2 | 0.23 | 0.0153 |
| 5% | 0.4 | 0.41 | 0.4 | 0.40 | 0.0033 |
| 10% | 0.55 | 0.59 | 0.55 | 0.56 | 0.0133 |
| 20% | 0.72 | 0.75 | 0.73 | 0.73 | 0.0088 |
| 25% | 0.83 | 0.85 | 0.81 | 0.83 | 0.0115 |

Compound 23

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.24 | 0.25 | 0.18 | 0.22 | 0.0219 |
| 5% | 0.4 | 0.38 | 0.4 | 0.39 | 0.0067 |
| 10% | 0.55 | 0.59 | 0.55 | 0.56 | 0.0133 |
| 20% | 0.72 | 0.75 | 0.73 | 0.73 | 0.0088 |
| 25% | 0.83 | 0.85 | 0.81 | 0.83 | 0.0115 |

Compound 24

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.4 | 0.4 | 0.45 | 0.42 | 0.0167 |
| 5% | 0.59 | 0.62 | 0.58 | 0.60 | 0.0167 |
| 10% | 0.68 | 0.68 | 0.69 | 0.68 | 0.0033 |
| 20% | 0.79 | 0.79 | 0.78 | 0.79 | 0.0033 |
| 25% | 0.84 | 0.83 | 0.84 | 0.84 | 0.0033 |

Compound 25

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.4 | 0.4 | 0.43 | 0.41 | 0.0100 |
| 5% | 0.62 | 0.61 | 0.62 | 0.62 | 0.0033 |
| 10% | 0.71 | 0.71 | 0.73 | 0.72 | 0.0067 |
| 20% | 0.81 | 0.81 | 0.81 | 0.81 | 0.0000 |
| 25% | 0.9 | 0.87 | 0.94 | 0.90 | 0.0203 |

Compound 26

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.66 | 0.66 | 0.68 | 0.67 | 0.0067 |
| 5% | 0.78 | 0.76 | 0.79 | 0.78 | 0.0088 |
| 10% | 0.8 | 0.81 | 0.83 | 0.81 | 0.0088 |
| 20% | 0.89 | 0.89 | 0.88 | 0.89 | 0.0033 |
| 25% | 0.96 | 0.93 | 0.96 | 0.95 | 0.0100 |

Compound 27

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.63 | 0.67 | 0.62 | 0.64 | 0.0153 |
| 5% | 0.78 | 0.78 | 0.83 | 0.80 | 0.0167 |
| 10% | 0.83 | 0.82 | 0.85 | 0.83 | 0.0088 |
| 20% | 0.9 | 0.91 | 0.89 | 0.90 | 0.0058 |
| 25% | 0.9 | 0.96 | 0.97 | 0.94 | 0.0219 |

Compound 28

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.53 | 0.54 | 0.54 | 0.54 | 0.0033 |
| 5% | 0.71 | 0.7 | 0.71 | 0.71 | 0.0033 |
| 10% | 0.77 | 0.78 | 0.81 | 0.79 | 0.0120 |
| 20% | 0.87 | 0.86 | 0.85 | 0.86 | 0.0058 |
| 25% | 0.9 | 0.88 | 0.87 | 0.88 | 0.0088 |

Compound 29

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.33 | 0.35 | 0.38 | 0.35 | 0.0145 |
| 5% | 0.5 | 0.5 | 0.51 | 0.50 | 0.0033 |
| 10% | 0.6 | 0.58 | 0.65 | 0.61 | 0.0208 |
| 20% | 0.84 | 0.78 | 0.76 | 0.79 | 0.0240 |
| 25% | 0.87 | 0.88 | 0.83 | 0.86 | 0.0153 |

Compound 30

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.35 | 0.4 | 0.35 | 0.37 | 0.0167 |
| 5% | 0.63 | 0.6 | 0.64 | 0.62 | 0.0120 |
| 10% | 0.75 | 0.72 | 0.74 | 0.74 | 0.0088 |
| 20% | 0.85 | 0.85 | 0.88 | 0.86 | 0.0100 |
| 25% | 0.91 | 0.91 | 0.91 | 0.91 | 0.0000 |

Compound 31

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 5% | 0.05 | 0.06 | 0.03 | 0.05 | 0.0088 |
| 10% | 0.18 | 0.15 | 0 | 0.11 | 0.0557 |
| 20% | 0.38 | 0.46 | 0.38 | 0.41 | 0.0267 |
| 25% | 0.68 | 0.64 | 0.67 | 0.66 | 0.0120 |

Compound 32

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.05 | 0.06 | 0.06 | 0.06 | 0.0033 |
| 5% | 0.15 | 0.2 | 0.17 | 0.17 | 0.0145 |
| 10% | 0.37 | 0.36 | 0.37 | 0.37 | 0.0033 |
| 20% | 0.88 | 0.91 | 0.75 | 0.85 | 0.0491 |
| 25% | 0.95 | 0.97 | 0.98 | 0.97 | 0.0088 |

Compound 33

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.28 | 0.27 | 0.25 | 0.27 | 0.0088 |
| 5% | 0.46 | 0.47 | 0.47 | 0.47 | 0.0033 |
| 10% | 0.64 | 0.57 | 0.7 | 0.64 | 0.0376 |
| 20% | 0.96 | 0.98 | 1 | 0.98 | 0.0115 |
| 25% | 1 | 1 | 1 | 1.00 | 0.0000 |

Compound 34

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.63 | 0.61 | 0.72 | 0.65 | 0.0338 |
| 5% | 0.73 | 0.73 | 0.75 | 0.74 | 0.0067 |
| 10% | 0.78 | 0.77 | 0.76 | 0.77 | 0.0058 |
| 20% | 0.9 | 0.91 | 0.89 | 0.90 | 0.0058 |
| 25% | 1 | 1 | 0.95 | 0.98 | 0.0167 |

Compound 35

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.11 | 0.12 | 0.12 | 0.12 | 0.0033 |
| 5% | 0.23 | 0.21 | 0.23 | 0.22 | 0.0067 |
| 10% | 0.34 | 0.34 | 0.39 | 0.36 | 0.0167 |
| 20% | 0.76 | 0.65 | 0.65 | 0.69 | 0.0367 |
| 25% | 0.75 | 0.76 | 0.79 | 0.77 | 0.0120 |

Compound 36

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 5% | 0.04 | 0.04 | 0.06 | 0.05 | 0.0067 |
| 10% | 0.32 | 0.36 | 0.36 | 0.35 | 0.0133 |
| 20% | 0.77 | 0.77 | 0.82 | 0.79 | 0.0167 |
| 25% | 0.85 | 0.84 | 0.83 | 0.84 | 0.0058 |

Compound 37

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.02 | 0.02 | 0.02 | 0.02 | 0.0000 |
| 5% | 0.09 | 0.09 | 0.05 | 0.08 | 0.0133 |
| 10% | 0.54 | 0.35 | 0.31 | 0.40 | 0.0709 |
| 20% | 0.85 | 0.85 | 0.85 | 0.85 | 0.0000 |
| 25% | 0.93 | 0.88 | 0.9 | 0.90 | 0.0145 |

Compound 38

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.3 | 0.31 | 0.36 | 0.32 | 0.0186 |
| 5% | 0.48 | 0.44 | 0.48 | 0.47 | 0.0133 |
| 10% | 0.58 | 0.59 | 0.57 | 0.58 | 0.0058 |
| 20% | 0.79 | 0.69 | 0.68 | 0.72 | 0.0351 |
| 25% | 0.79 | 0.81 | 0.83 | 0.81 | 0.0115 |

Compound 39

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.4 | 0.36 | 0.35 | 0.37 | 0.0153 |
| 5% | 0.5 | 0.48 | 0.52 | 0.50 | 0.0115 |
| 10% | 0.68 | 0.68 | 0.65 | 0.67 | 0.0100 |
| 20% | 0.79 | 0.84 | 0.8 | 0.81 | 0.0153 |
| 25% | 0.92 | 0.86 | 0.9 | 0.89 | 0.0176 |

Compound 40

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.25 | 0.22 | 0.24 | 0.24 | 0.0088 |
| 5% | 0.3 | 0.35 | 0.33 | 0.33 | 0.0145 |
| 10% | 0.44 | 0.47 | 0.45 | 0.45 | 0.0088 |
| 20% | 0.78 | 0.73 | 0.76 | 0.76 | 0.0145 |
| 25% | 0.92 | 0.9 | 0.89 | 0.90 | 0.0088 |

Compound 41

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 5% | 0.1 | 0.1 | 0.12 | 0.11 | 0.0067 |
| 10% | 0.26 | 0.33 | 0.3 | 0.30 | 0.0203 |
| 20% | 0.6 | 0.58 | 0.63 | 0.60 | 0.0145 |
| 25% | 0.73 | 0.77 | 0.89 | 0.80 | 0.0481 |

Compound 42

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.08 | 0.08 | 0.06 | 0.07 | 0.0067 |
| 5% | 0.22 | 0.23 | 0.23 | 0.23 | 0.0033 |
| 10% | 0.47 | 0.43 | 0.4 | 0.43 | 0.0203 |
| 20% | 0.78 | 0.83 | 0.85 | 0.82 | 0.0208 |
| 25% | 0.88 | 0.83 | 0.81 | 0.84 | 0.0208 |

Compound 43

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 5% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 10% | 0.07 | 0.09 | 0.07 | 0.08 | 0.0067 |
| 20% | 0.33 | 0.33 | 0.33 | 0.33 | 0.0000 |
| 25% | 0.42 | 0.44 | 0.46 | 0.44 | 0.0115 |

Compound 44

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.81 | 0.83 | 0.79 | 0.81 | 0.0115 |
| 5% | 0.83 | 0.82 | 0.84 | 0.83 | 0.0058 |
| 10% | 0.88 | 0.87 | 0.88 | 0.88 | 0.0033 |
| 20% | 1 | 1 | 0.94 | 0.98 | 0.0200 |
| 25% | 1 | 1 | 1 | 1.00 | 0.0000 |

Compound 45

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 5% | 0.09 | 0.05 | 0.03 | 0.06 | 0.0176 |
| 10% | 0.16 | 0.16 | 0.15 | 0.16 | 0.0033 |
| 20% | 0.35 | 0.35 | 0.38 | 0.36 | 0.0100 |
| 25% | 0.49 | 0.5 | 0.57 | 0.52 | 0.0252 |

Compound 46

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 5% | 0.04 | 0.08 | 0.1 | 0.07 | 0.0176 |
| 10% | 0.23 | 0.3 | 0.2 | 0.24 | 0.0296 |
| 20% | 0.7 | 0.72 | 0.77 | 0.73 | 0.0208 |
| 25% | 0.88 | 0.85 | 0.86 | 0.86 | 0.0088 |

Compound 47

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 5% | 0.05 | 0.03 | 0.03 | 0.04 | 0.0067 |
| 10% | 0.16 | 0.16 | 0.15 | 0.16 | 0.0033 |
| 20% | 0.45 | 0.48 | 0.47 | 0.47 | 0.0088 |
| 25% | 0.67 | 0.65 | 0.7 | 0.67 | 0.0145 |

Compound 48

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.06 | 0.1 | 0.04 | 0.07 | 0.0176 |
| 5% | 0.19 | 0.2 | 0.2 | 0.20 | 0.0033 |
| 10% | 0.48 | 0.45 | 0.4 | 0.44 | 0.0233 |
| 20% | 0.82 | 0.84 | 0.87 | 0.84 | 0.0145 |
| 25% | 0.9 | 0.89 | 0.86 | 0.88 | 0.0120 |

Compound 49

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.01 | 0.01 | 0.03 | 0.02 | 0.0067 |
| 5% | 0.14 | 0.13 | 0.17 | 0.15 | 0.0120 |
| 10% | 0.37 | 0.44 | 0.39 | 0.40 | 0.0208 |
| 20% | 0.81 | 0.8 | 0.85 | 0.82 | 0.0153 |
| 25% | 0.89 | 0.84 | 0.85 | 0.86 | 0.0153 |

Compound 50

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 5% | 0.04 | 0.06 | 0.03 | 0.04 | 0.0088 |
| 10% | 0.26 | 0.23 | 0.23 | 0.24 | 0.0100 |
| 20% | 0.75 | 0.81 | 0.75 | 0.77 | 0.0200 |
| 25% | 0.92 | 0.89 | 0.83 | 0.88 | 0.0265 |

Compound 51

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.03 | 0.02 | 0.02 | 0.02 | 0.0033 |
| 5% | 0.05 | 0.05 | 0.06 | 0.05 | 0.0033 |
| 10% | 0.18 | 0.19 | 0.2 | 0.19 | 0.0058 |
| 20% | 0.27 | 0.4 | 0.26 | 0.31 | 0.0451 |
| 25% | 0.28 | 0.37 | 0.38 | 0.34 | 0.0318 |

Compound 52

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.38 | 0.36 | 0.42 | 0.39 | 0.0176 |
| 5% | 0.61 | 0.6 | 0.63 | 0.61 | 0.0088 |
| 10% | 0.8 | 0.78 | 0.77 | 0.78 | 0.0088 |
| 20% | 0.98 | 0.96 | 0.96 | 0.97 | 0.0067 |
| 25% | 1 | 1 | 1 | 1.00 | 0.0000 |

Compound 53

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.02 | 0 | 0.02 | 0.01 | 0.0067 |
| 5% | 0.13 | 0.09 | 0.11 | 0.11 | 0.0115 |
| 10% | 0.45 | 0.5 | 0.48 | 0.48 | 0.0145 |
| 20% | 1 | 1 | 1 | 1.00 | 0.0000 |
| 25% | 1 | 1 | 1 | 1.00 | 0.0000 |

Compound 54

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.27 | 0.32 | 0.28 | 0.29 | 0.0153 |
| 5% | 0.51 | 0.45 | 0.48 | 0.48 | 0.0173 |
| 10% | 0.55 | 0.63 | 0.63 | 0.60 | 0.0267 |
| 20% | 0.83 | 0.78 | 0.75 | 0.79 | 0.0233 |
| 25% | 0.9 | 0.88 | 0.85 | 0.88 | 0.0145 |

Compound 55

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 5% | 0.04 | 0.02 | 0.04 | 0.03 | 0.0067 |
| 10% | 0.11 | 0.11 | 0.11 | 0.11 | 0.0000 |
| 20% | 0.26 | 0.27 | 0.25 | 0.26 | 0.0058 |
| 25% | 0.44 | 0.33 | 0.47 | 0.41 | 0.0426 |

Compound 56

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 5% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 10% | 0.07 | 0.04 | 0.04 | 0.05 | 0.0100 |
| 20% | 0.33 | 0.33 | 0.33 | 0.33 | 0.0000 |
| 25% | 0.4 | 0.35 | 0.44 | 0.40 | 0.0260 |

Compound 57

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 5% | 0.02 | 0.02 | 0.02 | 0.02 | 0.0000 |
| 10% | 0.06 | 0.07 | | 0.07 | 0.0050 |
| 20% | 0.14 | 0.13 | 0.14 | 0.14 | 0.0033 |
| 25% | 0.14 | 0.14 | 0.14 | 0.14 | 0.0000 |

Compound 58

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 5% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 10% | 0.09 | 0.07 | 0.06 | 0.07 | 0.0088 |
| 20% | 0.37 | 0.41 | 0.36 | 0.38 | 0.0153 |
| 25% | 0.56 | 0.38 | 0.47 | 0.47 | 0.0520 |

Compound 59

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.04 | 0.06 | 0.03 | 0.04 | 0.0088 |
| 5% | 0.07 | 0.04 | 0.07 | 0.06 | 0.0100 |
| 10% | 0.15 | 0.15 | 0.12 | 0.14 | 0.0100 |
| 20% | 0.24 | 0.19 | 0.2 | 0.21 | 0.0153 |
| 25% | 0.26 | 0.27 | 0.26 | 0.26 | 0.0033 |

Compound 60

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 5% | 0.07 | 0.08 | 0.09 | 0.08 | 0.0058 |
| 10% | 0.4 | 0.47 | 0.36 | 0.41 | 0.0321 |
| 20% | 0.85 | 0.88 | 0.79 | 0.84 | 0.0265 |
| 25% | 0.9 | 0.87 | 0.9 | 0.89 | 0.0100 |

Compound 61

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.33 | 0.33 | 0.28 | 0.31 | 0.0167 |
| 5% | 0.5 | 0.48 | 0.53 | 0.50 | 0.0145 |
| 10% | 0.69 | 0.67 | 0.7 | 0.69 | 0.0088 |
| 20% | 0.91 | 0.94 | 0.94 | 0.93 | 0.0100 |
| 25% | 1 | 1 | 1 | 1.00 | 0.0000 |

Compound 62

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.14 | 0.13 | 0.17 | 0.15 | 0.0120 |
| 5% | 0.47 | 0.42 | 0.56 | 0.48 | 0.0410 |
| 10% | 0.63 | 0.73 | 0.65 | 0.67 | 0.0306 |
| 20% | 0.97 | 0.95 | 0.97 | 0.96 | 0.0067 |
| 25% | 1 | 1 | 1 | 1.00 | 0.0000 |

Compound 63

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.04 | 0.04 | 0.04 | 0.04 | 0.0000 |
| 5% | 0.17 | 0.14 | 0.15 | 0.15 | 0.0088 |
| 10% | 0.45 | 0.46 | 0.48 | 0.46 | 0.0088 |
| 20% | 0.86 | 0.9 | 0.87 | 0.88 | 0.0120 |
| 25% | 0.89 | 0.93 | 0.96 | 0.93 | 0.0203 |

Compound 64

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 5% | 0.03 | 0.05 | 0.07 | 0.05 | 0.0115 |
| 10% | 0.26 | 0.33 | 0.3 | 0.30 | 0.0203 |
| 20% | 0.66 | 0.66 | 0.68 | 0.67 | 0.0067 |
| 25% | 0.85 | 0.83 | 0.79 | 0.82 | 0.0176 |

Compound 65

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.05 | 0.05 | 0.05 | 0.05 | 0.0000 |
| 5% | 0.17 | 0.15 | 0.15 | 0.16 | 0.0067 |
| 10% | 0.48 | 0.39 | 0.37 | 0.41 | 0.0338 |
| 20% | 0.77 | 0.75 | 0.73 | 0.75 | 0.0115 |
| 25% | 0.83 | 0.84 | 0.81 | 0.83 | 0.0088 |

Compound 66

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.07 | 0.06 | 0.11 | 0.08 | 0.0153 |
| 5% | 0.4 | 0.4 | 0.4 | 0.40 | 0.0000 |
| 10% | 0.6 | 0.58 | 0.63 | 0.60 | 0.0145 |
| 20% | 0.83 | 0.86 | 0.83 | 0.84 | 0.0100 |
| 25% | 1 | 1 | 0.99 | 1.00 | 0.0033 |

Compound 67

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.04 | 0.04 | 0.04 | 0.04 | 0.0000 |
| 5% | 0.16 | 0.14 | 0.14 | 0.15 | 0.0067 |
| 10% | 0.45 | 0.48 | 0.49 | 0.47 | 0.0120 |
| 20% | 0.9 | 1 | 0.93 | 0.94 | 0.0296 |
| 25% | 0.97 | 0.97 | 1 | 0.98 | 0.0100 |

Compound 68

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.06 | 0.08 | 0.08 | 0.07 | 0.0067 |
| 5% | 0.19 | 0.24 | 0.23 | 0.22 | 0.0153 |
| 10% | 0.3 | 0.42 | 0.4 | 0.37 | 0.0371 |
| 20% | 0.68 | 0.66 | 0.69 | 0.68 | 0.0088 |
| 25% | 0.8 | 0.81 | 0.85 | 0.82 | 0.0153 |

Compound 69

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.17 | 0.15 | 0.16 | 0.16 | 0.0058 |
| 5% | 0.34 | 0.35 | 0.33 | 0.34 | 0.0058 |
| 10% | 0.51 | 0.52 | 0.46 | 0.50 | 0.0186 |
| 20% | 0.83 | 0.85 | 0.84 | 0.84 | 0.0058 |
| 25% | 0.81 | 0.86 | 0.9 | 0.86 | 0.0260 |

Compound 70

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.35 | 0.33 | 0.37 | 0.35 | 0.0115 |
| 5% | 0.55 | 0.5 | 0.53 | 0.53 | 0.0145 |
| 10% | 0.65 | 0.68 | 0.67 | 0.67 | 0.0088 |
| 20% | 0.83 | 0.83 | 0.85 | 0.84 | 0.0067 |
| 25% | 0.9 | 0.95 | 0.93 | 0.93 | 0.0145 |

Compound 71

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.13 | 0.14 | 0.11 | 0.13 | 0.0088 |
| 5% | 0.3 | 0.3 | 0.3 | 0.30 | 0.0000 |
| 10% | 0.52 | 0.52 | 0.51 | 0.52 | 0.0033 |
| 20% | 0.7 | 0.67 | 0.65 | 0.67 | 0.0145 |
| 25% | 0.8 | 0.83 | 0.83 | 0.82 | 0.0100 |

Compound 72

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.13 | 0.23 | 0.2 | 0.19 | 0.0296 |
| 5% | 0.49 | 0.42 | 0.42 | 0.44 | 0.0233 |
| 10% | 0.63 | 0.73 | 0.6 | 0.65 | 0.0393 |
| 20% | 0.84 | 0.85 | 0.83 | 0.84 | 0.0058 |
| 25% | 0.91 | 0.89 | 0.91 | 0.90 | 0.0067 |

Compound 73

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 5% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 10% | 0.05 | 0.05 | 0.02 | 0.04 | 0.0100 |
| 20% | 0.19 | 0.21 | 0.2 | 0.20 | 0.0058 |
| 25% | 0.33 | 0.28 | 0.3 | 0.30 | 0.0145 |

Compound 74

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.26 | 0.22 | 0.24 | 0.24 | 0.0115 |
| 5% | 0.58 | 0.57 | 0.6 | 0.58 | 0.0088 |
| 10% | 0.7 | 0.72 | 0.71 | 0.71 | 0.0058 |
| 20% | 0.81 | 0.83 | 0.81 | 0.82 | 0.0067 |
| 25% | 0.87 | 0.87 | 0.91 | 0.88 | 0.0133 |

Compound 75

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 5% | 0.19 | 0.19 | 0.16 | 0.18 | 0.0100 |
| 10% | 0.56 | 0.44 | 0.42 | 0.47 | 0.0437 |
| 20% | 1 | 1 | 1 | 1.00 | 0.0000 |
| 25% | 1 | 1 | 1 | 1.00 | 0.0000 |

Compound 76

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.02 | 0.02 | 0.05 | 0.03 | 0.0000 |
| 5% | 0.28 | 0.3 | 0.32 | 0.30 | 0.0115 |
| 10% | 0.5 | 0.53 | 0.64 | 0.56 | 0.0426 |
| 20% | 0.84 | 0.88 | 0.86 | 0.86 | 0.0115 |
| 25% | 1 | 1 | 1 | 1.00 | 0.0000 |

Compound 77

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 5% | 0.07 | 0.09 | 0.09 | 0.08 | 0.0067 |
| 10% | 0.29 | 0.31 | 0.28 | 0.29 | 0.0088 |
| 20% | 0.73 | 0.72 | 0.76 | 0.74 | 0.0120 |
| 25% | 0.87 | 0.85 | 0.85 | 0.86 | 0.0067 |

Compound 78

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 5% | 0.03 | 0.02 | 0.03 | 0.03 | 0.0033 |
| 10% | 0.06 | 0.05 | 0.07 | 0.06 | 0.0058 |
| 20% | 0.14 | 0.14 | 0.11 | 0.13 | 0.0100 |
| 25% | 0.15 | 0.16 | 0.14 | 0.15 | 0.0058 |

Compound 79

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 5% | 0.04 | 0.05 | 0.05 | 0.05 | 0.0033 |
| 10% | 0.24 | 0.24 | 0.25 | 0.24 | 0.0033 |
| 20% | 0.62 | 0.66 | 0.67 | 0.65 | 0.0153 |
| 25% | 0.78 | 0.75 | 0.73 | 0.75 | 0.0145 |

Compound 80

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 5% | 0.03 | 0.03 | 0.06 | 0.04 | 0.0100 |
| 10% | 0.18 | 0.24 | 0.24 | 0.22 | 0.0200 |
| 20% | 0.54 | 0.56 | | 0.55 | 0.0100 |
| 25% | 0.61 | 0.63 | 0.65 | 0.63 | 0.0115 |

Compound 81

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.58 | 0.54 | 0.57 | 0.56 | 0.0120 |
| 5% | 0.67 | 0.63 | 0.64 | 0.65 | 0.0120 |
| 10% | 0.72 | 0.73 | 0.74 | 0.73 | 0.0058 |
| 20% | 0.81 | 0.84 | 0.78 | 0.81 | 0.0173 |
| 25% | 0.84 | 0.86 | 0.88 | 0.86 | 0.0115 |

Compound 82

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 5% | 0.06 | 0.1 | 0.1 | 0.09 | 0.0133 |
| 10% | 0.27 | 0.26 | 0.26 | 0.26 | 0.0033 |
| 20% | 0.59 | 0.6 | 0.57 | 0.59 | 0.0088 |
| 25% | 0.65 | 0.66 | 0.68 | 0.66 | 0.0088 |

Compound 83

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 5% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 10% | 0.11 | 0.11 | 0.12 | 0.11 | 0.0033 |
| 20% | 0.43 | 0.44 | 0.44 | 0.44 | 0.0033 |
| 25% | 0.53 | 0.53 | 0.54 | 0.53 | 0.0033 |

Compound 84

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 5% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 10% | 0.11 | 0.13 | 0.12 | 0.12 | 0.0058 |
| 20% | 0.45 | 0.48 | 0.41 | 0.45 | 0.0203 |
| 25% | 0.53 | 0.56 | 0.55 | 0.55 | 0.0088 |

Compound 85

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 5% | 0.09 | 0.11 | 0.1 | 0.10 | 0.0058 |
| 10% | 0.24 | 0.33 | 0.26 | 0.28 | 0.0273 |
| 20% | 0.59 | 0.58 | 0.6 | 0.59 | 0.0058 |
| 25% | 0.66 | 0.65 | 0.64 | 0.65 | 0.0058 |

Compound 86

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 5% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 10% | 0.01 | 0.01 | 0.02 | 0.01 | 0.0033 |
| 20% | 0.01 | 0.04 | 0.03 | 0.03 | 0.0088 |
| 25% | 0.05 | 0.04 | 0.05 | 0.05 | 0.0033 |

Compound 87

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.06 | 0.04 | 0.05 | 0.05 | 0.0058 |
| 5% | 0.11 | 0.11 | 0.1 | 0.11 | 0.0033 |
| 10% | 0.18 | 0.26 | 0.21 | 0.22 | 0.0233 |
| 20% | 0.5 | 0.47 | 0.47 | 0.48 | 0.0100 |
| 25% | 0.55 | 0.62 | 0.61 | 0.59 | 0.0219 |

Compound 88

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 5% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 10% | 0.13 | 0.09 | 0.1 | 0.11 | 0.0120 |
| 20% | 0.35 | 0.37 | 0.32 | 0.35 | 0.0145 |
| 25% | 0.45 | 0.47 | 0.5 | 0.47 | 0.0145 |

Compound 89

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 5% | 0.04 | 0.06 | 0.09 | 0.06 | 0.0145 |
| 10% | 0.38 | 0.31 | 0.26 | 0.32 | 0.0348 |
| 20% | 0.66 | 0.64 | 0.64 | 0.65 | 0.0067 |
| 25% | 0.7 | 0.84 | 0.7 | 0.75 | 0.0467 |

Compound 90

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.2 | 0.15 | 0.2 | 0.18 | 0.0167 |
| 5% | 0.41 | 0.36 | 0.34 | 0.37 | 0.0208 |
| 10% | 0.5 | 0.52 | 0.53 | 0.52 | 0.0088 |
| 20% | 0.68 | 0.68 | 0.78 | 0.71 | 0.0333 |
| 25% | 0.78 | 0.79 | 0.83 | 0.80 | 0.0153 |

Compound 91

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 5% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 10% | 0.16 | 0.15 | 0.16 | 0.16 | 0.0033 |
| 20% | 0.45 | 0.4 | 0.42 | 0.42 | 0.0145 |
| 25% | 0.48 | 0.5 | 0.53 | 0.50 | 0.0145 |

Compound 92

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.08 | 0.04 | 0.05 | 0.06 | 0.0120 |
| 5% | 0.19 | 0.18 | 0.21 | 0.19 | 0.0088 |
| 10% | 0.46 | 0.44 | 0.4 | 0.43 | 0.0176 |
| 20% | 0.66 | 0.61 | 0.62 | 0.63 | 0.0153 |
| 25% | 0.68 | 0.7 | 0.74 | 0.71 | 0.0176 |

Compound 93

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 5% | 0.03 | 0.03 | 0.07 | 0.04 | 0.0133 |
| 10% | 0.29 | 0.22 | 0.27 | 0.26 | 0.0208 |
| 20% | 0.63 | 0.62 | 0.64 | 0.63 | 0.0058 |
| 25% | 0.77 | 0.71 | 0.75 | 0.74 | 0.0176 |

Compound 94

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 5% | 0.04 | 0.04 | 0.04 | 0.04 | 0.0000 |
| 10% | 0.38 | 0.36 | 0.38 | 0.37 | 0.0067 |
| 20% | 0.82 | 0.83 | 0.84 | 0.83 | 0.0058 |
| 25% | 0.89 | 0.89 | 0.89 | 0.89 | 0.0000 |

Compound 95

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 5% | 0.01 | 0.01 | 0.01 | 0.01 | 0.0000 |
| 10% | 0.28 | 0.28 | 0.27 | 0.28 | 0.0033 |
| 20% | 0.77 | 0.77 | 0.79 | 0.78 | 0.0067 |
| 25% | 0.88 | 0.89 | 0.87 | 0.88 | 0.0058 |

3.2.2 MeOH/CPME R_f Data

| Compound 1 | | | | | |
|----------------|-------|-------|-------|---------|----------------|
| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
| 2% | 0.71 | 0.71 | 0.73 | 0.72 | 0.0067 |
| 5% | 0.72 | 0.76 | 0.74 | 0.74 | 0.0115 |
| 10% | 0.74 | 0.78 | 0.77 | 0.76 | 0.0120 |
| 20% | 0.78 | 0.79 | 0.78 | 0.78 | 0.0033 |
| 25% | 0.8 | 0.82 | 0.84 | 0.82 | 0.0115 |

| Compound 2 | | | | | |
|----------------|-------|-------|-------|---------|----------------|
| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
| 2% | 0.73 | 0.71 | 0.72 | 0.72 | 0.0058 |
| 5% | 0.77 | 0.71 | 0.77 | 0.75 | 0.0200 |
| 10% | 0.8 | 0.82 | 0.81 | 0.81 | 0.0058 |
| 20% | 0.87 | 0.83 | 0.86 | 0.85 | 0.0120 |
| 25% | 0.89 | 0.88 | 0.87 | 0.88 | 0.0058 |

| Compound 3 | | | | | |
|----------------|-------|-------|-------|---------|----------------|
| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
| 2% | 0.76 | 0.69 | 0.74 | 0.73 | 0.0208 |
| 5% | 0.74 | 0.75 | 0.73 | 0.74 | 0.0058 |
| 10% | 0.75 | 0.78 | 0.77 | 0.77 | 0.0088 |
| 20% | 0.78 | 0.79 | 0.79 | 0.79 | 0.0033 |
| 25% | 0.78 | 0.83 | 0.79 | 0.80 | 0.0153 |

| Compound 4 | | | | | |
|----------------|-------|-------|-------|---------|----------------|
| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
| 2% | 0.51 | 0.55 | 0.57 | 0.54 | 0.0176 |
| 5% | 0.54 | 0.56 | 0.56 | 0.55 | 0.0067 |
| 10% | 0.58 | 0.61 | 0.62 | 0.60 | 0.0120 |
| 20% | 0.63 | 0.64 | 0.63 | 0.63 | 0.0033 |
| 25% | 0.71 | 0.67 | 0.68 | 0.69 | 0.0120 |

| Compound 5 | | | | | |
|----------------|-------|-------|-------|---------|----------------|
| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
| 2% | 0.39 | 0.52 | 0.38 | 0.43 | 0.0451 |
| 5% | 0.35 | 0.41 | 0.45 | 0.40 | 0.0291 |
| 10% | 0.44 | 0.45 | 0.48 | 0.46 | 0.0120 |
| 20% | 0.56 | 0.56 | 0.6 | 0.57 | 0.0133 |
| 25% | 0.64 | 0.69 | 0.67 | 0.67 | 0.0145 |

| Compound 6 | | | | | |
|----------------|-------|-------|-------|---------|----------------|
| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
| 2% | 0.56 | 0.59 | 0.6 | 0.58 | 0.0120 |
| 5% | 0.6 | 0.61 | 0.63 | 0.61 | 0.0088 |
| 10% | 0.63 | 0.64 | 0.65 | 0.64 | 0.0058 |
| 20% | 0.67 | 0.67 | 0.68 | 0.67 | 0.0033 |
| 25% | 0.67 | 0.73 | 0.71 | 0.70 | 0.0176 |

Compound 7

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.53 | 0.62 | 0.64 | 0.60 | 0.0338 |
| 5% | 0.63 | 0.64 | 0.64 | 0.64 | 0.0033 |
| 10% | 0.65 | 0.66 | 0.64 | 0.65 | 0.0058 |
| 20% | 0.68 | 0.7 | 0.67 | 0.68 | 0.0088 |
| 25% | 0.66 | 0.7 | 0.71 | 0.69 | 0.0153 |

Compound 8

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.66 | 0.6 | 0.63 | 0.63 | 0.0173 |
| 5% | 0.63 | 0.65 | 0.64 | 0.64 | 0.0058 |
| 10% | 0.67 | 0.68 | 0.63 | 0.66 | 0.0153 |
| 20% | 0.66 | 0.69 | 0.68 | 0.68 | 0.0088 |
| 25% | 0.68 | 0.69 | 0.7 | 0.69 | 0.0058 |

Compound 9

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.6 | 0.63 | 0.65 | 0.63 | 0.0145 |
| 5% | 0.64 | 0.64 | 0.64 | 0.64 | 0.0000 |
| 10% | 0.65 | 0.66 | 0.68 | 0.66 | 0.0088 |
| 20% | 0.69 | 0.68 | 0.7 | 0.69 | 0.0058 |
| 25% | 0.71 | 0.68 | 0.7 | 0.70 | 0.0088 |

Compound 10

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.67 | 0.66 | 0.63 | 0.65 | 0.0120 |
| 5% | 0.69 | 0.68 | 0.68 | 0.68 | 0.0033 |
| 10% | 0.68 | 0.72 | 0.7 | 0.70 | 0.0115 |
| 20% | 0.77 | 0.75 | 0.75 | 0.76 | 0.0067 |
| 25% | 0.77 | 0.78 | 0.79 | 0.78 | 0.0058 |

Compound 11

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.12 | 0.09 | 0.09 | 0.10 | 0.0100 |
| 5% | 0.1 | 0.1 | 0.13 | 0.11 | 0.0100 |
| 10% | 0.16 | 0.12 | 0.18 | 0.15 | 0.0176 |
| 20% | 0.16 | 0.18 | 0.25 | 0.20 | 0.0273 |
| 25% | 0.24 | 0.26 | 0.2 | 0.23 | 0.0176 |

Compound 12

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.06 | 0.11 | 0.11 | 0.09 | 0.0167 |
| 5% | 0.1 | 0.12 | 0.1 | 0.11 | 0.0067 |
| 10% | 0.2 | 0.18 | 0.18 | 0.19 | 0.0067 |
| 20% | 0.25 | 0.24 | 0.25 | 0.25 | 0.0033 |
| 25% | 0.28 | 0.3 | 0.28 | 0.29 | 0.0067 |

Compound 13

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.03 | 0.06 | 0.05 | 0.05 | 0.0088 |
| 5% | 0.07 | 0.07 | 0.07 | 0.07 | 0.0000 |
| 10% | 0.14 | 0.17 | 0.15 | 0.15 | 0.0088 |
| 20% | 0.19 | 0.2 | 0.18 | 0.19 | 0.0058 |
| 25% | 0.26 | 0.26 | 0.23 | 0.25 | 0.0100 |

Compound 14

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.01 | 0 | 0 | 0.00 | 0.0033 |
| 5% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 10% | 0.03 | 0.02 | 0.06 | 0.04 | 0.0120 |
| 20% | 0.15 | 0.11 | 0.11 | 0.12 | 0.0133 |
| 25% | 0.23 | 0.18 | 0.2 | 0.20 | 0.0145 |

Compound 15

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.11 | 0.1 | 0.11 | 0.11 | 0.0033 |
| 5% | 0.17 | 0.18 | 0.16 | 0.17 | 0.0058 |
| 10% | 0.25 | 0.3 | 0.25 | 0.27 | 0.0167 |
| 20% | 0.36 | 0.31 | 0.5 | 0.39 | 0.0569 |
| 25% | 0.5 | 0.5 | 0.52 | 0.51 | 0.0067 |

Compound 16

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.05 | 0.07 | 0.05 | 0.06 | 0.0067 |
| 5% | 0.14 | 0.17 | 0.17 | 0.16 | 0.0100 |
| 10% | 0.22 | 0.23 | 0.23 | 0.23 | 0.0033 |
| 20% | 0.25 | 0.23 | 0.22 | 0.23 | 0.0088 |
| 25% | 0.29 | 0.26 | 0.23 | 0.26 | 0.0173 |

Compound 17

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.12 | 0.09 | 0.1 | 0.10 | 0.0088 |
| 5% | 0.11 | 0.13 | 0.13 | 0.12 | 0.0067 |
| 10% | 0.15 | 0.16 | 0.12 | 0.14 | 0.0120 |
| 20% | 0.2 | 0.22 | 0.18 | 0.20 | 0.0115 |
| 25% | 0.3 | 0.25 | 0.25 | 0.27 | 0.0167 |

Compound 18

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.63 | 0.66 | 0.64 | 0.64 | 0.0088 |
| 5% | 0.66 | 0.71 | 0.71 | 0.69 | 0.0167 |
| 10% | 0.7 | 0.73 | 0.71 | 0.71 | 0.0088 |
| 20% | 0.72 | 0.81 | 0.8 | 0.78 | 0.0285 |
| 25% | 0.79 | 0.81 | 0.8 | 0.80 | 0.0058 |

Compound 19

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.67 | 0.68 | 0.7 | 0.68 | 0.0088 |
| 5% | 0.67 | 0.7 | 0.71 | 0.69 | 0.0120 |
| 10% | 0.68 | 0.68 | 0.76 | 0.71 | 0.0267 |
| 20% | 0.8 | 0.81 | 0.84 | 0.82 | 0.0120 |
| 25% | 0.85 | 0.82 | 0.86 | 0.84 | 0.0120 |

Compound 20

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.49 | 0.54 | 0.54 | 0.52 | 0.0167 |
| 5% | 0.56 | 0.59 | 0.6 | 0.58 | 0.0120 |
| 10% | 0.63 | 0.59 | 0.67 | 0.63 | 0.0231 |
| 20% | 0.69 | 0.7 | 0.73 | 0.71 | 0.0120 |
| 25% | 0.7 | 0.79 | 0.76 | 0.75 | 0.0265 |

Compound 21

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.63 | 0.66 | 0.67 | 0.65 | 0.0120 |
| 5% | 0.66 | 0.74 | 0.71 | 0.70 | 0.0233 |
| 10% | 0.73 | 0.71 | 0.75 | 0.73 | 0.0115 |
| 20% | 0.75 | 0.84 | 0.84 | 0.81 | 0.0300 |
| 25% | 0.82 | 0.85 | 0.84 | 0.84 | 0.0088 |

Compound 22

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.63 | 0.66 | 0.67 | 0.65 | 0.0120 |
| 5% | 0.66 | 0.74 | 0.71 | 0.70 | 0.0233 |
| 10% | 0.74 | 0.73 | 0.73 | 0.73 | 0.0033 |
| 20% | 0.75 | 0.84 | 0.84 | 0.81 | 0.0300 |
| 25% | 0.82 | 0.85 | 0.84 | 0.84 | 0.0088 |

Compound 23

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.57 | 0.59 | 0.58 | 0.58 | 0.0058 |
| 5% | 0.61 | 0.66 | 0.68 | 0.65 | 0.0208 |
| 10% | 0.68 | 0.72 | 0.7 | 0.70 | 0.0115 |
| 20% | 0.74 | 0.81 | 0.78 | 0.78 | 0.0203 |
| 25% | 0.82 | 0.85 | 0.84 | 0.84 | 0.0088 |

Compound 24

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.67 | 0.68 | 0.69 | 0.68 | 0.0058 |
| 5% | 0.7 | 0.69 | 0.69 | 0.69 | 0.0033 |
| 10% | 0.71 | 0.7 | 0.74 | 0.72 | 0.0120 |
| 20% | 0.74 | 0.73 | 0.75 | 0.74 | 0.0058 |
| 25% | 0.73 | 0.79 | 0.76 | 0.76 | 0.0173 |

Compound 25

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.64 | 0.65 | 0.65 | 0.65 | 0.0033 |
| 5% | 0.67 | 0.67 | 0.68 | 0.67 | 0.0033 |
| 10% | 0.73 | 0.7 | 0.7 | 0.71 | 0.0100 |
| 20% | 0.73 | 0.74 | 0.73 | 0.73 | 0.0033 |
| 25% | 0.73 | 0.79 | 0.78 | 0.77 | 0.0186 |

Compound 26

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.74 | 0.75 | 0.75 | 0.75 | 0.0033 |
| 5% | 0.77 | 0.76 | 0.77 | 0.77 | 0.0033 |
| 10% | 0.8 | 0.77 | 0.78 | 0.78 | 0.0088 |
| 20% | 0.81 | 0.79 | 0.82 | 0.81 | 0.0088 |
| 25% | 0.83 | 0.85 | 0.84 | 0.84 | 0.0058 |

Compound 27

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.76 | 0.71 | 0.78 | 0.75 | 0.0208 |
| 5% | 0.76 | 0.73 | 0.78 | 0.76 | 0.0145 |
| 10% | 0.78 | 0.77 | 0.75 | 0.77 | 0.0088 |
| 20% | 0.77 | 0.78 | 0.8 | 0.78 | 0.0088 |
| 25% | 0.81 | 0.8 | 0.8 | 0.80 | 0.0033 |

Compound 28

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.68 | 0.71 | 0.7 | 0.70 | 0.0088 |
| 5% | 0.69 | 0.73 | 0.72 | 0.71 | 0.0120 |
| 10% | 0.7 | 0.71 | 0.77 | 0.73 | 0.0219 |
| 20% | 0.78 | 0.77 | 0.71 | 0.75 | 0.0219 |
| 25% | 0.74 | 0.78 | 0.79 | 0.77 | 0.0153 |

Compound 29

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.58 | 0.55 | 0.41 | 0.51 | 0.0524 |
| 5% | 0.59 | 0.59 | 0.54 | 0.57 | 0.0167 |
| 10% | 0.65 | 0.62 | 0.67 | 0.65 | 0.0145 |
| 20% | 0.72 | 0.7 | 0.75 | 0.72 | 0.0145 |
| 25% | 0.77 | 0.8 | 0.74 | 0.77 | 0.0173 |

Compound 30

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.57 | 0.57 | 0.53 | 0.56 | 0.0133 |
| 5% | 0.61 | 0.6 | 0.61 | 0.61 | 0.0033 |
| 10% | 0.63 | 0.64 | 0.63 | 0.63 | 0.0033 |
| 20% | 0.64 | 0.67 | 0.66 | 0.66 | 0.0088 |
| 25% | 0.68 | 0.68 | 0.67 | 0.68 | 0.0033 |

Compound 31

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.03 | 0.03 | 0.04 | 0.03 | 0.0033 |
| 5% | 0.07 | 0.07 | 0.05 | 0.06 | 0.0067 |
| 10% | 0.12 | 0.1 | 0.12 | 0.11 | 0.0067 |
| 20% | 0.14 | 0.15 | 0.15 | 0.15 | 0.0033 |
| 25% | 0.21 | 0.2 | 0.15 | 0.19 | 0.0186 |

Compound 32

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.33 | 0.31 | 0.24 | 0.29 | 0.0273 |
| 5% | 0.38 | 0.36 | 0.27 | 0.34 | 0.0338 |
| 10% | 0.45 | 0.48 | 0.43 | 0.45 | 0.0145 |
| 20% | 0.55 | 0.57 | 0.45 | 0.52 | 0.0371 |
| 25% | 0.64 | 0.6 | 0.48 | 0.57 | 0.0481 |

Compound 33

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.66 | 0.65 | 0.64 | 0.65 | 0.0058 |
| 5% | 0.67 | 0.66 | 0.71 | 0.68 | 0.0153 |
| 10% | 0.67 | 0.71 | 0.71 | 0.70 | 0.0133 |
| 20% | 0.7 | 0.73 | 0.71 | 0.71 | 0.0088 |
| 25% | 0.76 | 0.72 | 0.74 | 0.74 | 0.0115 |

Compound 34

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.89 | 0.91 | 0.91 | 0.90 | 0.0067 |
| 5% | 0.93 | 0.91 | 0.93 | 0.92 | 0.0067 |
| 10% | 0.95 | 0.94 | 0.93 | 0.94 | 0.0058 |
| 20% | 0.94 | 0.96 | 0.97 | 0.96 | 0.0088 |
| 25% | 0.95 | 1 | 1 | 0.98 | 0.0167 |

Compound 35

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.48 | 0.48 | 0.41 | 0.46 | 0.0233 |
| 5% | 0.5 | 0.52 | 0.51 | 0.51 | 0.0058 |
| 10% | 0.6 | 0.63 | 0.61 | 0.61 | 0.0088 |
| 20% | 0.65 | 0.7 | 0.74 | 0.70 | 0.0260 |
| 25% | 0.74 | 0.76 | 0.75 | 0.75 | 0.0058 |

Compound 36

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.18 | 0.16 | 0.16 | 0.17 | 0.0067 |
| 5% | 0.26 | 0.27 | 0.23 | 0.25 | 0.0120 |
| 10% | 0.37 | 0.33 | 0.33 | 0.34 | 0.0133 |
| 20% | 0.53 | 0.49 | 0.47 | 0.50 | 0.0176 |
| 25% | 0.56 | 0.57 | 0.59 | 0.57 | 0.0088 |

Compound 37

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.69 | 0.75 | 0.7 | 0.71 | 0.0186 |
| 5% | 0.7 | 0.75 | 0.78 | 0.74 | 0.0233 |
| 10% | 0.79 | 0.75 | 0.73 | 0.76 | 0.0176 |
| 20% | 0.81 | 0.78 | 0.83 | 0.81 | 0.0145 |
| 25% | 0.8 | 0.84 | 0.85 | 0.83 | 0.0153 |

Compound 38

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.57 | 0.56 | 0.52 | 0.55 | 0.0153 |
| 5% | 0.58 | 0.58 | 0.6 | 0.59 | 0.0067 |
| 10% | 0.65 | 0.65 | 0.68 | 0.66 | 0.0100 |
| 20% | 0.67 | 0.7 | 0.75 | 0.71 | 0.0233 |
| 25% | 0.71 | 0.75 | 0.77 | 0.74 | 0.0176 |

Compound 39

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.6 | 0.53 | 0.51 | 0.55 | 0.0273 |
| 5% | 0.62 | 0.65 | 0.63 | 0.63 | 0.0088 |
| 10% | 0.69 | 0.7 | 0.75 | 0.71 | 0.0186 |
| 20% | 0.83 | 0.8 | 0.75 | 0.79 | 0.0233 |
| 25% | 0.8 | 0.88 | 0.87 | 0.85 | 0.0252 |

Compound 40

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.38 | 0.36 | 0.33 | 0.36 | 0.0145 |
| 5% | 0.42 | 0.39 | 0.36 | 0.39 | 0.0173 |
| 10% | 0.45 | 0.55 | 0.48 | 0.49 | 0.0296 |
| 20% | 0.59 | 0.58 | 0.59 | 0.59 | 0.0033 |
| 25% | 0.66 | 0.63 | 0.63 | 0.64 | 0.0100 |

Compound 41

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.28 | 0.28 | 0.25 | 0.27 | 0.0100 |
| 5% | 0.37 | 0.31 | 0.34 | 0.34 | 0.0173 |
| 10% | 0.47 | 0.45 | 0.5 | 0.47 | 0.0145 |
| 20% | 0.55 | 0.55 | 0.6 | 0.57 | 0.0167 |
| 25% | 0.6 | 0.68 | 0.65 | 0.64 | 0.0233 |

Compound 42

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.27 | 0.27 | 0.27 | 0.27 | 0.0000 |
| 5% | 0.33 | 0.32 | 0.31 | 0.32 | 0.0058 |
| 10% | 0.44 | 0.45 | 0.44 | 0.44 | 0.0033 |
| 20% | 0.57 | 0.46 | 0.53 | 0.52 | 0.0321 |
| 25% | 0.65 | 0.64 | 0.58 | 0.62 | 0.0219 |

Compound 43

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 5% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 10% | 0.02 | 0.02 | 0.02 | 0.02 | 0.0000 |
| 20% | 0.07 | 0.1 | 0.1 | 0.09 | 0.0100 |
| 25% | 0.18 | 0.14 | 0.17 | 0.16 | 0.0120 |

Compound 44

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.64 | 0.59 | 0.66 | 0.63 | 0.0208 |
| 5% | 0.64 | 0.63 | 0.65 | 0.64 | 0.0058 |
| 10% | 0.66 | 0.69 | 0.68 | 0.68 | 0.0088 |
| 20% | 0.72 | 0.66 | 0.71 | 0.70 | 0.0186 |
| 25% | 0.71 | 0.75 | 0.72 | 0.73 | 0.0120 |

Compound 45

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.05 | 0.05 | 0.05 | 0.05 | 0.0000 |
| 5% | 0.06 | 0.05 | 0.06 | 0.06 | 0.0033 |
| 10% | 0.15 | 0.16 | 0.13 | 0.15 | 0.0088 |
| 20% | 0.28 | 0.19 | 0.17 | 0.21 | 0.0338 |
| 25% | 0.32 | 0.3 | 0.3 | 0.31 | 0.0067 |

Compound 46

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.2 | 0.14 | 0.18 | 0.17 | 0.0176 |
| 5% | 0.24 | 0.23 | 0.26 | 0.24 | 0.0088 |
| 10% | 0.32 | 0.39 | 0.38 | 0.36 | 0.0219 |
| 20% | 0.48 | 0.45 | 0.5 | 0.48 | 0.0145 |
| 25% | 0.51 | 0.55 | 0.59 | 0.55 | 0.0231 |

Compound 47

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.03 | 0.02 | 0.04 | 0.03 | 0.0058 |
| 5% | 0.03 | 0.02 | 0.03 | 0.03 | 0.0033 |
| 10% | 0.1 | 0.07 | 0.06 | 0.08 | 0.0120 |
| 20% | 0.1 | 0.15 | 0.16 | 0.14 | 0.0186 |
| 25% | 0.17 | 0.18 | 0.16 | 0.17 | 0.0058 |
| 28% | 0.21 | 0.23 | 0.23 | 0.22 | 0.0067 |
| 30% | 0.29 | 0.27 | 0.22 | 0.26 | 0.0208 |

Compound 48

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.38 | 0.36 | 0.38 | 0.37 | 0.0067 |
| 5% | 0.45 | 0.45 | 0.44 | 0.45 | 0.0033 |
| 10% | 0.46 | 0.5 | 0.46 | 0.47 | 0.0133 |
| 20% | 0.63 | 0.61 | 0.61 | 0.62 | 0.0067 |
| 25% | 0.69 | 0.71 | 0.66 | 0.69 | 0.0145 |

Compound 49

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.15 | 0.17 | 0.15 | 0.16 | 0.0067 |
| 5% | 0.24 | 0.23 | 0.17 | 0.21 | 0.0219 |
| 10% | 0.37 | 0.39 | 0.38 | 0.38 | 0.0058 |
| 20% | 0.49 | 0.51 | 0.5 | 0.50 | 0.0058 |
| 25% | 0.58 | 0.53 | 0.58 | 0.56 | 0.0167 |

Compound 50

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.17 | 0.2 | 0.19 | 0.19 | 0.0088 |
| 5% | 0.25 | 0.24 | 0.25 | 0.25 | 0.0033 |
| 10% | 0.4 | 0.42 | 0.42 | 0.41 | 0.0067 |
| 20% | 0.52 | 0.5 | 0.5 | 0.51 | 0.0067 |
| 25% | 0.63 | 0.62 | 0.51 | 0.59 | 0.0384 |

Compound 51

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.13 | 0.14 | 0.1 | 0.12 | 0.0120 |
| 5% | 0.17 | 0.15 | 0.17 | 0.16 | 0.0067 |
| 10% | 0.14 | 0.2 | 0.22 | 0.19 | 0.0240 |
| 20% | 0.23 | 0.28 | 0.23 | 0.25 | 0.0167 |
| 25% | 0.32 | 0.33 | 0.31 | 0.32 | 0.0058 |

Compound 52

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.69 | 0.66 | 0.65 | 0.67 | 0.0120 |
| 5% | 0.69 | 0.7 | 0.71 | 0.70 | 0.0058 |
| 10% | 0.7 | 0.73 | 0.71 | 0.71 | 0.0088 |
| 20% | 0.89 | 0.8 | 0.83 | 0.84 | 0.0265 |
| 25% | 0.85 | 0.83 | 0.85 | 0.84 | 0.0067 |

Compound 53

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.07 | 0.08 | 0.08 | 0.08 | 0.0033 |
| 5% | 0.17 | 0.15 | 0.14 | 0.15 | 0.0088 |
| 10% | 0.28 | 0.28 | 0.27 | 0.28 | 0.0033 |
| 20% | 0.61 | 0.57 | 0.55 | 0.58 | 0.0176 |
| 25% | 0.64 | 0.68 | 0.67 | 0.66 | 0.0120 |

Compound 54

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.49 | 0.51 | 0.49 | 0.50 | 0.0067 |
| 5% | 0.53 | 0.5 | 0.54 | 0.52 | 0.0120 |
| 10% | 0.7 | 0.68 | 0.65 | 0.68 | 0.0145 |
| 20% | 0.87 | 0.83 | 0.75 | 0.82 | 0.0353 |
| 25% | 0.9 | 0.85 | 0.8 | 0.85 | 0.0289 |

Compound 55

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 5% | 0.07 | 0.06 | 0.07 | 0.07 | 0.0033 |
| 10% | 0.13 | 0.14 | 0.12 | 0.13 | 0.0058 |
| 20% | 0.17 | 0.17 | 0.18 | 0.17 | 0.0033 |
| 25% | 0.16 | 0.16 | 0.25 | 0.19 | 0.0300 |

Compound 56

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 5% | 0.07 | 0.09 | 0.07 | 0.08 | 0.0067 |
| 10% | 0.13 | 0.14 | 0.14 | 0.14 | 0.0033 |
| 20% | 0.15 | 0.16 | 0.17 | 0.16 | 0.0058 |
| 25% | 0.2 | 0.23 | 0.23 | 0.22 | 0.0100 |
| 28% | 0.23 | 0.26 | 0.23 | 0.24 | 0.0100 |
| 30% | 0 | 0 | 0 | 0.00 | 0.0000 |

Compound 57

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.01 | 0 | 0 | 0.00 | 0.0033 |
| 5% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 10% | 0.02 | 0.02 | 0.02 | 0.02 | 0.0000 |
| 20% | 0.06 | 0.07 | 0.09 | 0.07 | 0.0088 |
| 25% | 0.1 | 0.13 | 0.1 | 0.11 | 0.0100 |

Compound 58

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 5% | 0.02 | 0.03 | 0.03 | 0.03 | 0.0033 |
| 10% | 0.03 | 0.03 | 0.06 | 0.04 | 0.0100 |
| 20% | 0.08 | 0.05 | 0.04 | 0.06 | 0.0120 |
| 25% | 0.07 | 0.07 | 0.08 | 0.07 | 0.0033 |
| 28% | 0.09 | 0.1 | 0.11 | 0.10 | 0.0058 |
| 30% | 0 | 0 | 0 | 0.00 | 0.0000 |

Compound 59

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 5% | 0.03 | 0.01 | 0.04 | 0.03 | 0.0088 |
| 10% | 0.05 | 0.04 | 0.04 | 0.04 | 0.0033 |
| 20% | 0.11 | 0.1 | 0.1 | 0.10 | 0.0033 |
| 25% | 0.14 | 0.14 | 0.15 | 0.14 | 0.0033 |

