

## Contents

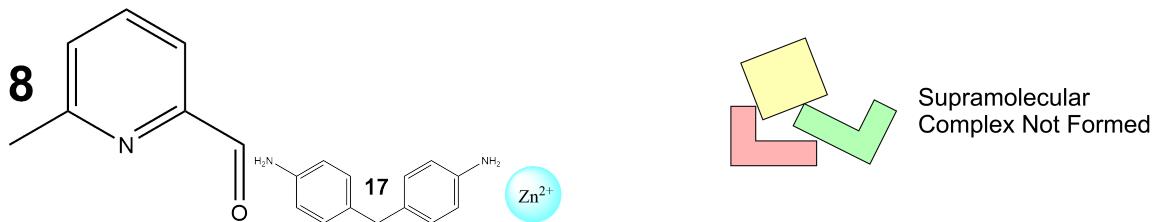
Reaction 1	5
Reaction 2	7
Reaction 3	8
Reaction 4	10
Reaction 5	11
Reaction 7	12
Reaction 8	14
Reaction 9	15
Reaction 10	17
Reaction 11	18
Reaction 12	19
Reaction 13	21
Reaction 14	22
Reaction 15	24
Reaction 16	25
Reaction 17	27
Reaction 18	28
Reaction 19	30
Reaction 20	31
Reaction 21	32
Reaction 23	34
Reaction 24	35
Reaction 26	36
Reaction 27	38
Reaction 28	39
Reaction 29	41
Reaction 30	42
Reaction 31	44
Reaction 32	45

<b>Reaction 33</b>	<b>46</b>
<b>Reaction 34</b>	<b>48</b>
<b>Reaction 35</b>	<b>49</b>
<b>Reaction 36</b>	<b>50</b>
<b>Reaction 37</b>	<b>52</b>
<b>Reaction 38</b>	<b>54</b>
<b>Reaction 39</b>	<b>56</b>
<b>Reaction 40</b>	<b>58</b>
<b>Reaction 41</b>	<b>59</b>
<b>Reaction 42</b>	<b>61</b>
<b>Reaction 44</b>	<b>63</b>
<b>Reaction 45</b>	<b>64</b>
<b>Reaction 47</b>	<b>65</b>
<b>Reaction 48</b>	<b>67</b>
<b>Reaction 49</b>	<b>69</b>
<b>Reaction 50</b>	<b>70</b>
<b>Reaction 51</b>	<b>72</b>
<b>Reaction 52</b>	<b>73</b>
<b>Reaction 54</b>	<b>75</b>
<b>Reaction 55</b>	<b>77</b>
<b>Reaction 56</b>	<b>79</b>
<b>Reaction 57</b>	<b>81</b>
<b>Reaction 58</b>	<b>82</b>
<b>Reaction 60</b>	<b>83</b>
<b>Reaction 63</b>	<b>85</b>
<b>Reaction 64</b>	<b>86</b>
<b>Reaction 66</b>	<b>87</b>
<b>Reaction 67</b>	<b>89</b>
<b>Reaction 68</b>	<b>90</b>
<b>Reaction 69</b>	<b>91</b>

<b>Reaction 70</b>	<b>93</b>
<b>Reaction 71</b>	<b>94</b>
<b>Reaction 72</b>	<b>96</b>
<b>Reaction 74</b>	<b>97</b>
<b>Reaction 78</b>	<b>99</b>
<b>Reaction 80</b>	<b>100</b>
<b>Reaction 81</b>	<b>101</b>
<b>Reaction 82</b>	<b>103</b>
<b>Reaction 83</b>	<b>104</b>
<b>Reaction 84</b>	<b>106</b>
<b>Reaction 85</b>	<b>107</b>
<b>Reaction 87</b>	<b>109</b>
<b>Reaction 88</b>	<b>110</b>
<b>Reaction 89</b>	<b>111</b>
<b>Reaction 90</b>	<b>113</b>
<b>Reaction 91</b>	<b>114</b>
<b>Reaction 92</b>	<b>115</b>
<b>Reaction 93</b>	<b>117</b>
<b>Reaction 94</b>	<b>118</b>
<b>Reaction 96</b>	<b>119</b>
<b>Reaction 97</b>	<b>121</b>
<b>Reaction 98</b>	<b>122</b>
<b>Reaction 99</b>	<b>123</b>
<b>Reaction 100</b>	<b>125</b>
<b>Reaction 101</b>	<b>126</b>
<b>Reaction 102</b>	<b>128</b>
<b>Reaction 103</b>	<b>129</b>
<b>Reaction 104</b>	<b>130</b>
<b>Reaction 105</b>	<b>132</b>
<b>Reaction 106</b>	<b>133</b>

<b>Reaction 107</b>	<b>135</b>
<b>Reaction 108</b>	<b>136</b>
<b>Reaction 109</b>	<b>137</b>
<b>Reaction 110</b>	<b>139</b>
<b>Reaction 111</b>	<b>140</b>
<b>Reaction 113</b>	<b>142</b>
<b>Reaction 114</b>	<b>143</b>
<b>Reaction 115</b>	<b>144</b>
<b>Reaction 116</b>	<b>146</b>
<b>Reaction 117</b>	<b>147</b>
<b>Reaction 118</b>	<b>148</b>
<b>Reaction 119</b>	<b>150</b>
<b>Reaction 120</b>	<b>151</b>
<b>Reaction 123</b>	<b>152</b>
<b>Reaction 124</b>	<b>154</b>
<b>Reaction 126</b>	<b>156</b>
<b>Reaction 127</b>	<b>158</b>
<b>Reaction 128</b>	<b>159</b>
<b>Reaction 129</b>	<b>161</b>
<b>Reaction 131</b>	<b>162</b>
<b>Reaction 132</b>	<b>164</b>
<b>Reaction 133</b>	<b>166</b>
<b>Reaction 134</b>	<b>167</b>
<b>Reaction 135</b>	<b>169</b>
<b>Reaction 136</b>	<b>170</b>
<b>Reaction 137</b>	<b>172</b>
<b>Reaction 138</b>	<b>173</b>
<b>Reaction 139</b>	<b>174</b>
<b>Reaction 140</b>	<b>176</b>
<b>Reaction 141</b>	<b>177</b>

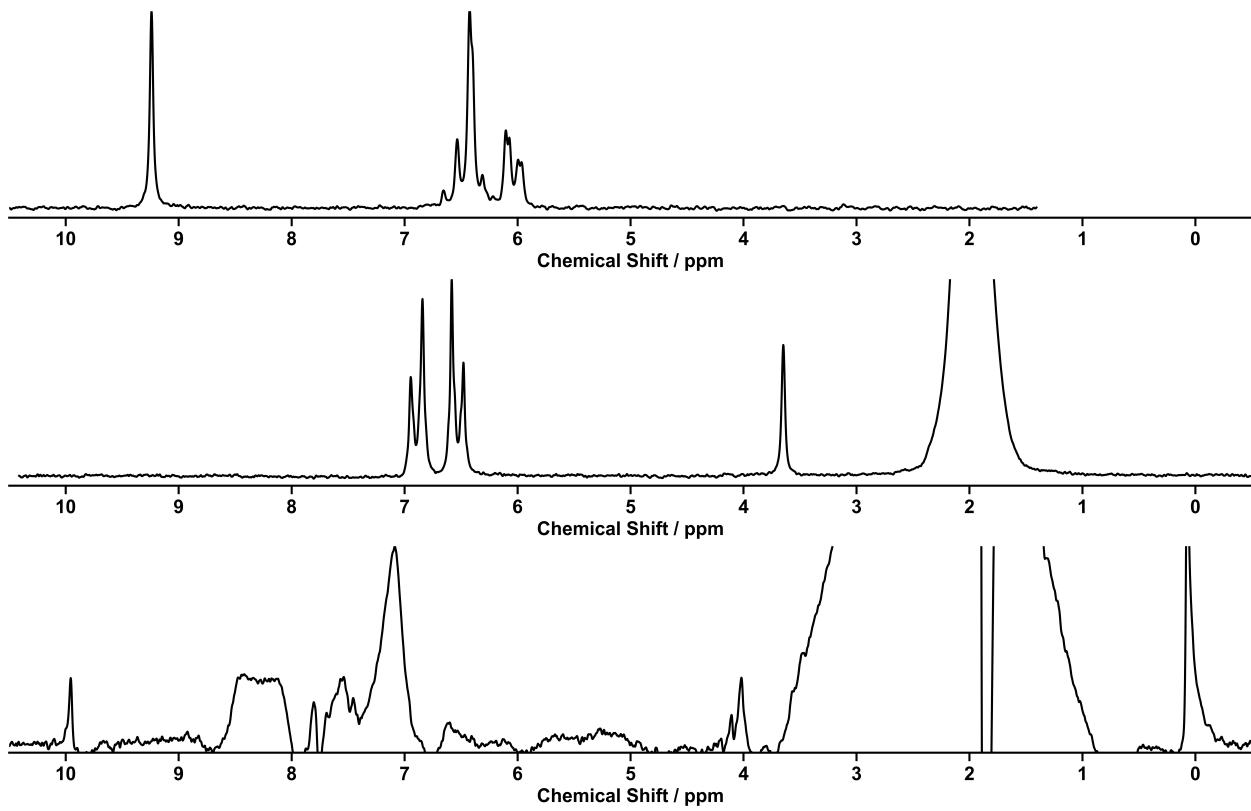
## Reaction 1



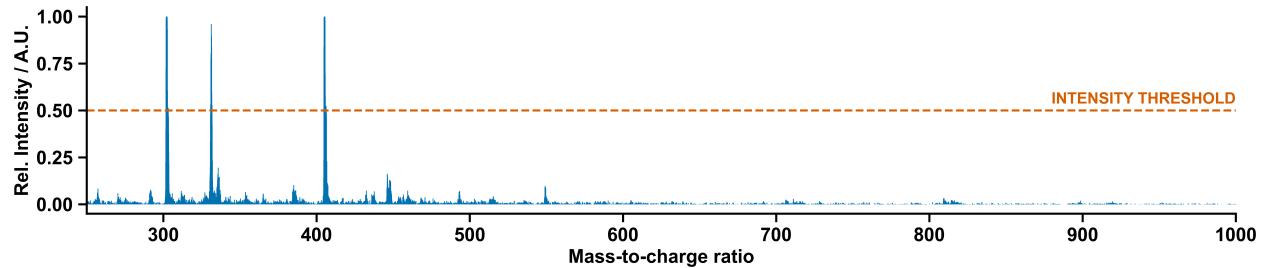
Scheme 1: Self-assembly of components 8, 17, with Zinc(II) in a 3.0:1.5:1.0 molar ratio in  $CH_3CN$  at 60°C for 40h. These are the reagents (starting materials) for reaction 1.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: Oligomers formed.
	Human MS Decision: Failed	MS Spectra Category: Reaction occurred, unknown product.
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A
	Decision Maker MS Decision: Pass	NMR Criteria 2: N/A
	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 0
	MS Criteria 3: Pass	Number of counter-ions found: 0

Decision Table 1: Human labeled and Decsision maker labeled outcomes for the  $^1H$  NMR spectroscopy and ULPC-MS spectrometry of reaction 1. Decision motivations are also given.

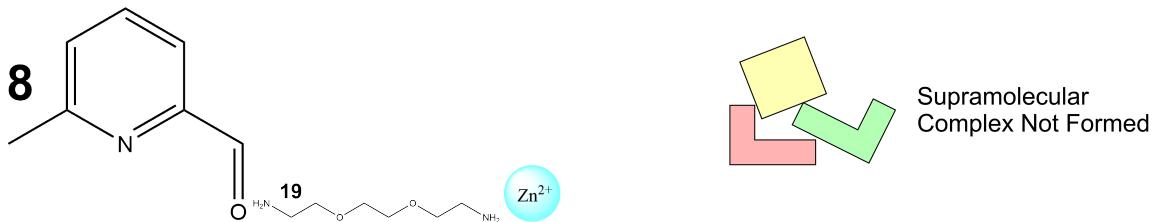


NMR Spectra 1: The stacked  $^1\text{H}$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 1.



MS Spectra 1: The ULPC-MS spectra of reaction 1. The intensity threshold is also shown.

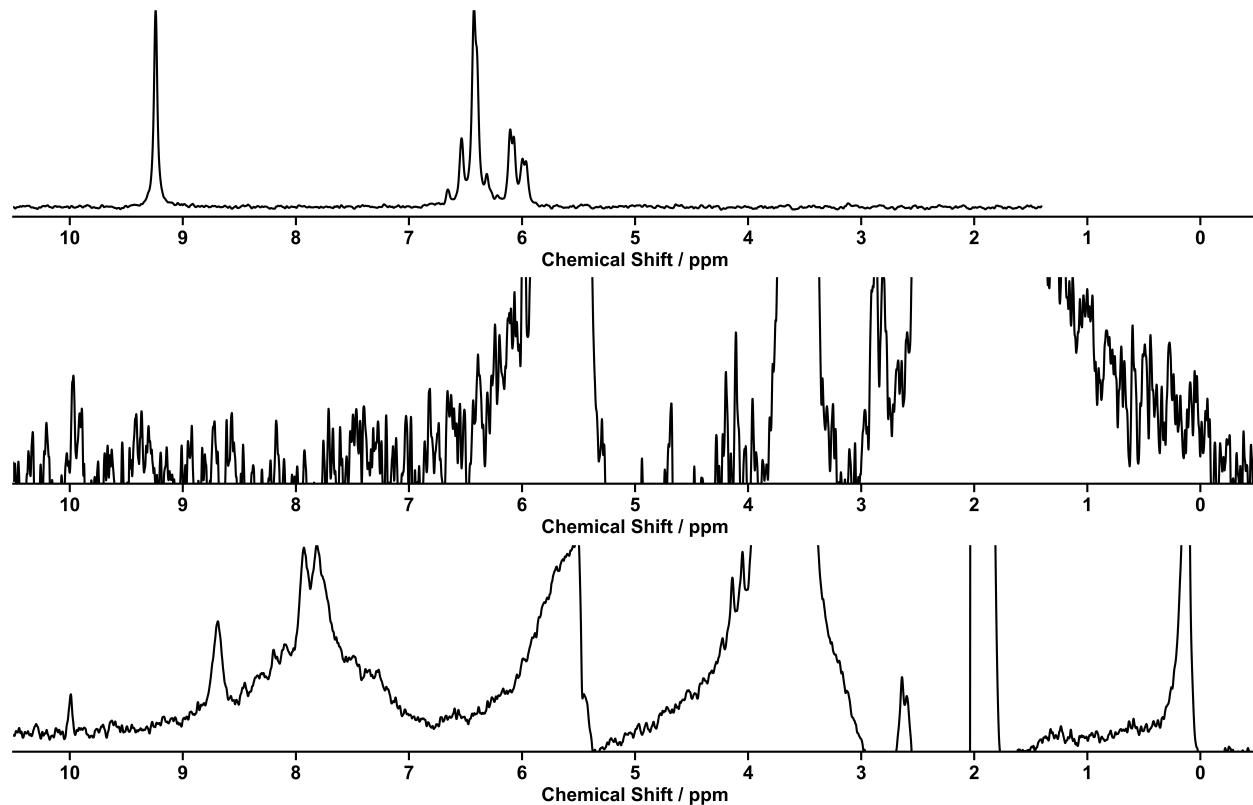
## Reaction 2



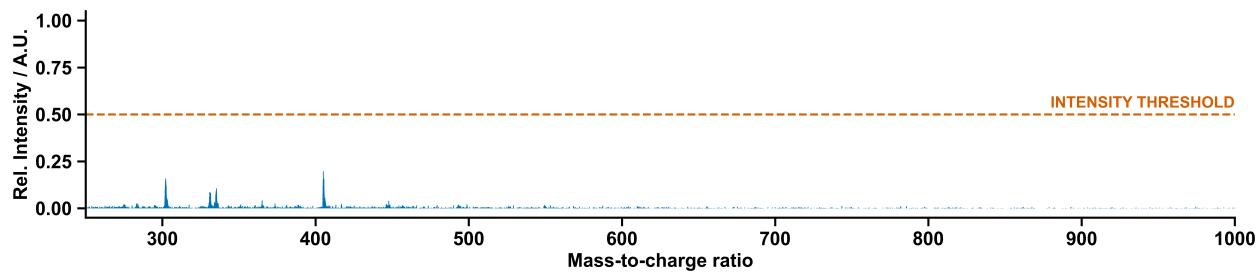
Scheme 2: Self-assembly of components 8, 19, with Zinc(II) in a 3.0:1.5:1.0 molar ratio in  $\text{CH}_3\text{CN}$  at  $60^\circ\text{C}$  for 40h. These are the reagents (starting materials) for reaction 2.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: Oligomers formed.	
	Human MS Decision: Failed	MS Spectra Category: Reaction failed.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	NMR Criteria 2: N/A
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 0
		MS Criteria 3: Pass	Number of counter-ions found: 0

Decision Table 2: Human labeled and Decision maker labeled outcomes for the  $^1\text{H}$  NMR spectroscopy and UPLC-MS spectrometry of reaction 2. Decision motivations are also given.

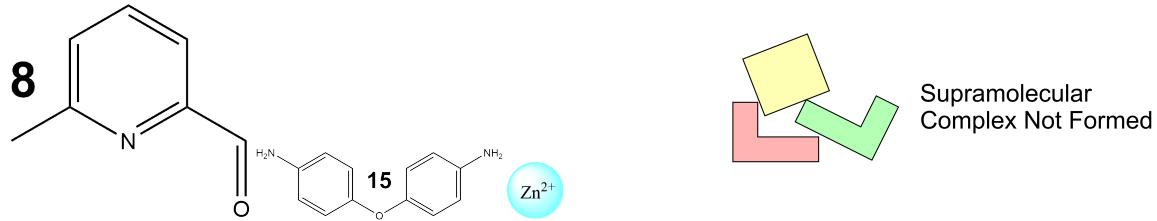


NMR Spectra 2: The stacked  $^1\text{H}$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 2.



MS Spectra 2: The ULPC-MS spectra of reaction 2. The intensity threshold is also shown.

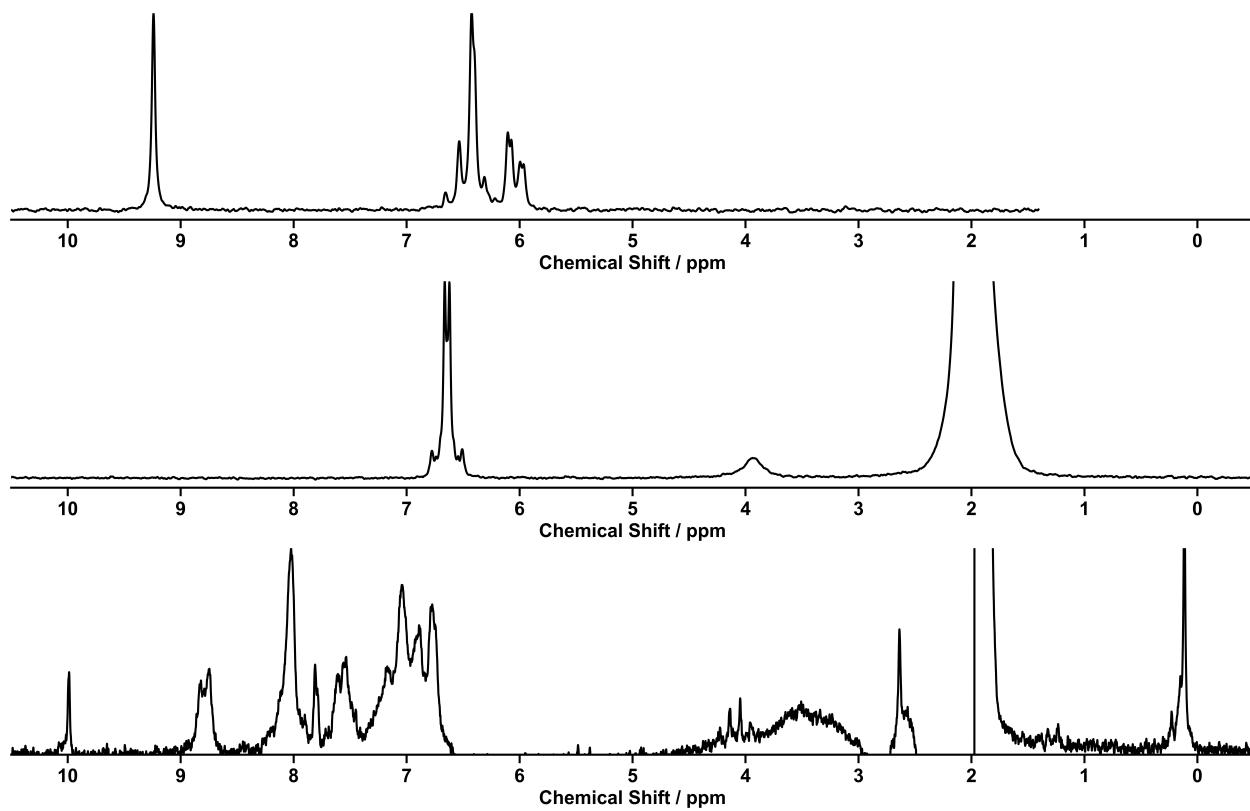
## Reaction 3



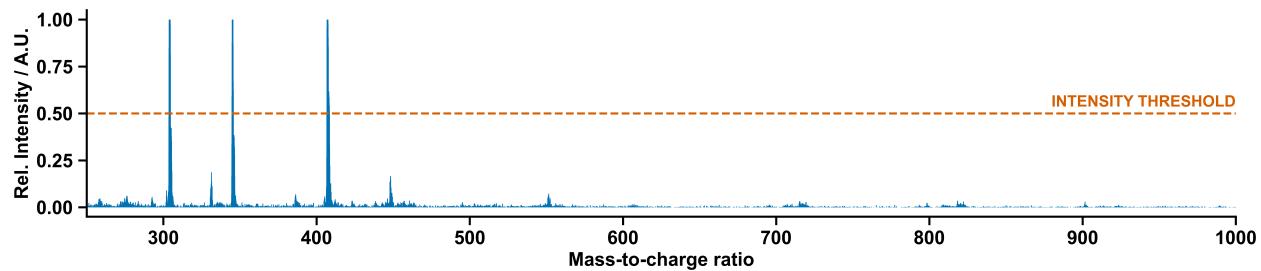
Scheme 3: Self-assembly of components 8, 15, with Zinc(II) in a 3.0:1.5:1.0 molar ratio in  $\text{CH}_3\text{CN}$  at  $60^\circ\text{C}$  for 40h. These are the reagents (starting materials) for reaction 3.

Human Reaction Decision: Failed	Human NMR Decision: Pass	NMR Spectra Category: Single discrete species formed.	
	Human MS Decision: Failed	MS Spectra Category: Reaction occurred, unknown product.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	NMR Criteria 2: N/A
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 0
		MS Criteria 3: Pass	Number of counter-ions found: 0

Decision Table 3: Human labeled and Decsision maker labeled outcomes for the  $^1\text{H}$  NMR spectroscopy and ULPC-MS spectrometry of reaction 3. Decision motivations are also given.

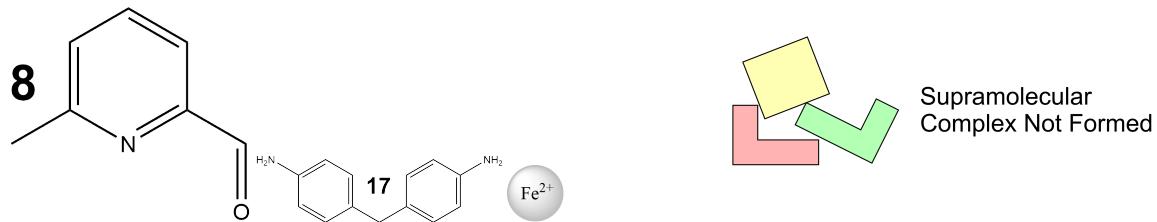


NMR Spectra 3: The stacked  $^1\text{H}$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 3.



MS Spectra 3: The ULPC-MS spectra of reaction 3. The intensity threshold is also shown.

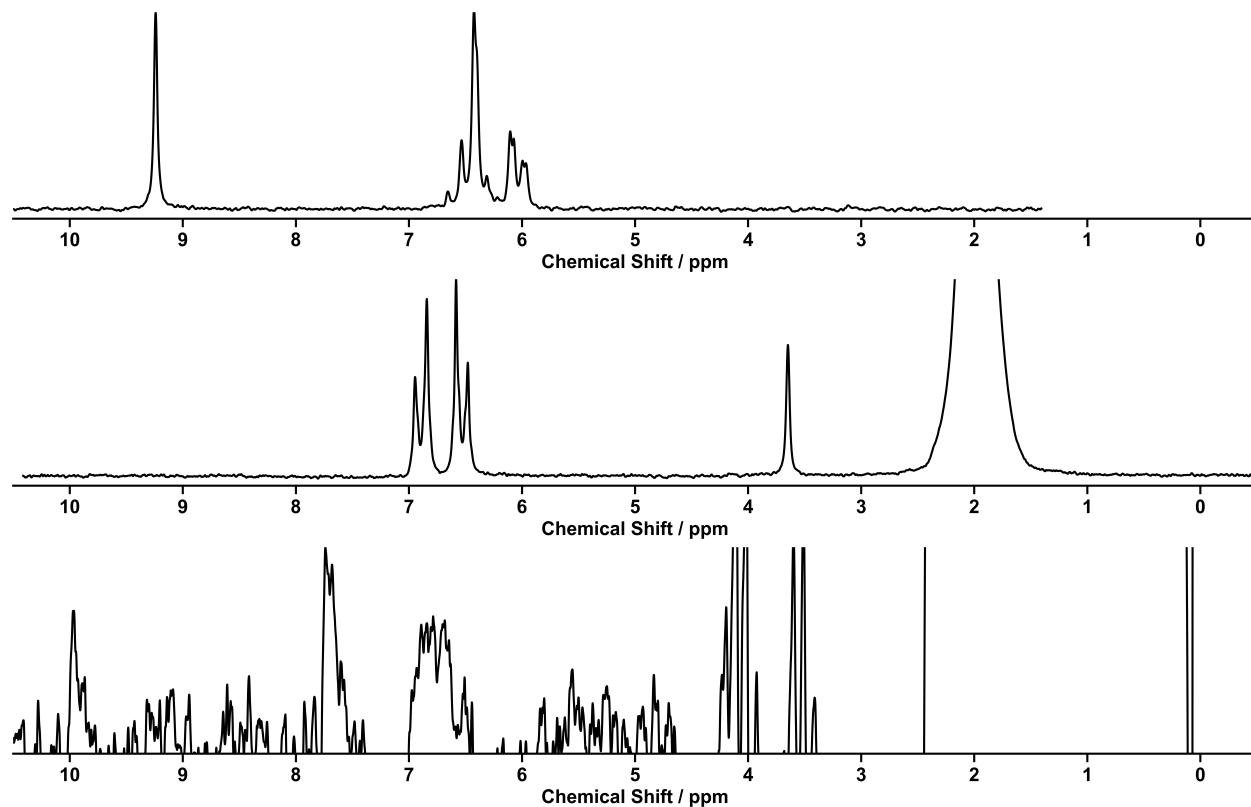
## Reaction 4



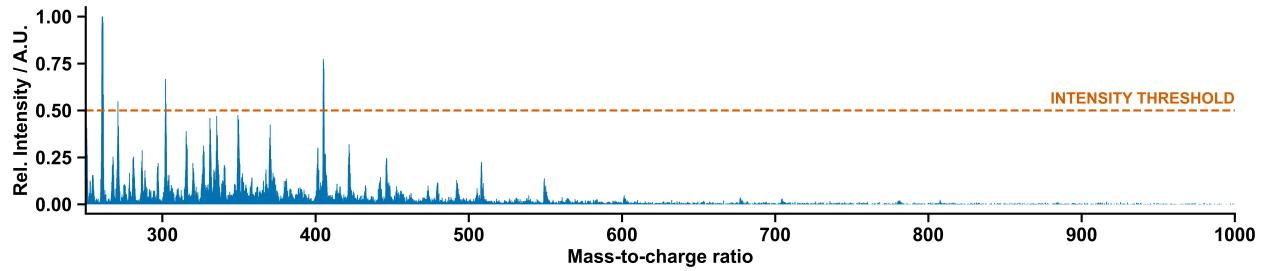
Scheme 4: Self-assembly of components 8, 17, with Iron(II) in a 3.0:1.5:1.0 molar ratio in  $\text{CH}_3\text{CN}$  at 60°C for 40h. These are the reagents (starting materials) for reaction 4.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: Paramagnetic species formed.	
	Human MS Decision: Failed	MS Spectra Category: Reaction occurred, unknown product.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	
	Decision Maker MS Decision: Pass	NMR Criteria 2: N/A	
		MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 1
	MS Criteria 3: Pass		Number of counter-ions found: 0

Decision Table 4: Human labeled and Decision maker labeled outcomes for the  $^1\text{H}$  NMR spectroscopy and UPLC-MS spectrometry of reaction 4. Decision motivations are also given.

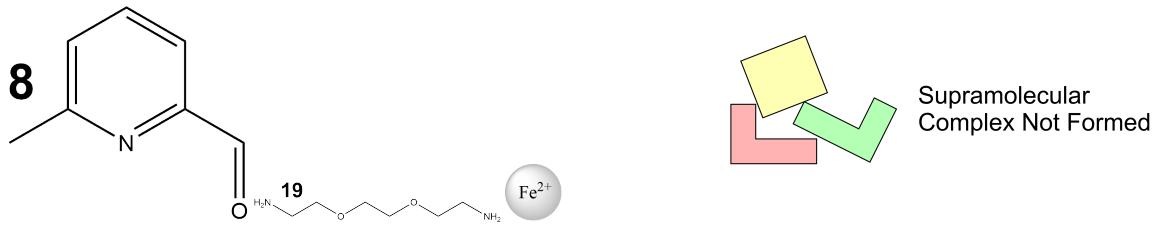


NMR Spectra 4: The stacked  $^1\text{H}$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 4.



MS Spectra 4: The UPLC-MS spectra of reaction 4. The intensity threshold is also shown.

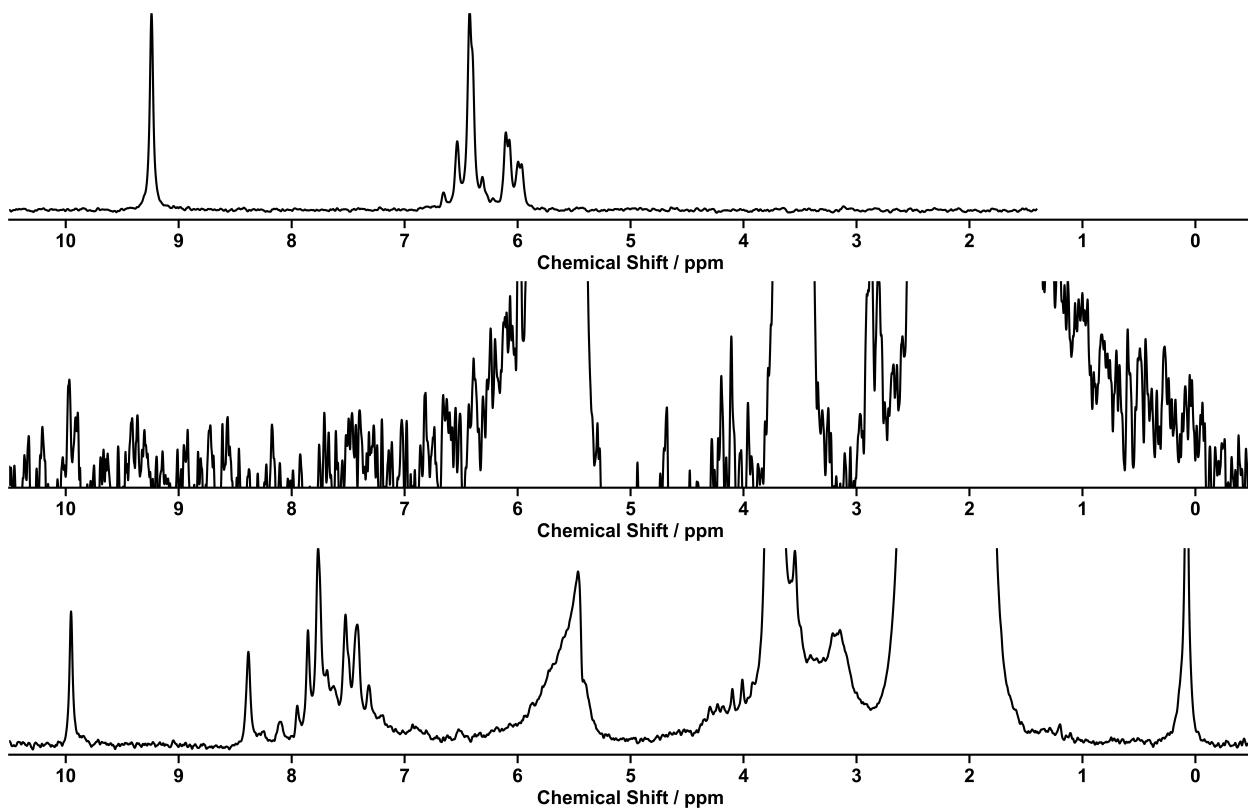
## Reaction 5



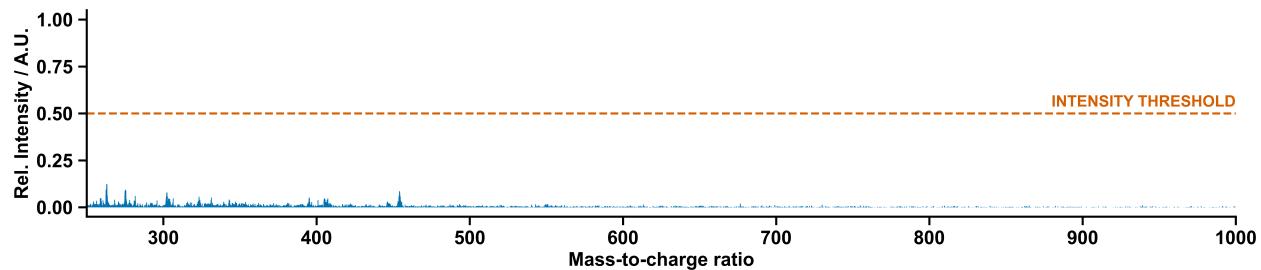
Scheme 5: Self-assembly of components 8, 19, with Iron(II) in a 3.0:1.5:1.0 molar ratio in CH<sub>3</sub>CN at 60°C for 40h. These are the reagents (starting materials) for reaction 5.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: No reaction occurred.	
	Human MS Decision: Failed	MS Spectra Category: Reaction failed.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	NMR Criteria 2: N/A
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 0
		MS Criteria 3: Pass	Number of counter-ions found: 0

Decision Table 5: Human labeled and Decsision maker labeled outcomes for the <sup>1</sup>H NMR spectroscopy and UPLC-MS spectrometry of reaction 5. Decision motivations are also given.

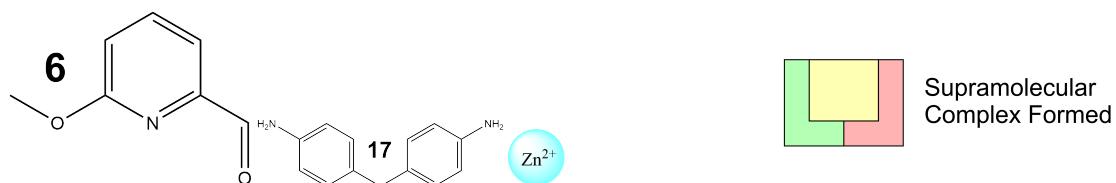


NMR Spectra 5: The stacked <sup>1</sup>H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 5.



MS Spectra 5: The ULPC-MS spectra of reaction 5. The intensity threshold is also shown.

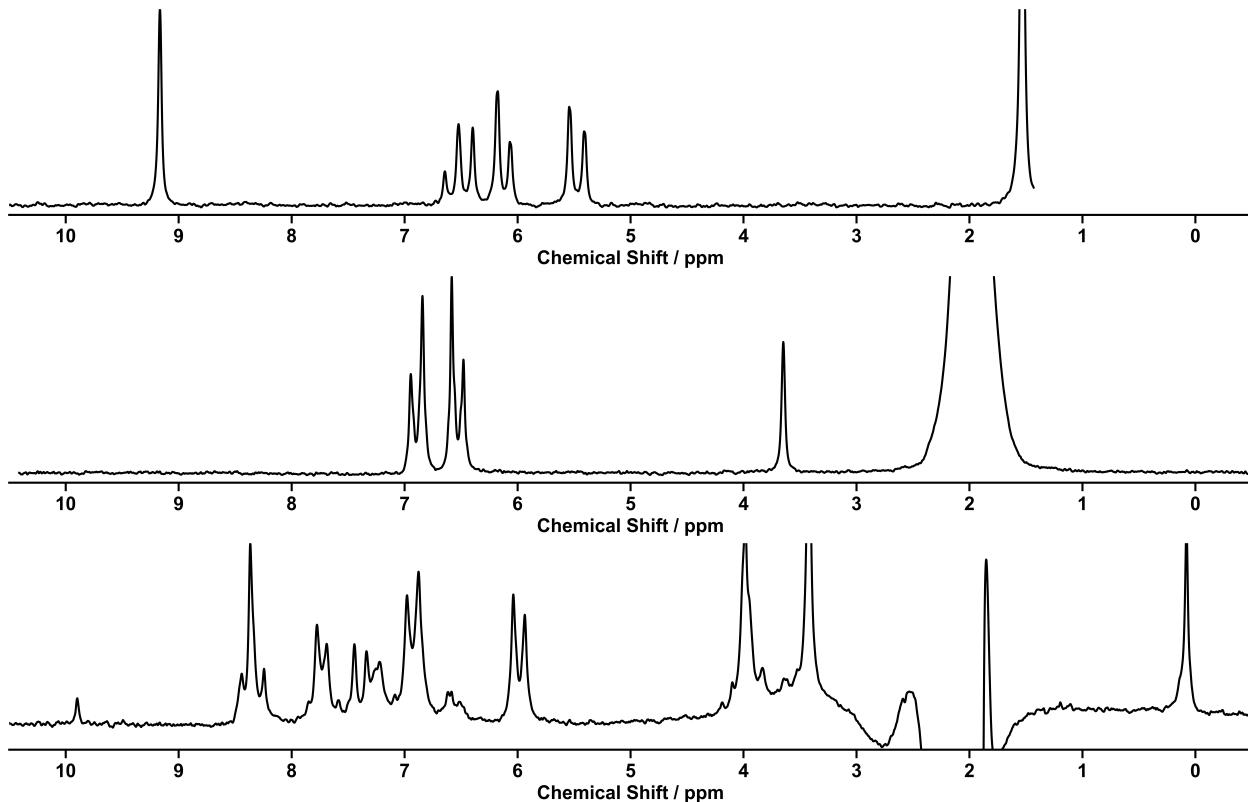
## Reaction 7



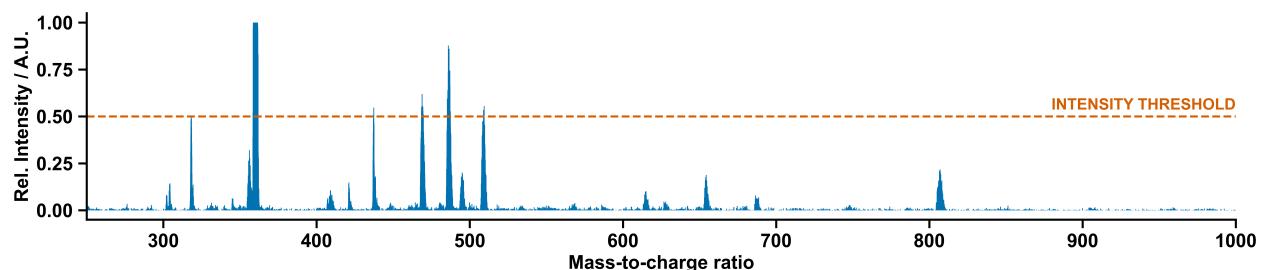
Scheme 6: Self-assembly of components 6, 17, with Zinc(II) in a 3.0:1.5:1.0 molar ratio in  $CH_3CN$  at 60°C for 40h. These are the reagents (starting materials) for reaction 7.

Human Reaction Decision: Pass	Human NMR Decision: Pass	NMR Spectra Category: Single discrete species formed.	
	Human MS Decision: Pass	MS Spectra Category: Reaction occurred, supramolecular product.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	
		NMR Criteria 2: N/A	
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 5
	MS Criteria 3: Pass	Number of counter-ions found: 4	

Decision Table 6: Human labeled and Decsision maker labeled outcomes for the  $^1\text{H}$  NMR spectroscopy and ULPC-MS spectrometry of reaction 7. Decision motivations are also given.

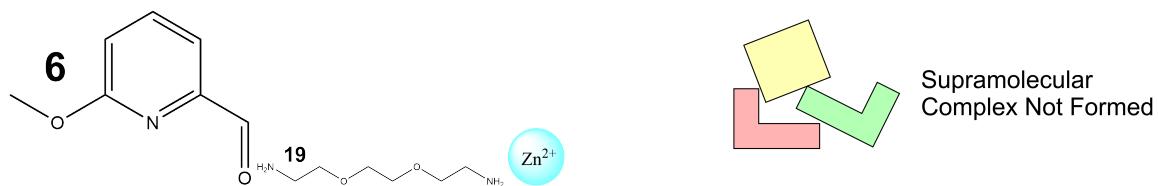


NMR Spectra 6: The stacked  $^1\text{H}$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 7.



MS Spectra 6: The ULPC-MS spectra of reaction 7. The intensity threshold is also shown.

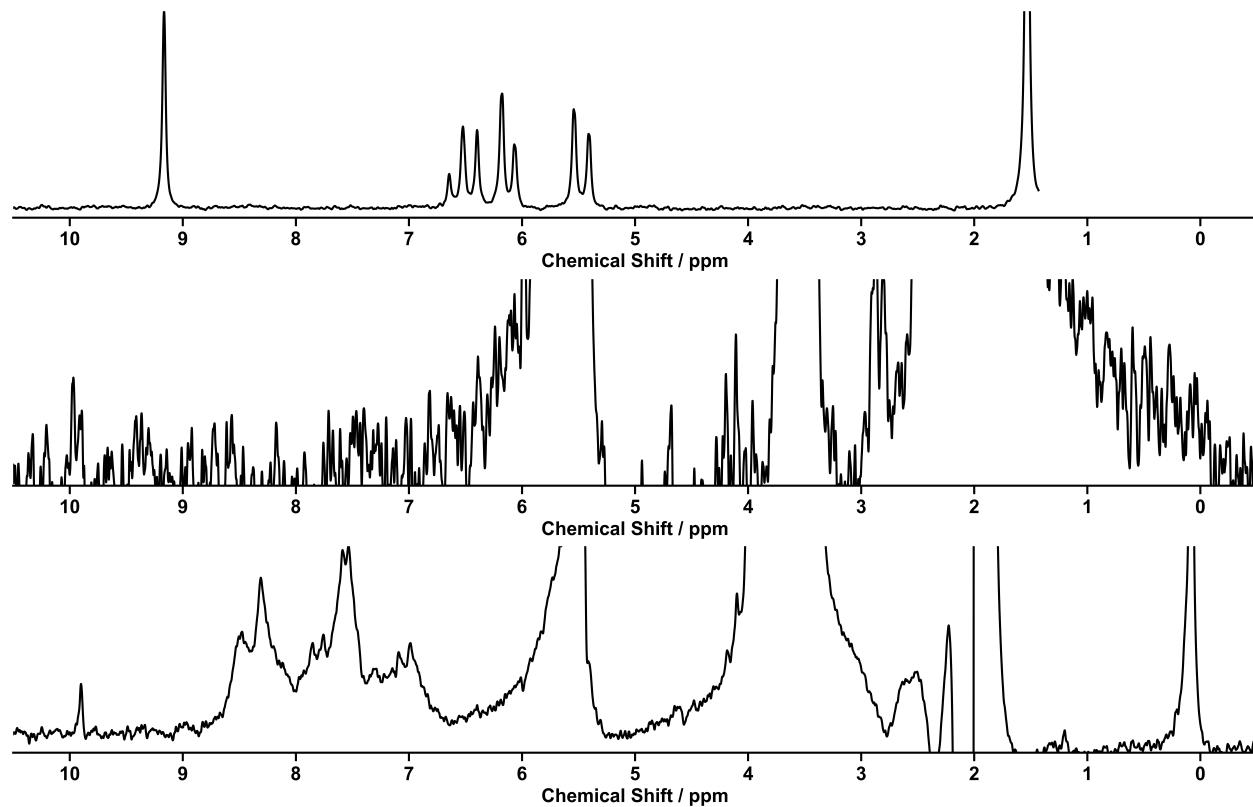
## Reaction 8



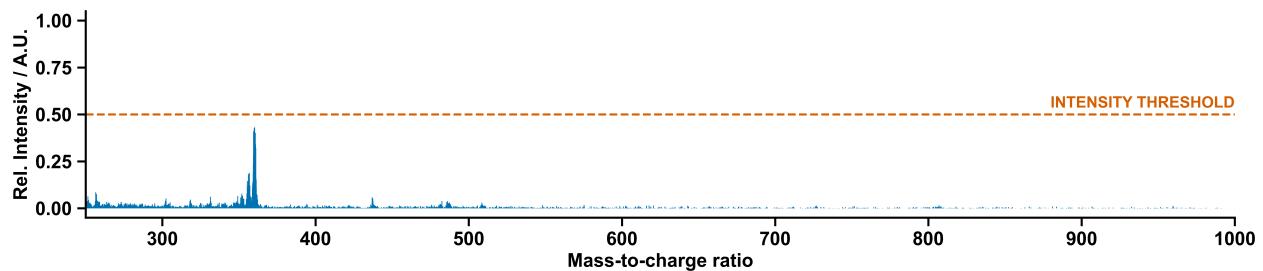
Scheme 7: Self-assembly of components 6, 19, with Zinc(II) in a 3.0:1.5:1.0 molar ratio in  $CH_3CN$  at  $60^\circ C$  for 40h. These are the reagents (starting materials) for reaction 8.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: Oligomers formed.	
	Human MS Decision: Failed	MS Spectra Category: Reaction failed.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	NMR Criteria 2: N/A
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 0
		MS Criteria 3: Pass	Number of counter-ions found: 0

Decision Table 7: Human labeled and Decision maker labeled outcomes for the  $^1H$  NMR spectroscopy and UPLC-MS spectrometry of reaction 8. Decision motivations are also given.

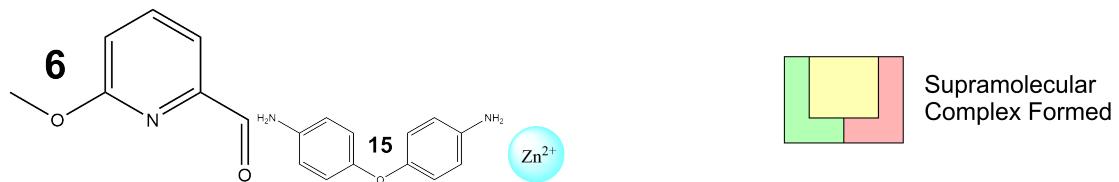


NMR Spectra 7: The stacked  $^1H$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 8.