Compound 60

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.18 | 0.19 | 0.19 | 0.19 | 0.0033 |
| 5% | 0.29 | 0.26 | 0.24 | 0.26 | 0.0145 |
| 10% | 0.37 | 0.41 | 0.4 | 0.39 | 0.0120 |
| 20% | 0.62 | 0.54 | 0.54 | 0.57 | 0.0267 |
| 25% | 0.71 | 0.71 | 0.65 | 0.69 | 0.0200 |

Compound 61

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.47 | 0.47 | 0.46 | 0.47 | 0.0033 |
| 5% | 0.54 | 0.53 | 0.56 | 0.54 | 0.0088 |
| 10% | 0.6 | 0.59 | 0.6 | 0.60 | 0.0033 |
| 20% | 0.6 | 0.66 | 0.66 | 0.64 | 0.0200 |
| 25% | 0.67 | 0.68 | 0.67 | 0.67 | 0.0033 |

Compound 62

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.44 | 0.45 | 0.46 | 0.45 | 0.0058 |
| 5% | 0.5 | 0.53 | 0.5 | 0.51 | 0.0100 |
| 10% | 0.57 | 0.54 | 0.54 | 0.55 | 0.0100 |
| 20% | 0.6 | 0.61 | 0.64 | 0.61 | 0.0120 |
| 25% | 0.67 | 0.68 | 0.7 | 0.68 | 0.0088 |

Compound 63

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.17 | 0.19 | 0.17 | 0.18 | 0.0067 |
| 5% | 0.26 | 0.22 | 0.24 | 0.24 | 0.0115 |
| 10% | 0.3 | 0.3 | 0.28 | 0.29 | 0.0067 |
| 20% | 0.47 | 0.44 | 0.4 | 0.44 | 0.0203 |
| 25% | 0.64 | 0.5 | 0.5 | 0.55 | 0.0467 |

Compound 64

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.07 | 0.07 | 0.05 | 0.06 | 0.0067 |
| 5% | 0.11 | 0.1 | 0.11 | 0.11 | 0.0033 |
| 10% | 0.29 | 0.36 | 0.28 | 0.31 | 0.0252 |
| 20% | 0.46 | 0.46 | 0.46 | 0.46 | 0.0000 |
| 25% | 0.54 | 0.59 | 0.6 | 0.58 | 0.0186 |

Compound 65

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.46 | 0.57 | 0.47 | 0.50 | 0.0351 |
| 5% | 0.44 | 0.46 | 0.53 | 0.48 | 0.0273 |
| 10% | 0.5 | 0.51 | 0.52 | 0.51 | 0.0058 |
| 20% | 0.58 | 0.56 | 0.6 | 0.58 | 0.0115 |
| 25% | 0.59 | 0.66 | 0.64 | 0.63 | 0.0208 |

Compound 66

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.07 | 0.05 | 0.08 | 0.07 | 0.0088 |
| 5% | 0.09 | 0.09 | 0.1 | 0.09 | 0.0033 |
| 10% | 0.22 | 0.29 | 0.22 | 0.24 | 0.0233 |
| 20% | 0.32 | 0.38 | 0.3 | 0.33 | 0.0240 |
| 25% | 0.5 | 0.47 | 0.52 | 0.50 | 0.0145 |

Compound 67

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.58 | 0.6 | 0.58 | 0.59 | 0.0067 |
| 5% | 0.66 | 0.64 | 0.66 | 0.65 | 0.0067 |
| 10% | 0.69 | 0.69 | 0.7 | 0.69 | 0.0033 |
| 20% | 0.73 | 0.74 | 0.7 | 0.72 | 0.0120 |
| 25% | 0.75 | 0.79 | 0.74 | 0.76 | 0.0153 |

Compound 68

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.21 | 0.21 | 0.2 | 0.21 | 0.0033 |
| 5% | 0.29 | 0.24 | 0.26 | 0.26 | 0.0145 |
| 10% | 0.44 | 0.44 | 0.41 | 0.43 | 0.0100 |
| 20% | 0.63 | 0.63 | 0.6 | 0.62 | 0.0100 |
| 25% | 0.75 | 0.72 | 0.77 | 0.75 | 0.0145 |

Compound 69

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.58 | 0.54 | 0.56 | 0.56 | 0.0115 |
| 5% | 0.63 | 0.6 | 0.65 | 0.63 | 0.0145 |
| 10% | 0.78 | 0.81 | 0.75 | 0.78 | 0.0173 |
| 20% | 0.96 | 0.93 | 0.77 | 0.89 | 0.0590 |
| 25% | 0.95 | 0.97 | 1 | 0.97 | 0.0145 |

Compound 70

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.32 | 0.32 | 0.29 | 0.31 | 0.0100 |
| 5% | 0.33 | 0.4 | 0.38 | 0.37 | 0.0208 |
| 10% | 0.51 | 0.51 | 0.55 | 0.52 | 0.0133 |
| 20% | 0.63 | 0.6 | 0.6 | 0.61 | 0.0100 |
| 25% | 0.7 | 0.77 | 0.7 | 0.72 | 0.0233 |

Compound 71

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.55 | 0.57 | 0.55 | 0.56 | 0.0067 |
| 5% | 0.61 | 0.63 | 0.6 | 0.61 | 0.0088 |
| 10% | 0.63 | 0.69 | 0.67 | 0.66 | 0.0176 |
| 20% | 0.71 | 0.73 | 0.7 | 0.71 | 0.0088 |
| 25% | 0.75 | 0.8 | 0.77 | 0.77 | 0.0145 |

Compound 72

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.42 | 0.38 | 0.42 | 0.41 | 0.0133 |
| 5% | 0.47 | 0.47 | 0.47 | 0.47 | 0.0000 |
| 10% | 0.53 | 0.52 | 0.5 | 0.52 | 0.0088 |
| 20% | 0.57 | 0.55 | 0.54 | 0.55 | 0.0088 |
| 25% | 0.57 | 0.58 | 0.61 | 0.59 | 0.0120 |

Compound 73

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 5% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 10% | 0.01 | 0.01 | 0.01 | 0.01 | 0.0000 |
| 20% | 0.03 | 0.03 | 0.03 | 0.03 | 0.0000 |
| 25% | 0.07 | 0.06 | 0.07 | 0.07 | 0.0033 |
| 28% | 0.08 | 0.1 | 0.09 | 0.09 | 0.0058 |
| 30% | 0 | 0 | 0 | 0.00 | 0.0000 |

Compound 74

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.79 | 0.77 | 0.8 | 0.79 | 0.0088 |
| 5% | 0.78 | 0.8 | 0.79 | 0.79 | 0.0058 |
| 10% | 0.84 | 0.8 | 0.83 | 0.82 | 0.0120 |
| 20% | 0.86 | 0.84 | 0.91 | 0.87 | 0.0208 |
| 25% | 0.9 | 0.93 | 0.89 | 0.91 | 0.0120 |

Compound 75

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.5 | 0.55 | 0.54 | 0.53 | 0.0153 |
| 5% | 0.54 | 0.54 | 0.54 | 0.54 | 0.0000 |
| 10% | 0.57 | 0.57 | 0.56 | 0.57 | 0.0033 |
| 20% | 0.64 | 0.7 | 0.68 | 0.67 | 0.0176 |
| 25% | 0.71 | 0.7 | 0.72 | 0.71 | 0.0058 |

Compound 76

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.34 | 0.32 | 0.35 | 0.34 | 0.0088 |
| 5% | 0.44 | 0.37 | 0.31 | 0.37 | 0.0376 |
| 10% | 0.49 | 0.47 | 0.46 | 0.47 | 0.0088 |
| 20% | 0.54 | 0.53 | 0.51 | 0.53 | 0.0088 |
| 25% | 0.64 | 0.57 | 0.65 | 0.62 | 0.0252 |

Compound 77

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.09 | 0.12 | 0.1 | 0.10 | 0.0088 |
| 5% | 0.1 | 0.11 | 0.1 | 0.10 | 0.0033 |
| 10% | 0.17 | 0.14 | 0.17 | 0.16 | 0.0100 |
| 20% | 0.28 | 0.33 | 0.31 | 0.31 | 0.0145 |
| 25% | 0.34 | 0.42 | 0.34 | 0.37 | 0.0267 |

Compound 78

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 5% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 10% | 0.03 | 0.04 | 0.03 | 0.03 | 0.0033 |
| 20% | 0.09 | 0.1 | 0.1 | 0.10 | 0.0033 |
| 25% | 0.13 | 0.19 | 0.13 | 0.15 | 0.0200 |

Compound 79

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 5% | 0.4 | 0.44 | 0.43 | 0.42 | 0.0120 |
| 10% | 0.42 | 0.46 | 0.44 | 0.44 | 0.0115 |
| 20% | 0.53 | 0.52 | 0.52 | 0.52 | 0.0033 |
| 25% | 0.53 | 0.55 | 0.53 | 0.54 | 0.0067 |

Compound 80

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 5% | 0.06 | 0.05 | 0.04 | 0.05 | 0.0058 |
| 10% | 0.05 | 0.07 | 0.12 | 0.08 | 0.0208 |
| 20% | 0.18 | 0.16 | 0.2 | 0.18 | 0.0115 |
| 25% | 0.22 | 0.23 | 0.25 | 0.23 | 0.0088 |

Compound 81

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.7 | 0.7 | 0.72 | 0.71 | 0.0067 |
| 5% | 0.71 | 0.73 | 0.73 | 0.72 | 0.0067 |
| 10% | 0.73 | 0.75 | 0.7 | 0.73 | 0.0145 |
| 20% | 0.71 | 0.79 | 0.74 | 0.75 | 0.0233 |
| 25% | 0.73 | 0.76 | 0.8 | 0.76 | 0.0203 |

Compound 82

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.14 | 0.14 | 0.12 | 0.13 | 0.0067 |
| 5% | 0.19 | 0.23 | 0.23 | 0.22 | 0.0133 |
| 10% | 0.36 | 0.38 | 0.39 | 0.38 | 0.0088 |
| 20% | 0.48 | 0.55 | 0.49 | 0.51 | 0.0219 |
| 25% | 0.55 | 0.58 | 0.6 | 0.58 | 0.0145 |

Compound 83

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 5% | 0.04 | 0.04 | 0.04 | 0.04 | 0.0000 |
| 10% | 0.09 | 0.09 | 0.09 | 0.09 | 0.0000 |
| 20% | 0.12 | 0.12 | 0.11 | 0.12 | 0.0033 |
| 25% | 0.15 | 0.13 | 0.15 | 0.14 | 0.0067 |

Compound 84

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 5% | 0.05 | 0.05 | 0.03 | 0.04 | 0.0067 |
| 10% | 0.07 | 0.08 | 0.09 | 0.08 | 0.0058 |
| 20% | 0.26 | 0.23 | 0.29 | 0.26 | 0.0173 |
| 25% | 0.33 | 0.35 | 0.33 | 0.34 | 0.0067 |

Compound 85

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.11 | 0.11 | 0.1 | 0.11 | 0.0033 |
| 5% | 0.14 | 0.14 | 0.16 | 0.15 | 0.0067 |
| 10% | 0.23 | 0.23 | 0.26 | 0.24 | 0.0100 |
| 20% | 0.35 | 0.32 | 0.33 | 0.33 | 0.0088 |
| 25% | 0.39 | 0.38 | 0.4 | 0.39 | 0.0058 |

Compound 86

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.02 | 0.03 | 0.02 | 0.02 | 0.0033 |
| 5% | 0.02 | 0.05 | 0.05 | 0.04 | 0.0100 |
| 10% | 0.13 | 0.1 | 0.12 | 0.12 | 0.0088 |
| 20% | 0.2 | 0.18 | 0.2 | 0.19 | 0.0067 |
| 25% | 0.2 | 0.23 | 0.24 | 0.22 | 0.0120 |

Compound 87

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.21 | 0.2 | 0.2 | 0.20 | 0.0033 |
| 5% | 0.26 | 0.25 | 0.26 | 0.26 | 0.0033 |
| 10% | 0.38 | 0.38 | 0.36 | 0.37 | 0.0067 |
| 20% | 0.4 | 0.42 | 0.48 | 0.43 | 0.0240 |
| 25% | 0.51 | 0.54 | 0.53 | 0.53 | 0.0088 |

Compound 88

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 5% | 0.02 | 0.03 | 0.03 | 0.03 | 0.0033 |
| 10% | 0.07 | 0.08 | 0.08 | 0.08 | 0.0033 |
| 20% | 0.15 | 0.24 | 0.22 | 0.20 | 0.0273 |
| 25% | 0.25 | 0.26 | 0.24 | 0.25 | 0.0058 |

Compound 89

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.08 | 0.07 | 0.08 | 0.08 | 0.0033 |
| 5% | 0.16 | 0.14 | 0.12 | 0.14 | 0.0115 |
| 10% | 0.31 | 0.31 | 0.36 | 0.33 | 0.0167 |
| 20% | 0.4 | 0.39 | 0.48 | 0.42 | 0.0285 |
| 25% | 0.5 | 0.55 | 0.53 | 0.53 | 0.0145 |

Compound 90

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.68 | 0.64 | 0.68 | 0.67 | 0.0133 |
| 5% | 0.68 | 0.68 | 0.71 | 0.69 | 0.0100 |
| 10% | 0.7 | 0.73 | 0.74 | 0.72 | 0.0120 |
| 20% | 0.73 | 0.79 | 0.78 | 0.77 | 0.0186 |
| 25% | 0.75 | 0.76 | 0.8 | 0.77 | 0.0153 |

Compound 91

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.48 | 0.48 | 0.47 | 0.48 | 0.0033 |
| 5% | 0.47 | 0.5 | 0.49 | 0.49 | 0.0088 |
| 10% | 0.55 | 0.58 | 0.56 | 0.56 | 0.0088 |
| 20% | 0.6 | 0.63 | 0.61 | 0.61 | 0.0088 |
| 25% | 0.63 | 0.66 | 0.62 | 0.64 | 0.0120 |

Compound 92

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.13 | 0.15 | 0.14 | 0.14 | 0.0058 |
| 5% | 0.2 | 0.2 | 0.23 | 0.21 | 0.0100 |
| 10% | 0.35 | 0.36 | 0.4 | 0.37 | 0.0153 |
| 20% | 0.46 | 0.53 | 0.49 | 0.49 | 0.0203 |
| 25% | 0.55 | 0.58 | 0.55 | 0.56 | 0.0100 |

Compound 93

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 5% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 10% | 0.05 | 0.07 | 0.07 | 0.06 | 0.0067 |
| 20% | 0.16 | 0.13 | 0.13 | 0.14 | 0.0100 |
| 25% | 0.17 | 0.16 | 0.2 | 0.18 | 0.0120 |

Compound 94

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 5% | 0.03 | 0.05 | 0.04 | 0.04 | 0.0058 |
| 10% | 0.13 | 0.12 | 0.11 | 0.12 | 0.0058 |
| 20% | 0.13 | 0.17 | 0.13 | 0.14 | 0.0133 |
| 25% | 0.17 | 0.23 | 0.19 | 0.20 | 0.0176 |

Compound 95

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 5% | 0.04 | 0.03 | 0.04 | 0.04 | 0.0033 |
| 10% | 0.1 | 0.09 | 0.08 | 0.09 | 0.0058 |
| 20% | 0.1 | 0.12 | 0.13 | 0.12 | 0.0088 |
| 25% | 0.13 | 0.17 | 0.15 | 0.15 | 0.0115 |

3.2.3 MeOH/TBME R_f Data

Compound 1

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.6 | 0.61 | 0.61 | 0.61 | 0.0033 |
| 5% | 0.66 | 0.61 | 0.6 | 0.62 | 0.0186 |
| 10% | 0.76 | 0.72 | 0.72 | 0.73 | 0.0133 |
| 20% | 0.87 | 0.91 | 0.83 | 0.87 | 0.0231 |
| 25% | 0.94 | 0.92 | 0.9 | 0.92 | 0.0115 |

Compound 2

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.48 | 0.48 | 0.48 | 0.48 | 0.0000 |
| 5% | 0.57 | 0.51 | 0.61 | 0.56 | 0.0291 |
| 10% | 0.69 | 0.6 | 0.62 | 0.64 | 0.0273 |
| 20% | 0.8 | 0.7 | 0.78 | 0.76 | 0.0306 |
| 25% | 0.87 | 0.87 | 0.83 | 0.86 | 0.0133 |

Compound 3

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.66 | 0.64 | 0.65 | 0.65 | 0.0058 |
| 5% | 0.68 | 0.66 | 0.63 | 0.66 | 0.0145 |
| 10% | 0.79 | 0.71 | 0.74 | 0.75 | 0.0233 |
| 20% | 0.89 | 0.91 | 0.86 | 0.89 | 0.0145 |
| 25% | 0.97 | 0.9 | 0.93 | 0.93 | 0.0203 |

Compound 4

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.52 | 0.52 | 0.53 | 0.52 | 0.0033 |
| 5% | 0.56 | 0.5 | 0.49 | 0.52 | 0.0219 |
| 10% | 0.63 | 0.56 | 0.61 | 0.60 | 0.0208 |
| 20% | 0.73 | 0.92 | 0.82 | 0.82 | 0.0549 |
| 25% | 0.89 | 0.83 | 0.87 | 0.86 | 0.0176 |

Compound 5

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.36 | 0.35 | 0.37 | 0.36 | 0.0058 |
| 5% | 0.38 | 0.38 | 0.44 | 0.40 | 0.0200 |
| 10% | 0.44 | 0.4 | 0.47 | 0.44 | 0.0203 |
| 20% | 0.58 | 0.55 | 0.56 | 0.56 | 0.0088 |
| 25% | 0.63 | 0.6 | 0.58 | 0.60 | 0.0145 |

Compound 6

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.55 | 0.52 | 0.52 | 0.53 | 0.0100 |
| 5% | 0.49 | 0.53 | 0.5 | 0.51 | 0.0120 |
| 10% | 0.67 | 0.62 | 0.63 | 0.64 | 0.0153 |
| 20% | 0.8 | 0.84 | 0.78 | 0.81 | 0.0176 |
| 25% | 0.87 | 0.85 | 0.83 | 0.85 | 0.0115 |

Compound 7

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.49 | 0.54 | 0.52 | 0.52 | 0.0100 |
| 5% | 0.57 | 0.56 | 0.57 | 0.57 | 0.0120 |
| 10% | 0.61 | 0.6 | 0.6 | 0.60 | 0.0153 |
| 20% | 0.73 | 0.73 | 0.71 | 0.72 | 0.0176 |
| 25% | 0.73 | 0.74 | 0.71 | 0.73 | 0.0115 |

Compound 8

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.55 | 0.57 | 0.55 | 0.56 | 0.0067 |
| 5% | 0.61 | 0.58 | 0.57 | 0.59 | 0.0120 |
| 10% | 0.71 | 0.61 | 0.64 | 0.65 | 0.0296 |
| 20% | 0.77 | 0.81 | 0.74 | 0.77 | 0.0203 |
| 25% | 0.89 | 0.82 | 0.83 | 0.85 | 0.0219 |

Compound 9

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.6 | 0.61 | 0.6 | 0.60 | 0.0033 |
| 5% | 0.62 | 0.64 | 0.68 | 0.65 | 0.0176 |
| 10% | 0.72 | 0.62 | 0.76 | 0.70 | 0.0416 |
| 20% | 0.73 | 0.77 | 0.82 | 0.77 | 0.0260 |
| 25% | 0.93 | 0.88 | 0.9 | 0.90 | 0.0145 |

Compound 10

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.47 | 0.5 | 0.49 | 0.49 | 0.0088 |
| 5% | 0.49 | 0.51 | 0.49 | 0.50 | 0.0067 |
| 10% | 0.5 | 0.63 | 0.57 | 0.57 | 0.0376 |
| 20% | 0.7 | 0.67 | 0.67 | 0.68 | 0.0100 |
| 25% | 0.8 | 0.75 | 0.78 | 0.78 | 0.0145 |

Compound 11

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.06 | 0.11 | 0.08 | 0.08 | 0.0145 |
| 5% | 0.09 | 0.15 | 0.13 | 0.12 | 0.0176 |
| 10% | 0.14 | 0.14 | 0.17 | 0.15 | 0.0100 |
| 20% | 0.32 | 0.27 | 0.27 | 0.29 | 0.0167 |
| 25% | 0.4 | 0.4 | 0.44 | 0.41 | 0.0133 |

Compound 12

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.1 | 0.08 | 0.05 | 0.08 | 0.0145 |
| 5% | 0.17 | 0.06 | 0.2 | 0.14 | 0.0426 |
| 10% | 0.22 | 0.2 | 0.22 | 0.21 | 0.0067 |
| 20% | 0.27 | 0.3 | 0.27 | 0.28 | 0.0100 |
| 25% | 0.36 | 0.35 | 0.4 | 0.37 | 0.0153 |

Compound 13

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.08 | 0.08 | 0.06 | 0.07 | 0.0067 |
| 5% | 0.11 | 0.09 | 0.09 | 0.10 | 0.0067 |
| 10% | 0.09 | 0.14 | 0.17 | 0.13 | 0.0233 |
| 20% | 0.27 | 0.27 | 0.27 | 0.27 | 0.0000 |
| 25% | 0.4 | 0.36 | 0.44 | 0.40 | 0.0231 |

Compound 14

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 5% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 10% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 20% | 0.13 | 0.11 | 0.13 | 0.12 | 0.0067 |
| 25% | 0.18 | 0.17 | 0.13 | 0.16 | 0.0153 |
| 30% | 0.17 | 0.19 | 0.23 | 0.20 | 0.0176 |

Compound 15

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.12 | 0.15 | 0.14 | 0.14 | 0.0088 |
| 5% | 0.18 | 0.16 | 0.16 | 0.17 | 0.0067 |
| 10% | 0.26 | 0.23 | 0.26 | 0.25 | 0.0100 |
| 20% | 0.34 | 0.38 | 0.42 | 0.38 | 0.0231 |
| 25% | 0.46 | 0.47 | 0.5 | 0.48 | 0.0120 |

Compound 16

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.17 | 0.17 | 0.16 | 0.17 | 0.0033 |
| 5% | 0.2 | 0.22 | 0.22 | 0.21 | 0.0067 |
| 10% | 0.27 | 0.26 | 0.3 | 0.28 | 0.0120 |
| 20% | 0.38 | 0.37 | 0.34 | 0.36 | 0.0120 |
| 25% | 0.35 | 0.4 | 0.45 | 0.40 | 0.0289 |

Compound 17

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.1 | 0.08 | 0.08 | 0.09 | 0.0067 |
| 5% | 0.11 | 0.14 | 0.09 | 0.11 | 0.0145 |
| 10% | 0.15 | 0.14 | 0.17 | 0.15 | 0.0088 |
| 20% | 0.23 | 0.23 | 0.3 | 0.25 | 0.0233 |
| 25% | 0.4 | 0.32 | 0.4 | 0.37 | 0.0267 |

Compound 18

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.6 | 0.63 | 0.65 | 0.63 | 0.0145 |
| 5% | 0.69 | 0.68 | 0.67 | 0.68 | 0.0058 |
| 10% | 0.7 | 0.7 | 0.71 | 0.70 | 0.0033 |
| 20% | 0.75 | 0.75 | 0.78 | 0.76 | 0.0100 |
| 25% | 0.8 | 0.74 | 0.8 | 0.78 | 0.0200 |

Compound 19

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.65 | 0.58 | 0.6 | 0.61 | 0.0208 |
| 5% | 0.67 | 0.65 | 0.62 | 0.65 | 0.0145 |
| 10% | 0.7 | 0.73 | 0.65 | 0.69 | 0.0233 |
| 20% | 0.75 | 0.75 | 0.72 | 0.74 | 0.0100 |
| 25% | 0.78 | 0.74 | 0.78 | 0.77 | 0.0133 |

Compound 20

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.56 | 0.55 | 0.5 | 0.54 | 0.0186 |
| 5% | 0.57 | 0.55 | 0.6 | 0.57 | 0.0145 |
| 10% | 0.64 | 0.62 | 0.6 | 0.62 | 0.0115 |
| 20% | 0.68 | 0.69 | 0.68 | 0.68 | 0.0033 |
| 25% | 0.7 | 0.7 | 0.72 | 0.71 | 0.0067 |

Compound 21

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.62 | 0.6 | 0.65 | 0.62 | 0.0145 |
| 5% | 0.67 | 0.65 | 0.63 | 0.65 | 0.0115 |
| 10% | 0.68 | 0.7 | 0.74 | 0.71 | 0.0176 |
| 20% | 0.75 | 0.75 | 0.78 | 0.76 | 0.0100 |
| 25% | 0.77 | 0.8 | 0.82 | 0.80 | 0.0145 |

Compound 22

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.68 | 0.65 | 0.6 | 0.64 | 0.0233 |
| 5% | 0.7 | 0.68 | 0.7 | 0.69 | 0.0067 |
| 10% | 0.71 | 0.72 | 0.71 | 0.71 | 0.0033 |
| 20% | 0.75 | 0.75 | 0.78 | 0.76 | 0.0100 |
| 25% | 0.77 | 0.8 | 0.82 | 0.80 | 0.0145 |

Compound 23

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.63 | 0.62 | 0.58 | 0.61 | 0.0153 |
| 5% | 0.63 | 0.65 | 0.67 | 0.65 | 0.0115 |
| 10% | 0.68 | 0.7 | 0.74 | 0.71 | 0.0176 |
| 20% | 0.75 | 0.75 | 0.76 | 0.75 | 0.0033 |
| 25% | 0.77 | 0.8 | 0.82 | 0.80 | 0.0145 |

Compound 24

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.63 | 0.62 | 0.64 | 0.63 | 0.0058 |
| 5% | 0.64 | 0.63 | 0.64 | 0.64 | 0.0033 |
| 10% | 0.68 | 0.67 | 0.71 | 0.69 | 0.0120 |
| 20% | 0.73 | 0.75 | 0.75 | 0.74 | 0.0067 |
| 25% | 0.8 | 0.8 | 0.76 | 0.79 | 0.0133 |

Compound 25

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.6 | 0.58 | 0.61 | 0.60 | 0.0088 |
| 5% | 0.61 | 0.62 | 0.62 | 0.62 | 0.0033 |
| 10% | 0.67 | 0.63 | 0.69 | 0.66 | 0.0176 |
| 20% | 0.73 | 0.73 | 0.74 | 0.73 | 0.0033 |
| 25% | 0.78 | 0.82 | 0.74 | 0.78 | 0.0231 |

Compound 26

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.68 | 0.65 | 0.68 | 0.67 | 0.0100 |
| 5% | 0.68 | 0.68 | 0.69 | 0.68 | 0.0033 |
| 10% | 0.7 | 0.68 | 0.74 | 0.71 | 0.0176 |
| 20% | 0.78 | 0.79 | 0.78 | 0.78 | 0.0033 |
| 25% | 0.81 | 0.86 | 0.77 | 0.81 | 0.0260 |

Compound 27

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.61 | 0.59 | 0.66 | 0.62 | 0.0208 |
| 5% | 0.67 | 0.68 | 0.66 | 0.67 | 0.0058 |
| 10% | 0.7 | 0.69 | 0.71 | 0.70 | 0.0058 |
| 20% | 0.8 | 0.82 | 0.81 | 0.81 | 0.0058 |
| 25% | 0.8 | 0.79 | 0.81 | 0.80 | 0.0058 |

Compound 28

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.59 | 0.61 | 0.56 | 0.59 | 0.0145 |
| 5% | 0.63 | 0.63 | 0.65 | 0.64 | 0.0067 |
| 10% | 0.67 | 0.69 | 0.68 | 0.68 | 0.0058 |
| 20% | 0.79 | 0.77 | 0.77 | 0.78 | 0.0067 |
| 25% | 0.78 | 0.81 | 0.76 | 0.78 | 0.0145 |

Compound 29

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.59 | 0.54 | 0.61 | 0.58 | 0.0208 |
| 5% | 0.62 | 0.59 | 0.63 | 0.61 | 0.0120 |
| 10% | 0.67 | 0.67 | 0.68 | 0.67 | 0.0033 |
| 20% | 0.85 | 0.74 | 0.73 | 0.77 | 0.0384 |
| 25% | 0.93 | 0.84 | 0.86 | 0.88 | 0.0273 |

Compound 30

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.5 | 0.5 | 0.53 | 0.51 | 0.0100 |
| 5% | 0.55 | 0.61 | 0.55 | 0.57 | 0.0200 |
| 10% | 0.65 | 0.68 | 0.63 | 0.65 | 0.0145 |
| 20% | 0.79 | 0.81 | 0.81 | 0.80 | 0.0067 |
| 25% | 0.87 | 0.87 | 0.88 | 0.87 | 0.0033 |

Compound 31

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.03 | 0.03 | 0.03 | 0.03 | 0.0000 |
| 5% | 0.06 | 0.04 | 0.03 | 0.04 | 0.0088 |
| 10% | 0.03 | 0.17 | 0.13 | 0.11 | 0.0416 |
| 20% | 0.3 | 0.27 | 0.27 | 0.28 | 0.0100 |
| 25% | 0.28 | 0.32 | 0.4 | 0.33 | 0.0353 |

Compound 32

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.25 | 0.28 | 0.23 | 0.25 | 0.0145 |
| 5% | 0.34 | 0.37 | 0.34 | 0.35 | 0.0100 |
| 10% | 0.45 | 0.49 | 0.47 | 0.47 | 0.0115 |
| 20% | 0.63 | 0.63 | 0.63 | 0.63 | 0.0000 |
| 25% | 0.74 | 0.78 | 0.78 | 0.77 | 0.0133 |

Compound 33

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.61 | 0.62 | 0.6 | 0.61 | 0.0058 |
| 5% | 0.68 | 0.7 | 0.69 | 0.69 | 0.0058 |
| 10% | 0.75 | 0.76 | 0.75 | 0.75 | 0.0033 |
| 20% | 0.87 | 0.8 | 0.82 | 0.83 | 0.0208 |
| 25% | 0.91 | 0.85 | 0.94 | 0.90 | 0.0265 |

Compound 34

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.68 | 0.65 | 0.67 | 0.67 | 0.0088 |
| 5% | 0.73 | 0.67 | 0.65 | 0.68 | 0.0240 |
| 10% | 0.77 | 0.72 | 0.71 | 0.73 | 0.0186 |
| 20% | 0.86 | 0.89 | 0.82 | 0.86 | 0.0203 |
| 25% | 0.94 | 0.93 | 0.9 | 0.92 | 0.0120 |

Compound 35

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.45 | 0.49 | 0.47 | 0.47 | 0.0115 |
| 5% | 0.5 | 0.55 | 0.61 | 0.55 | 0.0318 |
| 10% | 0.63 | 0.58 | 0.59 | 0.60 | 0.0153 |
| 20% | 0.76 | 0.75 | 0.68 | 0.73 | 0.0252 |
| 25% | 0.93 | 0.84 | 0.86 | 0.88 | 0.0273 |

Compound 36

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.21 | 0.21 | 0.21 | 0.21 | 0.0000 |
| 5% | 0.28 | 0.29 | 0.28 | 0.28 | 0.0033 |
| 10% | 0.5 | 0.54 | 0.46 | 0.50 | 0.0231 |
| 20% | 0.69 | 0.69 | 0.69 | 0.69 | 0.0000 |
| 25% | 0.78 | 0.77 | 0.8 | 0.78 | 0.0088 |

Compound 37

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.51 | 0.49 | 0.47 | 0.49 | 0.0115 |
| 5% | 0.59 | 0.63 | 0.58 | 0.60 | 0.0153 |
| 10% | 0.69 | 0.65 | 0.62 | 0.65 | 0.0203 |
| 20% | 0.76 | 0.84 | 0.78 | 0.79 | 0.0240 |
| 25% | 0.93 | 0.97 | 0.9 | 0.93 | 0.0203 |

Compound 38

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.55 | 0.57 | 0.55 | 0.56 | 0.0067 |
| 5% | 0.59 | 0.57 | 0.59 | 0.58 | 0.0067 |
| 10% | 0.64 | 0.62 | 0.65 | 0.64 | 0.0088 |
| 20% | 0.74 | 0.71 | 0.75 | 0.73 | 0.0120 |
| 25% | 0.95 | 0.83 | 0.82 | 0.87 | 0.0418 |

Compound 39

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.55 | 0.52 | 0.5 | 0.52 | 0.0145 |
| 5% | 0.55 | 0.58 | 0.58 | 0.57 | 0.0100 |
| 10% | 0.62 | 0.65 | 0.61 | 0.63 | 0.0120 |
| 20% | 0.75 | 0.73 | 0.65 | 0.71 | 0.0306 |
| 25% | 0.87 | 0.82 | 0.83 | 0.84 | 0.0153 |

Compound 40

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.38 | 0.39 | 0.36 | 0.38 | 0.0088 |
| 5% | 0.45 | 0.4 | 0.41 | 0.42 | 0.0153 |
| 10% | 0.51 | 0.5 | 0.53 | 0.51 | 0.0088 |
| 20% | 0.69 | 0.65 | 0.69 | 0.68 | 0.0133 |
| 25% | 0.86 | 0.76 | 0.73 | 0.78 | 0.0393 |

Compound 41

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.33 | 0.3 | 0.3 | 0.31 | 0.0100 |
| 5% | 0.46 | 0.47 | 0.4 | 0.44 | 0.0219 |
| 10% | 0.53 | 0.56 | 0.5 | 0.53 | 0.0173 |
| 20% | 0.73 | 0.71 | 0.64 | 0.69 | 0.0273 |
| 25% | 0.87 | 0.81 | 0.83 | 0.84 | 0.0176 |

Compound 42

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.16 | 0.17 | 0.19 | 0.17 | 0.0088 |
| 5% | 0.27 | 0.3 | 0.26 | 0.28 | 0.0120 |
| 10% | 0.39 | 0.42 | 0.35 | 0.39 | 0.0203 |
| 20% | 0.58 | 0.58 | 0.58 | 0.58 | 0.0000 |
| 25% | 0.67 | 0.66 | 0.67 | 0.67 | 0.0033 |

Compound 43

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 5% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 10% | 0.06 | 0.03 | 0.05 | 0.05 | 0.0088 |
| 20% | 0.29 | 0.15 | 0.11 | 0.18 | 0.0546 |
| 25% | 0.24 | 0.24 | 0.19 | 0.22 | 0.0167 |

Compound 44

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.51 | 0.49 | 0.54 | 0.51 | 0.0145 |
| 5% | 0.59 | 0.61 | 0.6 | 0.60 | 0.0058 |
| 10% | 0.65 | 0.64 | 0.65 | 0.65 | 0.0033 |
| 20% | 0.76 | 0.78 | 0.78 | 0.77 | 0.0067 |
| 25% | 0.77 | 0.79 | 0.77 | 0.78 | 0.0067 |

Compound 45

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.03 | 0.03 | 0.03 | 0.03 | 0.0000 |
| 5% | 0.06 | 0.06 | 0.06 | 0.06 | 0.0000 |
| 10% | 0.17 | 0.13 | 0.15 | 0.15 | 0.0115 |
| 20% | 0.28 | 0.32 | 0.32 | 0.31 | 0.0133 |
| 25% | 0.41 | 0.42 | 0.38 | 0.40 | 0.0120 |

Compound 46

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.21 | 0.18 | 0.2 | 0.20 | 0.0088 |
| 5% | 0.34 | 0.34 | 0.27 | 0.32 | 0.0233 |
| 10% | 0.37 | 0.36 | 0.32 | 0.35 | 0.0153 |
| 20% | 0.61 | 0.58 | 0.51 | 0.57 | 0.0296 |
| 25% | 0.75 | 0.73 | 0.7 | 0.73 | 0.0145 |

Compound 47

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 5% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 10% | 0.03 | 0.02 | 0.03 | 0.03 | 0.0033 |
| 20% | 0.19 | 0.21 | 0.24 | 0.21 | 0.0145 |
| 25% | 0.3 | 0.33 | 0.32 | 0.32 | 0.0088 |

Compound 48

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.26 | 0.29 | 0.33 | 0.29 | 0.0203 |
| 5% | 0.39 | 0.43 | 0.39 | 0.40 | 0.0133 |
| 10% | 0.52 | 0.57 | 0.49 | 0.53 | 0.0233 |
| 20% | 0.66 | 0.69 | 0.68 | 0.68 | 0.0088 |
| 25% | 0.77 | 0.76 | 0.78 | 0.77 | 0.0058 |

Compound 49

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.17 | 0.17 | 0.16 | 0.17 | 0.0033 |
| 5% | 0.27 | 0.26 | 0.4 | 0.31 | 0.0451 |
| 10% | 0.34 | 0.36 | 0.34 | 0.35 | 0.0067 |
| 20% | 0.65 | 0.6 | 0.64 | 0.63 | 0.0153 |
| 25% | 0.79 | 0.68 | 0.71 | 0.73 | 0.0328 |

Compound 50

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.2 | 0.21 | 0.19 | 0.20 | 0.0058 |
| 5% | 0.29 | 0.28 | 0.29 | 0.29 | 0.0033 |
| 10% | 0.4 | 0.4 | 0.4 | 0.40 | 0.0000 |
| 20% | 0.6 | 0.6 | 0.58 | 0.59 | 0.0067 |
| 25% | 0.68 | 0.65 | 0.75 | 0.69 | 0.0296 |

Compound 51

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.02 | 0.01 | 0.01 | 0.01 | 0.0033 |
| 5% | 0.02 | 0.03 | 0.03 | 0.03 | 0.0033 |
| 10% | 0.05 | 0.05 | 0.05 | 0.05 | 0.0000 |
| 20% | 0.07 | 0.08 | 0.11 | 0.09 | 0.0120 |
| 25% | 0.12 | 0.09 | 0.13 | 0.11 | 0.0120 |

Compound 52

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.43 | 0.42 | 0.44 | 0.43 | 0.0058 |
| 5% | 0.51 | 0.53 | 0.51 | 0.52 | 0.0067 |
| 10% | 0.6 | 0.64 | 0.6 | 0.61 | 0.0133 |
| 20% | 0.71 | 0.75 | 0.71 | 0.72 | 0.0133 |
| 25% | 0.74 | 0.76 | 0.73 | 0.74 | 0.0088 |

Compound 53

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.08 | 0.07 | 0.08 | 0.08 | 0.0033 |
| 5% | 0.19 | 0.18 | 0.21 | 0.19 | 0.0088 |
| 10% | 0.45 | 0.38 | 0.35 | 0.39 | 0.0296 |
| 20% | 0.71 | 0.64 | 0.63 | 0.66 | 0.0252 |
| 25% | 0.76 | 0.64 | 0.73 | 0.71 | 0.0361 |

Compound 54

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.47 | 0.46 | 0.42 | 0.45 | 0.0153 |
| 5% | 0.5 | 0.58 | 0.56 | 0.55 | 0.0240 |
| 10% | 0.61 | 0.61 | 0.53 | 0.58 | 0.0267 |
| 20% | 0.75 | 0.69 | 0.66 | 0.70 | 0.0265 |
| 25% | 0.86 | 0.81 | 0.8 | 0.82 | 0.0186 |

Compound 55

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 5% | 0.02 | 0.01 | 0 | 0.01 | 0.0058 |
| 10% | 0.02 | 0.02 | 0.02 | 0.02 | 0.0000 |
| 20% | 0.14 | 0.1 | 0.11 | 0.12 | 0.0120 |
| 25% | 0.21 | 0.12 | 0.19 | 0.17 | 0.0273 |

Compound 56

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 5% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 10% | 0.08 | 0.1 | 0.07 | 0.08 | 0.0088 |
| 20% | 0.24 | 0.21 | 0.16 | 0.20 | 0.0233 |
| 25% | 0.3 | 0.27 | 0.3 | 0.29 | 0.0100 |

Compound 57

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 5% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 10% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 20% | 0.1 | 0.11 | 0.13 | 0.11 | 0.0088 |
| 25% | 0.17 | 0.19 | 0.17 | 0.18 | 0.0067 |
| 30% | 0.19 | 0.22 | 0.23 | 0.21 | 0.0120 |

Compound 58

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 5% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 10% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 20% | 0.03 | 0.03 | 0.02 | 0.03 | 0.0033 |
| 25% | 0.04 | 0.04 | 0.05 | 0.04 | 0.0033 |
| 30% | 0.07 | 0.06 | 0.09 | 0.07 | 0.0088 |

Compound 59

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.02 | 0.01 | 0.01 | 0.01 | 0.0033 |
| 5% | 0.04 | 0.03 | 0.04 | 0.04 | 0.0033 |
| 10% | 0.08 | 0.06 | 0.07 | 0.07 | 0.0058 |
| 20% | 0.14 | 0.13 | 0.13 | 0.13 | 0.0033 |
| 25% | 0.15 | 0.15 | 0.16 | 0.15 | 0.0033 |

Compound 60

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.16 | 0.16 | 0.16 | 0.16 | 0.0000 |
| 5% | 0.33 | 0.37 | 0.32 | 0.34 | 0.0153 |
| 10% | 0.43 | 0.5 | 0.39 | 0.44 | 0.0321 |
| 20% | 0.7 | 0.71 | 0.71 | 0.71 | 0.0033 |
| 25% | 0.78 | 0.79 | 0.8 | 0.79 | 0.0058 |

Compound 61

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.46 | 0.42 | 0.42 | 0.43 | 0.0133 |
| 5% | 0.49 | 0.52 | 0.52 | 0.51 | 0.0100 |
| 10% | 0.63 | 0.6 | 0.62 | 0.62 | 0.0088 |
| 20% | 0.69 | 0.67 | 0.74 | 0.70 | 0.0208 |
| 25% | 0.76 | 0.75 | 0.79 | 0.77 | 0.0120 |

Compound 62

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.48 | 0.48 | 0.49 | 0.48 | 0.0033 |
| 5% | 0.5 | 0.49 | 0.5 | 0.50 | 0.0033 |
| 10% | 0.56 | 0.6 | 0.57 | 0.58 | 0.0120 |
| 20% | 0.78 | 0.72 | 0.79 | 0.76 | 0.0219 |
| 25% | 0.8 | 0.79 | 0.86 | 0.82 | 0.0219 |

Compound 63

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.17 | 0.17 | 0.16 | 0.17 | 0.0033 |
| 5% | 0.26 | 0.27 | 0.27 | 0.27 | 0.0033 |
| 10% | 0.36 | 0.37 | 0.36 | 0.36 | 0.0033 |
| 20% | 0.51 | 0.49 | 0.47 | 0.49 | 0.0115 |
| 25% | 0.58 | 0.46 | 0.52 | 0.52 | 0.0346 |

Compound 64

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.09 | 0.09 | 0.08 | 0.09 | 0.0033 |
| 5% | 0.21 | 0.2 | 0.18 | 0.20 | 0.0088 |
| 10% | 0.35 | 0.34 | 0.31 | 0.33 | 0.0120 |
| 20% | 0.59 | 0.63 | 0.51 | 0.58 | 0.0353 |
| 25% | 0.77 | 0.71 | 0.74 | 0.74 | 0.0173 |

Compound 65

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.45 | 0.49 | 0.43 | 0.46 | 0.0176 |
| 5% | 0.46 | 0.48 | 0.54 | 0.49 | 0.0240 |
| 10% | 0.62 | 0.59 | 0.55 | 0.59 | 0.0203 |
| 20% | 0.64 | 0.8 | 0.68 | 0.71 | 0.0481 |
| 25% | 0.83 | 0.83 | 0.77 | 0.81 | 0.0200 |

Compound 66

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.06 | 0.06 | 0.07 | 0.06 | 0.0033 |
| 5% | 0.14 | 0.11 | 0.11 | 0.12 | 0.0100 |
| 10% | 0.27 | 0.22 | 0.24 | 0.24 | 0.0145 |
| 20% | 0.49 | 0.53 | 0.49 | 0.50 | 0.0133 |
| 25% | 0.6 | 0.57 | 0.53 | 0.57 | 0.0203 |

Compound 67

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.57 | 0.55 | 0.57 | 0.56 | 0.0067 |
| 5% | 0.65 | 0.65 | 0.66 | 0.65 | 0.0033 |
| 10% | 0.81 | 0.7 | 0.7 | 0.74 | 0.0367 |
| 20% | 0.88 | 0.8 | 0.84 | 0.84 | 0.0231 |
| 25% | 0.94 | 0.85 | 0.92 | 0.90 | 0.0273 |

Compound 68

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.29 | 0.27 | 0.27 | 0.28 | 0.0067 |
| 5% | 0.41 | 0.39 | 0.35 | 0.38 | 0.0176 |
| 10% | 0.47 | 0.5 | 0.44 | 0.47 | 0.0173 |
| 20% | 0.63 | 0.63 | 0.56 | 0.61 | 0.0233 |
| 25% | 0.78 | 0.77 | 0.78 | 0.78 | 0.0033 |

Compound 69

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.53 | 0.53 | 0.53 | 0.53 | 0.0000 |
| 5% | 0.59 | 0.57 | 0.6 | 0.59 | 0.0088 |
| 10% | 0.68 | 0.69 | 0.64 | 0.67 | 0.0153 |
| 20% | 0.79 | 0.79 | 0.7 | 0.76 | 0.0300 |
| 25% | 0.93 | 0.87 | 0.87 | 0.89 | 0.0200 |

Compound 70

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.28 | 0.3 | 0.32 | 0.30 | 0.0115 |
| 5% | 0.33 | 0.45 | 0.38 | 0.39 | 0.0348 |
| 10% | 0.45 | 0.5 | 0.49 | 0.48 | 0.0153 |
| 20% | 0.67 | 0.63 | 0.51 | 0.60 | 0.0481 |
| 25% | 0.75 | 0.72 | 0.73 | 0.73 | 0.0088 |

Compound 71

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.5 | 0.5 | 0.53 | 0.51 | 0.0100 |
| 5% | 0.55 | 0.54 | 0.55 | 0.55 | 0.0033 |
| 10% | 0.7 | 0.74 | 0.64 | 0.69 | 0.0291 |
| 20% | 0.8 | 0.81 | 0.84 | 0.82 | 0.0120 |
| 25% | 0.88 | 0.89 | 0.88 | 0.88 | 0.0033 |

Compound 72

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.41 | 0.45 | 0.4 | 0.42 | 0.0153 |
| 5% | 0.52 | 0.47 | 0.51 | 0.50 | 0.0153 |
| 10% | 0.62 | 0.59 | 0.61 | 0.61 | 0.0088 |
| 20% | 0.64 | 0.71 | 0.73 | 0.69 | 0.0273 |
| 25% | 0.88 | 0.8 | 0.78 | 0.82 | 0.0306 |

Compound 73

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 5% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 10% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 20% | 0.03 | 0.05 | 0.05 | 0.04 | 0.0067 |
| 25% | 0.07 | 0.07 | 0.07 | 0.07 | 0.0000 |
| 30% | 0.11 | 0.11 | 0.1 | 0.11 | 0.0033 |

Compound 74

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.54 | 0.53 | 0.55 | 0.54 | 0.0058 |
| 5% | 0.57 | 0.58 | 0.57 | 0.57 | 0.0033 |
| 10% | 0.58 | 0.6 | 0.65 | 0.61 | 0.0208 |
| 20% | 0.7 | 0.69 | 0.67 | 0.69 | 0.0088 |
| 25% | 0.74 | 0.74 | 0.71 | 0.73 | 0.0100 |

Compound 75

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.43 | 0.42 | 0.43 | 0.43 | 0.0033 |
| 5% | 0.5 | 0.44 | 0.46 | 0.47 | 0.0176 |
| 10% | 0.58 | 0.53 | 0.57 | 0.56 | 0.0153 |
| 20% | 0.74 | 0.71 | 0.78 | 0.74 | 0.0203 |
| 25% | 0.82 | 0.8 | 0.76 | 0.79 | 0.0176 |

Compound 76

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.35 | 0.33 | 0.36 | 0.35 | 0.0088 |
| 5% | 0.28 | 0.37 | 0.37 | 0.34 | 0.0300 |
| 10% | 0.49 | 0.47 | 0.43 | 0.46 | 0.0176 |
| 20% | 0.6 | 0.59 | 0.58 | 0.59 | 0.0058 |
| 25% | 0.68 | 0.67 | 0.66 | 0.67 | 0.0058 |

Compound 77

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.16 | 0.17 | 0.17 | 0.17 | 0.0033 |
| 5% | 0.22 | 0.22 | 0.22 | 0.22 | 0.0000 |
| 10% | 0.27 | 0.29 | 0.33 | 0.30 | 0.0176 |
| 20% | 0.45 | 0.43 | 0.46 | 0.45 | 0.0088 |
| 25% | 0.53 | 0.5 | 0.48 | 0.50 | 0.0145 |

Compound 78

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.02 | 0.02 | 0.03 | 0.02 | 0.0033 |
| 5% | 0.04 | 0.04 | 0.07 | 0.05 | 0.0100 |
| 10% | 0.06 | 0.05 | 0.07 | 0.06 | 0.0058 |
| 20% | 0.1 | 0.11 | 0.1 | 0.10 | 0.0033 |
| 25% | 0.17 | 0.14 | 0.13 | 0.15 | 0.0120 |

Compound 79

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.04 | 0.04 | 0.03 | 0.04 | 0.0033 |
| 5% | 0.1 | 0.08 | 0.14 | 0.11 | 0.0176 |
| 10% | 0.19 | 0.19 | 0.18 | 0.19 | 0.0033 |
| 20% | 0.5 | 0.54 | 0.5 | 0.51 | 0.0133 |
| 25% | 0.73 | 0.72 | 0.7 | 0.72 | 0.0088 |

Compound 80

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 5% | 0.09 | 0.06 | 0.06 | 0.07 | 0.0100 |
| 10% | 0.15 | 0.18 | 0.13 | 0.15 | 0.0145 |
| 20% | 0.34 | 0.33 | 0.28 | 0.32 | 0.0186 |
| 25% | 0.32 | 0.36 | 0.4 | 0.36 | 0.0231 |

Compound 81

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.64 | 0.61 | 0.59 | 0.61 | 0.0145 |
| 5% | 0.65 | 0.67 | 0.66 | 0.66 | 0.0058 |
| 10% | 0.73 | 0.68 | 0.71 | 0.71 | 0.0145 |
| 20% | 0.79 | 0.76 | 0.77 | 0.77 | 0.0088 |
| 25% | 0.79 | 0.8 | 0.79 | 0.79 | 0.0033 |

Compound 82

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.15 | 0.16 | 0.16 | 0.16 | 0.0033 |
| 5% | 0.26 | 0.29 | 0.29 | 0.28 | 0.0100 |
| 10% | 0.42 | 0.44 | 0.38 | 0.41 | 0.0176 |
| 20% | 0.62 | 0.57 | 0.61 | 0.60 | 0.0153 |
| 25% | 0.64 | 0.67 | 0.63 | 0.65 | 0.0120 |

Compound 83

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 5% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 10% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 20% | 0.14 | 0.1 | 0.09 | 0.11 | 0.0153 |
| 25% | 0.18 | 0.18 | 0.17 | 0.18 | 0.0033 |
| 30% | 0.18 | 0.17 | 0.2 | 0.18 | 0.0088 |

Compound 84

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 5% | 0.03 | 0.03 | 0.04 | 0.03 | 0.0033 |
| 10% | 0.09 | 0.09 | 0.12 | 0.10 | 0.0100 |
| 20% | 0.3 | 0.29 | 0.29 | 0.29 | 0.0033 |
| 25% | 0.32 | 0.33 | 0.33 | 0.33 | 0.0033 |

Compound 85

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.1 | 0.1 | 0.12 | 0.11 | 0.0067 |
| 5% | 0.15 | 0.16 | 0.17 | 0.16 | 0.0058 |
| 10% | 0.3 | 0.31 | 0.23 | 0.28 | 0.0252 |
| 20% | 0.38 | 0.37 | 0.37 | 0.37 | 0.0033 |
| 25% | 0.4 | 0.45 | 0.4 | 0.42 | 0.0167 |

Compound 86

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.03 | 0.01 | 0.06 | 0.03 | 0.0145 |
| 5% | 0.06 | 0.07 | 0.03 | 0.05 | 0.0120 |
| 10% | 0.11 | 0.12 | 0.09 | 0.11 | 0.0088 |
| 20% | 0.17 | 0.17 | 0.15 | 0.16 | 0.0067 |
| 25% | 0.22 | 0.13 | 0.18 | 0.18 | 0.0260 |

Compound 87

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.18 | 0.17 | 0.14 | 0.16 | 0.0120 |
| 5% | 0.24 | 0.29 | 0.27 | 0.27 | 0.0145 |
| 10% | 0.45 | 0.48 | 0.43 | 0.45 | 0.0145 |
| 20% | 0.61 | 0.63 | 0.6 | 0.61 | 0.0088 |
| 25% | 0.56 | 0.54 | 0.56 | 0.55 | 0.0067 |

Compound 88

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 5% | 0.03 | 0.03 | 0.06 | 0.04 | 0.0100 |
| 10% | 0.11 | 0.11 | 0.1 | 0.11 | 0.0033 |
| 20% | 0.28 | 0.27 | 0.28 | 0.28 | 0.0033 |
| 25% | 0.36 | 0.39 | 0.41 | 0.39 | 0.0145 |

Compound 89

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.14 | 0.16 | 0.13 | 0.14 | 0.0088 |
| 5% | 0.22 | 0.26 | 0.21 | 0.23 | 0.0153 |
| 10% | 0.48 | 0.5 | 0.43 | 0.47 | 0.0208 |
| 20% | 0.66 | 0.68 | 0.65 | 0.66 | 0.0088 |
| 25% | 0.68 | 0.74 | 0.73 | 0.72 | 0.0186 |

Compound 90

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.6 | 0.58 | 0.58 | 0.59 | 0.0067 |
| 5% | 0.63 | 0.66 | 0.65 | 0.65 | 0.0088 |
| 10% | 0.73 | 0.7 | 0.71 | 0.71 | 0.0088 |
| 20% | 0.75 | 0.77 | 0.82 | 0.78 | 0.0208 |
| 25% | 0.79 | 0.83 | 0.82 | 0.81 | 0.0120 |

Compound 91

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.49 | 0.47 | 0.45 | 0.47 | 0.0115 |
| 5% | 0.5 | 0.56 | 0.6 | 0.55 | 0.0291 |
| 10% | 0.62 | 0.59 | 0.62 | 0.61 | 0.0100 |
| 20% | 0.7 | 0.67 | 0.71 | 0.69 | 0.0120 |
| 25% | 0.68 | 0.72 | 0.82 | 0.74 | 0.0416 |

Compound 92

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.17 | 0.18 | 0.18 | 0.18 | 0.0033 |
| 5% | 0.23 | 0.26 | 0.26 | 0.25 | 0.0100 |
| 10% | 0.41 | 0.41 | 0.38 | 0.40 | 0.0100 |
| 20% | 0.57 | 0.55 | 0.59 | 0.57 | 0.0115 |
| 25% | 0.57 | 0.6 | 0.59 | 0.59 | 0.0088 |

Compound 93

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|-----------------------|--------------|--------------|--------------|----------------|-----------------------|
| 2% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 5% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 10% | 0.07 | 0.07 | 0.05 | 0.06 | 0.0067 |
| 20% | 0.14 | 0.14 | 0.14 | 0.14 | 0.0000 |
| 25% | 0.16 | 0.19 | 0.19 | 0.18 | 0.0100 |

Compound 94

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|-----------------------|--------------|--------------|--------------|----------------|-----------------------|
| 2% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 5% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 10% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 20% | 0.05 | 0.06 | 0.11 | 0.07 | 0.0186 |
| 25% | 0.18 | 0.14 | 0.17 | 0.16 | 0.0120 |
| 30% | 0.24 | 0.21 | 0.23 | 0.23 | 0.0088 |

Compound 95

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|-----------------------|--------------|--------------|--------------|----------------|-----------------------|
| 2% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 5% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 10% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 20% | 0.05 | 0.06 | 0.04 | 0.05 | 0.0058 |
| 25% | 0.1 | 0.09 | 0.09 | 0.09 | 0.0033 |
| 30% | 0.11 | 0.11 | 0.14 | 0.12 | 0.0100 |