MS Spectra 7: The ULPC-MS spectra of reaction 8. The intensity threshold is also shown.

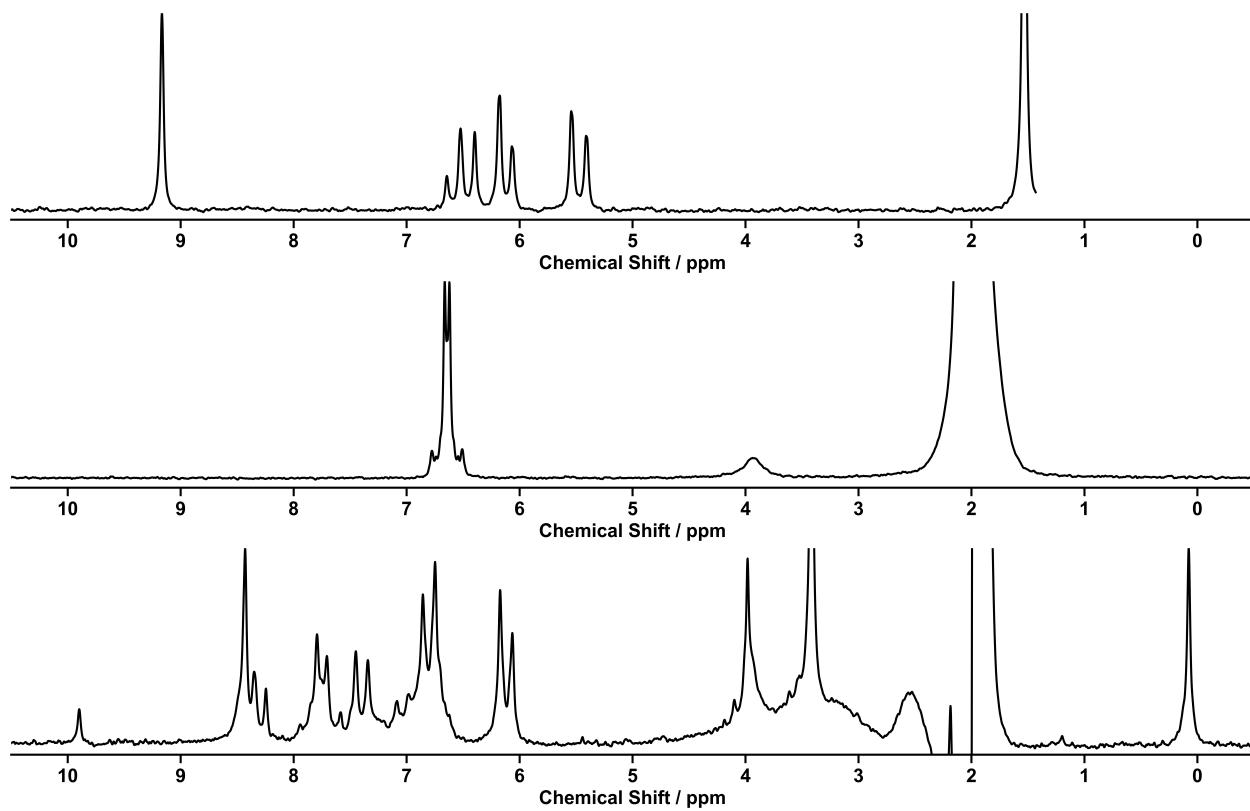
## Reaction 9



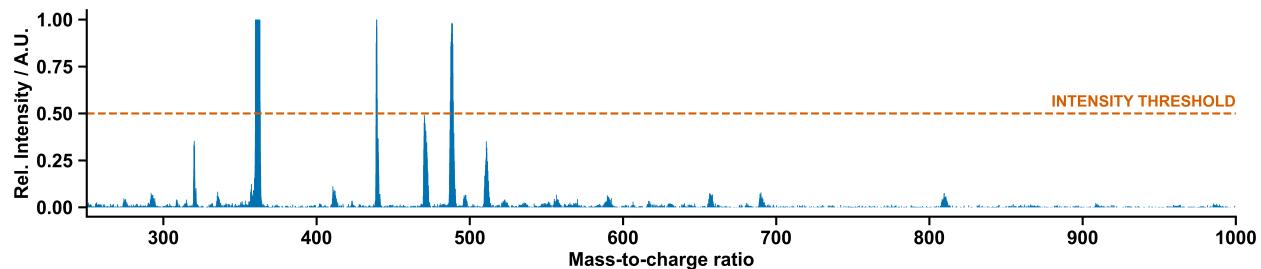
Scheme 8: Self-assembly of components 6, 15, with Zinc(II) in a 3.0:1.5:1.0 molar ratio in  $CH_3CN$  at  $60^\circ C$  for 40h. These are the reagents (starting materials) for reaction 9.

Human Reaction Decision: Pass	Human NMR Decision: Pass	NMR Spectra Category: Single discrete species formed.	
	Human MS Decision: Pass	MS Spectra Category: Reaction occurred, supramolecular product.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	NMR Criteria 2: N/A
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 2
		MS Criteria 3: Pass	Number of counter-ions found: 2

Decision Table 8: Human labeled and Decsision maker labeled outcomes for the  $^1H$  NMR spectroscopy and ULPC-MS spectrometry of reaction 9. Decision motivations are also given.

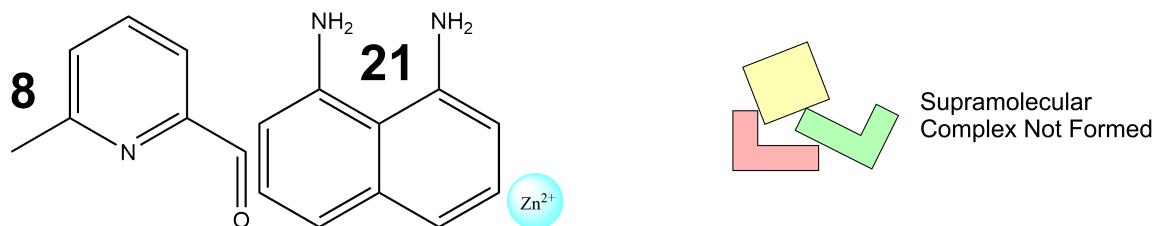


NMR Spectra 8: The stacked  $^1\text{H}$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 9.



MS Spectra 8: The ULPC-MS spectra of reaction 9. The intensity threshold is also shown.

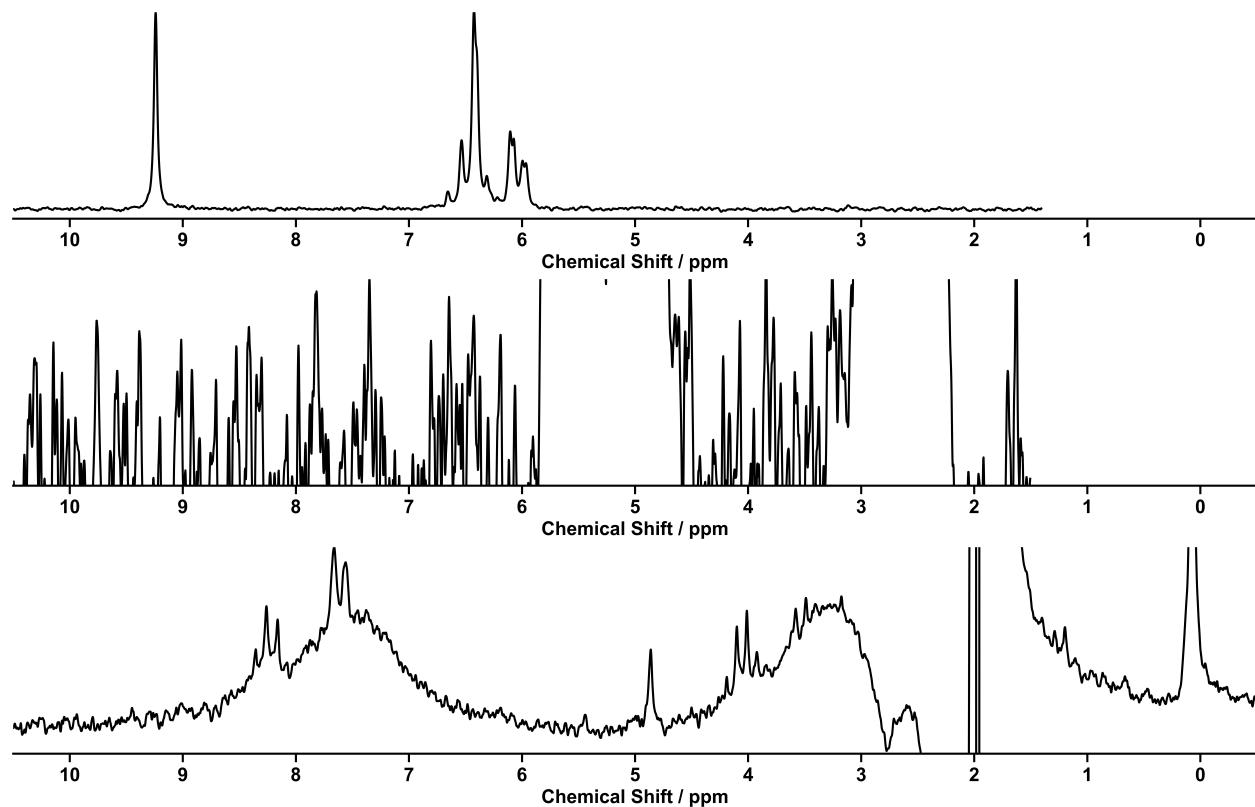
## Reaction 10



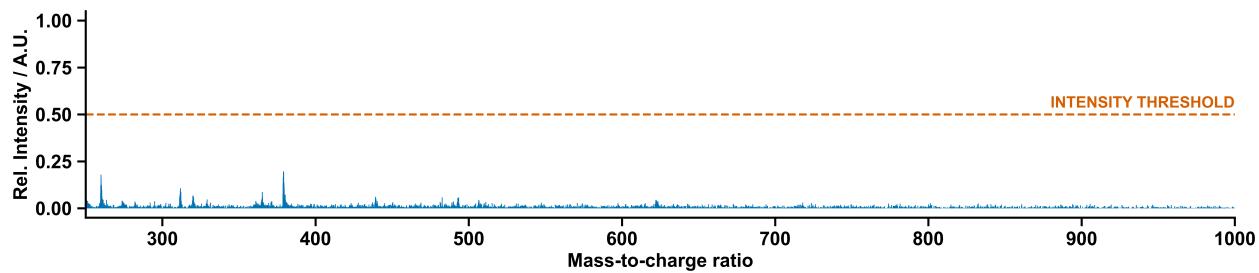
Scheme 9: Self-assembly of components 8, 21, with Zinc(II) in a 3.0:1.5:1.0 molar ratio in  $CH_3CN$  at  $60^\circ C$  for 40h. These are the reagents (starting materials) for reaction 10.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: Oligomers formed.	
	Human MS Decision: Failed	MS Spectra Category: Reaction failed.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	NMR Criteria 2: N/A
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 0
		MS Criteria 3: Pass	Number of counter-ions found: 0

Decision Table 9: Human labeled and Decision maker labeled outcomes for the  $^1H$  NMR spectroscopy and UPLC-MS spectrometry of reaction 10. Decision motivations are also given.

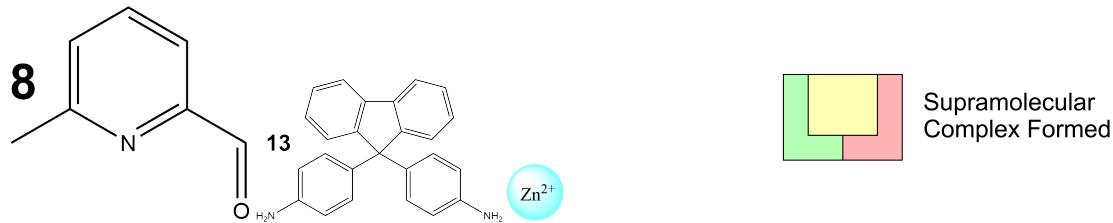


NMR Spectra 9: The stacked  $^1H$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 10.



MS Spectra 9: The ULPC-MS spectra of reaction 10. The intensity threshold is also shown.

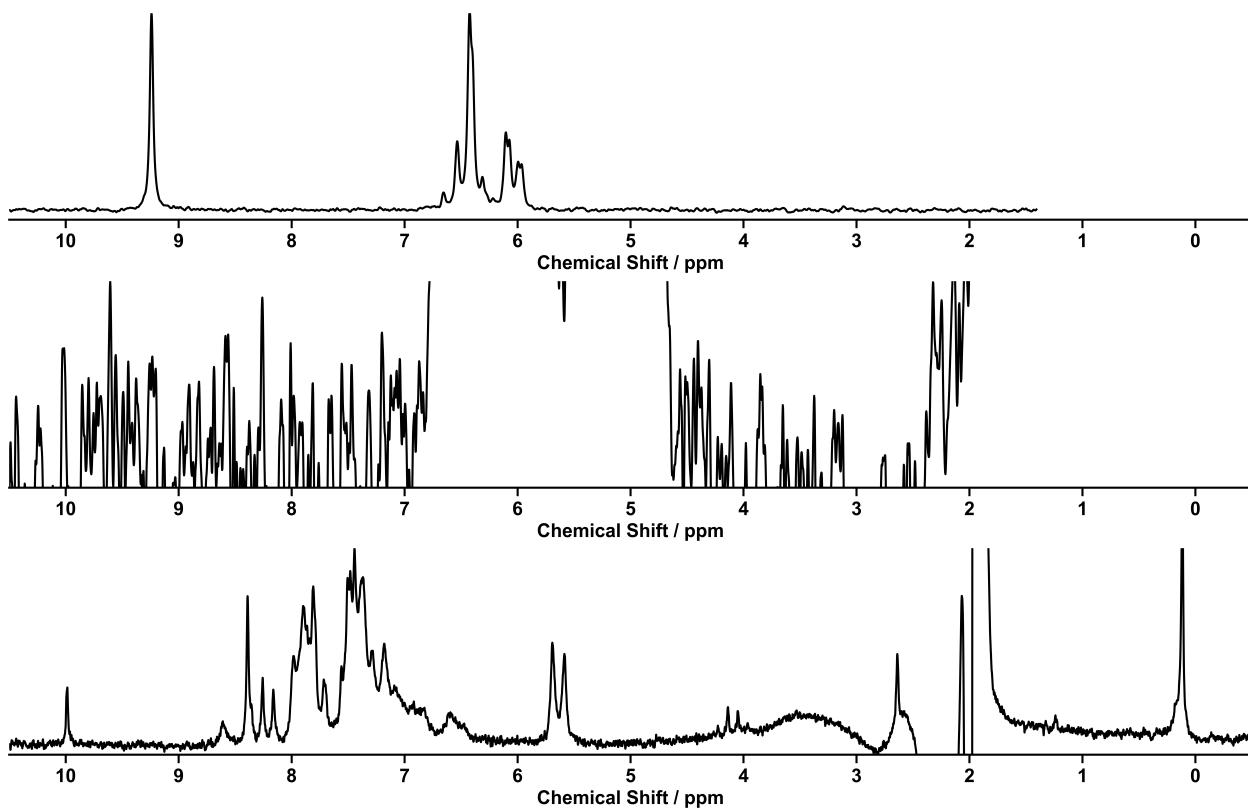
## Reaction 11



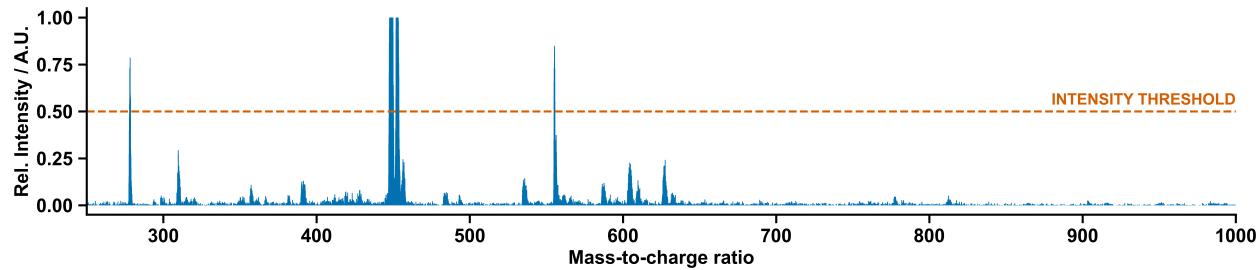
Scheme 10: Self-assembly of components 8, 13, with Zinc(II) in a 3.0:1.5:1.0 molar ratio in CH<sub>3</sub>CN at 60°C for 40h. These are the reagents (starting materials) for reaction 11.

Human Reaction Decision: Pass	Human NMR Decision: Pass	NMR Spectra Category: Single discrete species formed.	
	Human MS Decision: Pass	MS Spectra Category: Reaction occurred, supramolecular product.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	NMR Criteria 2: N/A
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 3
		MS Criteria 3: Pass	Number of counter-ions found: 1

Decision Table 10: Human labeled and Decsision maker labeled outcomes for the <sup>1</sup>H NMR spectroscopy and ULPC-MS spectrometry of reaction 11. Decision motivations are also given.

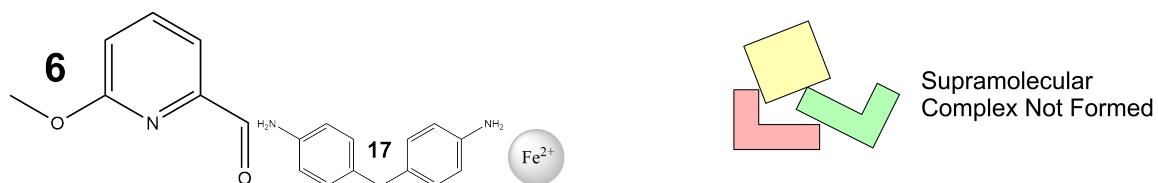


NMR Spectra 10: The stacked <sup>1</sup>H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 11.



MS Spectra 10: The ULPC-MS spectra of reaction 11. The intensity threshold is also shown.

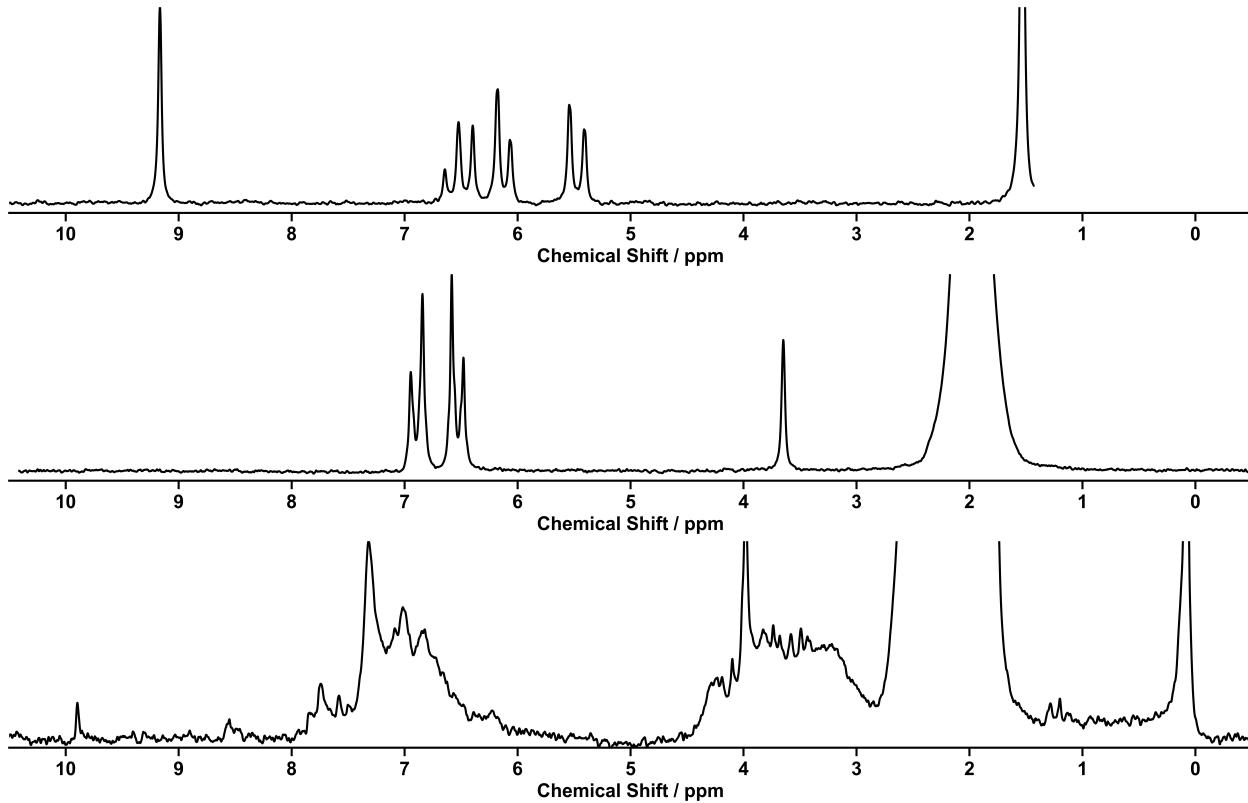
## Reaction 12



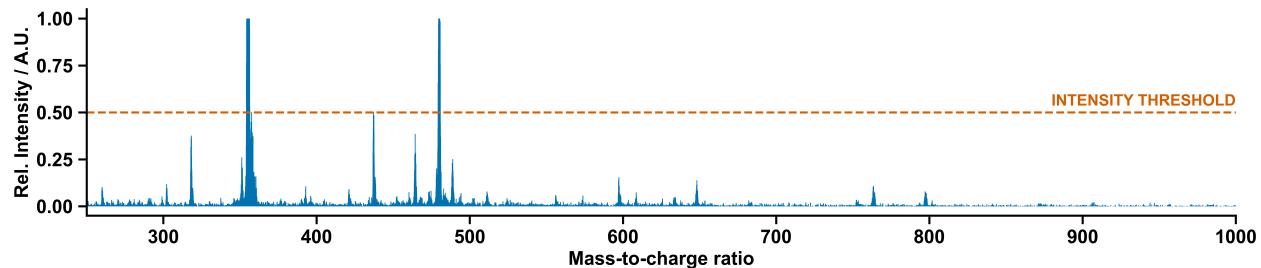
Scheme 11: Self-assembly of components 6, 17, with Iron(II) in a 3.0:1.5:1.0 molar ratio in CH<sub>3</sub>CN at 60°C for 40h. These are the reagents (starting materials) for reaction 12.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: Paramagnetic species formed.	
	Human MS Decision: Pass	MS Spectra Category: Reaction occurred, supramolecular product.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	
		NMR Criteria 2: N/A	
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 5
		MS Criteria 3: Pass	Number of counter-ions found: 3

Decision Table 11: Human labeled and Decsision maker labeled outcomes for the  $^1\text{H}$  NMR spectroscopy and ULPC-MS spectrometry of reaction 12. Decision motivations are also given.

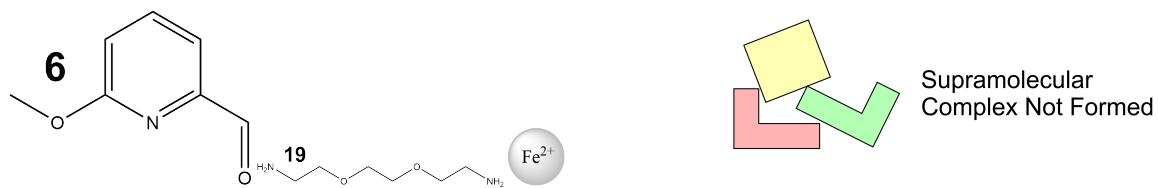


NMR Spectra 11: The stacked  $^1\text{H}$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 12.



MS Spectra 11: The ULPC-MS spectra of reaction 12. The intensity threshold is also shown.

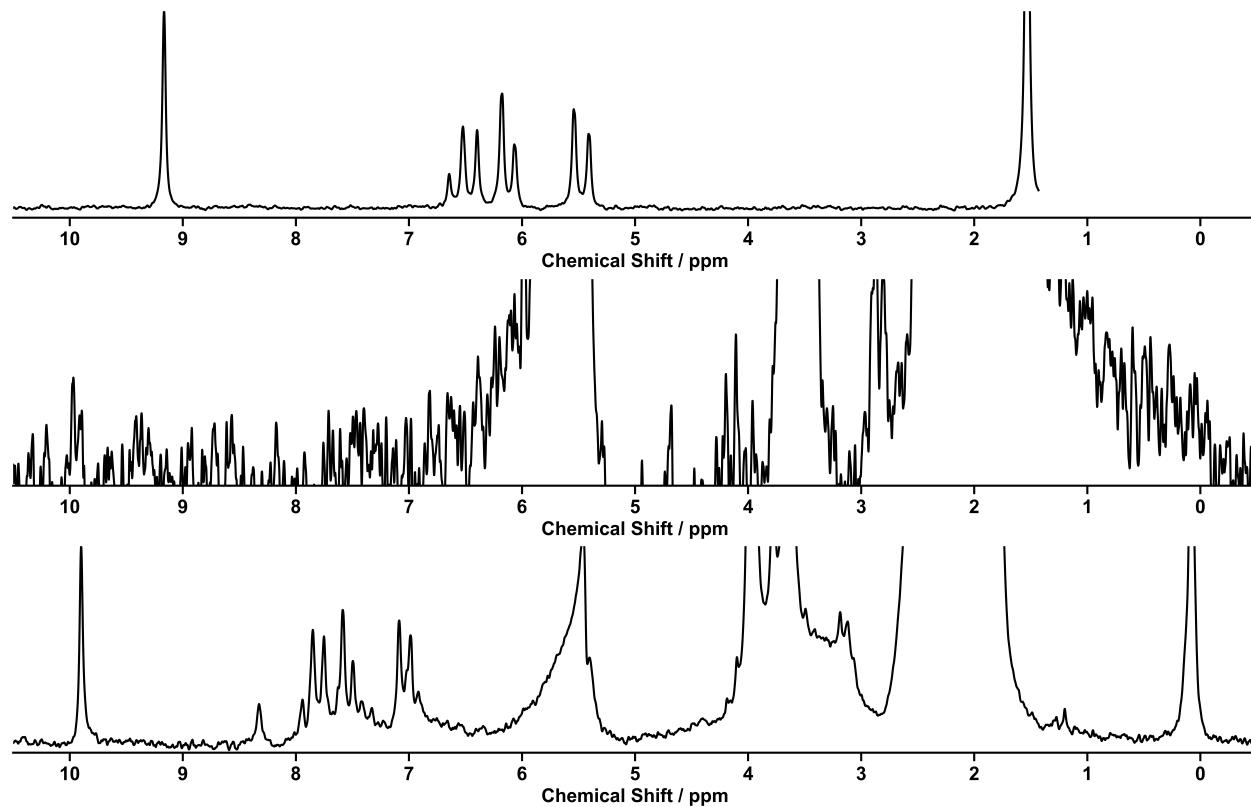
## Reaction 13



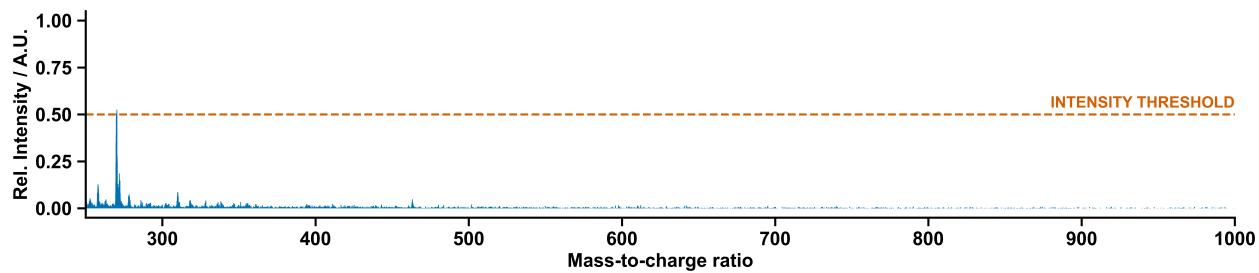
Scheme 12: Self-assembly of components 6, 19, with Iron(II) in a 3.0:1.5:1.0 molar ratio in  $\text{CH}_3\text{CN}$  at  $60^\circ\text{C}$  for 40h. These are the reagents (starting materials) for reaction 13.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: No reaction occurred.	
	Human MS Decision: Failed	MS Spectra Category: Reaction failed.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	NMR Criteria 2: N/A
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 0
		MS Criteria 3: Pass	Number of counter-ions found: 0

Decision Table 12: Human labeled and Decsision maker labeled outcomes for the  $^1\text{H}$  NMR spectroscopy and UPLC-MS spectrometry of reaction 13. Decision motivations are also given.

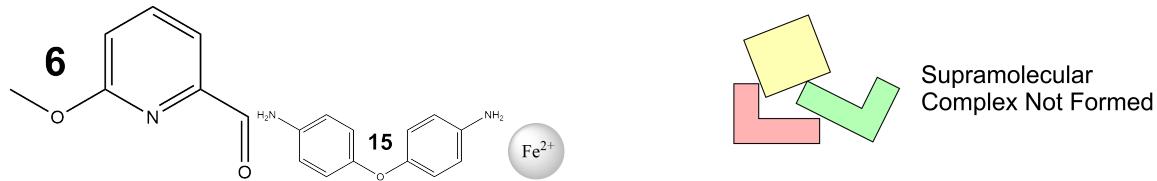


NMR Spectra 12: The stacked  $^1\text{H}$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 13.



MS Spectra 12: The ULPC-MS spectra of reaction 13. The intensity threshold is also shown.

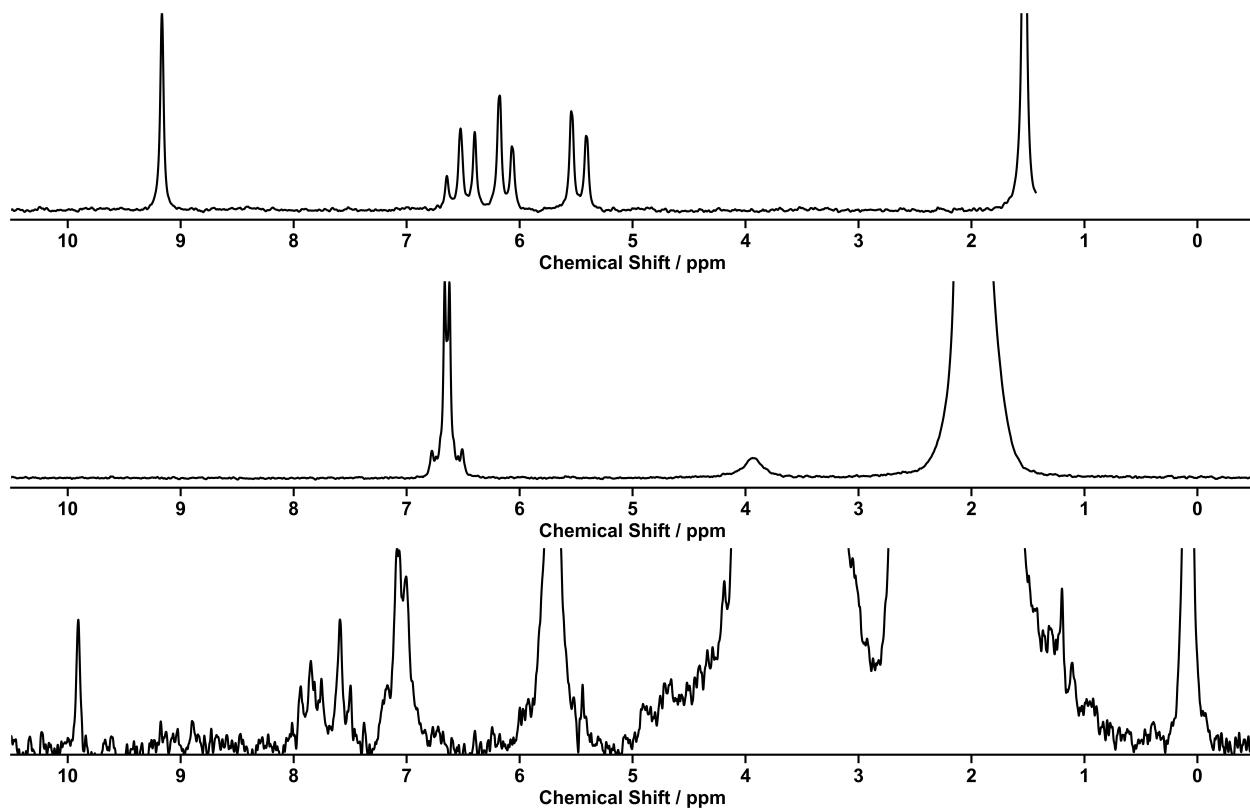
## Reaction 14



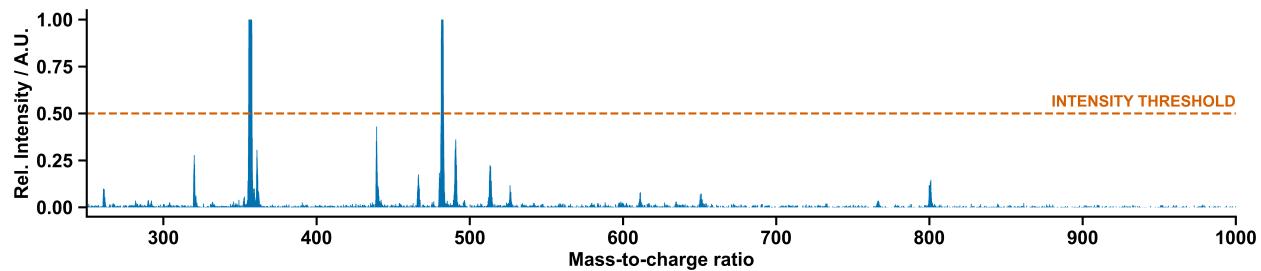
Scheme 13: Self-assembly of components 6, 15, with Iron(II) in a 3.0:1.5:1.0 molar ratio in CH<sub>3</sub>CN at 60°C for 40h. These are the reagents (starting materials) for reaction 14.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: Paramagnetic species formed.	
	Human MS Decision: Pass	MS Spectra Category: Reaction occurred, supramolecular product.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	NMR Criteria 2: N/A
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 5
		MS Criteria 3: Pass	Number of counter-ions found: 3

Decision Table 13: Human labeled and Decsision maker labeled outcomes for the <sup>1</sup>H NMR spectroscopy and ULPC-MS spectrometry of reaction 14. Decision motivations are also given.

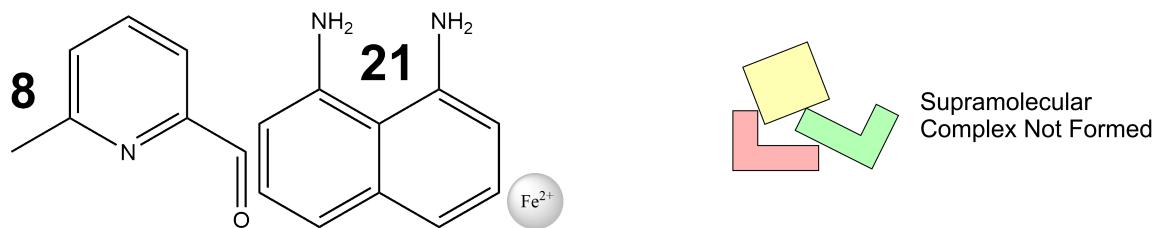


NMR Spectra 13: The stacked  $^1\text{H}$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 14.



MS Spectra 13: The ULPC-MS spectra of reaction 14. The intensity threshold is also shown.

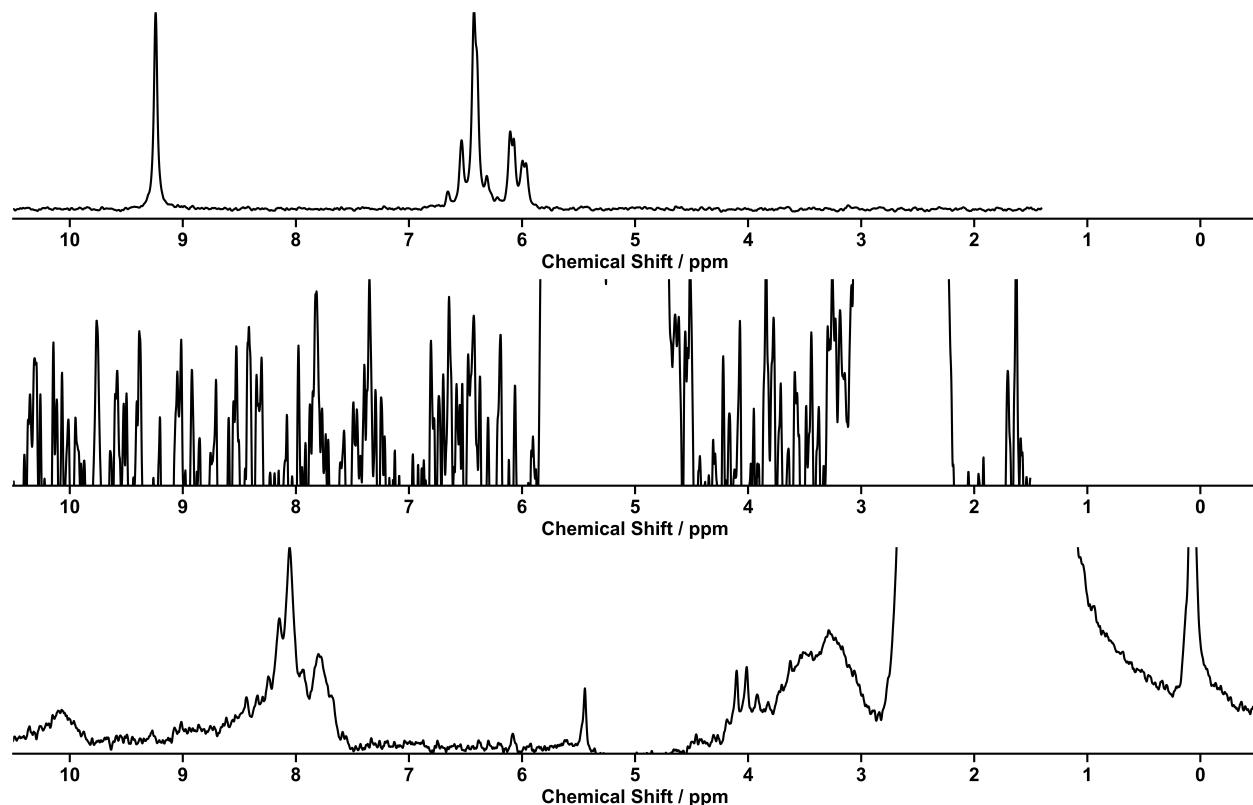
## Reaction 15



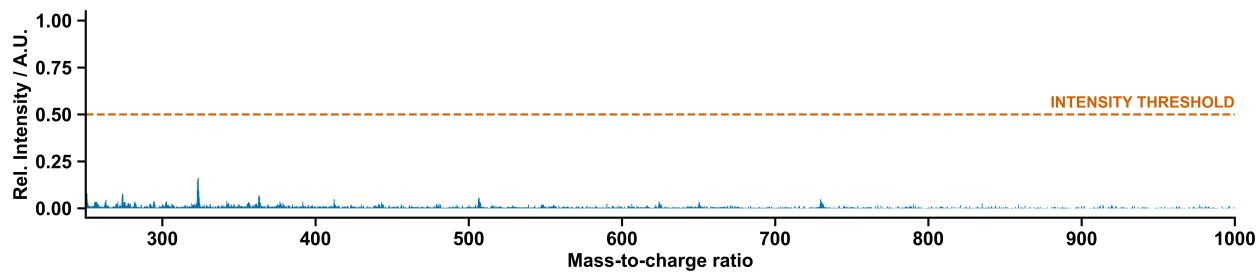
Scheme 14: Self-assembly of components 8, 21, with Iron(II) in a 3.0:1.5:1.0 molar ratio in  $\text{CH}_3\text{CN}$  at  $60^\circ\text{C}$  for 40h. These are the reagents (starting materials) for reaction 15.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: Paramagnetic species formed.	
	Human MS Decision: Failed	MS Spectra Category: Reaction failed.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	NMR Criteria 2: N/A
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 0
		MS Criteria 3: Pass	Number of counter-ions found: 0

Decision Table 14: Human labeled and Decsision maker labeled outcomes for the  $^1\text{H}$  NMR spectroscopy and ULP-MS spectrometry of reaction 15. Decision motivations are also given.

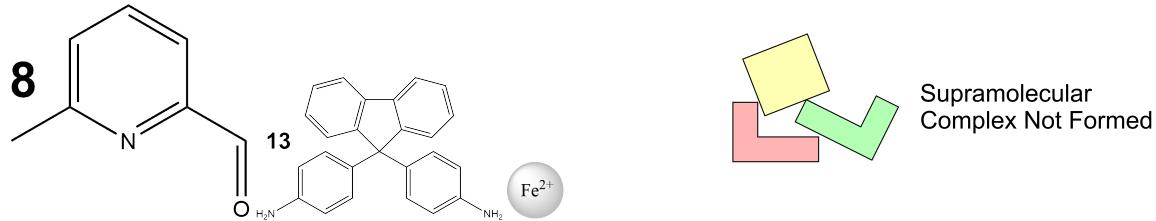


NMR Spectra 14: The stacked  $^1\text{H}$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 15.



MS Spectra 14: The ULPC-MS spectra of reaction 15. The intensity threshold is also shown.

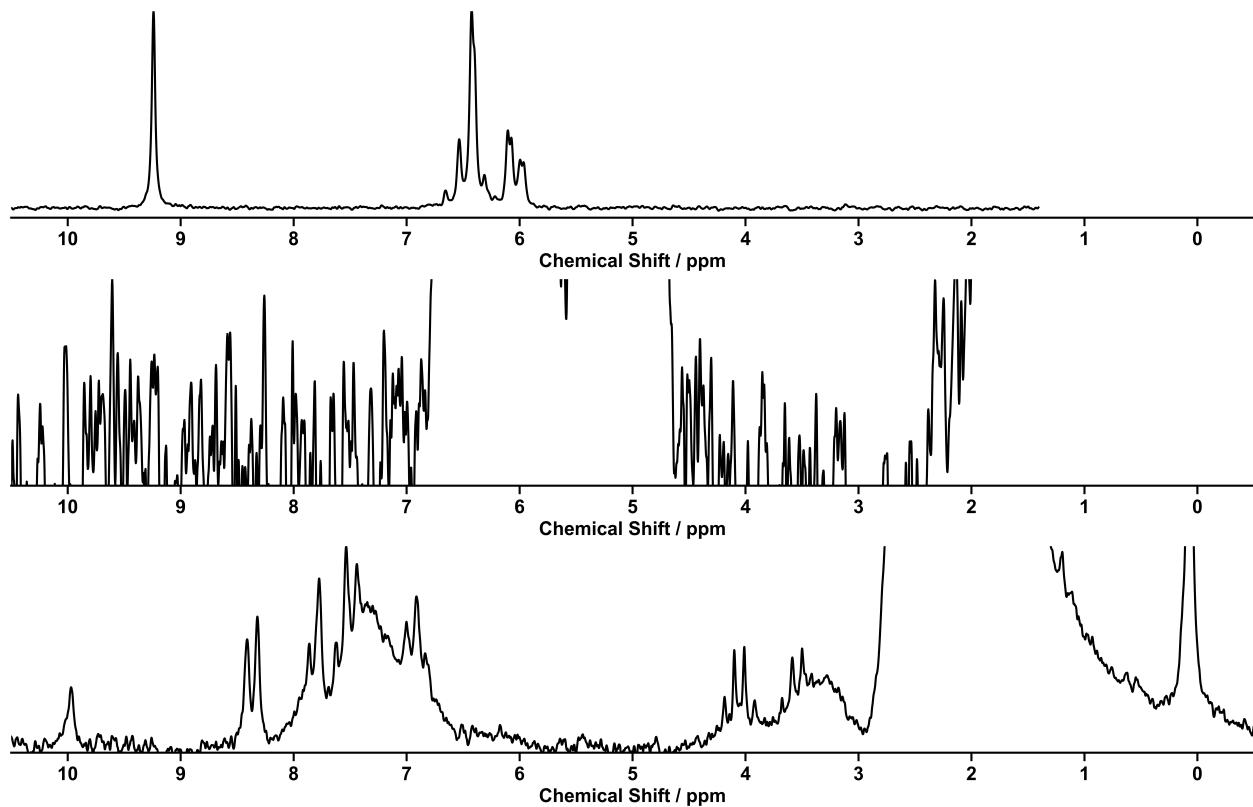
## Reaction 16



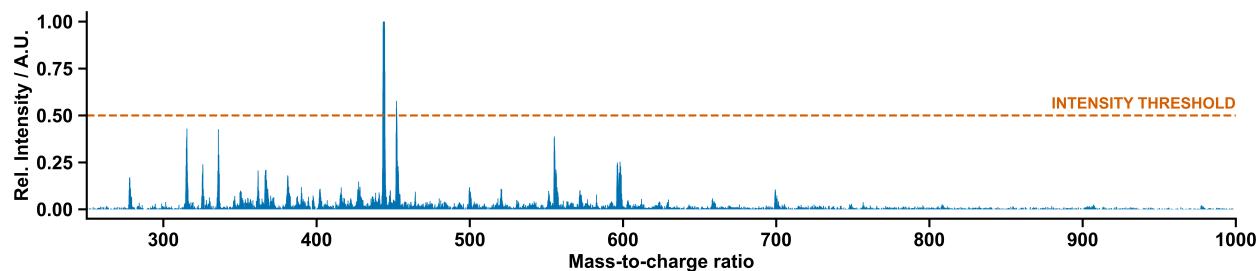
Scheme 15: Self-assembly of components 8, 13, with Iron(II) in a 3.0:1.5:1.0 molar ratio in CH<sub>3</sub>CN at 60°C for 40h. These are the reagents (starting materials) for reaction 16.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: Paramagnetic species formed.	
	Human MS Decision: Failed	MS Spectra Category: Reaction occurred, unknown product.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	NMR Criteria 2: N/A
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 5
		MS Criteria 3: Pass	Number of counter-ions found: 3

Decision Table 15: Human labeled and Decsision maker labeled outcomes for the <sup>1</sup>H NMR spectroscopy and ULPC-MS spectrometry of reaction 16. Decision motivations are also given.

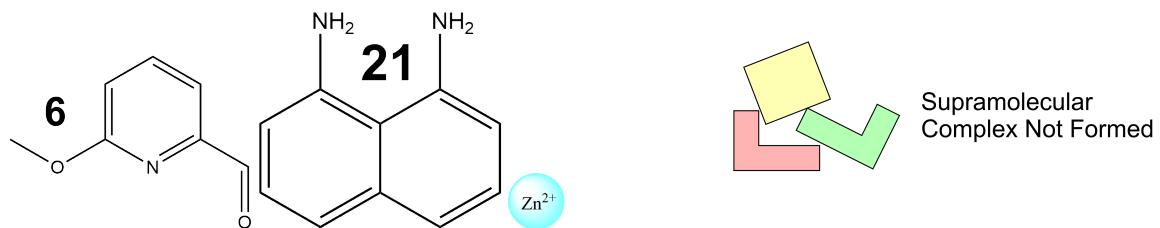


NMR Spectra 15: The stacked  $^1\text{H}$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 16.



MS Spectra 15: The ULPC-MS spectra of reaction 16. The intensity threshold is also shown.

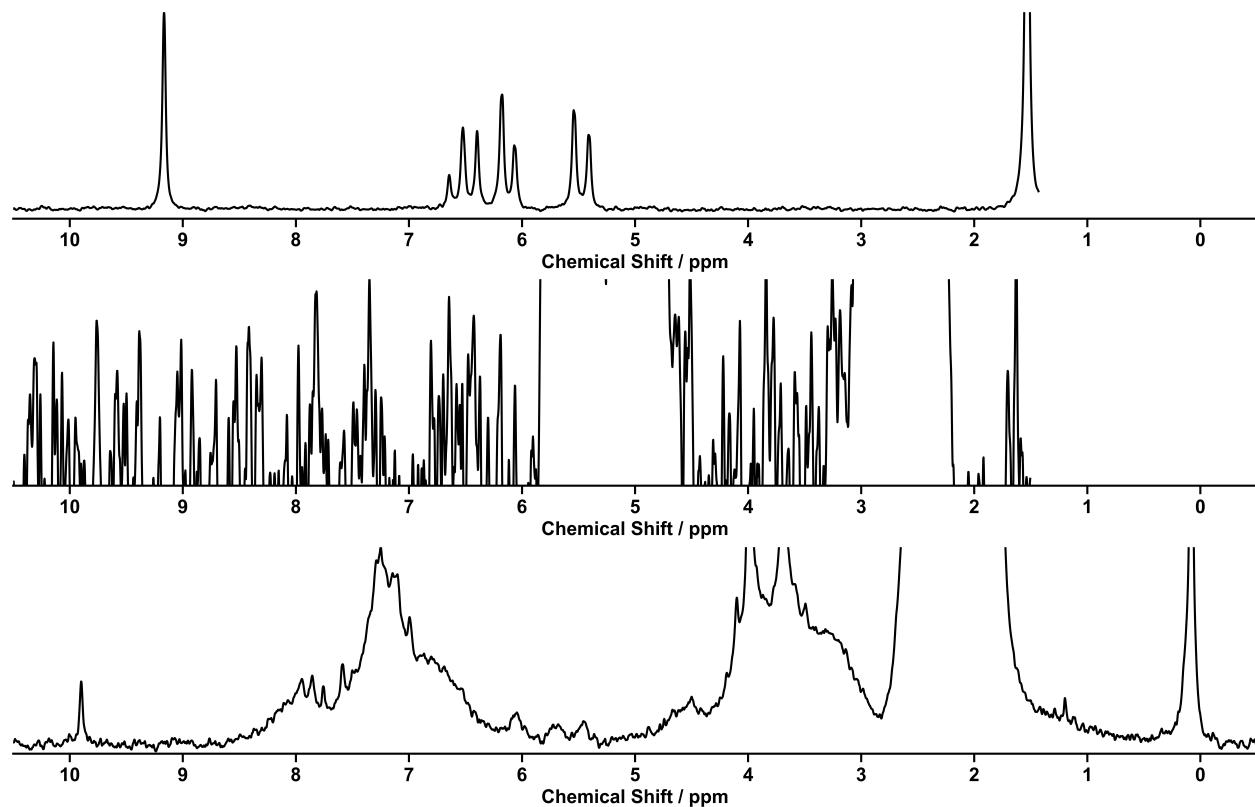
## Reaction 17



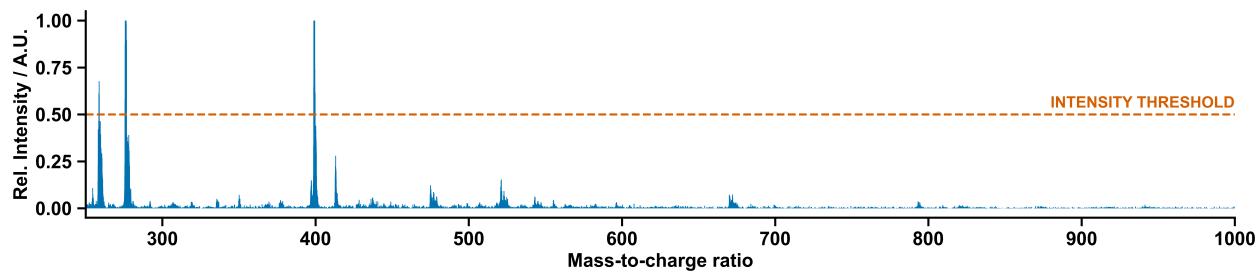
Scheme 16: Self-assembly of components 6, 21, with Zinc(II) in a 3.0:1.5:1.0 molar ratio in  $CH_3CN$  at  $60^\circ C$  for 40h. These are the reagents (starting materials) for reaction 17.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: Oligomers formed.	
	Human MS Decision: Failed	MS Spectra Category: Reaction occurred, unknown product.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	NMR Criteria 2: N/A
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 0
		MS Criteria 3: Pass	Number of counter-ions found: 0

Decision Table 16: Human labeled and Decsision maker labeled outcomes for the  $^1H$  NMR spectroscopy and ULP-MS spectrometry of reaction 17. Decision motivations are also given.

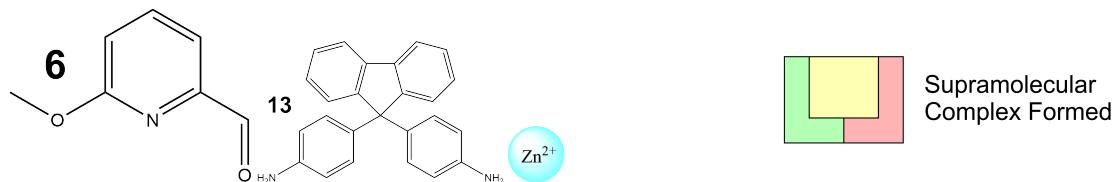


NMR Spectra 16: The stacked  $^1H$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 17.



MS Spectra 16: The ULPC-MS spectra of reaction 17. The intensity threshold is also shown.

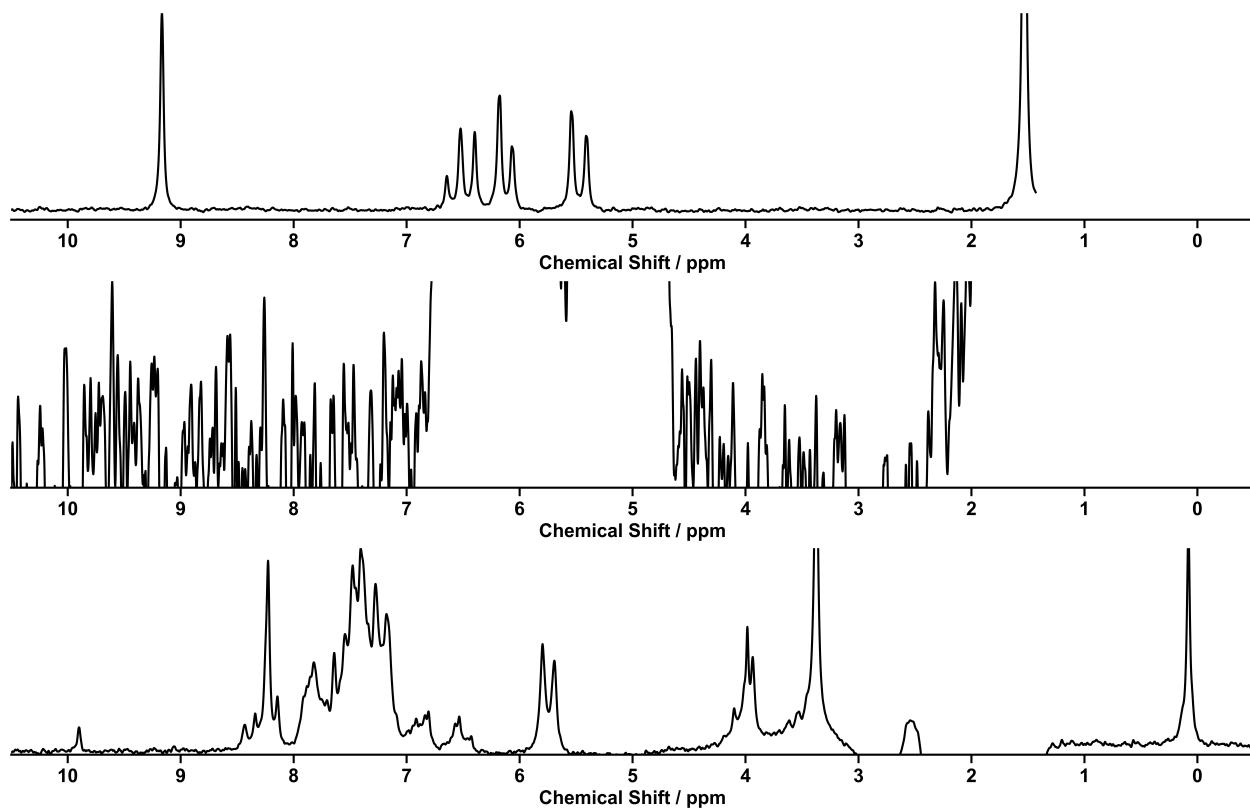
## Reaction 18



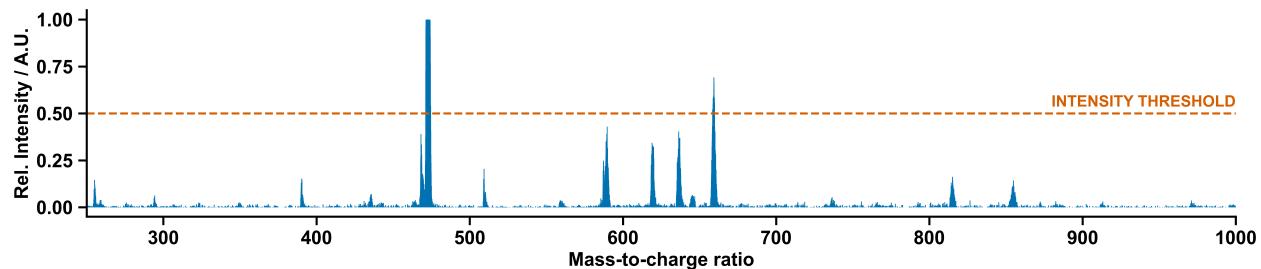
Scheme 17: Self-assembly of components 6, 13, with Zinc(II) in a 3.0:1.5:1.0 molar ratio in CH<sub>3</sub>CN at 60°C for 40h. These are the reagents (starting materials) for reaction 18.

Human Reaction Decision: Pass	Human NMR Decision: Pass	NMR Spectra Category: Single discrete species formed.	
	Human MS Decision: Pass	MS Spectra Category: Reaction occurred, supramolecular product.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	NMR Criteria 2: N/A
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 4
		MS Criteria 3: Pass	Number of counter-ions found: 2

Decision Table 17: Human labeled and Decsision maker labeled outcomes for the <sup>1</sup>H NMR spectroscopy and ULPC-MS spectrometry of reaction 18. Decision motivations are also given.

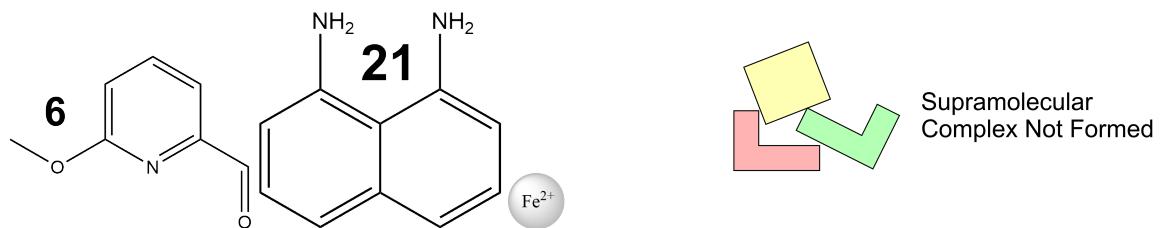


NMR Spectra 17: The stacked  $^1\text{H}$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 18.



MS Spectra 17: The ULPC-MS spectra of reaction 18. The intensity threshold is also shown.

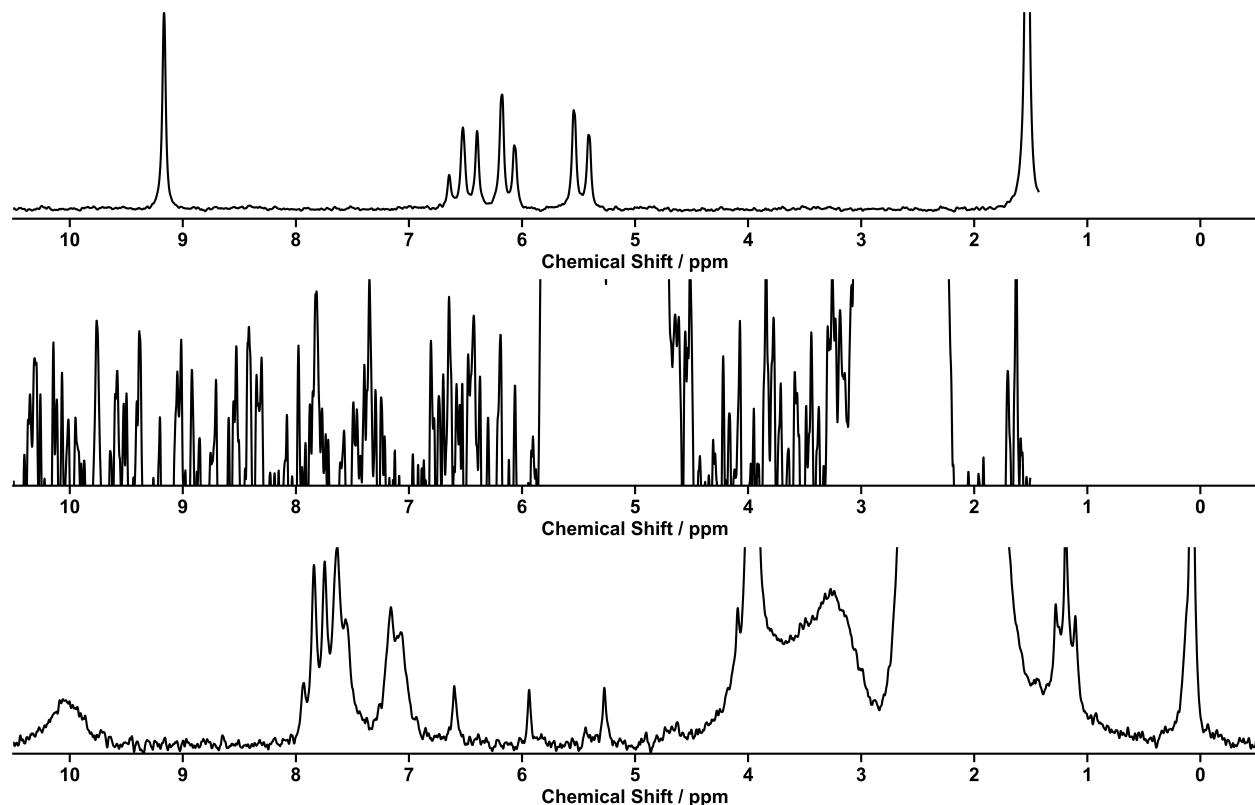
## Reaction 19



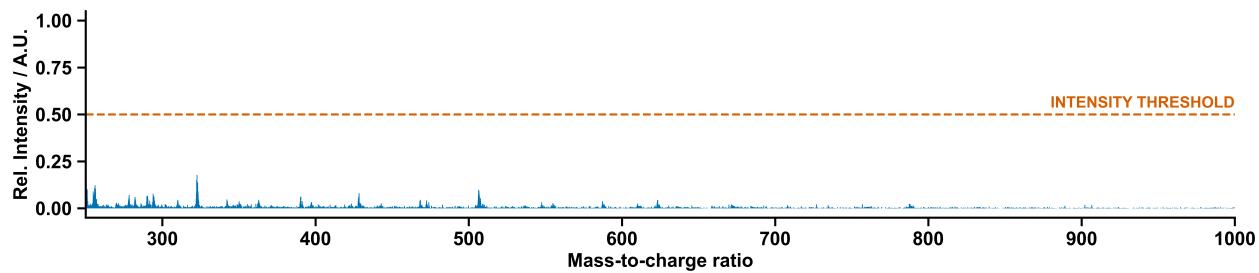
Scheme 18: Self-assembly of components 6, 21, with Iron(II) in a 3.0:1.5:1.0 molar ratio in CH<sub>3</sub>CN at 60°C for 40h. These are the reagents (starting materials) for reaction 19.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: Oligomers formed.	
	Human MS Decision: Failed	MS Spectra Category: Reaction failed.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	NMR Criteria 2: N/A
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 0
		MS Criteria 3: Pass	Number of counter-ions found: 0

Decision Table 18: Human labeled and Decsision maker labeled outcomes for the <sup>1</sup>H NMR spectroscopy and ULP-MS spectrometry of reaction 19. Decision motivations are also given.

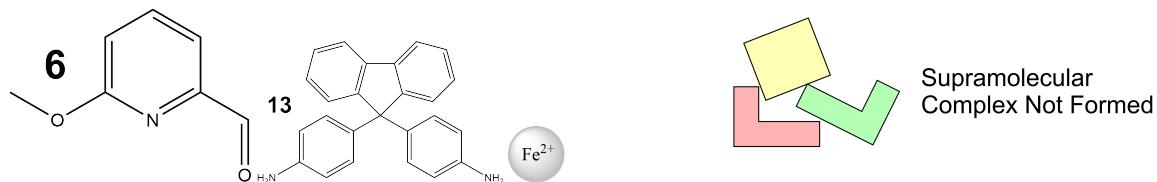


NMR Spectra 18: The stacked <sup>1</sup>H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 19.



MS Spectra 18: The ULPC-MS spectra of reaction 19. The intensity threshold is also shown.

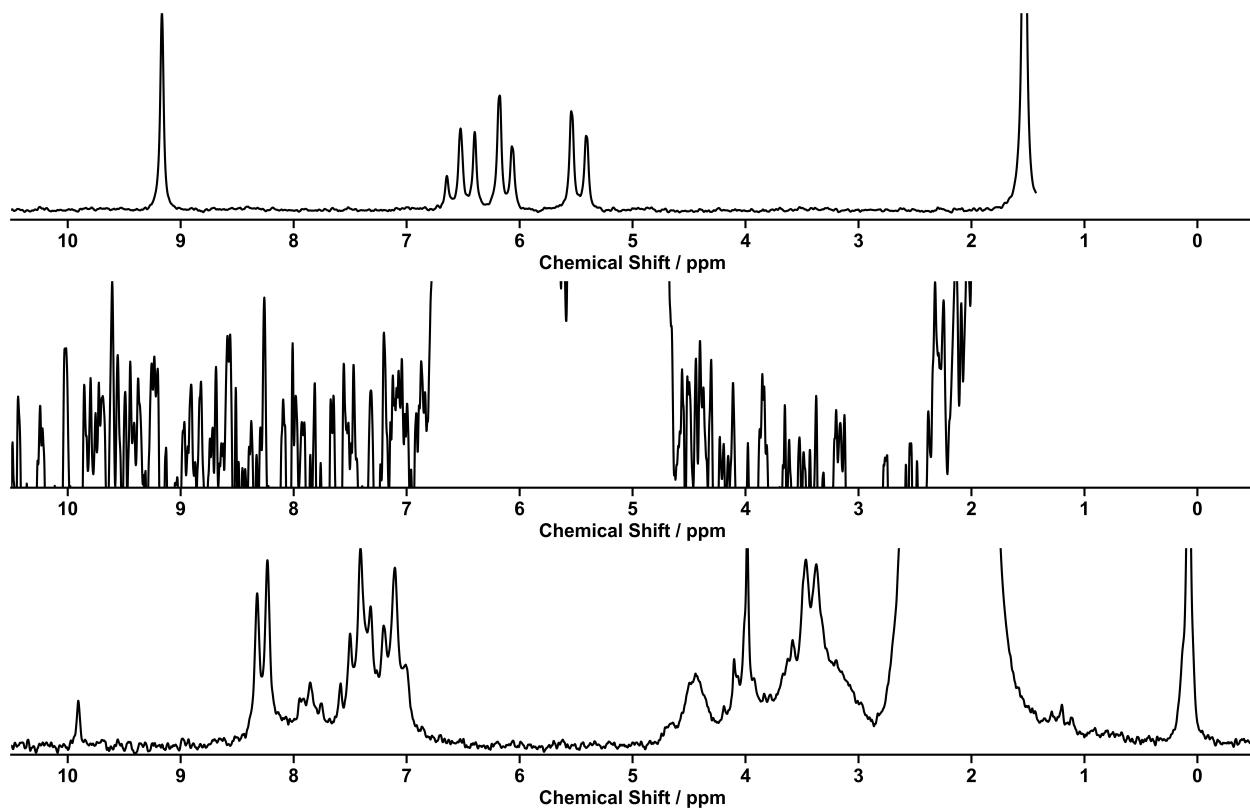
## Reaction 20



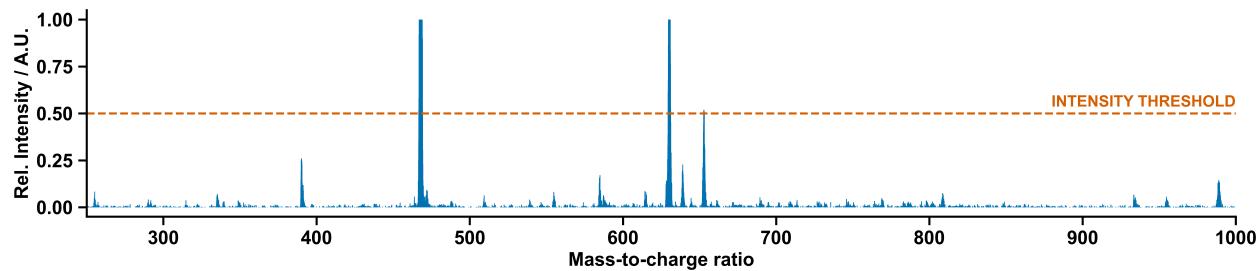
Scheme 19: Self-assembly of components 6, 13, with Iron(II) in a 3.0:1.5:1.0 molar ratio in CH<sub>3</sub>CN at 60°C for 40h. These are the reagents (starting materials) for reaction 20.

Human Reaction Decision: Failed	Human NMR Decision: Pass	NMR Spectra Category: Single discrete species formed.	
	Human MS Decision: Failed	MS Spectra Category: Reaction occurred, unknown product.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	NMR Criteria 2: N/A
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 9
		MS Criteria 3: Pass	Number of counter-ions found: 6

Decision Table 19: Human labeled and Decsision maker labeled outcomes for the <sup>1</sup>H NMR spectroscopy and ULPC-MS spectrometry of reaction 20. Decision motivations are also given.

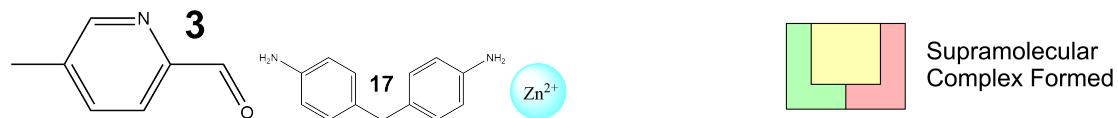


NMR Spectra 19: The stacked <sup>1</sup>H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 20.



MS Spectra 19: The ULPC-MS spectra of reaction 20. The intensity threshold is also shown.

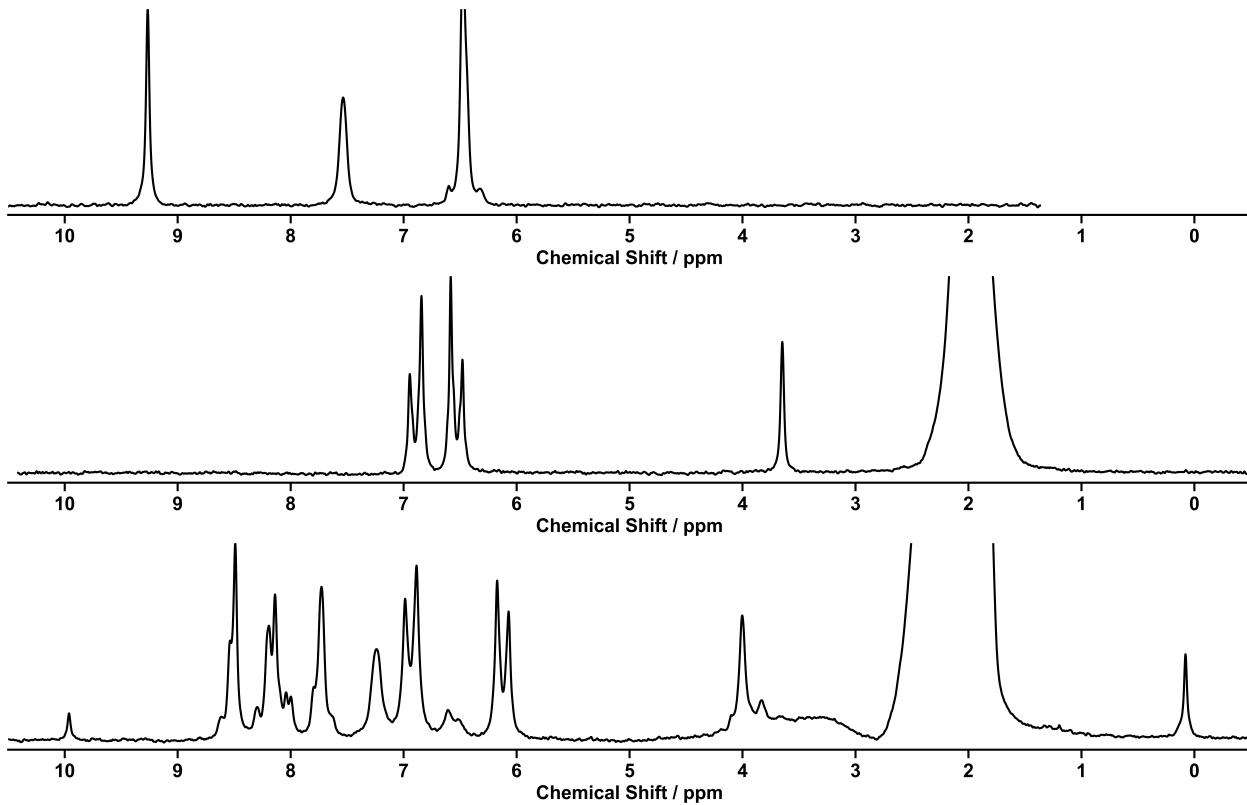
## Reaction 21



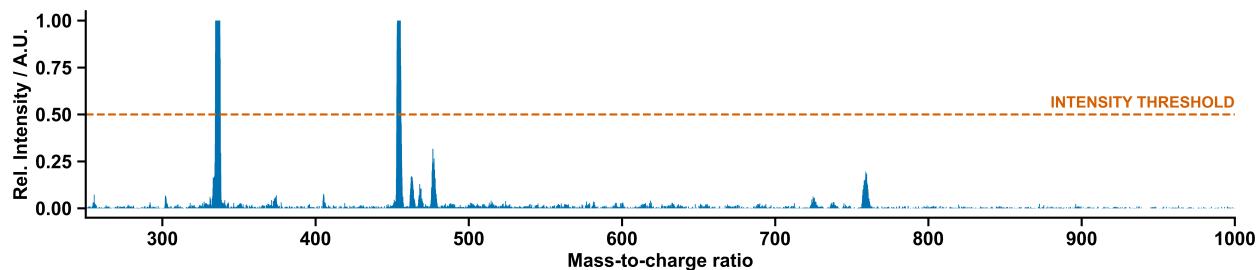
Scheme 20: Self-assembly of components 3, 17, with Zinc(II) in a 3.0:1.5:1.0 molar ratio in  $\text{CH}_3\text{CN}$  at 60°C for 40h. These are the reagents (starting materials) for reaction 21.

Human Reaction Decision: Pass	Human NMR Decision: Pass	NMR Spectra Category: Single discrete species formed.
	Human MS Decision: Pass	MS Spectra Category: Reaction occurred, supramolecular product.
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A
		NMR Criteria 2: N/A
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass  MS Criteria 3: Pass
		Number of predicted peaks found in MS spectra with appropriate intensity: 1  Number of counter-ions found: 1

Decision Table 20: Human labeled and Decsision maker labeled outcomes for the  $^1\text{H}$  NMR spectroscopy and ULPC-MS spectrometry of reaction 21. Decision motivations are also given.

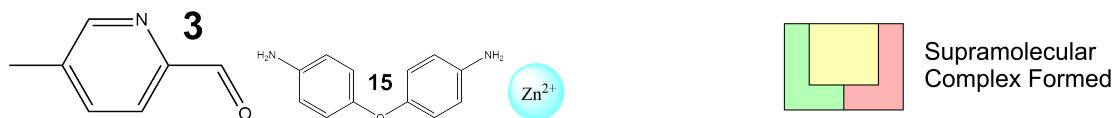


NMR Spectra 20: The stacked  $^1\text{H}$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 21.



MS Spectra 20: The ULPC-MS spectra of reaction 21. The intensity threshold is also shown.

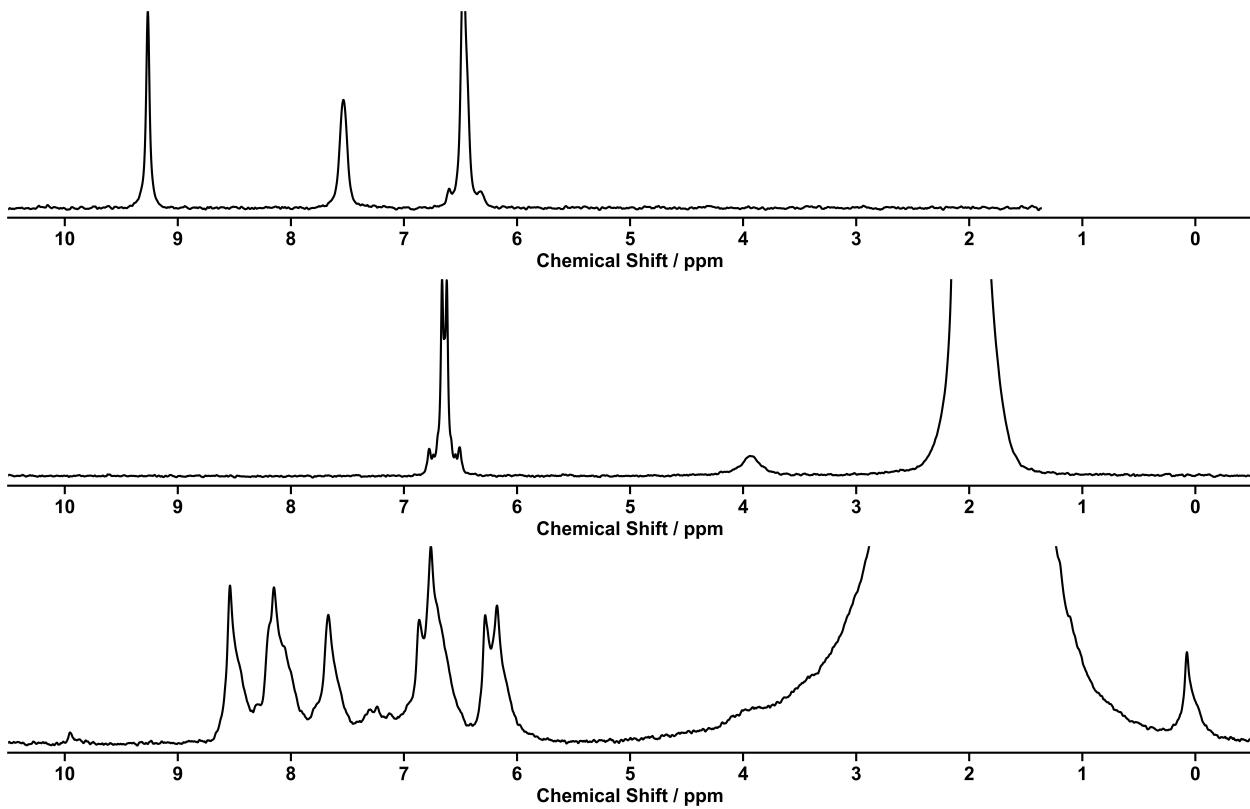
## Reaction 23



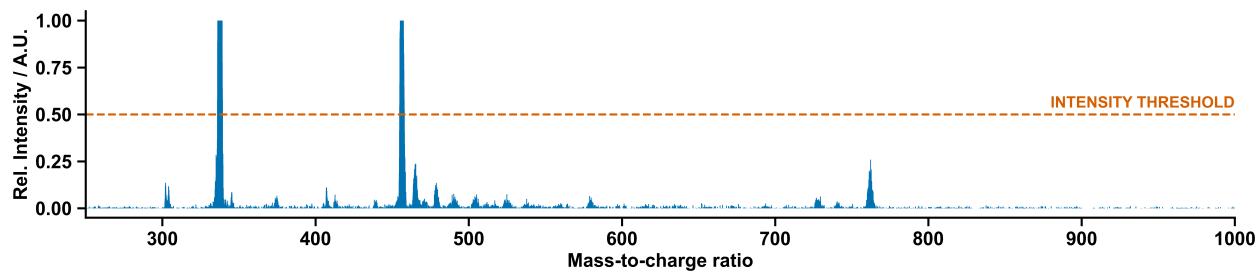
Scheme 21: Self-assembly of components 3, 15, with Zinc(II) in a 3.0:1.5:1.0 molar ratio in  $CH_3CN$  at  $60^\circ C$  for 40h. These are the reagents (starting materials) for reaction 23.

Human Reaction Decision: Pass	Human NMR Decision: Pass	NMR Spectra Category: Single discrete species formed.	
	Human MS Decision: Pass	MS Spectra Category: Reaction occurred, supramolecular product.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	NMR Criteria 2: N/A
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 1
	MS Criteria 3: Pass	MS Criteria 3: Pass	Number of counter-ions found: 1

Decision Table 21: Human labeled and Decision maker labeled outcomes for the  $^1H$  NMR spectroscopy and UPLC-MS spectrometry of reaction 23. Decision motivations are also given.

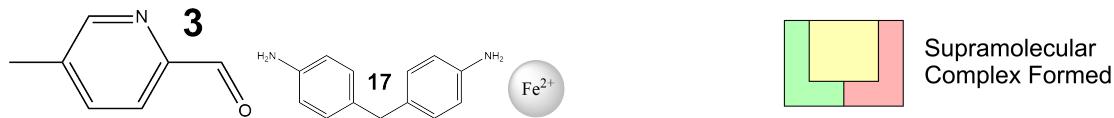


NMR Spectra 21: The stacked  $^1H$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 23.



MS Spectra 21: The ULPC-MS spectra of reaction 23. The intensity threshold is also shown.

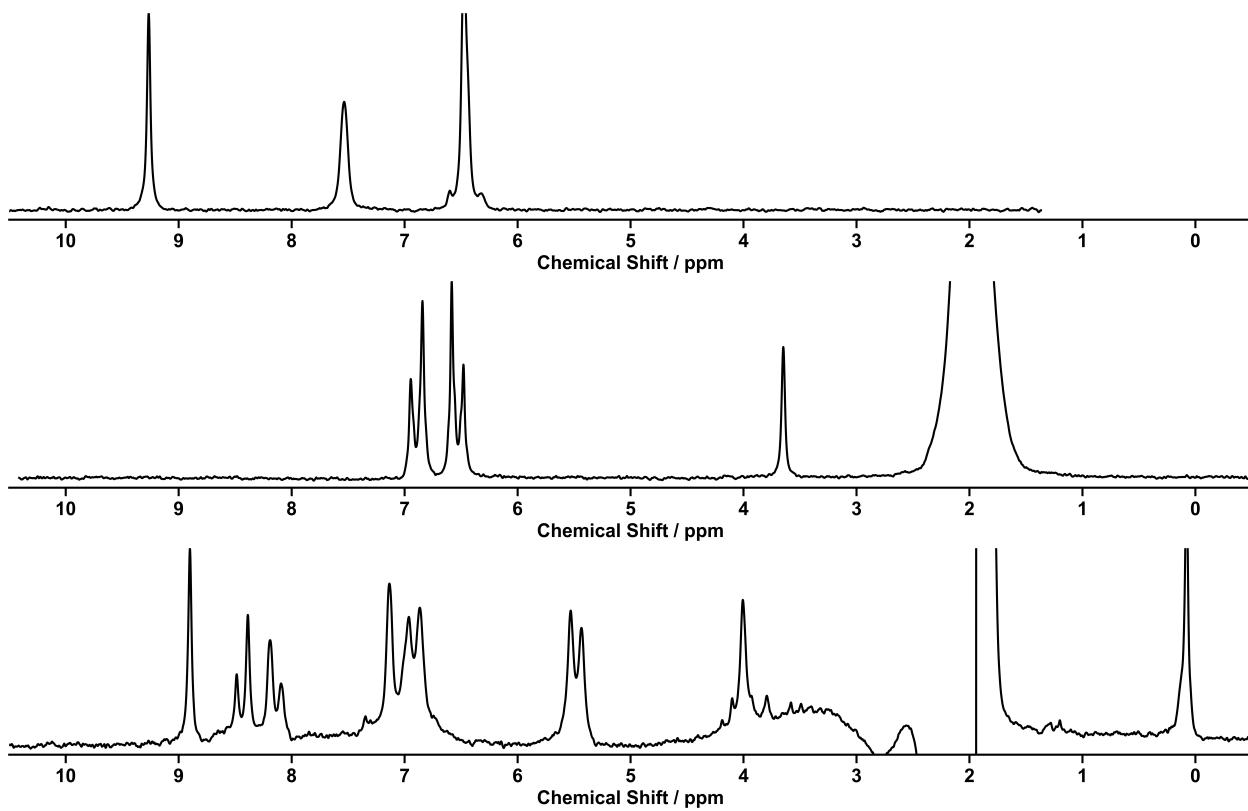
## Reaction 24



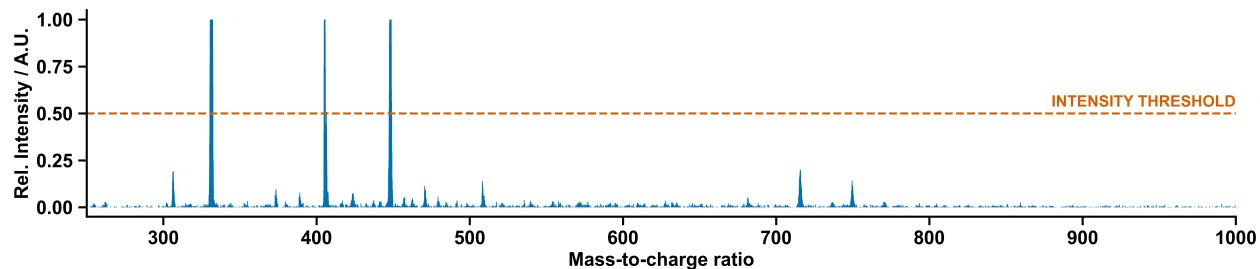
Scheme 22: Self-assembly of components 3, 17, with Iron(II) in a 3.0:1.5:1.0 molar ratio in  $\text{CH}_3\text{CN}$  at 60°C for 40h. These are the reagents (starting materials) for reaction 24.

Human Reaction Decision: Pass	Human NMR Decision: Pass	NMR Spectra Category: Single discrete species formed.	
	Human MS Decision: Pass	MS Spectra Category: Reaction occurred, supramolecular product.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	
	Decision Maker MS Decision: Pass	NMR Criteria 2: N/A	MS Criteria 1 and 2: Pass
		Number of predicted peaks found in MS spectra with appropriate intensity: 6	MS Criteria 3: Pass
		Number of counter-ions found: 3	

Decision Table 22: Human labeled and Decision maker labeled outcomes for the  $^1\text{H}$  NMR spectroscopy and ULPC-MS spectrometry of reaction 24. Decision motivations are also given.

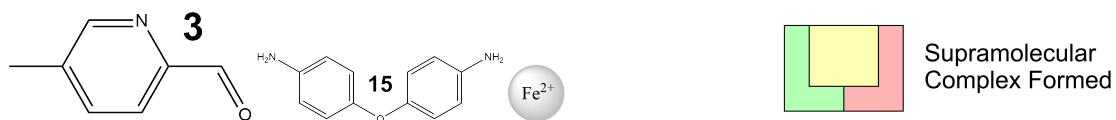


NMR Spectra 22: The stacked <sup>1</sup>H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 24.



MS Spectra 22: The ULPC-MS spectra of reaction 24. The intensity threshold is also shown.

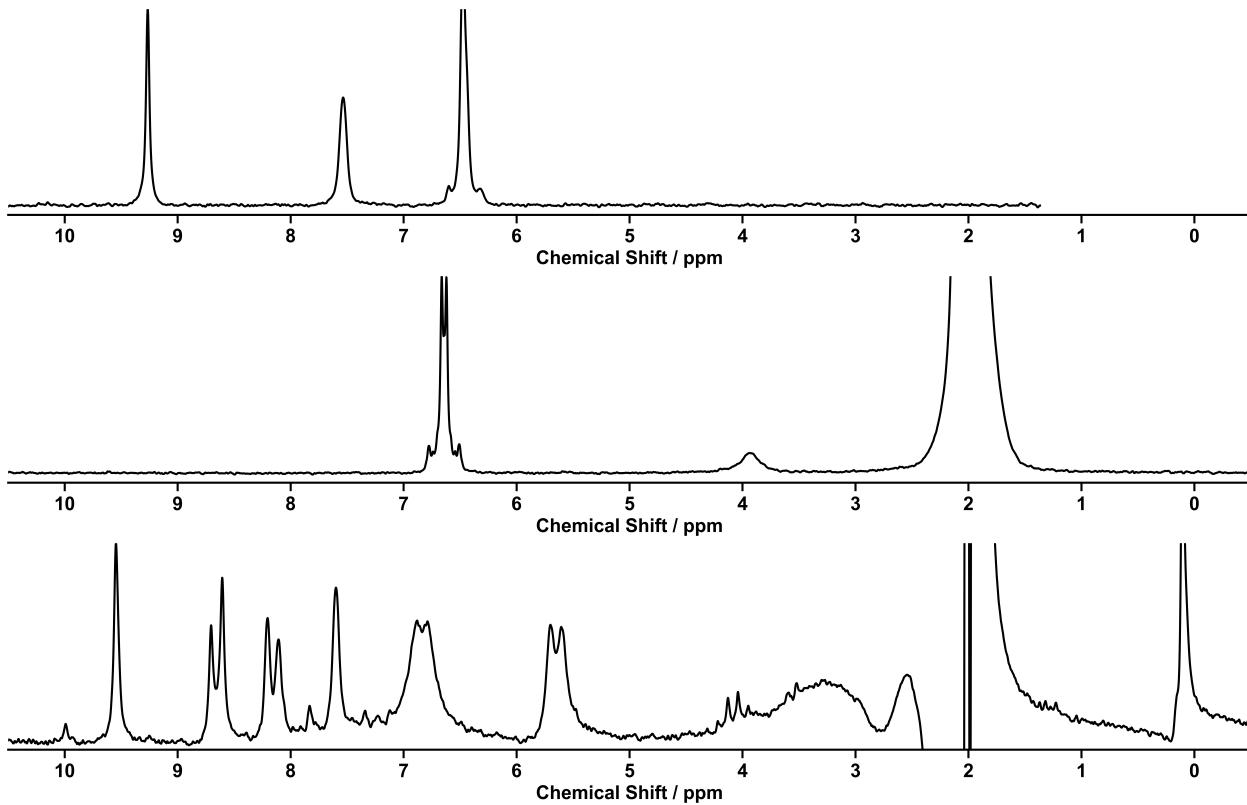
## Reaction 26



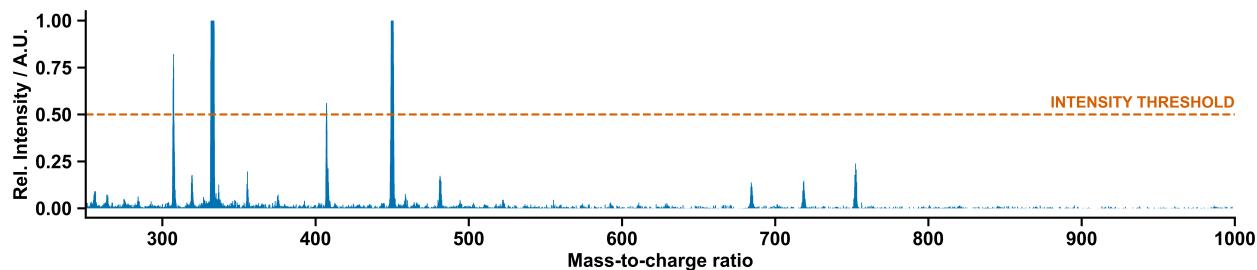
Scheme 23: Self-assembly of components 3, 15, with Iron(II) in a 3.0:1.5:1.0 molar ratio in  $\text{CH}_3\text{CN}$  at 60°C for 40h. These are the reagents (starting materials) for reaction 26.

Human Reaction Decision: Pass	Human NMR Decision: Pass	NMR Spectra Category: Single discrete species formed.	
	Human MS Decision: Pass	MS Spectra Category: Reaction occurred, supramolecular product.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	
		NMR Criteria 2: N/A	
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 5
		MS Criteria 3: Pass	Number of counter-ions found: 3

Decision Table 23: Human labeled and Decsision maker labeled outcomes for the  $^1\text{H}$  NMR spectroscopy and ULPC-MS spectrometry of reaction 26. Decision motivations are also given.

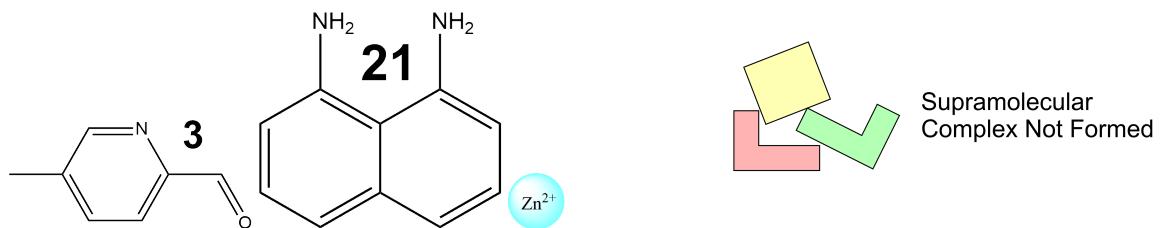


NMR Spectra 23: The stacked  $^1\text{H}$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 26.



MS Spectra 23: The ULPC-MS spectra of reaction 26. The intensity threshold is also shown.