3.2.4 MeOH/2-MeTHF R_f Data

| Compound 1 | | | | | |
|----------------|-------|-------|-------|---------|----------------|
| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
| 2% | 0.62 | 0.65 | 0.7 | 0.66 | 0.0233 |
| 5% | 0.72 | 0.78 | 0.73 | 0.74 | 0.0186 |
| 10% | 0.81 | 0.78 | 0.81 | 0.80 | 0.0100 |
| 20% | 0.82 | 0.85 | 0.85 | 0.84 | 0.0100 |
| 25% | 0.91 | 0.89 | 0.85 | 0.88 | 0.0176 |

| Compound 2 | | | | | |
|----------------|-------|-------|-------|---------|----------------|
| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
| 2% | 0.68 | 0.67 | 0.65 | 0.67 | 0.0088 |
| 5% | 0.73 | 0.73 | 0.66 | 0.71 | 0.0233 |
| 10% | 0.77 | 0.73 | 0.76 | 0.75 | 0.0120 |
| 20% | 0.77 | 0.76 | 0.83 | 0.79 | 0.0219 |
| 25% | 0.89 | 0.83 | 0.81 | 0.84 | 0.0240 |

| Compound 3 | | | | | |
|----------------|-------|-------|-------|---------|----------------|
| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
| 2% | 0.73 | 0.74 | 0.73 | 0.73 | 0.0033 |
| 5% | 0.72 | 0.8 | 0.74 | 0.75 | 0.0240 |
| 10% | 0.82 | 0.77 | 0.8 | 0.80 | 0.0145 |
| 20% | 0.82 | 0.82 | 0.85 | 0.83 | 0.0100 |
| 25% | 0.93 | 0.83 | 0.85 | 0.87 | 0.0306 |

| Compound 4 | | | | | |
|----------------|-------|-------|-------|---------|----------------|
| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
| 2% | 0.63 | 0.63 | 0.62 | 0.63 | 0.0033 |
| 5% | 0.66 | 0.64 | 0.64 | 0.65 | 0.0067 |
| 10% | 0.68 | 0.64 | 0.64 | 0.65 | 0.0133 |
| 20% | 0.74 | 0.76 | 0.72 | 0.74 | 0.0115 |
| 25% | 0.78 | 0.74 | 0.74 | 0.75 | 0.0133 |

| Compound 5 | | | | | |
|----------------|-------|-------|-------|---------|----------------|
| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
| 2% | 0.56 | 0.56 | 0.58 | 0.57 | 0.0067 |
| 5% | 0.66 | 0.64 | 0.64 | 0.65 | 0.0067 |
| 10% | 0.69 | 0.68 | 0.66 | 0.68 | 0.0088 |
| 20% | 0.71 | 0.69 | 0.7 | 0.70 | 0.0058 |
| 25% | 0.71 | 0.72 | 0.73 | 0.72 | 0.0058 |

| Compound 6 | | | | | |
|----------------|-------|-------|-------|---------|----------------|
| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
| 2% | 0.66 | 0.64 | 0.64 | 0.65 | 0.0067 |
| 5% | 0.66 | 0.73 | 0.65 | 0.68 | 0.0252 |
| 10% | 0.75 | 0.73 | 0.71 | 0.73 | 0.0115 |
| 20% | 0.76 | 0.78 | 0.77 | 0.77 | 0.0058 |
| 25% | 0.84 | 0.82 | 0.79 | 0.82 | 0.0145 |

Compound 7

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.65 | 0.64 | 0.67 | 0.65 | 0.0088 |
| 5% | 0.67 | 0.65 | 0.67 | 0.66 | 0.0067 |
| 10% | 0.68 | 0.66 | 0.69 | 0.68 | 0.0088 |
| 20% | 0.68 | 0.71 | 0.68 | 0.69 | 0.0100 |
| 25% | 0.72 | 0.72 | 0.69 | 0.71 | 0.0100 |

Compound 8

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.65 | 0.66 | 0.65 | 0.65 | 0.0033 |
| 5% | 0.67 | 0.71 | 0.64 | 0.67 | 0.0203 |
| 10% | 0.71 | 0.73 | 0.69 | 0.71 | 0.0115 |
| 20% | 0.71 | 0.75 | 0.75 | 0.74 | 0.0133 |
| 25% | 0.8 | 0.76 | 0.77 | 0.78 | 0.0120 |

Compound 9

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.64 | 0.61 | 0.6 | 0.62 | 0.0120 |
| 5% | 0.64 | 0.63 | 0.64 | 0.64 | 0.0033 |
| 10% | 0.66 | 0.66 | 0.69 | 0.67 | 0.0100 |
| 20% | 0.65 | 0.71 | 0.72 | 0.69 | 0.0219 |
| 25% | 0.71 | 0.69 | 0.74 | 0.71 | 0.0145 |

Compound 10

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.6 | 0.58 | 0.58 | 0.59 | 0.0067 |
| 5% | 0.58 | 0.6 | 0.63 | 0.60 | 0.0145 |
| 10% | 0.63 | 0.7 | 0.64 | 0.66 | 0.0219 |
| 20% | 0.71 | 0.7 | 0.68 | 0.70 | 0.0088 |
| 25% | 0.73 | 0.7 | 0.73 | 0.72 | 0.0100 |

Compound 11

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.34 | 0.26 | 0.25 | 0.28 | 0.0285 |
| 5% | 0.29 | 0.25 | 0.28 | 0.27 | 0.0120 |
| 10% | 0.42 | 0.34 | 0.38 | 0.38 | 0.0231 |
| 20% | 0.54 | 0.51 | 0.53 | 0.53 | 0.0088 |
| 25% | 0.61 | 0.55 | 0.63 | 0.60 | 0.0240 |

Compound 12

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.2 | 0.2 | 0.13 | 0.18 | 0.0233 |
| 5% | 0.17 | 0.23 | 0.2 | 0.20 | 0.0173 |
| 10% | 0.26 | 0.24 | 0.29 | 0.26 | 0.0145 |
| 20% | 0.31 | 0.31 | 0.3 | 0.31 | 0.0033 |
| 25% | 0.36 | 0.33 | 0.38 | 0.36 | 0.0145 |

Compound 13

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.26 | 0.24 | 0.2 | 0.23 | 0.0176 |
| 5% | 0.27 | 0.2 | 0.25 | 0.24 | 0.0208 |
| 10% | 0.26 | 0.25 | 0.27 | 0.26 | 0.0058 |
| 20% | 0.35 | 0.34 | 0.32 | 0.34 | 0.0088 |
| 25% | 0.45 | 0.35 | 0.4 | 0.40 | 0.0289 |

Compound 14

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.08 | 0.12 | 0.12 | 0.11 | 0.0133 |
| 5% | 0.16 | 0.17 | 0.14 | 0.16 | 0.0088 |
| 10% | 0.2 | 0.2 | 0.18 | 0.19 | 0.0067 |
| 20% | 0.24 | 0.24 | 0.26 | 0.25 | 0.0067 |
| 25% | 0.25 | 0.31 | 0.28 | 0.28 | 0.0173 |

Compound 15

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.35 | 0.38 | 0.38 | 0.37 | 0.0100 |
| 5% | 0.4 | 0.4 | 0.38 | 0.39 | 0.0067 |
| 10% | 0.44 | 0.44 | 0.49 | 0.46 | 0.0167 |
| 20% | 0.5 | 0.5 | 0.5 | 0.50 | 0.0000 |
| 25% | 0.53 | 0.52 | 0.52 | 0.52 | 0.0033 |

Compound 16

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.24 | 0.25 | 0.28 | 0.26 | 0.0120 |
| 5% | 0.31 | 0.3 | 0.26 | 0.29 | 0.0153 |
| 10% | 0.3 | 0.32 | 0.33 | 0.32 | 0.0088 |
| 20% | 0.37 | 0.41 | 0.31 | 0.36 | 0.0291 |
| 25% | 0.44 | 0.38 | 0.39 | 0.40 | 0.0186 |

Compound 17

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.29 | 0.26 | 0.24 | 0.26 | 0.0145 |
| 5% | 0.28 | 0.28 | 0.31 | 0.29 | 0.0100 |
| 10% | 0.38 | 0.46 | 0.35 | 0.40 | 0.0328 |
| 20% | 0.59 | 0.6 | 0.57 | 0.59 | 0.0088 |
| 25% | 0.65 | 0.73 | 0.73 | 0.70 | 0.0267 |

Compound 18

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.68 | 0.65 | 0.68 | 0.67 | 0.0100 |
| 5% | 0.65 | 0.73 | 0.69 | 0.69 | 0.0231 |
| 10% | 0.73 | 0.71 | 0.73 | 0.72 | 0.0067 |
| 20% | 0.75 | 0.77 | 0.75 | 0.76 | 0.0067 |
| 25% | 0.77 | 0.8 | 0.84 | 0.80 | 0.0203 |

Compound 19

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.62 | 0.66 | 0.63 | 0.64 | 0.0120 |
| 5% | 0.65 | 0.7 | 0.69 | 0.68 | 0.0153 |
| 10% | 0.73 | 0.71 | 0.7 | 0.71 | 0.0088 |
| 20% | 0.75 | 0.77 | 0.73 | 0.75 | 0.0115 |
| 25% | 0.77 | 0.8 | 0.84 | 0.80 | 0.0203 |

Compound 20

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.59 | 0.65 | 0.68 | 0.64 | 0.0265 |
| 5% | 0.65 | 0.68 | 0.69 | 0.67 | 0.0120 |
| 10% | 0.73 | 0.71 | 0.7 | 0.71 | 0.0088 |
| 20% | 0.75 | 0.77 | 0.74 | 0.75 | 0.0088 |
| 25% | 0.77 | 0.8 | 0.84 | 0.80 | 0.0203 |

Compound 21

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.65 | 0.65 | 0.66 | 0.65 | 0.0033 |
| 5% | 0.65 | 0.73 | 0.69 | 0.69 | 0.0231 |
| 10% | 0.73 | 0.71 | 0.73 | 0.72 | 0.0067 |
| 20% | 0.75 | 0.77 | 0.75 | 0.76 | 0.0067 |
| 25% | 0.77 | 0.8 | 0.84 | 0.80 | 0.0203 |

Compound 22

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.65 | 0.65 | 0.66 | 0.65 | 0.0033 |
| 5% | 0.65 | 0.73 | 0.69 | 0.69 | 0.0231 |
| 10% | 0.73 | 0.71 | 0.73 | 0.72 | 0.0067 |
| 20% | 0.75 | 0.77 | 0.75 | 0.76 | 0.0067 |
| 25% | 0.77 | 0.8 | 0.84 | 0.80 | 0.0203 |

Compound 23

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.59 | 0.66 | 0.63 | 0.63 | 0.0203 |
| 5% | 0.65 | 0.7 | 0.69 | 0.68 | 0.0153 |
| 10% | 0.69 | 0.71 | 0.73 | 0.71 | 0.0115 |
| 20% | 0.75 | 0.77 | 0.75 | 0.76 | 0.0067 |
| 25% | 0.77 | 0.8 | 0.84 | 0.80 | 0.0203 |

Compound 24

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.7 | 0.65 | 0.68 | 0.68 | 0.0145 |
| 5% | 0.71 | 0.69 | 0.67 | 0.69 | 0.0115 |
| 10% | 0.74 | 0.73 | 0.76 | 0.74 | 0.0088 |
| 20% | 0.79 | 0.78 | 0.79 | 0.79 | 0.0033 |
| 25% | 0.79 | 0.8 | 0.81 | 0.80 | 0.0058 |

Compound 25

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.64 | 0.67 | 0.66 | 0.66 | 0.0088 |
| 5% | 0.67 | 0.68 | 0.7 | 0.68 | 0.0088 |
| 10% | 0.75 | 0.74 | 0.76 | 0.75 | 0.0058 |
| 20% | 0.79 | 0.81 | 0.8 | 0.80 | 0.0058 |
| 25% | 0.77 | 0.74 | 0.74 | 0.75 | 0.0100 |

Compound 26

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.7 | 0.7 | 0.68 | 0.69 | 0.0067 |
| 5% | 0.69 | 0.71 | 0.71 | 0.70 | 0.0067 |
| 10% | 0.75 | 0.76 | 0.79 | 0.77 | 0.0120 |
| 20% | 0.8 | 0.83 | 0.81 | 0.81 | 0.0088 |
| 25% | 0.75 | 0.76 | 0.8 | 0.77 | 0.0153 |

Compound 27

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.75 | 0.73 | 0.7 | 0.73 | 0.0145 |
| 5% | 0.74 | 0.74 | 0.73 | 0.74 | 0.0033 |
| 10% | 0.79 | 0.75 | 0.77 | 0.77 | 0.0115 |
| 20% | 0.8 | 0.78 | 0.8 | 0.79 | 0.0067 |
| 25% | 0.81 | 0.82 | 0.8 | 0.81 | 0.0058 |

Compound 28

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.73 | 0.7 | 0.69 | 0.71 | 0.0120 |
| 5% | 0.74 | 0.7 | 0.72 | 0.72 | 0.0115 |
| 10% | 0.75 | 0.74 | 0.72 | 0.74 | 0.0088 |
| 20% | 0.71 | 0.81 | 0.73 | 0.75 | 0.0306 |
| 25% | 0.78 | 0.77 | 0.77 | 0.77 | 0.0033 |

Compound 29

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.68 | 0.67 | 0.68 | 0.68 | 0.0033 |
| 5% | 0.66 | 0.72 | 0.69 | 0.69 | 0.0173 |
| 10% | 0.68 | 0.69 | 0.74 | 0.70 | 0.0186 |
| 20% | 0.73 | 0.75 | 0.73 | 0.74 | 0.0067 |
| 25% | 0.77 | 0.79 | 0.77 | 0.78 | 0.0067 |

Compound 30

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.64 | 0.63 | 0.65 | 0.64 | 0.0058 |
| 5% | 0.68 | 0.64 | 0.66 | 0.66 | 0.0115 |
| 10% | 0.69 | 0.7 | 0.72 | 0.70 | 0.0088 |
| 20% | 0.72 | 0.71 | 0.76 | 0.73 | 0.0153 |
| 25% | 0.74 | 0.76 | 0.77 | 0.76 | 0.0088 |

Compound 31

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.12 | 0.14 | 0.15 | 0.14 | 0.0088 |
| 5% | 0.16 | 0.16 | 0.2 | 0.17 | 0.0133 |
| 10% | 0.26 | 0.22 | 0.2 | 0.23 | 0.0176 |
| 20% | 0.29 | 0.29 | 0.27 | 0.28 | 0.0067 |
| 25% | 0.32 | 0.28 | 0.33 | 0.31 | 0.0153 |

Compound 32

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.51 | 0.53 | 0.52 | 0.52 | 0.0058 |
| 5% | 0.57 | 0.56 | 0.58 | 0.57 | 0.0058 |
| 10% | 0.64 | 0.59 | 0.65 | 0.63 | 0.0186 |
| 20% | 0.69 | 0.7 | 0.69 | 0.69 | 0.0033 |
| 25% | 0.73 | 0.73 | 0.74 | 0.73 | 0.0033 |

Compound 33

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.66 | 0.67 | 0.66 | 0.66 | 0.0033 |
| 5% | 0.65 | 0.71 | 0.68 | 0.68 | 0.0173 |
| 10% | 0.7 | 0.71 | 0.7 | 0.70 | 0.0033 |
| 20% | 0.71 | 0.73 | 0.73 | 0.72 | 0.0067 |
| 25% | 0.75 | 0.71 | 0.74 | 0.73 | 0.0120 |

Compound 34

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.71 | 0.74 | 0.75 | 0.73 | 0.0120 |
| 5% | 0.71 | 0.75 | 0.76 | 0.74 | 0.0153 |
| 10% | 0.77 | 0.74 | 0.78 | 0.76 | 0.0120 |
| 20% | 0.82 | 0.8 | 0.77 | 0.80 | 0.0145 |
| 25% | 0.82 | 0.8 | 0.8 | 0.81 | 0.0067 |

Compound 35

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.61 | 0.63 | 0.65 | 0.63 | 0.0115 |
| 5% | 0.67 | 0.73 | 0.63 | 0.68 | 0.0291 |
| 10% | 0.7 | 0.74 | 0.7 | 0.71 | 0.0133 |
| 20% | 0.77 | 0.76 | 0.76 | 0.76 | 0.0033 |
| 25% | 0.8 | 0.79 | 0.77 | 0.79 | 0.0088 |

Compound 36

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.47 | 0.49 | 0.45 | 0.47 | 0.0115 |
| 5% | 0.51 | 0.51 | 0.53 | 0.52 | 0.0067 |
| 10% | 0.54 | 0.59 | 0.57 | 0.57 | 0.0145 |
| 20% | 0.61 | 0.63 | 0.6 | 0.61 | 0.0088 |
| 25% | 0.62 | 0.65 | 0.66 | 0.64 | 0.0120 |

Compound 37

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.73 | 0.71 | 0.71 | 0.72 | 0.0067 |
| 5% | 0.74 | 0.7 | 0.75 | 0.73 | 0.0153 |
| 10% | 0.77 | 0.71 | 0.73 | 0.74 | 0.0176 |
| 20% | 0.76 | 0.77 | 0.75 | 0.76 | 0.0058 |
| 25% | 0.76 | 0.81 | 0.77 | 0.78 | 0.0153 |

Compound 38

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.69 | 0.66 | 0.65 | 0.67 | 0.0120 |
| 5% | 0.75 | 0.68 | 0.65 | 0.69 | 0.0296 |
| 10% | 0.73 | 0.71 | 0.72 | 0.72 | 0.0058 |
| 20% | 0.74 | 0.78 | 0.73 | 0.75 | 0.0153 |
| 25% | 0.8 | 0.79 | 0.79 | 0.79 | 0.0033 |

Compound 39

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.63 | 0.61 | 0.65 | 0.63 | 0.0115 |
| 5% | 0.63 | 0.69 | 0.66 | 0.66 | 0.0173 |
| 10% | 0.71 | 0.74 | 0.67 | 0.71 | 0.0203 |
| 20% | 0.77 | 0.74 | 0.71 | 0.74 | 0.0173 |
| 25% | 0.75 | 0.81 | 0.77 | 0.78 | 0.0176 |

Compound 40

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.53 | 0.56 | 0.58 | 0.56 | 0.0145 |
| 5% | 0.6 | 0.62 | 0.59 | 0.60 | 0.0088 |
| 10% | 0.67 | 0.63 | 0.65 | 0.65 | 0.0115 |
| 20% | 0.71 | 0.69 | 0.7 | 0.70 | 0.0058 |
| 25% | 0.77 | 0.74 | 0.74 | 0.75 | 0.0100 |

Compound 41

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.57 | 0.57 | 0.6 | 0.58 | 0.0100 |
| 5% | 0.6 | 0.63 | 0.64 | 0.62 | 0.0120 |
| 10% | 0.69 | 0.68 | 0.63 | 0.67 | 0.0186 |
| 20% | 0.68 | 0.74 | 0.73 | 0.72 | 0.0186 |
| 25% | 0.71 | 0.8 | 0.74 | 0.75 | 0.0265 |

Compound 42

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.43 | 0.44 | 0.46 | 0.44 | 0.0088 |
| 5% | 0.44 | 0.46 | 0.49 | 0.46 | 0.0145 |
| 10% | 0.56 | 0.54 | 0.52 | 0.54 | 0.0115 |
| 20% | 0.63 | 0.61 | 0.64 | 0.63 | 0.0088 |
| 25% | 0.64 | 0.63 | 0.64 | 0.64 | 0.0033 |

Compound 43

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.03 | 0.03 | 0.03 | 0.03 | 0.0000 |
| 5% | 0.05 | 0.08 | 0.07 | 0.07 | 0.0088 |
| 10% | 0.1 | 0.1 | 0.08 | 0.09 | 0.0067 |
| 20% | 0.13 | 0.16 | 0.13 | 0.14 | 0.0100 |
| 25% | 0.14 | 0.17 | 0.16 | 0.16 | 0.0088 |

Compound 44

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.7 | 0.68 | 0.69 | 0.69 | 0.0058 |
| 5% | 0.68 | 0.71 | 0.72 | 0.70 | 0.0120 |
| 10% | 0.73 | 0.72 | 0.73 | 0.73 | 0.0033 |
| 20% | 0.74 | 0.76 | 0.73 | 0.74 | 0.0088 |
| 25% | 0.77 | 0.75 | 0.77 | 0.76 | 0.0067 |

Compound 45

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.19 | 0.22 | 0.21 | 0.21 | 0.0088 |
| 5% | 0.26 | 0.29 | 0.25 | 0.27 | 0.0120 |
| 10% | 0.34 | 0.3 | 0.34 | 0.33 | 0.0133 |
| 20% | 0.4 | 0.46 | 0.41 | 0.42 | 0.0186 |
| 25% | 0.46 | 0.46 | 0.44 | 0.45 | 0.0067 |

Compound 46

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.5 | 0.49 | 0.48 | 0.49 | 0.0058 |
| 5% | 0.5 | 0.51 | 0.53 | 0.51 | 0.0088 |
| 10% | 0.59 | 0.57 | 0.57 | 0.58 | 0.0067 |
| 20% | 0.62 | 0.62 | 0.68 | 0.64 | 0.0200 |
| 25% | 0.66 | 0.73 | 0.73 | 0.71 | 0.0233 |

Compound 47

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.04 | 0.04 | 0.04 | 0.04 | 0.0000 |
| 5% | 0.04 | 0.07 | 0.07 | 0.06 | 0.0100 |
| 10% | 0.09 | 0.12 | 0.08 | 0.10 | 0.0120 |
| 20% | 0.18 | 0.2 | 0.17 | 0.18 | 0.0088 |
| 25% | 0.33 | 0.24 | 0.23 | 0.27 | 0.0318 |

Compound 48

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.54 | 0.54 | 0.57 | 0.55 | 0.0100 |
| 5% | 0.54 | 0.56 | 0.57 | 0.56 | 0.0088 |
| 10% | 0.64 | 0.61 | 0.63 | 0.63 | 0.0088 |
| 20% | 0.69 | 0.7 | 0.69 | 0.69 | 0.0033 |
| 25% | 0.7 | 0.71 | 0.72 | 0.71 | 0.0058 |

Compound 49

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.41 | 0.39 | 0.42 | 0.41 | 0.0088 |
| 5% | 0.46 | 0.46 | 0.46 | 0.46 | 0.0000 |
| 10% | 0.54 | 0.56 | 0.54 | 0.55 | 0.0067 |
| 20% | 0.65 | 0.63 | 0.62 | 0.63 | 0.0088 |
| 25% | 0.63 | 0.6 | 0.66 | 0.63 | 0.0173 |

Compound 50

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.47 | 0.51 | 0.48 | 0.49 | 0.0120 |
| 5% | 0.55 | 0.53 | 0.5 | 0.53 | 0.0145 |
| 10% | 0.61 | 0.61 | | 0.61 | 0.0000 |
| 20% | 0.66 | 0.67 | 0.64 | 0.66 | 0.0088 |
| 25% | 0.68 | 0.73 | 0.71 | 0.71 | 0.0145 |

Compound 51

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.04 | 0.05 | 0.04 | 0.04 | 0.0033 |
| 5% | 0.05 | 0.05 | 0.05 | 0.05 | 0.0000 |
| 10% | 0.07 | 0.08 | 0.07 | 0.07 | 0.0033 |
| 20% | 0.11 | 0.11 | 0.16 | 0.13 | 0.0167 |
| 25% | 0.14 | 0.15 | 0.15 | 0.15 | 0.0033 |

Compound 52

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.66 | 0.66 | 0.64 | 0.65 | 0.0067 |
| 5% | 0.64 | 0.69 | 0.69 | 0.67 | 0.0167 |
| 10% | 0.73 | 0.72 | 0.7 | 0.72 | 0.0088 |
| 20% | 0.77 | 0.73 | 0.74 | 0.75 | 0.0120 |
| 25% | 0.76 | 0.76 | 0.77 | 0.76 | 0.0033 |

Compound 53

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.63 | 0.66 | 0.65 | 0.65 | 0.0088 |
| 5% | 0.74 | 0.64 | 0.63 | 0.67 | 0.0351 |
| 10% | 0.73 | 0.7 | 0.68 | 0.70 | 0.0145 |
| 20% | 0.72 | 0.76 | 0.71 | 0.73 | 0.0153 |
| 25% | 0.7 | 0.73 | 0.81 | 0.75 | 0.0328 |

Compound 54

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.6 | 0.63 | 0.6 | 0.61 | 0.0100 |
| 5% | 0.63 | 0.63 | 0.66 | 0.64 | 0.0100 |
| 10% | 0.69 | 0.65 | 0.64 | 0.66 | 0.0153 |
| 20% | 0.7 | 0.68 | 0.7 | 0.69 | 0.0067 |
| 25% | 0.73 | 0.74 | 0.74 | 0.74 | 0.0033 |

Compound 55

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 5% | 0.04 | 0.04 | 0.07 | 0.05 | 0.0100 |
| 10% | 0.07 | 0.07 | 0.07 | 0.07 | 0.0000 |
| 20% | 0.11 | 0.11 | 0.1 | 0.11 | 0.0033 |
| 25% | 0.12 | 0.12 | 0.11 | 0.12 | 0.0033 |

Compound 56

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 5% | 0.03 | 0.03 | 0.03 | 0.03 | 0.0000 |
| 10% | 0.08 | 0.08 | 0.08 | 0.08 | 0.0000 |
| 20% | 0.16 | 0.16 | 0.16 | 0.16 | 0.0000 |
| 25% | 0.28 | 0.22 | 0.24 | 0.25 | 0.0176 |

Compound 57

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0 | 0 | | 0.00 | 0.0000 |
| 5% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 10% | 0.06 | 0.04 | 0.08 | 0.06 | 0.0115 |
| 20% | 0.11 | 0.13 | 0.11 | 0.12 | 0.0067 |
| 25% | 0.13 | 0.17 | | 0.15 | 0.0200 |

Compound 58

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 22% | 0.06 | 0.05 | 0.08 | 0.06 | 0.0088 |
| 25% | 0.06 | 0.1 | 0.08 | 0.08 | 0.0115 |
| 28% | 0.1 | 0.17 | 0.13 | 0.13 | 0.0203 |
| 30% | 0.16 | 0.17 | 0.15 | 0.16 | 0.0058 |

Compound 59

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.48 | 0.43 | 0.48 | 0.46 | 0.0167 |
| 5% | 0.43 | 0.52 | 0.48 | 0.48 | 0.0260 |
| 10% | 0.53 | 0.52 | 0.54 | 0.53 | 0.0058 |
| 20% | 0.56 | 0.61 | 0.6 | 0.59 | 0.0153 |
| 25% | 0.59 | 0.63 | 0.64 | 0.62 | 0.0153 |

Compound 60

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.64 | 0.58 | 0.65 | 0.62 | 0.0219 |
| 5% | 0.68 | 0.65 | 0.66 | 0.66 | 0.0088 |
| 10% | 0.71 | 0.71 | 0.67 | 0.70 | 0.0133 |
| 20% | 0.74 | 0.73 | 0.73 | 0.73 | 0.0033 |
| 25% | 0.75 | 0.75 | 0.77 | 0.76 | 0.0067 |

Compound 61

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.6 | 0.56 | 0.58 | 0.58 | 0.0115 |
| 5% | 0.59 | 0.61 | 0.61 | 0.60 | 0.0067 |
| 10% | 0.66 | 0.69 | 0.64 | 0.66 | 0.0145 |
| 20% | 0.71 | 0.68 | 0.72 | 0.70 | 0.0120 |
| 25% | 0.71 | 0.71 | 0.75 | 0.72 | 0.0133 |

Compound 62

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.54 | 0.57 | 0.55 | 0.55 | 0.0088 |
| 5% | 0.56 | 0.56 | 0.57 | 0.56 | 0.0033 |
| 10% | 0.64 | 0.66 | 0.65 | 0.65 | 0.0058 |
| 20% | 0.7 | 0.71 | 0.68 | 0.70 | 0.0088 |
| 25% | 0.66 | 0.79 | 0.75 | 0.73 | 0.0384 |

Compound 63

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 5% | 0.5 | 0.48 | 0.46 | 0.48 | 0.0115 |
| 10% | 0.6 | 0.6 | 0.62 | 0.61 | 0.0067 |
| 20% | 0.72 | 0.7 | 0.74 | 0.72 | 0.0115 |
| 25% | 0.78 | 0.79 | 0.81 | 0.79 | 0.0088 |

Compound 64

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.4 | 0.4 | 0.38 | 0.39 | 0.0067 |
| 5% | 0.45 | 0.46 | 0.46 | 0.46 | 0.0033 |
| 10% | 0.51 | 0.51 | 0.51 | 0.51 | 0.0000 |
| 20% | 0.61 | 0.64 | 0.65 | 0.63 | 0.0120 |
| 25% | 0.67 | 0.71 | 0.69 | 0.69 | 0.0115 |

Compound 65

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.65 | 0.6 | 0.61 | 0.62 | 0.0153 |
| 5% | 0.62 | 0.66 | 0.62 | 0.63 | 0.0133 |
| 10% | 0.74 | 0.68 | 0.7 | 0.71 | 0.0176 |
| 20% | 0.76 | 0.74 | 0.82 | 0.77 | 0.0240 |
| 25% | 0.8 | 0.76 | 0.85 | 0.80 | 0.0260 |

Compound 66

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.26 | 0.28 | 0.28 | 0.27 | 0.0067 |
| 5% | 0.31 | 0.35 | 0.3 | 0.32 | 0.0153 |
| 10% | 0.43 | 0.42 | 0.43 | 0.43 | 0.0033 |
| 20% | 0.5 | 0.54 | 0.54 | 0.53 | 0.0133 |
| 25% | 0.59 | 0.59 | 0.56 | 0.58 | 0.0100 |

Compound 67

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.68 | 0.67 | 0.68 | 0.68 | 0.0033 |
| 5% | 0.72 | 0.68 | 0.7 | 0.70 | 0.0115 |
| 10% | 0.73 | 0.76 | 0.74 | 0.74 | 0.0088 |
| 20% | 0.77 | 0.76 | 0.8 | 0.78 | 0.0120 |
| 25% | 0.78 | 0.8 | 0.81 | 0.80 | 0.0088 |

Compound 68

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.51 | 0.51 | 0.5 | 0.51 | 0.0033 |
| 5% | 0.53 | 0.57 | 0.54 | 0.55 | 0.0120 |
| 10% | 0.63 | 0.62 | 0.6 | 0.62 | 0.0088 |
| 20% | 0.66 | 0.68 | 0.68 | 0.67 | 0.0067 |
| 25% | 0.68 | 0.74 | 0.69 | 0.70 | 0.0186 |

Compound 69

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.66 | 0.65 | 0.68 | 0.66 | 0.0088 |
| 5% | 0.68 | 0.7 | 0.7 | 0.69 | 0.0067 |
| 10% | 0.74 | 0.73 | 0.69 | 0.72 | 0.0153 |
| 20% | 0.73 | 0.77 | 0.76 | 0.75 | 0.0120 |
| 25% | 0.77 | 0.83 | 0.8 | 0.80 | 0.0173 |

Compound 70

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.54 | 0.54 | 0.58 | 0.55 | 0.0133 |
| 5% | 0.58 | 0.57 | 0.6 | 0.58 | 0.0088 |
| 10% | 0.63 | 0.62 | 0.57 | 0.61 | 0.0186 |
| 20% | 0.65 | 0.64 | 0.68 | 0.66 | 0.0120 |
| 25% | 0.68 | 0.71 | 0.69 | 0.69 | 0.0088 |

Compound 71

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.65 | 0.63 | 0.64 | 0.64 | 0.0058 |
| 5% | 0.66 | 0.69 | 0.64 | 0.66 | 0.0145 |
| 10% | 0.69 | 0.72 | 0.73 | 0.71 | 0.0120 |
| 20% | 0.77 | 0.74 | 0.74 | 0.75 | 0.0100 |
| 25% | 0.76 | 0.78 | 0.77 | 0.77 | 0.0058 |

Compound 72

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.54 | 0.48 | 0.5 | 0.51 | 0.0176 |
| 5% | 0.5 | 0.52 | 0.54 | 0.52 | 0.0115 |
| 10% | 0.57 | 0.58 | 0.54 | 0.56 | 0.0120 |
| 20% | 0.65 | 0.61 | 0.63 | 0.63 | 0.0115 |
| 25% | 0.67 | 0.64 | 0.63 | 0.65 | 0.0120 |

Compound 73

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.06 | 0.05 | 0.05 | 0.05 | 0.0033 |
| 5% | 0.08 | 0.06 | 0.08 | 0.07 | 0.0067 |
| 10% | 0.12 | 0.13 | 0.13 | 0.13 | 0.0033 |
| 20% | 0.16 | 0.17 | 0.16 | 0.16 | 0.0033 |
| 25% | 0.06 | 0.05 | 0.05 | 0.05 | 0.0033 |

Compound 74

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.61 | 0.64 | 0.63 | 0.63 | 0.0088 |
| 5% | 0.64 | 0.61 | 0.66 | 0.64 | 0.0145 |
| 10% | 0.67 | 0.64 | 0.67 | 0.66 | 0.0100 |
| 20% | 0.67 | 0.68 | 0.71 | 0.69 | 0.0120 |
| 25% | 0.73 | 0.74 | 0.72 | 0.73 | 0.0058 |

Compound 75

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.68 | 0.68 | 0.66 | 0.67 | 0.0067 |
| 5% | 0.68 | 0.68 | 0.69 | 0.68 | 0.0033 |
| 10% | 0.69 | 0.68 | 0.71 | 0.69 | 0.0088 |
| 20% | 0.7 | 0.72 | 0.71 | 0.71 | 0.0058 |
| 25% | 0.71 | 0.73 | 0.71 | 0.72 | 0.0067 |

Compound 76

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.62 | 0.62 | 0.58 | 0.61 | 0.0133 |
| 5% | 0.6 | 0.61 | 0.65 | 0.62 | 0.0153 |
| 10% | 0.63 | 0.63 | 0.61 | 0.62 | 0.0067 |
| 20% | 0.68 | 0.67 | 0.69 | 0.68 | 0.0058 |
| 25% | 0.74 | 0.68 | 0.68 | 0.70 | 0.0200 |

Compound 77

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.29 | 0.22 | 0.31 | 0.27 | 0.0273 |
| 5% | 0.28 | 0.32 | 0.29 | 0.30 | 0.0120 |
| 10% | 0.36 | 0.42 | 0.42 | 0.40 | 0.0200 |
| 20% | 0.52 | 0.43 | 0.5 | 0.48 | 0.0273 |
| 25% | 0.52 | 0.54 | 0.52 | 0.53 | 0.0067 |

Compound 78

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.04 | 0.03 | 0.03 | 0.03 | 0.0033 |
| 5% | 0.05 | 0.05 | 0.05 | 0.05 | 0.0000 |
| 10% | 0.07 | 0.06 | 0.07 | 0.07 | 0.0033 |
| 20% | 0.11 | 0.15 | 0.13 | 0.13 | 0.0115 |
| 25% | 0.14 | 0.12 | 0.19 | 0.15 | 0.0208 |

Compound 79

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.47 | 0.46 | 0.45 | 0.46 | 0.0058 |
| 5% | 0.51 | 0.49 | 0.5 | 0.50 | 0.0058 |
| 10% | 0.55 | 0.56 | 0.57 | 0.56 | 0.0058 |
| 20% | 0.59 | 0.66 | 0.61 | 0.62 | 0.0208 |
| 25% | 0.65 | 0.67 | 0.61 | 0.64 | 0.0176 |

Compound 80

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.13 | 0.11 | 0.15 | 0.13 | 0.0115 |
| 5% | 0.2 | 0.23 | 0.25 | 0.23 | 0.0145 |
| 10% | 0.34 | 0.32 | 0.33 | 0.33 | 0.0058 |
| 20% | 0.42 | 0.4 | 0.41 | 0.41 | 0.0058 |
| 25% | 0.49 | 0.49 | 0.55 | 0.51 | 0.0200 |

Compound 81

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.73 | 0.68 | 0.68 | 0.70 | 0.0167 |
| 5% | 0.72 | 0.73 | 0.7 | 0.72 | 0.0088 |
| 10% | 0.72 | 0.74 | 0.72 | 0.73 | 0.0067 |
| 20% | 0.76 | 0.74 | 0.78 | 0.76 | 0.0115 |
| 25% | 0.8 | 0.78 | 0.8 | 0.79 | 0.0067 |

Compound 82

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.53 | 0.49 | 0.47 | 0.50 | 0.0176 |
| 5% | 0.51 | 0.51 | 0.56 | 0.53 | 0.0167 |
| 10% | 0.58 | 0.6 | 0.61 | 0.60 | 0.0088 |
| 20% | 0.65 | 0.66 | 0.63 | 0.65 | 0.0088 |
| 25% | 0.65 | 0.74 | 0.66 | 0.68 | 0.0285 |

Compound 83

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.04 | 0.03 | 0.03 | 0.03 | 0.0033 |
| 5% | 0.07 | 0.05 | 0.05 | 0.06 | 0.0067 |
| 10% | 0.12 | 0.11 | 0.13 | 0.12 | 0.0058 |
| 20% | 0.25 | 0.26 | 0.24 | 0.25 | 0.0058 |
| 25% | 0.28 | 0.26 | 0.25 | 0.26 | 0.0088 |

Compound 84

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.1 | 0.13 | 0.13 | 0.12 | 0.0100 |
| 5% | 0.19 | 0.17 | 0.16 | 0.17 | 0.0088 |
| 10% | 0.21 | 0.21 | 0.24 | 0.22 | 0.0100 |
| 20% | 0.28 | 0.26 | 0.27 | 0.27 | 0.0058 |
| 25% | 0.32 | 0.31 | 0.31 | 0.31 | 0.0033 |

Compound 85

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | | 0.36 | 0.33 | 0.35 | 0.0150 |
| 5% | 0.38 | 0.38 | 0.39 | 0.38 | 0.0033 |
| 10% | 0.43 | 0.44 | 0.45 | 0.44 | 0.0058 |
| 20% | 0.47 | 0.48 | 0.49 | 0.48 | 0.0058 |
| 25% | 0.5 | 0.52 | 0.53 | 0.52 | 0.0088 |

Compound 86

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.26 | 0.22 | | 0.24 | 0.0200 |
| 5% | 0.25 | 0.26 | 0.29 | 0.27 | 0.0120 |
| 10% | 0.32 | 0.32 | 0.29 | 0.31 | 0.0100 |
| 20% | 0.33 | 0.37 | 0.35 | 0.35 | 0.0115 |
| 25% | 0.4 | 0.38 | 0.4 | 0.39 | 0.0067 |

Compound 87

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.52 | 0.51 | 0.47 | 0.50 | 0.0153 |
| 5% | 0.53 | 0.53 | 0.53 | 0.53 | 0.0000 |
| 10% | 0.6 | 0.58 | 0.61 | 0.60 | 0.0088 |
| 20% | 0.63 | 0.64 | 0.65 | 0.64 | 0.0058 |
| 25% | 0.64 | 0.68 | 0.68 | 0.67 | 0.0133 |

Compound 88

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.28 | 0.28 | 0.27 | 0.28 | 0.0033 |
| 5% | 0.32 | 0.34 | 0.38 | 0.35 | 0.0176 |
| 10% | 0.39 | 0.39 | 0.42 | 0.40 | 0.0100 |
| 20% | 0.49 | 0.5 | 0.47 | 0.49 | 0.0088 |
| 25% | 0.49 | 0.55 | 0.51 | 0.52 | 0.0176 |

Compound 89

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.51 | 0.5 | 0.53 | 0.51 | 0.0088 |
| 5% | 0.53 | 0.55 | 0.56 | 0.55 | 0.0088 |
| 10% | 0.6 | 0.62 | 0.62 | 0.61 | 0.0067 |
| 20% | 0.68 | 0.65 | 0.65 | 0.66 | 0.0100 |
| 25% | 0.65 | 0.7 | 0.71 | 0.69 | 0.0186 |

Compound 90

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.78 | 0.73 | 0.68 | 0.73 | 0.0289 |
| 5% | 0.74 | 0.75 | 0.75 | 0.75 | 0.0033 |
| 10% | 0.76 | 0.78 | 0.77 | 0.77 | 0.0058 |
| 20% | 0.76 | 0.81 | 0.8 | 0.79 | 0.0153 |
| 25% | 0.82 | 0.83 | 0.8 | 0.82 | 0.0088 |

Compound 91

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.65 | 0.64 | 0.66 | 0.65 | 0.0058 |
| 5% | 0.67 | 0.69 | 0.67 | 0.68 | 0.0067 |
| 10% | 0.69 | 0.7 | 0.71 | 0.70 | 0.0058 |
| 20% | 0.72 | 0.74 | 0.72 | 0.73 | 0.0067 |
| 25% | 0.74 | 0.74 | 0.76 | 0.75 | 0.0067 |

Compound 92

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|-----------------------|--------------|--------------|--------------|----------------|-----------------------|
| 2% | 0.48 | 0.48 | 0.5 | 0.49 | 0.0067 |
| 5% | 0.56 | 0.54 | 0.5 | 0.53 | 0.0176 |
| 10% | 0.58 | 0.55 | 0.58 | 0.57 | 0.0100 |
| 20% | 0.63 | 0.65 | 0.61 | 0.63 | 0.0115 |
| 25% | 0.64 | 0.68 | 0.62 | 0.65 | 0.0176 |

Compound 93

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|-----------------------|--------------|--------------|--------------|----------------|-----------------------|
| 2% | 0.11 | 0.11 | 0.14 | 0.12 | 0.0100 |
| 5% | 0.15 | 0.15 | 0.16 | 0.15 | 0.0033 |
| 10% | 0.21 | 0.24 | 0.22 | 0.22 | 0.0088 |
| 20% | 0.28 | 0.28 | 0.27 | 0.28 | 0.0033 |
| 25% | 0.36 | 0.33 | 0.39 | 0.36 | 0.0173 |

Compound 94

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|-----------------------|--------------|--------------|--------------|----------------|-----------------------|
| 2% | 0.08 | 0.05 | 0.08 | 0.07 | 0.0100 |
| 5% | 0.11 | 0.08 | 0.09 | 0.09 | 0.0088 |
| 10% | 0.2 | 0.19 | 0.19 | 0.19 | 0.0033 |
| 20% | 0.28 | 0.3 | 0.28 | 0.29 | 0.0067 |
| 25% | 0.38 | 0.37 | 0.37 | 0.37 | 0.0033 |

Compound 95

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|-----------------------|--------------|--------------|--------------|----------------|-----------------------|
| 2% | 0.03 | 0.04 | 0.03 | 0.03 | 0.0033 |
| 5% | 0.06 | 0.04 | 0.04 | 0.05 | 0.0067 |
| 10% | 0.12 | 0.11 | 0.14 | 0.12 | 0.0088 |
| 20% | 0.22 | 0.22 | 0.21 | 0.22 | 0.0033 |
| 25% | 0.28 | 0.3 | 0.35 | 0.31 | 0.0208 |

3.2.5 MeOH/DMC R_f Data

Compound 1

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.81 | 0.81 | 0.8 | 0.81 | 0.0033 |
| 5% | 0.82 | 0.82 | 0.81 | 0.82 | 0.0033 |
| 10% | 0.81 | 0.83 | 0.82 | 0.82 | 0.0058 |
| 20% | 0.84 | 0.83 | 0.83 | 0.83 | 0.0033 |
| 25% | 0.86 | 0.85 | 0.83 | 0.85 | 0.0088 |

Compound 2

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0 | 0.01 | 0.01 | 0.01 | 0.0033 |
| 5% | 0.03 | 0.01 | 0.03 | 0.02 | 0.0067 |
| 10% | 0.06 | 0.05 | 0.05 | 0.05 | 0.0033 |
| 20% | 0.3 | 0.25 | 0.26 | 0.27 | 0.0153 |
| 25% | 0.3 | 0.35 | 0.35 | 0.33 | 0.0167 |

Compound 3

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.81 | 0.81 | 0.8 | 0.81 | 0.0033 |
| 5% | 0.81 | 0.83 | 0.82 | 0.82 | 0.0058 |
| 10% | 0.81 | 0.83 | 0.83 | 0.82 | 0.0067 |
| 20% | 0.85 | 0.84 | 0.83 | 0.84 | 0.0058 |
| 25% | 0.86 | 0.85 | 0.83 | 0.85 | 0.0088 |

Compound 4

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.38 | 0.42 | 0.44 | 0.41 | 0.0176 |
| 5% | 0.56 | 0.53 | 0.4 | 0.50 | 0.0491 |
| 10% | 0.53 | 0.51 | 0.58 | 0.54 | 0.0208 |
| 20% | 0.63 | 0.61 | 0.59 | 0.61 | 0.0115 |
| 25% | 0.72 | 0.72 | 0.62 | 0.69 | 0.0333 |

Compound 5

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.34 | 0.37 | 0.47 | 0.39 | 0.0393 |
| 5% | 0.4 | 0.44 | 0.39 | 0.41 | 0.0153 |
| 10% | 0.46 | 0.44 | 0.46 | 0.45 | 0.0067 |
| 20% | 0.5 | 0.53 | 0.55 | 0.53 | 0.0145 |
| 25% | 0.58 | 0.58 | 0.57 | 0.58 | 0.0033 |

Compound 6

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.73 | 0.73 | 0.75 | 0.74 | 0.0067 |
| 5% | 0.72 | 0.78 | 0.76 | 0.75 | 0.0176 |
| 10% | 0.78 | 0.75 | 0.8 | 0.78 | 0.0145 |
| 20% | 0.81 | 0.81 | 0.91 | 0.84 | 0.0333 |
| 25% | 0.86 | 0.83 | 0.91 | 0.87 | 0.0233 |

Compound 7

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.71 | 0.76 | 0.7 | 0.72 | 0.0186 |
| 5% | 0.73 | 0.75 | 0.71 | 0.73 | 0.0115 |
| 10% | 0.73 | 0.76 | 0.75 | 0.75 | 0.0088 |
| 20% | 0.77 | 0.78 | 0.77 | 0.77 | 0.0033 |
| 25% | 0.8 | 0.79 | 0.83 | 0.81 | 0.0120 |

Compound 8

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.6 | 0.63 | 0.67 | 0.63 | 0.0203 |
| 5% | 0.68 | 0.64 | 0.65 | 0.66 | 0.0120 |
| 10% | 0.71 | 0.65 | 0.65 | 0.67 | 0.0200 |
| 20% | 0.68 | 0.7 | 0.7 | 0.69 | 0.0067 |
| 25% | 0.7 | 0.75 | 0.73 | 0.73 | 0.0145 |

Compound 9

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.81 | 0.79 | 0.8 | 0.80 | 0.0058 |
| 5% | 0.83 | 0.81 | 0.8 | 0.81 | 0.0088 |
| 10% | 0.82 | 0.8 | 0.83 | 0.82 | 0.0088 |
| 20% | 0.84 | 0.83 | 0.82 | 0.83 | 0.0058 |
| 25% | 0.86 | 0.85 | 0.83 | 0.85 | 0.0088 |

Compound 10

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.52 | 0.57 | 0.5 | 0.53 | 0.0208 |
| 5% | 0.55 | 0.58 | 0.58 | 0.57 | 0.0100 |
| 10% | 0.65 | 0.64 | 0.68 | 0.66 | 0.0120 |
| 20% | 0.67 | 0.7 | 0.76 | 0.71 | 0.0265 |
| 25% | 0.79 | 0.74 | 0.79 | 0.77 | 0.0167 |

Compound 11

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.06 | 0.08 | 0.1 | 0.08 | 0.0115 |
| 5% | 0.14 | 0.11 | 0.16 | 0.14 | 0.0145 |
| 10% | 0.23 | 0.2 | 0.22 | 0.22 | 0.0088 |
| 20% | 0.28 | 0.26 | 0.28 | 0.27 | 0.0067 |
| 25% | 0.34 | 0.34 | 0.33 | 0.34 | 0.0033 |

Compound 12

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.32 | 0.34 | 0.31 | 0.32 | 0.0088 |
| 5% | 0.34 | 0.38 | 0.34 | 0.35 | 0.0133 |
| 10% | 0.4 | 0.42 | 0.4 | 0.41 | 0.0067 |
| 20% | 0.45 | 0.46 | 0.41 | 0.44 | 0.0153 |
| 25% | 0.45 | 0.51 | 0.45 | 0.47 | 0.0200 |

Compound 13

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.25 | 0.23 | 0.2 | 0.23 | 0.0145 |
| 5% | 0.21 | 0.25 | 0.27 | 0.24 | 0.0176 |
| 10% | 0.36 | 0.24 | 0.3 | 0.30 | 0.0346 |
| 20% | 0.37 | 0.35 | 0.33 | 0.35 | 0.0115 |
| 25% | 0.4 | 0.44 | 0.39 | 0.41 | 0.0153 |

Compound 14

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.09 | 0.08 | 0.09 | 0.09 | 0.0033 |
| 5% | 0.19 | 0.16 | 0.13 | 0.16 | 0.0173 |
| 10% | 0.26 | 0.21 | 0.25 | 0.24 | 0.0153 |
| 20% | 0.38 | 0.28 | 0.27 | 0.31 | 0.0351 |
| 25% | 0.39 | 0.43 | 0.31 | 0.38 | 0.0353 |

Compound 15

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.3 | 0.28 | 0.35 | 0.31 | 0.0208 |
| 5% | 0.42 | 0.39 | 0.4 | 0.40 | 0.0088 |
| 10% | 0.46 | 0.42 | 0.44 | 0.44 | 0.0115 |
| 20% | 0.55 | 0.51 | 0.53 | 0.53 | 0.0115 |
| 25% | 0.66 | 0.64 | 0.57 | 0.62 | 0.0273 |

Compound 16

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.09 | 0.11 | 0.07 | 0.09 | 0.0115 |
| 5% | 0.09 | 0.11 | 0.11 | 0.10 | 0.0067 |
| 10% | 0.12 | 0.14 | 0.11 | 0.12 | 0.0088 |
| 20% | 0.15 | 0.13 | 0.14 | 0.14 | 0.0058 |
| 25% | 0.14 | 0.18 | 0.19 | 0.17 | 0.0153 |

Compound 17

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.14 | 0.12 | 0.13 | 0.13 | 0.0058 |
| 5% | 0.18 | 0.22 | 0.14 | 0.18 | 0.0231 |
| 10% | 0.28 | 0.2 | 0.25 | 0.24 | 0.0233 |
| 20% | 0.29 | 0.29 | 0.28 | 0.29 | 0.0033 |
| 25% | 0.35 | 0.35 | 0.37 | 0.36 | 0.0067 |

Compound 18

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.69 | 0.71 | 0.67 | 0.69 | 0.0115 |
| 5% | 0.65 | 0.73 | 0.74 | 0.71 | 0.0285 |
| 10% | 0.73 | 0.72 | 0.73 | 0.73 | 0.0033 |
| 20% | 0.73 | 0.76 | 0.74 | 0.74 | 0.0088 |
| 25% | 0.79 | 0.8 | 0.73 | 0.77 | 0.0219 |

Compound 19

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.69 | 0.71 | 0.67 | 0.69 | 0.0115 |
| 5% | 0.65 | 0.73 | 0.74 | 0.71 | 0.0285 |
| 10% | 0.73 | 0.72 | 0.73 | 0.73 | 0.0033 |
| 20% | 0.73 | 0.76 | 0.74 | 0.74 | 0.0088 |
| 25% | 0.79 | 0.8 | 0.73 | 0.77 | 0.0219 |

Compound 20

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.69 | 0.71 | 0.67 | 0.69 | 0.0115 |
| 5% | 0.65 | 0.73 | 0.74 | 0.71 | 0.0285 |
| 10% | 0.73 | 0.72 | 0.73 | 0.73 | 0.0033 |
| 20% | 0.73 | 0.76 | 0.74 | 0.74 | 0.0088 |
| 25% | 0.79 | 0.8 | 0.73 | 0.77 | 0.0219 |

Compound 21

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.69 | 0.71 | 0.67 | 0.69 | 0.0115 |
| 5% | 0.65 | 0.73 | 0.74 | 0.71 | 0.0285 |
| 10% | 0.73 | 0.72 | 0.73 | 0.73 | 0.0033 |
| 20% | 0.73 | 0.76 | 0.74 | 0.74 | 0.0088 |
| 25% | 0.79 | 0.8 | 0.73 | 0.77 | 0.0219 |

Compound 22

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.69 | 0.71 | 0.67 | 0.69 | 0.0115 |
| 5% | 0.65 | 0.73 | 0.74 | 0.71 | 0.0285 |
| 10% | 0.73 | 0.72 | 0.73 | 0.73 | 0.0033 |
| 20% | 0.73 | 0.76 | 0.74 | 0.74 | 0.0088 |
| 25% | 0.79 | 0.8 | 0.73 | 0.77 | 0.0219 |

Compound 23

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.69 | 0.71 | 0.67 | 0.69 | 0.0115 |
| 5% | 0.65 | 0.73 | 0.74 | 0.71 | 0.0285 |
| 10% | 0.73 | 0.72 | 0.73 | 0.73 | 0.0033 |
| 20% | 0.73 | 0.76 | 0.74 | 0.74 | 0.0088 |
| 25% | 0.79 | 0.8 | 0.73 | 0.77 | 0.0219 |

Compound 24

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.77 | 0.74 | 0.73 | 0.75 | 0.0120 |
| 5% | 0.75 | 0.77 | 0.76 | 0.76 | 0.0058 |
| 10% | 0.76 | 0.76 | 0.78 | 0.77 | 0.0067 |
| 20% | 0.78 | 0.79 | 0.8 | 0.79 | 0.0058 |
| 25% | 0.82 | 0.79 | 0.8 | 0.80 | 0.0088 |

Compound 25

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.74 | 0.73 | 0.7 | 0.72 | 0.0120 |
| 5% | 0.72 | 0.78 | 0.76 | 0.75 | 0.0176 |
| 10% | 0.79 | 0.73 | 0.8 | 0.77 | 0.0219 |
| 20% | 0.8 | 0.79 | 0.81 | 0.80 | 0.0058 |
| 25% | 0.82 | 0.84 | 0.85 | 0.84 | 0.0088 |

Compound 26

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.81 | 0.82 | 0.84 | 0.82 | 0.0088 |
| 5% | 0.83 | 0.82 | 0.84 | 0.83 | 0.0058 |
| 10% | 0.85 | 0.81 | 0.85 | 0.84 | 0.0133 |
| 20% | 0.86 | 0.89 | 0.84 | 0.86 | 0.0145 |
| 25% | 0.88 | 0.86 | 0.88 | 0.87 | 0.0067 |

Compound 27

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.87 | 0.86 | 0.83 | 0.85 | 0.0120 |
| 5% | 0.89 | 0.85 | 0.87 | 0.87 | 0.0115 |
| 10% | 0.87 | 0.89 | 0.88 | 0.88 | 0.0058 |
| 20% | 0.92 | 0.87 | 0.9 | 0.90 | 0.0145 |
| 25% | 0.9 | 0.95 | 0.92 | 0.92 | 0.0145 |

Compound 28

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.81 | 0.8 | 0.81 | 0.81 | 0.0033 |
| 5% | 0.83 | 0.8 | 0.8 | 0.81 | 0.0100 |
| 10% | 0.78 | 0.86 | 0.81 | 0.82 | 0.0233 |
| 20% | 0.85 | 0.84 | 0.83 | 0.84 | 0.0058 |
| 25% | 0.86 | 0.85 | 0.83 | 0.85 | 0.0088 |

Compound 29

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.71 | 0.75 | 0.73 | 0.73 | 0.0115 |
| 5% | 0.76 | 0.78 | 0.76 | 0.77 | 0.0067 |
| 10% | 0.8 | 0.83 | 0.78 | 0.80 | 0.0145 |
| 20% | 0.86 | 0.85 | 0.82 | 0.84 | 0.0120 |
| 25% | 0.85 | 0.89 | 0.88 | 0.87 | 0.0120 |

Compound 30

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.71 | 0.7 | 0.69 | 0.70 | 0.0058 |
| 5% | 0.72 | 0.71 | 0.74 | 0.72 | 0.0088 |
| 10% | 0.73 | 0.74 | 0.78 | 0.75 | 0.0153 |
| 20% | 0.77 | 0.74 | 0.8 | 0.77 | 0.0173 |
| 25% | 0.8 | 0.83 | 0.79 | 0.81 | 0.0120 |

Compound 31

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.34 | 0.29 | 0.22 | 0.28 | 0.0348 |
| 5% | 0.29 | 0.28 | 0.27 | 0.28 | 0.0058 |
| 10% | 0.36 | 0.32 | 0.3 | 0.33 | 0.0176 |
| 20% | 0.37 | 0.38 | 0.42 | 0.39 | 0.0153 |
| 25% | 0.42 | 0.46 | 0.39 | 0.42 | 0.0203 |

Compound 32

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.23 | 0.25 | 0.2 | 0.23 | 0.0145 |
| 5% | 0.29 | 0.28 | 0.27 | 0.28 | 0.0058 |
| 10% | 0.37 | 0.35 | 0.3 | 0.34 | 0.0208 |
| 20% | 0.45 | 0.48 | 0.43 | 0.45 | 0.0145 |
| 25% | 0.63 | 0.64 | 0.6 | 0.62 | 0.0120 |

Compound 33

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.71 | 0.69 | 0.68 | 0.69 | 0.0088 |
| 5% | 0.74 | 0.73 | 0.7 | 0.72 | 0.0120 |
| 10% | 0.74 | 0.74 | 0.74 | 0.74 | 0.0000 |
| 20% | 0.74 | 0.76 | 0.8 | 0.77 | 0.0176 |
| 25% | 0.8 | 0.77 | 0.82 | 0.80 | 0.0145 |