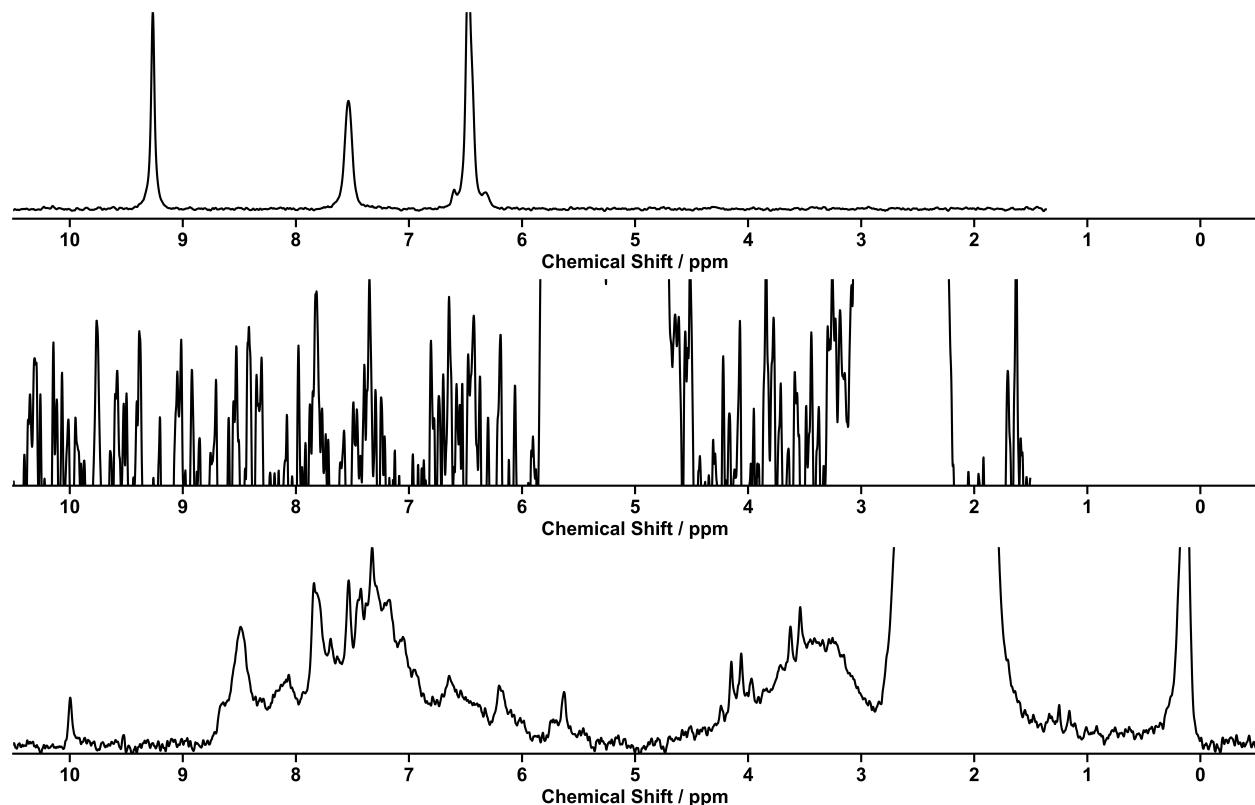
## Reaction 27



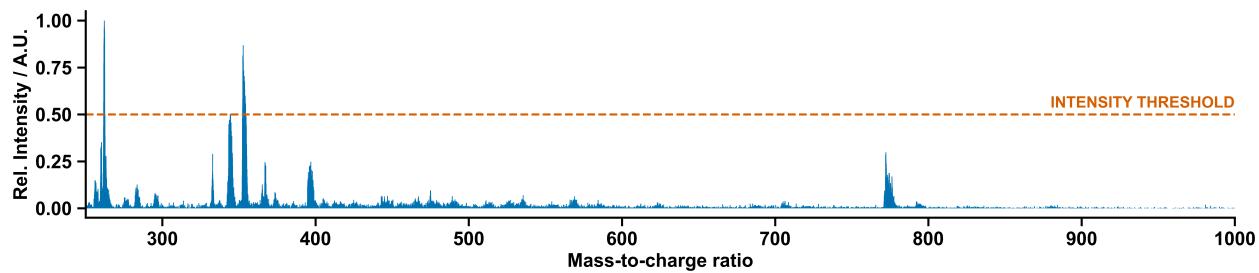
Scheme 24: Self-assembly of components 3, 21, with Zinc(II) in a 3.0:1.5:1.0 molar ratio in  $CH_3CN$  at  $60^\circ C$  for 40h. These are the reagents (starting materials) for reaction 27.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: Oligomers formed.	
	Human MS Decision: Failed	MS Spectra Category: Reaction occurred, unknown product.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	NMR Criteria 2: N/A
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 0
		MS Criteria 3: Pass	Number of counter-ions found: 0

Decision Table 24: Human labeled and Decsision maker labeled outcomes for the  $^1H$  NMR spectroscopy and ULP-MS spectrometry of reaction 27. Decision motivations are also given.

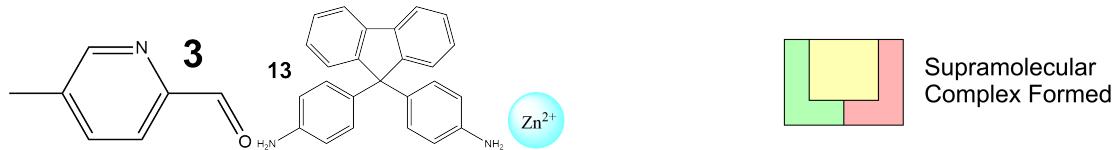


NMR Spectra 24: The stacked  $^1H$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 27.



MS Spectra 24: The ULPC-MS spectra of reaction 27. The intensity threshold is also shown.

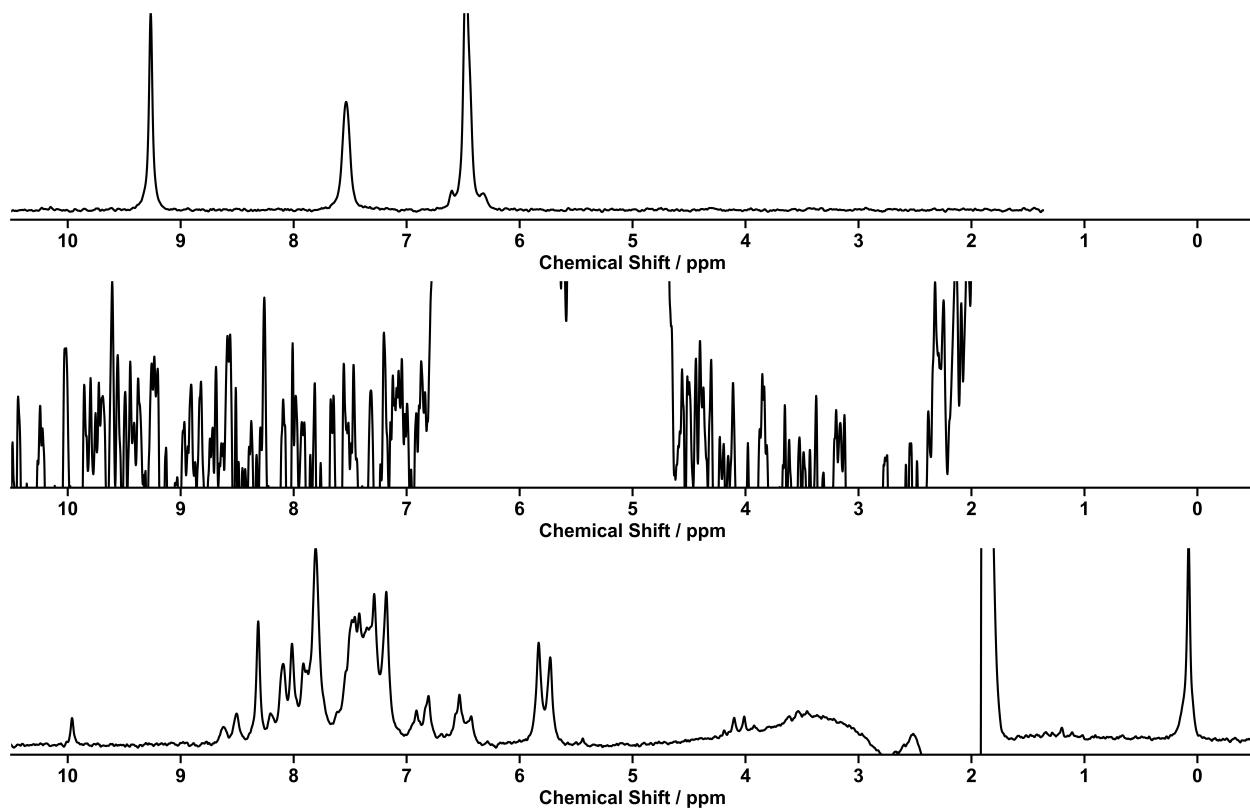
## Reaction 28



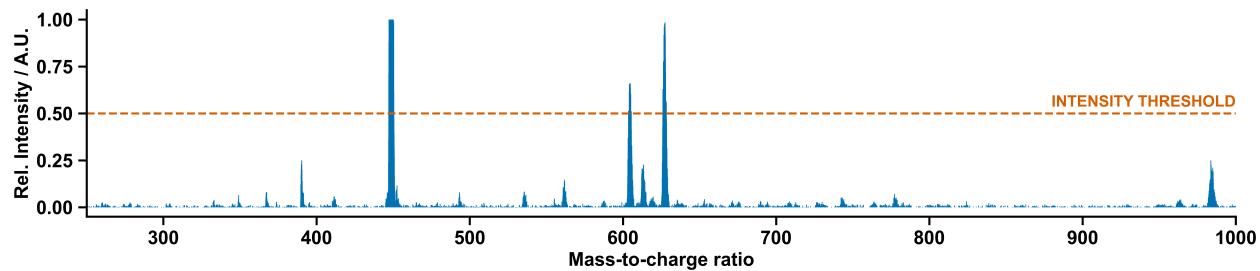
Scheme 25: Self-assembly of components 3, 13, with Zinc(II) in a 3.0:1.5:1.0 molar ratio in  $\text{CH}_3\text{CN}$  at  $60^\circ\text{C}$  for 40h. These are the reagents (starting materials) for reaction 28.

Human Reaction Decision: Pass	Human NMR Decision: Pass	NMR Spectra Category: Single discrete species formed.	
	Human MS Decision: Pass	MS Spectra Category: Reaction occurred, supramolecular product.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	
	Decision Maker MS Decision: Pass	NMR Criteria 2: N/A	MS Criteria 1 and 2: Pass
		Number of predicted peaks found in MS spectra with appropriate intensity: 4	Number of counter-ions found: 3
		MS Criteria 3: Pass	

Decision Table 25: Human labeled and Decision maker labeled outcomes for the  $^1\text{H}$  NMR spectroscopy and ULPC-MS spectrometry of reaction 28. Decision motivations are also given.

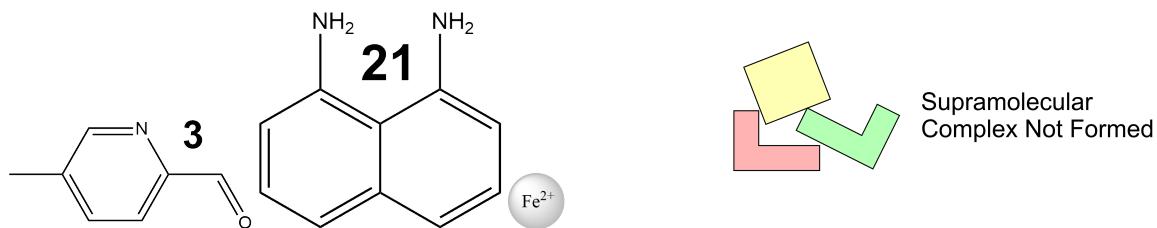


NMR Spectra 25: The stacked  $^1\text{H}$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 28.



MS Spectra 25: The ULPC-MS spectra of reaction 28. The intensity threshold is also shown.

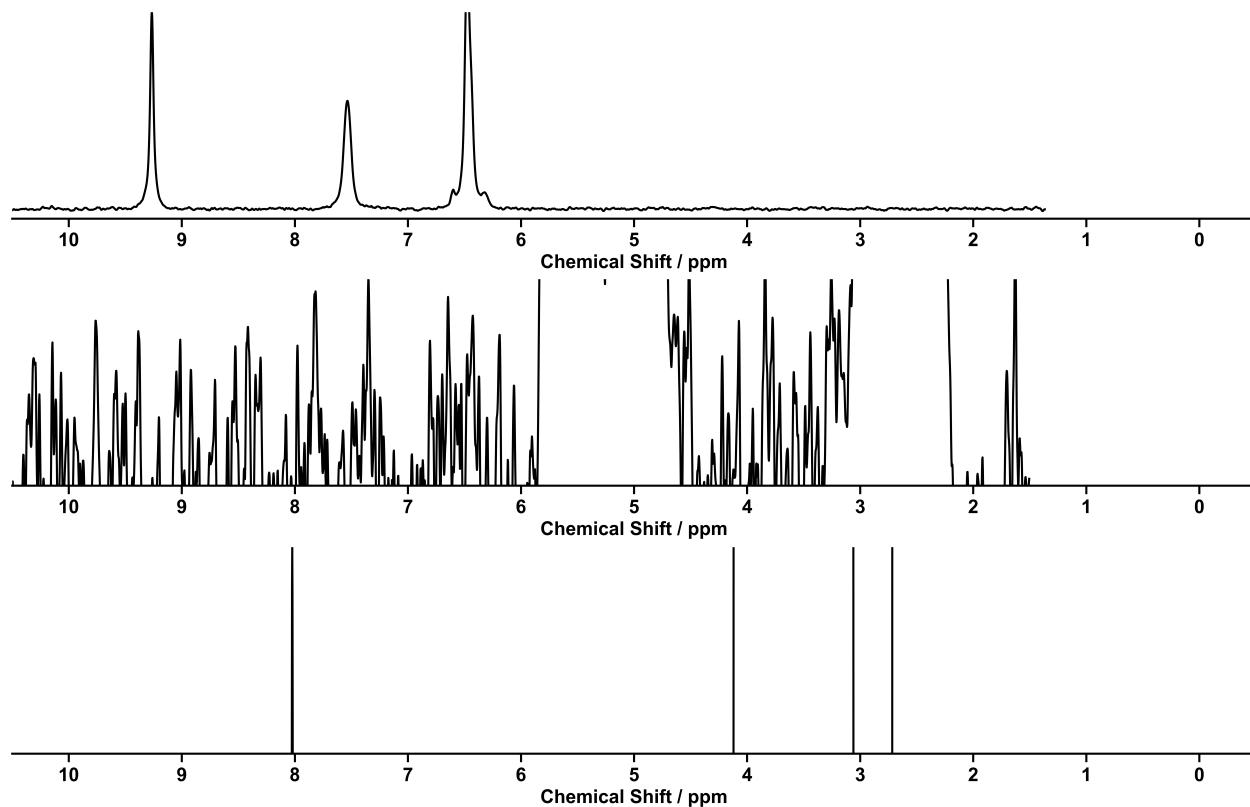
## Reaction 29



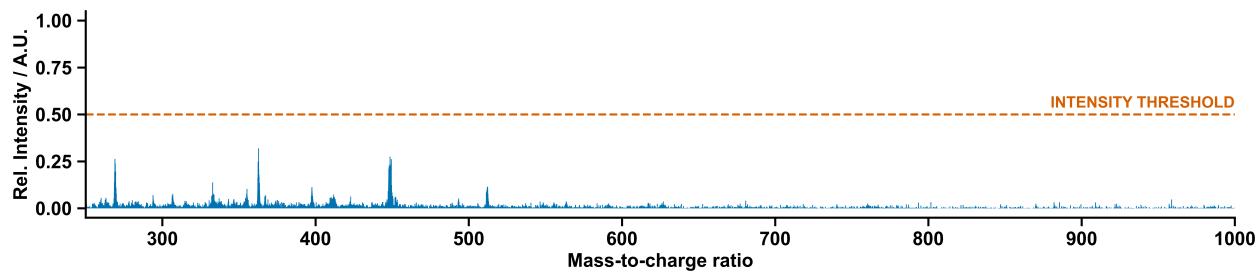
Scheme 26: Self-assembly of components **3**, **21**, with Iron(II) in a 3.0:1.5:1.0 molar ratio in  $\text{CH}_3\text{CN}$  at  $60^\circ\text{C}$  for 40h. These are the reagents (starting materials) for reaction 29.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: Paramagnetic species formed.	
	Human MS Decision: Failed	MS Spectra Category: Reaction failed.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	NMR Criteria 2: N/A
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 0
		MS Criteria 3: Pass	Number of counter-ions found: 0

Decision Table 26: Human labeled and Decsision maker labeled outcomes for the  $^1\text{H}$  NMR spectroscopy and ULP-MS spectrometry of reaction 29. Decision motivations are also given.

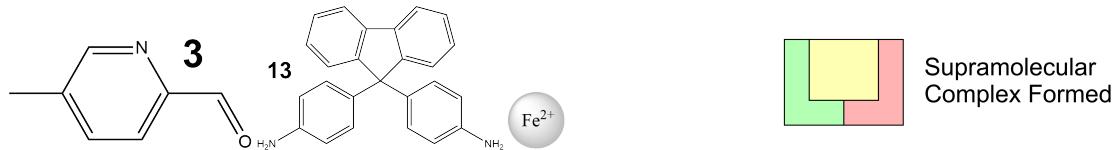


NMR Spectra 26: The stacked  $^1\text{H}$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 29.



MS Spectra 26: The ULPC-MS spectra of reaction 29. The intensity threshold is also shown.

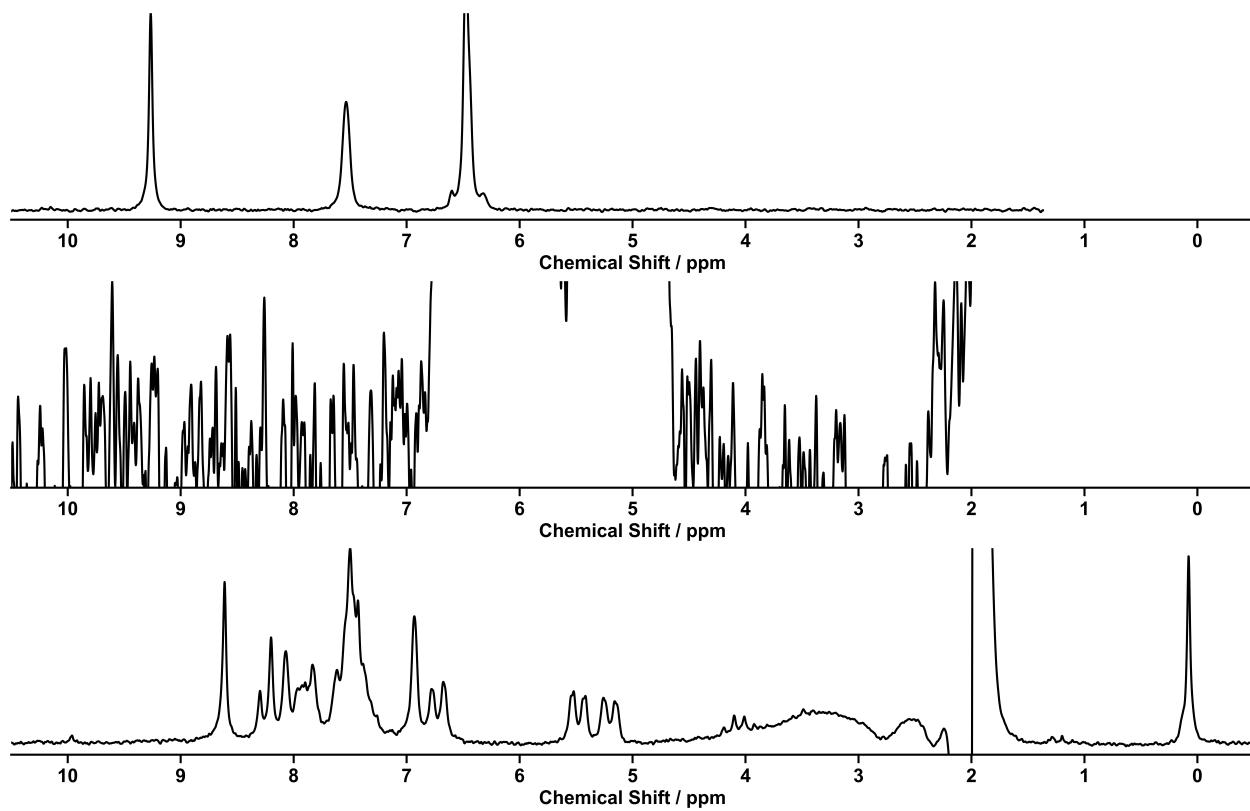
## Reaction 30



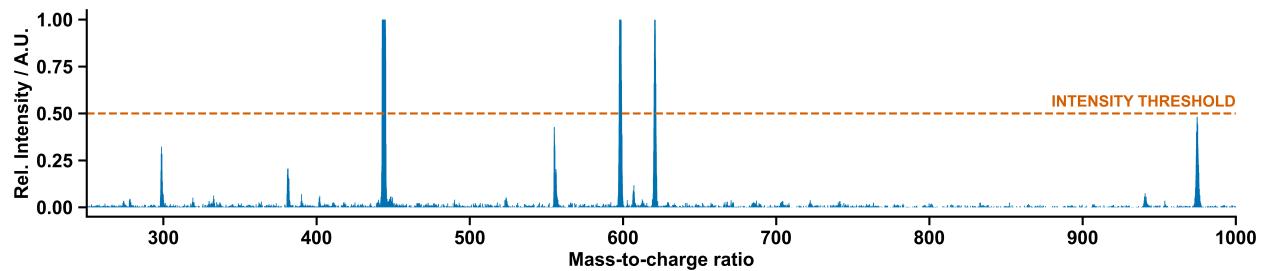
Scheme 27: Self-assembly of components 3, 13, with Iron(II) in a 3.0:1.5:1.0 molar ratio in  $\text{CH}_3\text{CN}$  at  $60^\circ\text{C}$  for 40h. These are the reagents (starting materials) for reaction 30.

Human Reaction Decision: Pass	Human NMR Decision: Pass	NMR Spectra Category: Single discrete species formed.	
	Human MS Decision: Pass	MS Spectra Category: Reaction occurred, supramolecular product.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	
	Decision Maker MS Decision: Pass	NMR Criteria 2: N/A	MS Criteria 1 and 2: Pass
		Number of predicted peaks found in MS spectra with appropriate intensity: 10	Number of counter-ions found: 6
		MS Criteria 3: Pass	

Decision Table 27: Human labeled and Decision maker labeled outcomes for the  $^1\text{H}$  NMR spectroscopy and ULPC-MS spectrometry of reaction 30. Decision motivations are also given.

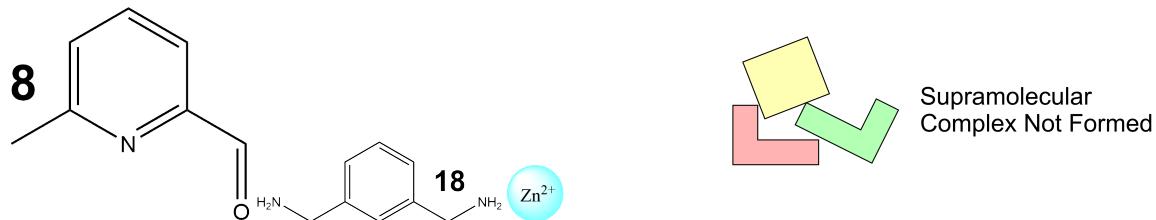


NMR Spectra 27: The stacked  $^1\text{H}$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 30.



MS Spectra 27: The ULPC-MS spectra of reaction 30. The intensity threshold is also shown.

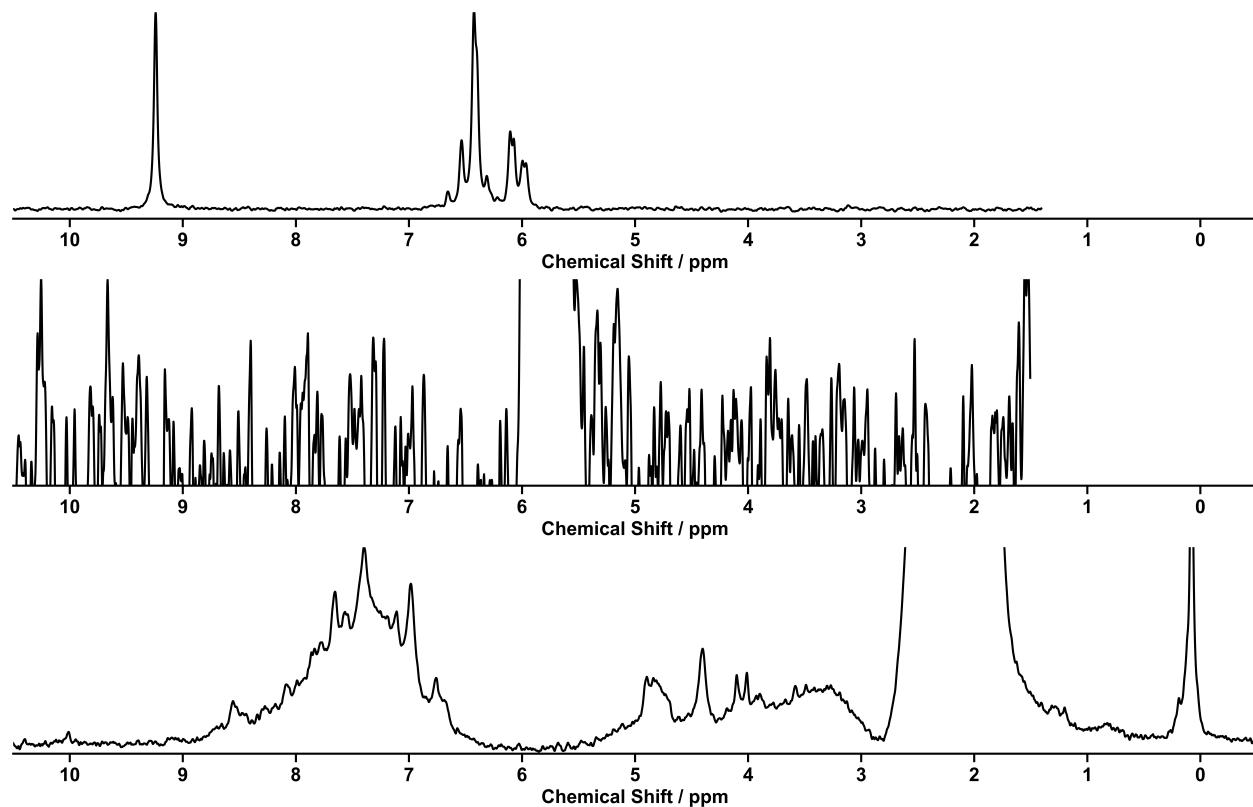
## Reaction 31



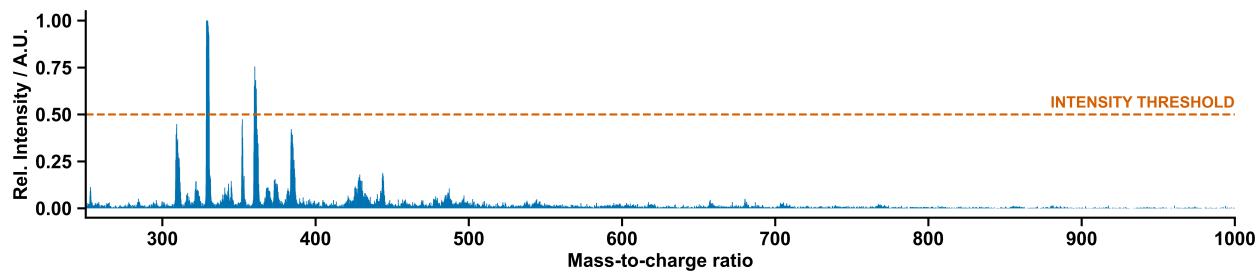
Scheme 28: Self-assembly of components 8, 18, with Zinc(II) in a 3.0:1.5:1.0 molar ratio in  $CH_3CN$  at  $60^\circ C$  for 40h. These are the reagents (starting materials) for reaction 31.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: Oligomers formed.	
	Human MS Decision: Failed	MS Spectra Category: Reaction occurred, unknown product.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	NMR Criteria 2: N/A
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 0
		MS Criteria 3: Pass	Number of counter-ions found: 0

Decision Table 28: Human labeled and Decsision maker labeled outcomes for the  $^1H$  NMR spectroscopy and UPLC-MS spectrometry of reaction 31. Decision motivations are also given.

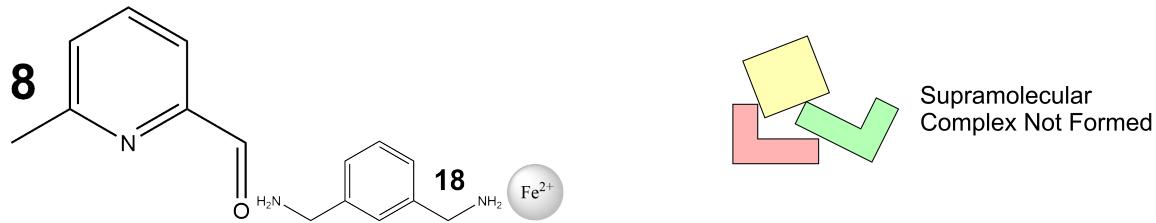


NMR Spectra 28: The stacked  $^1H$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 31.



MS Spectra 28: The ULPC-MS spectra of reaction 31. The intensity threshold is also shown.

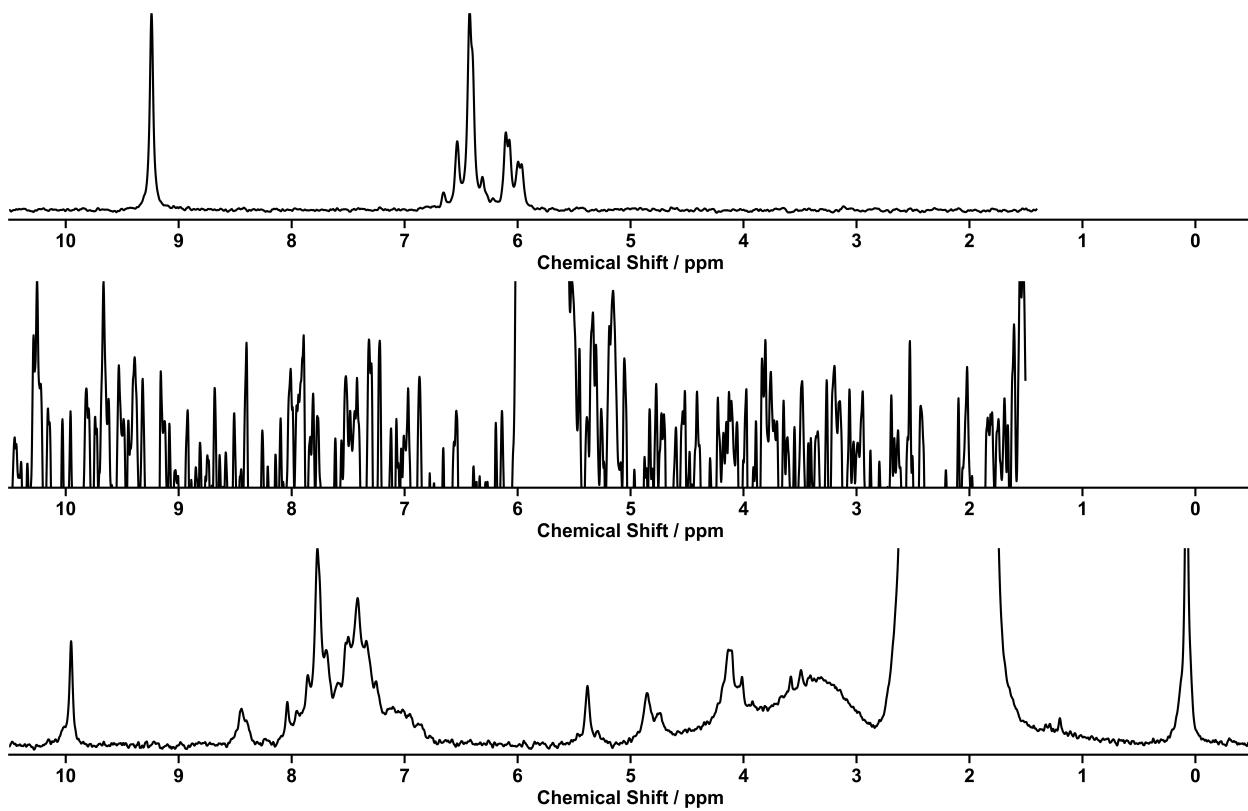
## Reaction 32



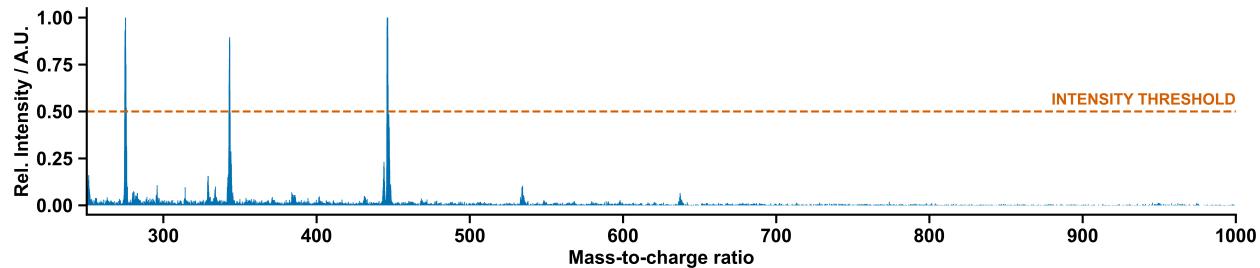
Scheme 29: Self-assembly of components 8, 18, with Iron(II) in a 3.0:1.5:1.0 molar ratio in CH<sub>3</sub>CN at 60°C for 40h. These are the reagents (starting materials) for reaction 32.

Human Reaction Decision: Failed	Human NMR Decision: Pass	NMR Spectra Category: Single discrete species formed.	
	Human MS Decision: Failed	MS Spectra Category: Reaction occurred, unknown product.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	NMR Criteria 2: N/A
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 0
		MS Criteria 3: Pass	Number of counter-ions found: 0

Decision Table 29: Human labeled and Decsision maker labeled outcomes for the <sup>1</sup>H NMR spectroscopy and ULPC-MS spectrometry of reaction 32. Decision motivations are also given.

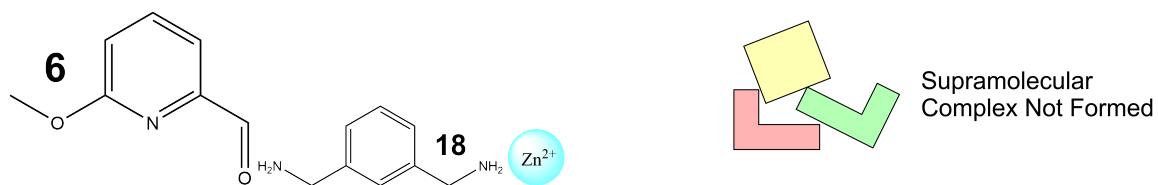


NMR Spectra 29: The stacked <sup>1</sup>H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 32.



MS Spectra 29: The ULPC-MS spectra of reaction 32. The intensity threshold is also shown.

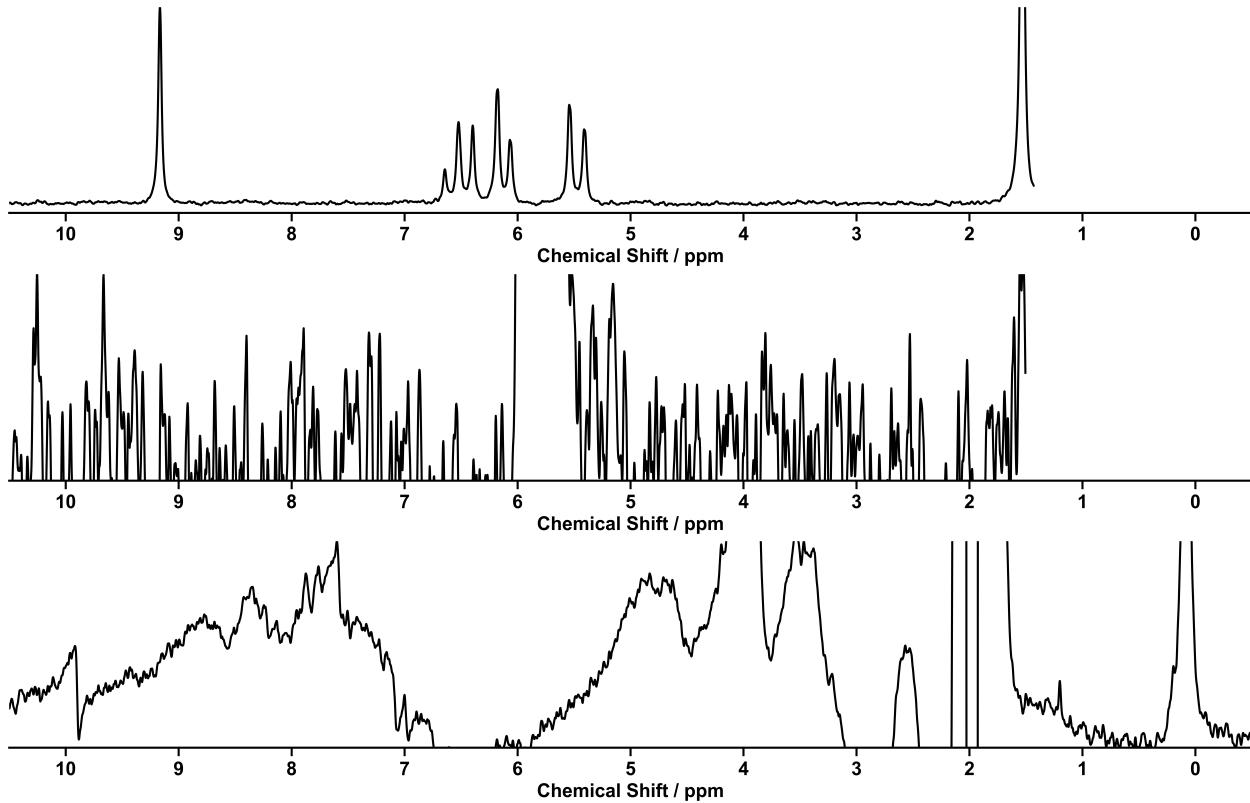
## Reaction 33



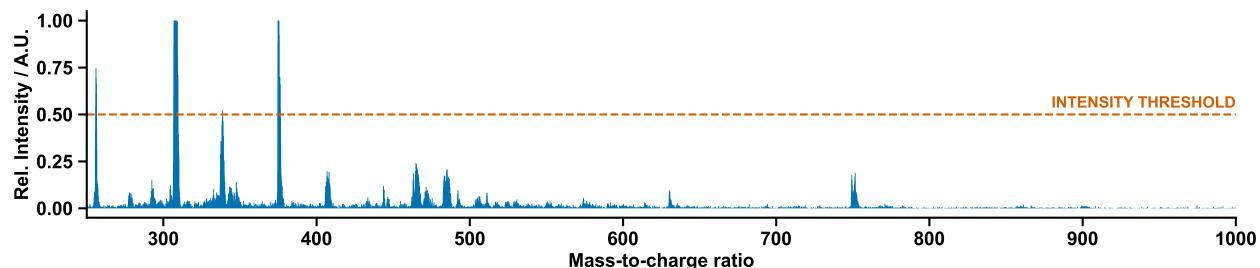
Scheme 30: Self-assembly of components 6, 18, with Zinc(II) in a 3.0:1.5:1.0 molar ratio in  $CH_3CN$  at 60°C for 40h. These are the reagents (starting materials) for reaction 33.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: Oligomers formed.	
	Human MS Decision: Pass	MS Spectra Category: Reaction occurred, supramolecular product.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	
	Decision Maker MS Decision: Pass	NMR Criteria 2: N/A	MS Criteria 1 and 2: Pass Number of predicted peaks found in MS spectra with appropriate intensity: 0
	MS Criteria 3: Pass	Number of counter-ions found: 0	

Decision Table 30: Human labeled and Decsision maker labeled outcomes for the  $^1\text{H}$  NMR spectroscopy and ULPC-MS spectrometry of reaction 33. Decision motivations are also given.

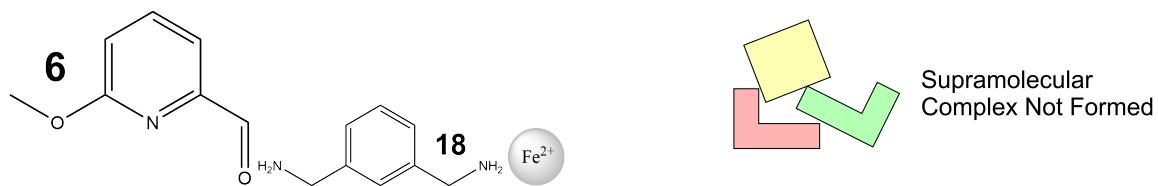


NMR Spectra 30: The stacked  $^1\text{H}$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 33.



MS Spectra 30: The ULPC-MS spectra of reaction 33. The intensity threshold is also shown.

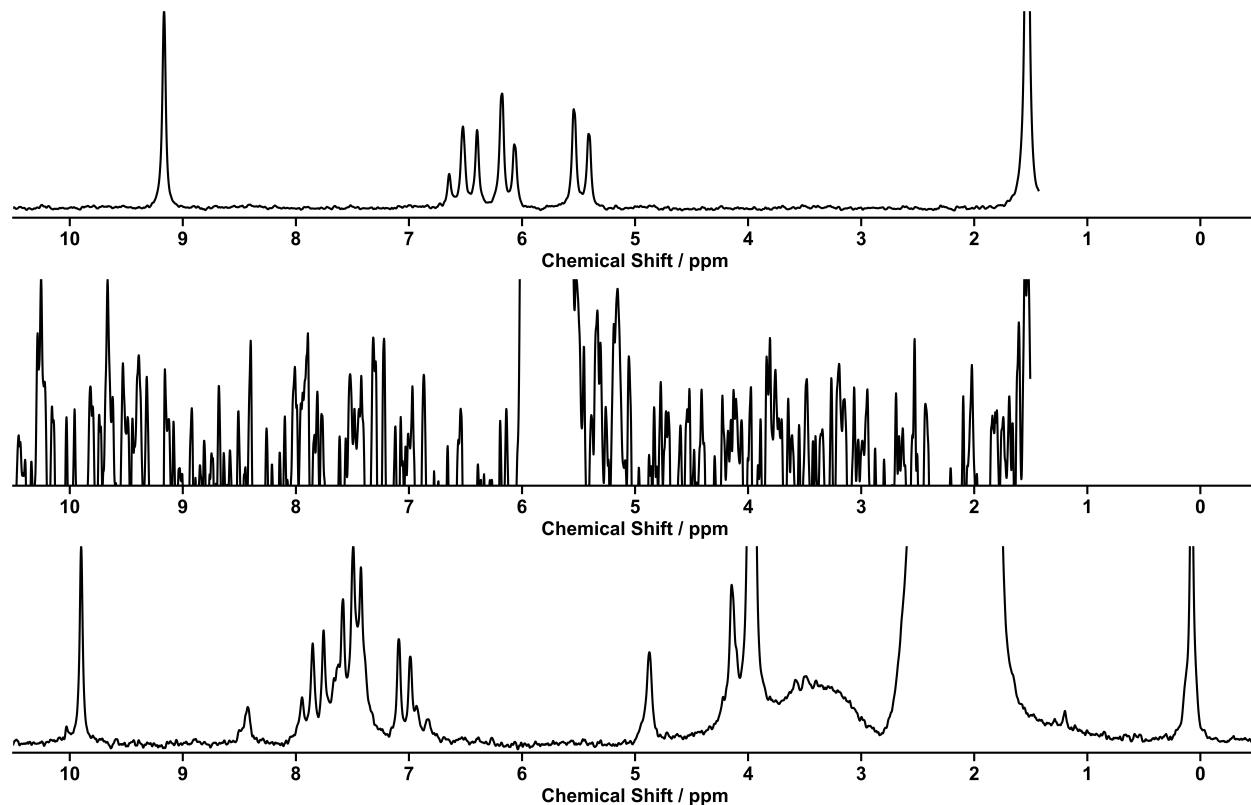
## Reaction 34



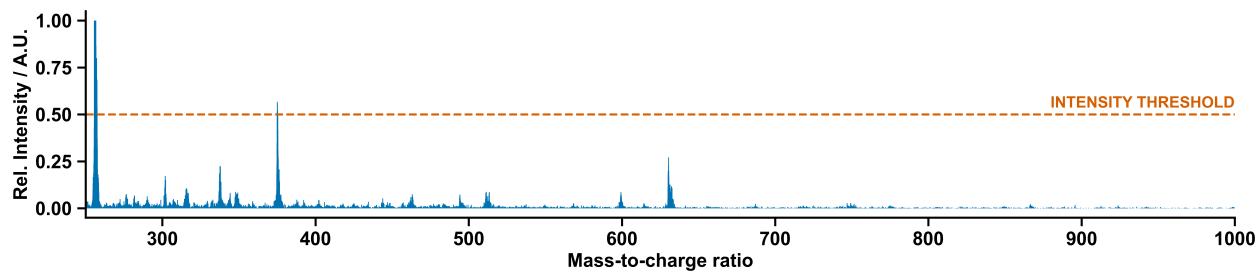
Scheme 31: Self-assembly of components 6, 18, with Iron(II) in a 3.0:1.5:1.0 molar ratio in  $\text{CH}_3\text{CN}$  at  $60^\circ\text{C}$  for 40h. These are the reagents (starting materials) for reaction 34.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: No reaction occurred.	
	Human MS Decision: Failed	MS Spectra Category: Reaction occurred, unknown product.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	NMR Criteria 2: N/A
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 0
		MS Criteria 3: Pass	Number of counter-ions found: 0

Decision Table 31: Human labeled and Decsision maker labeled outcomes for the  $^1\text{H}$  NMR spectroscopy and UPLC-MS spectrometry of reaction 34. Decision motivations are also given.



NMR Spectra 31: The stacked  $^1\text{H}$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 34.



MS Spectra 31: The ULPC-MS spectra of reaction 34. The intensity threshold is also shown.

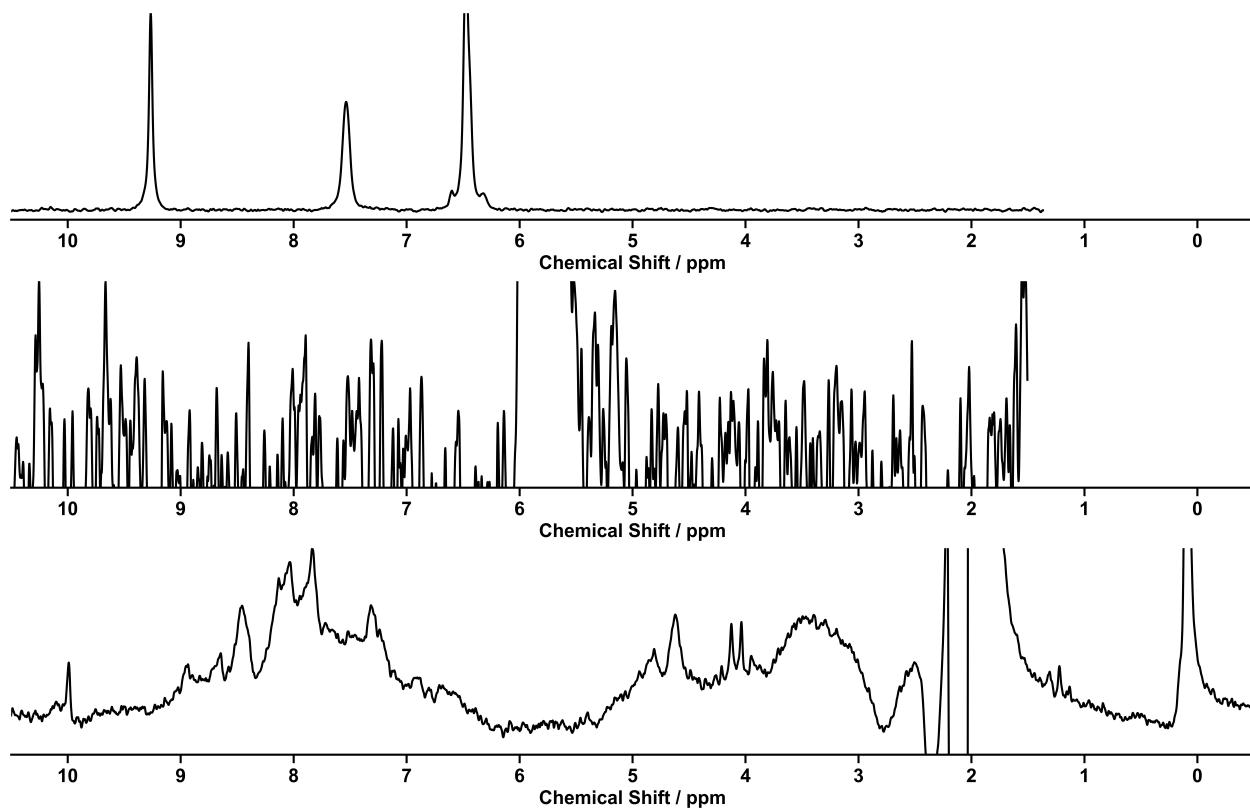
## Reaction 35



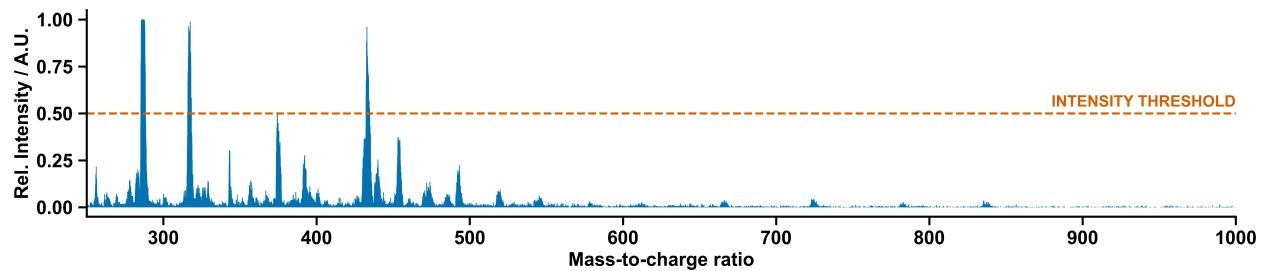
Scheme 32: Self-assembly of components 3, 18, with Zinc(II) in a 3.0:1.5:1.0 molar ratio in  $\text{CH}_3\text{CN}$  at  $60^\circ\text{C}$  for 40h. These are the reagents (starting materials) for reaction 35.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: Oligomers formed.	
	Human MS Decision: Pass	MS Spectra Category: Reaction occurred, supramolecular product.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	NMR Criteria 2: N/A
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 1
		MS Criteria 3: Pass	Number of counter-ions found: 0

Decision Table 32: Human labeled and Decision maker labeled outcomes for the  $^1\text{H}$  NMR spectroscopy and ULPC-MS spectrometry of reaction 35. Decision motivations are also given.

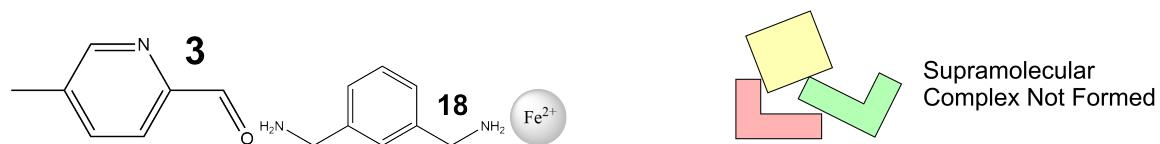


NMR Spectra 32: The stacked <sup>1</sup>H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 35.



MS Spectra 32: The ULPC-MS spectra of reaction 35. The intensity threshold is also shown.

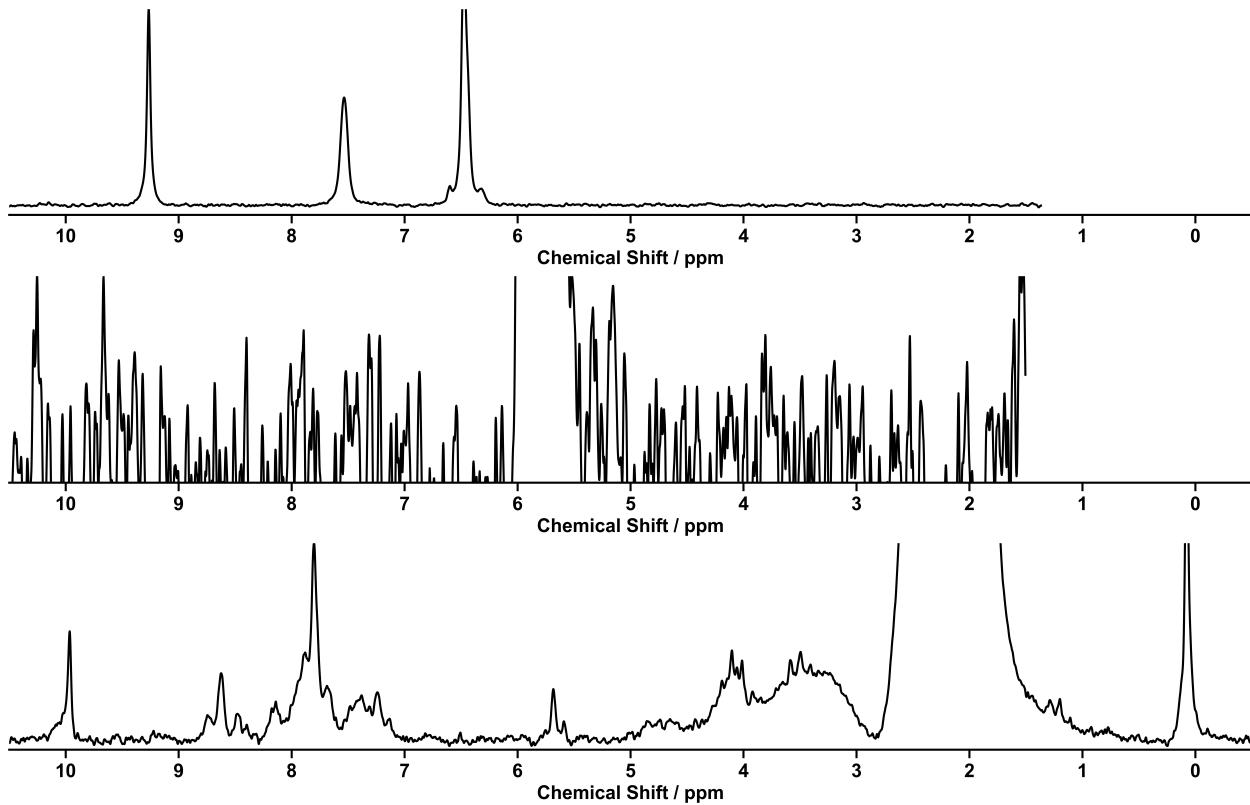
## Reaction 36



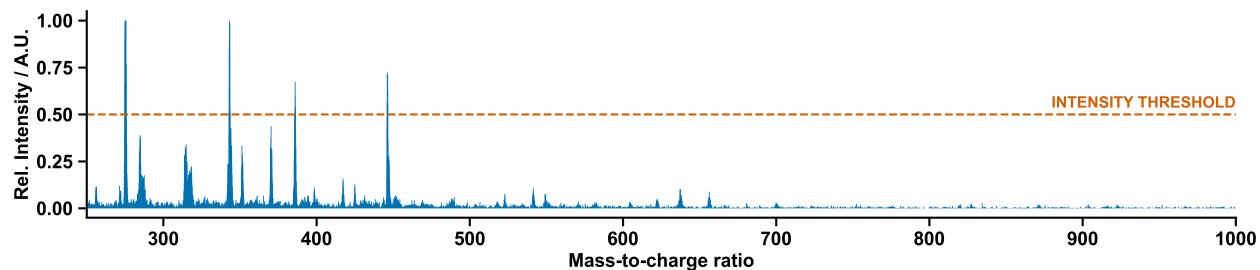
Scheme 33: Self-assembly of components 3, 18, with Iron(II) in a 3.0:1.5:1.0 molar ratio in  $\text{CH}_3\text{CN}$  at 60°C for 40h. These are the reagents (starting materials) for reaction 36.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: Paramagnetic species formed.	
	Human MS Decision: Failed	MS Spectra Category: Reaction occurred, unknown product.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	
		NMR Criteria 2: N/A	
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 0
		MS Criteria 3: Pass	Number of counter-ions found: 0

Decision Table 33: Human labeled and Decsision maker labeled outcomes for the  $^1\text{H}$  NMR spectroscopy and UPLC-MS spectrometry of reaction 36. Decision motivations are also given.

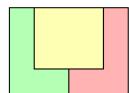
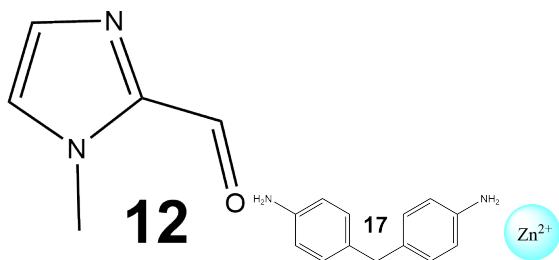


NMR Spectra 33: The stacked  $^1\text{H}$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 36.



MS Spectra 33: The ULPC-MS spectra of reaction 36. The intensity threshold is also shown.

## Reaction 37

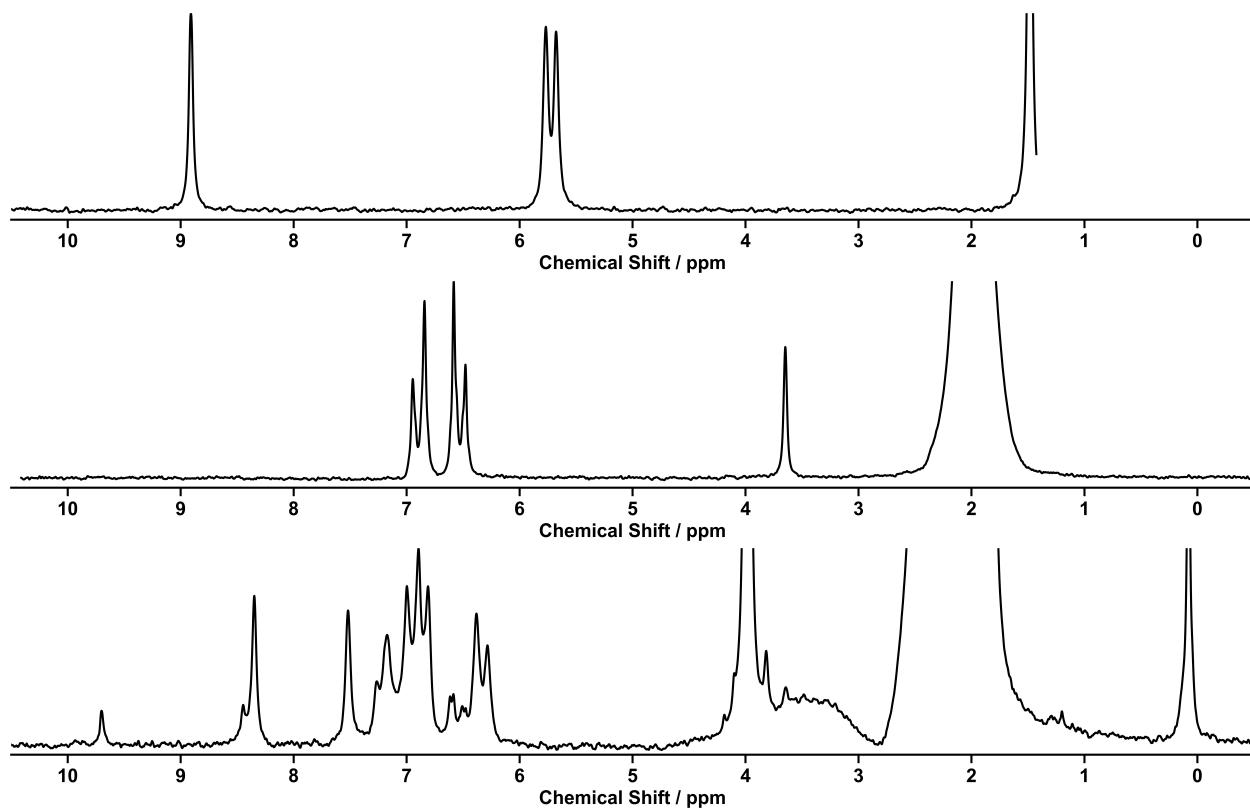


# Supramolecular Complex Formed

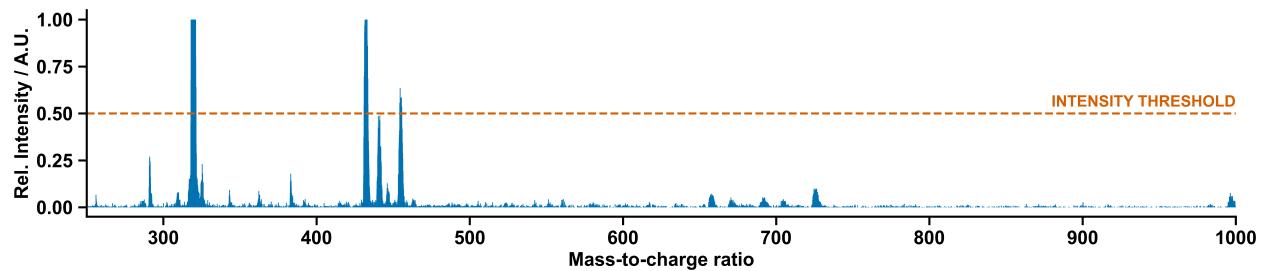
Scheme 34: Self-assembly of components 12, 17, with Zinc(II) in a 3.0:1.5:1.0 molar ratio in CH<sub>3</sub>CN at 60°C for 40h. These are the reagents (starting materials) for reaction 37.

Human Reaction Decision: Pass	Human NMR Decision: Pass	NMR Spectra Category: Single discrete species formed.	
	Human MS Decision: Pass	MS Spectra Category: Reaction occurred, supramolecular product.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	
		NMR Criteria 2: N/A	
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 4
		MS Criteria 3: Pass	Number of counter-ions found: 3

Decision Table 34: Human labeled and Decsision maker labeled outcomes for the  $^1\text{H}$  NMR spectroscopy and ULPC-MS spectrometry of reaction 37. Decision motivations are also given.

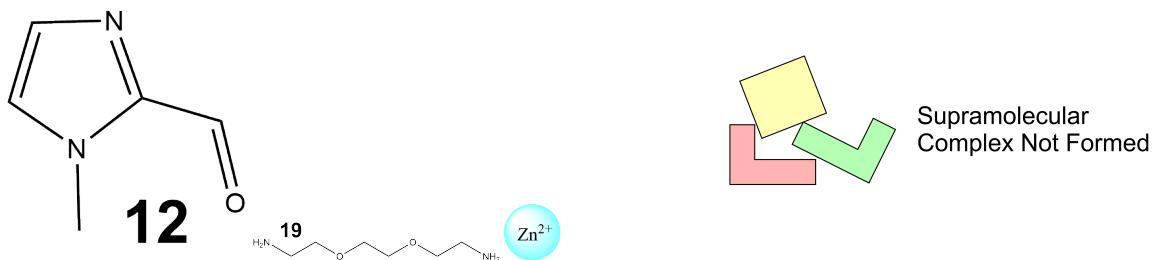


NMR Spectra 34: The stacked  $^1\text{H}$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 37.



MS Spectra 34: The ULPC-MS spectra of reaction 37. The intensity threshold is also shown.

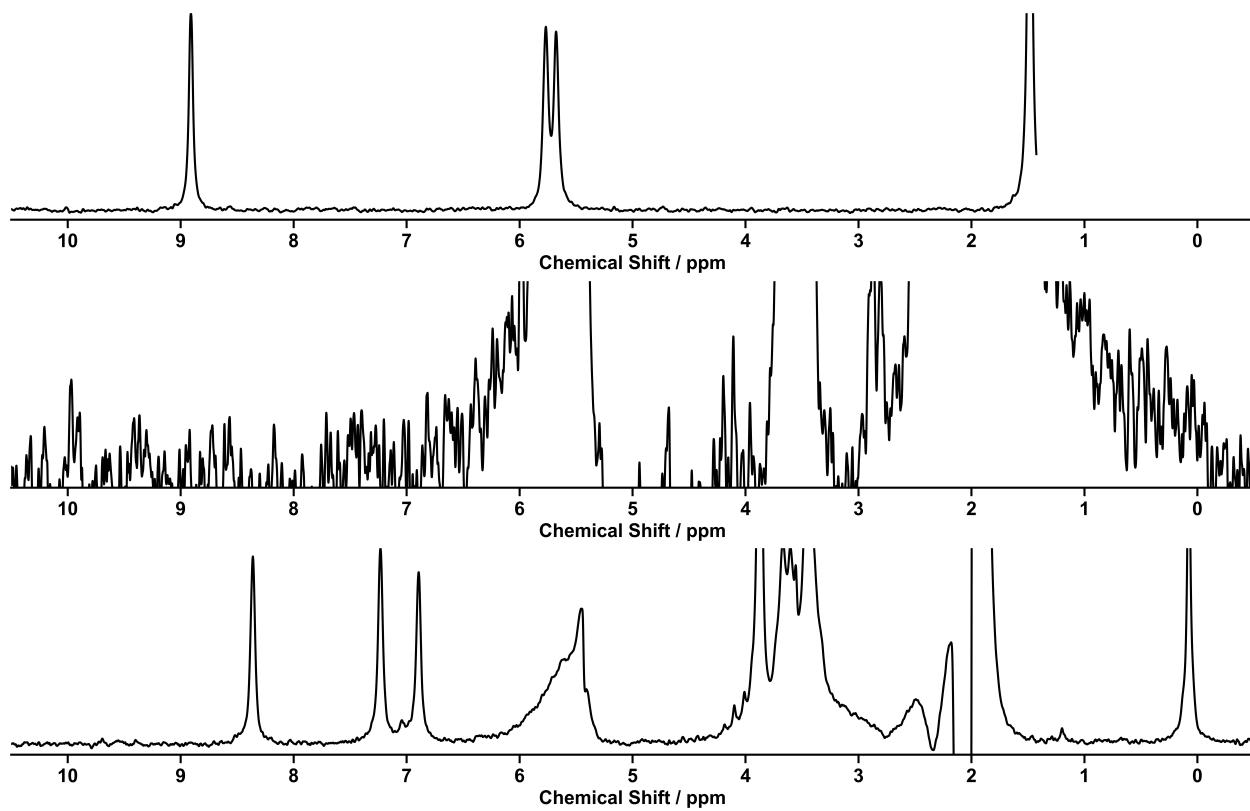
## Reaction 38



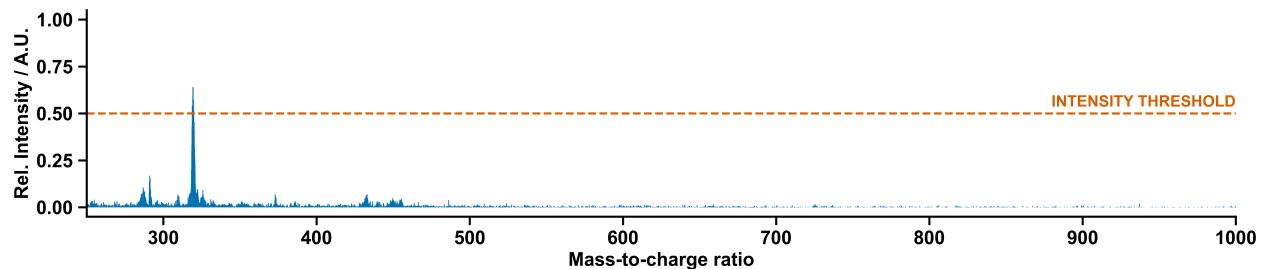
Scheme 35: Self-assembly of components 12, 19, with Zinc(II) in a 3.0:1.5:1.0 molar ratio in  $CH_3CN$  at 60°C for 40h. These are the reagents (starting materials) for reaction 38.

Human Reaction Decision: Failed	Human NMR Decision: Pass	NMR Spectra Category: Single discrete species formed.	
	Human MS Decision: Failed	MS Spectra Category: Reaction occurred, unknown product.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	
	Decision Maker MS Decision: Pass	NMR Criteria 2: N/A	MS Criteria 1 and 2: Pass
		Number of predicted peaks found in MS spectra with appropriate intensity: 0	Number of counter-ions found: 0
	MS Criteria 3: Pass		

Decision Table 35: Human labeled and Decsision maker labeled outcomes for the  $^1H$  NMR spectroscopy and UPLC-MS spectrometry of reaction 38. Decision motivations are also given.

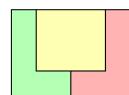
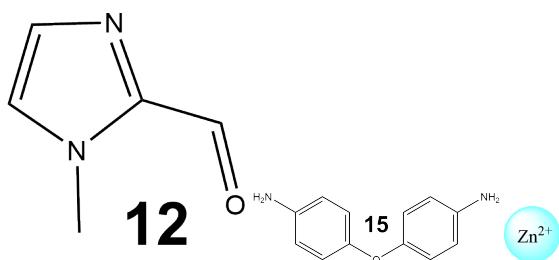


NMR Spectra 35: The stacked  $^1\text{H}$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 38.



MS Spectra 35: The ULPC-MS spectra of reaction 38. The intensity threshold is also shown.

## Reaction 39

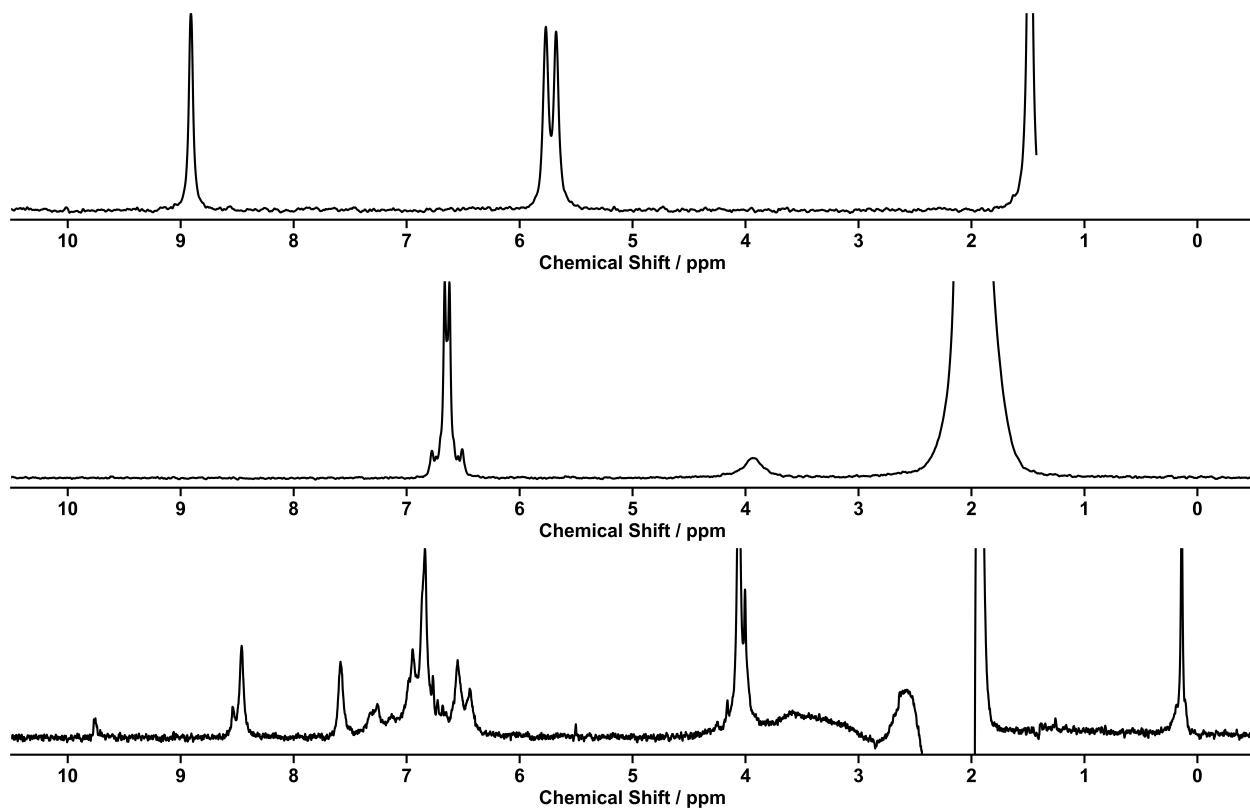


# Supramolecular Complex Formed

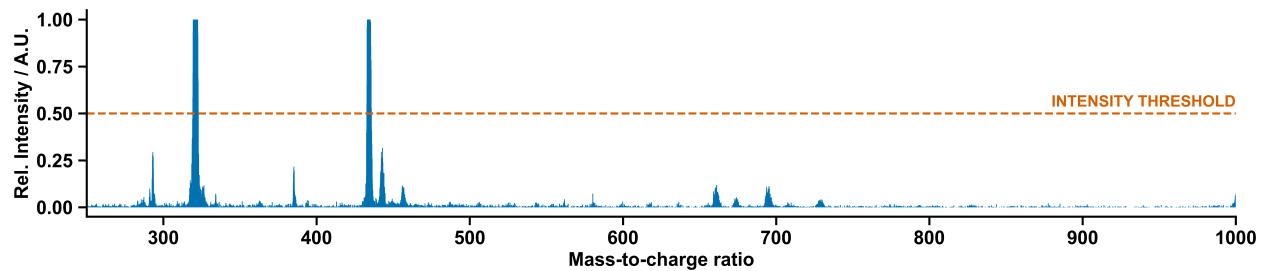
Scheme 36: Self-assembly of components 12, 15, with Zinc(II) in a 3.0:1.5:1.0 molar ratio in CH<sub>3</sub>CN at 60°C for 40h. These are the reagents (starting materials) for reaction 39.

Human Reaction Decision: Pass	Human NMR Decision: Pass	NMR Spectra Category: Single discrete species formed.
	Human MS Decision: Pass	MS Spectra Category: Reaction occurred, supramolecular product.
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A
		NMR Criteria 2: N/A
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass
		Number of predicted peaks found in MS spectra with appropriate intensity: 2
	MS Criteria 3: Pass	Number of counter-ions found: 1

Decision Table 36: Human labeled and Decsision maker labeled outcomes for the  $^1\text{H}$  NMR spectroscopy and ULPC-MS spectrometry of reaction 39. Decision motivations are also given.

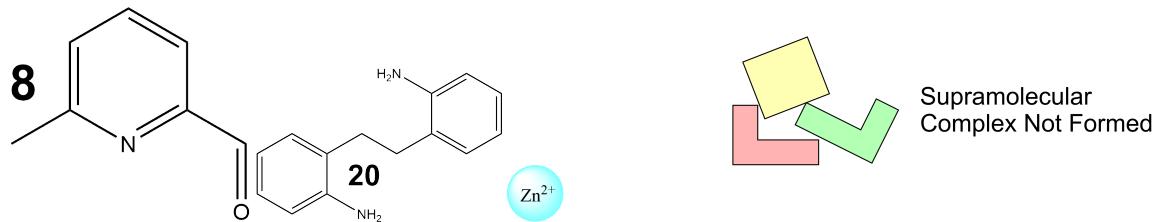


NMR Spectra 36: The stacked  $^1\text{H}$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 39.



MS Spectra 36: The ULPC-MS spectra of reaction 39. The intensity threshold is also shown.

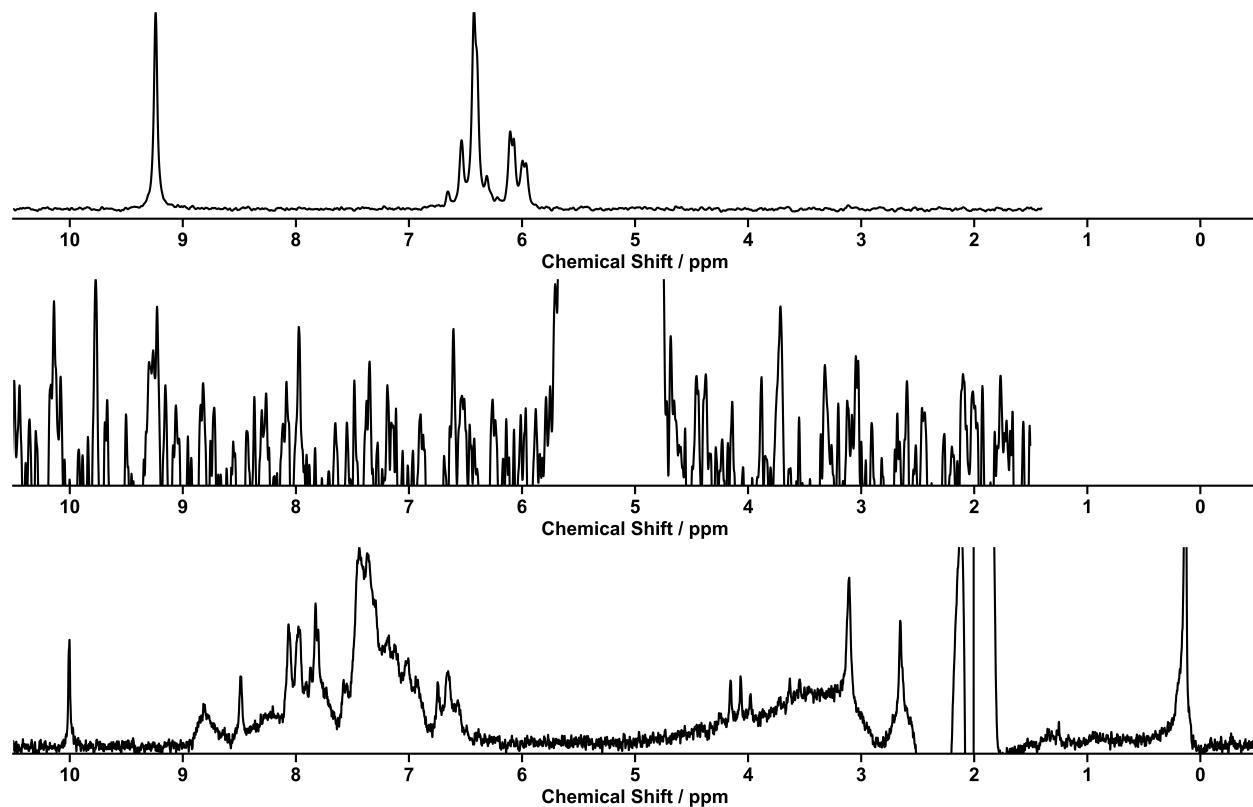
## Reaction 40



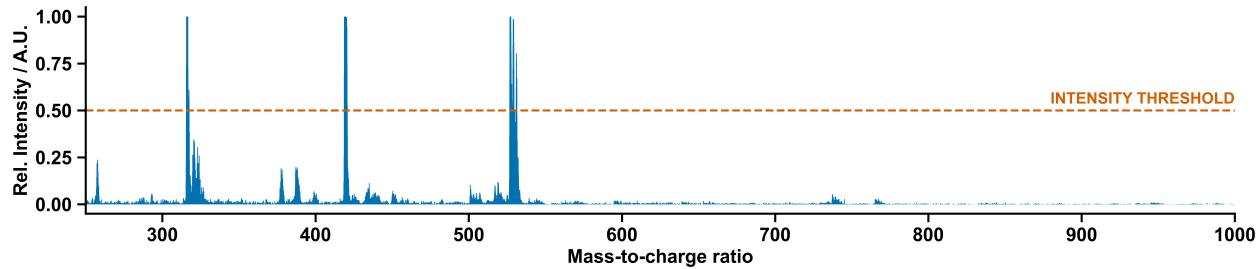
Scheme 37: Self-assembly of components 8, 20, with Zinc(II) in a 3.0:1.5:1.0 molar ratio in  $CH_3CN$  at  $60^\circ C$  for 40h. These are the reagents (starting materials) for reaction 40.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: Oligomers formed.	
	Human MS Decision: Pass	MS Spectra Category: Reaction occurred, supramolecular product.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	NMR Criteria 2: N/A
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 2
		MS Criteria 3: Pass	Number of counter-ions found: 1

Decision Table 37: Human labeled and Decsision maker labeled outcomes for the  $^1H$  NMR spectroscopy and UPLC-MS spectrometry of reaction 40. Decision motivations are also given.

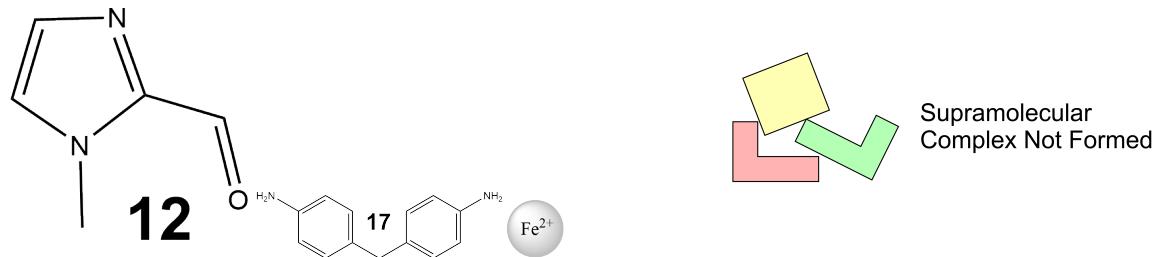


NMR Spectra 37: The stacked  $^1H$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 40.



MS Spectra 37: The ULPC-MS spectra of reaction 40. The intensity threshold is also shown.

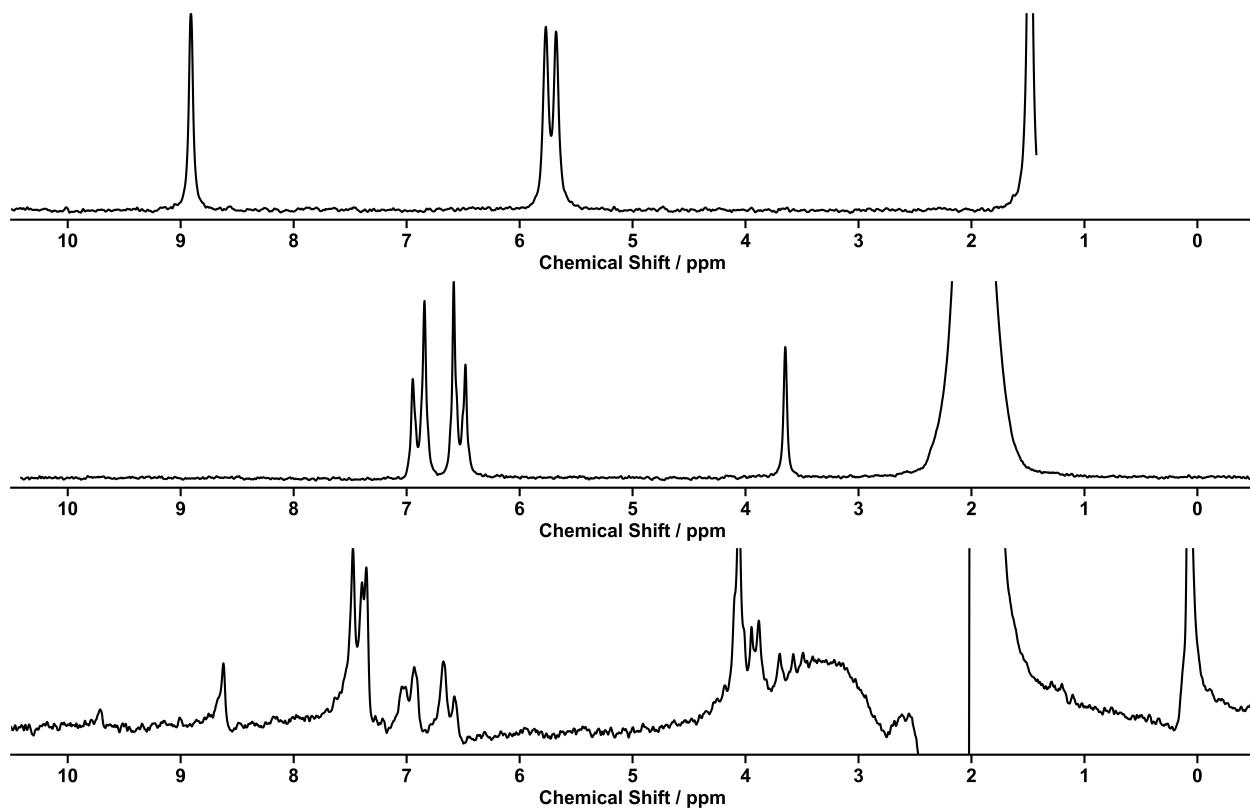
## Reaction 41



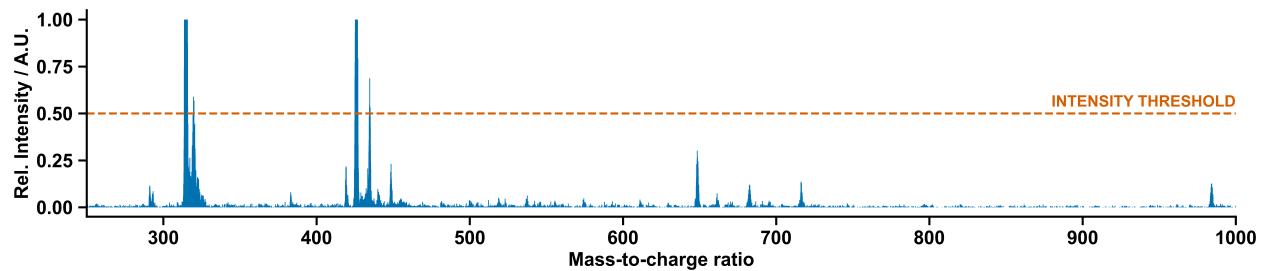
Scheme 38: Self-assembly of components 12, 17, with Iron(II) in a 3.0:1.5:1.0 molar ratio in CH<sub>3</sub>CN at 60°C for 40h. These are the reagents (starting materials) for reaction 41.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: Paramagnetic species formed.	
	Human MS Decision: Pass	MS Spectra Category: Reaction occurred, supramolecular product.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	NMR Criteria 2: N/A
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 5
		MS Criteria 3: Pass	Number of counter-ions found: 3

Decision Table 38: Human labeled and Decision maker labeled outcomes for the <sup>1</sup>H NMR spectroscopy and ULPC-MS spectrometry of reaction 41. Decision motivations are also given.

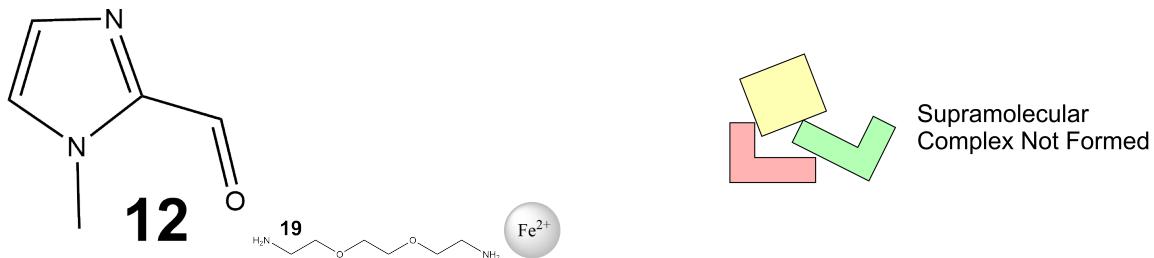


NMR Spectra 38: The stacked  $^1\text{H}$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 41.



MS Spectra 38: The ULPC-MS spectra of reaction 41. The intensity threshold is also shown.

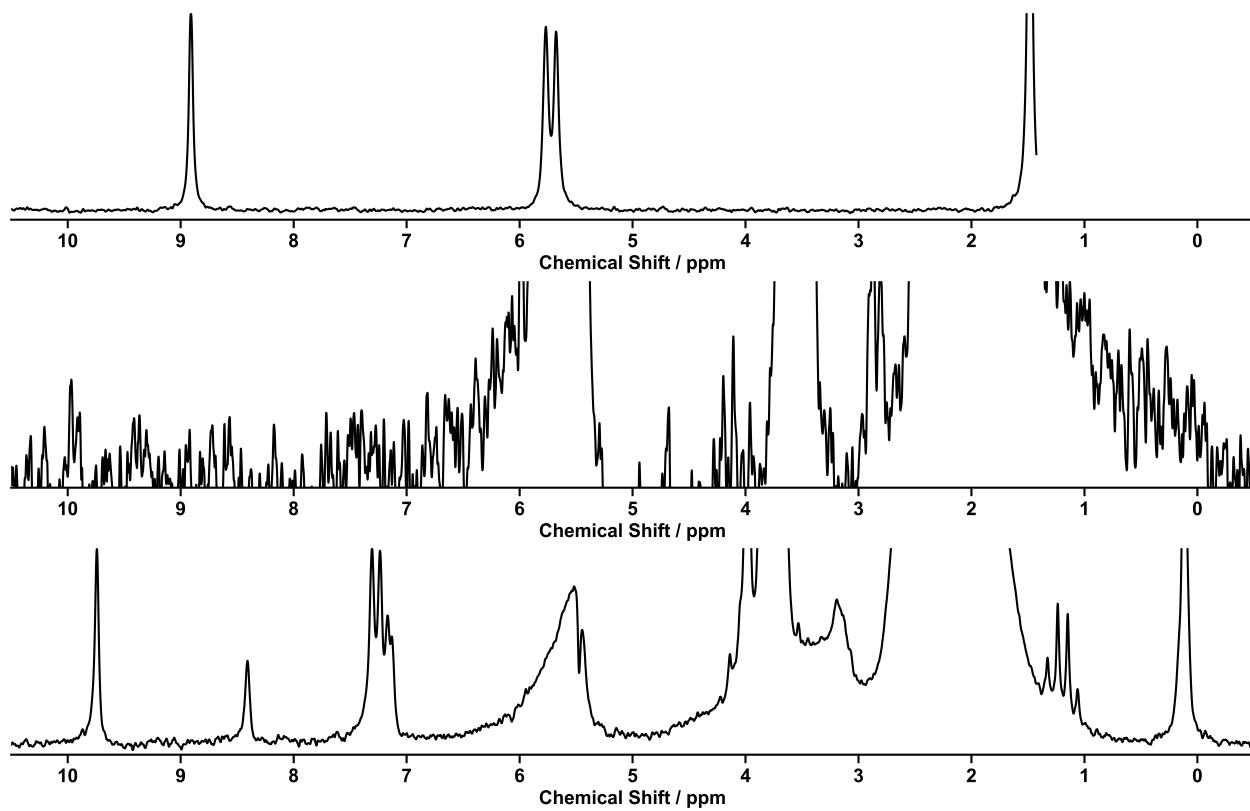
## Reaction 42



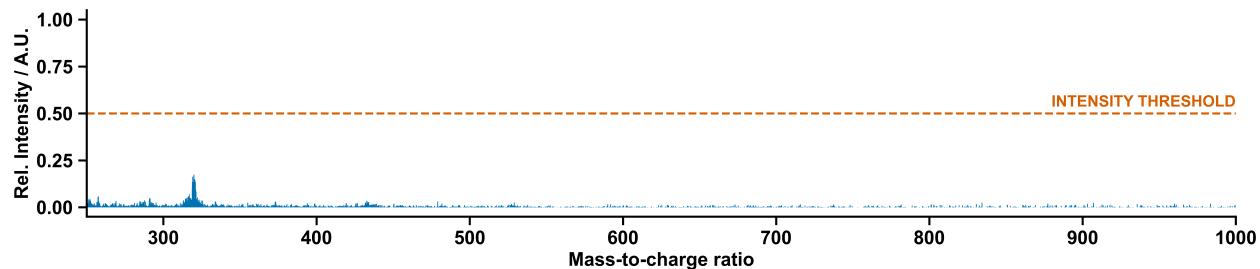
Scheme 39: Self-assembly of components 12, 19, with Iron(II) in a 3.0:1.5:1.0 molar ratio in  $\text{CH}_3\text{CN}$  at 60°C for 40h. These are the reagents (starting materials) for reaction 42.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: No reaction occurred.	
	Human MS Decision: Failed	MS Spectra Category: Reaction failed.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	
	Decision Maker MS Decision: Pass	NMR Criteria 2: N/A	MS Criteria 1 and 2: Pass
		Number of predicted peaks found in MS spectra with appropriate intensity: 0	
		MS Criteria 3: Pass	Number of counter-ions found: 0

Decision Table 39: Human labeled and Decsision maker labeled outcomes for the  $^1\text{H}$  NMR spectroscopy and UPLC-MS spectrometry of reaction 42. Decision motivations are also given.

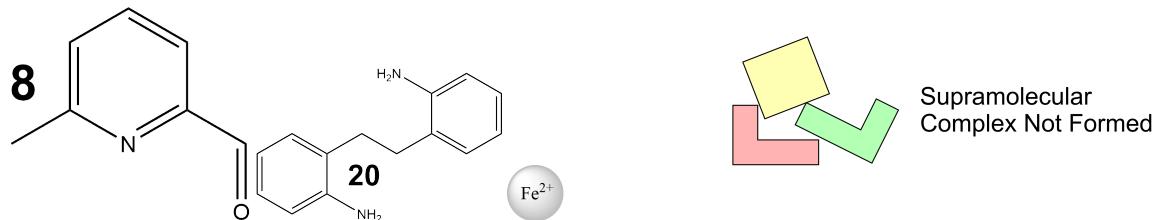


NMR Spectra 39: The stacked  $^1\text{H}$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 42.



MS Spectra 39: The ULPC-MS spectra of reaction 42. The intensity threshold is also shown.