Compound 34

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.03 | 0.01 | 0.03 | 0.02 | 0.0067 |
| 5% | 0.03 | 0.03 | 0.04 | 0.03 | 0.0033 |
| 10% | 0.03 | 0.05 | 0.03 | 0.04 | 0.0067 |
| 20% | 0.03 | 0.06 | 0.05 | 0.05 | 0.0088 |
| 25% | 0.05 | 0.07 | 0.05 | 0.06 | 0.0067 |

Compound 35

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.76 | 0.71 | 0.73 | 0.73 | 0.0145 |
| 5% | 0.76 | 0.78 | 0.76 | 0.77 | 0.0067 |
| 10% | 0.8 | 0.83 | 0.76 | 0.80 | 0.0203 |
| 20% | 0.86 | 0.85 | 0.82 | 0.84 | 0.0120 |
| 25% | 0.9 | 0.85 | 0.88 | 0.88 | 0.0145 |

Compound 36

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.35 | 0.34 | 0.33 | 0.34 | 0.0058 |
| 5% | 0.44 | 0.45 | 0.32 | 0.40 | 0.0418 |
| 10% | 0.48 | 0.44 | 0.43 | 0.45 | 0.0153 |
| 20% | 0.5 | 0.55 | 0.51 | 0.52 | 0.0153 |
| 25% | 0.6 | 0.6 | 0.55 | 0.58 | 0.0167 |

Compound 37

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.7 | 0.68 | 0.68 | 0.69 | 0.0067 |
| 5% | 0.7 | 0.74 | 0.71 | 0.72 | 0.0120 |
| 10% | 0.73 | 0.76 | 0.75 | 0.75 | 0.0088 |
| 20% | 0.77 | 0.78 | 0.77 | 0.77 | 0.0033 |
| 25% | 0.8 | 0.79 | 0.83 | 0.81 | 0.0120 |

Compound 38

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.75 | 0.71 | 0.73 | 0.73 | 0.0115 |
| 5% | 0.76 | 0.78 | 0.76 | 0.77 | 0.0067 |
| 10% | 0.76 | 0.83 | 0.8 | 0.80 | 0.0203 |
| 20% | 0.86 | 0.85 | 0.82 | 0.84 | 0.0120 |
| 25% | 0.85 | 0.85 | 0.88 | 0.86 | 0.0100 |

Compound 39

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.75 | 0.71 | 0.7 | 0.72 | 0.0153 |
| 5% | 0.73 | 0.78 | 0.76 | 0.76 | 0.0145 |
| 10% | 0.78 | 0.83 | 0.8 | 0.80 | 0.0145 |
| 20% | 0.86 | 0.85 | 0.82 | 0.84 | 0.0120 |
| 25% | 0.85 | 0.87 | 0.88 | 0.87 | 0.0088 |

Compound 40

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.57 | 0.59 | 0.6 | 0.59 | 0.0088 |
| 5% | 0.6 | 0.62 | 0.65 | 0.62 | 0.0145 |
| 10% | 0.62 | 0.71 | 0.64 | 0.66 | 0.0273 |
| 20% | 0.71 | 0.71 | 0.69 | 0.70 | 0.0067 |
| 25% | 0.71 | 0.74 | 0.72 | 0.72 | 0.0088 |

Compound 41

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.55 | 0.55 | 0.53 | 0.54 | 0.0067 |
| 5% | 0.59 | 0.54 | 0.54 | 0.56 | 0.0167 |
| 10% | 0.59 | 0.66 | 0.54 | 0.60 | 0.0348 |
| 20% | 0.66 | 0.6 | 0.66 | 0.64 | 0.0200 |
| 25% | 0.69 | 0.69 | 0.62 | 0.67 | 0.0233 |

Compound 42

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.5 | 0.47 | 0.55 | 0.51 | 0.0233 |
| 5% | 0.56 | 0.5 | 0.53 | 0.53 | 0.0173 |
| 10% | 0.6 | 0.57 | 0.54 | 0.57 | 0.0173 |
| 20% | 0.56 | 0.61 | 0.63 | 0.60 | 0.0208 |
| 25% | 0.66 | 0.64 | 0.6 | 0.63 | 0.0176 |

Compound 43

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.01 | 0.01 | 0.02 | 0.01 | 0.0033 |
| 5% | 0.05 | 0.05 | 0.01 | 0.04 | 0.0133 |
| 10% | 0.08 | 0.06 | 0.06 | 0.07 | 0.0067 |
| 20% | 0.09 | 0.09 | 0.11 | 0.10 | 0.0067 |
| 25% | 0.11 | 0.14 | 0.11 | 0.12 | 0.0100 |

Compound 44

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.78 | 0.76 | 0.75 | 0.76 | 0.0088 |
| 5% | 0.76 | 0.79 | 0.75 | 0.77 | 0.0120 |
| 10% | 0.8 | 0.82 | 0.76 | 0.79 | 0.0176 |
| 20% | 0.82 | 0.8 | 0.83 | 0.82 | 0.0088 |
| 25% | 0.84 | 0.86 | 0.84 | 0.85 | 0.0067 |

Compound 45

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.05 | 0.05 | 0.06 | 0.05 | 0.0033 |
| 5% | 0.09 | 0.08 | 0.09 | 0.09 | 0.0033 |
| 10% | 0.13 | 0.11 | 0.13 | 0.12 | 0.0067 |
| 20% | 0.21 | 0.11 | 0.17 | 0.16 | 0.0291 |
| 25% | 0.18 | 0.19 | 0.2 | 0.19 | 0.0058 |

Compound 46

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.38 | 0.41 | 0.4 | 0.40 | 0.0088 |
| 5% | 0.41 | 0.43 | 0.43 | 0.42 | 0.0067 |
| 10% | 0.47 | 0.51 | 0.48 | 0.49 | 0.0120 |
| 20% | 0.57 | 0.53 | 0.54 | 0.55 | 0.0120 |
| 25% | 0.59 | 0.57 | 0.6 | 0.59 | 0.0088 |

Compound 47

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.3 | 0.26 | 0.31 | 0.29 | 0.0153 |
| 5% | 0.52 | 0.42 | 0.29 | 0.41 | 0.0666 |
| 10% | 0.54 | 0.43 | 0.5 | 0.49 | 0.0321 |
| 20% | 0.59 | 0.57 | 0.6 | 0.59 | 0.0088 |
| 25% | 0.74 | 0.75 | 0.6 | 0.70 | 0.0484 |

Compound 48

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.54 | 0.58 | 0.54 | 0.55 | 0.0133 |
| 5% | 0.59 | 0.59 | 0.57 | 0.58 | 0.0067 |
| 10% | 0.6 | 0.65 | 0.63 | 0.63 | 0.0145 |
| 20% | 0.63 | 0.66 | 0.7 | 0.66 | 0.0203 |
| 25% | 0.66 | 0.69 | 0.7 | 0.68 | 0.0120 |

Compound 49

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.42 | 0.39 | 0.39 | 0.40 | 0.0100 |
| 5% | 0.46 | 0.48 | 0.43 | 0.46 | 0.0145 |
| 10% | 0.53 | 0.52 | 0.46 | 0.50 | 0.0219 |
| 20% | 0.5 | 0.63 | 0.54 | 0.56 | 0.0384 |
| 25% | 0.65 | 0.63 | 0.58 | 0.62 | 0.0208 |

Compound 50

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.4 | 0.41 | 0.39 | 0.40 | 0.0058 |
| 5% | 0.47 | 0.45 | 0.43 | 0.45 | 0.0115 |
| 10% | 0.51 | 0.46 | 0.48 | 0.48 | 0.0145 |
| 20% | 0.53 | 0.57 | 0.58 | 0.56 | 0.0153 |
| 25% | 0.66 | 0.74 | 0.63 | 0.68 | 0.0328 |

Compound 51

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.03 | 0.06 | 0.03 | 0.04 | 0.0100 |
| 5% | 0.06 | 0.03 | 0.06 | 0.05 | 0.0100 |
| 10% | 0.08 | 0.11 | 0.09 | 0.09 | 0.0088 |
| 20% | 0.14 | 0.11 | 0.11 | 0.12 | 0.0100 |
| 25% | 0.14 | 0.17 | 0.13 | 0.15 | 0.0120 |

Compound 52

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.73 | 0.7 | 0.69 | 0.71 | 0.0120 |
| 5% | 0.76 | 0.7 | 0.77 | 0.74 | 0.0219 |
| 10% | 0.76 | 0.78 | 0.74 | 0.76 | 0.0115 |
| 20% | 0.8 | 0.78 | 0.8 | 0.79 | 0.0067 |
| 25% | 0.78 | 0.83 | 0.84 | 0.82 | 0.0186 |

Compound 53

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.26 | 0.24 | 0.29 | 0.26 | 0.0145 |
| 5% | 0.37 | 0.37 | 0.34 | 0.36 | 0.0100 |
| 10% | 0.38 | 0.41 | 0.38 | 0.39 | 0.0100 |
| 20% | 0.53 | 0.5 | 0.53 | 0.52 | 0.0100 |
| 25% | 0.63 | 0.62 | 0.63 | 0.63 | 0.0033 |

Compound 54

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.71 | 0.71 | 0.71 | 0.71 | 0.0000 |
| 5% | 0.78 | 0.73 | 0.75 | 0.75 | 0.0145 |
| 10% | 0.75 | 0.8 | 0.75 | 0.77 | 0.0167 |
| 20% | 0.8 | 0.82 | 0.85 | 0.82 | 0.0145 |
| 25% | 0.85 | 0.8 | 0.87 | 0.84 | 0.0208 |

Compound 55

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.03 | 0.03 | 0.03 | 0.03 | 0.0000 |
| 5% | 0.05 | 0.03 | 0.05 | 0.04 | 0.0067 |
| 10% | 0.05 | 0.05 | 0.06 | 0.05 | 0.0033 |
| 20% | 0.13 | 0.1 | 0.13 | 0.12 | 0.0100 |
| 25% | 0.13 | 0.14 | 0.16 | 0.14 | 0.0088 |

Compound 56

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0 | 0.01 | 0.01 | 0.01 | 0.0033 |
| 5% | 0.03 | 0.03 | 0.03 | 0.03 | 0.0000 |
| 10% | 0.05 | 0.05 | 0.06 | 0.05 | 0.0033 |
| 20% | 0.09 | 0.11 | 0.09 | 0.10 | 0.0067 |
| 25% | 0.14 | 0.17 | 0.13 | 0.15 | 0.0120 |

Compound 57

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.01 | 0.01 | 0.01 | 0.01 | 0.0000 |
| 5% | 0.03 | 0.01 | 0.03 | 0.02 | 0.0067 |
| 10% | 0.08 | 0.11 | 0.08 | 0.09 | 0.0100 |
| 20% | 0.23 | 0.24 | 0.23 | 0.23 | 0.0033 |
| 25% | 0.24 | 0.23 | 0.25 | 0.24 | 0.0058 |

Compound 58

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 5% | 0.03 | 0.01 | 0.03 | 0.02 | 0.0067 |
| 10% | 0.05 | 0.05 | 0.04 | 0.05 | 0.0033 |
| 20% | 0.06 | 0.06 | 0.08 | 0.07 | 0.0067 |
| 25% | 0.08 | 0.1 | 0.11 | 0.10 | 0.0088 |

Compound 59

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.05 | 0.09 | 0.06 | 0.06 | 0.0050 |
| 5% | 0.08 | 0.11 | 0.11 | 0.10 | 0.0100 |
| 10% | 0.14 | 0.17 | 0.2 | 0.17 | 0.0173 |
| 20% | 0.29 | 0.29 | 0.26 | 0.28 | 0.0100 |
| 25% | 0.34 | 0.31 | 0.34 | 0.33 | 0.0100 |

Compound 60

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.5 | 0.47 | 0.5 | 0.49 | 0.0100 |
| 5% | 0.58 | 0.56 | 0.47 | 0.54 | 0.0338 |
| 10% | 0.6 | 0.57 | 0.61 | 0.59 | 0.0120 |
| 20% | 0.63 | 0.68 | 0.66 | 0.66 | 0.0145 |
| 25% | 0.79 | 0.69 | 0.65 | 0.71 | 0.0416 |

Compound 61

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.61 | 0.61 | 0.54 | 0.59 | 0.0233 |
| 5% | 0.63 | 0.62 | 0.61 | 0.62 | 0.0058 |
| 10% | 0.63 | 0.63 | 0.65 | 0.64 | 0.0067 |
| 20% | 0.66 | 0.67 | 0.71 | 0.68 | 0.0153 |
| 25% | 0.69 | 0.7 | 0.77 | 0.72 | 0.0252 |

Compound 62

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.5 | 0.57 | 0.58 | 0.55 | 0.0252 |
| 5% | 0.55 | 0.62 | 0.6 | 0.59 | 0.0208 |
| 10% | 0.63 | 0.62 | 0.57 | 0.61 | 0.0186 |
| 20% | 0.64 | 0.65 | 0.66 | 0.65 | 0.0058 |
| 25% | 0.73 | 0.7 | 0.64 | 0.69 | 0.0265 |

Compound 63

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.26 | 0.23 | 0.22 | 0.24 | 0.0120 |
| 5% | 0.32 | 0.26 | 0.29 | 0.29 | 0.0173 |
| 10% | 0.33 | 0.37 | 0.4 | 0.37 | 0.0203 |
| 20% | 0.43 | 0.45 | 0.4 | 0.43 | 0.0145 |
| 25% | 0.5 | 0.44 | 0.46 | 0.47 | 0.0176 |

Compound 64

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.34 | 0.4 | 0.31 | 0.35 | 0.0265 |
| 5% | 0.39 | 0.42 | 0.4 | 0.40 | 0.0088 |
| 10% | 0.5 | 0.44 | 0.45 | 0.46 | 0.0186 |
| 20% | 0.55 | 0.53 | 0.55 | 0.54 | 0.0067 |
| 25% | 0.6 | 0.63 | 0.62 | 0.62 | 0.0088 |

Compound 65

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.66 | 0.63 | 0.69 | 0.66 | 0.0173 |
| 5% | 0.65 | 0.68 | 0.69 | 0.67 | 0.0120 |
| 10% | 0.67 | 0.7 | 0.71 | 0.69 | 0.0120 |
| 20% | 0.7 | 0.7 | 0.72 | 0.71 | 0.0067 |
| 25% | 0.75 | 0.73 | 0.71 | 0.73 | 0.0115 |

Compound 66

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.6 | 0.58 | 0.55 | 0.58 | 0.0145 |
| 5% | 0.6 | 0.62 | 0.63 | 0.62 | 0.0088 |
| 10% | 0.68 | 0.63 | 0.62 | 0.64 | 0.0186 |
| 20% | 0.69 | 0.68 | 0.68 | 0.68 | 0.0033 |
| 25% | 0.76 | 0.73 | 0.74 | 0.74 | 0.0088 |

Compound 67

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.66 | 0.57 | 0.66 | 0.63 | 0.0300 |
| 5% | 0.68 | 0.62 | 0.66 | 0.65 | 0.0176 |
| 10% | 0.68 | 0.69 | 0.71 | 0.69 | 0.0088 |
| 20% | 0.75 | 0.7 | 0.71 | 0.72 | 0.0153 |
| 25% | 0.74 | 0.76 | 0.75 | 0.75 | 0.0058 |

Compound 68

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.44 | 0.45 | 0.43 | 0.44 | 0.0058 |
| 5% | 0.5 | 0.47 | 0.49 | 0.49 | 0.0088 |
| 10% | 0.5 | 0.53 | 0.54 | 0.52 | 0.0120 |
| 20% | 0.57 | 0.59 | 0.57 | 0.58 | 0.0067 |
| 25% | 0.65 | 0.63 | 0.59 | 0.62 | 0.0176 |

Compound 69

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.75 | 0.74 | 0.71 | 0.73 | 0.0120 |
| 5% | 0.73 | 0.76 | 0.74 | 0.74 | 0.0088 |
| 10% | 0.76 | 0.73 | 0.76 | 0.75 | 0.0100 |
| 20% | 0.78 | 0.76 | 0.78 | 0.77 | 0.0067 |
| 25% | 0.78 | 0.8 | 0.79 | 0.79 | 0.0058 |

Compound 70

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.63 | 0.6 | 0.65 | 0.63 | 0.0145 |
| 5% | 0.65 | 0.62 | 0.64 | 0.64 | 0.0088 |
| 10% | 0.64 | 0.68 | 0.63 | 0.65 | 0.0153 |
| 20% | 0.68 | 0.71 | 0.7 | 0.70 | 0.0088 |
| 25% | 0.7 | 0.7 | 0.75 | 0.72 | 0.0167 |

Compound 71

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.67 | 0.64 | 0.65 | 0.65 | 0.0088 |
| 5% | 0.65 | 0.67 | 0.7 | 0.67 | 0.0145 |
| 10% | 0.69 | 0.71 | 0.74 | 0.71 | 0.0145 |
| 20% | 0.69 | 0.76 | 0.77 | 0.74 | 0.0252 |
| 25% | 0.82 | 0.75 | 0.75 | 0.77 | 0.0233 |

Compound 72

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.81 | 0.83 | 0.8 | 0.81 | 0.0088 |
| 5% | 0.83 | 0.81 | 0.82 | 0.82 | 0.0058 |
| 10% | 0.84 | 0.8 | 0.83 | 0.82 | 0.0120 |
| 20% | 0.84 | 0.83 | 0.83 | 0.83 | 0.0033 |
| 25% | 0.86 | 0.85 | 0.83 | 0.85 | 0.0088 |

Compound 73

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.03 | 0.03 | 0.06 | 0.04 | 0.0100 |
| 5% | 0.07 | 0.08 | 0.06 | 0.07 | 0.0058 |
| 10% | 0.09 | 0.09 | 0.13 | 0.10 | 0.0133 |
| 20% | 0.12 | 0.16 | 0.13 | 0.14 | 0.0120 |
| 25% | 0.17 | 0.17 | 0.2 | 0.18 | 0.0100 |

Compound 74

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.4 | 0.42 | 0.45 | 0.42 | 0.0145 |
| 5% | 0.51 | 0.45 | 0.48 | 0.48 | 0.0173 |
| 10% | 0.53 | 0.5 | 0.52 | 0.52 | 0.0088 |
| 20% | 0.58 | 0.57 | 0.55 | 0.57 | 0.0088 |
| 25% | 0.66 | 0.66 | 0.57 | 0.63 | 0.0300 |

Compound 75

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.46 | 0.47 | 0.5 | 0.48 | 0.0120 |
| 5% | 0.54 | 0.5 | 0.52 | 0.52 | 0.0115 |
| 10% | 0.56 | 0.58 | 0.58 | 0.57 | 0.0067 |
| 20% | 0.65 | 0.66 | 0.6 | 0.64 | 0.0186 |
| 25% | 0.75 | 0.69 | 0.71 | 0.72 | 0.0176 |

Compound 76

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.78 | 0.78 | 0.72 | 0.76 | 0.0200 |
| 5% | 0.8 | 0.75 | 0.8 | 0.78 | 0.0167 |
| 10% | 0.8 | 0.82 | 0.82 | 0.81 | 0.0067 |
| 20% | 0.85 | 0.83 | 0.85 | 0.84 | 0.0067 |
| 25% | 0.83 | 0.85 | 0.89 | 0.86 | 0.0176 |

Compound 77

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.11 | 0.11 | 0.11 | 0.11 | 0.0000 |
| 5% | 0.11 | 0.13 | 0.14 | 0.13 | 0.0088 |
| 10% | 0.18 | 0.24 | 0.26 | 0.23 | 0.0240 |
| 20% | 0.35 | 0.33 | 0.37 | 0.35 | 0.0115 |
| 25% | 0.44 | 0.46 | 0.4 | 0.43 | 0.0176 |

Compound 78

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.03 | 0.01 | 0.03 | 0.02 | 0.0067 |
| 5% | 0.03 | 0.07 | 0.04 | 0.05 | 0.0120 |
| 10% | 0.08 | 0.06 | 0.06 | 0.07 | 0.0067 |
| 20% | 0.1 | 0.08 | 0.09 | 0.09 | 0.0058 |
| 25% | 0.12 | 0.09 | 0.11 | 0.11 | 0.0088 |

Compound 79

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.23 | 0.24 | 0.2 | 0.22 | 0.0120 |
| 5% | 0.35 | 0.3 | 0.28 | 0.31 | 0.0208 |
| 10% | 0.38 | 0.4 | 0.37 | 0.38 | 0.0088 |
| 20% | 0.48 | 0.47 | 0.49 | 0.48 | 0.0058 |
| 25% | 0.58 | 0.58 | 0.57 | 0.58 | 0.0033 |

Compound 80

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.01 | 0.01 | 0.03 | 0.02 | 0.0067 |
| 5% | 0.05 | 0.03 | 0.03 | 0.04 | 0.0067 |
| 10% | 0.05 | 0.06 | 0.05 | 0.05 | 0.0033 |
| 20% | 0.21 | 0.26 | 0.25 | 0.24 | 0.0153 |
| 25% | 0.35 | 0.33 | 0.32 | 0.33 | 0.0088 |

Compound 81

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.83 | 0.78 | 0.8 | 0.80 | 0.0145 |
| 5% | 0.8 | 0.83 | 0.8 | 0.81 | 0.0100 |
| 10% | 0.83 | 0.8 | 0.83 | 0.82 | 0.0100 |
| 20% | 0.84 | 0.84 | 0.85 | 0.84 | 0.0033 |
| 25% | 0.83 | 0.87 | 0.87 | 0.86 | 0.0133 |

Compound 82

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.83 | 0.78 | 0.8 | 0.80 | 0.0145 |
| 5% | 0.8 | 0.83 | 0.8 | 0.81 | 0.0100 |
| 10% | 0.83 | 0.8 | 0.83 | 0.82 | 0.0100 |
| 20% | 0.84 | 0.84 | 0.85 | 0.84 | 0.0033 |
| 25% | 0.83 | 0.87 | 0.87 | 0.86 | 0.0133 |

Compound 83

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.01 | 0.01 | 0.01 | 0.01 | 0.0000 |
| 5% | 0.03 | 0.03 | 0.03 | 0.03 | 0.0000 |
| 10% | 0.04 | 0.05 | 0.05 | 0.05 | 0.0033 |
| 20% | 0.11 | 0.11 | 0.12 | 0.11 | 0.0033 |
| 25% | 0.2 | 0.2 | 0.1 | 0.17 | 0.0333 |

Compound 84

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.06 | 0.05 | 0.03 | 0.05 | 0.0088 |
| 5% | 0.06 | 0.06 | 0.08 | 0.07 | 0.0067 |
| 10% | 0.12 | 0.11 | 0.08 | 0.10 | 0.0120 |
| 20% | 0.29 | 0.24 | 0.25 | 0.26 | 0.0153 |
| 25% | 0.28 | 0.34 | 0.39 | 0.34 | 0.0318 |

Compound 85

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.05 | 0.05 | 0.03 | 0.04 | 0.0067 |
| 5% | 0.13 | 0.13 | 0.11 | 0.12 | 0.0067 |
| 10% | 0.13 | 0.16 | 0.14 | 0.14 | 0.0088 |
| 20% | 0.32 | 0.28 | 0.25 | 0.28 | 0.0203 |
| 25% | 0.49 | 0.4 | 0.42 | 0.44 | 0.0273 |

Compound 86

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.04 | 0.06 | 0.03 | 0.04 | 0.0088 |
| 5% | 0.06 | 0.06 | 0.06 | 0.06 | 0.0000 |
| 10% | 0.09 | 0.05 | 0.08 | 0.07 | 0.0120 |
| 20% | 0.08 | 0.09 | 0.1 | 0.09 | 0.0058 |
| 25% | 0.1 | 0.11 | 0.1 | 0.10 | 0.0033 |

Compound 87

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.23 | 0.24 | 0.23 | 0.23 | 0.0033 |
| 5% | 0.27 | 0.29 | 0.32 | 0.29 | 0.0145 |
| 10% | 0.37 | 0.37 | 0.33 | 0.36 | 0.0133 |
| 20% | 0.48 | 0.5 | 0.48 | 0.49 | 0.0067 |
| 25% | 0.58 | 0.55 | 0.53 | 0.55 | 0.0145 |

Compound 88

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.06 | 0.06 | 0.03 | 0.05 | 0.0100 |
| 5% | 0.09 | 0.09 | 0.06 | 0.08 | 0.0100 |
| 10% | 0.14 | 0.11 | 0.13 | 0.13 | 0.0088 |
| 20% | 0.24 | 0.24 | 0.2 | 0.23 | 0.0133 |
| 25% | 0.28 | 0.26 | 0.32 | 0.29 | 0.0176 |

Compound 89

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.37 | 0.37 | 0.43 | 0.39 | 0.0200 |
| 5% | 0.37 | 0.42 | 0.46 | 0.42 | 0.0260 |
| 10% | 0.5 | 0.5 | 0.45 | 0.48 | 0.0167 |
| 20% | 0.6 | 0.5 | 0.55 | 0.55 | 0.0289 |
| 25% | 0.63 | 0.65 | 0.63 | 0.64 | 0.0067 |

Compound 90

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.8 | 0.77 | 0.77 | 0.78 | 0.0100 |
| 5% | 0.79 | 0.82 | 0.8 | 0.80 | 0.0088 |
| 10% | 0.82 | 0.81 | 0.82 | 0.82 | 0.0033 |
| 20% | 0.86 | 0.82 | 0.84 | 0.84 | 0.0115 |
| 25% | 0.83 | 0.88 | 0.87 | 0.86 | 0.0153 |

Compound 91

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.54 | 0.6 | 0.54 | 0.56 | 0.0200 |
| 5% | 0.58 | 0.58 | 0.6 | 0.59 | 0.0067 |
| 10% | 0.63 | 0.61 | 0.6 | 0.61 | 0.0088 |
| 20% | 0.64 | 0.66 | 0.63 | 0.64 | 0.0088 |
| 25% | 0.63 | 0.67 | 0.71 | 0.67 | 0.0231 |

Compound 92

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.46 | 0.49 | 0.46 | 0.47 | 0.0100 |
| 5% | 0.5 | 0.55 | 0.54 | 0.53 | 0.0153 |
| 10% | 0.57 | 0.54 | 0.53 | 0.55 | 0.0120 |
| 20% | 0.66 | 0.58 | 0.59 | 0.61 | 0.0252 |
| 25% | 0.63 | 0.66 | 0.68 | 0.66 | 0.0145 |

Compound 93

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.03 | 0.01 | 0.03 | 0.02 | 0.0067 |
| 5% | 0.05 | 0.05 | 0.03 | 0.04 | 0.0067 |
| 10% | 0.05 | 0.06 | 0.07 | 0.06 | 0.0058 |
| 20% | 0.08 | 0.1 | 0.1 | 0.09 | 0.0067 |
| 25% | 0.14 | 0.15 | 0.13 | 0.14 | 0.0058 |

Compound 94

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.04 | 0.06 | 0.06 | 0.05 | 0.0067 |
| 5% | 0.07 | 0.08 | 0.06 | 0.07 | 0.0058 |
| 10% | 0.1 | 0.08 | 0.11 | 0.10 | 0.0088 |
| 20% | 0.25 | 0.24 | 0.23 | 0.24 | 0.0058 |
| 25% | 0.36 | 0.31 | 0.37 | 0.35 | 0.0186 |

Compound 95

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.01 | 0.01 | 0.01 | 0.01 | 0.0000 |
| 5% | 0.03 | 0.03 | 0.03 | 0.03 | 0.0000 |
| 10% | 0.05 | 0.05 | 0.06 | 0.05 | 0.0033 |
| 20% | 0.11 | 0.11 | 0.14 | 0.12 | 0.0100 |
| 25% | 0.22 | 0.22 | 0.15 | 0.20 | 0.0233 |

3.2.6 *i*-PrOH/EtOAc R_f Data

Compound 1

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.8 | 0.79 | 0.81 | 0.80 | 0.0058 |
| 5% | 0.81 | 0.78 | 0.82 | 0.80 | 0.0120 |
| 10% | 0.79 | 0.82 | 0.82 | 0.81 | 0.0100 |
| 20% | 0.83 | 0.84 | 0.8 | 0.82 | 0.0120 |
| 25% | 0.85 | 0.83 | 0.8 | 0.83 | 0.0145 |

Compound 2

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.01 | 0.03 | 0.01 | 0.02 | 0.0067 |
| 5% | 0.03 | 0.03 | 0.03 | 0.03 | 0.0000 |
| 10% | 0.03 | 0.06 | 0.05 | 0.05 | 0.0088 |
| 20% | 0.11 | 0.14 | 0.11 | 0.12 | 0.0100 |
| 25% | 0.11 | 0.14 | 0.14 | 0.13 | 0.0100 |

Compound 3

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.71 | 0.75 | 0.79 | 0.75 | 0.0231 |
| 5% | 0.74 | 0.75 | 0.78 | 0.76 | 0.0120 |
| 10% | 0.79 | 0.79 | 0.76 | 0.78 | 0.0100 |
| 20% | 0.82 | 0.8 | 0.83 | 0.82 | 0.0088 |
| 25% | 0.85 | 0.8 | 0.84 | 0.83 | 0.0153 |

Compound 4

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.24 | 0.24 | 0.24 | 0.24 | 0.0000 |
| 5% | 0.38 | 0.35 | 0.34 | 0.36 | 0.0120 |
| 10% | 0.45 | 0.37 | 0.4 | 0.41 | 0.0233 |
| 20% | 0.5 | 0.5 | 0.52 | 0.51 | 0.0067 |
| 25% | 0.63 | 0.59 | 0.57 | 0.60 | 0.0176 |

Compound 5

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.44 | 0.48 | 0.41 | 0.44 | 0.0203 |
| 5% | 0.43 | 0.47 | 0.49 | 0.46 | 0.0176 |
| 10% | 0.5 | 0.58 | 0.5 | 0.53 | 0.0267 |
| 20% | 0.63 | 0.6 | 0.63 | 0.62 | 0.0100 |
| 25% | 0.66 | 0.69 | 0.74 | 0.70 | 0.0233 |

Compound 6

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.75 | 0.72 | 0.78 | 0.75 | 0.0173 |
| 5% | 0.77 | 0.75 | 0.76 | 0.76 | 0.0058 |
| 10% | 0.74 | 0.8 | 0.8 | 0.78 | 0.0200 |
| 20% | 0.8 | 0.82 | 0.81 | 0.81 | 0.0058 |
| 25% | 0.8 | 0.86 | 0.89 | 0.85 | 0.0265 |

Compound 7

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.63 | 0.62 | 0.65 | 0.63 | 0.0088 |
| 5% | 0.65 | 0.62 | 0.7 | 0.66 | 0.0233 |
| 10% | 0.69 | 0.69 | 0.67 | 0.68 | 0.0067 |
| 20% | 0.7 | 0.73 | 0.74 | 0.72 | 0.0120 |
| 25% | 0.79 | 0.77 | 0.77 | 0.78 | 0.0067 |

Compound 8

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.63 | 0.62 | 0.65 | 0.63 | 0.0088 |
| 5% | 0.65 | 0.62 | 0.7 | 0.66 | 0.0233 |
| 10% | 0.69 | 0.65 | 0.7 | 0.68 | 0.0153 |
| 20% | 0.7 | 0.73 | 0.74 | 0.72 | 0.0120 |
| 25% | 0.79 | 0.77 | 0.77 | 0.78 | 0.0067 |

Compound 9

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.76 | 0.79 | 0.81 | 0.79 | 0.0145 |
| 5% | 0.81 | 0.78 | 0.8 | 0.80 | 0.0088 |
| 10% | 0.79 | 0.83 | 0.82 | 0.81 | 0.0120 |
| 20% | 0.83 | 0.82 | 0.85 | 0.83 | 0.0088 |
| 25% | 0.85 | 0.84 | 0.84 | 0.84 | 0.0033 |

Compound 10

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.52 | 0.54 | 0.53 | 0.53 | 0.0058 |
| 5% | 0.56 | 0.56 | 0.53 | 0.55 | 0.0100 |
| 10% | 0.66 | 0.66 | 0.57 | 0.63 | 0.0300 |
| 20% | 0.69 | 0.67 | 0.73 | 0.70 | 0.0176 |
| 25% | 0.81 | 0.77 | 0.77 | 0.78 | 0.0133 |

Compound 11

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.19 | 0.24 | 0.27 | 0.23 | 0.0233 |
| 5% | 0.26 | 0.25 | 0.28 | 0.26 | 0.0088 |
| 10% | 0.3 | 0.28 | 0.3 | 0.29 | 0.0067 |
| 20% | 0.33 | 0.33 | 0.33 | 0.33 | 0.0000 |
| 25% | 0.35 | 0.38 | 0.44 | 0.39 | 0.0265 |

Compound 12

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.27 | 0.28 | 0.26 | 0.27 | 0.0058 |
| 5% | 0.3 | 0.32 | 0.33 | 0.32 | 0.0088 |
| 10% | 0.3 | 0.41 | 0.34 | 0.35 | 0.0321 |
| 20% | 0.43 | 0.43 | 0.32 | 0.39 | 0.0367 |
| 25% | 0.47 | 0.43 | 0.43 | 0.44 | 0.0133 |

Compound 13

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.18 | 0.24 | 0.14 | 0.19 | 0.0291 |
| 5% | 0.24 | 0.18 | 0.25 | 0.22 | 0.0219 |
| 10% | 0.25 | 0.3 | 0.29 | 0.28 | 0.0153 |
| 20% | 0.31 | 0.34 | 0.33 | 0.33 | 0.0088 |
| 25% | 0.4 | 0.33 | 0.35 | 0.36 | 0.0208 |

Compound 14

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.09 | 0.12 | 0.09 | 0.10 | 0.0100 |
| 5% | 0.12 | 0.14 | 0.15 | 0.14 | 0.0088 |
| 10% | 0.12 | 0.23 | 0.18 | 0.18 | 0.0318 |
| 20% | 0.22 | 0.21 | 0.2 | 0.21 | 0.0058 |
| 25% | 0.26 | 0.23 | 0.26 | 0.25 | 0.0100 |

Compound 15

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.38 | 0.34 | 0.29 | 0.34 | 0.0260 |
| 5% | 0.38 | 0.42 | 0.4 | 0.40 | 0.0115 |
| 10% | 0.41 | 0.43 | 0.45 | 0.43 | 0.0115 |
| 20% | 0.5 | 0.48 | 0.48 | 0.49 | 0.0067 |
| 25% | 0.54 | 0.55 | 0.52 | 0.54 | 0.0088 |

Compound 16

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.13 | 0.12 | 0.15 | 0.13 | 0.0088 |
| 5% | 0.13 | 0.17 | 0.18 | 0.16 | 0.0153 |
| 10% | 0.2 | 0.21 | 0.17 | 0.19 | 0.0120 |
| 20% | 0.27 | 0.28 | 0.26 | 0.27 | 0.0058 |
| 25% | 0.35 | 0.3 | 0.33 | 0.33 | 0.0145 |

Compound 17

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.23 | 0.2 | 0.24 | 0.22 | 0.0120 |
| 5% | 0.3 | 0.24 | 0.25 | 0.26 | 0.0186 |
| 10% | 0.28 | 0.3 | 0.3 | 0.29 | 0.0067 |
| 20% | 0.4 | 0.33 | 0.33 | 0.35 | 0.0233 |
| 25% | 0.42 | 0.39 | 0.39 | 0.40 | 0.0100 |

Compound 18

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.61 | 0.6 | 0.63 | 0.61 | 0.0088 |
| 5% | 0.68 | 0.63 | 0.6 | 0.64 | 0.0233 |
| 10% | 0.67 | 0.75 | 0.65 | 0.69 | 0.0306 |
| 20% | 0.75 | 0.72 | 0.72 | 0.73 | 0.0100 |
| 25% | 0.8 | 0.77 | 0.75 | 0.77 | 0.0145 |

Compound 19

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.61 | 0.6 | 0.63 | 0.61 | 0.0088 |
| 5% | 0.68 | 0.63 | 0.6 | 0.64 | 0.0233 |
| 10% | 0.67 | 0.75 | 0.65 | 0.69 | 0.0306 |
| 20% | 0.75 | 0.72 | 0.72 | 0.73 | 0.0100 |
| 25% | 0.8 | 0.77 | 0.75 | 0.77 | 0.0145 |

Compound 20

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.61 | 0.6 | 0.63 | 0.61 | 0.0088 |
| 5% | 0.68 | 0.63 | 0.6 | 0.64 | 0.0233 |
| 10% | 0.67 | 0.75 | 0.65 | 0.69 | 0.0306 |
| 20% | 0.75 | 0.72 | 0.72 | 0.73 | 0.0100 |
| 25% | 0.8 | 0.77 | 0.75 | 0.77 | 0.0145 |

Compound 21

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.61 | 0.6 | 0.63 | 0.61 | 0.0088 |
| 5% | 0.68 | 0.63 | 0.6 | 0.64 | 0.0233 |
| 10% | 0.67 | 0.75 | 0.65 | 0.69 | 0.0306 |
| 20% | 0.75 | 0.72 | 0.72 | 0.73 | 0.0100 |
| 25% | 0.8 | 0.77 | 0.75 | 0.77 | 0.0145 |

Compound 22

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.61 | 0.6 | 0.63 | 0.61 | 0.0088 |
| 5% | 0.68 | 0.63 | 0.6 | 0.64 | 0.0233 |
| 10% | 0.67 | 0.75 | 0.65 | 0.69 | 0.0306 |
| 20% | 0.75 | 0.72 | 0.72 | 0.73 | 0.0100 |
| 25% | 0.8 | 0.77 | 0.75 | 0.77 | 0.0145 |

Compound 23

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.61 | 0.6 | 0.63 | 0.61 | 0.0088 |
| 5% | 0.68 | 0.63 | 0.6 | 0.64 | 0.0233 |
| 10% | 0.67 | 0.75 | 0.65 | 0.69 | 0.0306 |
| 20% | 0.75 | 0.72 | 0.72 | 0.73 | 0.0100 |
| 25% | 0.8 | 0.77 | 0.75 | 0.77 | 0.0145 |

Compound 24

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.75 | 0.72 | 0.77 | 0.75 | 0.0145 |
| 5% | 0.75 | 0.77 | 0.76 | 0.76 | 0.0058 |
| 10% | 0.77 | 0.79 | 0.78 | 0.78 | 0.0058 |
| 20% | 0.8 | 0.82 | 0.83 | 0.82 | 0.0088 |
| 25% | 0.83 | 0.85 | 0.86 | 0.85 | 0.0088 |

Compound 25

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.7 | 0.73 | 0.68 | 0.70 | 0.0145 |
| 5% | 0.75 | 0.7 | 0.73 | 0.73 | 0.0145 |
| 10% | 0.76 | 0.78 | 0.72 | 0.75 | 0.0176 |
| 20% | 0.8 | 0.78 | 0.78 | 0.79 | 0.0067 |
| 25% | 0.85 | 0.83 | 0.84 | 0.84 | 0.0058 |

Compound 26

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.83 | 0.78 | 0.8 | 0.80 | 0.0145 |
| 5% | 0.84 | 0.8 | 0.79 | 0.81 | 0.0153 |
| 10% | 0.85 | 0.8 | 0.86 | 0.84 | 0.0186 |
| 20% | 0.84 | 0.88 | 0.86 | 0.86 | 0.0115 |
| 25% | 0.86 | 0.88 | 0.9 | 0.88 | 0.0115 |

Compound 27

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.77 | 0.77 | 0.78 | 0.77 | 0.0033 |
| 5% | 0.79 | 0.83 | 0.75 | 0.79 | 0.0231 |
| 10% | 0.81 | 0.83 | 0.8 | 0.81 | 0.0088 |
| 20% | 0.88 | 0.81 | 0.85 | 0.85 | 0.0203 |
| 25% | 0.89 | 0.84 | 0.9 | 0.88 | 0.0186 |

Compound 28

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.71 | 0.75 | 0.79 | 0.75 | 0.0231 |
| 5% | 0.74 | 0.75 | 0.78 | 0.76 | 0.0120 |
| 10% | 0.79 | 0.79 | 0.76 | 0.78 | 0.0100 |
| 20% | 0.8 | 0.83 | 0.81 | 0.81 | 0.0088 |
| 25% | 0.83 | 0.84 | 0.8 | 0.82 | 0.0120 |

Compound 29

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.65 | 0.63 | 0.67 | 0.65 | 0.0115 |
| 5% | 0.68 | 0.7 | 0.67 | 0.68 | 0.0088 |
| 10% | 0.72 | 0.73 | 0.74 | 0.73 | 0.0058 |
| 20% | 0.77 | 0.74 | 0.77 | 0.76 | 0.0100 |
| 25% | 0.77 | 0.81 | 0.84 | 0.81 | 0.0203 |

Compound 30

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.62 | 0.64 | 0.64 | 0.63 | 0.0067 |
| 5% | 0.67 | 0.65 | 0.7 | 0.67 | 0.0145 |
| 10% | 0.7 | 0.67 | 0.69 | 0.69 | 0.0088 |
| 20% | 0.79 | 0.72 | 0.74 | 0.75 | 0.0208 |
| 25% | 0.79 | 0.76 | 0.82 | 0.79 | 0.0173 |

Compound 31

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.21 | 0.28 | 0.21 | 0.23 | 0.0233 |
| 5% | 0.25 | 0.24 | 0.3 | 0.26 | 0.0186 |
| 10% | 0.31 | 0.29 | 0.26 | 0.29 | 0.0145 |
| 20% | 0.31 | 0.38 | 0.37 | 0.35 | 0.0219 |
| 25% | 0.4 | 0.39 | 0.39 | 0.39 | 0.0033 |

Compound 32

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.44 | 0.48 | 0.44 | 0.45 | 0.0133 |
| 5% | 0.53 | 0.49 | 0.5 | 0.51 | 0.0120 |
| 10% | 0.53 | 0.53 | 0.56 | 0.54 | 0.0100 |
| 20% | 0.6 | 0.58 | 0.59 | 0.59 | 0.0058 |
| 25% | 0.67 | 0.67 | 0.63 | 0.66 | 0.0133 |

Compound 33

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.58 | 0.61 | 0.64 | 0.61 | 0.0173 |
| 5% | 0.61 | 0.64 | 0.67 | 0.64 | 0.0173 |
| 10% | 0.77 | 0.67 | 0.65 | 0.70 | 0.0371 |
| 20% | 0.81 | 0.75 | 0.71 | 0.76 | 0.0291 |
| 25% | 0.84 | 0.82 | 0.83 | 0.83 | 0.0058 |

Compound 34

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.03 | 0.01 | 0.01 | 0.02 | 0.0067 |
| 5% | 0.05 | 0.02 | 0.03 | 0.03 | 0.0088 |
| 10% | 0.06 | 0.03 | 0.04 | 0.04 | 0.0088 |
| 20% | 0.07 | 0.07 | 0.07 | 0.07 | 0.0000 |
| 25% | 0.06 | 0.09 | 0.09 | 0.08 | 0.0100 |

Compound 35

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.67 | 0.63 | 0.67 | 0.66 | 0.0133 |
| 5% | 0.69 | 0.7 | 0.67 | 0.69 | 0.0088 |
| 10% | 0.72 | 0.73 | 0.74 | 0.73 | 0.0058 |
| 20% | 0.77 | 0.73 | 0.77 | 0.76 | 0.0133 |
| 25% | 0.77 | 0.81 | 0.84 | 0.81 | 0.0203 |

Compound 36

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.35 | 0.3 | 0.32 | 0.32 | 0.0145 |
| 5% | 0.36 | 0.41 | 0.38 | 0.38 | 0.0145 |
| 10% | 0.42 | 0.44 | 0.45 | 0.44 | 0.0088 |
| 20% | 0.49 | 0.49 | 0.53 | 0.50 | 0.0133 |
| 25% | 0.56 | 0.57 | 0.57 | 0.57 | 0.0033 |

Compound 37

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.63 | 0.62 | 0.65 | 0.63 | 0.0088 |
| 5% | 0.65 | 0.62 | 0.7 | 0.66 | 0.0233 |
| 10% | 0.69 | 0.69 | 0.67 | 0.68 | 0.0067 |
| 20% | 0.7 | 0.73 | 0.74 | 0.72 | 0.0120 |
| 25% | 0.79 | 0.77 | 0.77 | 0.78 | 0.0067 |

Compound 38

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.65 | 0.63 | 0.67 | 0.65 | 0.0115 |
| 5% | 0.69 | 0.7 | 0.67 | 0.69 | 0.0088 |
| 10% | 0.72 | 0.73 | 0.75 | 0.73 | 0.0088 |
| 20% | 0.77 | 0.75 | 0.77 | 0.76 | 0.0067 |
| 25% | 0.77 | 0.81 | 0.84 | 0.81 | 0.0203 |

Compound 39

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.65 | 0.63 | 0.67 | 0.65 | 0.0115 |
| 5% | 0.68 | 0.7 | 0.67 | 0.68 | 0.0088 |
| 10% | 0.72 | 0.73 | 0.72 | 0.72 | 0.0033 |
| 20% | 0.77 | 0.73 | 0.77 | 0.76 | 0.0133 |
| 25% | 0.77 | 0.81 | 0.84 | 0.81 | 0.0203 |

Compound 40

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.5 | 0.51 | 0.54 | 0.52 | 0.0120 |
| 5% | 0.57 | 0.58 | 0.53 | 0.56 | 0.0153 |
| 10% | 0.58 | 0.6 | 0.62 | 0.60 | 0.0115 |
| 20% | 0.68 | 0.63 | 0.63 | 0.65 | 0.0167 |
| 25% | 0.68 | 0.74 | 0.71 | 0.71 | 0.0173 |

Compound 41

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.5 | 0.54 | 0.54 | 0.53 | 0.0133 |
| 5% | 0.55 | 0.58 | 0.55 | 0.56 | 0.0100 |
| 10% | 0.59 | 0.63 | 0.6 | 0.61 | 0.0120 |
| 20% | 0.68 | 0.63 | 0.62 | 0.64 | 0.0186 |
| 25% | 0.68 | 0.72 | 0.72 | 0.71 | 0.0133 |

Compound 42

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.45 | 0.44 | 0.4 | 0.43 | 0.0153 |
| 5% | 0.4 | 0.48 | 0.44 | 0.44 | 0.0231 |
| 10% | 0.53 | 0.47 | 0.47 | 0.49 | 0.0200 |
| 20% | 0.52 | 0.49 | 0.56 | 0.52 | 0.0203 |
| 25% | 0.57 | 0.57 | 0.6 | 0.58 | 0.0100 |

Compound 43

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 5% | 0.01 | 0.01 | 0.01 | 0.01 | 0.0000 |
| 10% | 0.03 | 0.03 | 0.09 | 0.05 | 0.0200 |
| 20% | 0.1 | 0.12 | 0.12 | 0.11 | 0.0067 |
| 25% | 0.14 | 0.13 | 0.2 | 0.16 | 0.0219 |

Compound 44

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.67 | 0.65 | 0.7 | 0.67 | 0.0145 |
| 5% | 0.73 | 0.68 | 0.65 | 0.69 | 0.0233 |
| 10% | 0.72 | 0.7 | 0.72 | 0.71 | 0.0067 |
| 20% | 0.8 | 0.75 | 0.77 | 0.77 | 0.0145 |
| 25% | 0.82 | 0.83 | 0.8 | 0.82 | 0.0088 |

Compound 45

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.06 | 0.05 | 0.05 | 0.05 | 0.0033 |
| 5% | 0.09 | 0.09 | 0.09 | 0.09 | 0.0000 |
| 10% | 0.09 | 0.12 | 0.11 | 0.11 | 0.0088 |
| 20% | 0.13 | 0.17 | 0.17 | 0.16 | 0.0133 |
| 25% | 0.14 | 0.27 | 0.2 | 0.20 | 0.0376 |

Compound 46

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.34 | 0.29 | 0.35 | 0.33 | 0.0186 |
| 5% | 0.4 | 0.39 | 0.41 | 0.40 | 0.0058 |
| 10% | 0.42 | 0.47 | 0.47 | 0.45 | 0.0167 |
| 20% | 0.53 | 0.55 | 0.57 | 0.55 | 0.0115 |
| 25% | 0.58 | 0.56 | 0.63 | 0.59 | 0.0208 |

Compound 47

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.18 | 0.19 | 0.2 | 0.19 | 0.0058 |
| 5% | 0.36 | 0.3 | 0.32 | 0.33 | 0.0176 |
| 10% | 0.35 | 0.37 | 0.39 | 0.37 | 0.0115 |
| 20% | 0.47 | 0.52 | 0.53 | 0.51 | 0.0186 |
| 25% | 0.53 | 0.59 | 0.66 | 0.59 | 0.0376 |

Compound 48

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.5 | 0.48 | 0.5 | 0.49 | 0.0067 |
| 5% | 0.55 | 0.6 | 0.55 | 0.57 | 0.0167 |
| 10% | 0.61 | 0.6 | 0.56 | 0.59 | 0.0153 |
| 20% | 0.67 | 0.64 | 0.66 | 0.66 | 0.0088 |
| 25% | 0.71 | 0.71 | 0.71 | 0.71 | 0.0000 |

Compound 49

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.33 | 0.38 | 0.33 | 0.35 | 0.0167 |
| 5% | 0.41 | 0.41 | 0.41 | 0.41 | 0.0000 |
| 10% | 0.4 | 0.41 | 0.47 | 0.43 | 0.0219 |
| 20% | 0.51 | 0.5 | 0.53 | 0.51 | 0.0088 |
| 25% | 0.57 | 0.6 | 0.57 | 0.58 | 0.0100 |

Compound 50

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.33 | 0.36 | 0.34 | 0.34 | 0.0088 |
| 5% | 0.41 | 0.38 | 0.4 | 0.40 | 0.0088 |
| 10% | 0.42 | 0.44 | 0.46 | 0.44 | 0.0115 |
| 20% | 0.5 | 0.49 | 0.52 | 0.50 | 0.0088 |
| 25% | 0.6 | 0.6 | 0.58 | 0.59 | 0.0067 |

Compound 51

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 5% | 0.03 | 0.01 | 0.03 | 0.02 | 0.0067 |
| 10% | 0.02 | 0.03 | 0.06 | 0.04 | 0.0120 |
| 20% | 0.1 | 0.06 | 0.06 | 0.07 | 0.0133 |
| 25% | 0.06 | 0.09 | 0.12 | 0.09 | 0.0173 |

Compound 52

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.63 | 0.6 | 0.68 | 0.64 | 0.0233 |
| 5% | 0.64 | 0.63 | 0.68 | 0.65 | 0.0153 |
| 10% | 0.65 | 0.7 | 0.7 | 0.68 | 0.0167 |
| 20% | 0.78 | 0.73 | 0.72 | 0.74 | 0.0186 |
| 25% | 0.78 | 0.78 | 0.77 | 0.78 | 0.0033 |

Compound 53

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.21 | 0.2 | 0.19 | 0.20 | 0.0058 |
| 5% | 0.24 | 0.27 | 0.27 | 0.26 | 0.0100 |
| 10% | 0.3 | 0.25 | 0.27 | 0.27 | 0.0145 |
| 20% | 0.38 | 0.4 | 0.4 | 0.39 | 0.0067 |
| 25% | 0.5 | 0.48 | 0.47 | 0.48 | 0.0088 |

Compound 54

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.66 | 0.63 | 0.63 | 0.64 | 0.0100 |
| 5% | 0.64 | 0.7 | 0.66 | 0.67 | 0.0176 |
| 10% | 0.72 | 0.73 | 0.72 | 0.72 | 0.0033 |
| 20% | 0.77 | 0.79 | 0.76 | 0.77 | 0.0088 |
| 25% | 0.78 | 0.83 | 0.77 | 0.79 | 0.0186 |

Compound 55

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.1 | 0.1 | 0.11 | 0.10 | 0.0033 |
| 5% | 0.12 | 0.1 | 0.12 | 0.11 | 0.0067 |
| 10% | 0.13 | 0.1 | 0.13 | 0.12 | 0.0100 |
| 20% | 0.15 | 0.13 | 0.13 | 0.14 | 0.0067 |
| 25% | 0.15 | 0.13 | 0.16 | 0.15 | 0.0088 |

Compound 56

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 5% | 0.01 | 0.03 | 0.01 | 0.02 | 0.0067 |
| 10% | 0.03 | 0.03 | 0.03 | 0.03 | 0.0000 |
| 20% | 0.13 | 0.13 | 0.12 | 0.13 | 0.0033 |
| 25% | 0.18 | 0.2 | 0.16 | 0.18 | 0.0115 |

Compound 57

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.01 | 0.03 | 0.01 | 0.02 | 0.0067 |
| 5% | 0.03 | 0.05 | 0.03 | 0.04 | 0.0067 |
| 10% | 0.06 | 0.06 | 0.03 | 0.05 | 0.0100 |
| 20% | 0.09 | 0.12 | 0.05 | 0.09 | 0.0203 |
| 25% | 0.12 | 0.11 | 0.09 | 0.11 | 0.0088 |

Compound 58

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 5% | 0.03 | 0.01 | 0.03 | 0.02 | 0.0067 |
| 10% | 0.03 | 0.03 | 0.04 | 0.03 | 0.0033 |
| 20% | 0.06 | 0.06 | 0.06 | 0.06 | 0.0000 |
| 25% | 0.06 | 0.1 | 0.1 | 0.09 | 0.0133 |

Compound 59

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.03 | 0.01 | 0.03 | 0.02 | 0.0067 |
| 5% | 0.06 | 0.05 | 0.06 | 0.06 | 0.0033 |
| 10% | 0.1 | 0.07 | 0.09 | 0.09 | 0.0088 |
| 20% | 0.16 | 0.16 | 0.14 | 0.15 | 0.0067 |
| 25% | 0.21 | 0.18 | 0.17 | 0.19 | 0.0120 |

Compound 60

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.28 | 0.28 | 0.27 | 0.28 | 0.0033 |
| 5% | 0.37 | 0.34 | 0.34 | 0.35 | 0.0100 |
| 10% | 0.39 | 0.4 | 0.44 | 0.41 | 0.0153 |
| 20% | 0.51 | 0.53 | 0.5 | 0.51 | 0.0088 |
| 25% | 0.54 | 0.6 | 0.6 | 0.58 | 0.0200 |

Compound 61

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.53 | 0.6 | 0.51 | 0.55 | 0.0273 |
| 5% | 0.53 | 0.6 | 0.58 | 0.57 | 0.0208 |
| 10% | 0.6 | 0.58 | 0.61 | 0.60 | 0.0088 |
| 20% | 0.63 | 0.63 | 0.63 | 0.63 | 0.0000 |
| 25% | 0.67 | 0.66 | 0.7 | 0.68 | 0.0120 |

Compound 62

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.45 | 0.48 | 0.5 | 0.48 | 0.0145 |
| 5% | 0.48 | 0.52 | 0.49 | 0.50 | 0.0120 |
| 10% | 0.54 | 0.55 | 0.47 | 0.52 | 0.0252 |
| 20% | 0.55 | 0.58 | 0.55 | 0.56 | 0.0100 |
| 25% | 0.57 | 0.63 | 0.67 | 0.62 | 0.0291 |

Compound 63

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.21 | 0.21 | 0.24 | 0.22 | 0.0100 |
| 5% | 0.21 | 0.3 | 0.25 | 0.25 | 0.0260 |
| 10% | 0.3 | 0.27 | 0.28 | 0.28 | 0.0088 |
| 20% | 0.32 | 0.3 | 0.35 | 0.32 | 0.0145 |
| 25% | 0.39 | 0.4 | 0.39 | 0.39 | 0.0033 |

Compound 64

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.28 | 0.28 | 0.27 | 0.28 | 0.0033 |
| 5% | 0.34 | 0.34 | 0.3 | 0.33 | 0.0133 |
| 10% | 0.43 | 0.42 | 0.43 | 0.43 | 0.0033 |
| 20% | 0.53 | 0.6 | 0.53 | 0.55 | 0.0233 |
| 25% | 0.62 | 0.6 | 0.6 | 0.61 | 0.0067 |

Compound 65

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.5 | 0.51 | 0.53 | 0.51 | 0.0088 |
| 5% | 0.58 | 0.56 | 0.55 | 0.56 | 0.0088 |
| 10% | 0.59 | 0.6 | 0.58 | 0.59 | 0.0058 |
| 20% | 0.68 | 0.65 | 0.63 | 0.65 | 0.0145 |
| 25% | 0.77 | 0.69 | 0.74 | 0.73 | 0.0233 |