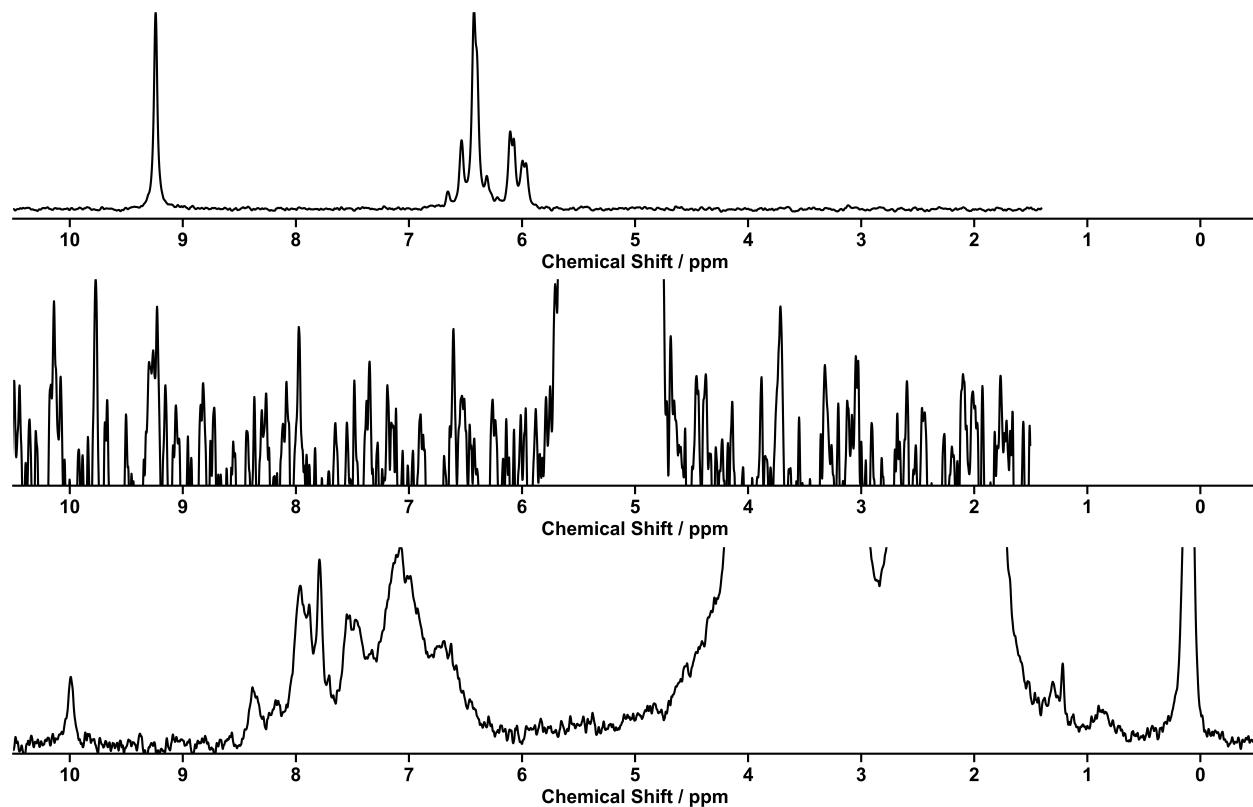
## Reaction 44



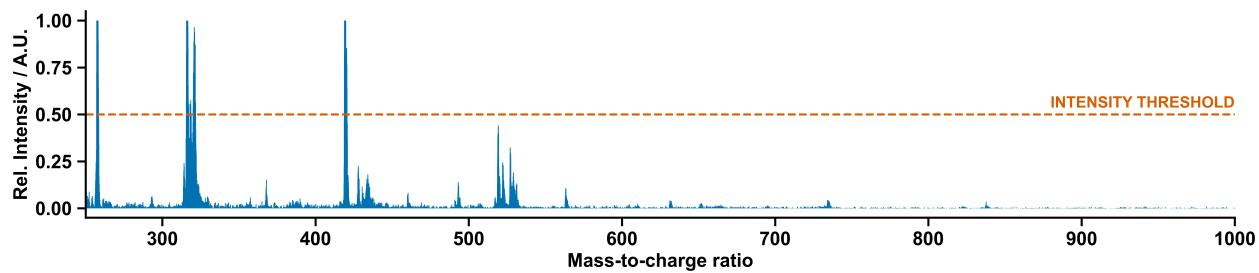
Scheme 40: Self-assembly of components 8, 20, with Iron(II) in a 3.0:1.5:1.0 molar ratio in  $\text{CH}_3\text{CN}$  at  $60^\circ\text{C}$  for 40h. These are the reagents (starting materials) for reaction 44.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: Paramagnetic species formed.	
	Human MS Decision: Failed	MS Spectra Category: Reaction occurred, unknown product.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	NMR Criteria 2: N/A
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 0
		MS Criteria 3: Pass	Number of counter-ions found: 0

Decision Table 40: Human labeled and Decsision maker labeled outcomes for the  $^1\text{H}$  NMR spectroscopy and UPLC-MS spectrometry of reaction 44. Decision motivations are also given.

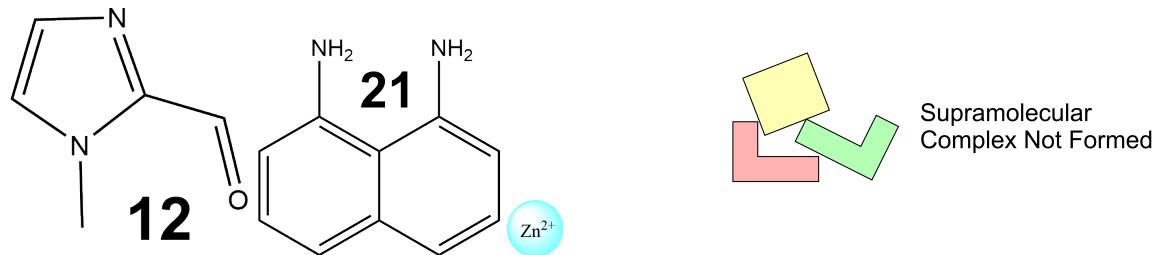


NMR Spectra 40: The stacked  $^1\text{H}$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 44.



MS Spectra 40: The ULPC-MS spectra of reaction 44. The intensity threshold is also shown.

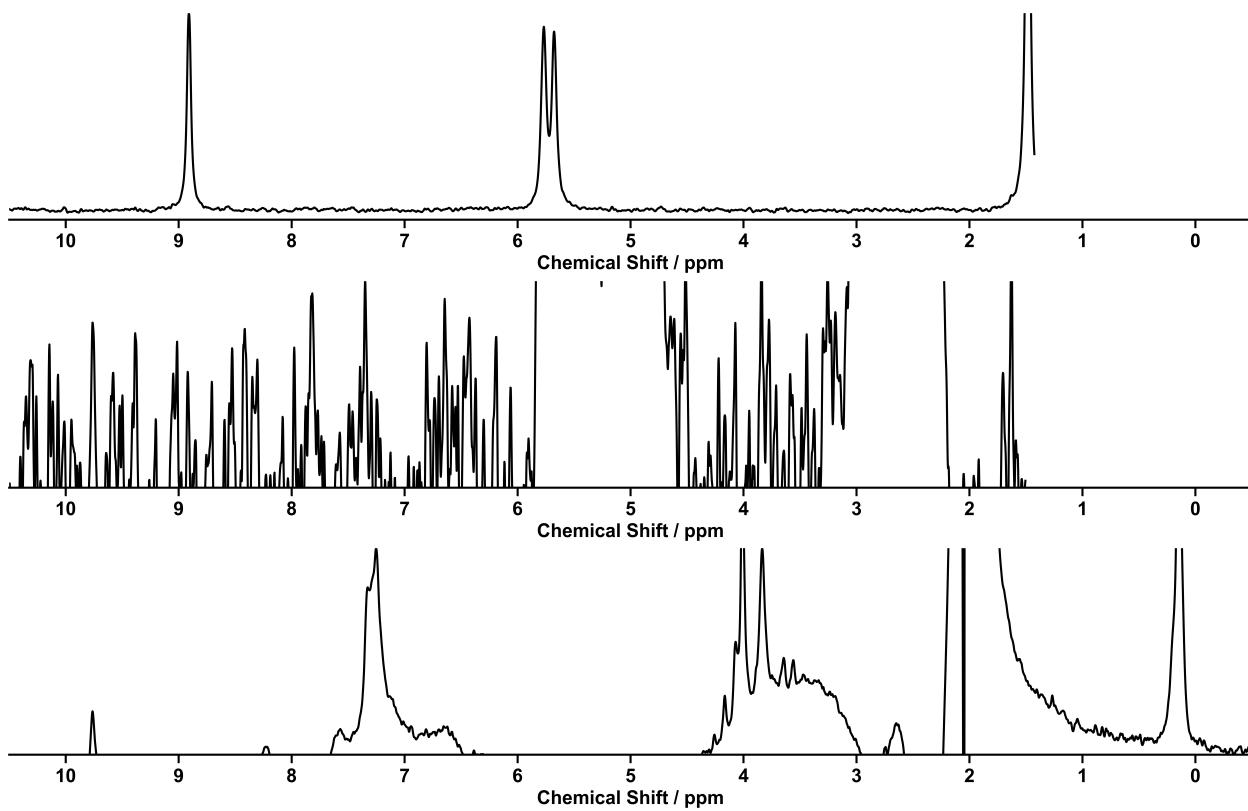
## Reaction 45



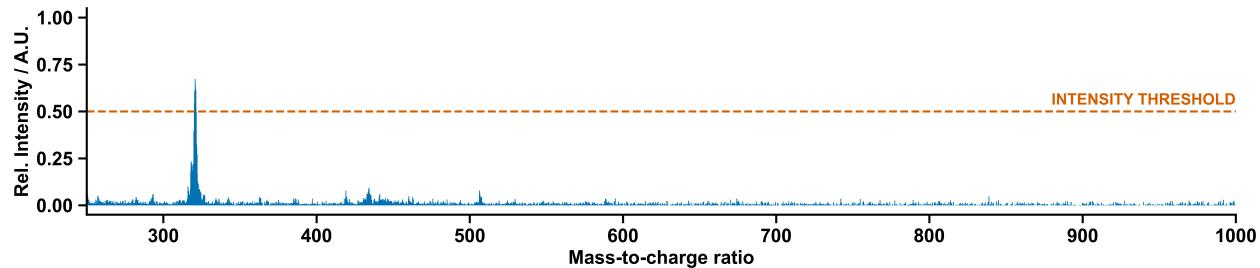
Scheme 41: Self-assembly of components 12, 21, with Zinc(II) in a 3.0:1.5:1.0 molar ratio in CH<sub>3</sub>CN at 60°C for 40h. These are the reagents (starting materials) for reaction 45.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: Oligomers formed.	
	Human MS Decision: Failed	MS Spectra Category: Reaction failed.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	NMR Criteria 2: N/A
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 0
		MS Criteria 3: Pass	Number of counter-ions found: 0

Decision Table 41: Human labeled and Decision maker labeled outcomes for the <sup>1</sup>H NMR spectroscopy and ULPC-MS spectrometry of reaction 45. Decision motivations are also given.

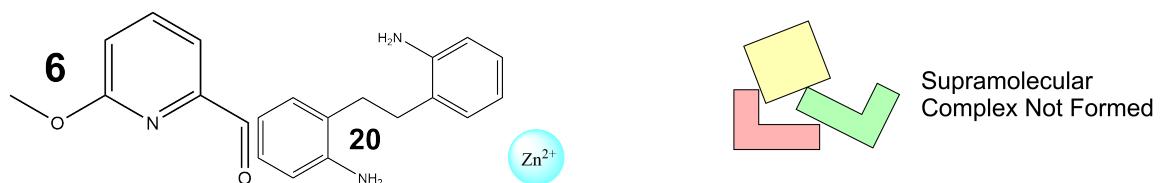


NMR Spectra 41: The stacked <sup>1</sup>H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 45.



MS Spectra 41: The ULPC-MS spectra of reaction 45. The intensity threshold is also shown.

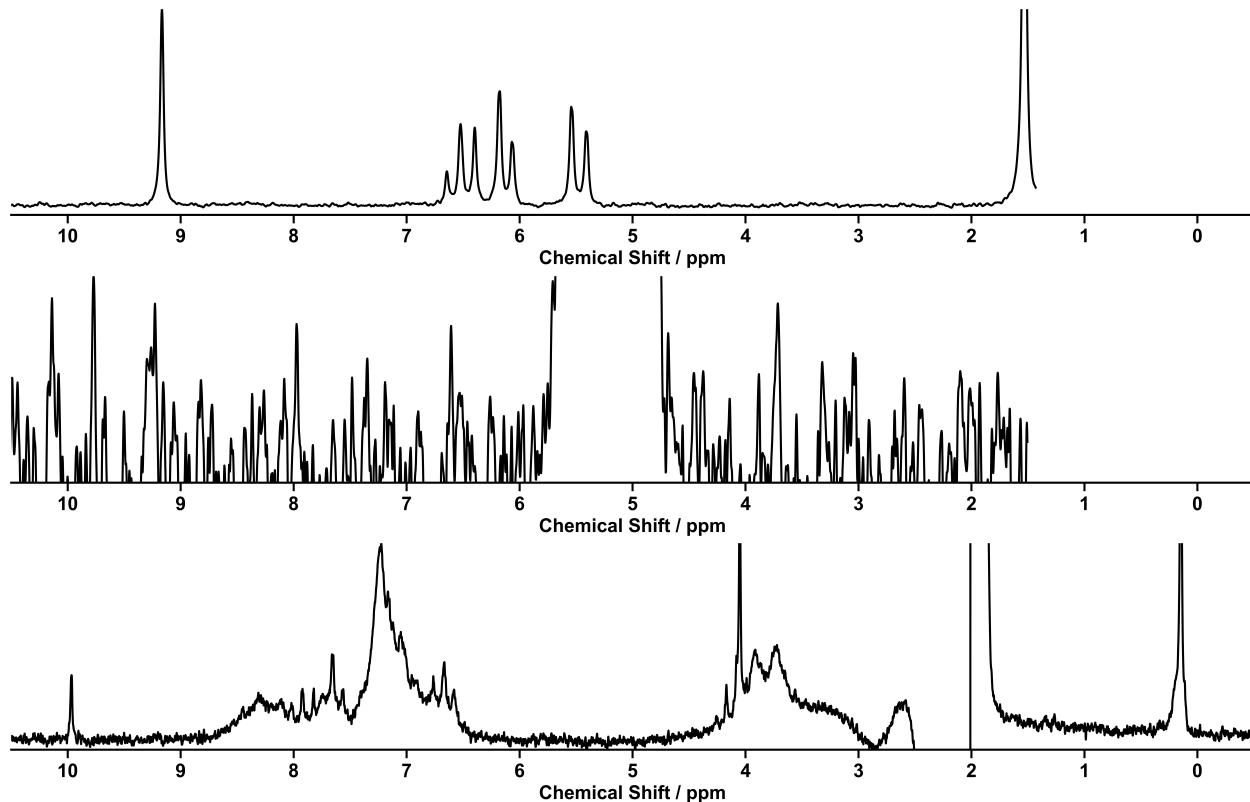
## Reaction 47



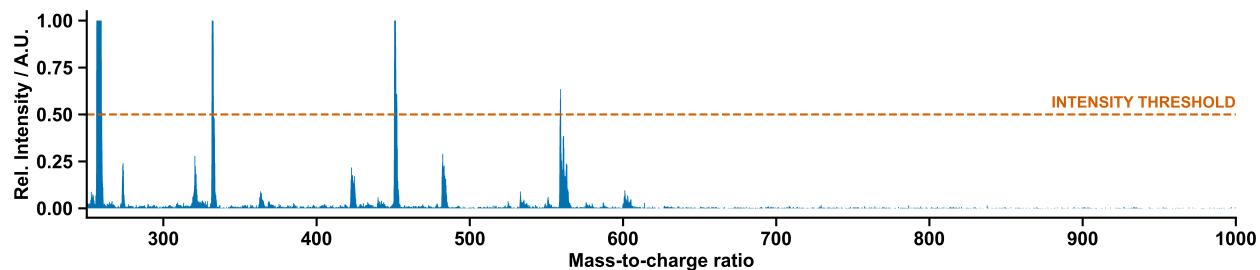
Scheme 42: Self-assembly of components 6, 20, with Zinc(II) in a 3.0:1.5:1.0 molar ratio in  $CH_3CN$  at 60°C for 40h. These are the reagents (starting materials) for reaction 47.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: Oligomers formed.	
	Human MS Decision: Failed	MS Spectra Category: Reaction occurred, unknown product.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	
		NMR Criteria 2: N/A	
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 1
	MS Criteria 3: Pass	Number of counter-ions found: 0	

Decision Table 42: Human labeled and Decsision maker labeled outcomes for the  $^1\text{H}$  NMR spectroscopy and UPLC-MS spectrometry of reaction 47. Decision motivations are also given.

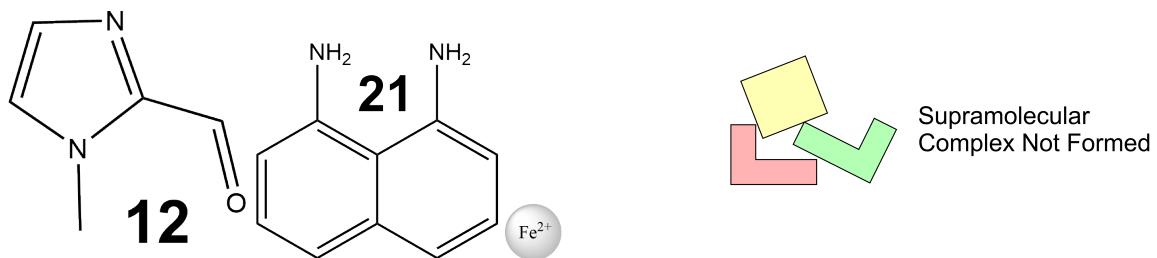


NMR Spectra 42: The stacked  $^1\text{H}$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 47.



MS Spectra 42: The UPLC-MS spectra of reaction 47. The intensity threshold is also shown.

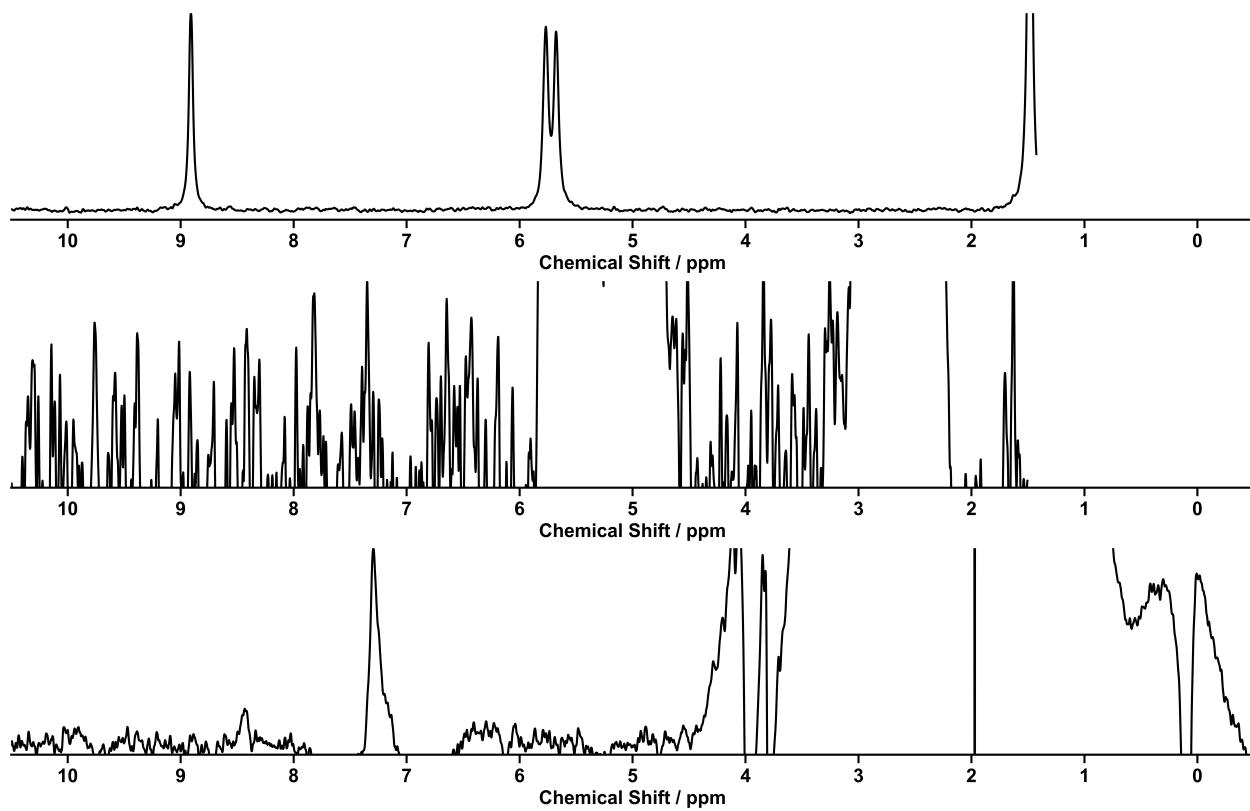
## Reaction 48



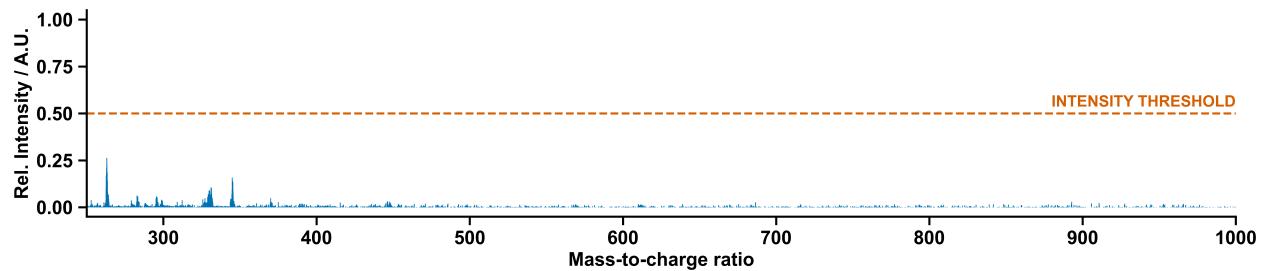
Scheme 43: Self-assembly of components 12, 21, with Iron(II) in a 3.0:1.5:1.0 molar ratio in CH<sub>3</sub>CN at 60°C for 40h. These are the reagents (starting materials) for reaction 48.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: Paramagnetic species formed.	
	Human MS Decision: Failed	MS Spectra Category: Reaction failed.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	NMR Criteria 2: N/A
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 0
		MS Criteria 3: Pass	Number of counter-ions found: 0

Decision Table 43: Human labeled and Decsision maker labeled outcomes for the <sup>1</sup>H NMR spectroscopy and UPLC-MS spectrometry of reaction 48. Decision motivations are also given.

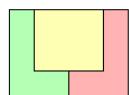
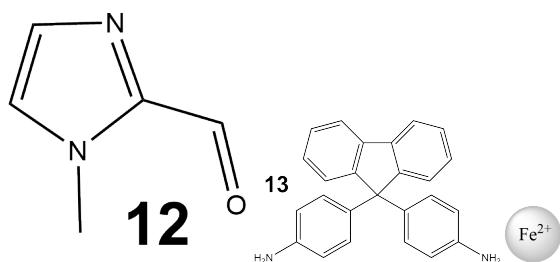


NMR Spectra 43: The stacked  $^1\text{H}$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 48.



MS Spectra 43: The ULPC-MS spectra of reaction 48. The intensity threshold is also shown.

## Reaction 49

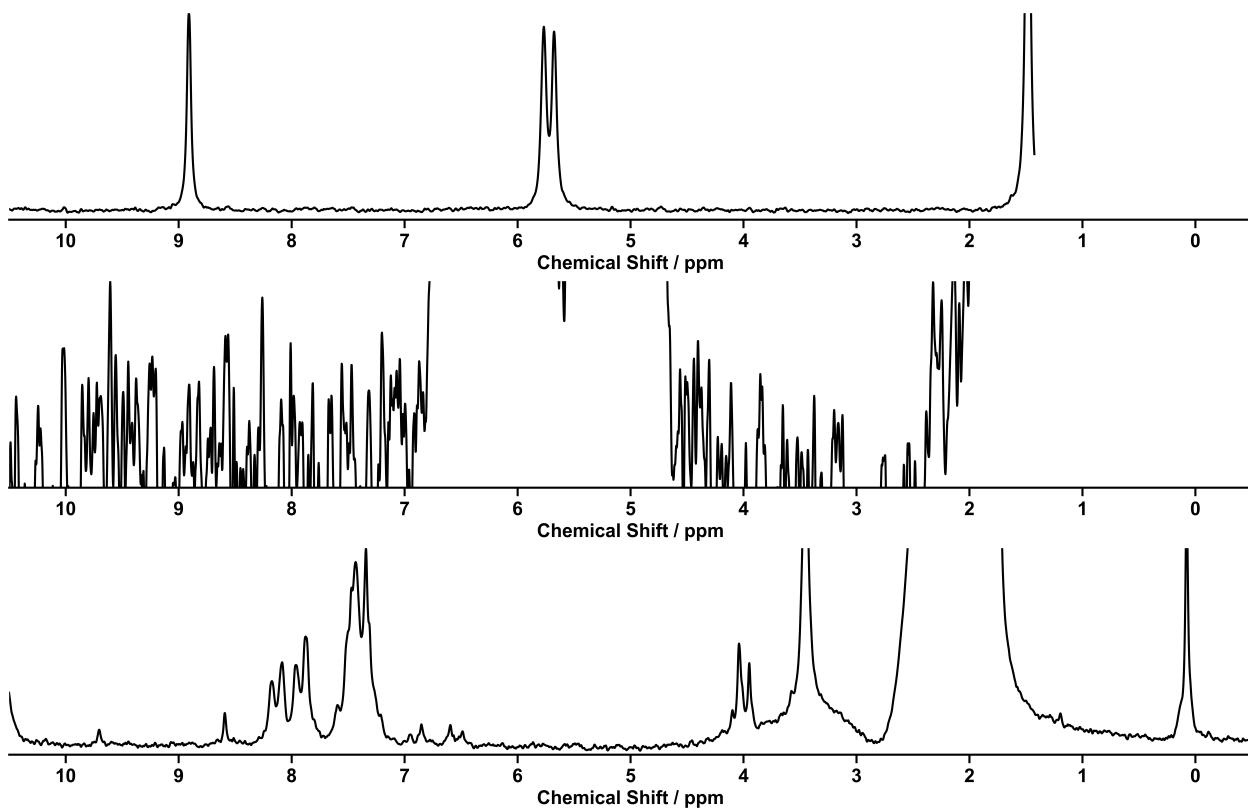


## Supramolecular Complex Formed

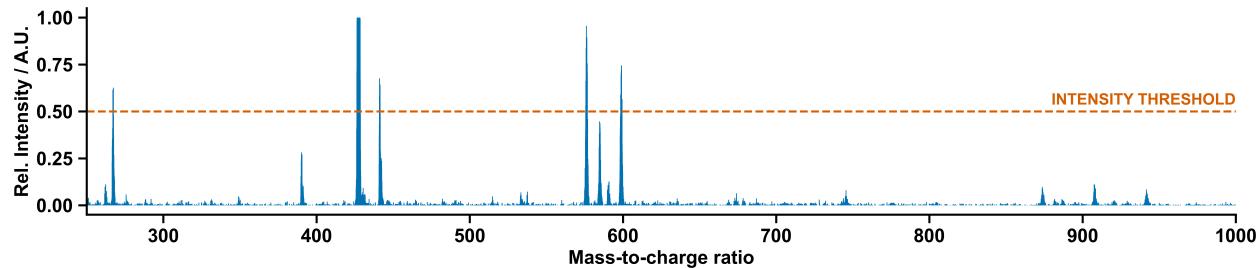
Scheme 44: Self-assembly of components 12, 13, with Iron(II) in a 3.0:1.5:1.0 molar ratio in CH<sub>3</sub>CN at 60°C for 40h. These are the reagents (starting materials) for reaction 49.

Human Reaction Decision: Pass	Human NMR Decision: Pass	NMR Spectra Category: Single discrete species formed.
	Human MS Decision: Pass	MS Spectra Category: Reaction occurred, supramolecular product.
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A
		NMR Criteria 2: N/A
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass
		Number of predicted peaks found in MS spectra with appropriate intensity: 9
	MS Criteria 3: Pass	Number of counter-ions found: 6

Decision Table 44: Human labeled and Decsision maker labeled outcomes for the  $^1\text{H}$  NMR spectroscopy and ULPC-MS spectrometry of reaction 49. Decision motivations are also given.

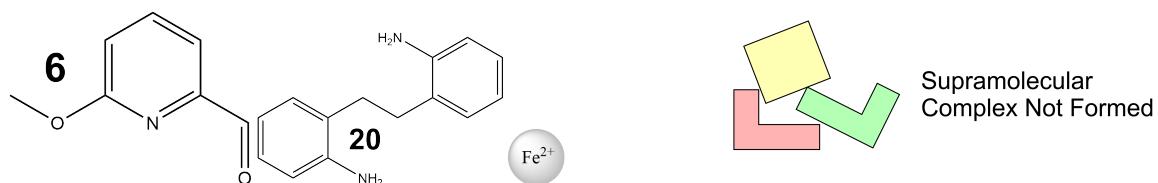


NMR Spectra 44: The stacked <sup>1</sup>H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 49.



MS Spectra 44: The ULPC-MS spectra of reaction 49. The intensity threshold is also shown.

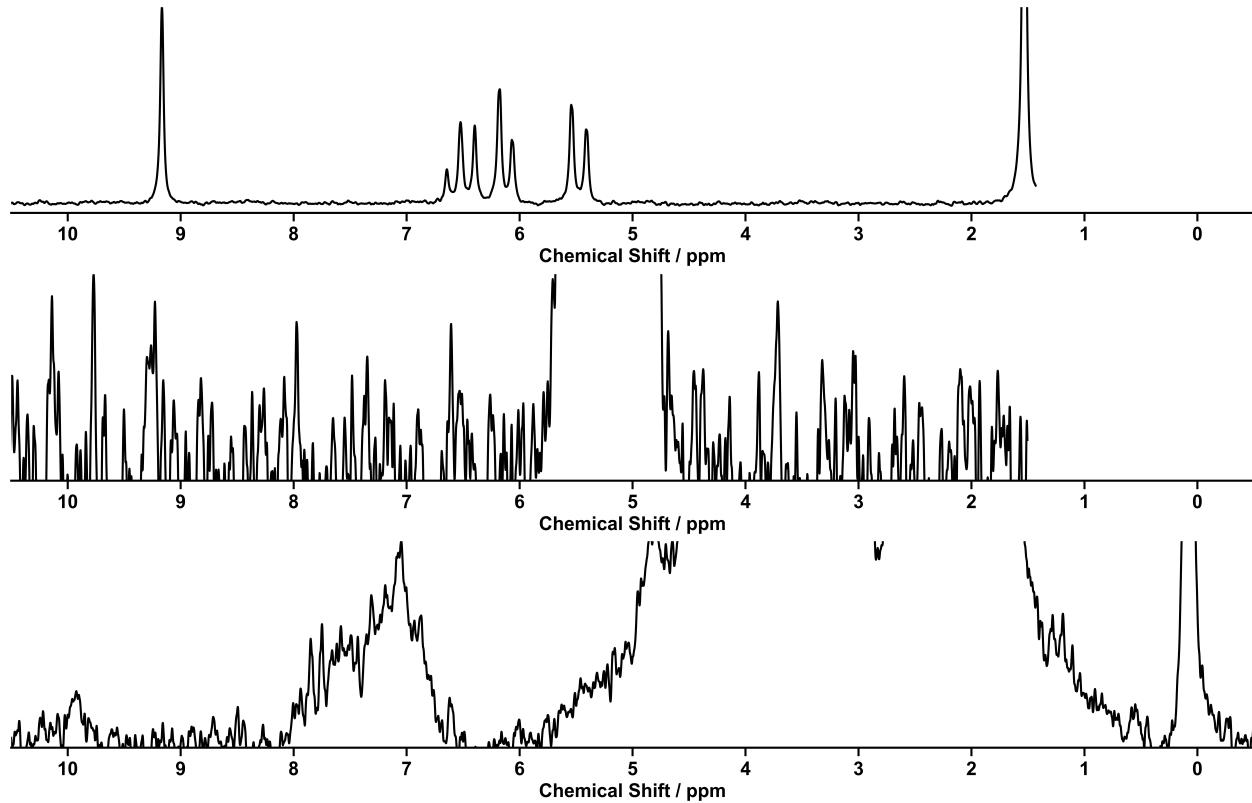
## Reaction 50



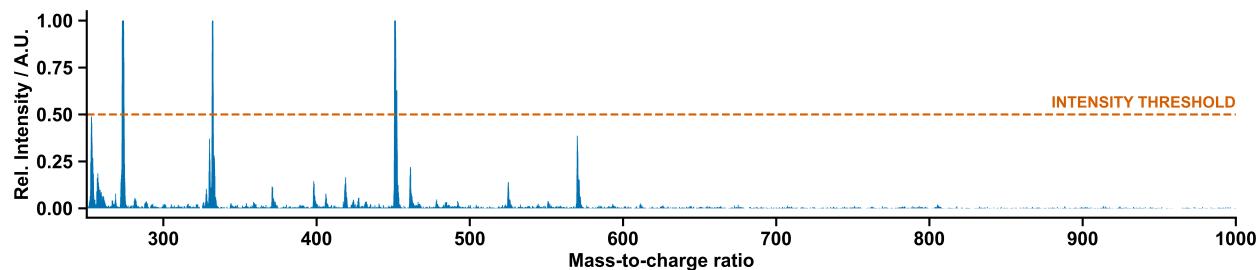
Scheme 45: Self-assembly of components 6, 20, with Iron(II) in a 3.0:1.5:1.0 molar ratio in  $\text{CH}_3\text{CN}$  at 60°C for 40h. These are the reagents (starting materials) for reaction 50.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: Paramagnetic species formed.	
	Human MS Decision: Failed	MS Spectra Category: Reaction occurred, unknown product.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	
		NMR Criteria 2: N/A	
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 0
	MS Criteria 3: Pass	Number of counter-ions found: 0	

Decision Table 45: Human labeled and Decsision maker labeled outcomes for the  $^1\text{H}$  NMR spectroscopy and ULPC-MS spectrometry of reaction 50. Decision motivations are also given.

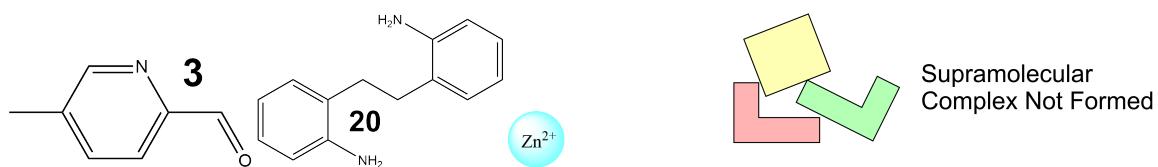


NMR Spectra 45: The stacked  $^1\text{H}$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 50.



MS Spectra 45: The ULPC-MS spectra of reaction 50. The intensity threshold is also shown.

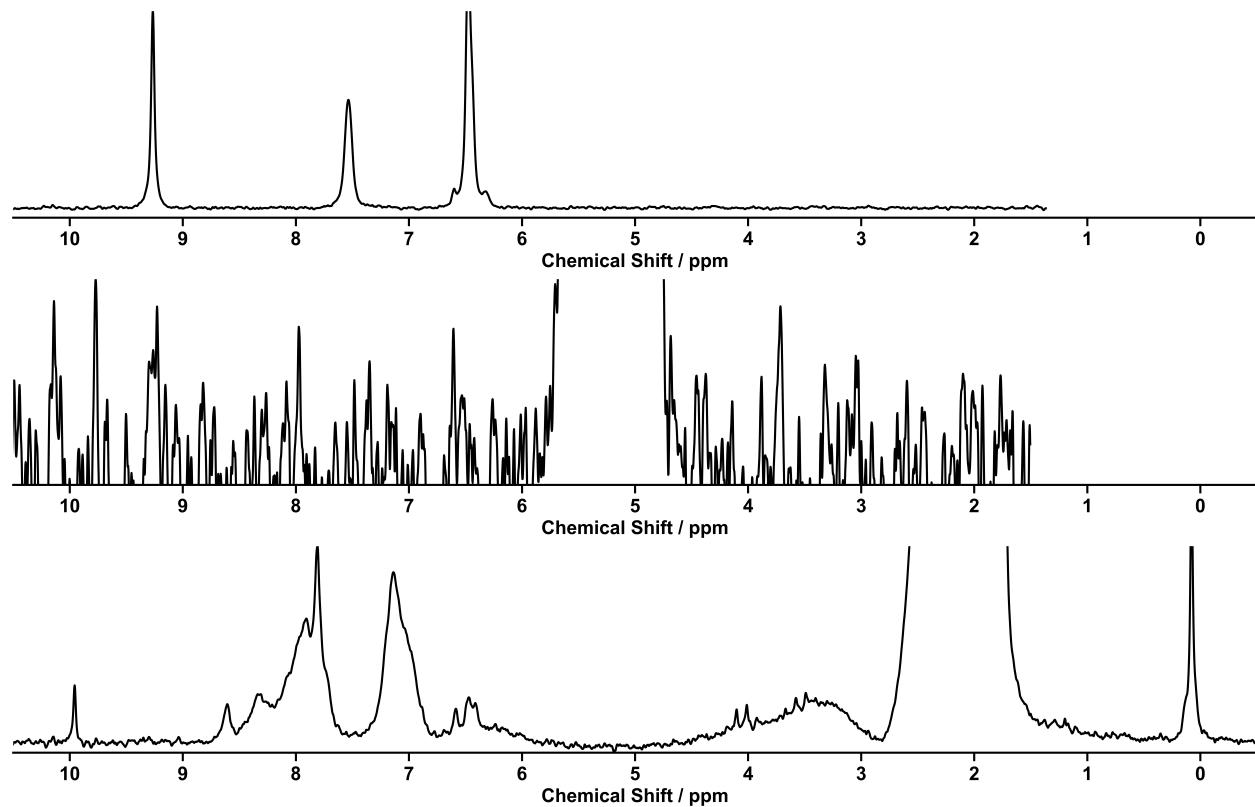
## Reaction 51



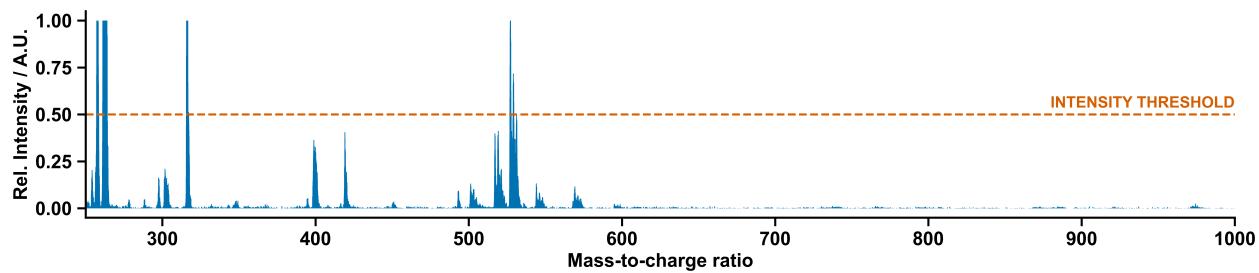
Scheme 46: Self-assembly of components 3, 20, with Zinc(II) in a 3.0:1.5:1.0 molar ratio in  $CH_3CN$  at  $60^\circ C$  for 40h. These are the reagents (starting materials) for reaction 51.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: Oligomers formed.	
	Human MS Decision: Failed	MS Spectra Category: Reaction occurred, unknown product.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	NMR Criteria 2: N/A
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 1
		MS Criteria 3: Pass	Number of counter-ions found: 0

Decision Table 46: Human labeled and Decision maker labeled outcomes for the  $^1H$  NMR spectroscopy and UPLC-MS spectrometry of reaction 51. Decision motivations are also given.

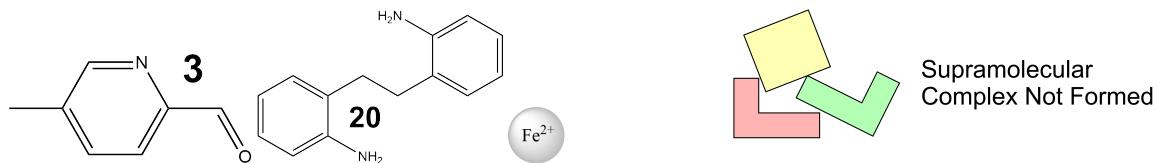


NMR Spectra 46: The stacked  $^1H$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 51.



MS Spectra 46: The ULPC-MS spectra of reaction 51. The intensity threshold is also shown.

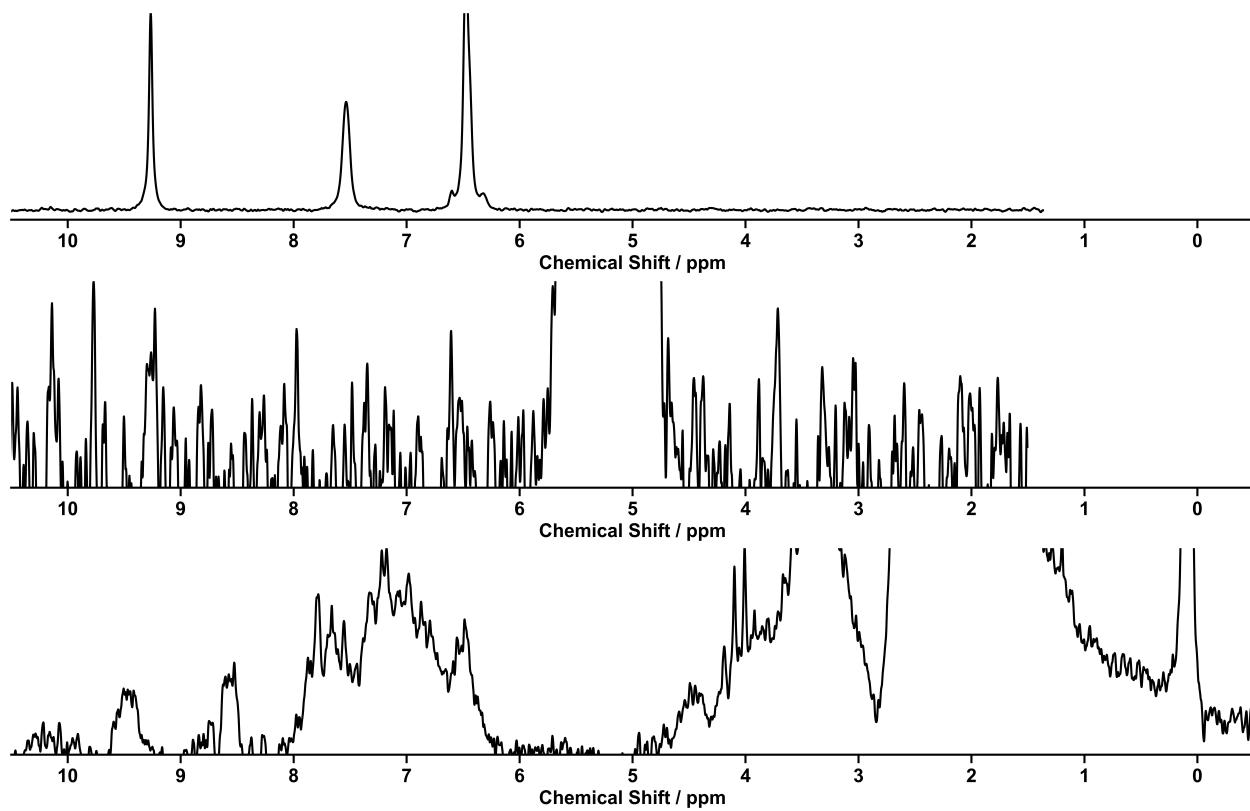
## Reaction 52



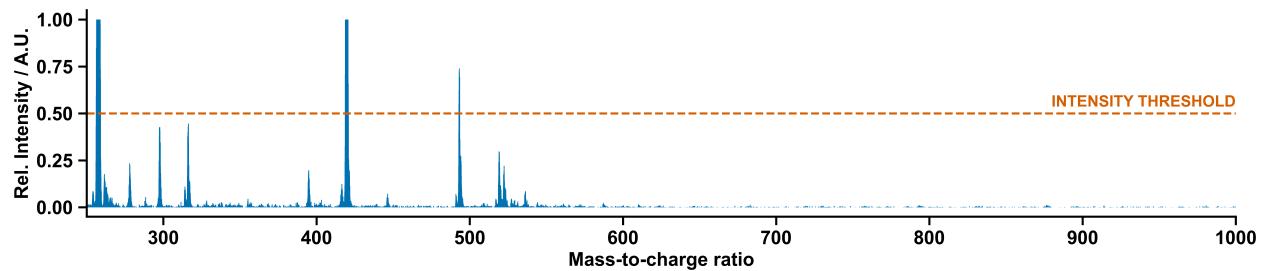
Scheme 47: Self-assembly of components 3, 20, with Iron(II) in a 3.0:1.5:1.0 molar ratio in CH<sub>3</sub>CN at 60°C for 40h. These are the reagents (starting materials) for reaction 52.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: Paramagnetic species formed.	
	Human MS Decision: Failed	MS Spectra Category: Reaction occurred, unknown product.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	NMR Criteria 2: N/A
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 0
		MS Criteria 3: Pass	Number of counter-ions found: 0

Decision Table 47: Human labeled and Decsision maker labeled outcomes for the <sup>1</sup>H NMR spectroscopy and ULPC-MS spectrometry of reaction 52. Decision motivations are also given.

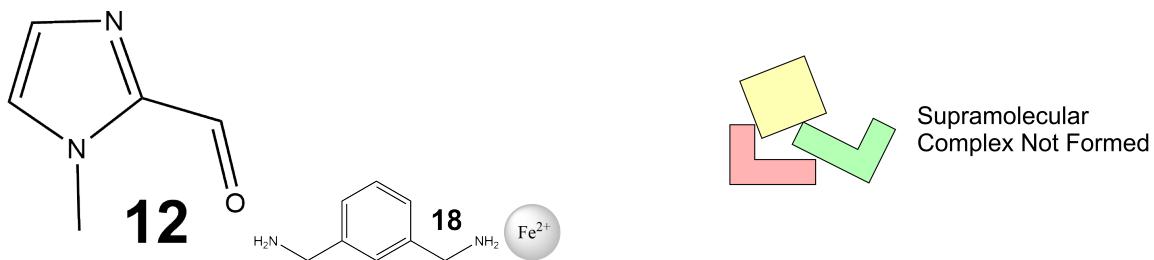


NMR Spectra 47: The stacked  $^1\text{H}$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 52.



MS Spectra 47: The ULPC-MS spectra of reaction 52. The intensity threshold is also shown.