Compound 66

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.62 | 0.6 | 0.64 | 0.62 | 0.0115 |
| 5% | 0.66 | 0.64 | 0.7 | 0.67 | 0.0176 |
| 10% | 0.69 | 0.69 | 0.7 | 0.69 | 0.0033 |
| 20% | 0.72 | 0.76 | 0.71 | 0.73 | 0.0153 |
| 25% | 0.82 | 0.79 | 0.75 | 0.79 | 0.0203 |

Compound 67

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.64 | 0.61 | 0.67 | 0.64 | 0.0173 |
| 5% | 0.65 | 0.67 | 0.69 | 0.67 | 0.0115 |
| 10% | 0.7 | 0.72 | 0.71 | 0.71 | 0.0058 |
| 20% | 0.75 | 0.78 | 0.76 | 0.76 | 0.0088 |
| 25% | 0.79 | 0.85 | 0.86 | 0.83 | 0.0219 |

Compound 68

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.37 | 0.4 | 0.43 | 0.40 | 0.0173 |
| 5% | 0.43 | 0.44 | 0.44 | 0.44 | 0.0033 |
| 10% | 0.46 | 0.5 | 0.5 | 0.49 | 0.0133 |
| 20% | 0.55 | 0.61 | 0.57 | 0.58 | 0.0176 |
| 25% | 0.61 | 0.63 | 0.63 | 0.62 | 0.0067 |

Compound 69

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.63 | 0.67 | 0.65 | 0.65 | 0.0115 |
| 5% | 0.68 | 0.67 | 0.65 | 0.67 | 0.0088 |
| 10% | 0.71 | 0.7 | 0.7 | 0.70 | 0.0033 |
| 20% | 0.73 | 0.79 | 0.73 | 0.75 | 0.0200 |
| 25% | 0.8 | 0.8 | 0.76 | 0.79 | 0.0133 |

Compound 70

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.47 | 0.5 | 0.52 | 0.50 | 0.0145 |
| 5% | 0.53 | 0.52 | 0.6 | 0.55 | 0.0252 |
| 10% | 0.6 | 0.63 | 0.58 | 0.60 | 0.0145 |
| 20% | 0.64 | 0.7 | 0.64 | 0.66 | 0.0200 |
| 25% | 0.67 | 0.7 | 0.71 | 0.69 | 0.0120 |

Compound 71

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.59 | 0.63 | 0.65 | 0.62 | 0.0176 |
| 5% | 0.63 | 0.66 | 0.64 | 0.64 | 0.0088 |
| 10% | 0.67 | 0.66 | 0.67 | 0.67 | 0.0033 |
| 20% | 0.69 | 0.75 | 0.73 | 0.72 | 0.0176 |
| 25% | 0.77 | 0.77 | 0.8 | 0.78 | 0.0100 |

Compound 72

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.76 | 0.79 | 0.81 | 0.79 | 0.0145 |
| 5% | 0.81 | 0.78 | 0.8 | 0.80 | 0.0088 |
| 10% | 0.79 | 0.83 | 0.82 | 0.81 | 0.0120 |
| 20% | 0.83 | 0.83 | 0.84 | 0.83 | 0.0033 |
| 25% | 0.85 | 0.84 | 0.84 | 0.84 | 0.0033 |

Compound 73

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.03 | 0.05 | 0.06 | 0.05 | 0.0088 |
| 5% | 0.05 | 0.06 | 0.06 | 0.06 | 0.0033 |
| 10% | 0.06 | 0.06 | 0.08 | 0.07 | 0.0067 |
| 20% | 0.08 | 0.07 | 0.09 | 0.08 | 0.0058 |
| 25% | 0.1 | 0.09 | 0.09 | 0.09 | 0.0033 |

Compound 74

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.33 | 0.34 | 0.38 | 0.35 | 0.0153 |
| 5% | 0.42 | 0.4 | 0.35 | 0.39 | 0.0208 |
| 10% | 0.42 | 0.45 | 0.38 | 0.42 | 0.0203 |
| 20% | 0.5 | 0.45 | 0.48 | 0.48 | 0.0145 |
| 25% | 0.53 | 0.51 | 0.55 | 0.53 | 0.0115 |

Compound 75

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.31 | 0.3 | 0.36 | 0.32 | 0.0186 |
| 5% | 0.4 | 0.42 | 0.43 | 0.42 | 0.0088 |
| 10% | 0.43 | 0.44 | 0.45 | 0.44 | 0.0058 |
| 20% | 0.5 | 0.53 | 0.55 | 0.53 | 0.0145 |
| 25% | 0.61 | 0.59 | 0.63 | 0.61 | 0.0115 |

Compound 76

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.74 | 0.73 | 0.72 | 0.73 | 0.0058 |
| 5% | 0.79 | 0.73 | 0.75 | 0.76 | 0.0176 |
| 10% | 0.77 | 0.75 | 0.78 | 0.77 | 0.0088 |
| 20% | 0.77 | 0.81 | 0.81 | 0.80 | 0.0133 |
| 25% | 0.82 | 0.83 | 0.83 | 0.83 | 0.0033 |

Compound 77

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.12 | 0.12 | 0.13 | 0.12 | 0.0033 |
| 5% | 0.12 | 0.13 | 0.13 | 0.13 | 0.0033 |
| 10% | 0.12 | 0.18 | 0.12 | 0.14 | 0.0200 |
| 20% | 0.17 | 0.16 | 0.17 | 0.17 | 0.0033 |
| 25% | 0.17 | 0.2 | 0.22 | 0.20 | 0.0145 |

Compound 78

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.01 | 0.03 | 0.01 | 0.02 | 0.0067 |
| 5% | 0.03 | 0.06 | 0.03 | 0.04 | 0.0100 |
| 10% | 0.05 | 0.06 | 0.03 | 0.05 | 0.0088 |
| 20% | 0.08 | 0.07 | 0.08 | 0.08 | 0.0033 |
| 25% | 0.1 | 0.08 | 0.09 | 0.09 | 0.0058 |

Compound 79

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.2 | 0.16 | 0.17 | 0.18 | 0.0120 |
| 5% | 0.27 | 0.23 | 0.23 | 0.24 | 0.0133 |
| 10% | 0.3 | 0.33 | 0.27 | 0.30 | 0.0173 |
| 20% | 0.43 | 0.47 | 0.47 | 0.46 | 0.0133 |
| 25% | 0.49 | 0.54 | 0.49 | 0.51 | 0.0167 |

Compound 80

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0 | 0.01 | 0.01 | 0.01 | 0.0033 |
| 5% | 0.03 | 0.03 | 0.01 | 0.02 | 0.0067 |
| 10% | 0.06 | 0.06 | 0.06 | 0.06 | 0.0000 |
| 20% | 0.08 | 0.15 | 0.2 | 0.14 | 0.0348 |
| 25% | 0.23 | 0.22 | 0.26 | 0.24 | 0.0120 |

Compound 81

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.76 | 0.72 | 0.72 | 0.73 | 0.0133 |
| 5% | 0.76 | 0.73 | 0.77 | 0.75 | 0.0120 |
| 10% | 0.77 | 0.84 | 0.73 | 0.78 | 0.0321 |
| 20% | 0.79 | 0.86 | 0.82 | 0.82 | 0.0203 |
| 25% | 0.83 | 0.87 | 0.83 | 0.84 | 0.0133 |

Compound 82

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.3 | 0.32 | 0.31 | 0.31 | 0.0058 |
| 5% | 0.39 | 0.39 | 0.33 | 0.37 | 0.0200 |
| 10% | 0.4 | 0.43 | 0.4 | 0.41 | 0.0100 |
| 20% | 0.55 | 0.58 | 0.52 | 0.55 | 0.0173 |
| 25% | 0.6 | 0.6 | 0.6 | 0.60 | 0.0000 |

Compound 83

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 5% | 0.01 | 0.01 | 0.01 | 0.01 | 0.0000 |
| 10% | 0.03 | 0.01 | 0.02 | 0.02 | 0.0058 |
| 20% | 0.06 | 0.05 | 0.06 | 0.06 | 0.0033 |
| 25% | 0.06 | 0.08 | 0.12 | 0.09 | 0.0176 |

Compound 84

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.06 | 0.03 | 0.02 | 0.04 | 0.0120 |
| 5% | 0.06 | 0.09 | 0.07 | 0.07 | 0.0088 |
| 10% | 0.11 | 0.09 | 0.09 | 0.10 | 0.0067 |
| 20% | 0.24 | 0.21 | 0.25 | 0.23 | 0.0120 |
| 25% | 0.33 | 0.3 | 0.24 | 0.29 | 0.0265 |

Compound 85

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.07 | 0.07 | 0.08 | 0.07 | 0.0033 |
| 5% | 0.09 | 0.07 | 0.1 | 0.09 | 0.0088 |
| 10% | 0.13 | 0.15 | 0.13 | 0.14 | 0.0067 |
| 20% | 0.23 | 0.18 | 0.2 | 0.20 | 0.0145 |
| 25% | 0.26 | 0.27 | 0.27 | 0.27 | 0.0033 |

Compound 86

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.05 | 0.07 | 0.1 | 0.07 | 0.0145 |
| 5% | 0.09 | 0.06 | 0.1 | 0.08 | 0.0120 |
| 10% | 0.13 | 0.1 | 0.13 | 0.12 | 0.0100 |
| 20% | 0.13 | 0.16 | 0.14 | 0.14 | 0.0088 |
| 25% | 0.17 | 0.17 | 0.17 | 0.17 | 0.0000 |

Compound 87

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.23 | 0.23 | 0.21 | 0.22 | 0.0067 |
| 5% | 0.28 | 0.27 | 0.31 | 0.29 | 0.0120 |
| 10% | 0.3 | 0.35 | 0.33 | 0.33 | 0.0145 |
| 20% | 0.48 | 0.42 | 0.4 | 0.43 | 0.0240 |
| 25% | 0.46 | 0.5 | 0.5 | 0.49 | 0.0133 |

Compound 88

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.01 | 0.03 | 0.01 | 0.02 | 0.0067 |
| 5% | 0.13 | 0.06 | 0.07 | 0.09 | 0.0219 |
| 10% | 0.19 | 0.16 | 0.12 | 0.16 | 0.0203 |
| 20% | 0.24 | 0.21 | 0.24 | 0.23 | 0.0100 |
| 25% | 0.27 | 0.3 | 0.31 | 0.29 | 0.0120 |

Compound 89

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.27 | 0.27 | 0.34 | 0.29 | 0.0233 |
| 5% | 0.33 | 0.33 | 0.37 | 0.34 | 0.0133 |
| 10% | 0.4 | 0.38 | 0.37 | 0.38 | 0.0088 |
| 20% | 0.58 | 0.49 | 0.53 | 0.53 | 0.0260 |
| 25% | 0.6 | 0.59 | 0.6 | 0.60 | 0.0033 |

Compound 90

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.73 | 0.75 | 0.72 | 0.73 | 0.0088 |
| 5% | 0.75 | 0.73 | 0.76 | 0.75 | 0.0088 |
| 10% | 0.8 | 0.8 | 0.73 | 0.78 | 0.0233 |
| 20% | 0.83 | 0.81 | 0.82 | 0.82 | 0.0058 |
| 25% | 0.83 | 0.85 | 0.86 | 0.85 | 0.0088 |

Compound 91

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.54 | 0.52 | 0.56 | 0.54 | 0.0115 |
| 5% | 0.6 | 0.58 | 0.6 | 0.59 | 0.0067 |
| 10% | 0.61 | 0.63 | 0.71 | 0.65 | 0.0306 |
| 20% | 0.69 | 0.74 | 0.67 | 0.70 | 0.0208 |
| 25% | 0.77 | 0.77 | 0.7 | 0.75 | 0.0233 |

Compound 92

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.32 | 0.33 | 0.28 | 0.31 | 0.0153 |
| 5% | 0.41 | 0.38 | 0.33 | 0.37 | 0.0233 |
| 10% | 0.47 | 0.43 | 0.4 | 0.43 | 0.0203 |
| 20% | 0.55 | 0.58 | 0.53 | 0.55 | 0.0145 |
| 25% | 0.63 | 0.6 | 0.6 | 0.61 | 0.0100 |

Compound 93

| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.03 | 0.03 | 0.03 | 0.03 | 0.0000 |
| 5% | 0.03 | 0.05 | 0.05 | 0.04 | 0.0067 |
| 10% | 0.06 | 0.08 | 0.06 | 0.07 | 0.0067 |
| 20% | 0.08 | 0.1 | 0.12 | 0.10 | 0.0115 |
| 25% | 0.16 | 0.13 | 0.13 | 0.14 | 0.0100 |

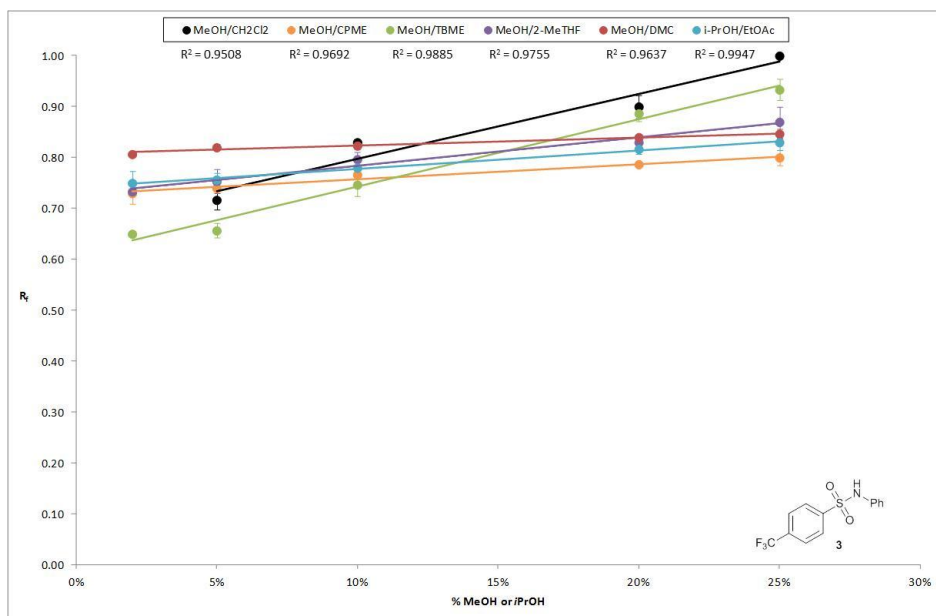
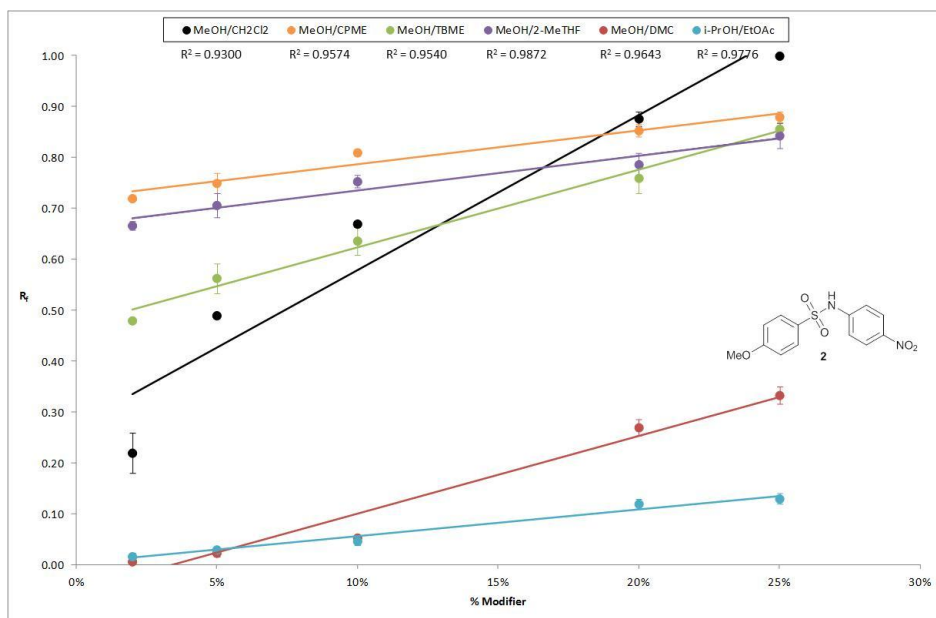
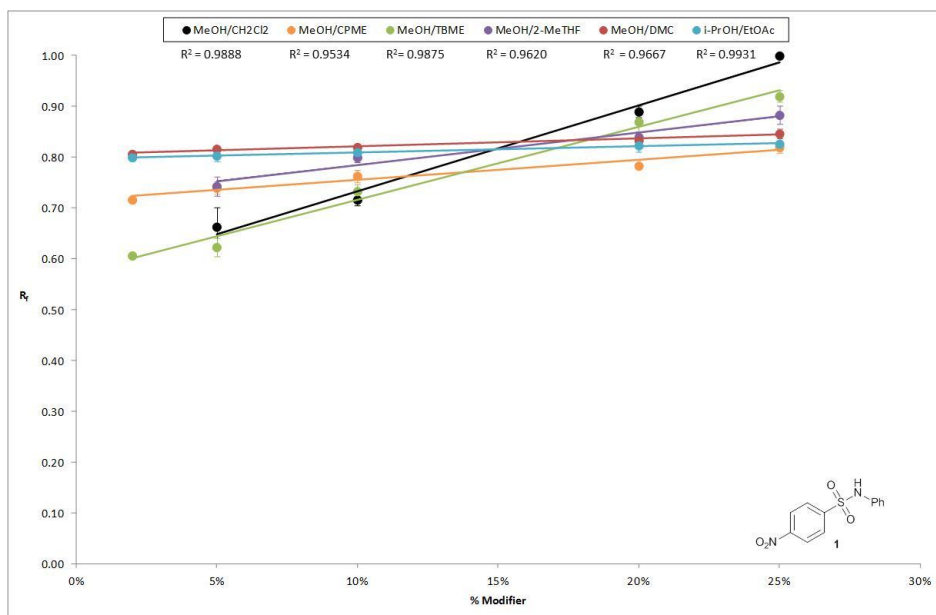
Compound 94

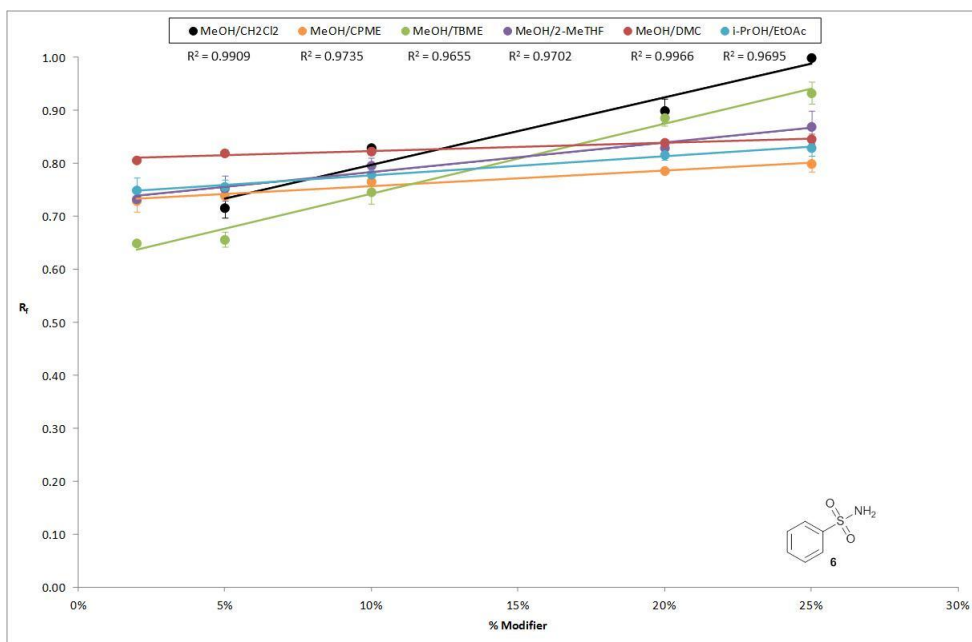
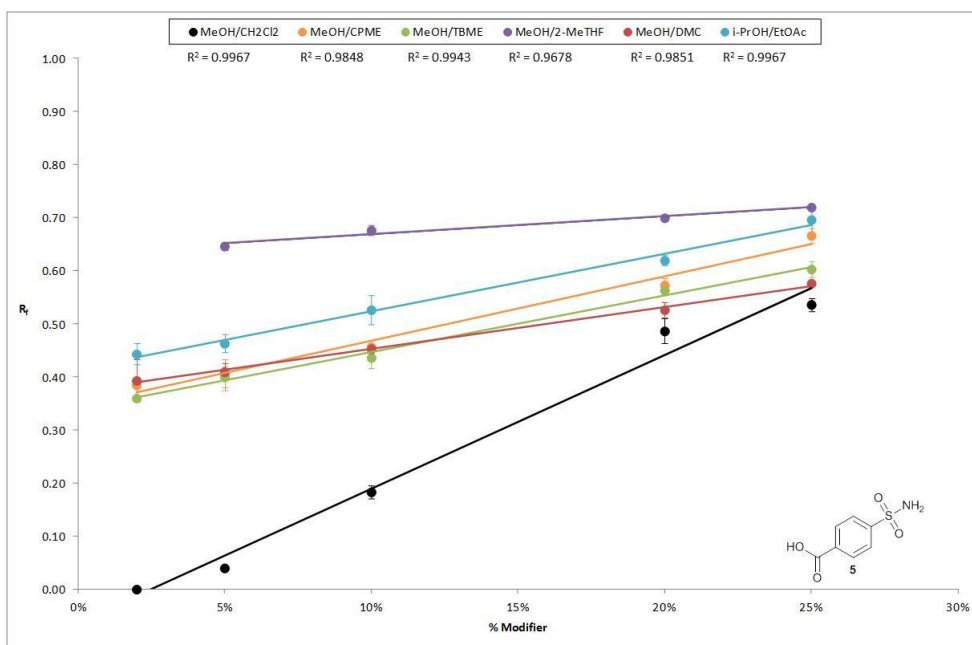
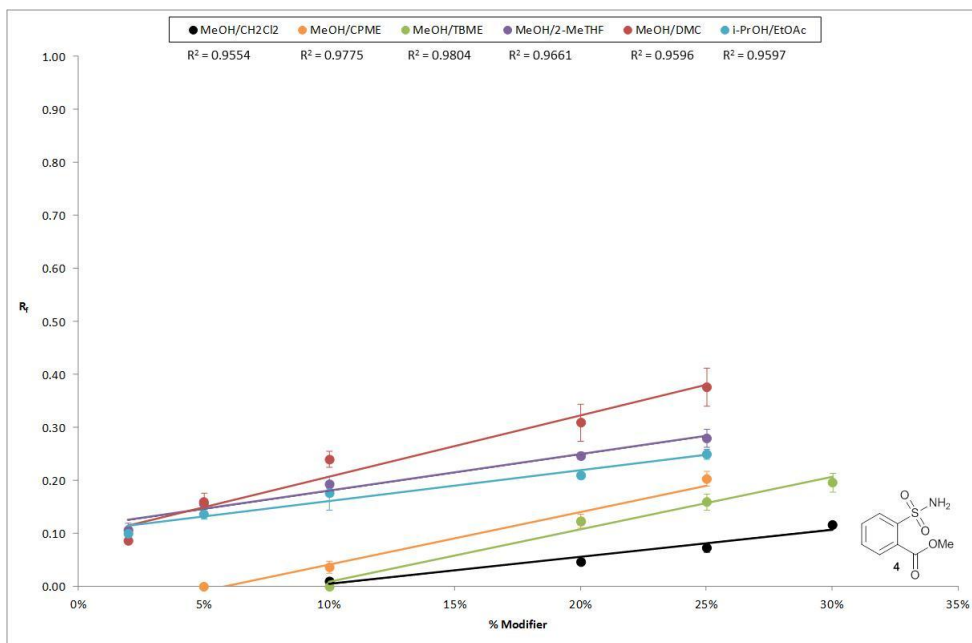
| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0.03 | 0.02 | 0.01 | 0.02 | 0.0058 |
| 5% | 0.07 | 0.03 | 0.04 | 0.05 | 0.0120 |
| 10% | 0.07 | 0.08 | 0.04 | 0.06 | 0.0120 |
| 20% | 0.1 | 0.08 | 0.1 | 0.09 | 0.0067 |
| 25% | 0.09 | 0.11 | 0.12 | 0.11 | 0.0088 |

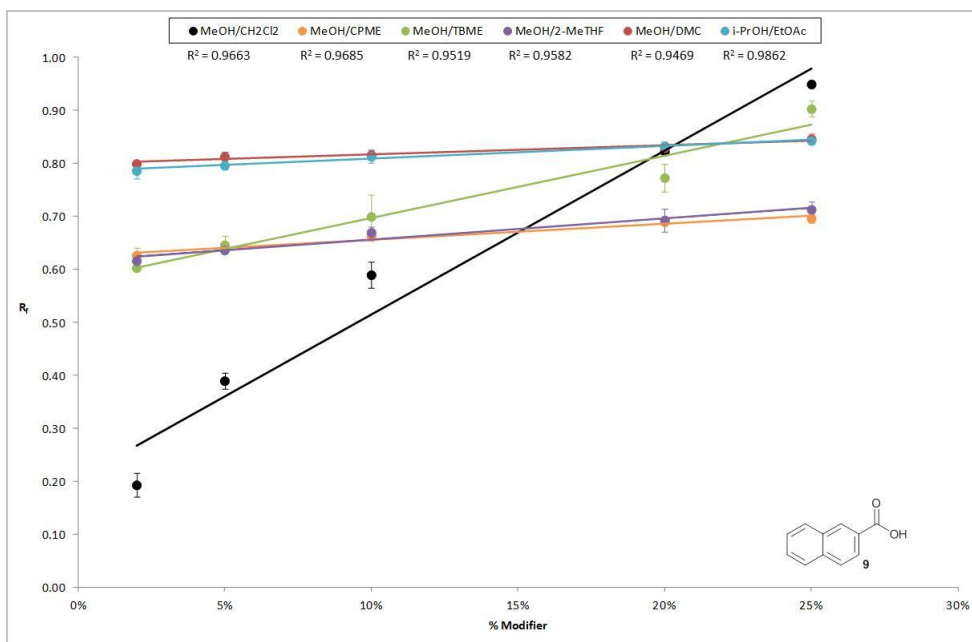
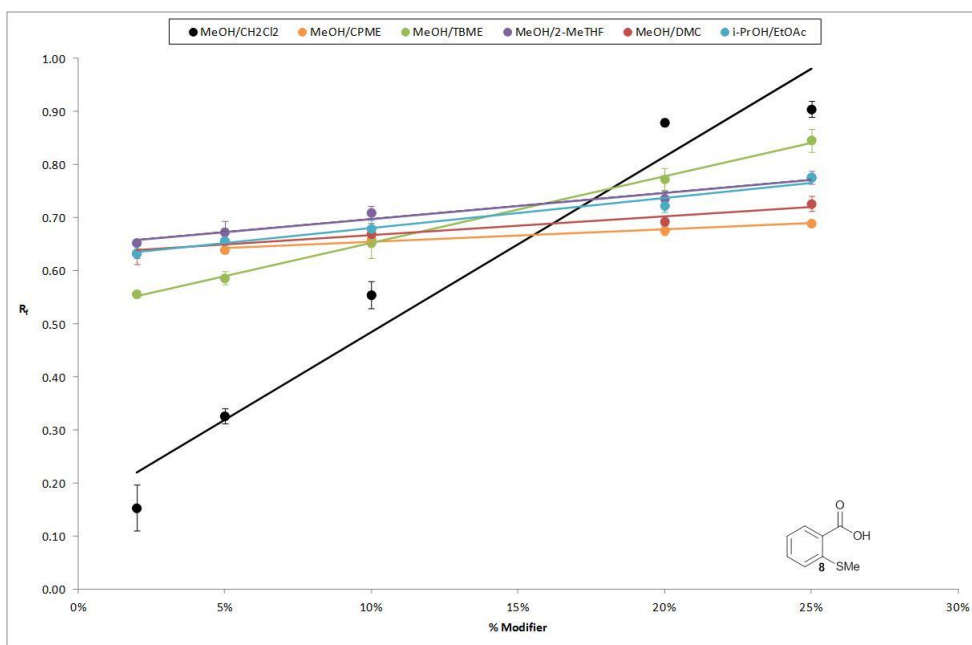
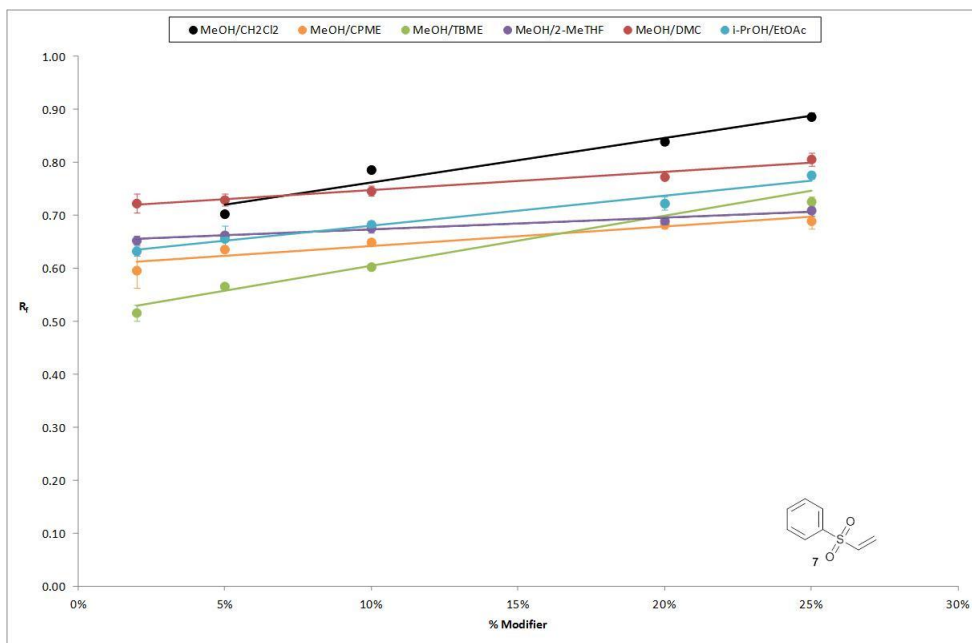
Compound 95

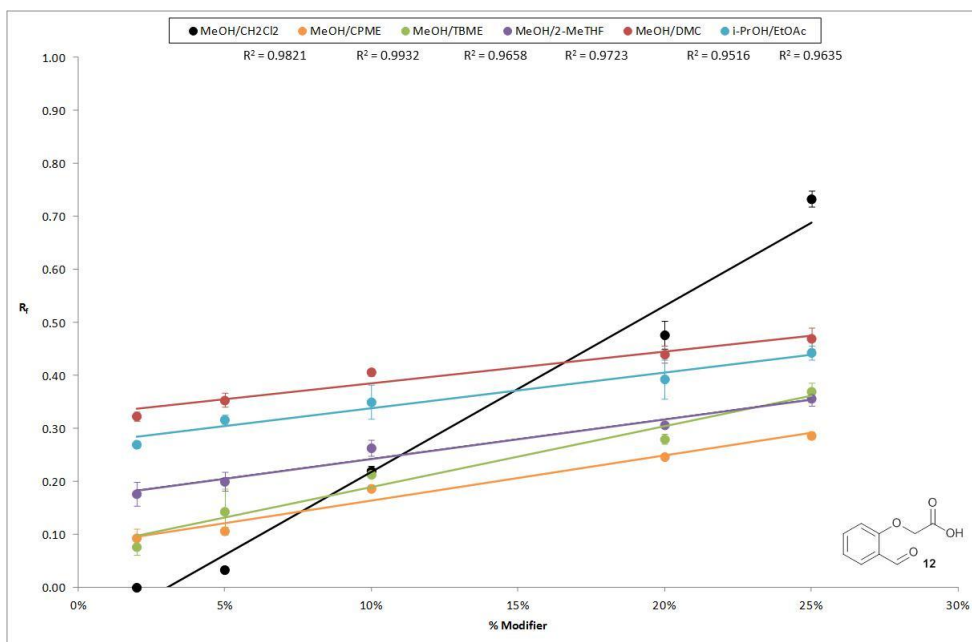
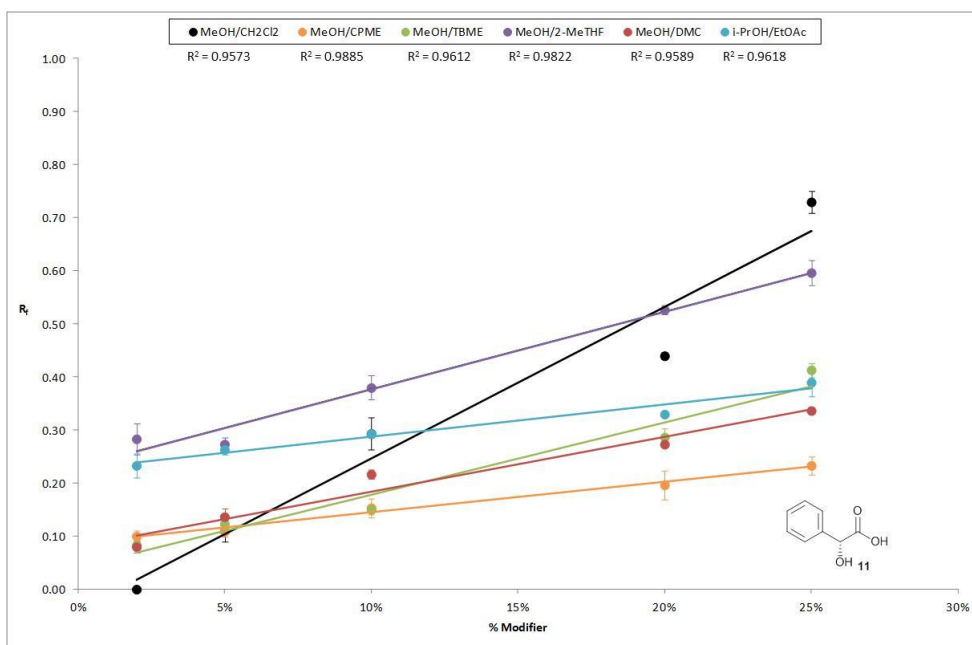
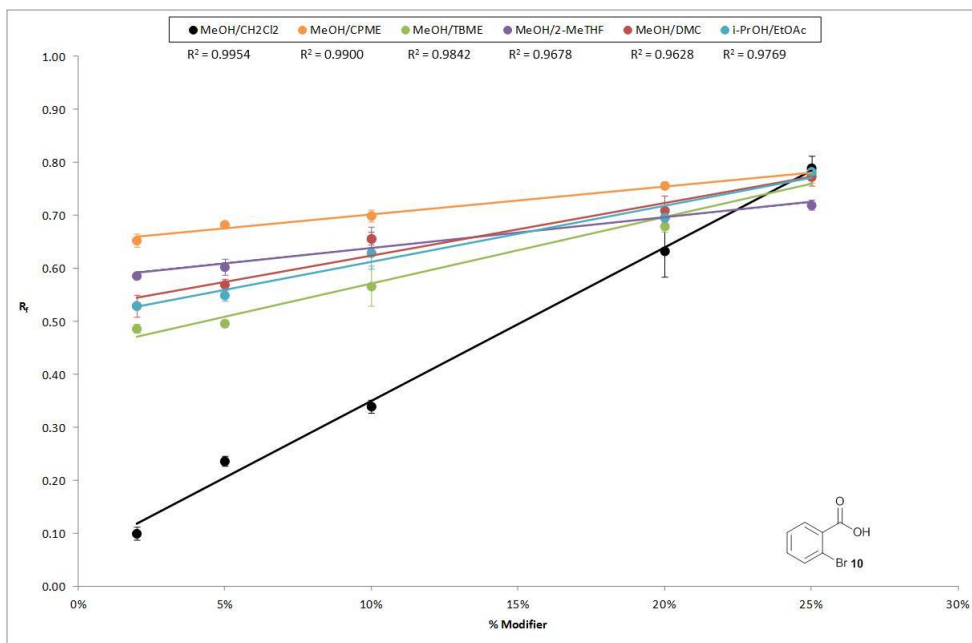
| Modifier Level | Run 1 | Run 2 | Run 3 | Average | Standard Error |
|----------------|-------|-------|-------|---------|----------------|
| 2% | 0 | 0 | 0 | 0.00 | 0.0000 |
| 5% | 0.01 | 0.01 | 0.01 | 0.01 | 0.0000 |
| 10% | 0.02 | 0.04 | 0.02 | 0.03 | 0.0067 |
| 20% | 0.06 | 0.05 | 0.06 | 0.06 | 0.0033 |
| 25% | 0.06 | 0.07 | 0.1 | 0.08 | 0.0120 |

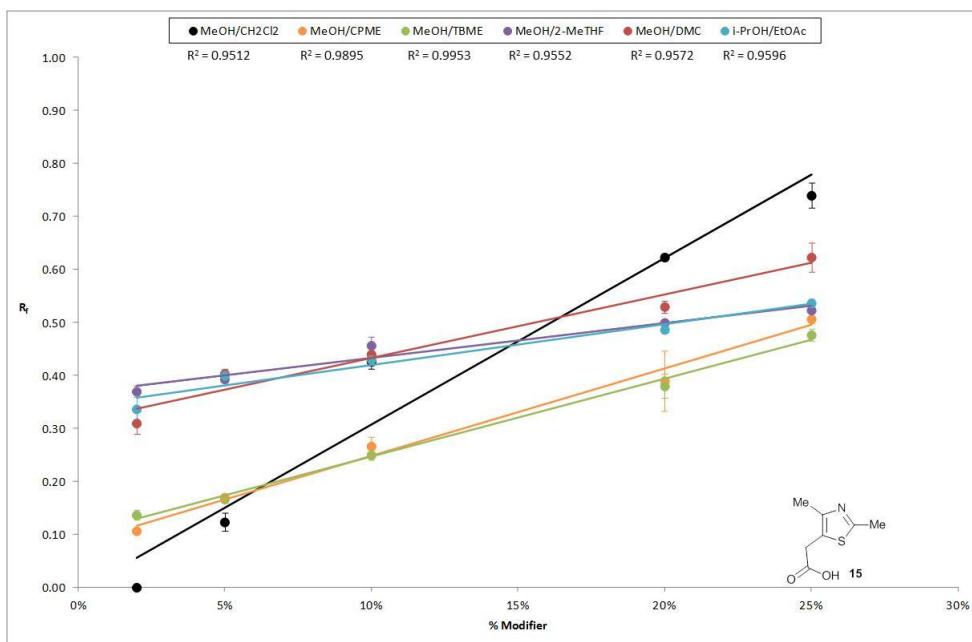
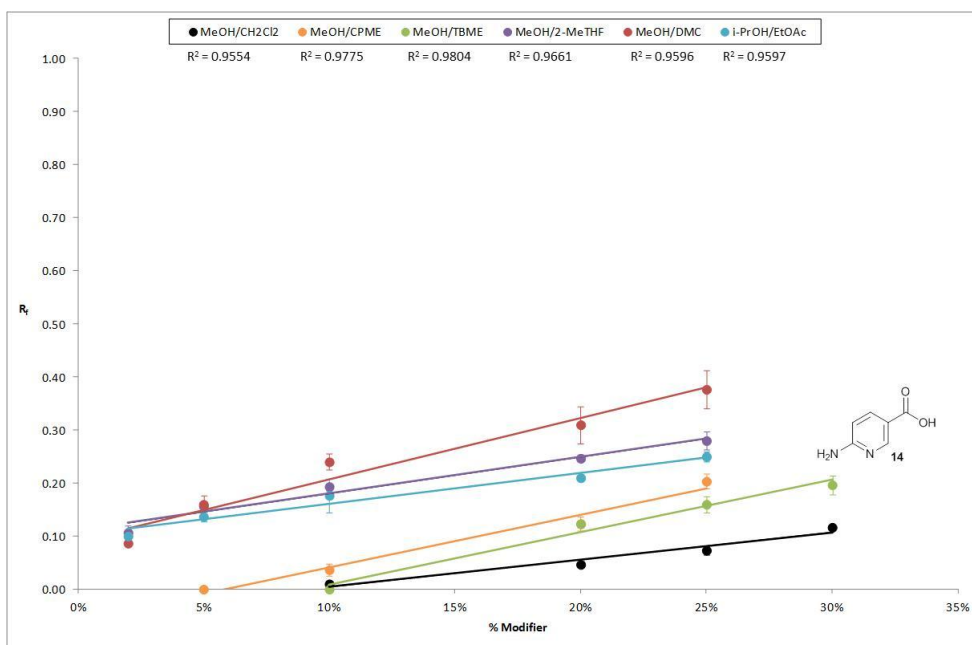
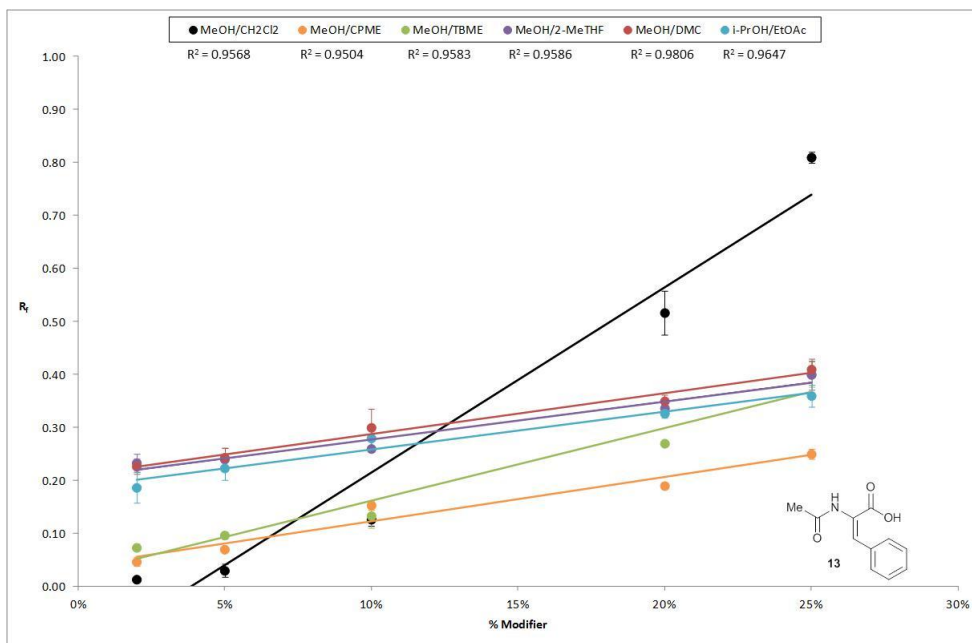
3.3 Compound Library – Plots of R_f vs. % Modifier

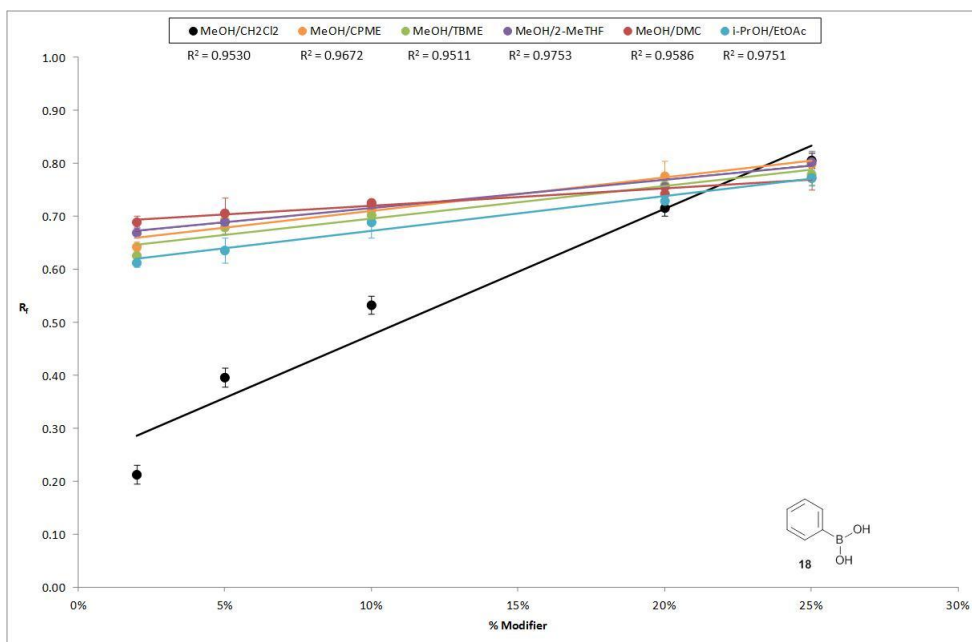
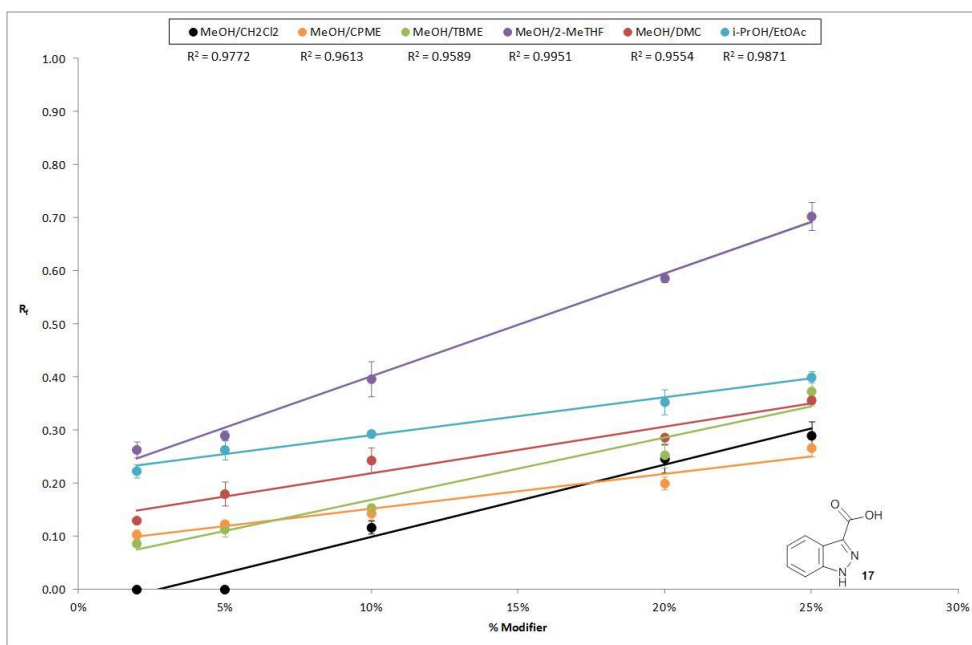
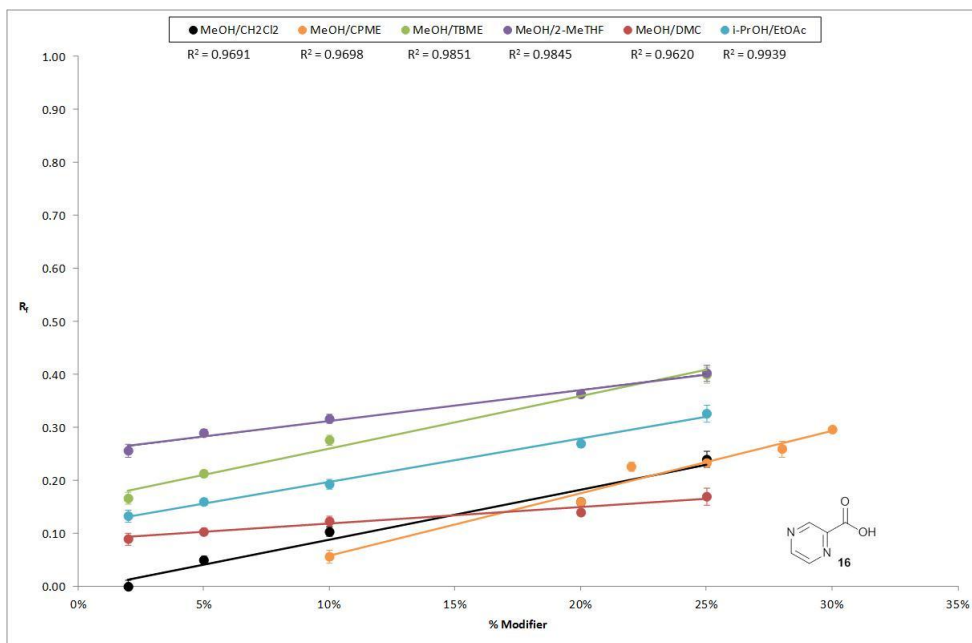


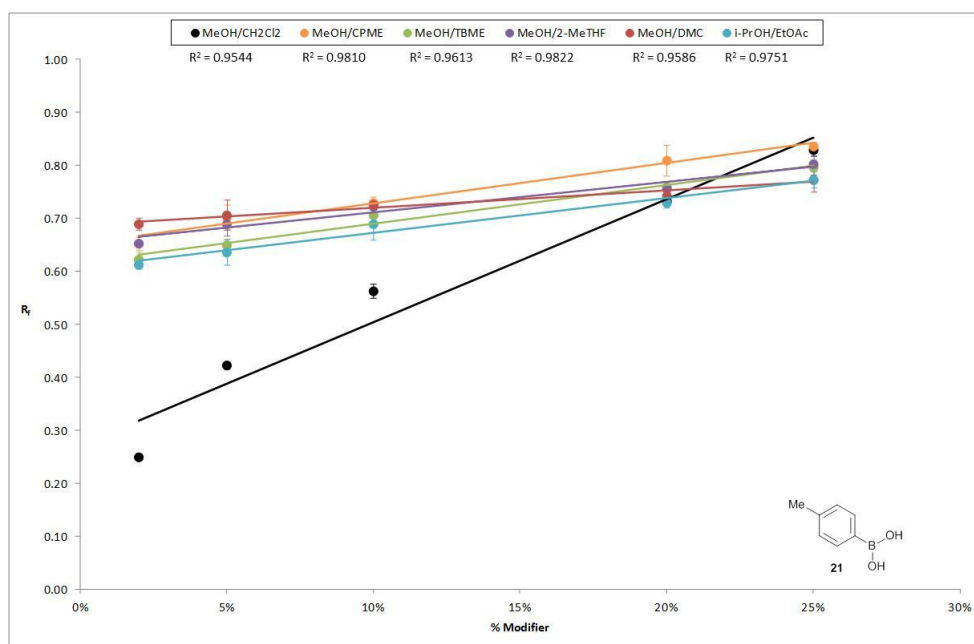
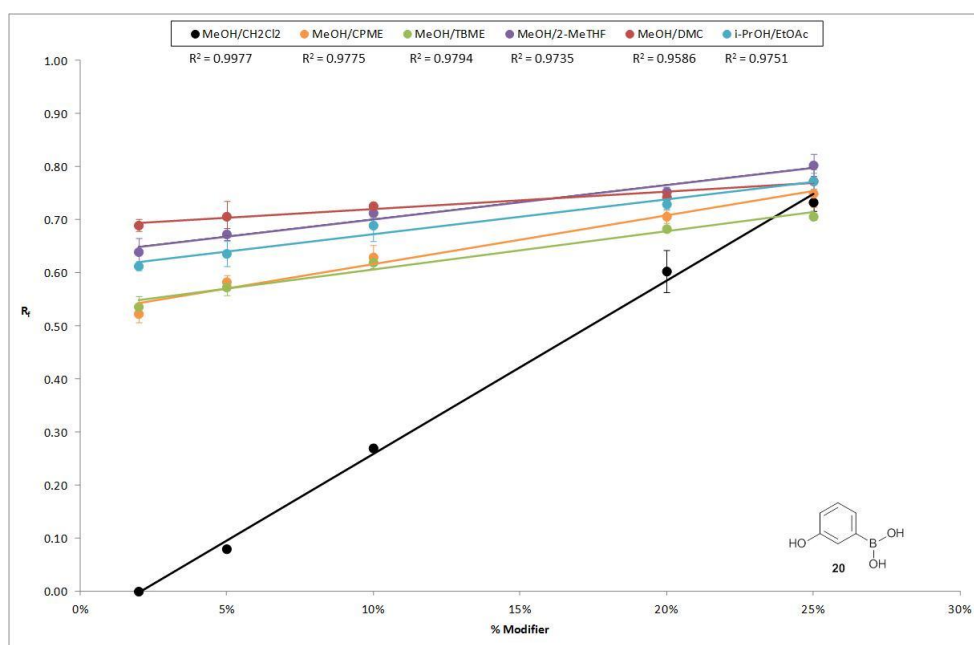
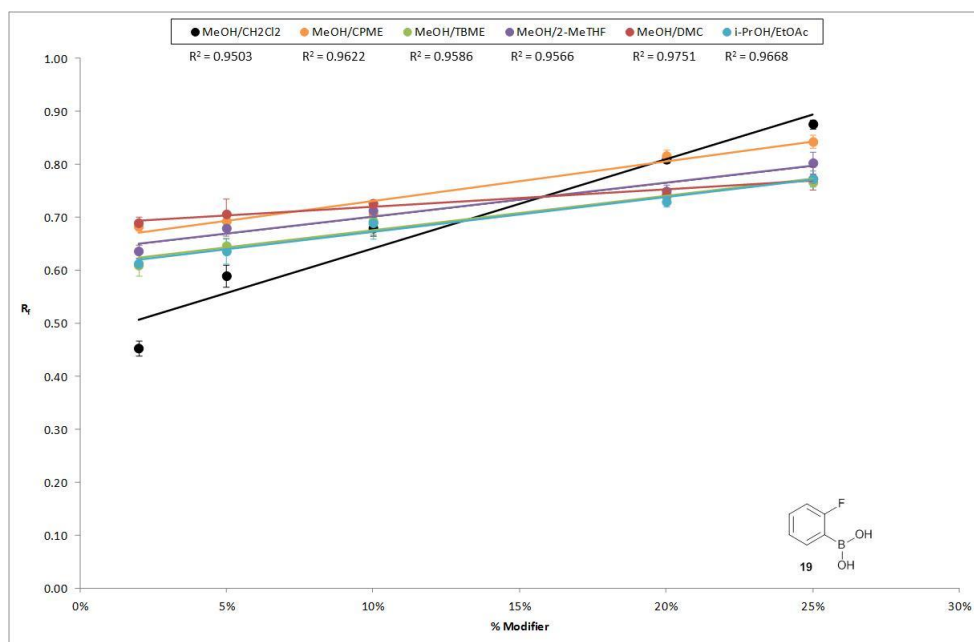


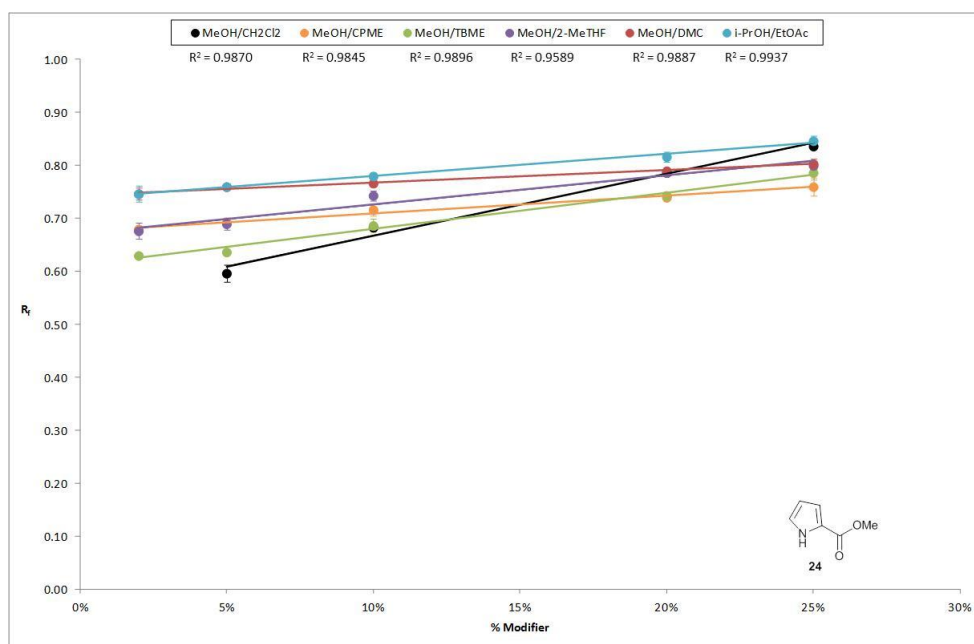
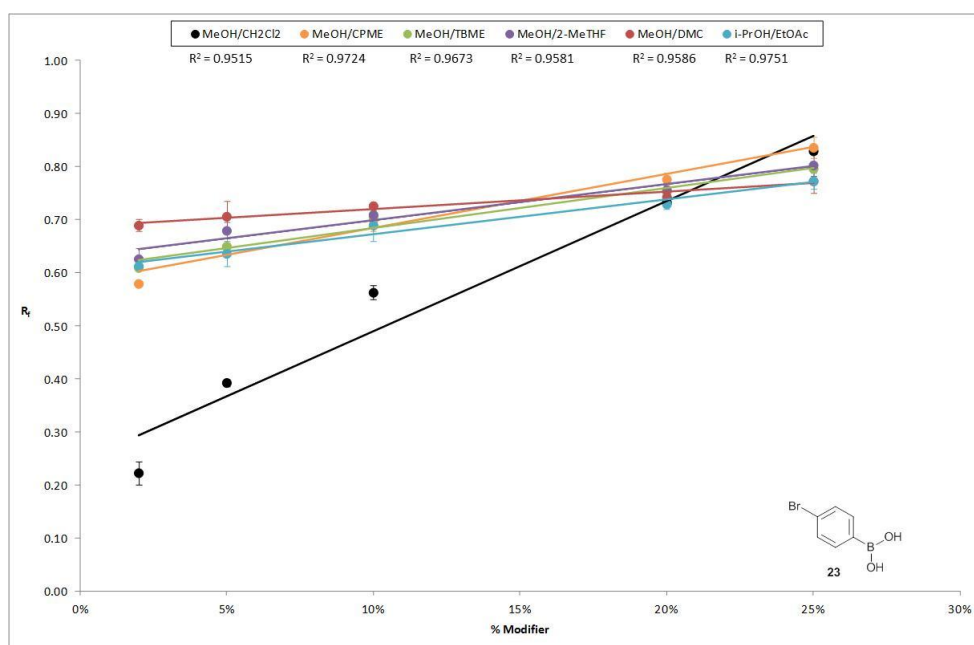
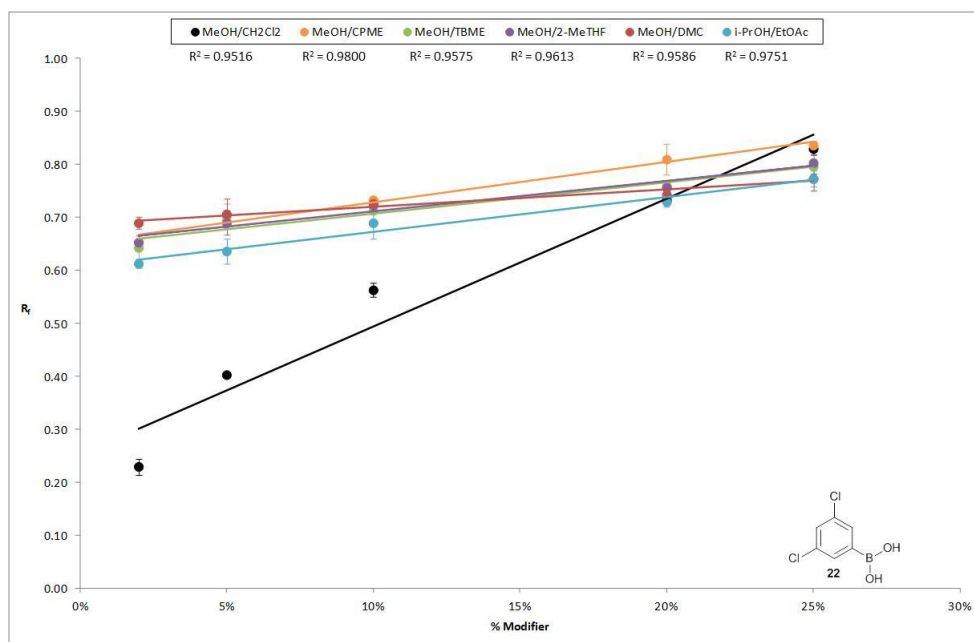


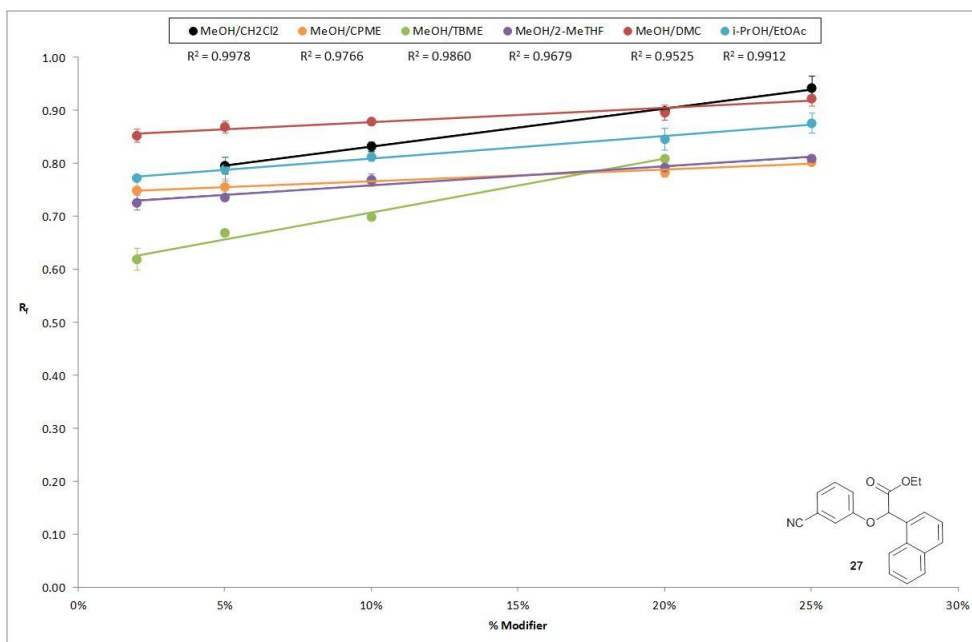
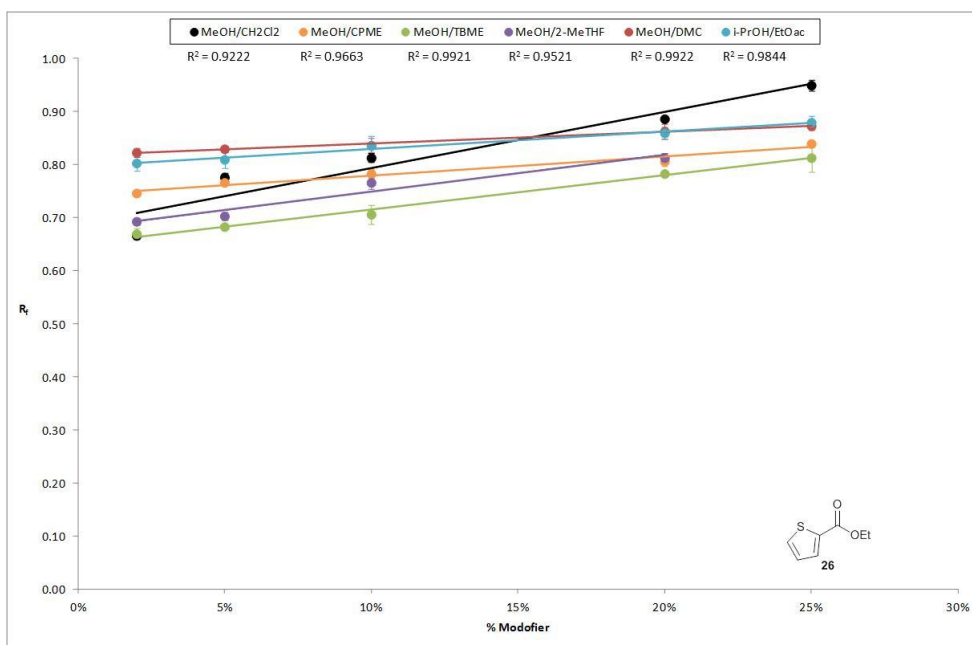
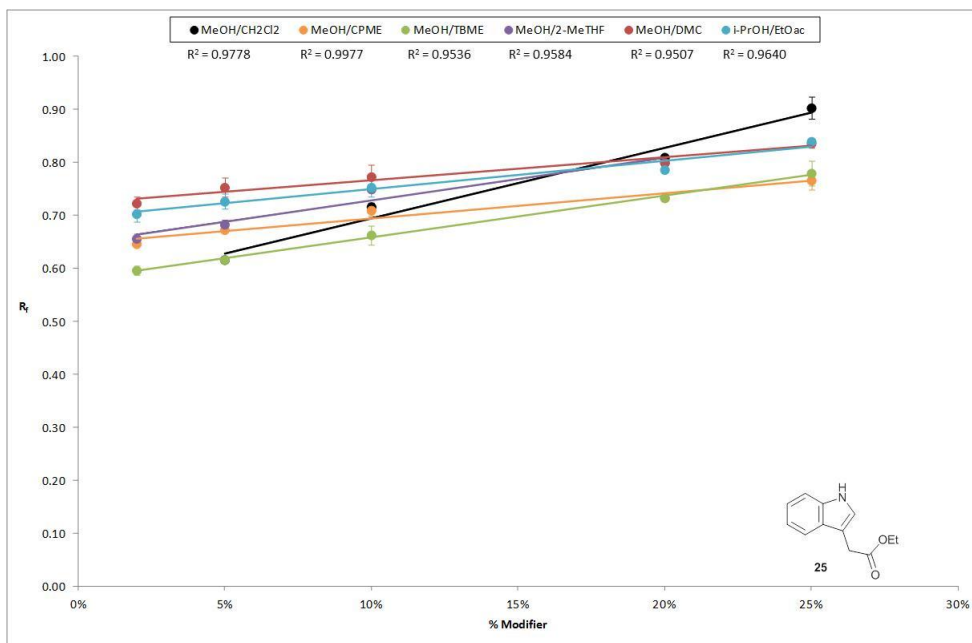


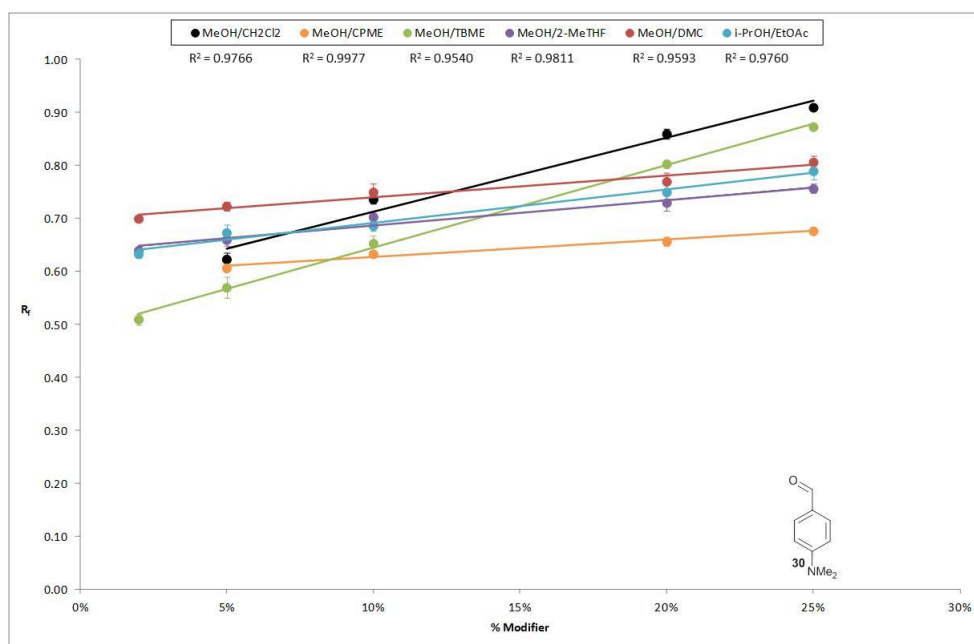
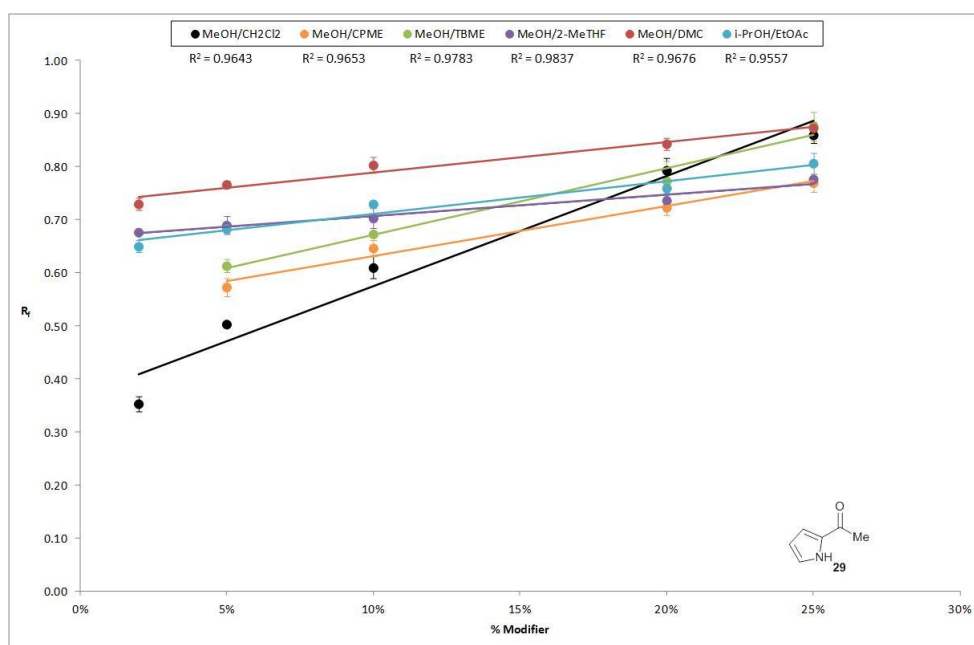
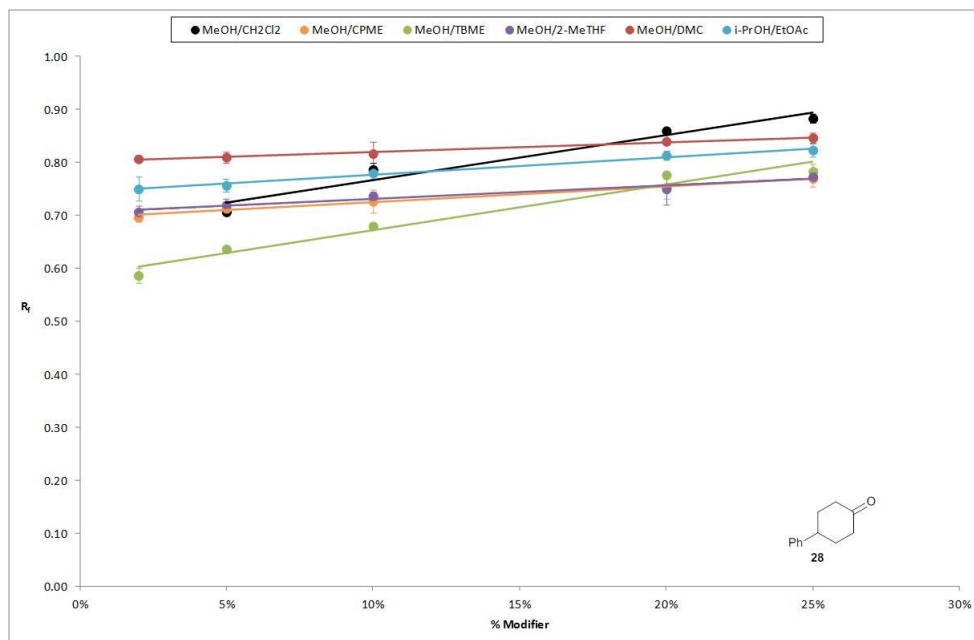


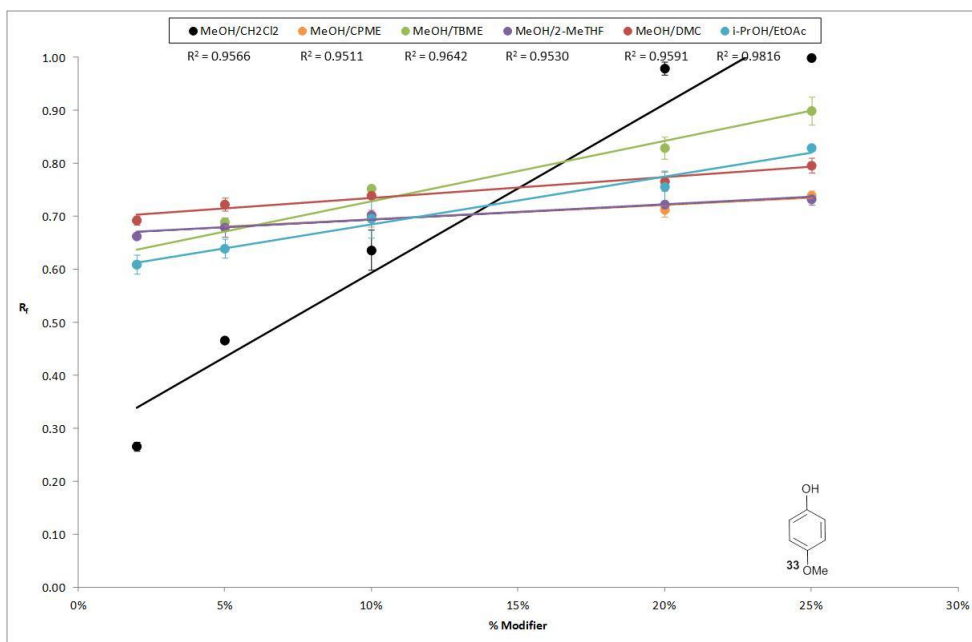
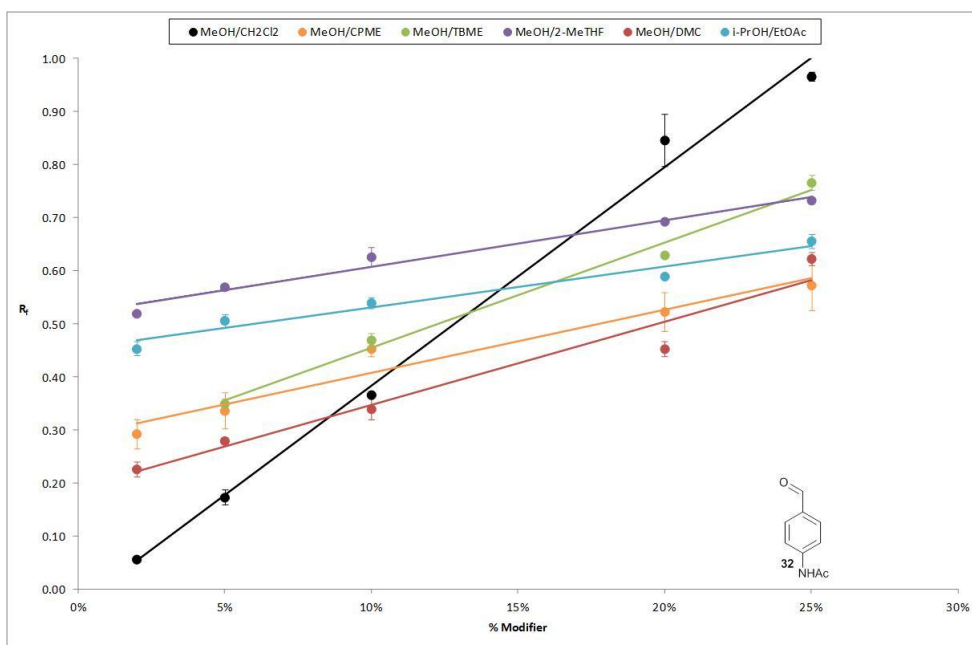
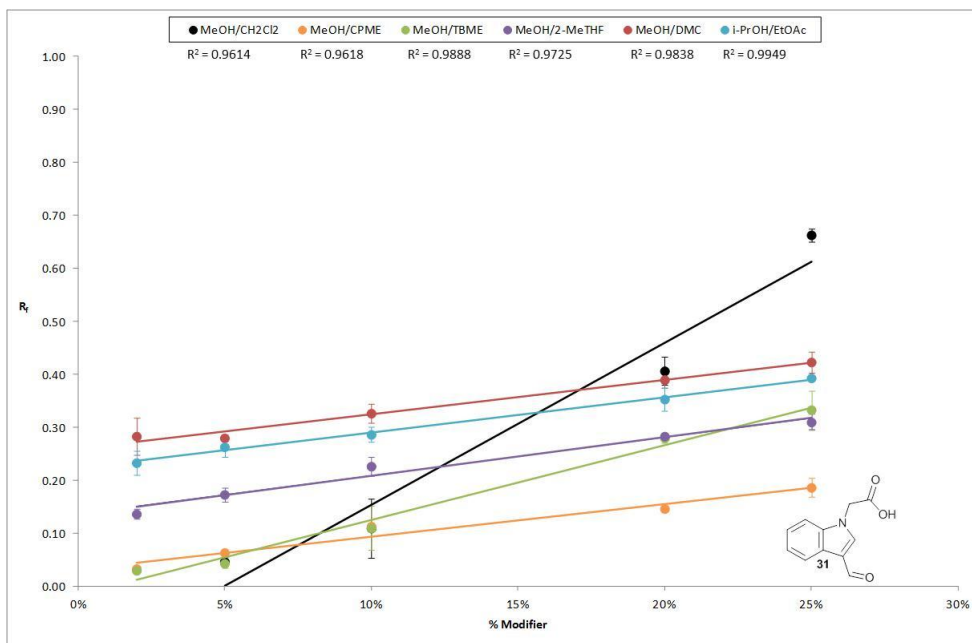


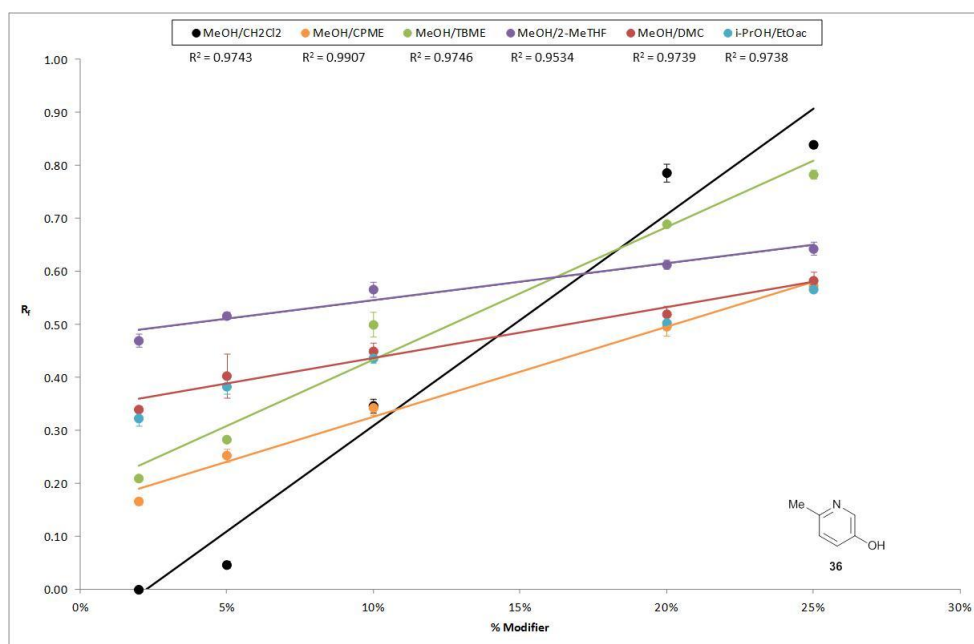
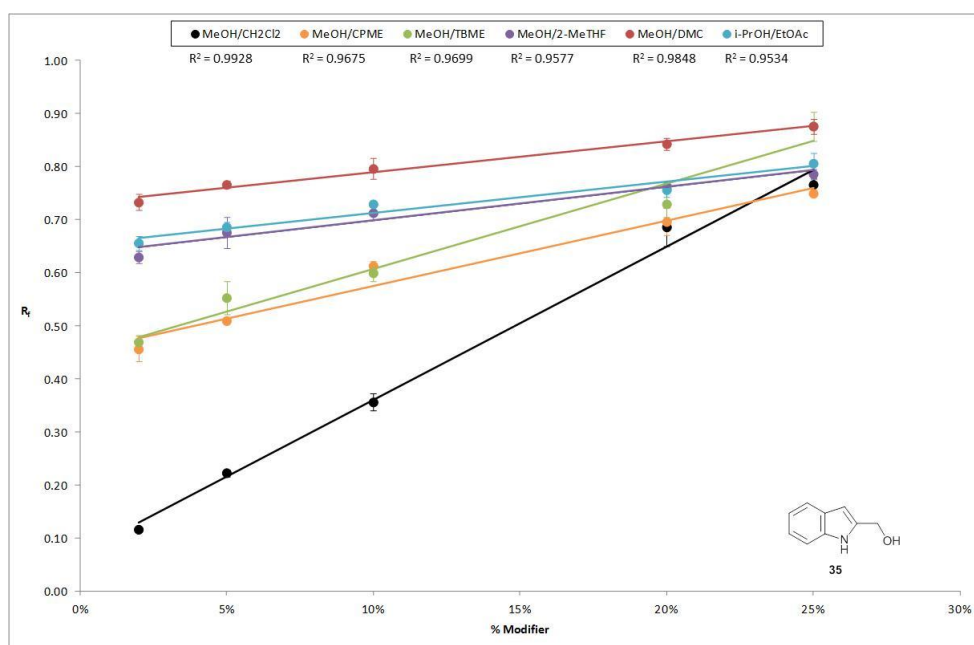
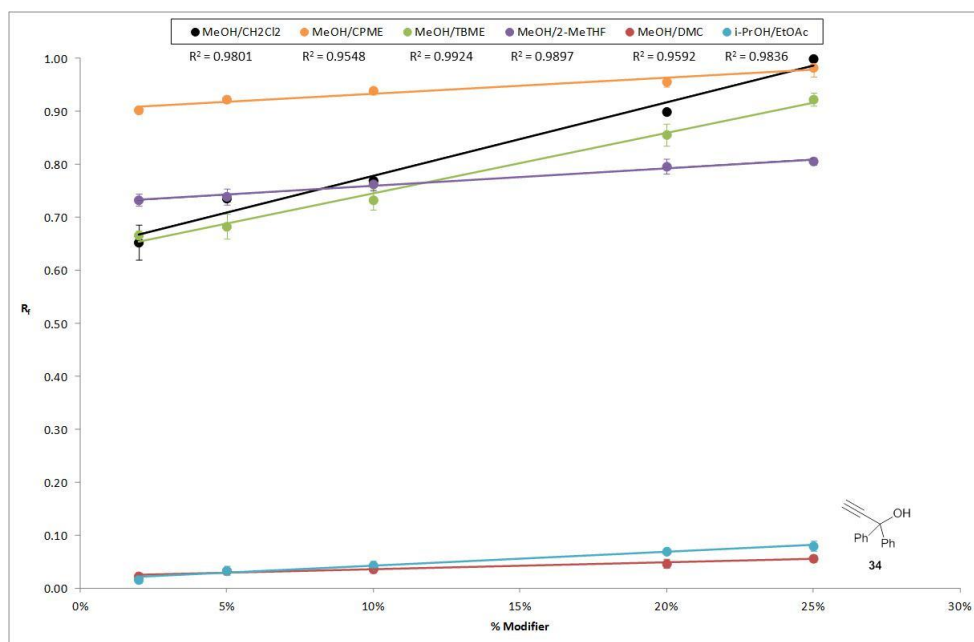


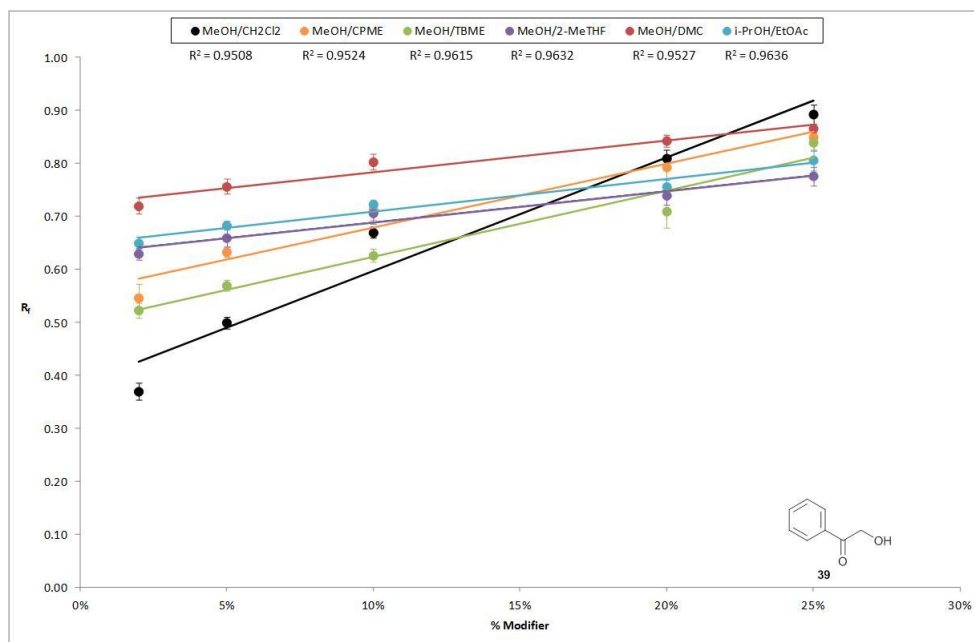
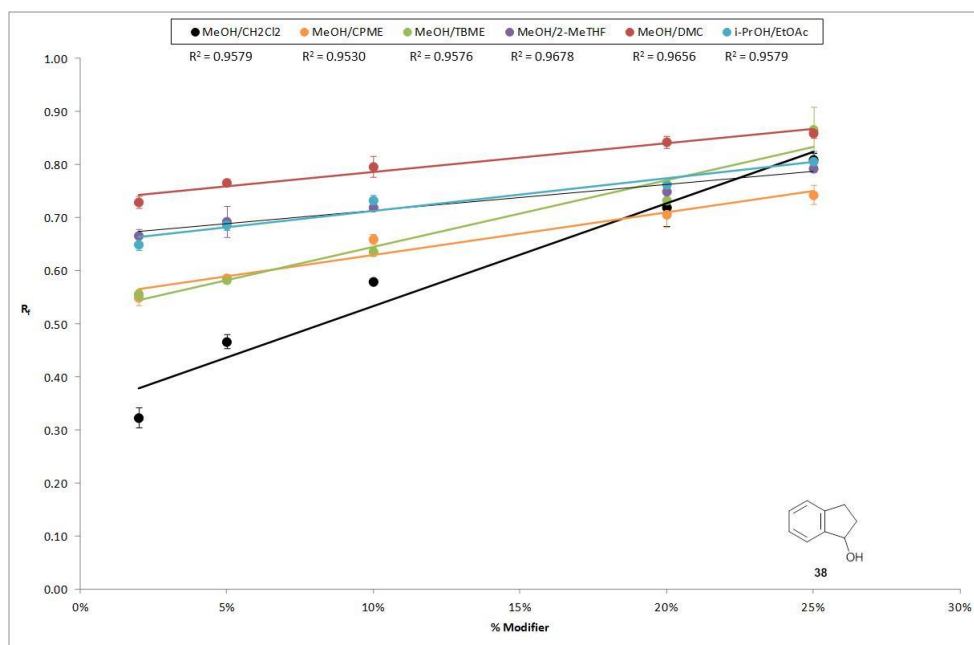
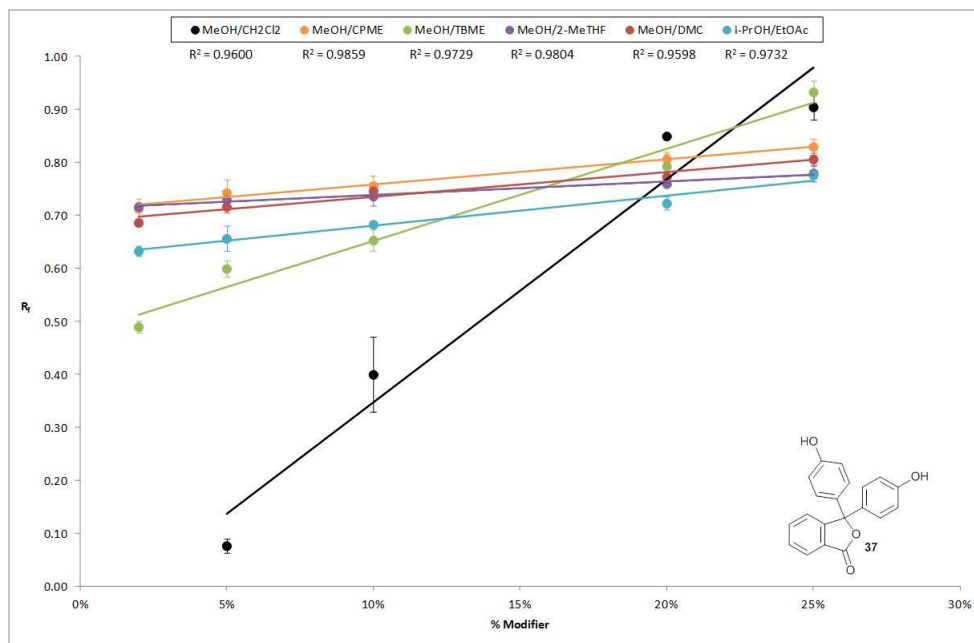


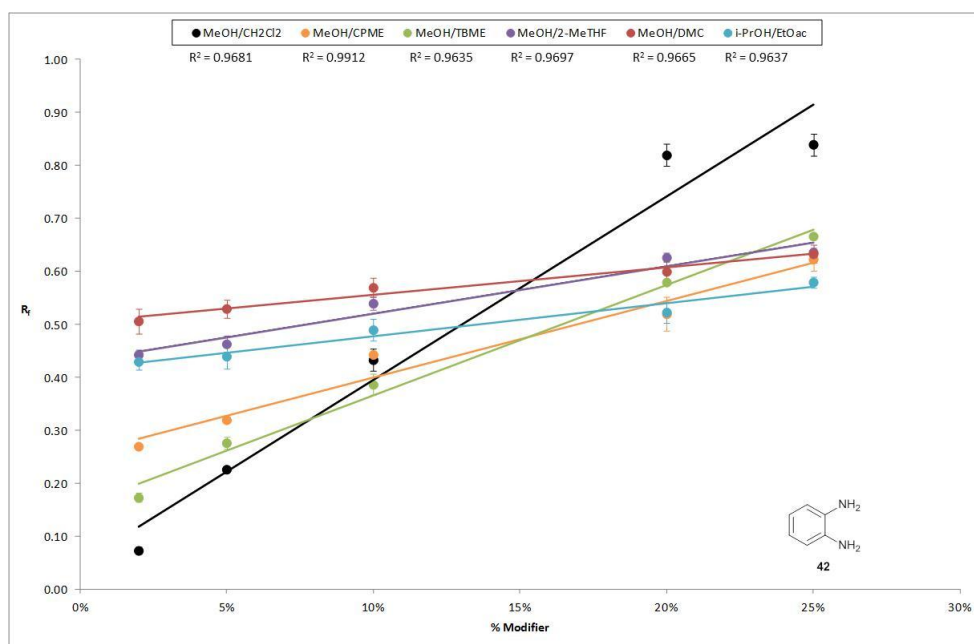
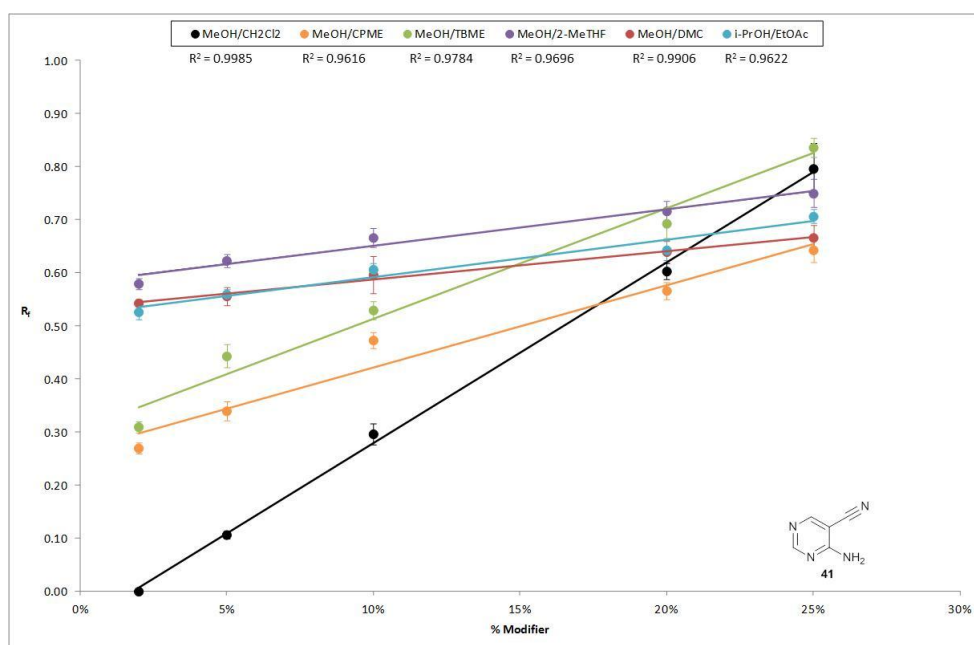
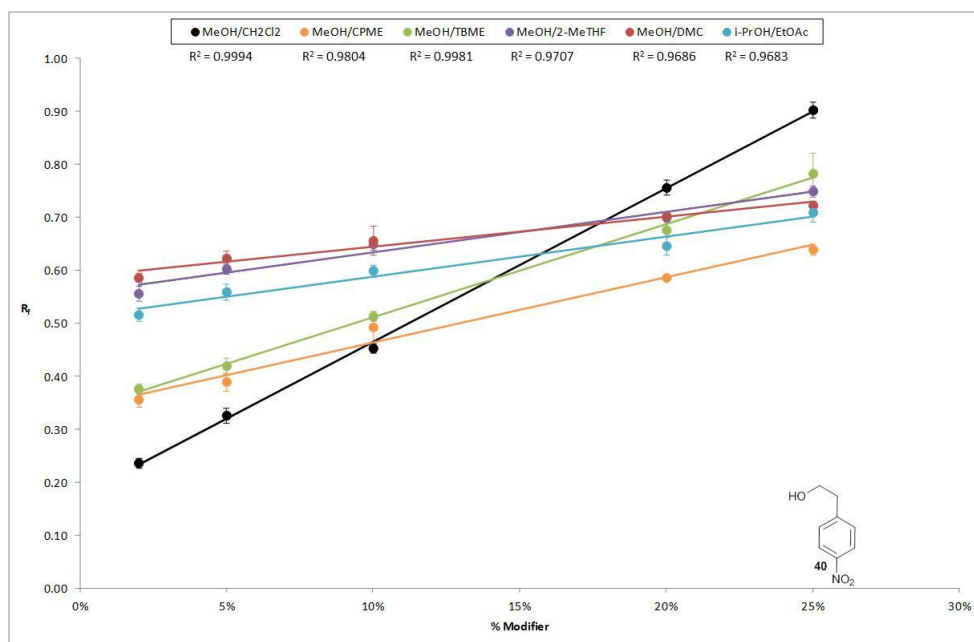


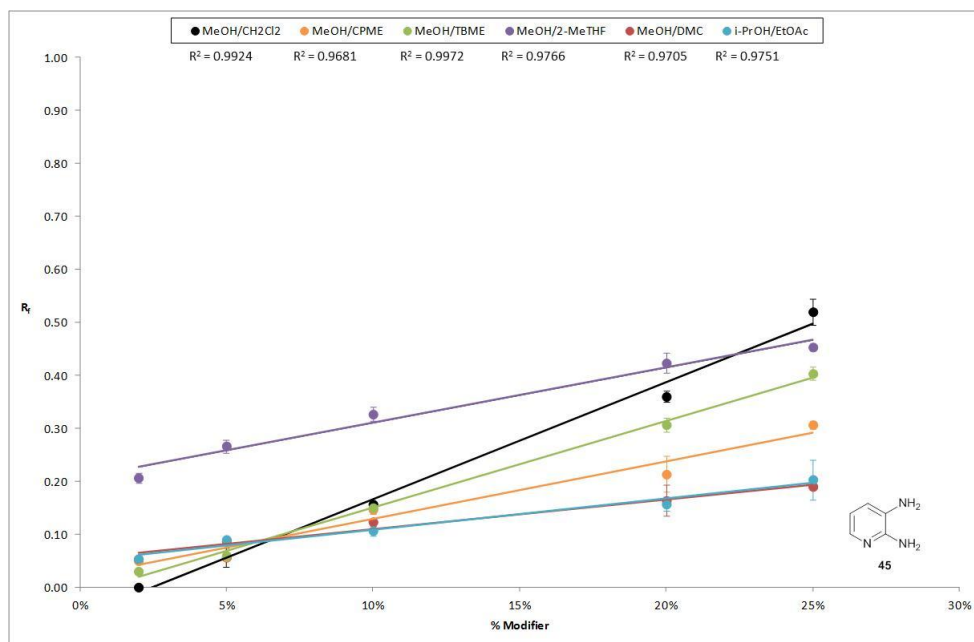
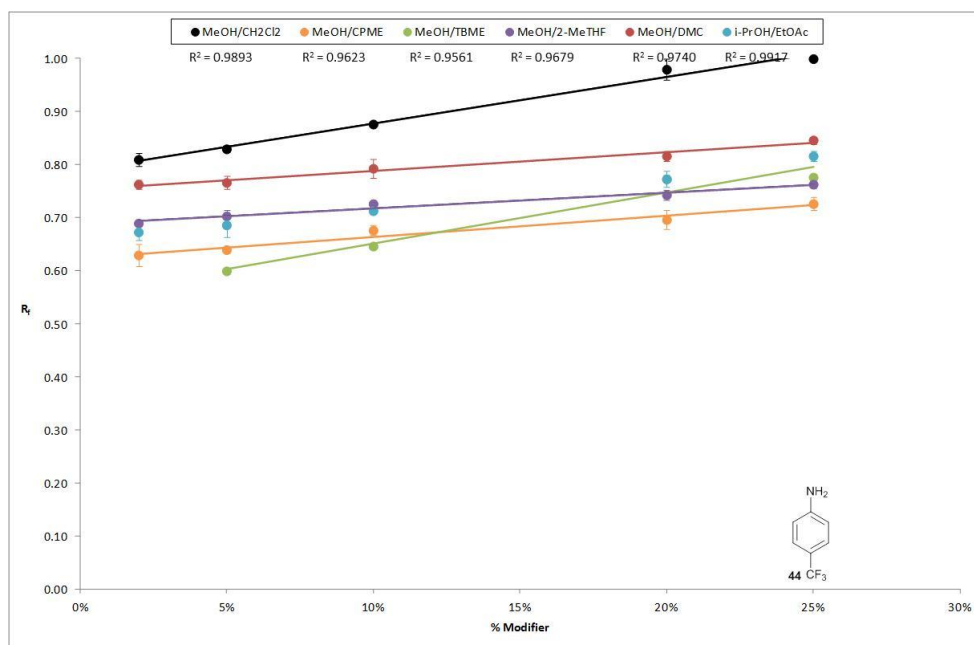
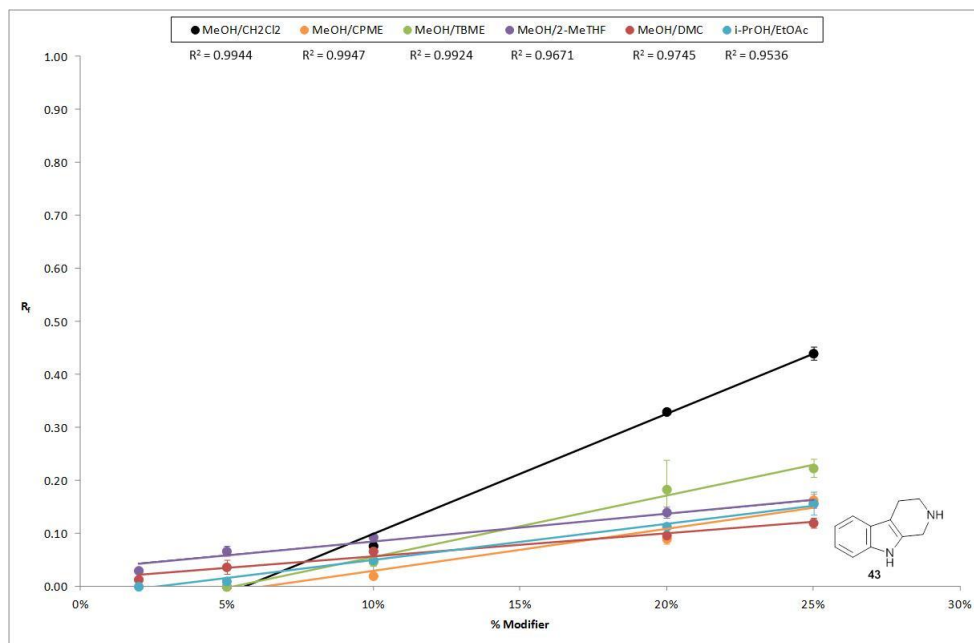


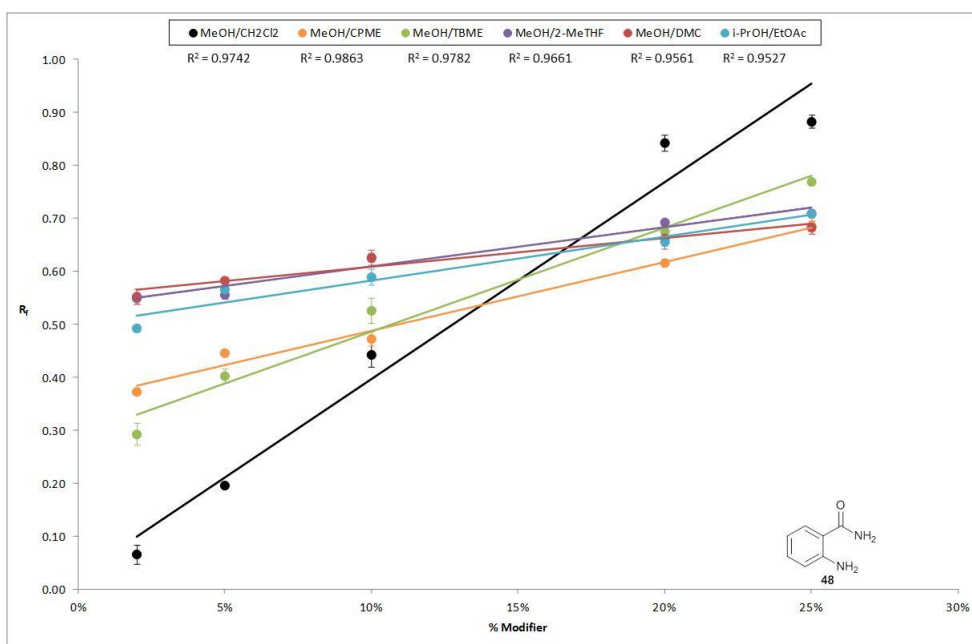
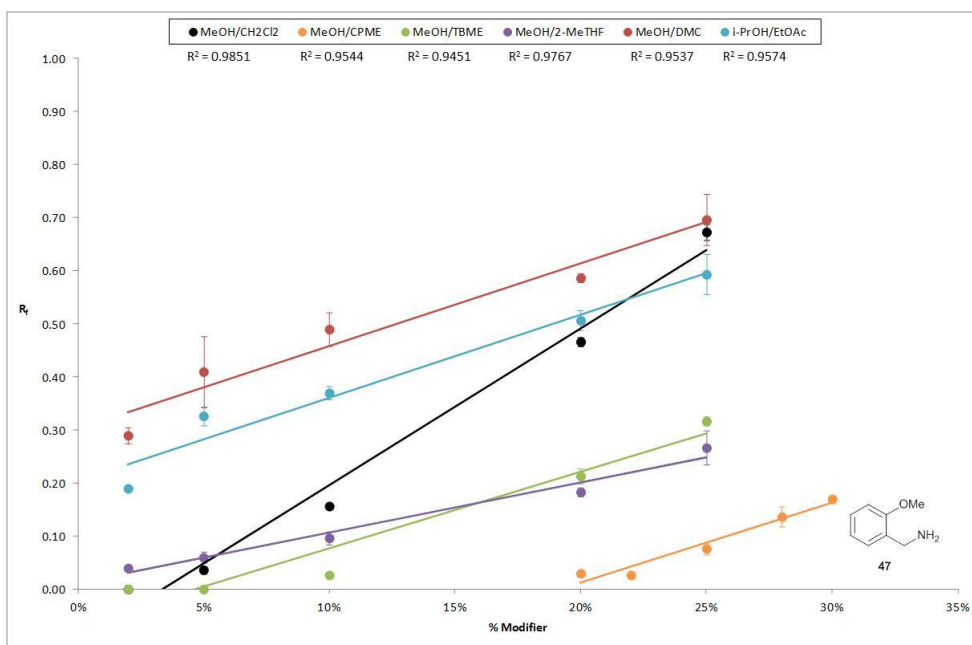
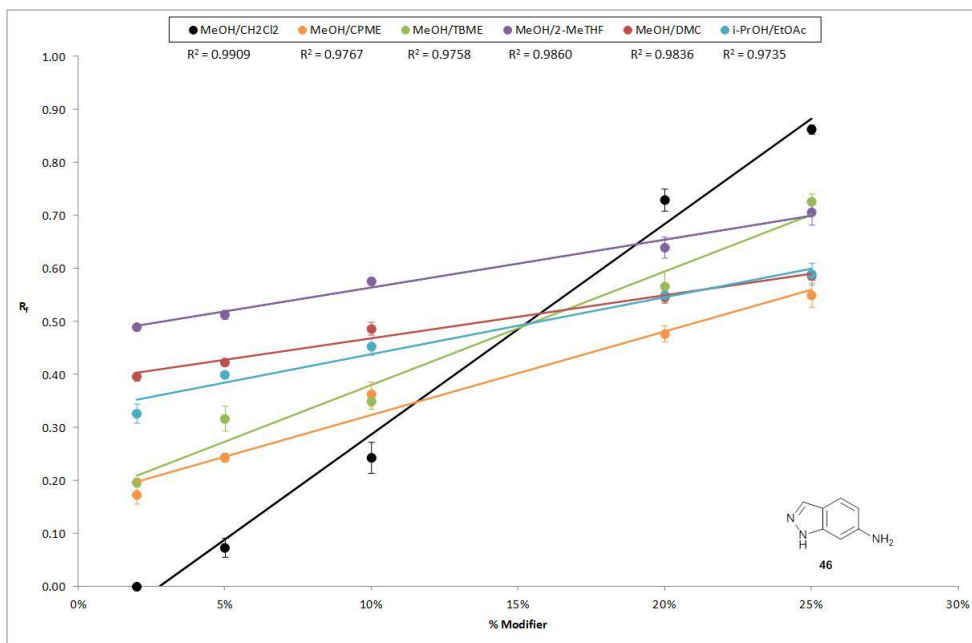


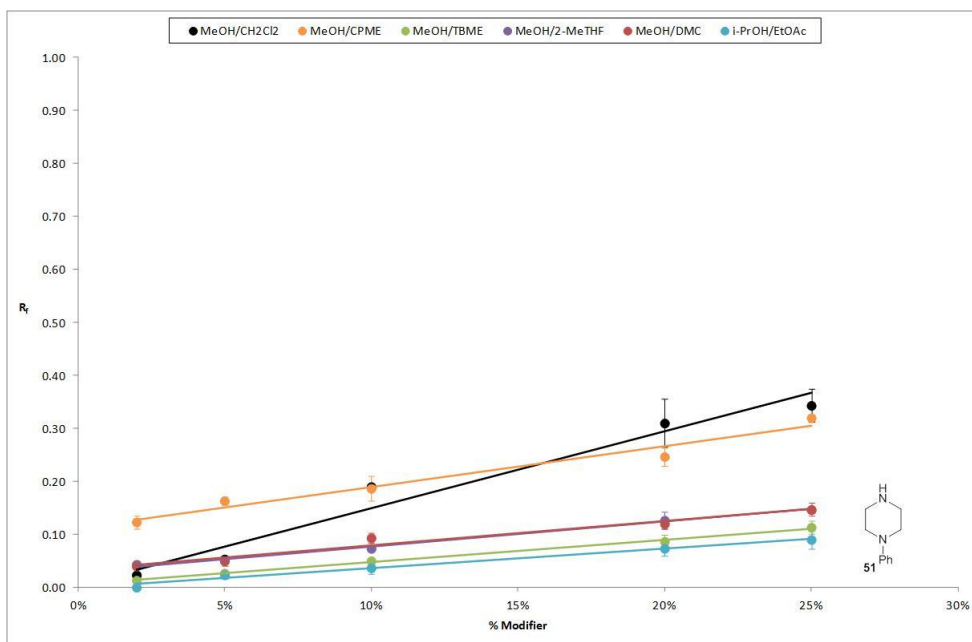
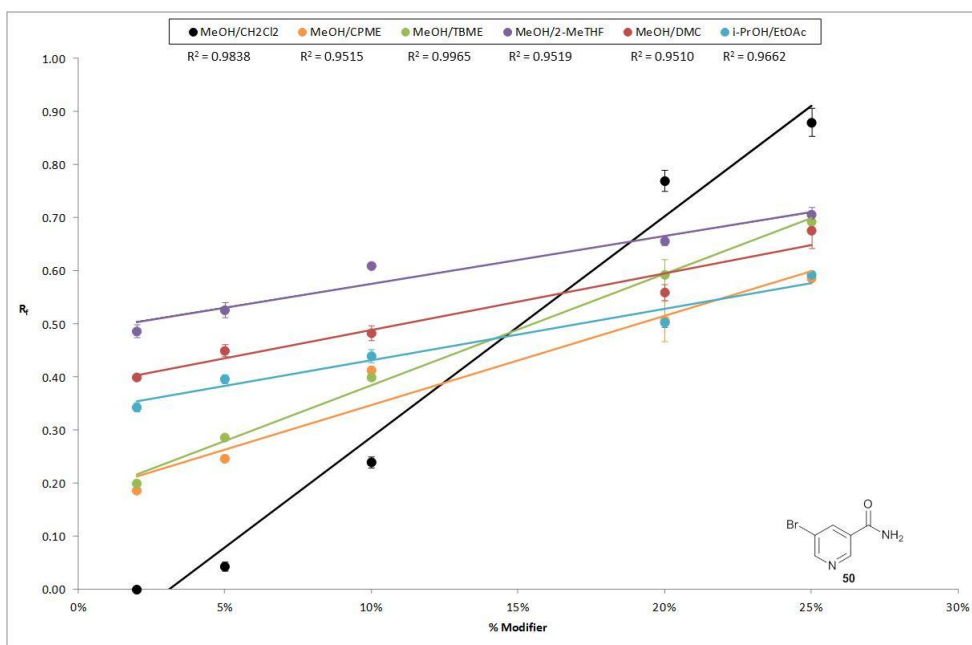
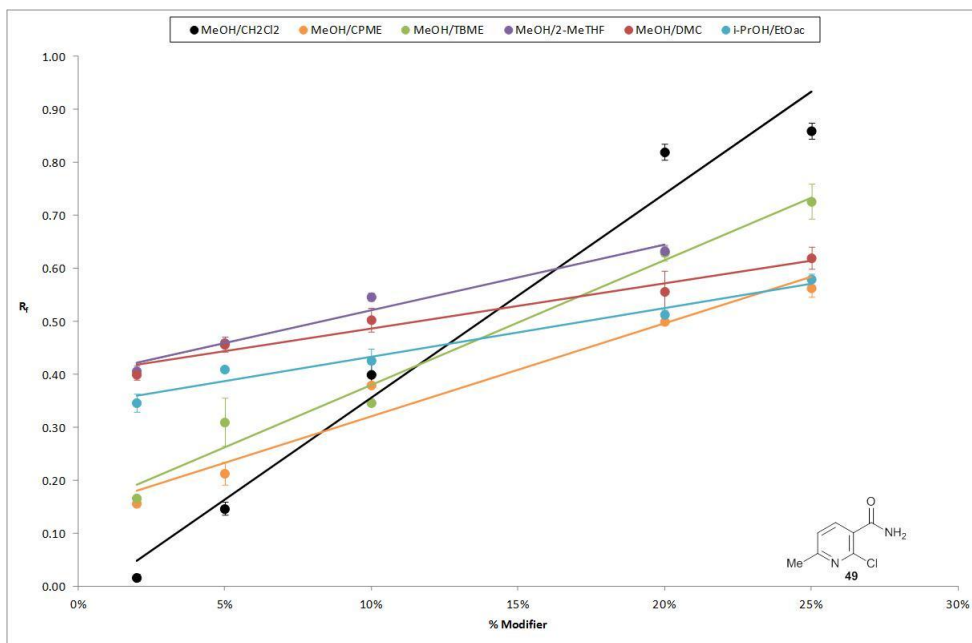