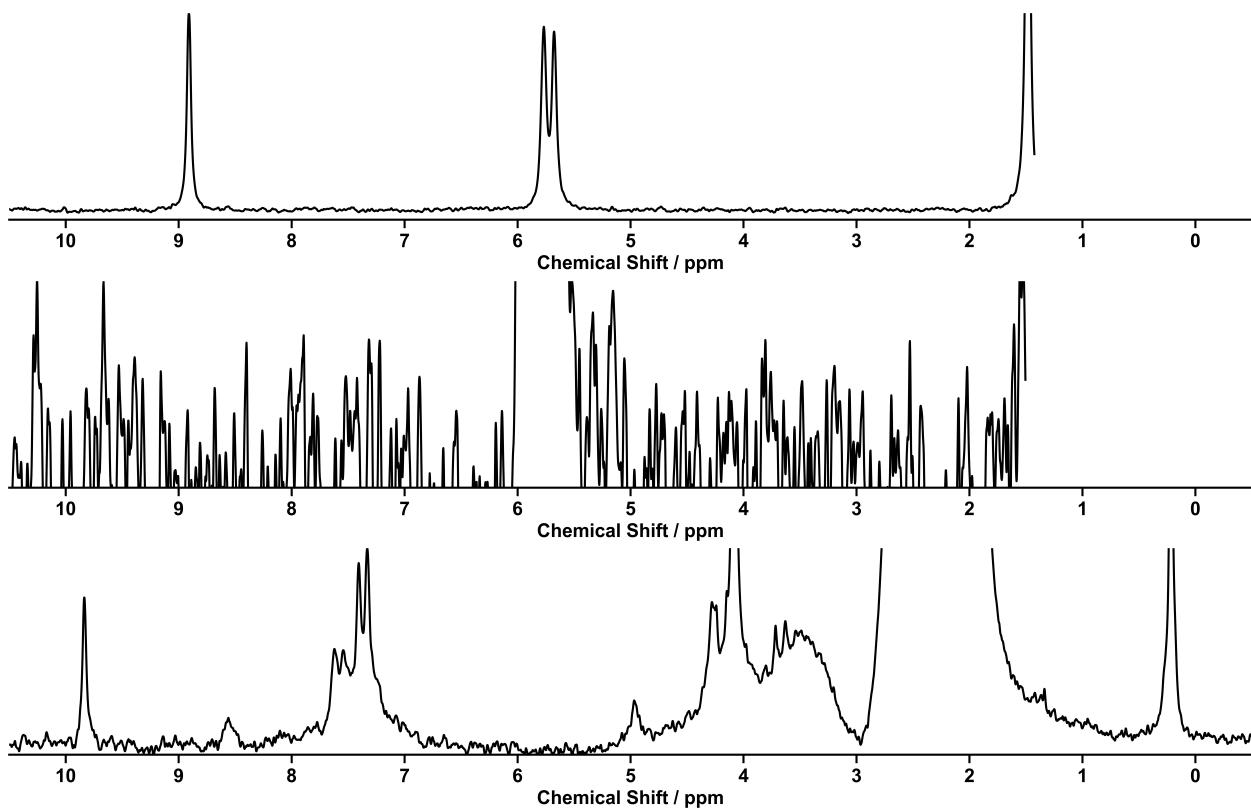
## Reaction 54



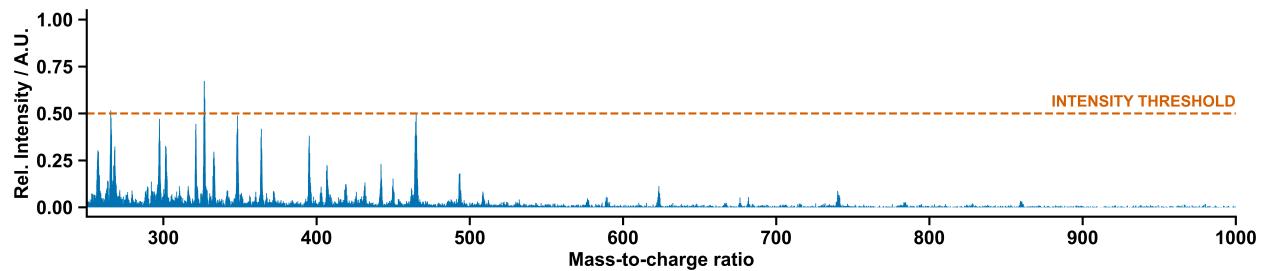
Scheme 48: Self-assembly of components 12, 18, with Iron(II) in a 3.0:1.5:1.0 molar ratio in CH<sub>3</sub>CN at 60°C for 40h. These are the reagents (starting materials) for reaction 54.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: No reaction occurred.	
	Human MS Decision: Failed	MS Spectra Category: Reaction failed.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	
	Decision Maker MS Decision: Pass	NMR Criteria 2: N/A	MS Criteria 1 and 2: Pass
		Number of predicted peaks found in MS spectra with appropriate intensity: 0	
		MS Criteria 3: Pass	Number of counter-ions found: 0

Decision Table 48: Human labeled and Decsision maker labeled outcomes for the <sup>1</sup>H NMR spectroscopy and UPLC-MS spectrometry of reaction 54. Decision motivations are also given.

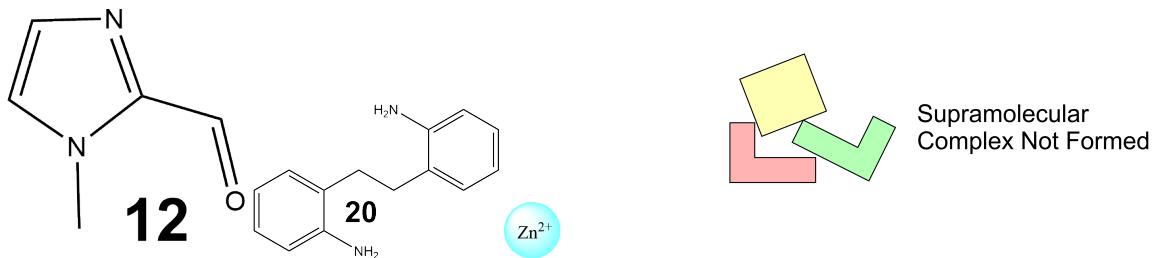


NMR Spectra 48: The stacked  $^1\text{H}$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 54.



MS Spectra 48: The ULPC-MS spectra of reaction 54. The intensity threshold is also shown.

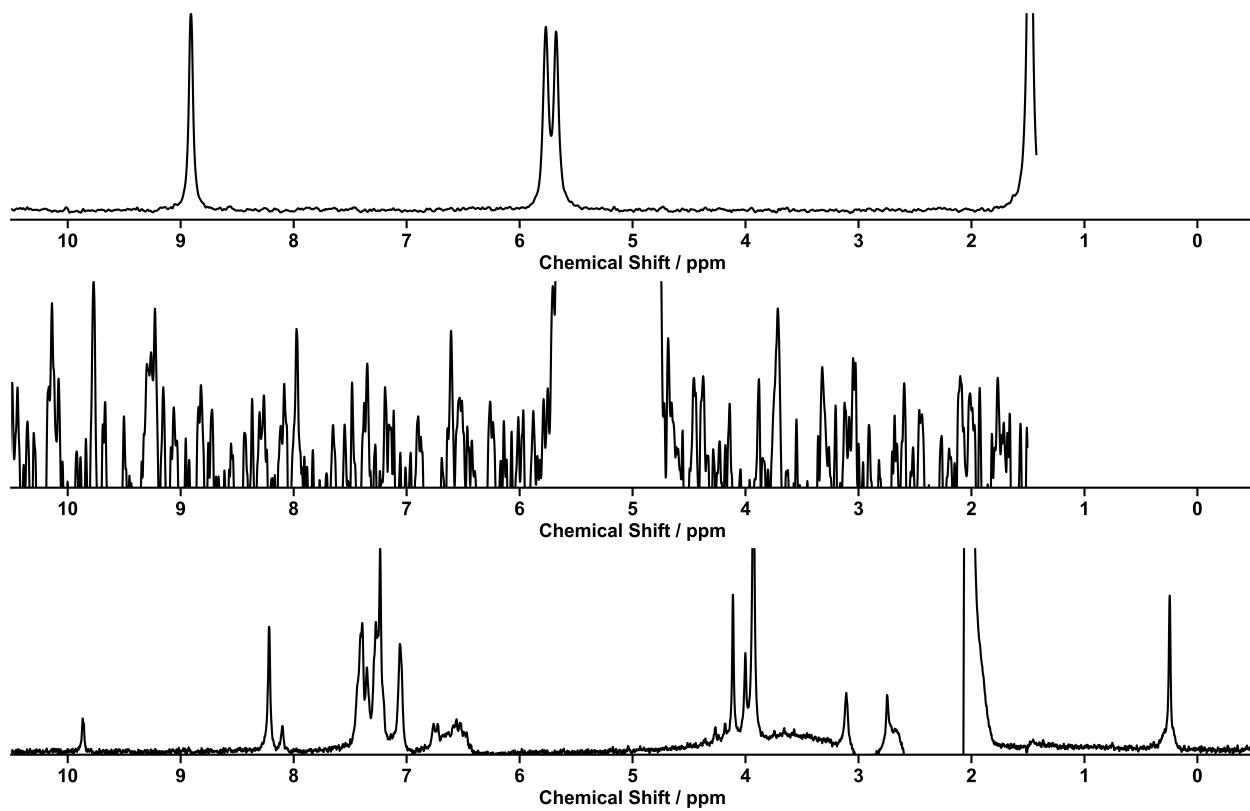
## Reaction 55



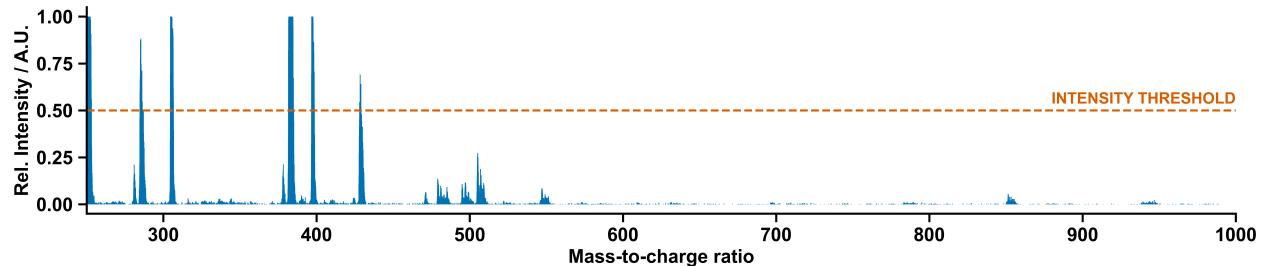
Scheme 49: Self-assembly of components 12, 20, with Zinc(II) in a 3.0:1.5:1.0 molar ratio in  $CH_3CN$  at 60°C for 40h. These are the reagents (starting materials) for reaction 55.

Human Reaction Decision: Failed	Human NMR Decision: Pass	NMR Spectra Category: Single discrete species formed.	
	Human MS Decision: Failed	MS Spectra Category: Reaction occurred, unknown product.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	
	Decision Maker MS Decision: Pass	NMR Criteria 2: N/A	MS Criteria 1 and 2: Pass
		Number of predicted peaks found in MS spectra with appropriate intensity: 0	
		MS Criteria 3: Pass	Number of counter-ions found: 0

Decision Table 49: Human labeled and Decsision maker labeled outcomes for the  $^1H$  NMR spectroscopy and UPLC-MS spectrometry of reaction 55. Decision motivations are also given.

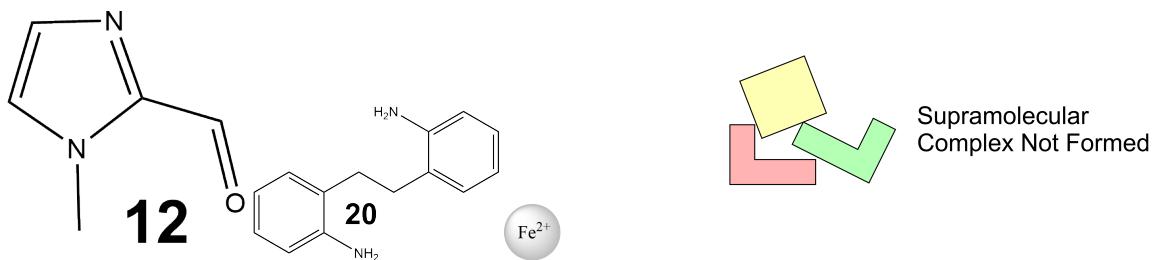


NMR Spectra 49: The stacked  $^1\text{H}$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 55.



MS Spectra 49: The ULPC-MS spectra of reaction 55. The intensity threshold is also shown.

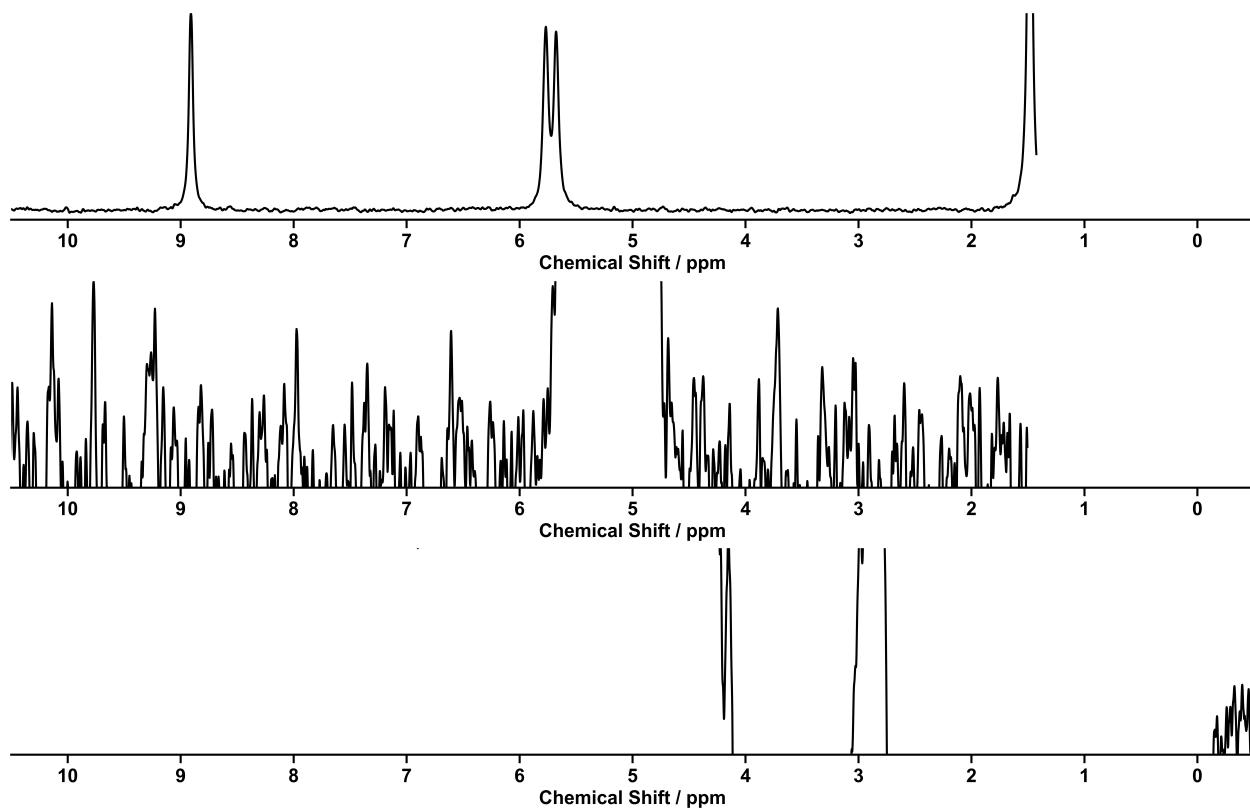
## Reaction 56



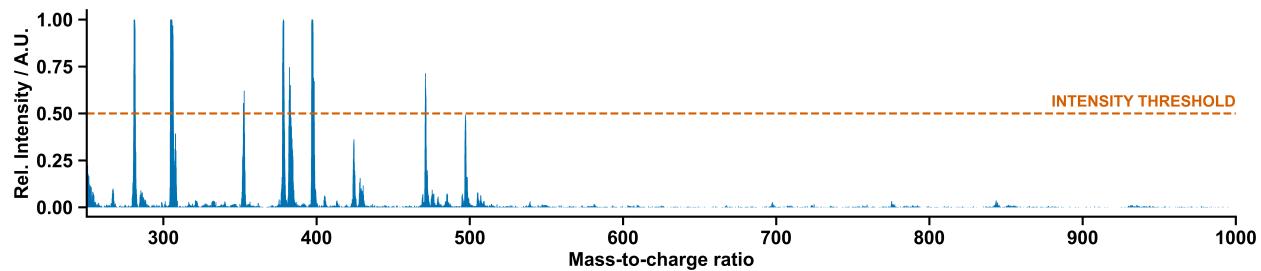
Scheme 50: Self-assembly of components **12**, **20**, with Iron(II) in a 3.0:1.5:1.0 molar ratio in CH<sub>3</sub>CN at 60°C for 40h. These are the reagents (starting materials) for reaction 56.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: Paramagnetic species formed.	
	Human MS Decision: Failed	MS Spectra Category: Reaction occurred, unknown product.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	
	Decision Maker MS Decision: Pass	NMR Criteria 2: N/A	Number of predicted peaks found in MS spectra with appropriate intensity: 2
	MS Criteria 1 and 2: Pass	MS Criteria 3: Pass	Number of counter-ions found: 1

Decision Table 50: Human labeled and Decsision maker labeled outcomes for the <sup>1</sup>H NMR spectroscopy and UPLC-MS spectrometry of reaction 56. Decision motivations are also given.

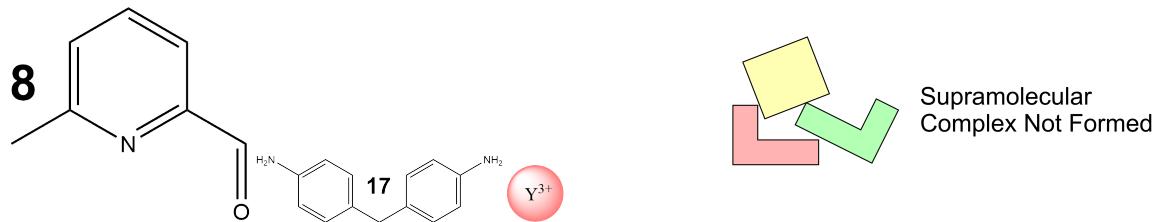


NMR Spectra 50: The stacked  $^1\text{H}$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 56.



MS Spectra 50: The ULPC-MS spectra of reaction 56. The intensity threshold is also shown.

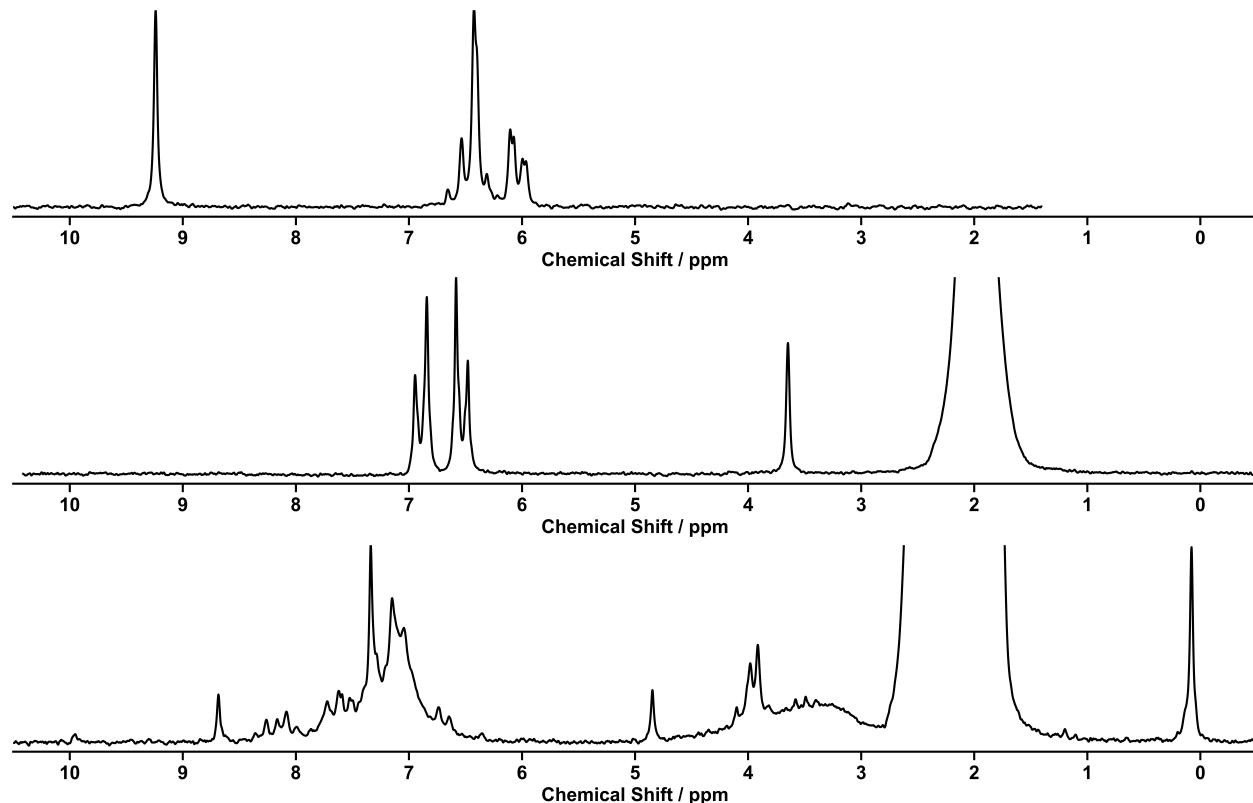
## Reaction 57



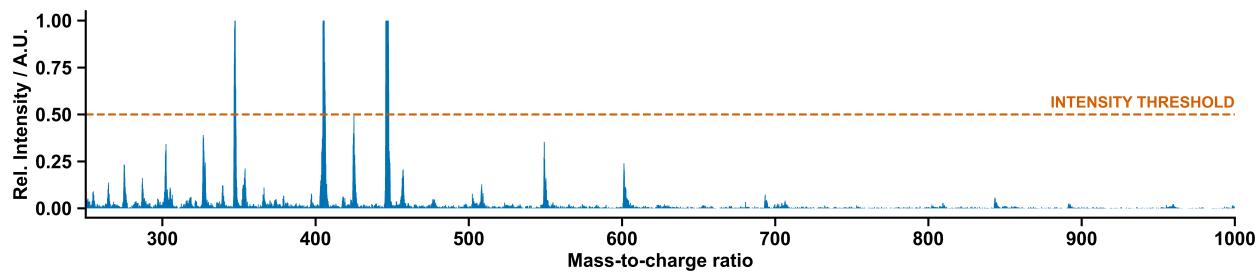
Scheme 51: Self-assembly of components 8, 17, with Yttrium(III) in a 3.0:1.5:1.0 molar ratio in  $\text{CH}_3\text{CN}$  at 60°C for 40h. These are the reagents (starting materials) for reaction 57.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: Oligomers formed.	
	Human MS Decision: Failed	MS Spectra Category: Reaction occurred, unknown product.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	NMR Criteria 2: N/A
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 1
		MS Criteria 3: Pass	Number of counter-ions found: 0

Decision Table 51: Human labeled and Decsision maker labeled outcomes for the  $^1\text{H}$  NMR spectroscopy and UPLC-MS spectrometry of reaction 57. Decision motivations are also given.

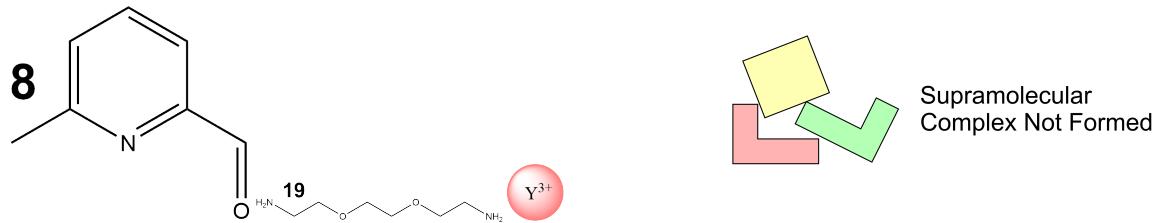


NMR Spectra 51: The stacked  $^1\text{H}$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 57.



MS Spectra 51: The ULPC-MS spectra of reaction 57. The intensity threshold is also shown.

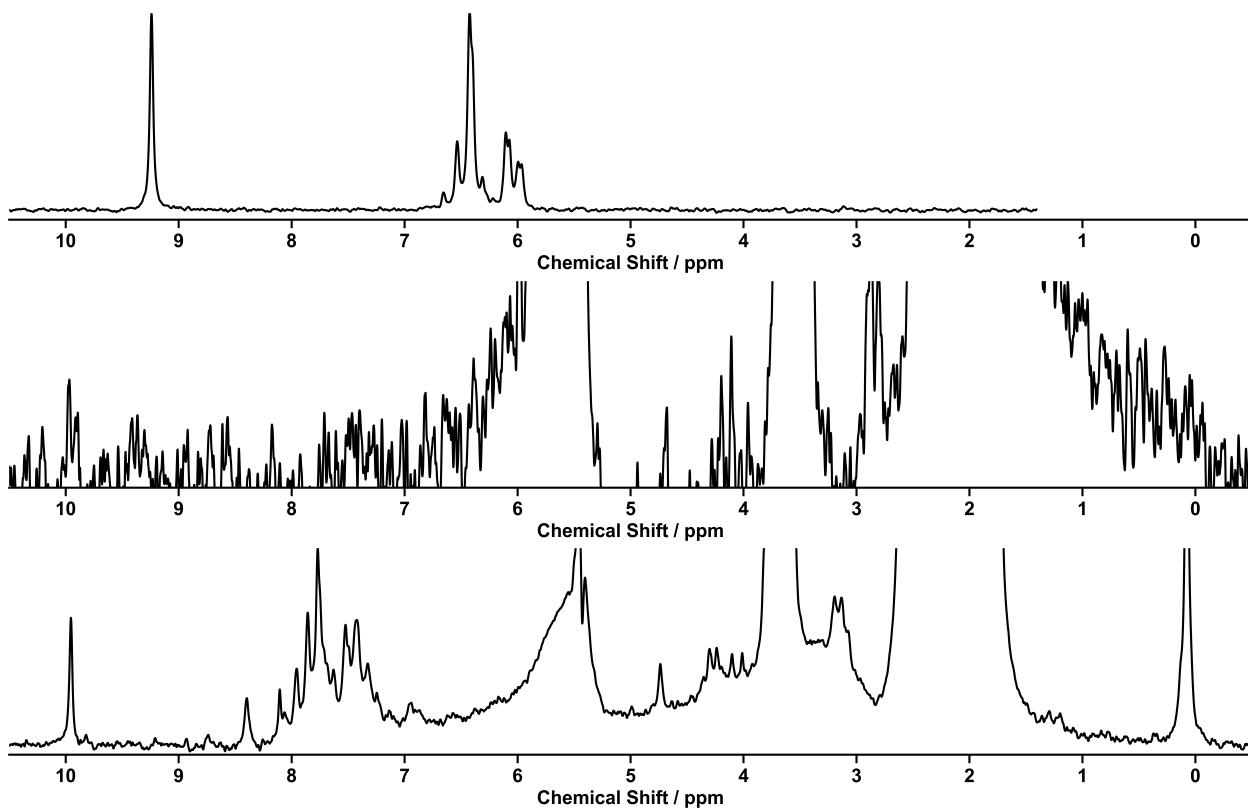
## Reaction 58



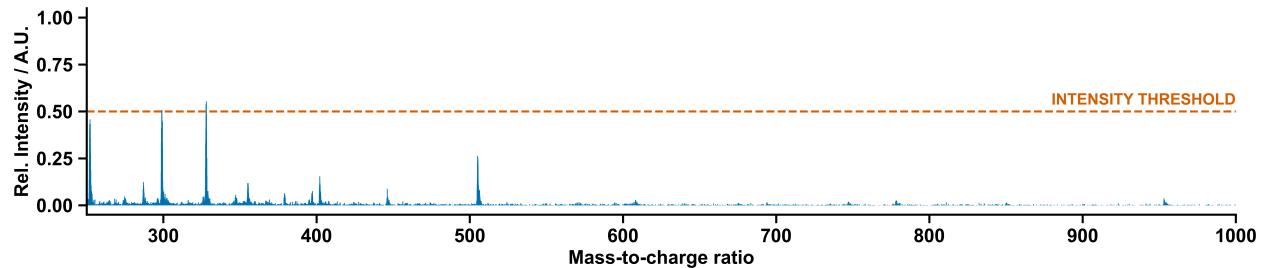
Scheme 52: Self-assembly of components 8, 19, with Yttrium(III) in a 3.0:1.5:1.0 molar ratio in CH<sub>3</sub>CN at 60°C for 40h. These are the reagents (starting materials) for reaction 58.

Human Reaction Decision: Failed	Human NMR Decision: Pass	NMR Spectra Category: Single discrete species formed.	
	Human MS Decision: Failed	MS Spectra Category: Reaction failed.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	NMR Criteria 2: N/A
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 0
		MS Criteria 3: Pass	Number of counter-ions found: 0

Decision Table 52: Human labeled and Decsision maker labeled outcomes for the <sup>1</sup>H NMR spectroscopy and ULPC-MS spectrometry of reaction 58. Decision motivations are also given.

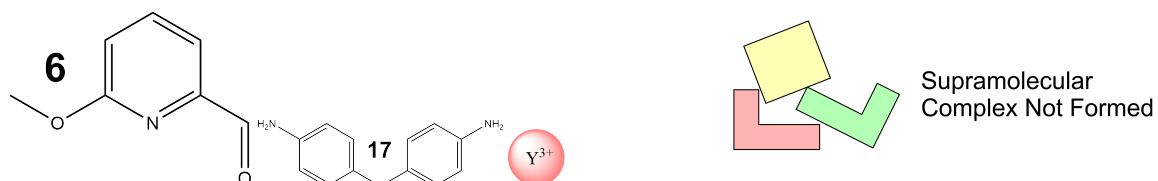


NMR Spectra 52: The stacked <sup>1</sup>H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 58.



MS Spectra 52: The ULPC-MS spectra of reaction 58. The intensity threshold is also shown.

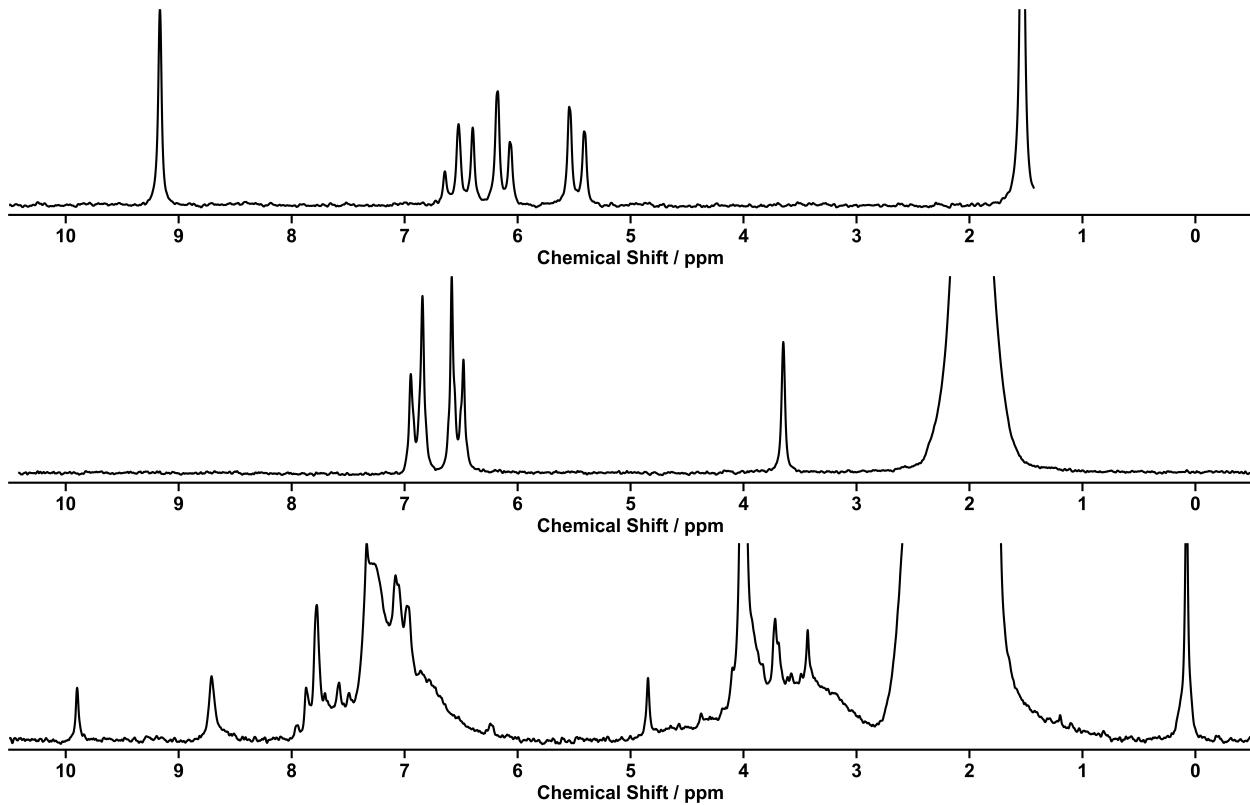
## Reaction 60



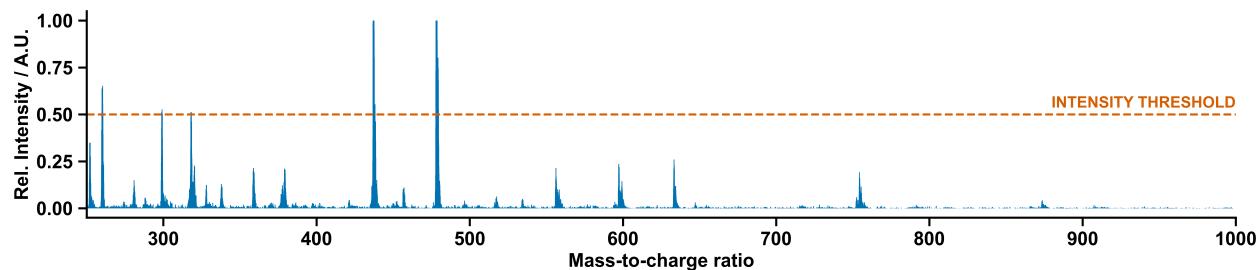
Scheme 53: Self-assembly of components 6, 17, with Yttrium(III) in a 3.0:1.5:1.0 molar ratio in CH<sub>3</sub>CN at 60°C for 40h. These are the reagents (starting materials) for reaction 60.

Human Reaction Decision: Failed	Human NMR Decision: Pass	NMR Spectra Category: Single discrete species formed.	
	Human MS Decision: Failed	MS Spectra Category: Reaction occurred, unknown product.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	
	Decision Maker MS Decision: Pass	NMR Criteria 2: N/A	MS Criteria 1 and 2: Pass Number of predicted peaks found in MS spectra with appropriate intensity: 0
	MS Criteria 3: Pass	Number of counter-ions found: 0	

Decision Table 53: Human labeled and Decsision maker labeled outcomes for the  $^1\text{H}$  NMR spectroscopy and UPLC-MS spectrometry of reaction 60. Decision motivations are also given.

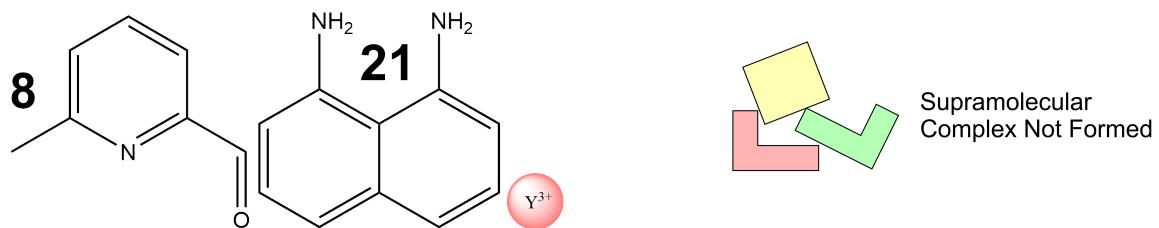


NMR Spectra 53: The stacked  $^1\text{H}$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 60.



MS Spectra 53: The UPLC-MS spectra of reaction 60. The intensity threshold is also shown.

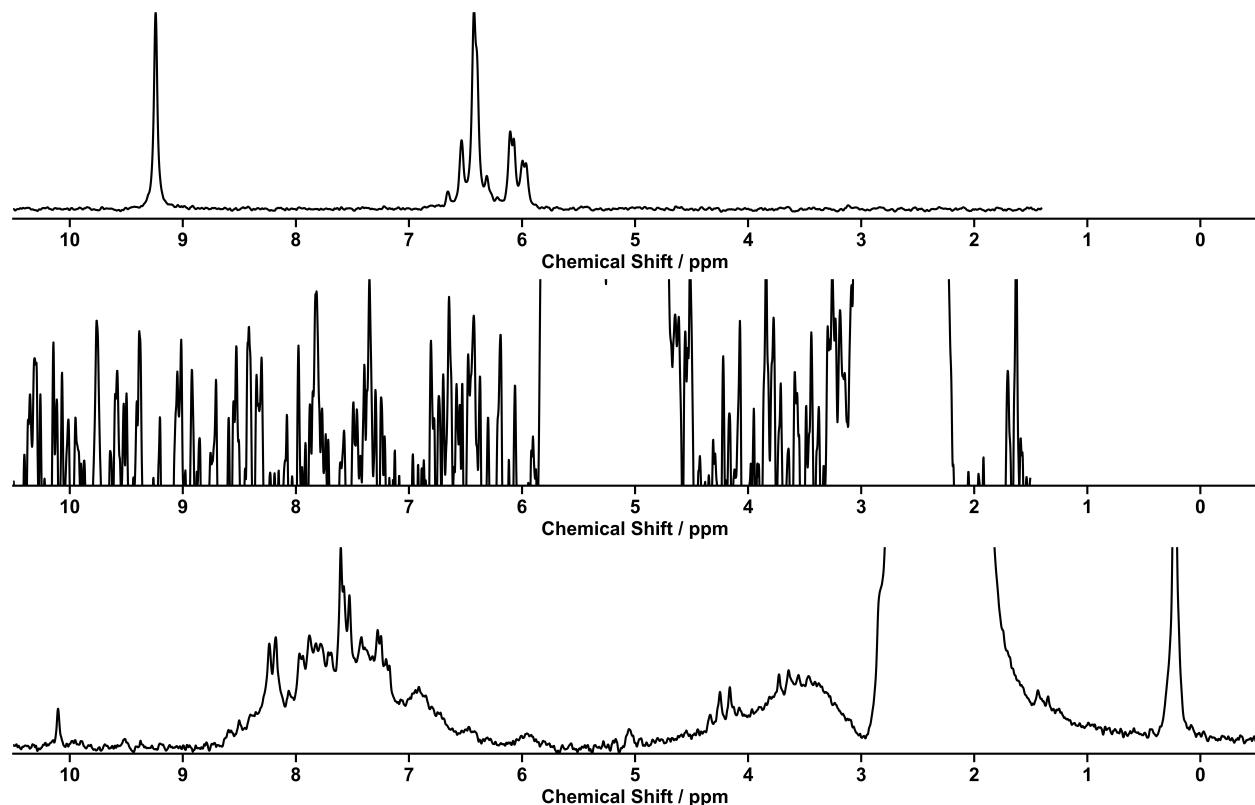
## Reaction 63



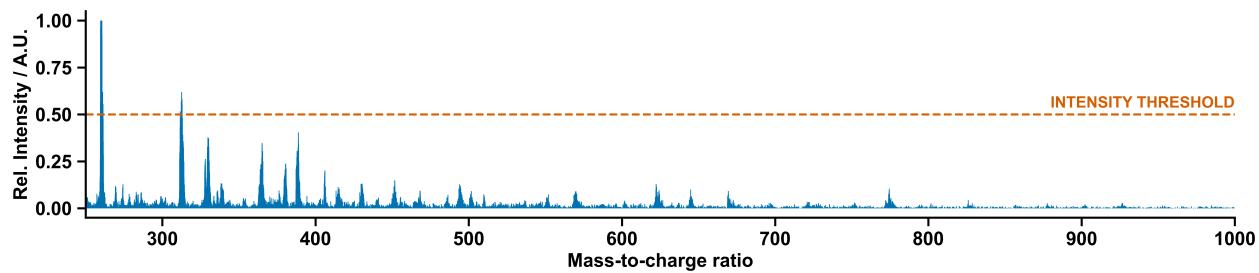
Scheme 54: Self-assembly of components 8, 21, with Yttrium(III) in a 3.0:1.5:1.0 molar ratio in  $\text{CH}_3\text{CN}$  at 60°C for 40h. These are the reagents (starting materials) for reaction 63.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: Oligomers formed.	
	Human MS Decision: Failed	MS Spectra Category: Reaction failed.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	NMR Criteria 2: N/A
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 0
		MS Criteria 3: Pass	Number of counter-ions found: 0

Decision Table 54: Human labeled and Decsision maker labeled outcomes for the  $^1\text{H}$  NMR spectroscopy and UPLC-MS spectrometry of reaction 63. Decision motivations are also given.

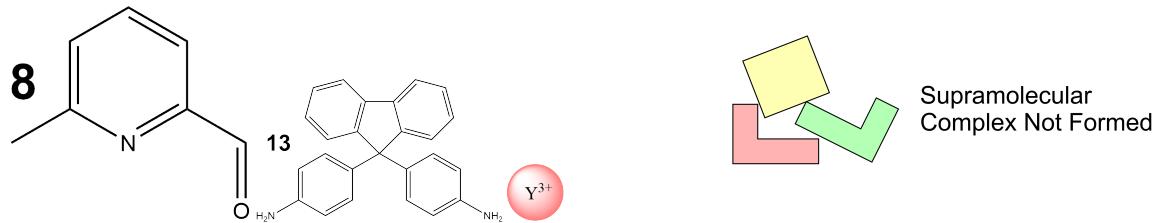


NMR Spectra 54: The stacked  $^1\text{H}$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 63.



MS Spectra 54: The ULPC-MS spectra of reaction 63. The intensity threshold is also shown.

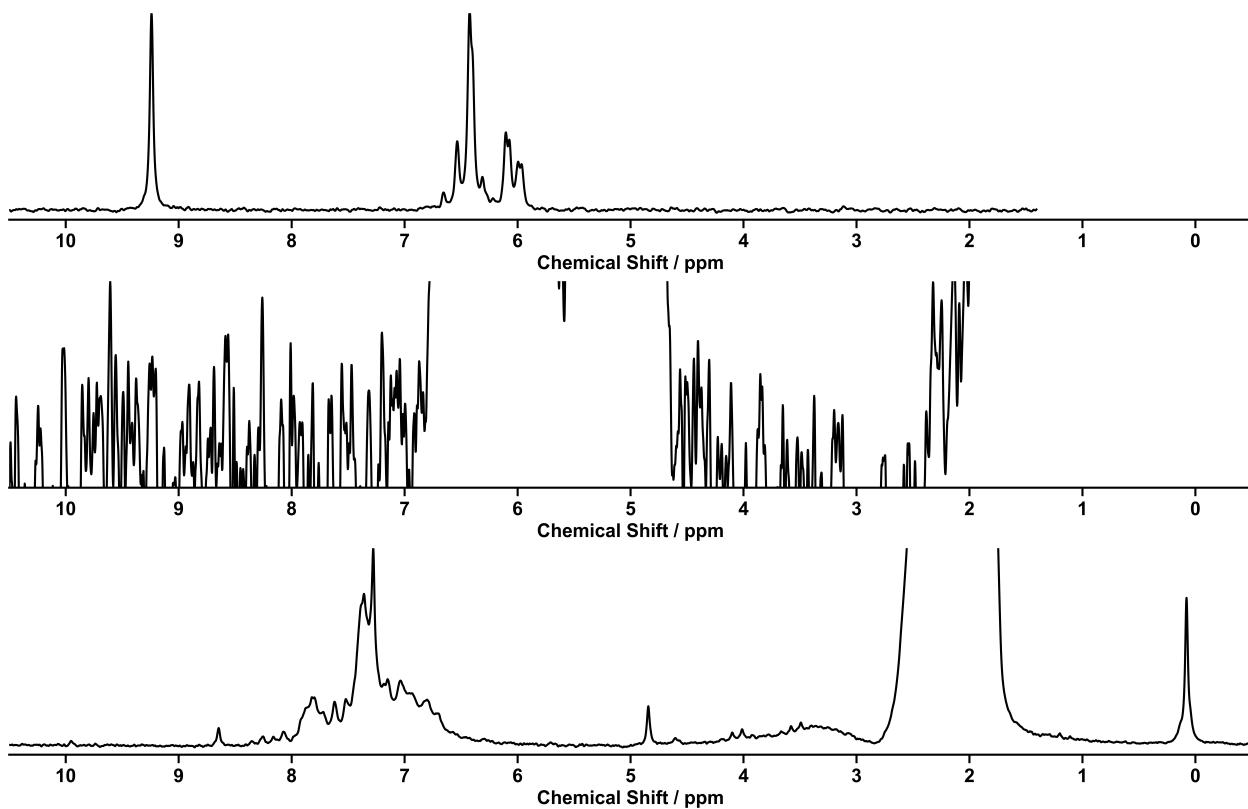
## Reaction 64



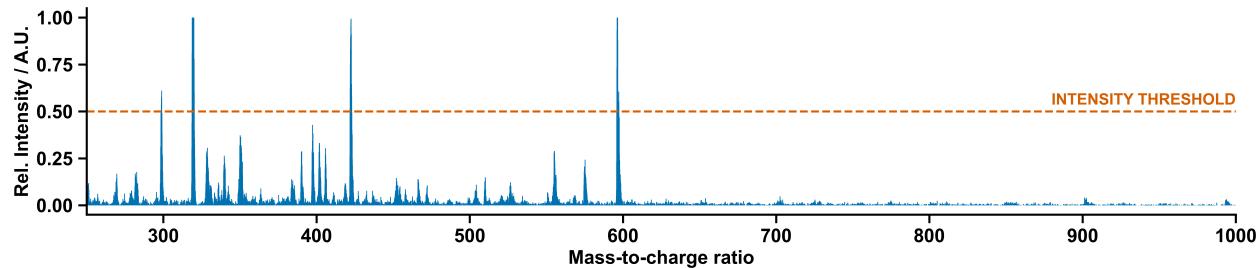
Scheme 55: Self-assembly of components 8, 13, with Yttrium(III) in a 3.0:1.5:1.0 molar ratio in CH<sub>3</sub>CN at 60°C for 40h. These are the reagents (starting materials) for reaction 64.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: Oligomers formed.	
	Human MS Decision: Failed	MS Spectra Category: Reaction occurred, unknown product.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	NMR Criteria 2: N/A
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 0
		MS Criteria 3: Pass	Number of counter-ions found: 0

Decision Table 55: Human labeled and Decsision maker labeled outcomes for the <sup>1</sup>H NMR spectroscopy and ULPC-MS spectrometry of reaction 64. Decision motivations are also given.

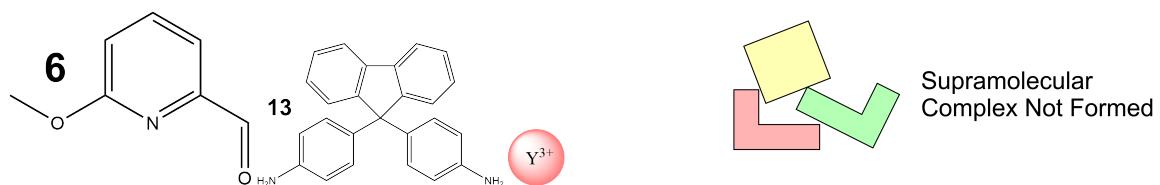


NMR Spectra 55: The stacked  $^1\text{H}$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 64.