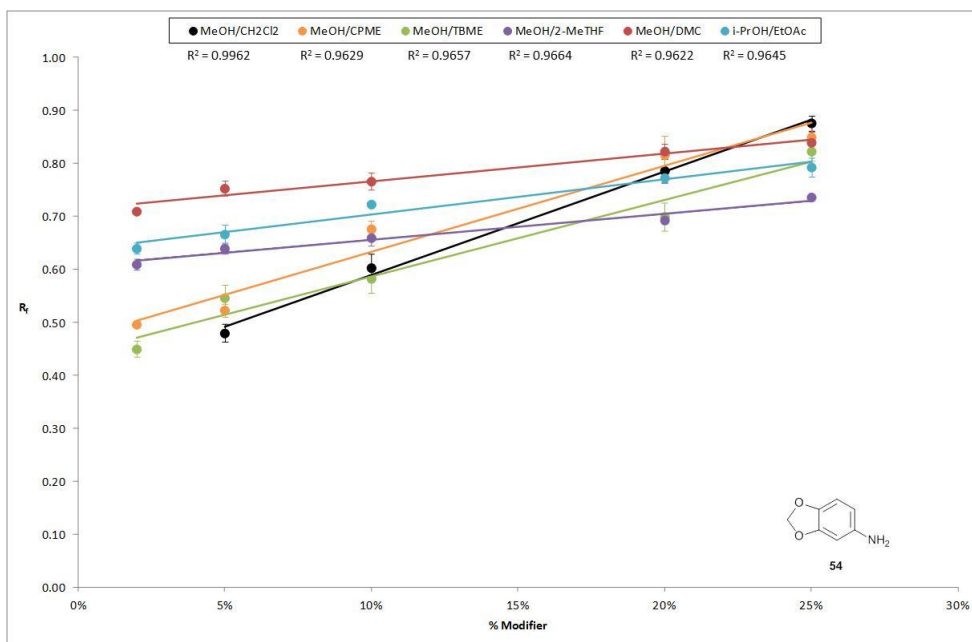
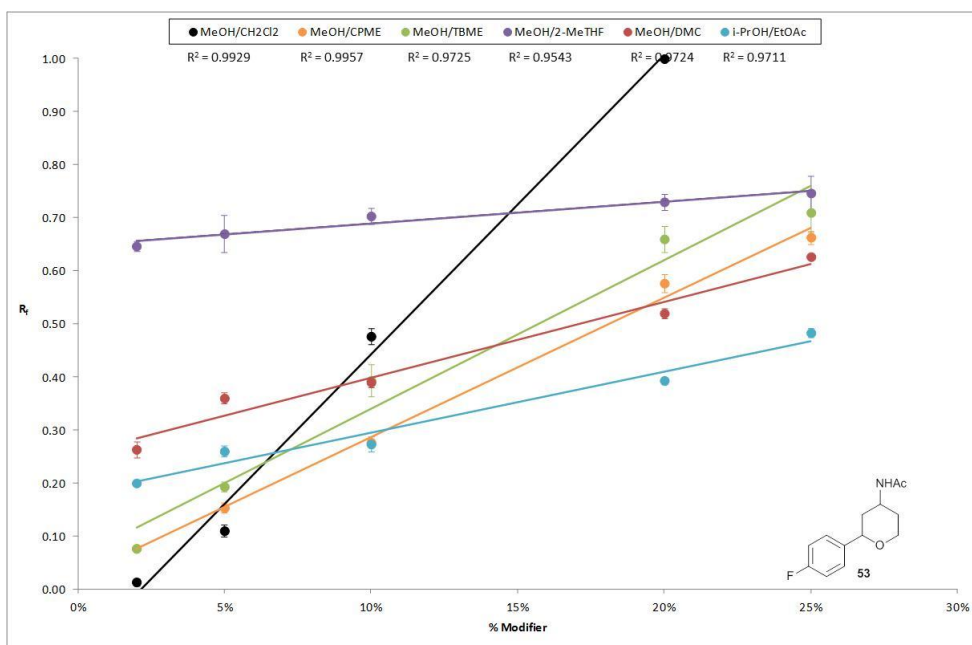
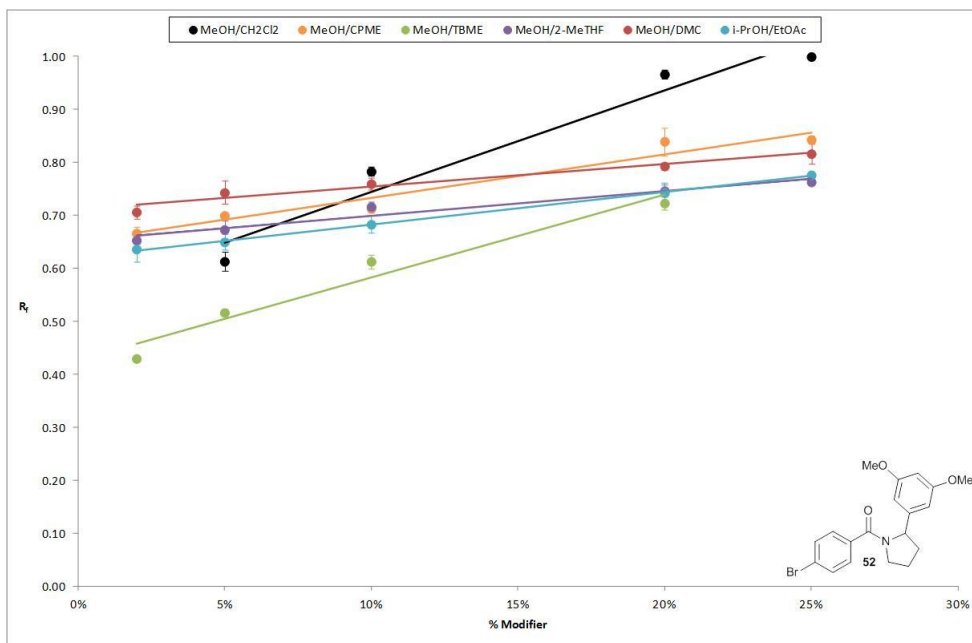


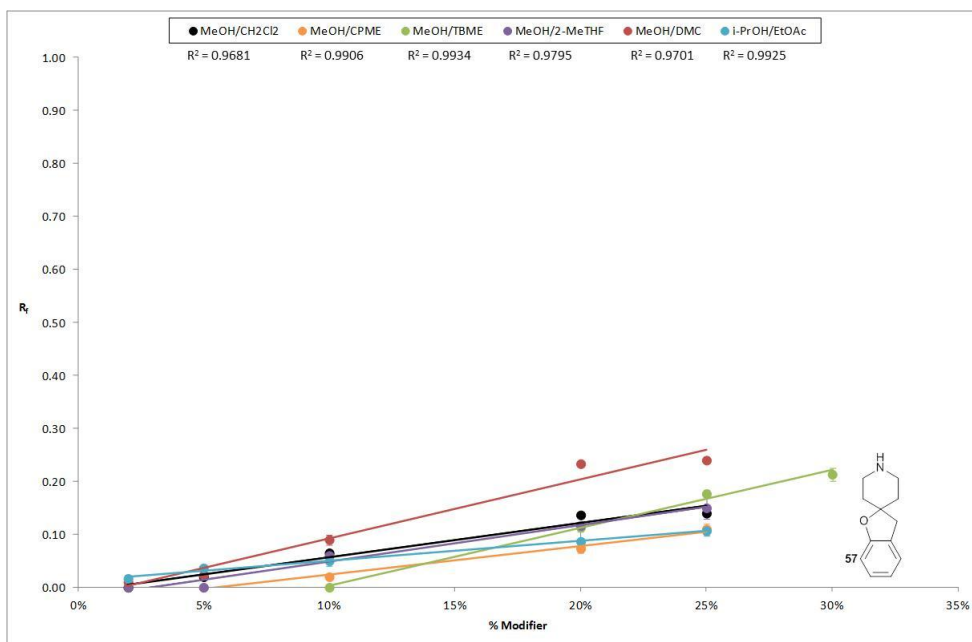
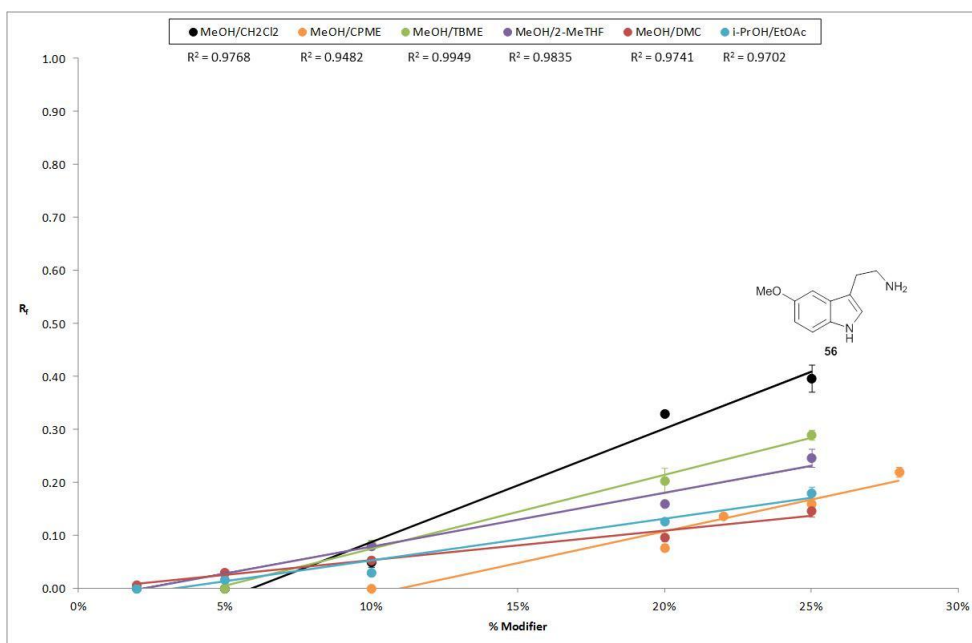
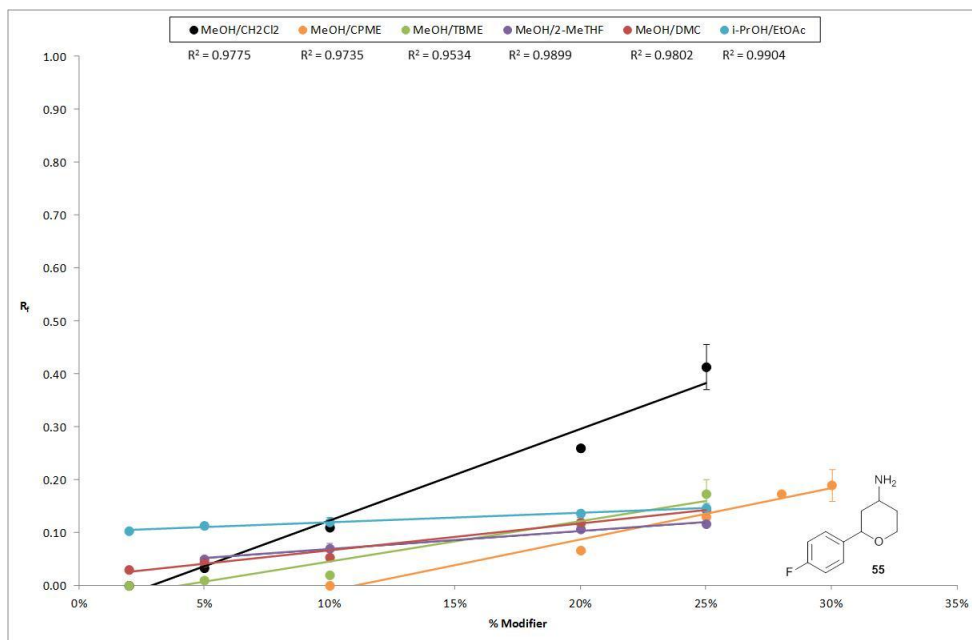


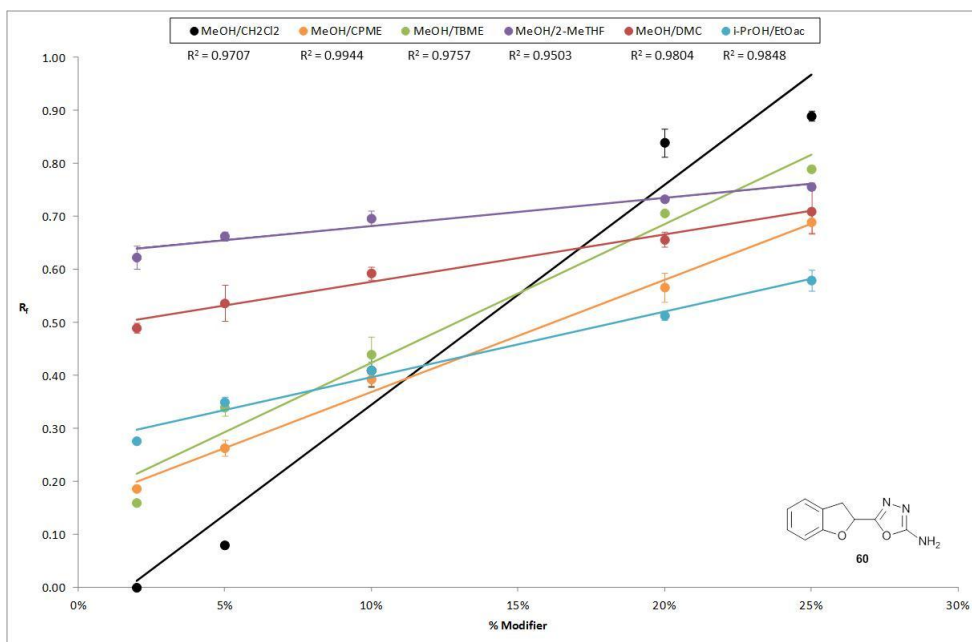
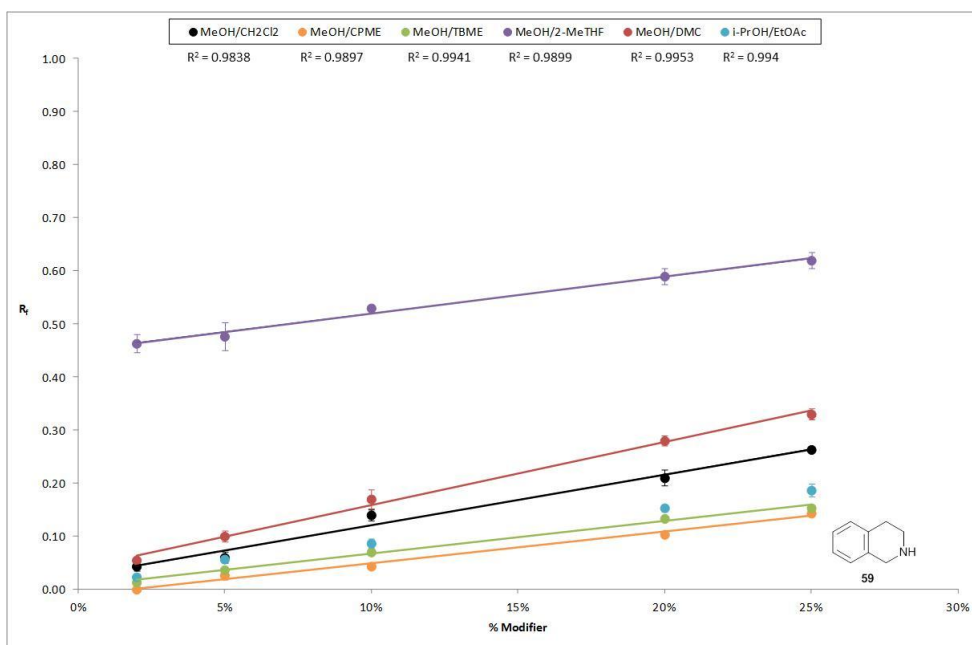
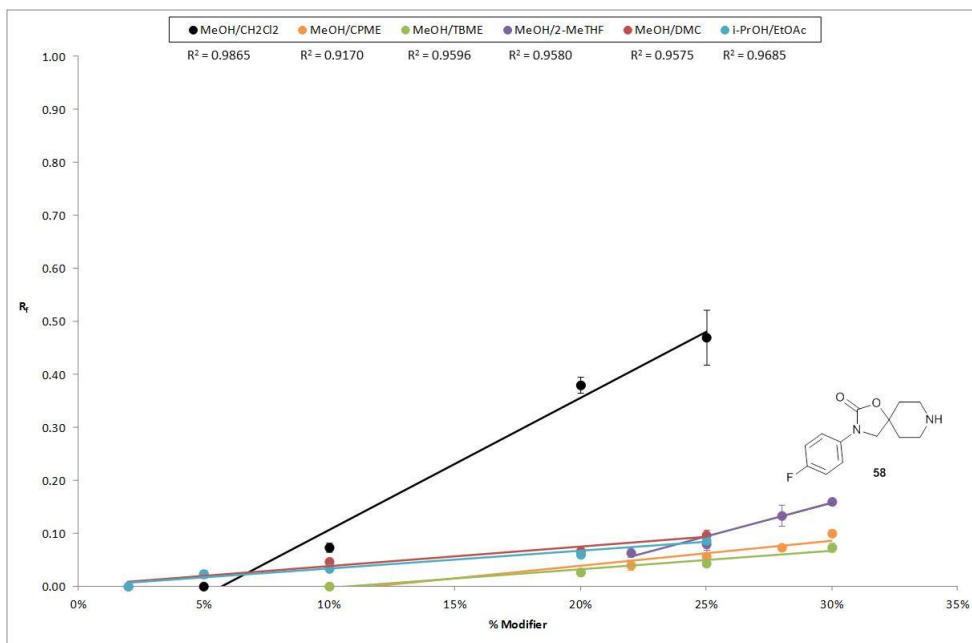


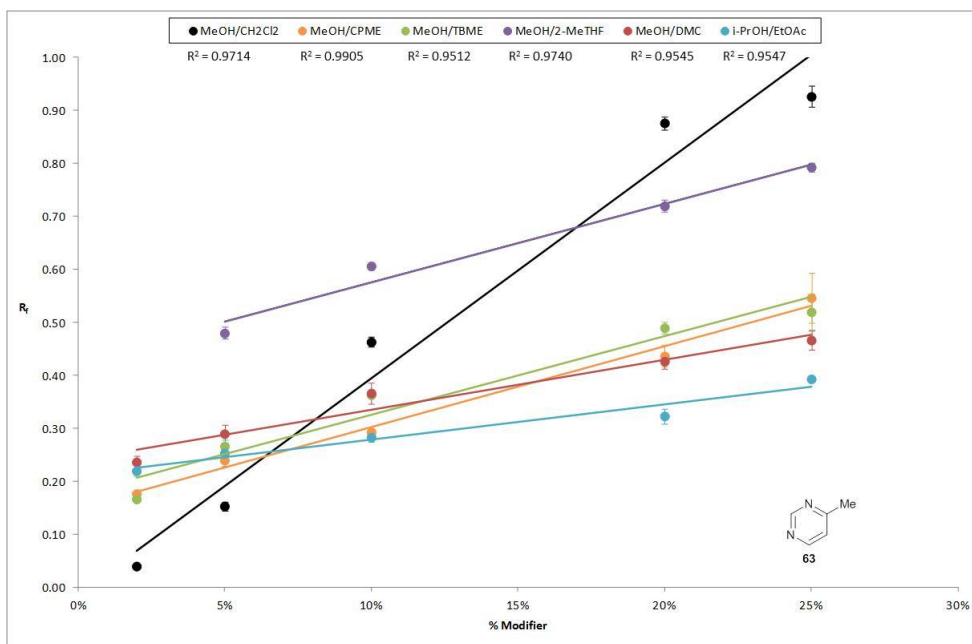
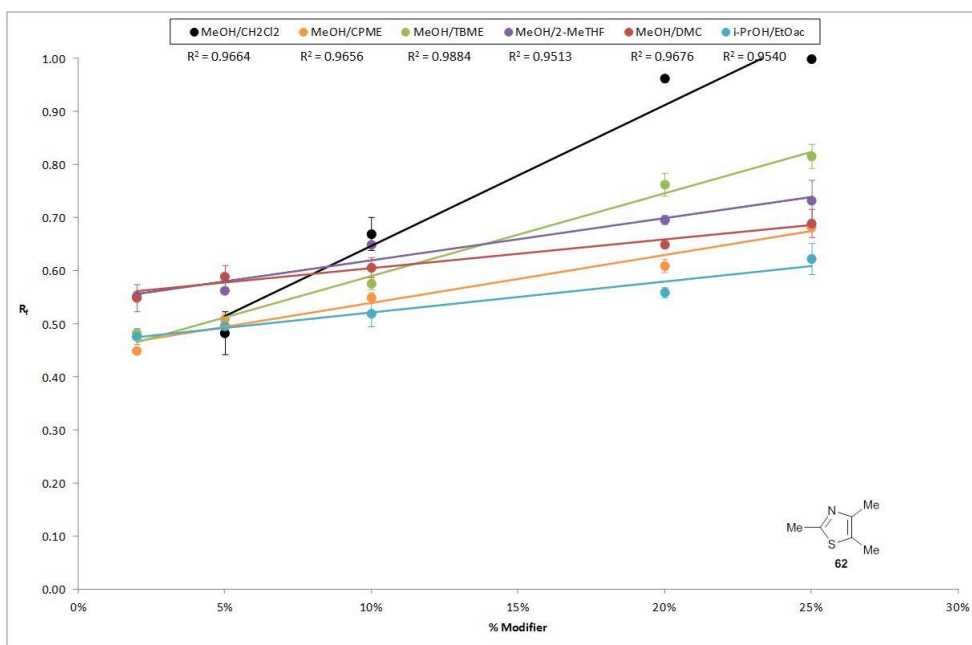
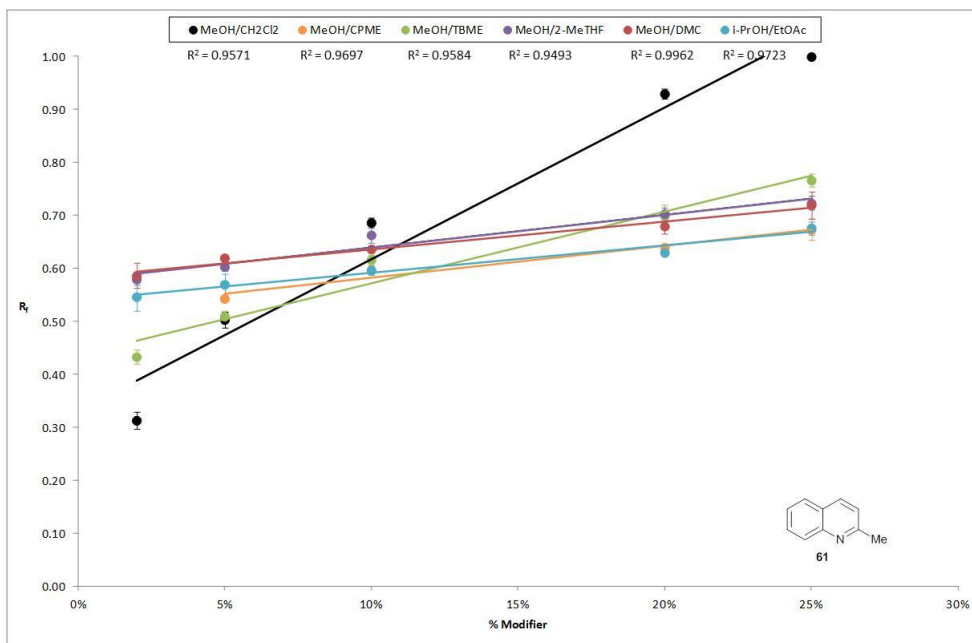


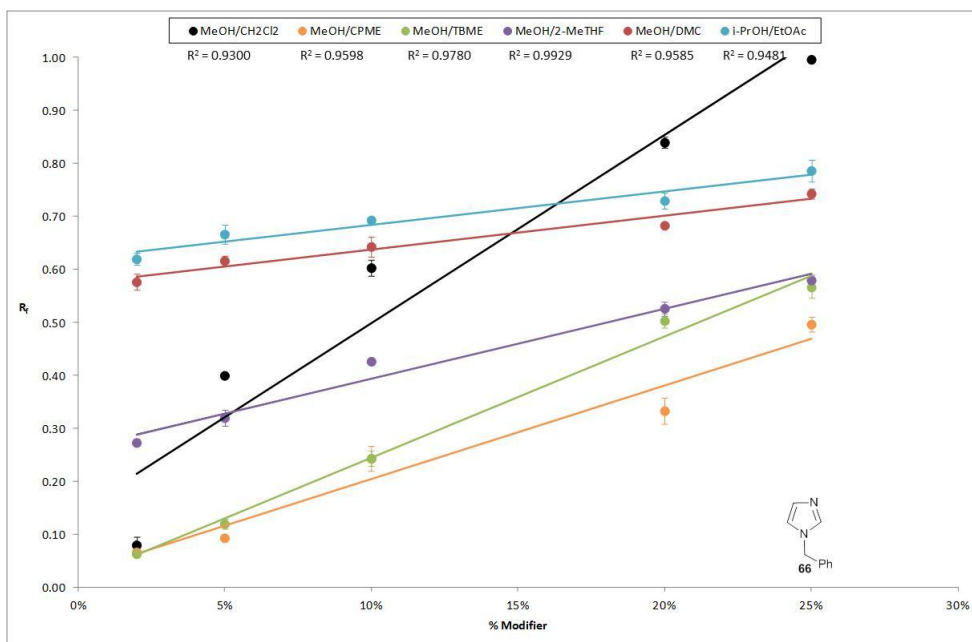
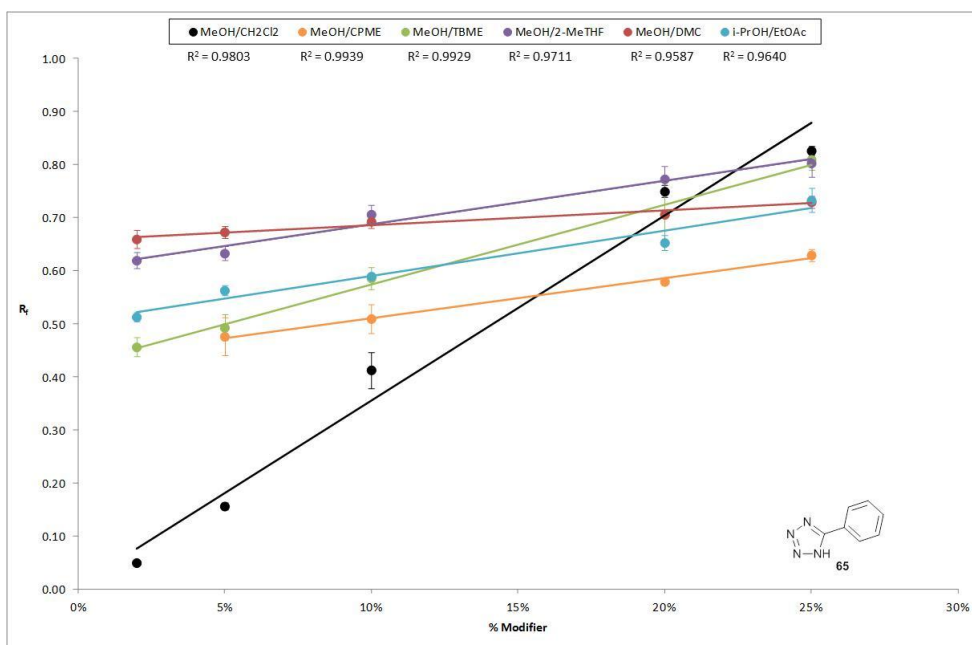
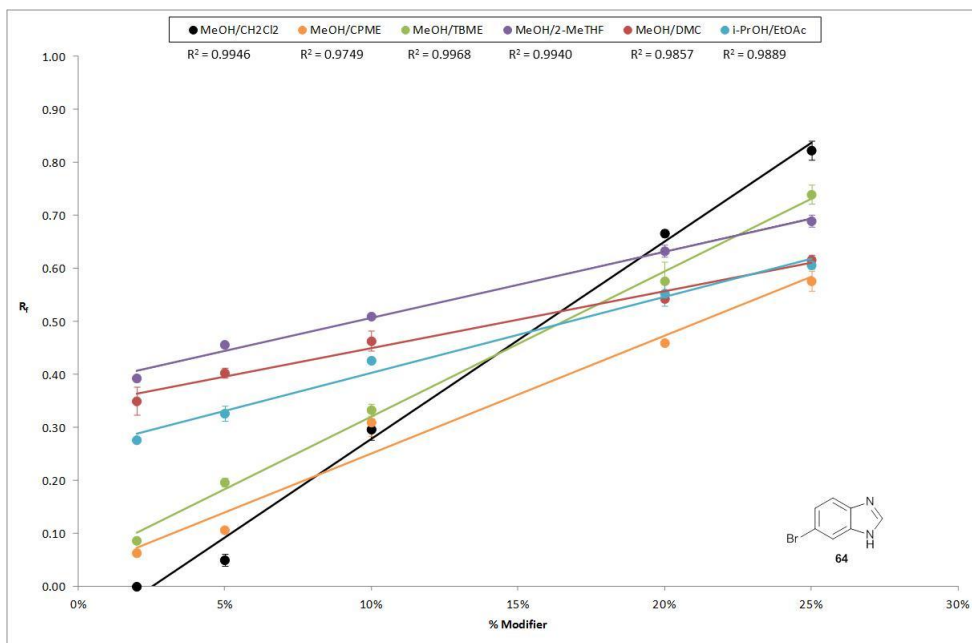


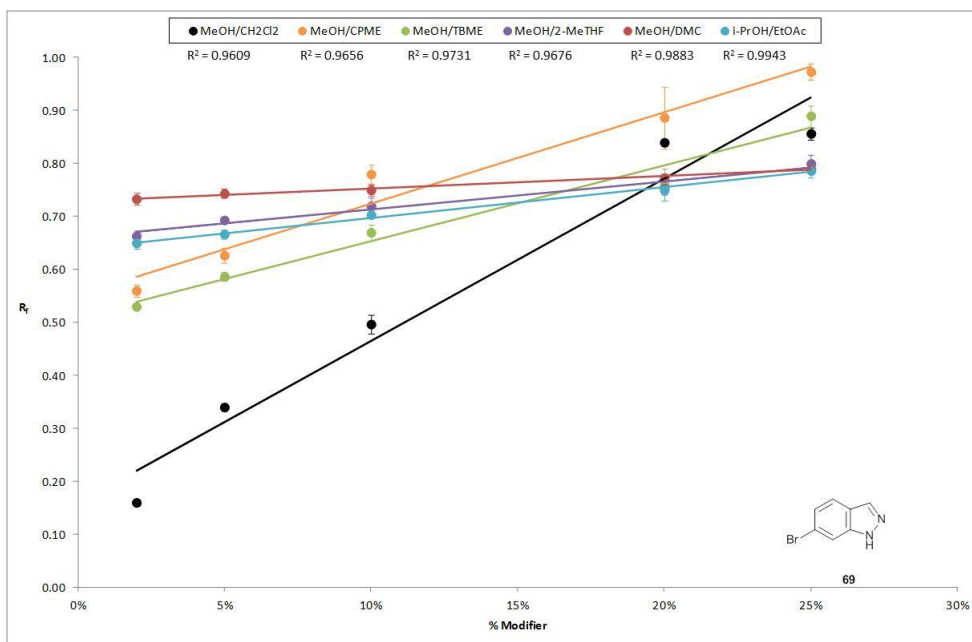
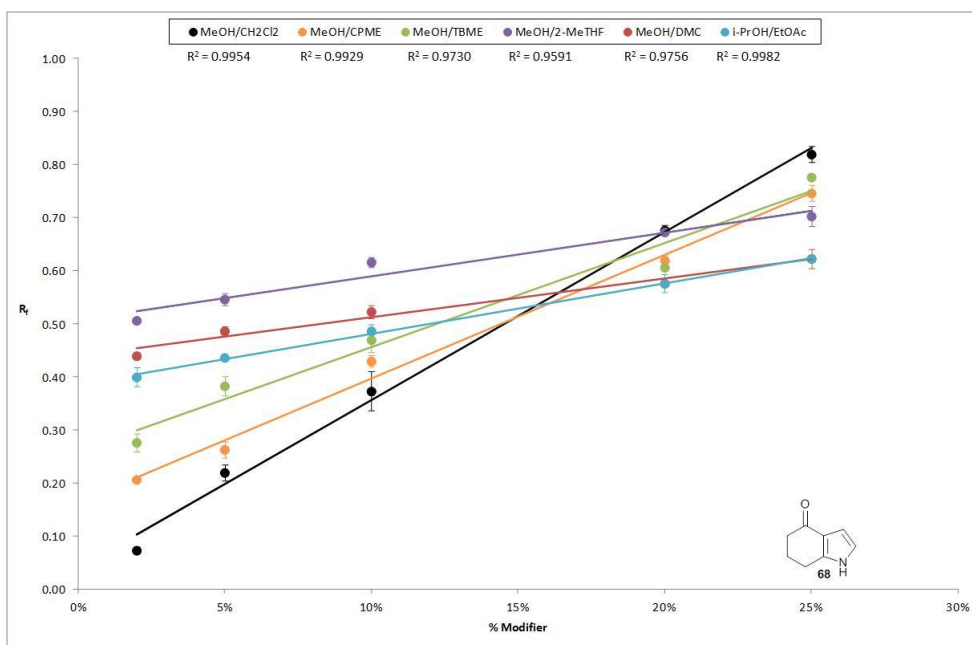
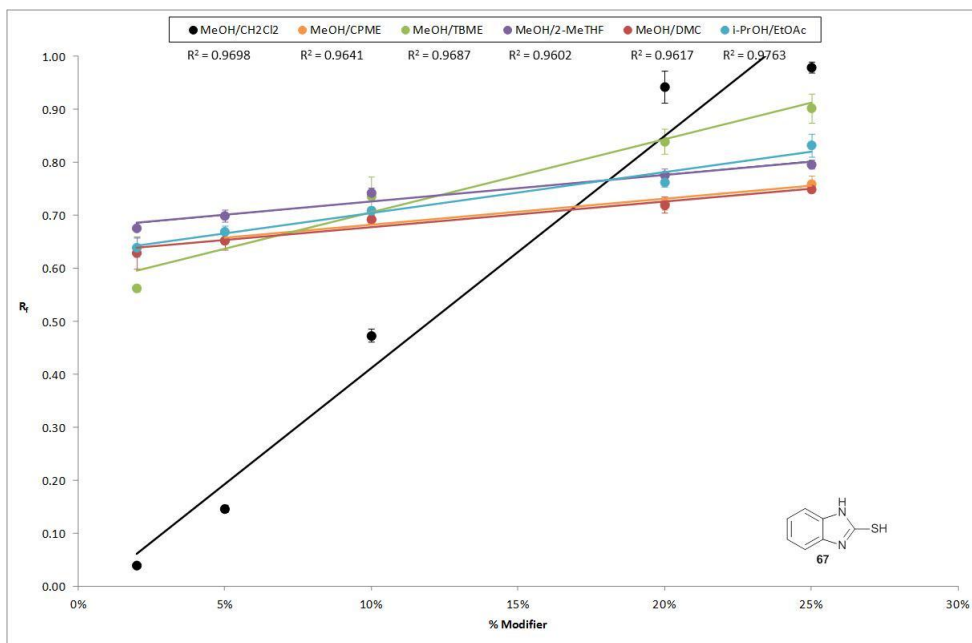


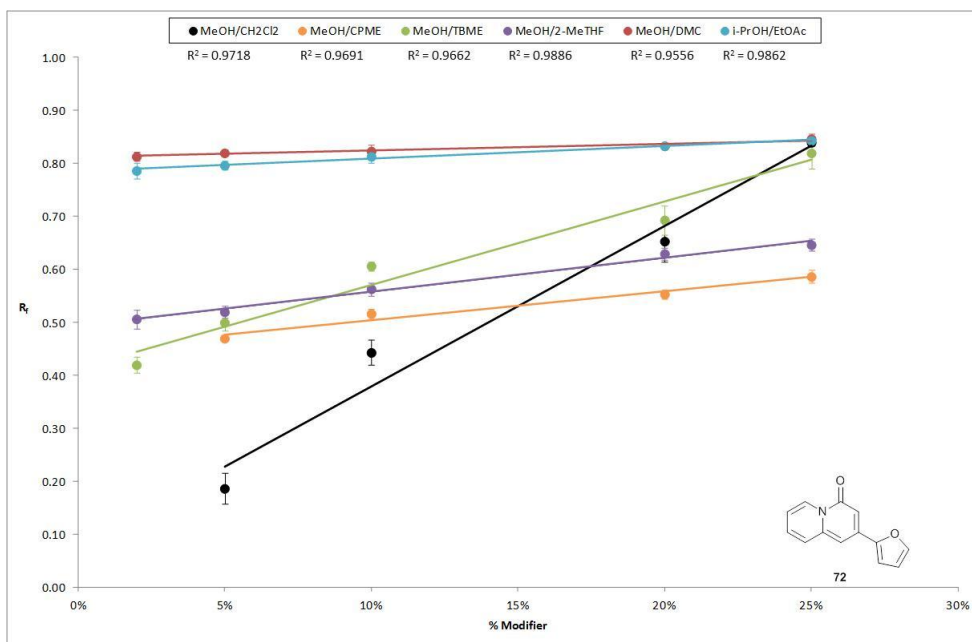
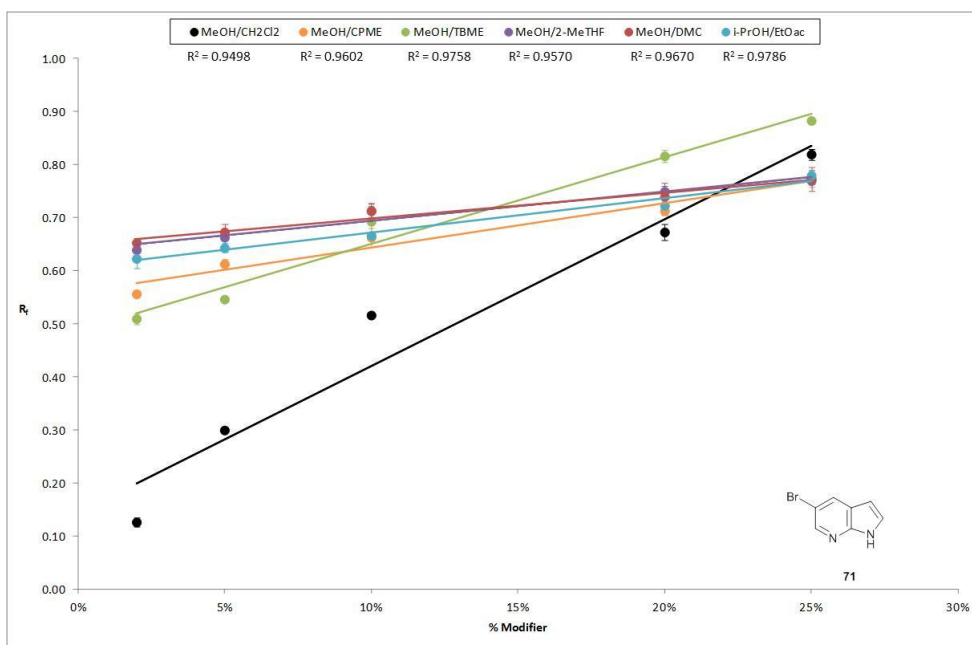
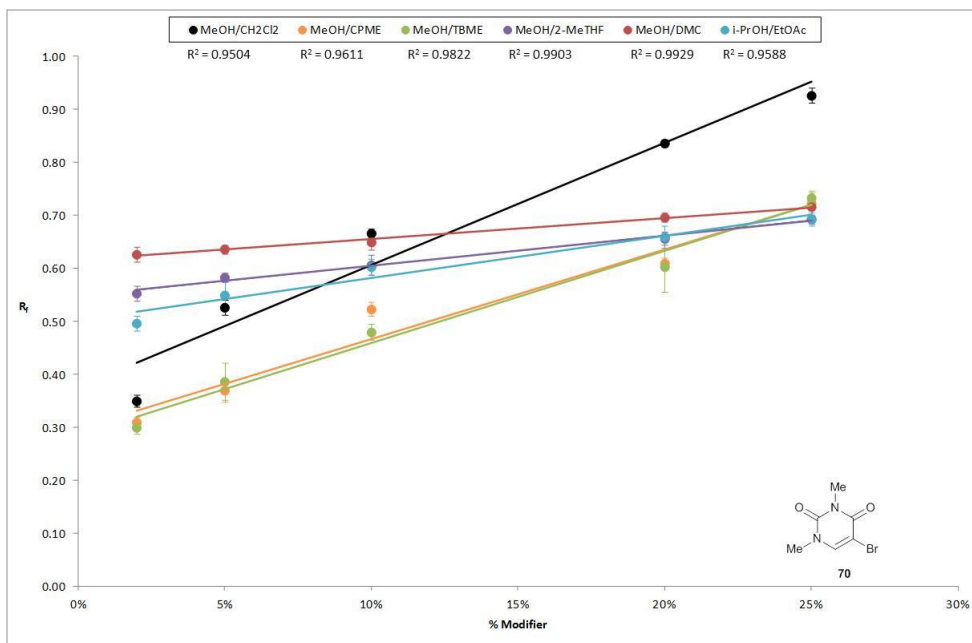


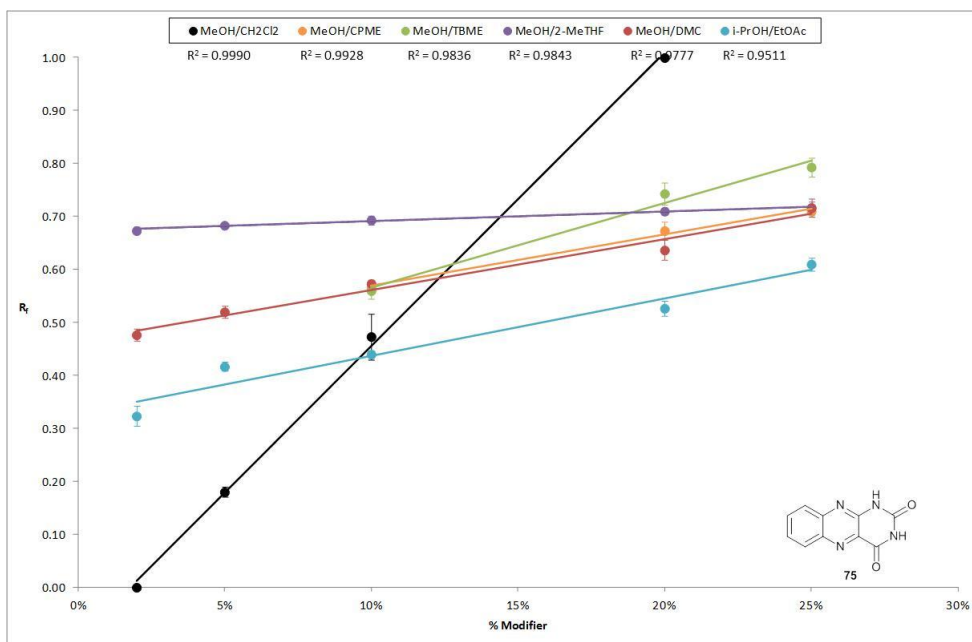
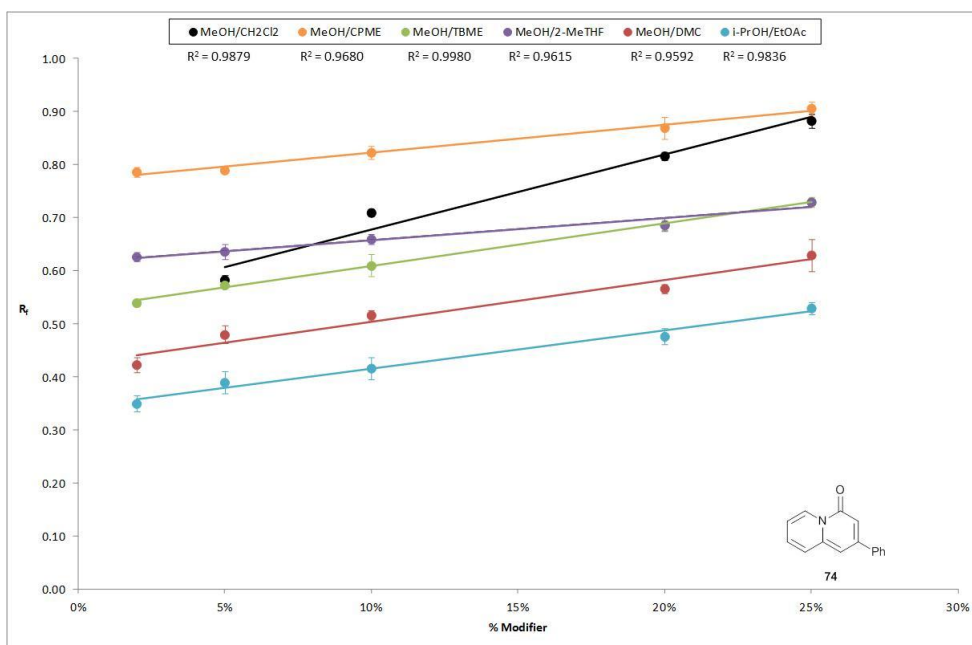
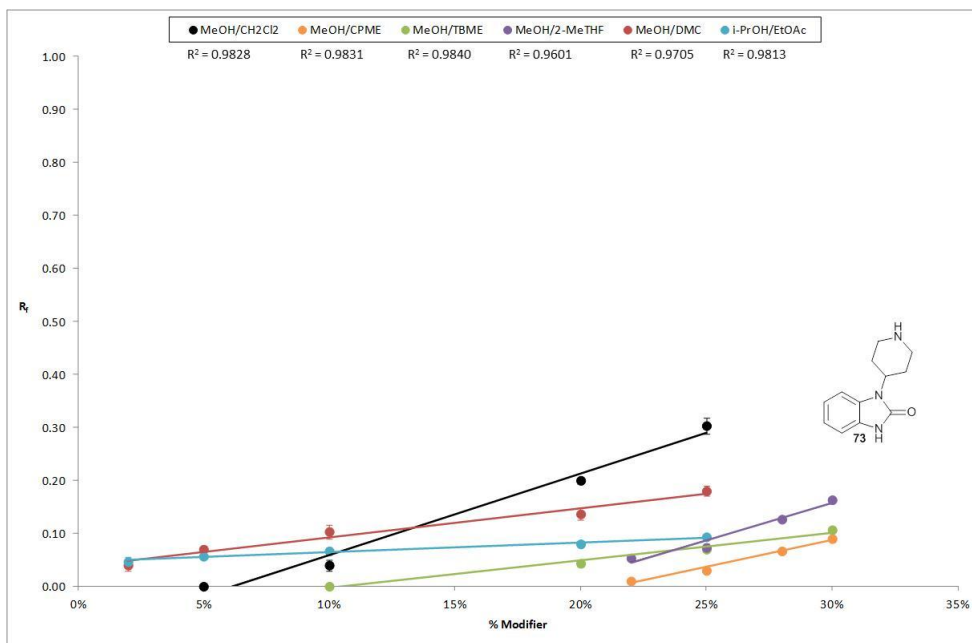


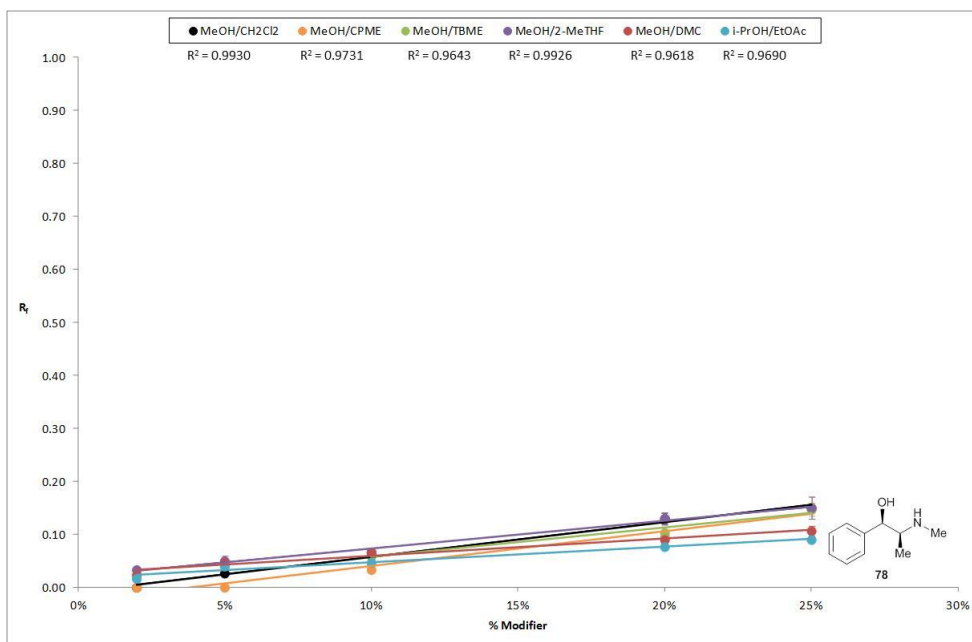
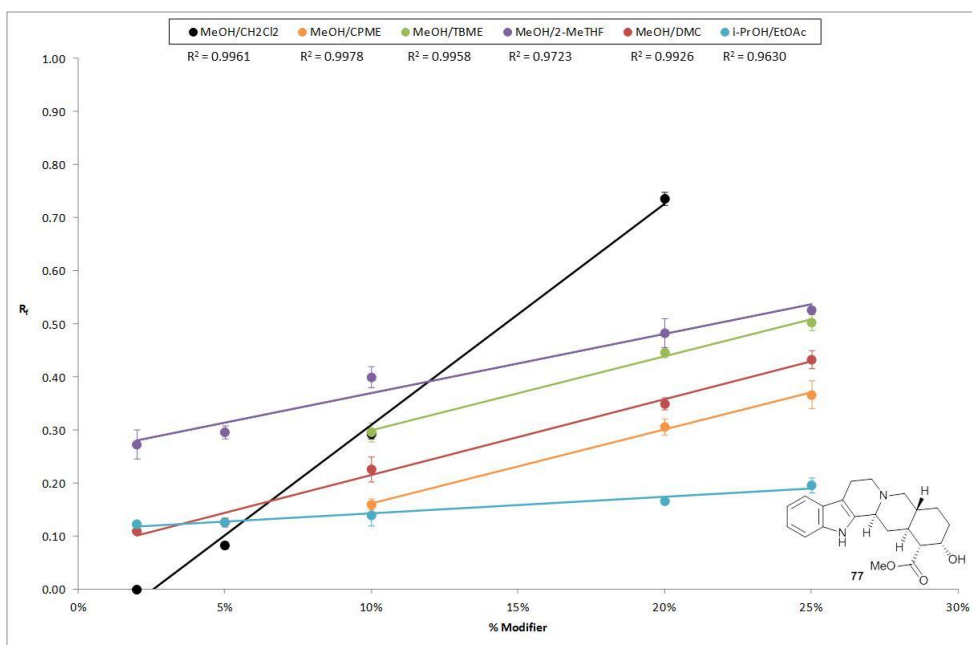
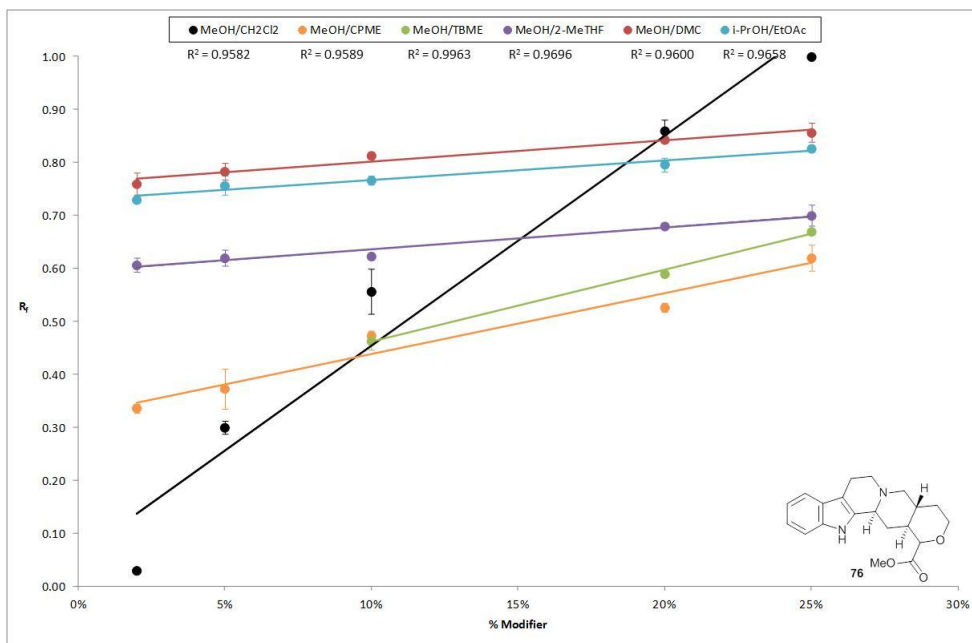


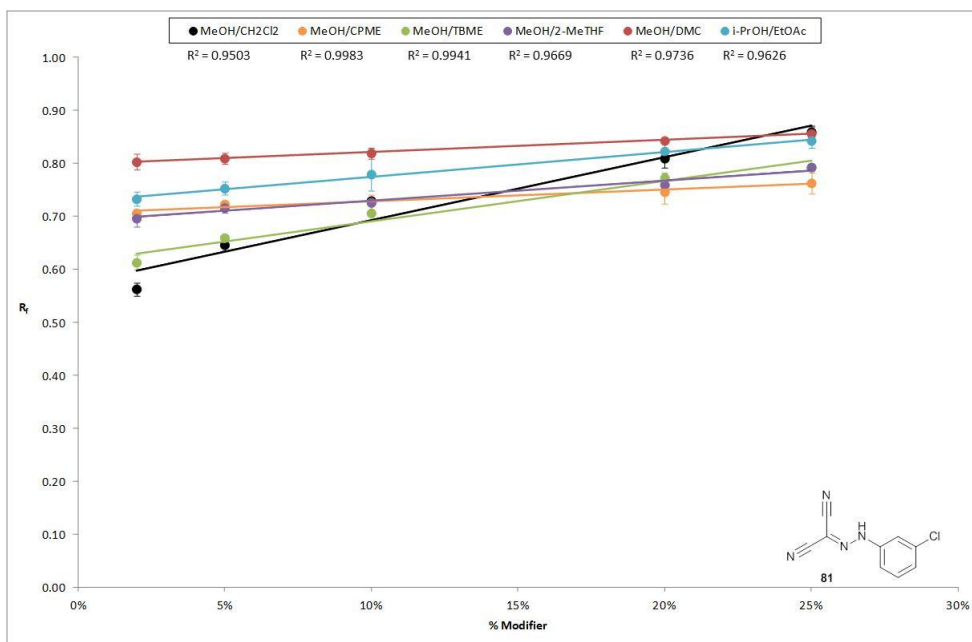
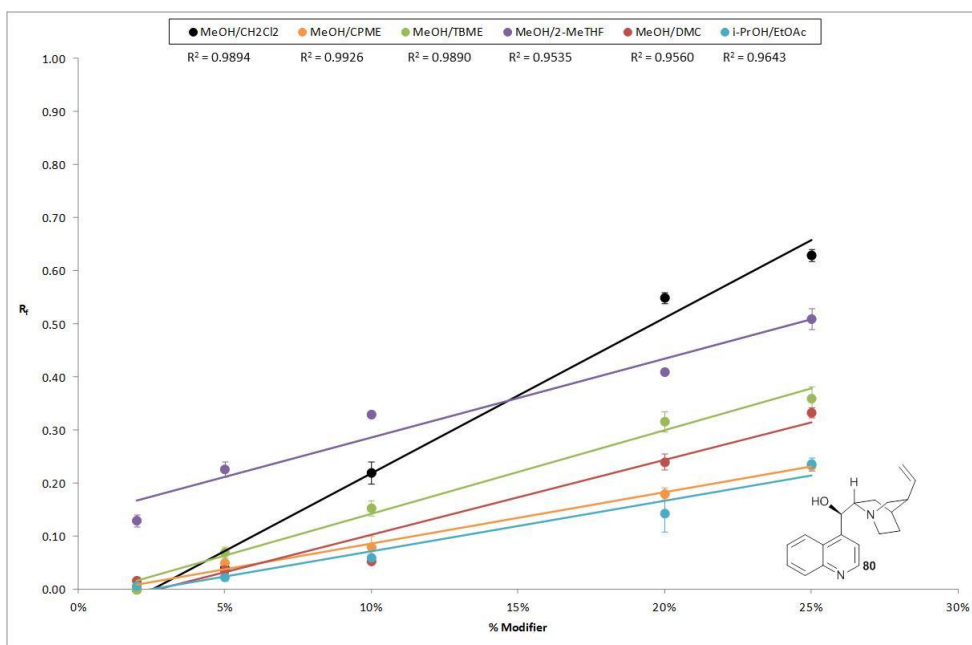
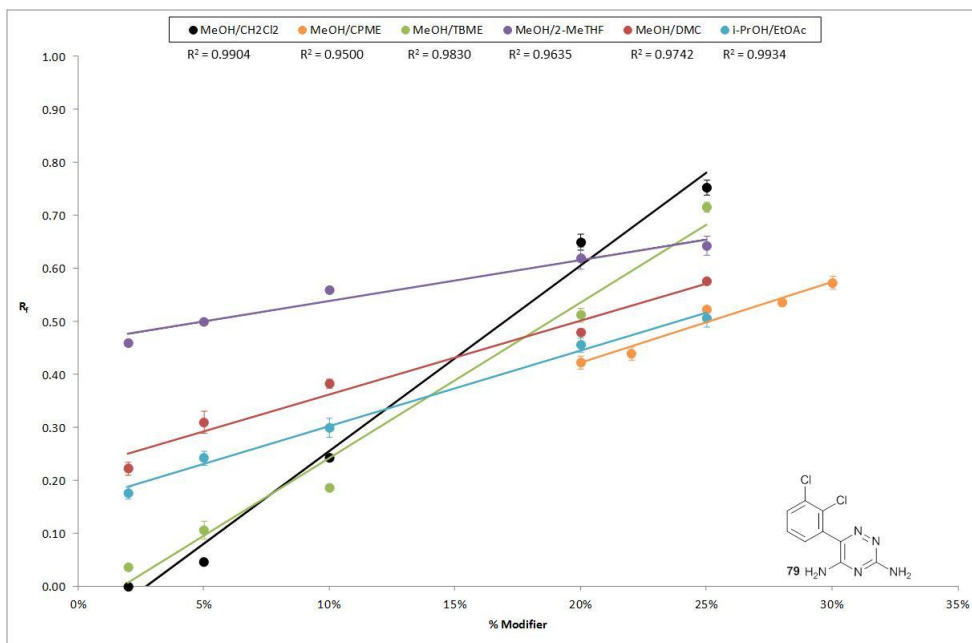


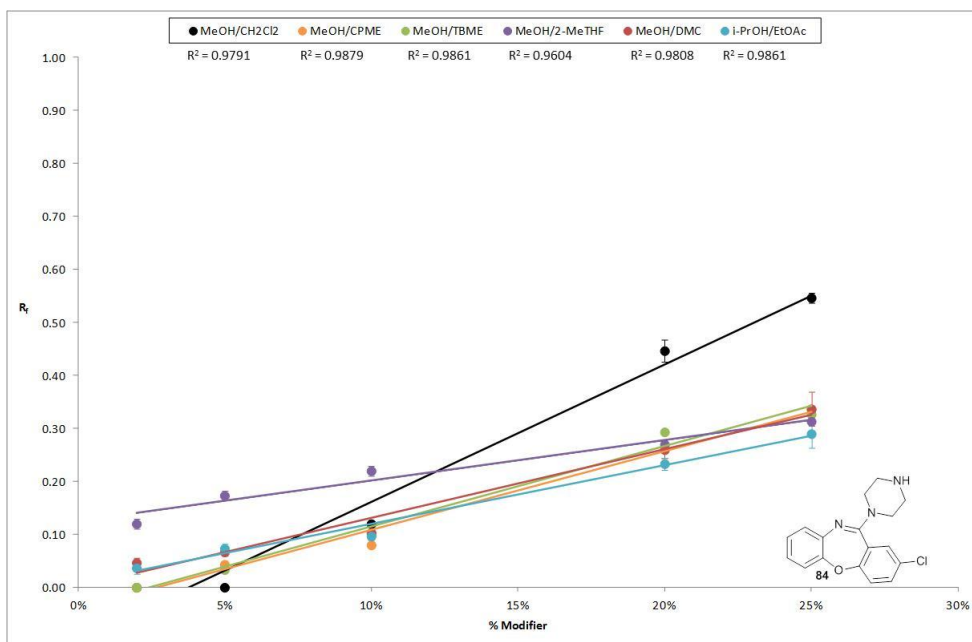
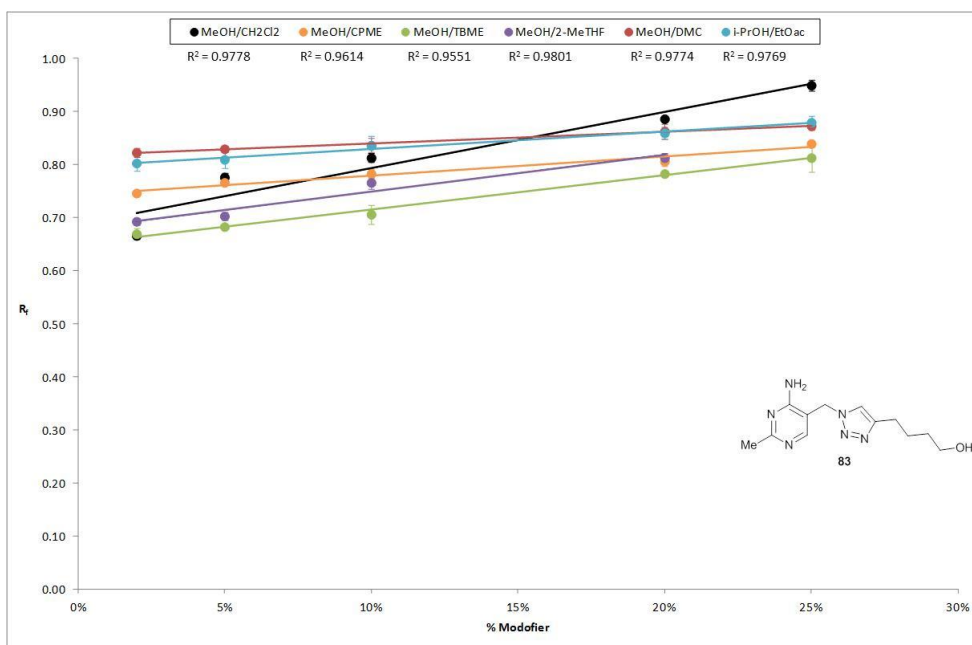
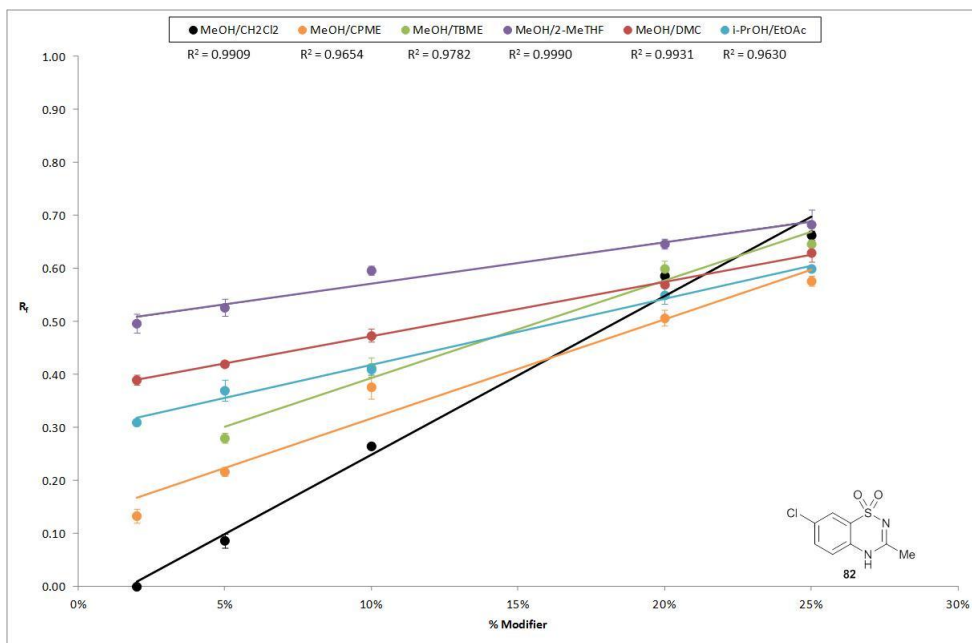


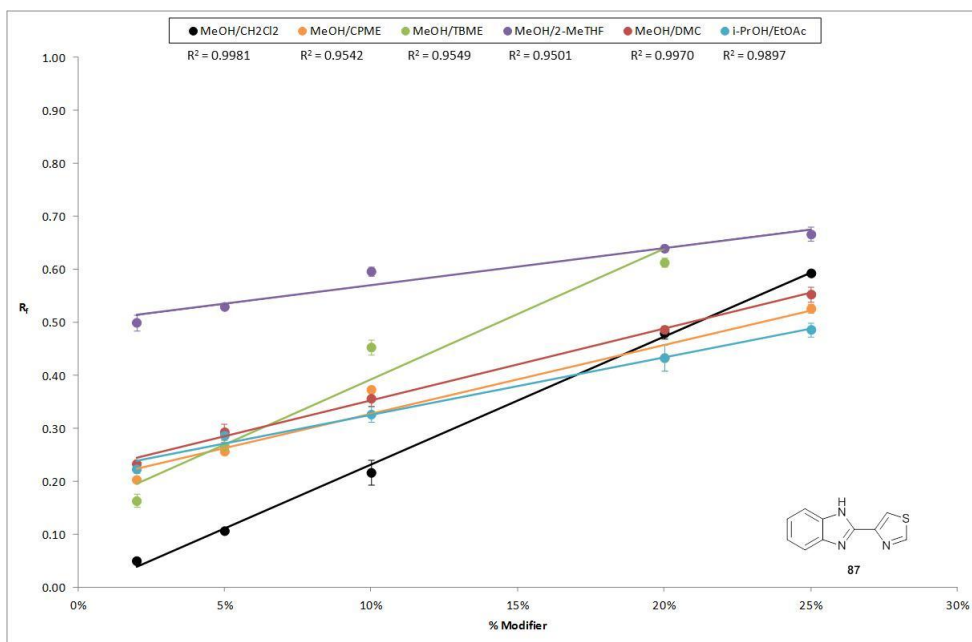
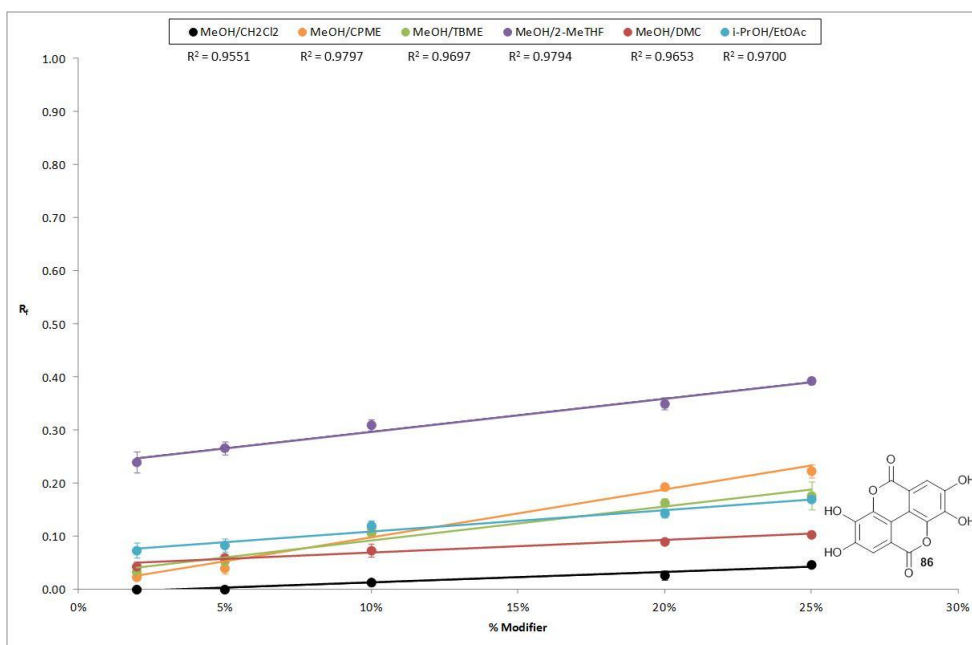
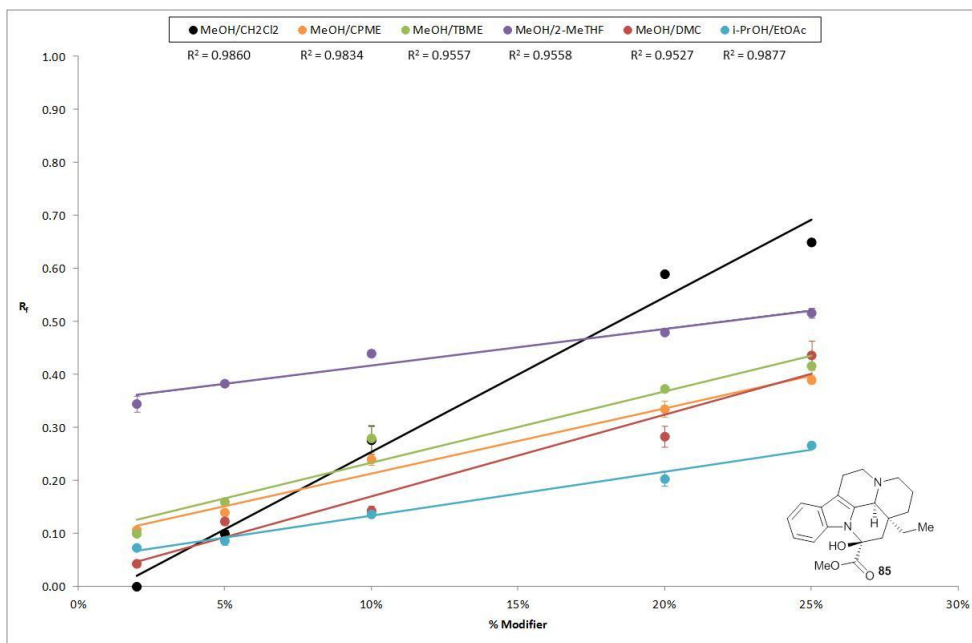


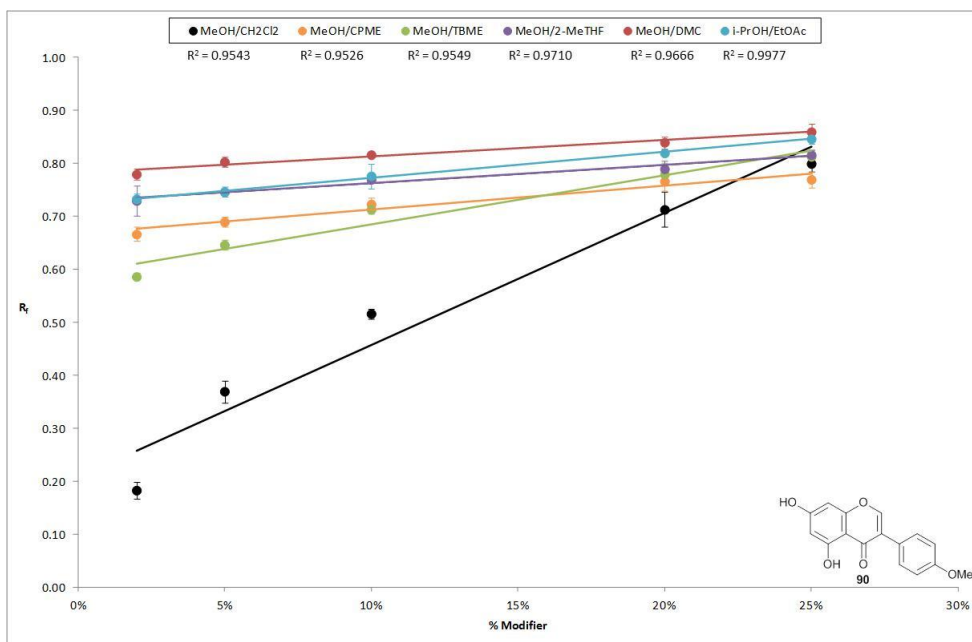
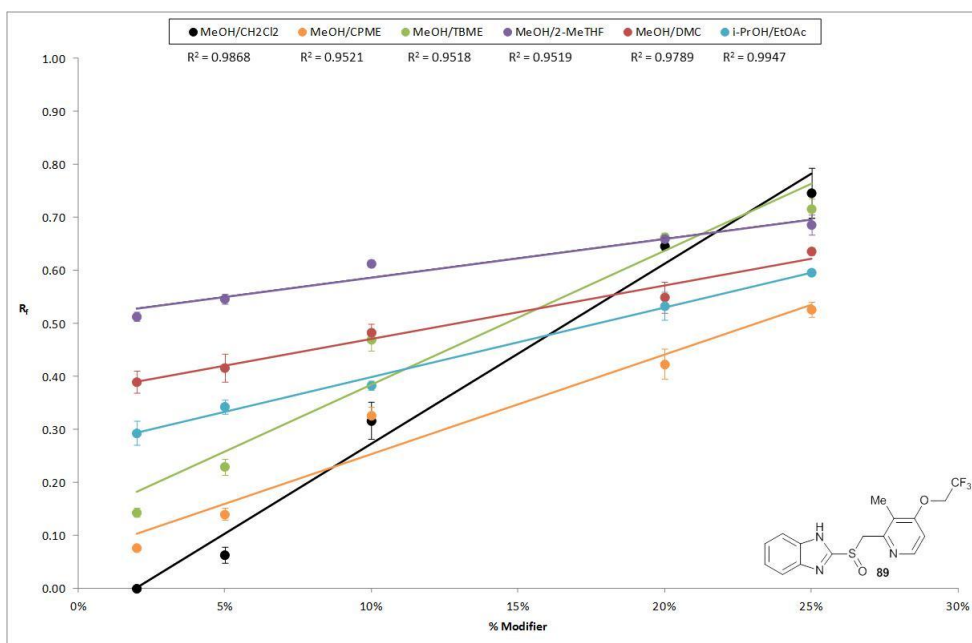
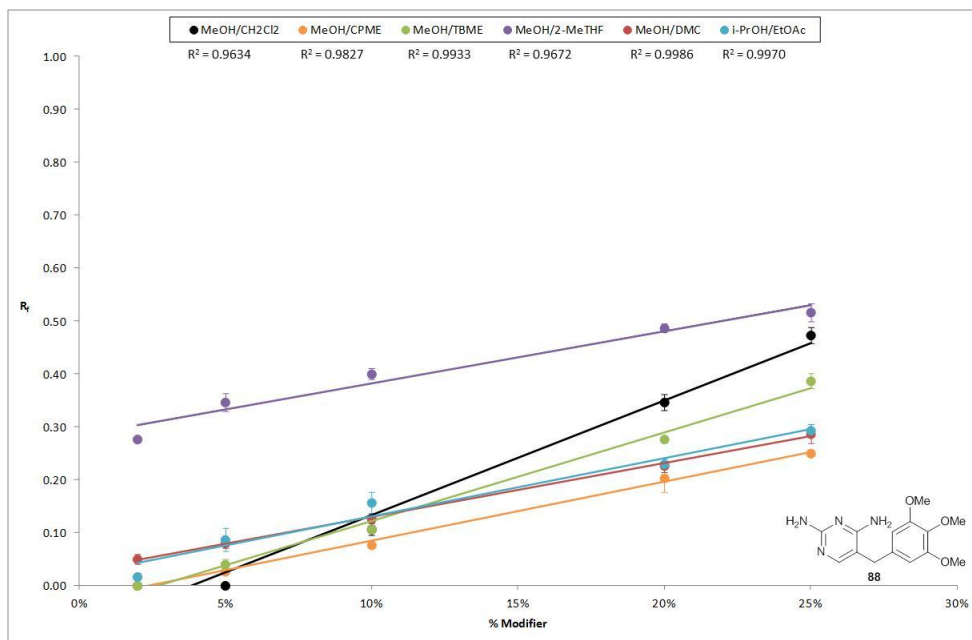


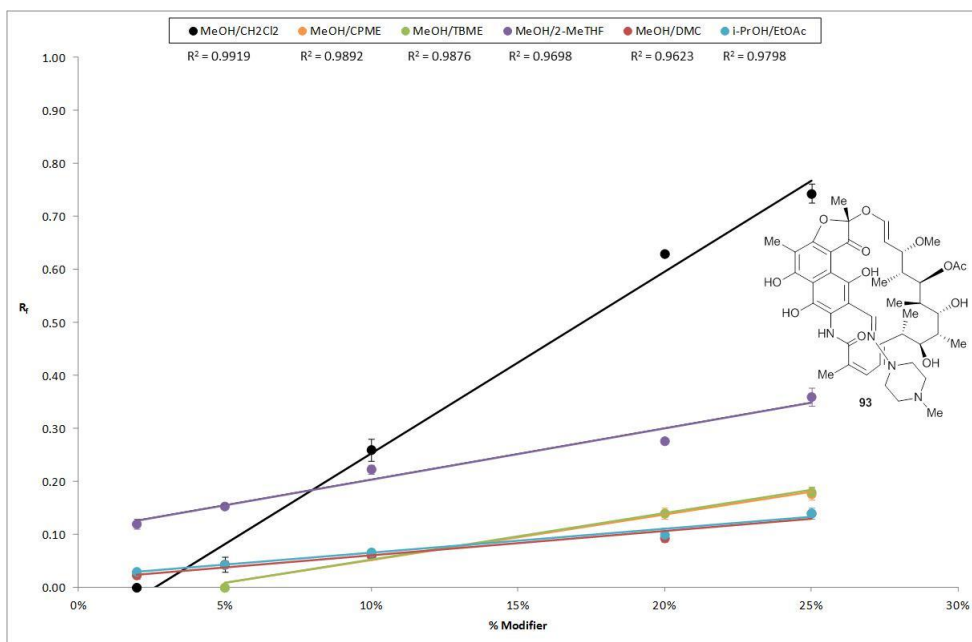
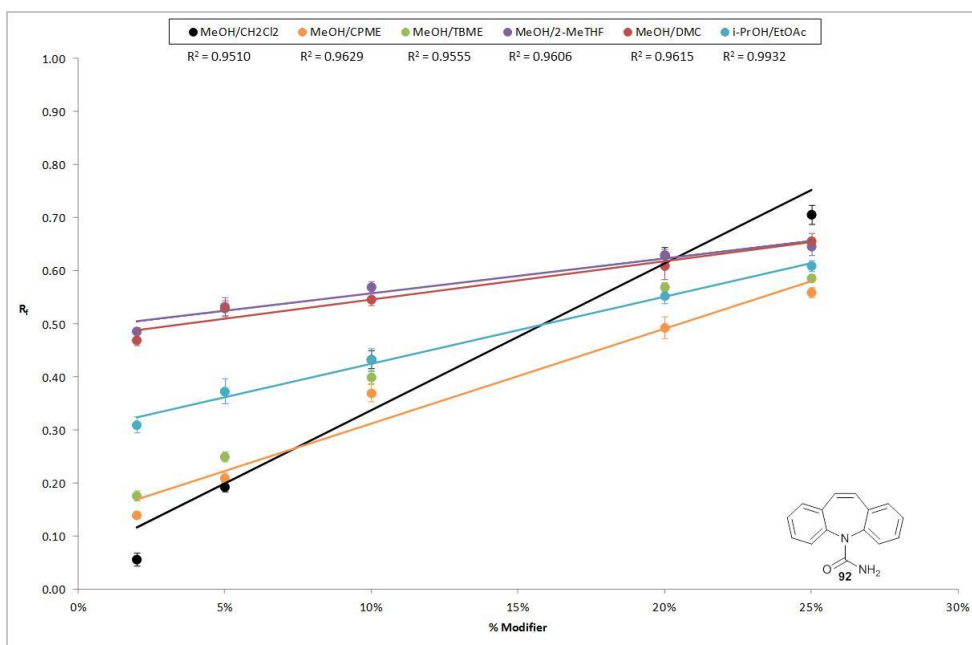
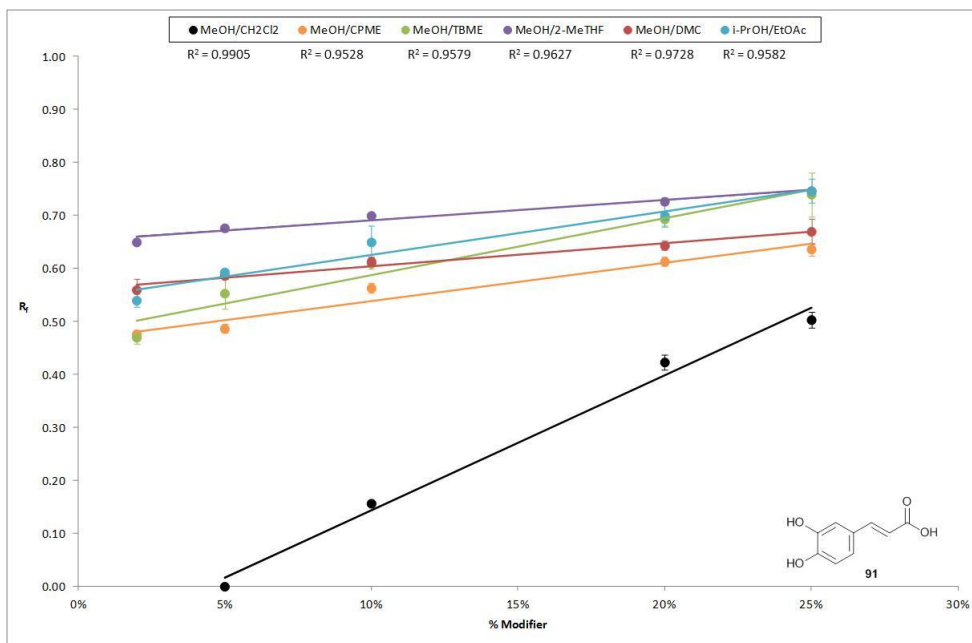


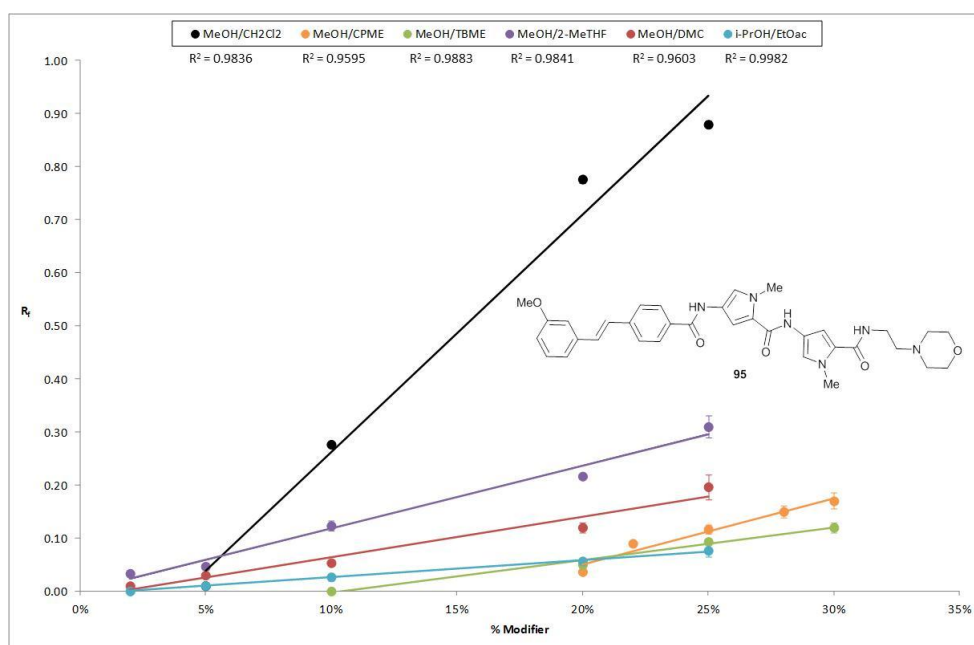
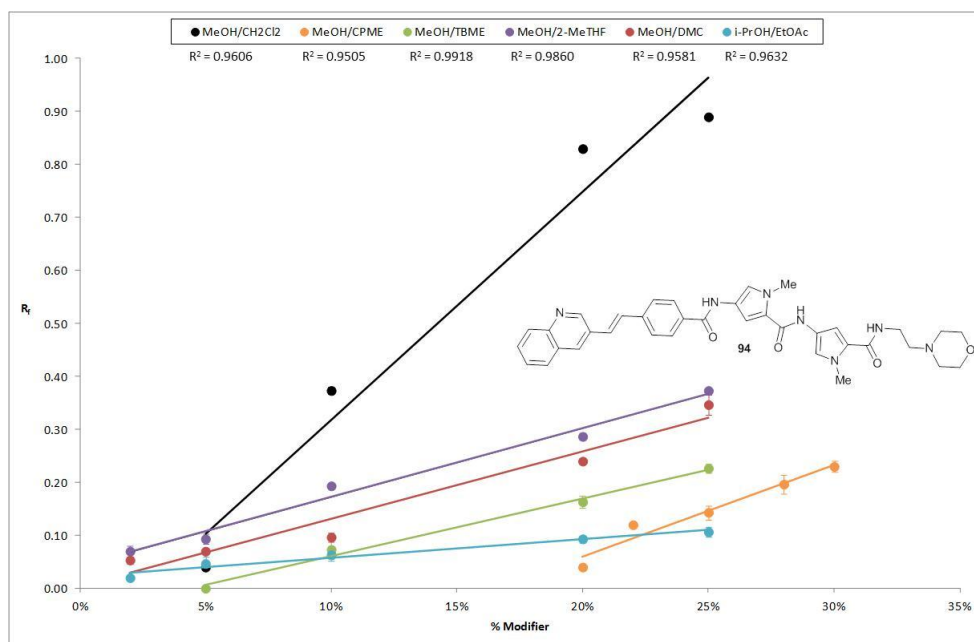






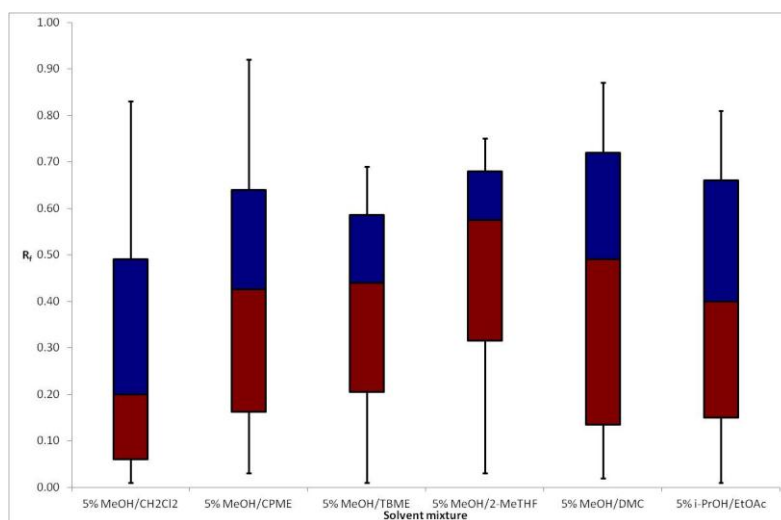




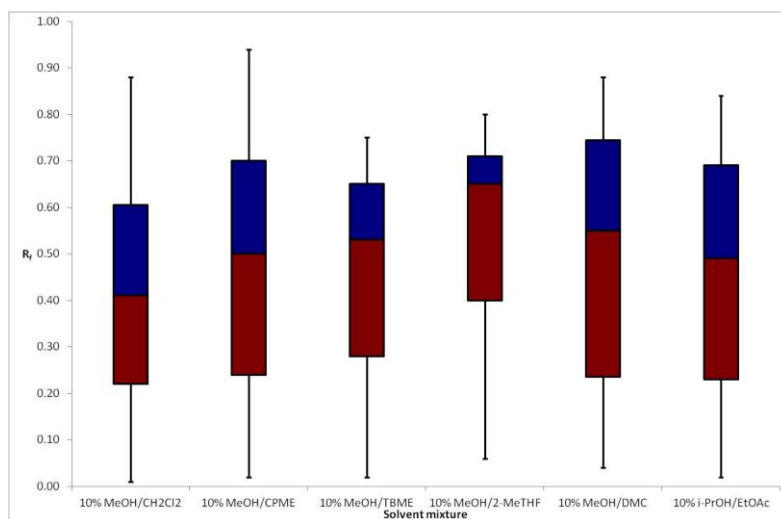


3.3 Box Plot Analyses

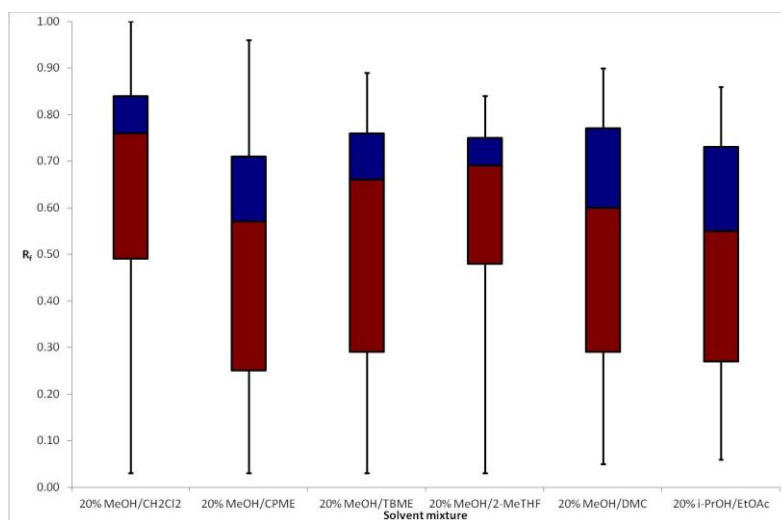
3.3.1 5% Modifier



3.3.2 10% Modifier

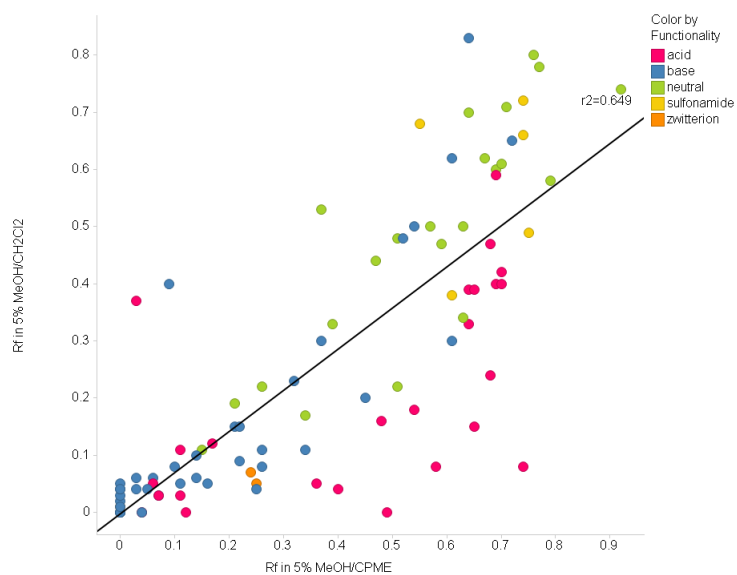


3.3.3 20% Modifier

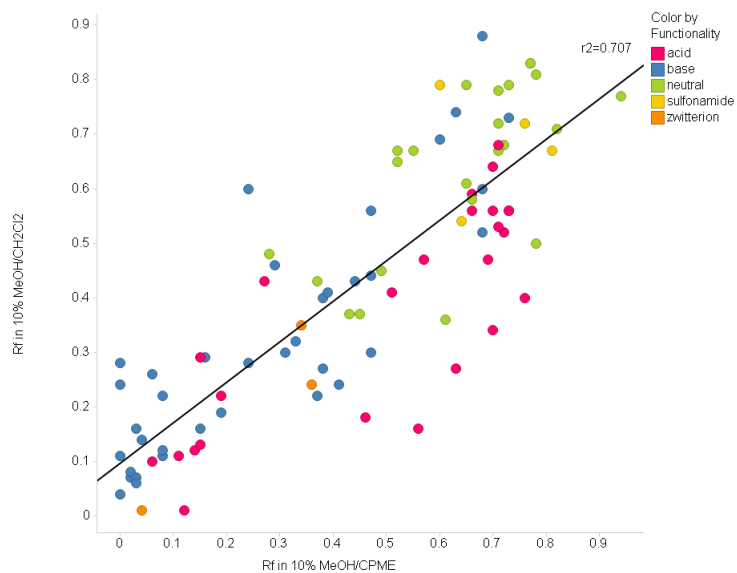


3.4 Spotfire Comparisons for All Eluents vs. MeOH/CH₂Cl₂

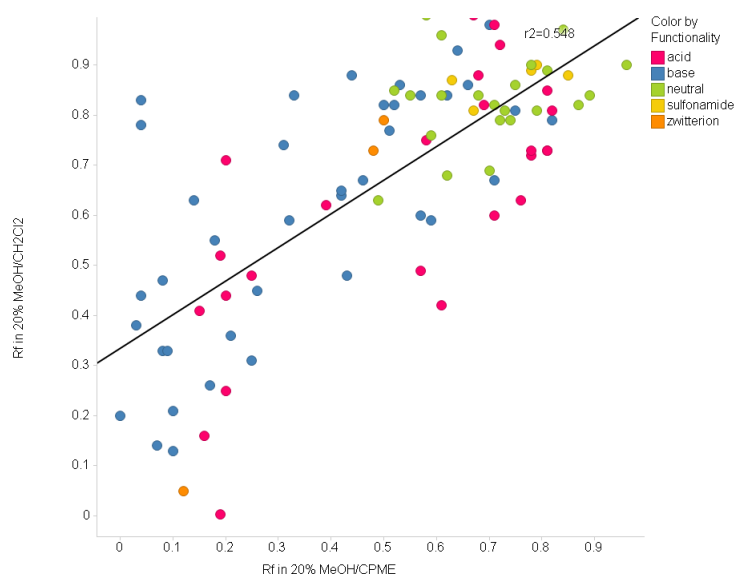
3.4.1 5% MeOH/CH₂Cl₂ vs. 5% MeOH/CPME



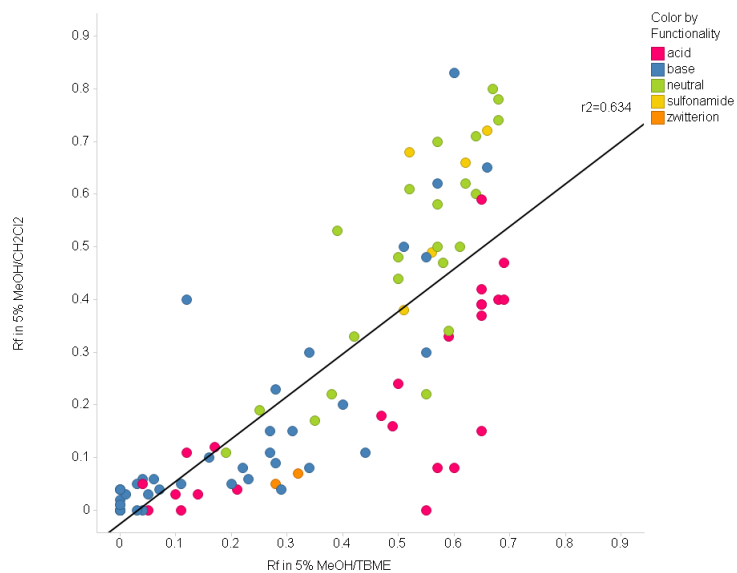
3.4.2 10% MeOH/CH₂Cl₂ vs. 10% MeOH/CPME



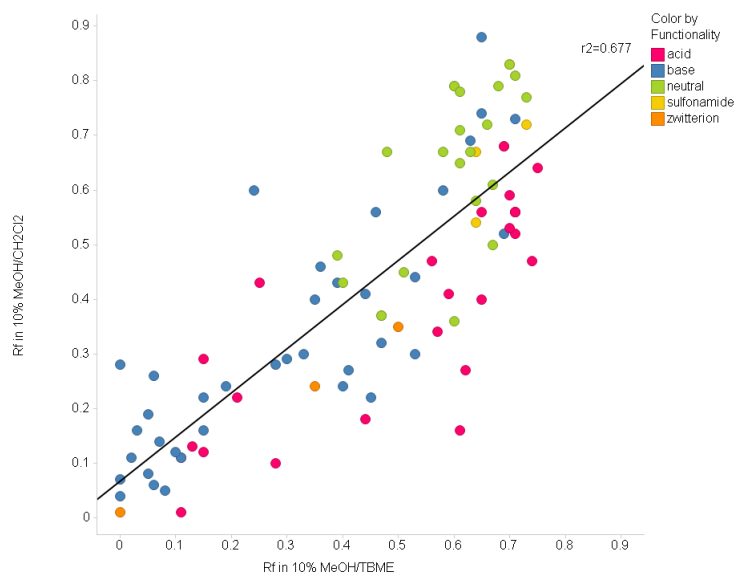
3.4.3 20% MeOH/CH₂Cl₂ vs. 20% MeOH/CPME



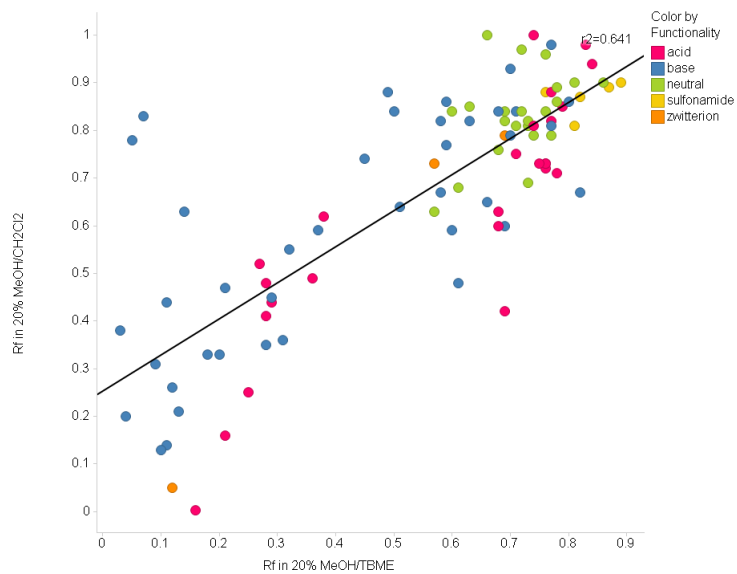
3.4.4 5% MeOH/CH₂Cl₂ vs. 5% MeOH/TBME



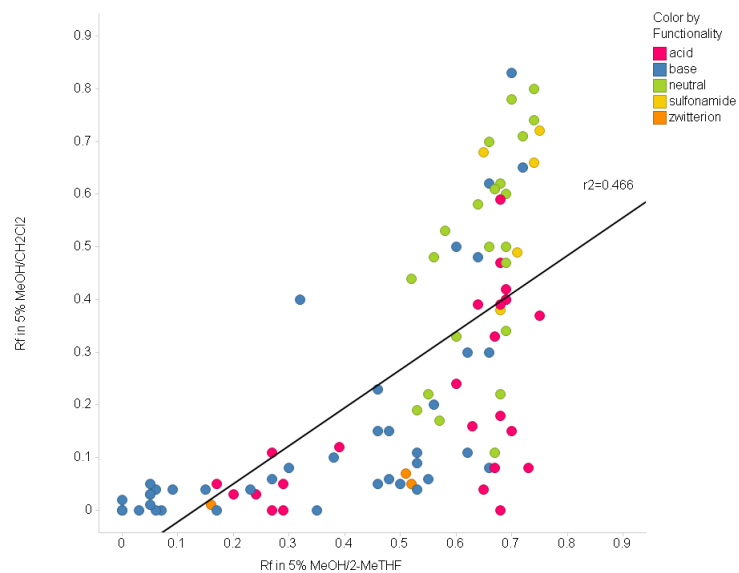
3.4.5 10% MeOH/CH₂Cl₂ vs. 10% MeOH/TBME



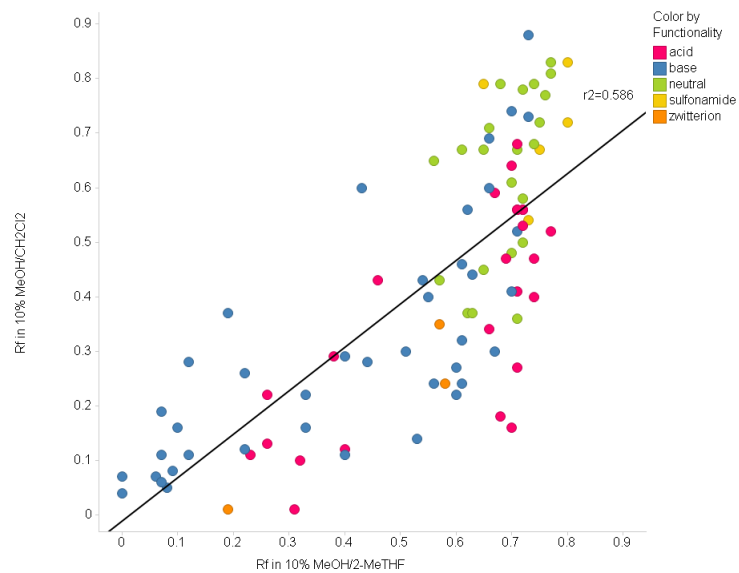
3.4.6 20% MeOH/CH₂Cl₂ vs. 20% MeOH/TBME



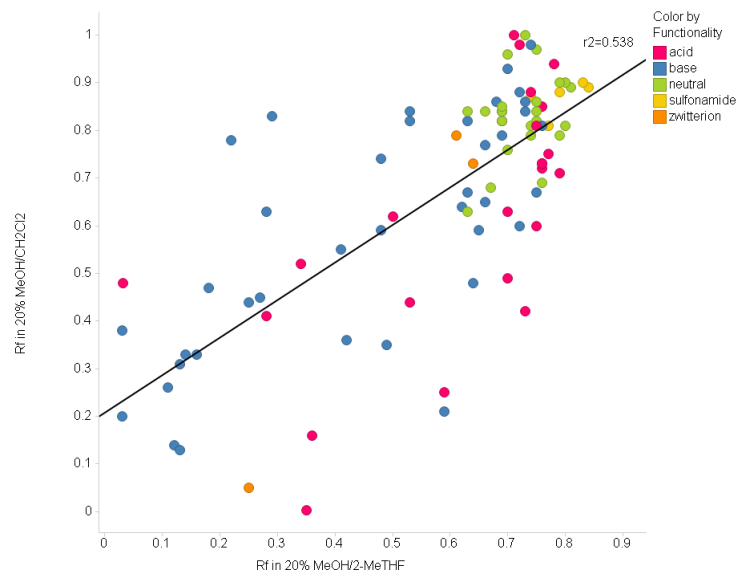
3.4.7 5% MeOH/CH₂Cl₂ vs. 5% MeOH/2-MeTHF



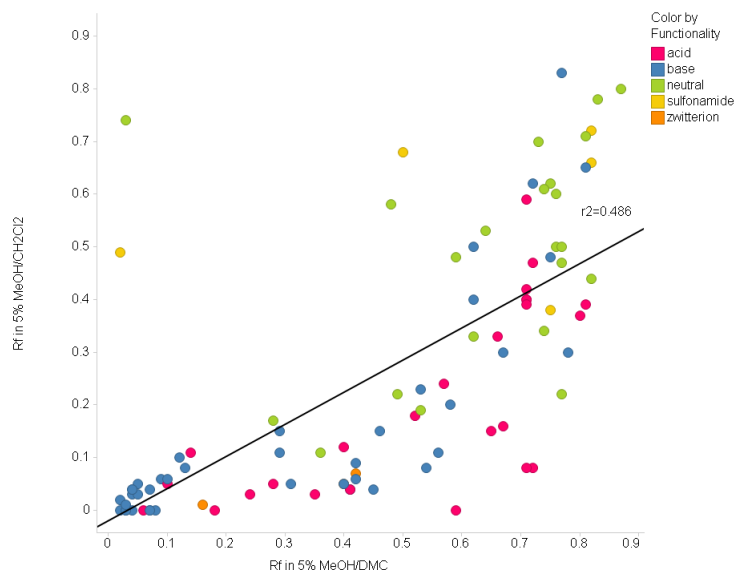
3.4.8 10% MeOH/CH₂Cl₂ vs. 10% MeOH/2-MeTHF



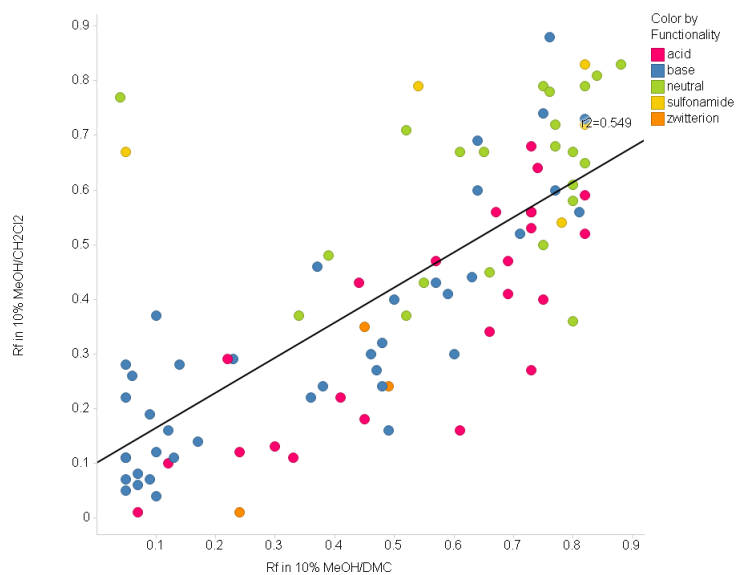
3.4.9 20% MeOH/CH₂Cl₂ vs. 20% MeOH/2-MeTHF



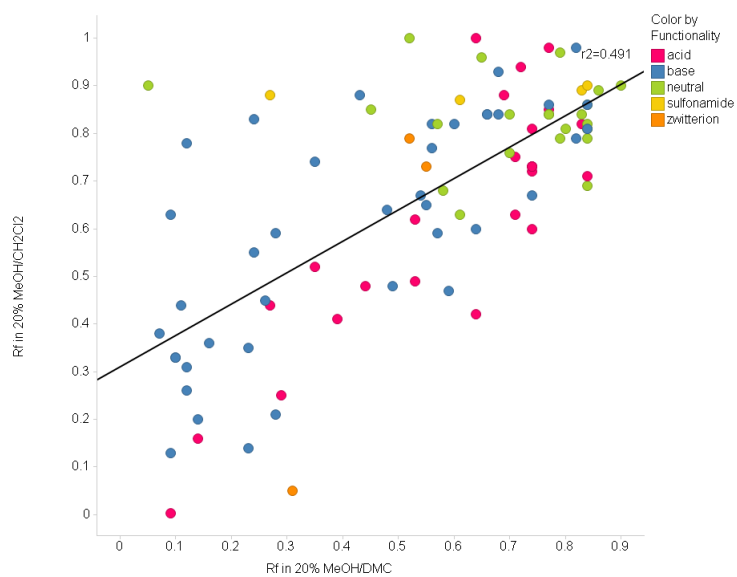
3.4.10 5% MeOH/CH₂Cl₂ vs. 5% MeOH/DMC



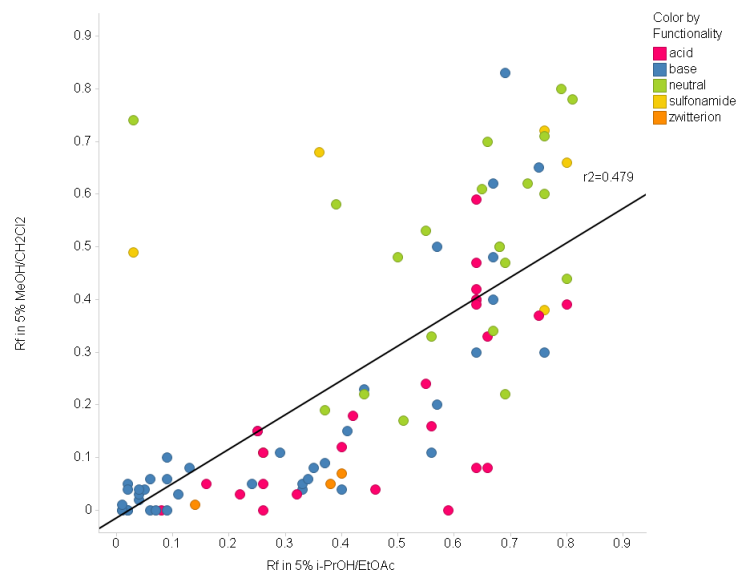
3.4.11 10% MeOH/CH₂Cl₂ vs. 10% MeOH/DMC



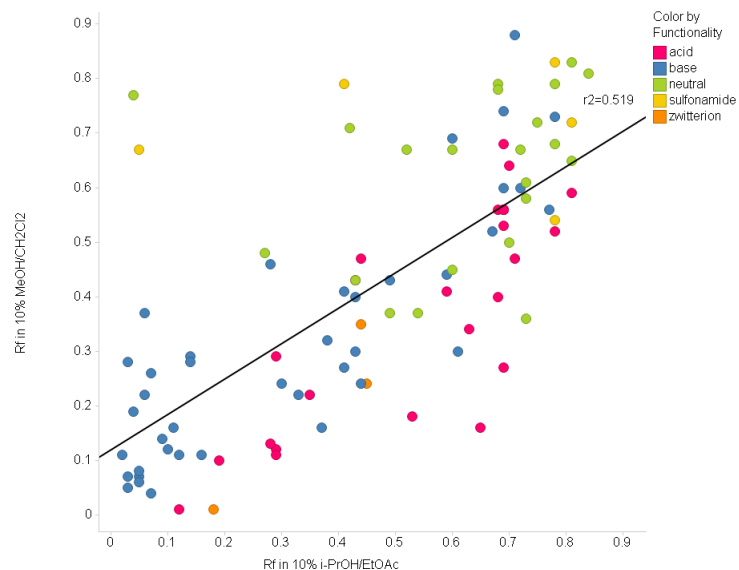
3.4.12 20% MeOH/CH₂Cl₂ vs. 20% MeOH/DMC



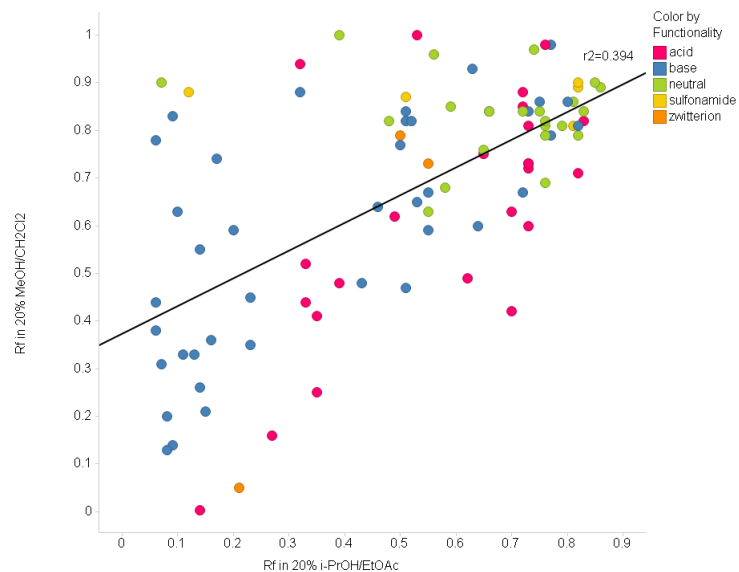
3.4.13 5% MeOH/CH₂Cl₂ vs. 5% *i*-PrOH/EtOAc



3.4.14 10% MeOH/CH₂Cl₂ vs. 10% *i*-PrOH/EtOAc



3.4.15 20% MeOH/CH₂Cl₂ vs. 20% *i*-PrOH/EtOAc



4. References

1. www.knime.org.