MS Spectra 55: The ULPC-MS spectra of reaction 64. The intensity threshold is also shown.

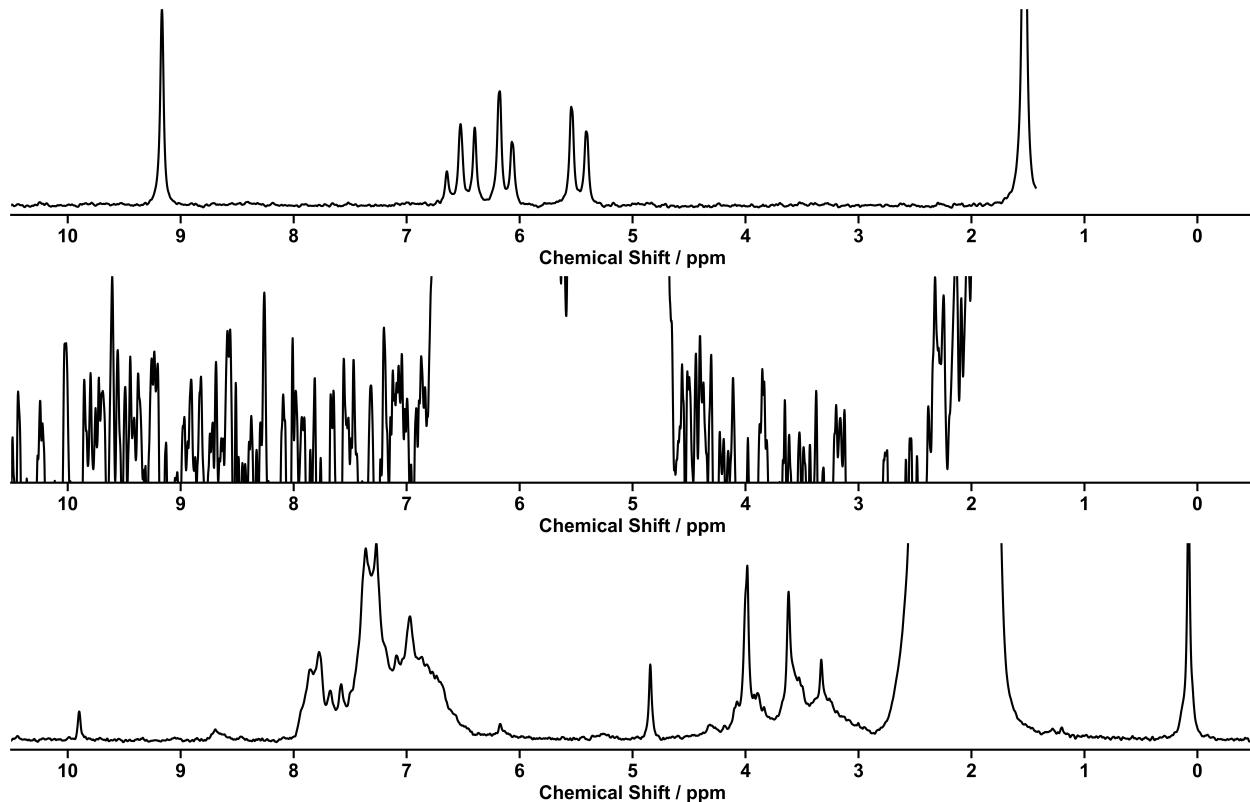
## Reaction 66



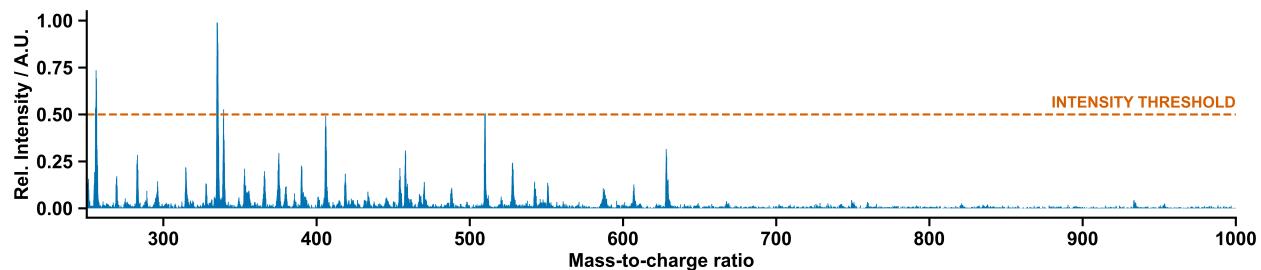
Scheme 56: Self-assembly of components 6, 13, with Yttrium(III) in a 3.0:1.5:1.0 molar ratio in  $\text{CH}_3\text{CN}$  at  $60^\circ\text{C}$  for 40h. These are the reagents (starting materials) for reaction 66.

Human Reaction Decision: Failed	Human NMR Decision: Pass	NMR Spectra Category: Single discrete species formed.	
	Human MS Decision: Failed	MS Spectra Category: Reaction occurred, unknown product.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	
	Decision Maker MS Decision: Pass	NMR Criteria 2: N/A	MS Criteria 1 and 2: Pass Number of predicted peaks found in MS spectra with appropriate intensity: 1
	MS Criteria 3: Pass	MS Criteria 3: Pass	Number of counter-ions found: 0

Decision Table 56: Human labeled and Decsision maker labeled outcomes for the  $^1\text{H}$  NMR spectroscopy and ULPC-MS spectrometry of reaction 66. Decision motivations are also given.

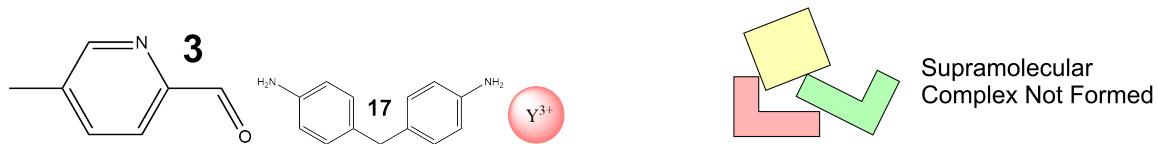


NMR Spectra 56: The stacked  $^1\text{H}$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 66.



MS Spectra 56: The ULPC-MS spectra of reaction 66. The intensity threshold is also shown.

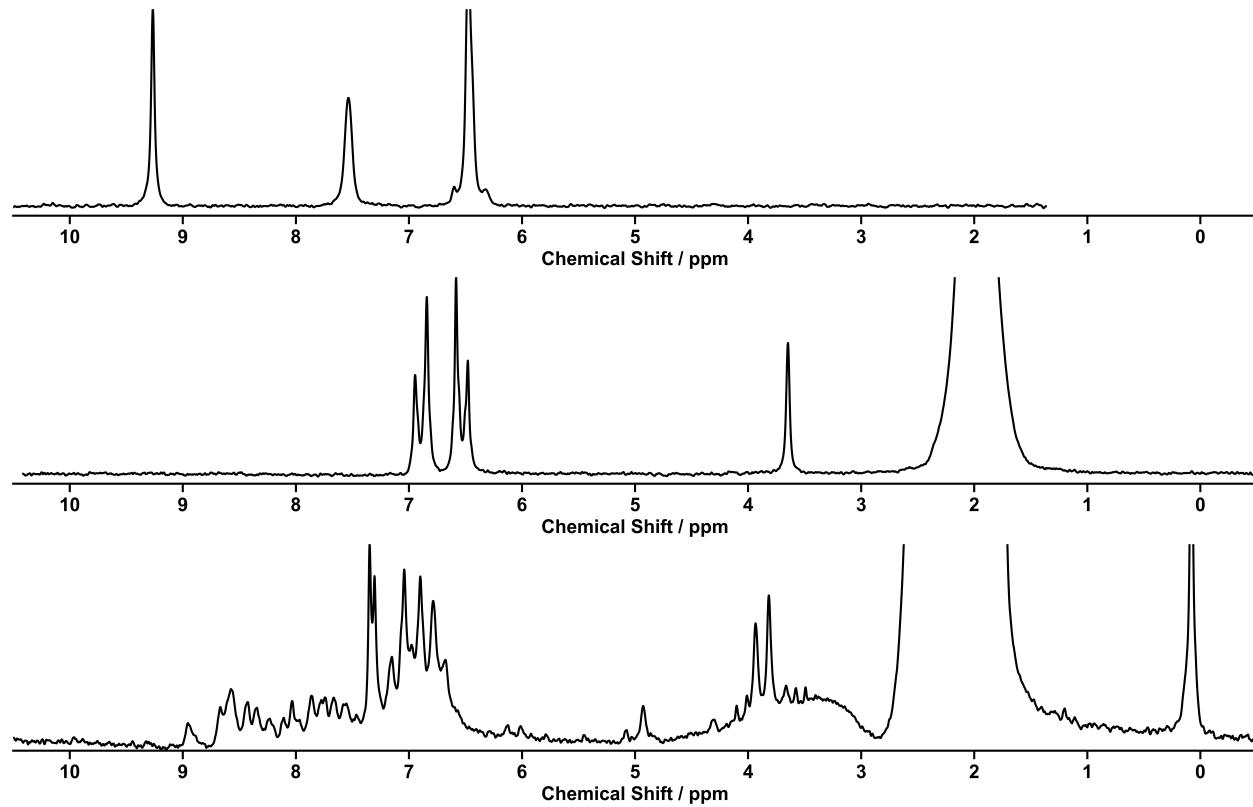
## Reaction 67



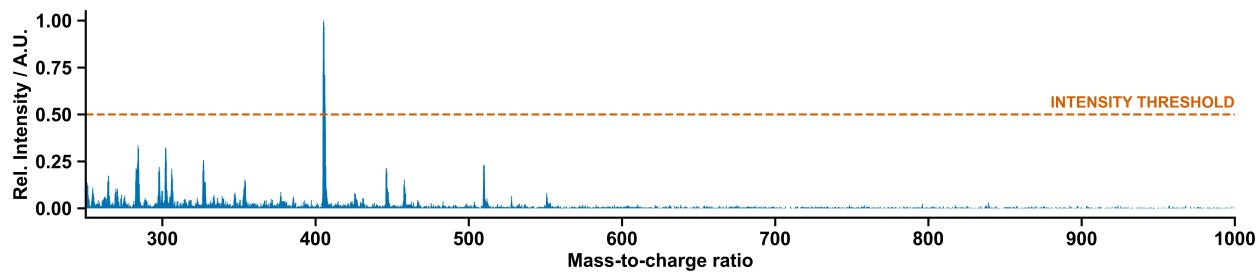
Scheme 57: Self-assembly of components 3, 17, with Yttrium(III) in a 3.0:1.5:1.0 molar ratio in  $\text{CH}_3\text{CN}$  at 60°C for 40h. These are the reagents (starting materials) for reaction 67.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: Oligomers formed.	
	Human MS Decision: Failed	MS Spectra Category: Reaction occurred, unknown product.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	NMR Criteria 2: N/A
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 0
		MS Criteria 3: Pass	Number of counter-ions found: 0

Decision Table 57: Human labeled and Decision maker labeled outcomes for the  $^1\text{H}$  NMR spectroscopy and UPLC-MS spectrometry of reaction 67. Decision motivations are also given.

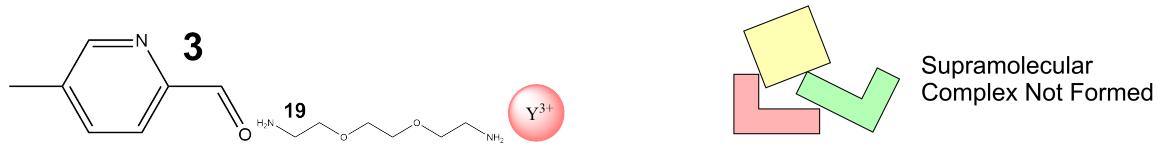


NMR Spectra 57: The stacked  $^1\text{H}$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 67.



MS Spectra 57: The ULPC-MS spectra of reaction 67. The intensity threshold is also shown.

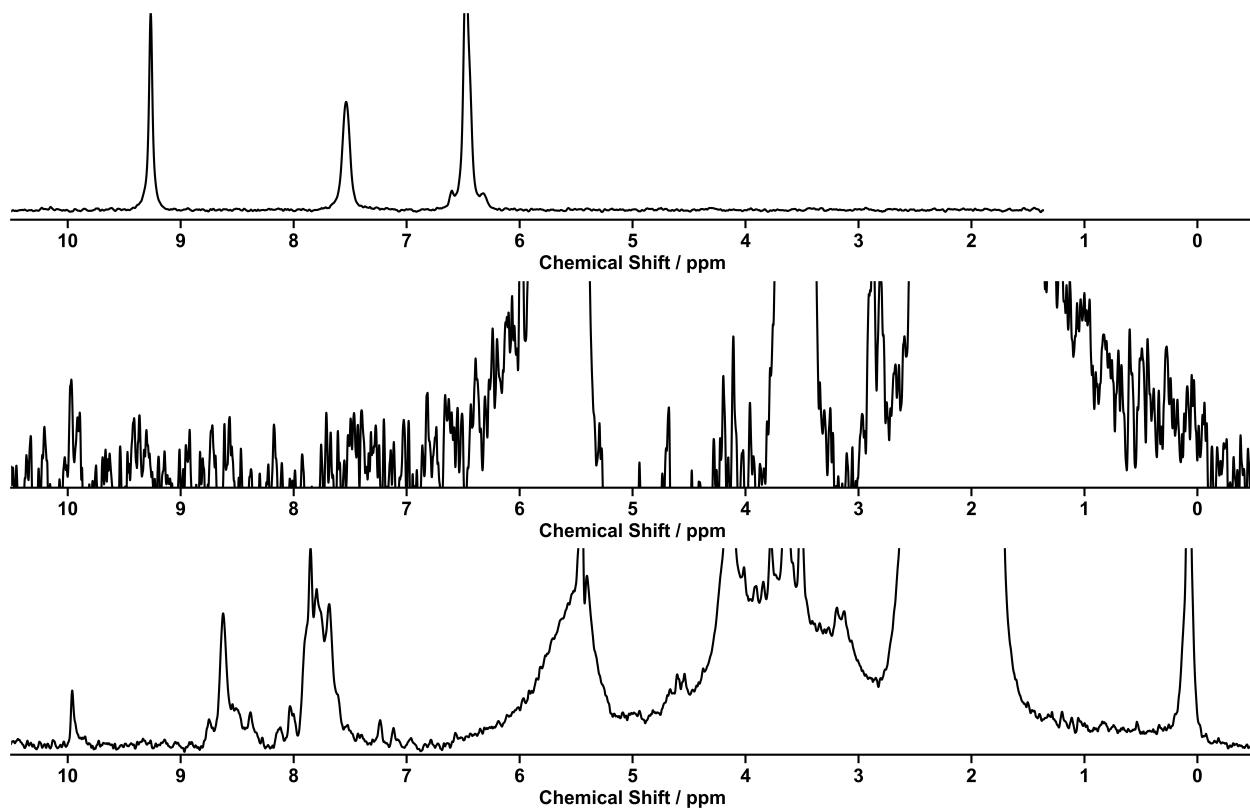
## Reaction 68



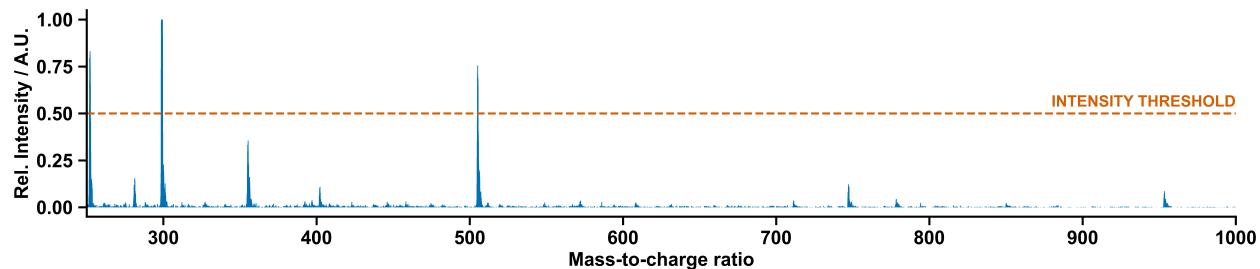
Scheme 58: Self-assembly of components 3, 19, with Yttrium(III) in a 3.0:1.5:1.0 molar ratio in CH<sub>3</sub>CN at 60°C for 40h. These are the reagents (starting materials) for reaction 68.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: Oligomers formed.	
	Human MS Decision: Failed	MS Spectra Category: Reaction occurred, unknown product.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	NMR Criteria 2: N/A
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 0
		MS Criteria 3: Pass	Number of counter-ions found: 0

Decision Table 58: Human labeled and Decsision maker labeled outcomes for the <sup>1</sup>H NMR spectroscopy and ULPC-MS spectrometry of reaction 68. Decision motivations are also given.

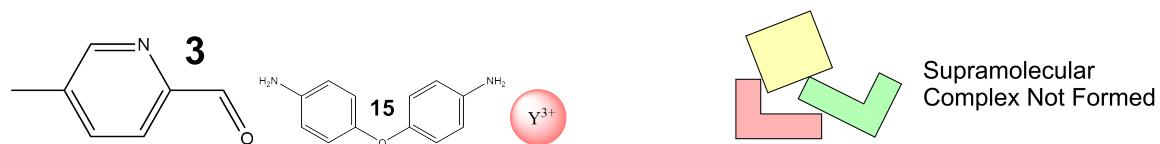


NMR Spectra 58: The stacked <sup>1</sup>H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 68.



MS Spectra 58: The ULPC-MS spectra of reaction 68. The intensity threshold is also shown.

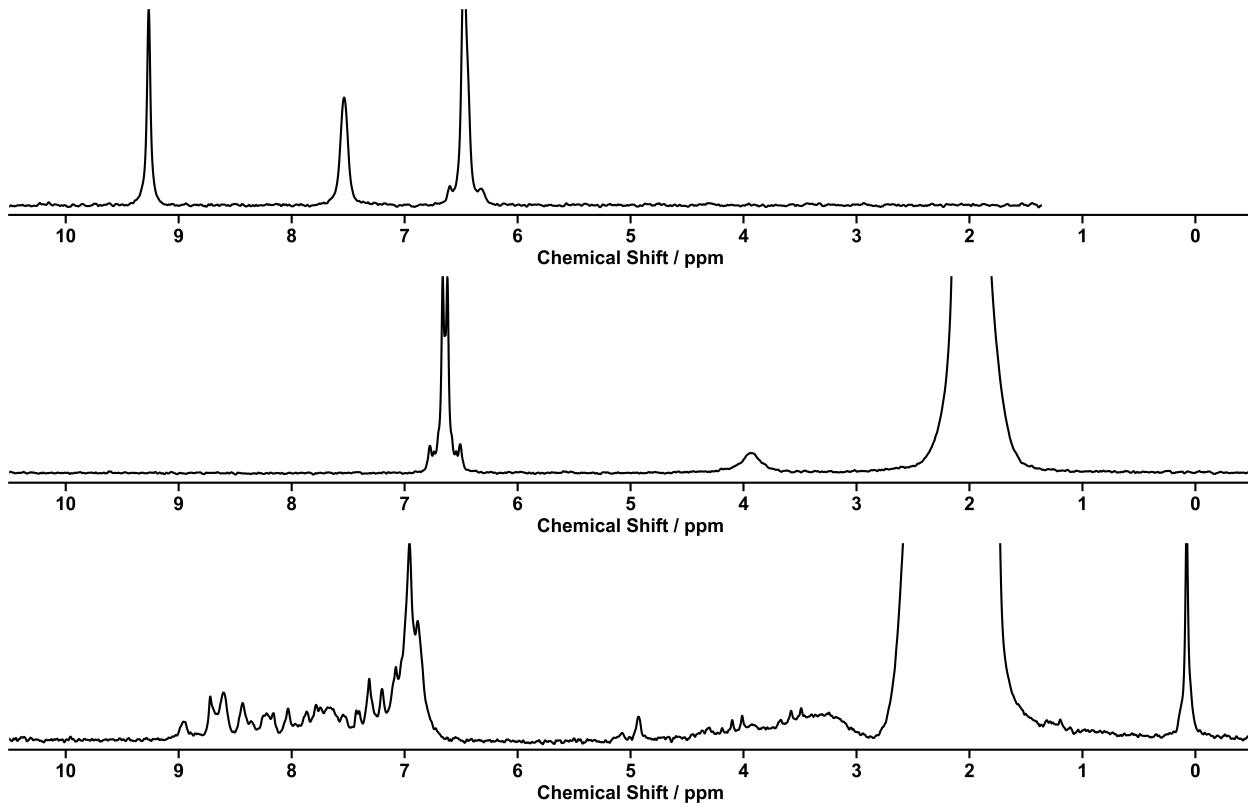
## Reaction 69



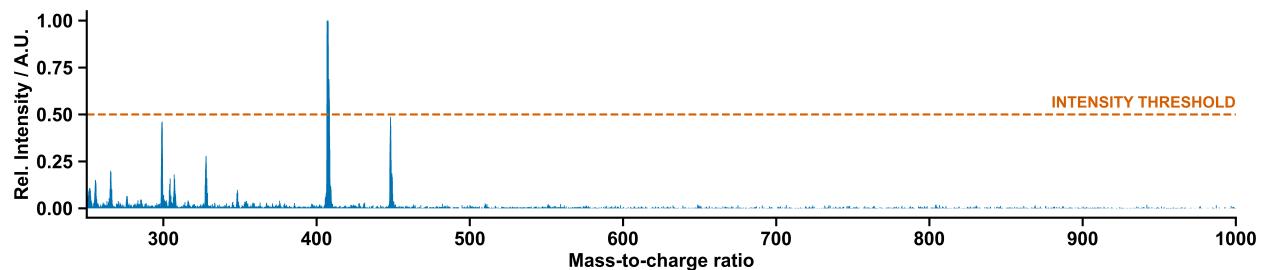
Scheme 59: Self-assembly of components 3, 15, with Yttrium(III) in a 3.0:1.5:1.0 molar ratio in  $\text{CH}_3\text{CN}$  at 60°C for 40h. These are the reagents (starting materials) for reaction 69.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: Oligomers formed.	
	Human MS Decision: Failed	MS Spectra Category: Reaction occurred, unknown product.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	
	Decision Maker MS Decision: Pass	NMR Criteria 2: N/A	MS Criteria 1 and 2: Pass Number of predicted peaks found in MS spectra with appropriate intensity: 0
	MS Criteria 3: Pass	Number of counter-ions found: 0	MS Criteria 3: Pass

Decision Table 59: Human labeled and Decsision maker labeled outcomes for the  $^1\text{H}$  NMR spectroscopy and UPLC-MS spectrometry of reaction 69. Decision motivations are also given.

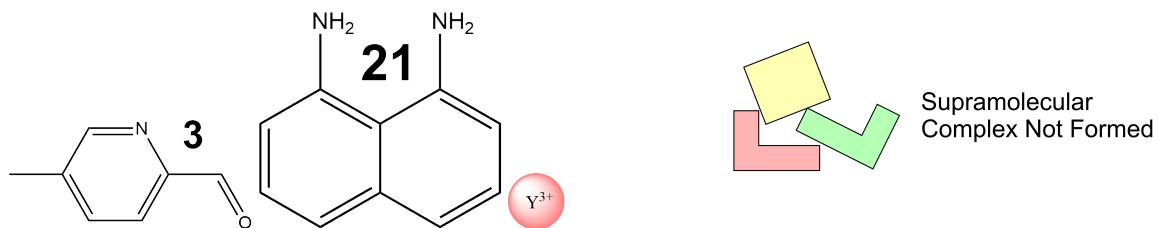


NMR Spectra 59: The stacked  $^1\text{H}$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 69.



MS Spectra 59: The ULPC-MS spectra of reaction 69. The intensity threshold is also shown.

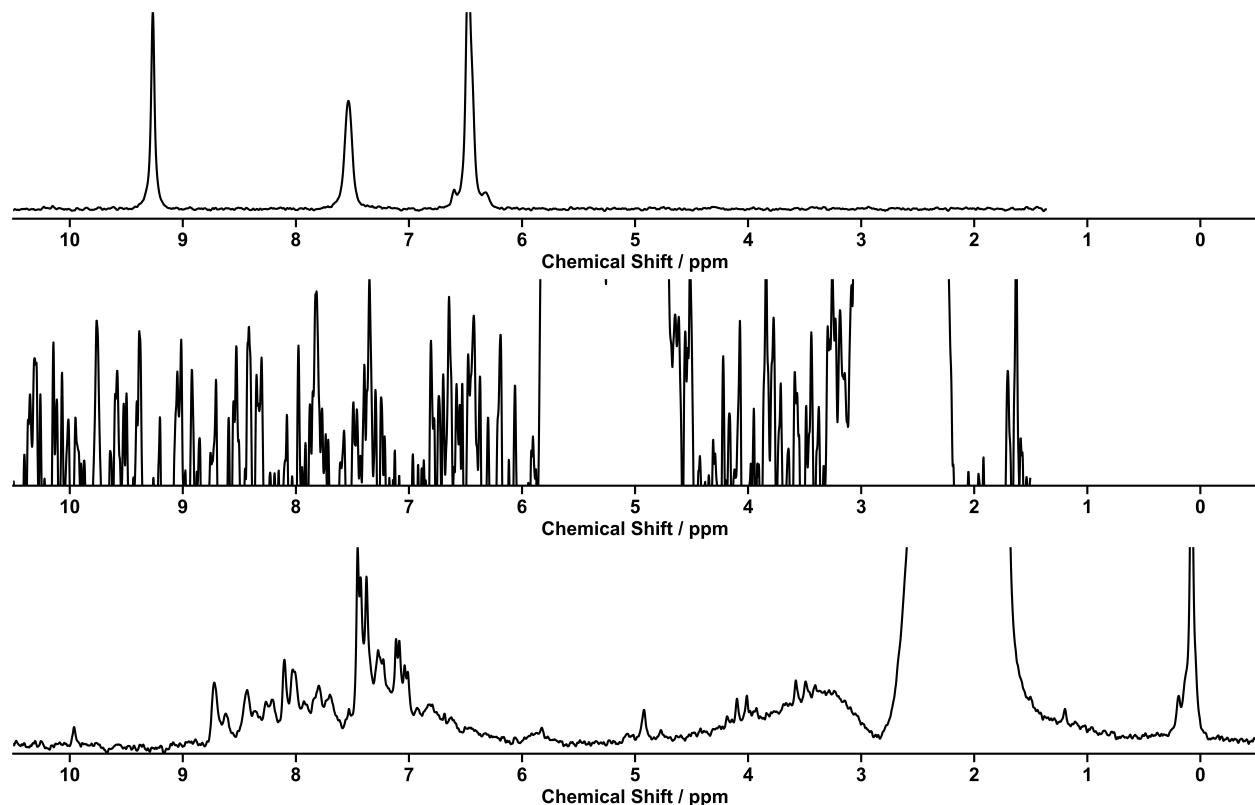
## Reaction 70



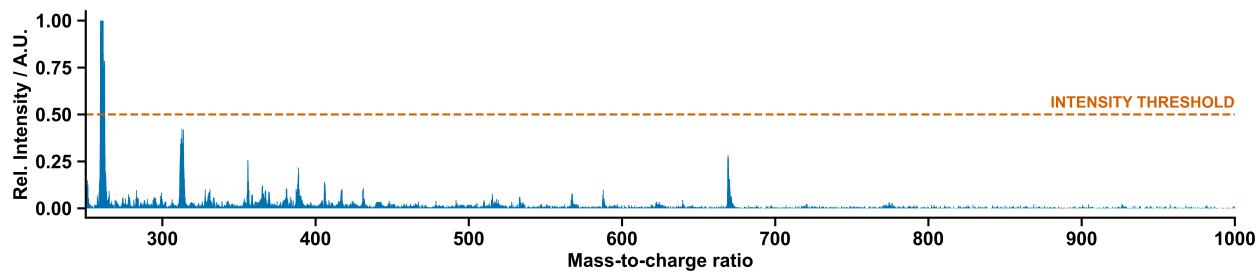
Scheme 60: Self-assembly of components 3, 21, with Yttrium(III) in a 3.0:1.5:1.0 molar ratio in  $\text{CH}_3\text{CN}$  at 60°C for 40h. These are the reagents (starting materials) for reaction 70.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: Oligomers formed.	
	Human MS Decision: Failed	MS Spectra Category: Reaction occurred, unknown product.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	NMR Criteria 2: N/A
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 0
		MS Criteria 3: Pass	Number of counter-ions found: 0

Decision Table 60: Human labeled and Decsision maker labeled outcomes for the  $^1\text{H}$  NMR spectroscopy and ULP-MS spectrometry of reaction 70. Decision motivations are also given.

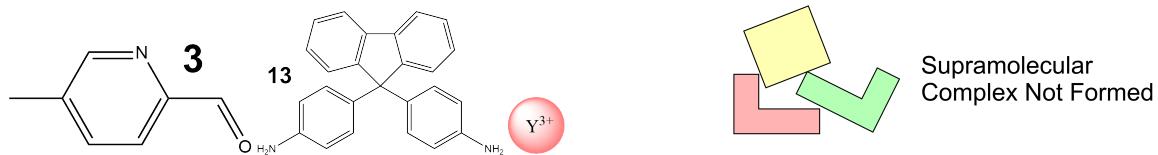


NMR Spectra 60: The stacked  $^1\text{H}$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 70.



MS Spectra 60: The ULPC-MS spectra of reaction 70. The intensity threshold is also shown.

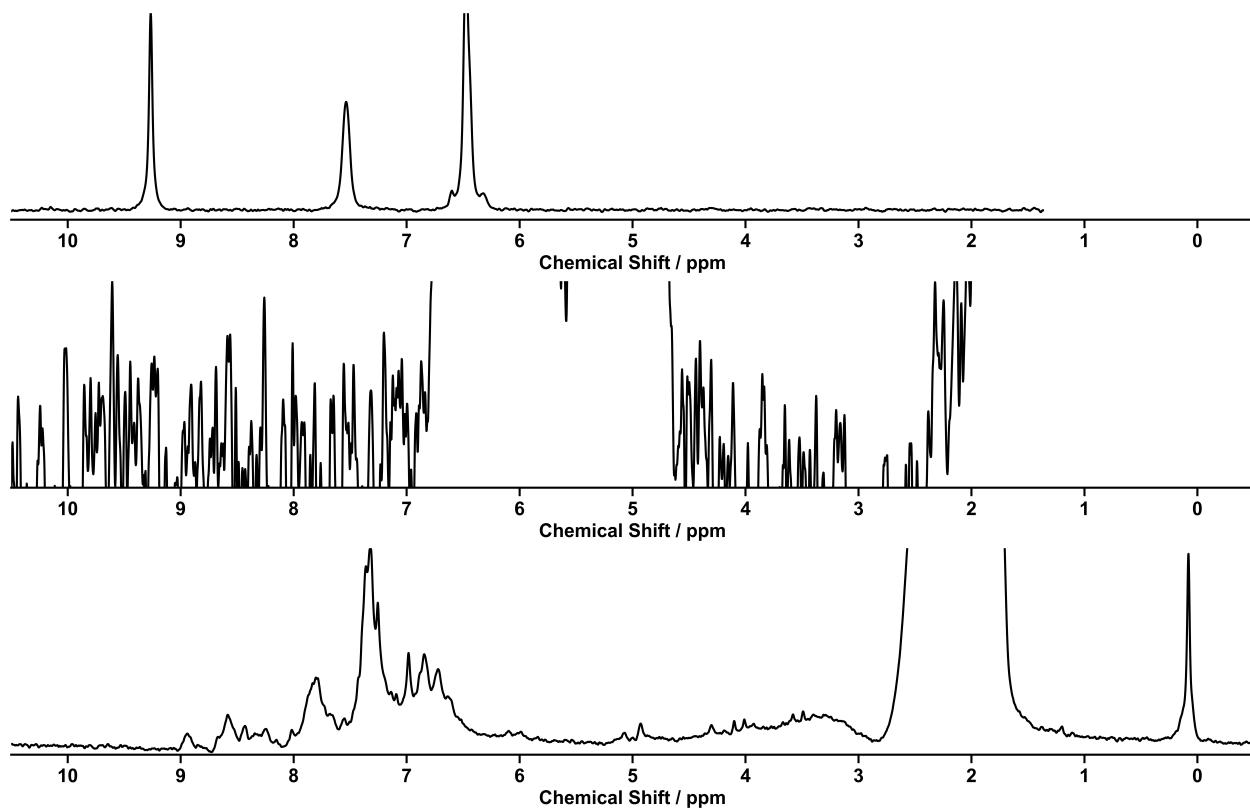
## Reaction 71



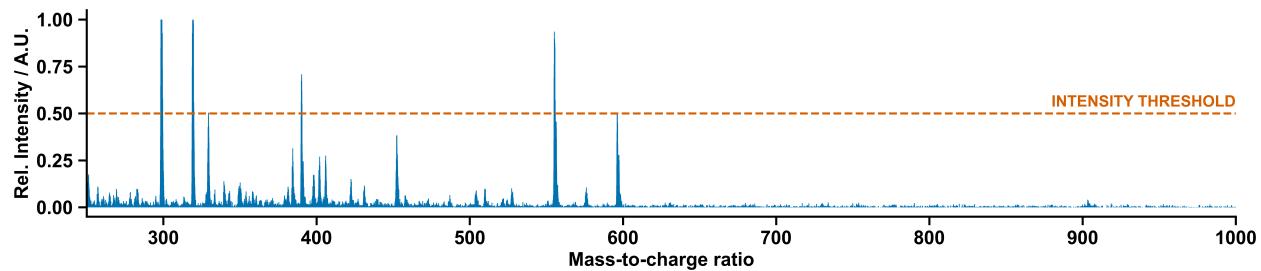
Scheme 61: Self-assembly of components 3, 13, with Yttrium(III) in a 3.0:1.5:1.0 molar ratio in CH<sub>3</sub>CN at 60°C for 40h. These are the reagents (starting materials) for reaction 71.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: Oligomers formed.	
	Human MS Decision: Failed	MS Spectra Category: Reaction occurred, unknown product.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	NMR Criteria 2: N/A
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 0
		MS Criteria 3: Pass	Number of counter-ions found: 0

Decision Table 61: Human labeled and Decsision maker labeled outcomes for the <sup>1</sup>H NMR spectroscopy and ULPC-MS spectrometry of reaction 71. Decision motivations are also given.

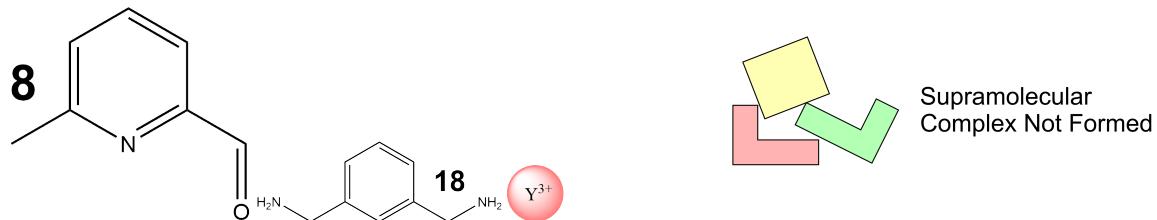


NMR Spectra 61: The stacked  $^1\text{H}$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 71.



MS Spectra 61: The ULPC-MS spectra of reaction 71. The intensity threshold is also shown.

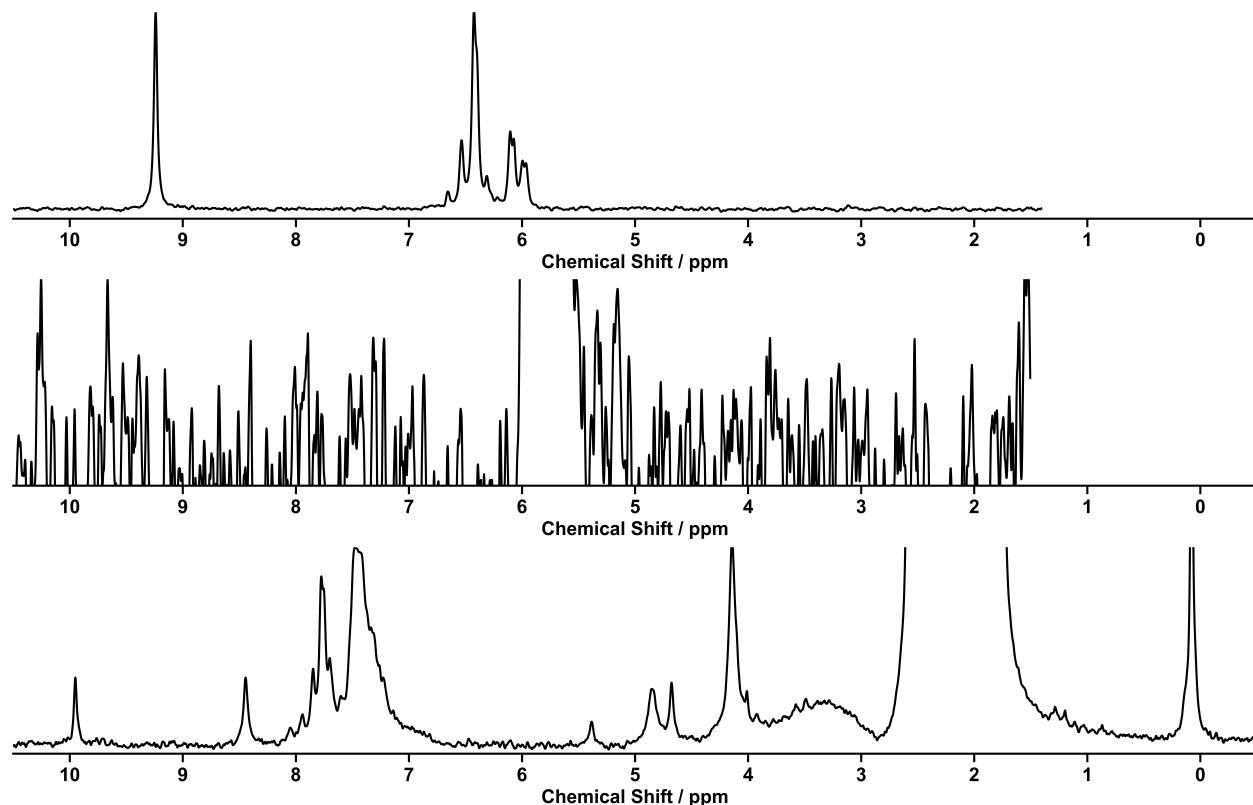
## Reaction 72



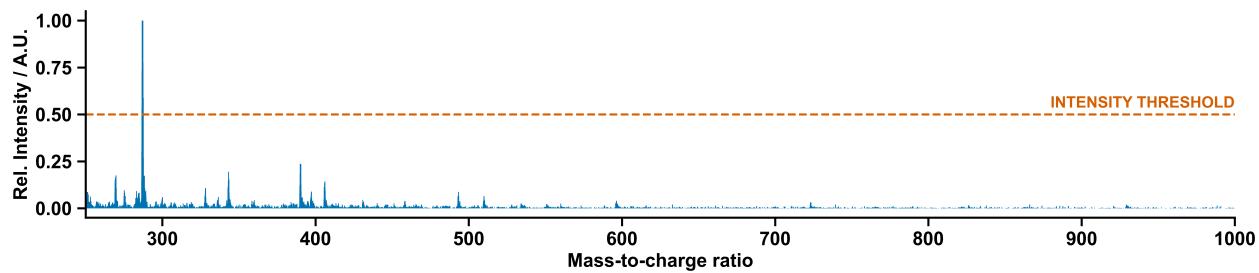
Scheme 62: Self-assembly of components 8, 18, with Yttrium(III) in a 3.0:1.5:1.0 molar ratio in  $\text{CH}_3\text{CN}$  at 60°C for 40h. These are the reagents (starting materials) for reaction 72.

Human Reaction Decision: Failed	Human NMR Decision: Pass	NMR Spectra Category: Single discrete species formed.	
	Human MS Decision: Failed	MS Spectra Category: Reaction occurred, unknown product.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	NMR Criteria 2: N/A
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 1
		MS Criteria 3: Pass	Number of counter-ions found: 0

Decision Table 62: Human labeled and Decsision maker labeled outcomes for the  $^1\text{H}$  NMR spectroscopy and UPLC-MS spectrometry of reaction 72. Decision motivations are also given.

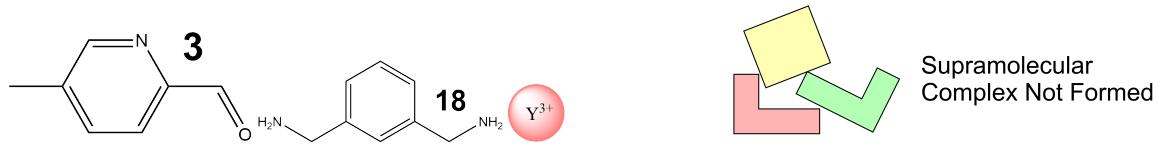


NMR Spectra 62: The stacked  $^1\text{H}$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 72.



MS Spectra 62: The ULPC-MS spectra of reaction 72. The intensity threshold is also shown.

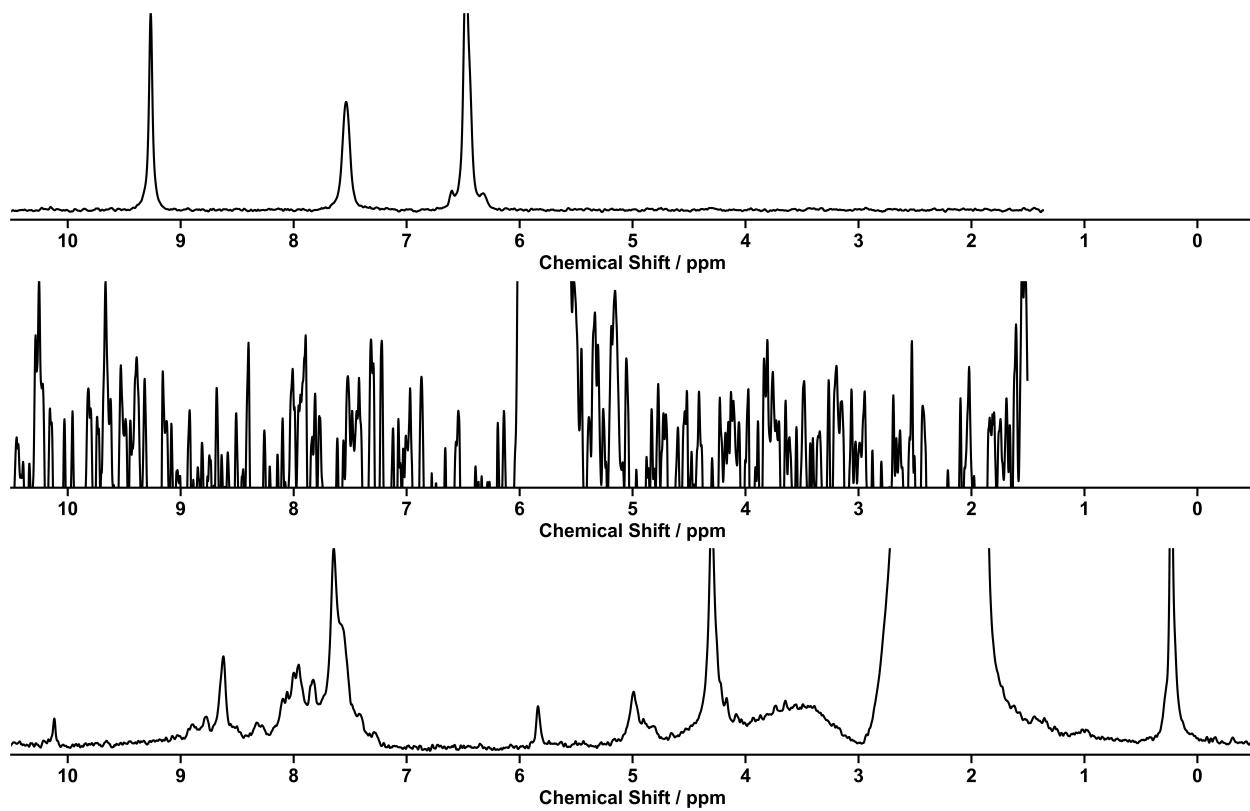
## Reaction 74



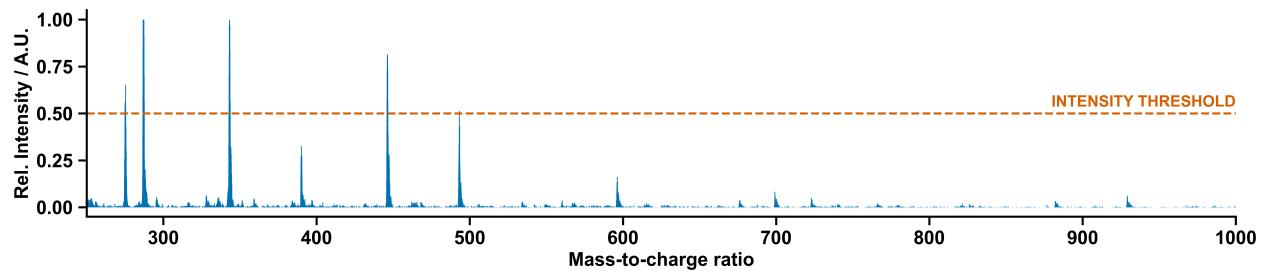
Scheme 63: Self-assembly of components 3, 18, with Yttrium(III) in a 3.0:1.5:1.0 molar ratio in  $\text{CH}_3\text{CN}$  at  $60^\circ\text{C}$  for 40h. These are the reagents (starting materials) for reaction 74.

Human Reaction Decision: Failed	Human NMR Decision: Pass	NMR Spectra Category: Single discrete species formed.	
	Human MS Decision: Failed	MS Spectra Category: Reaction occurred, unknown product.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	NMR Criteria 2: N/A
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 0
		MS Criteria 3: Pass	Number of counter-ions found: 0

Decision Table 63: Human labeled and Decision maker labeled outcomes for the  $^1\text{H}$  NMR spectroscopy and ULPC-MS spectrometry of reaction 74. Decision motivations are also given.

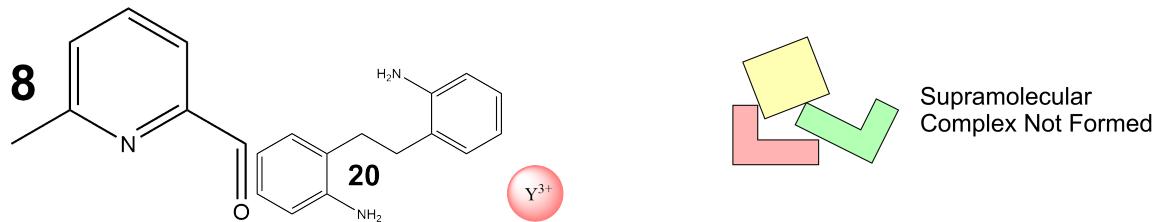


NMR Spectra 63: The stacked  $^1\text{H}$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 74.



MS Spectra 63: The ULPC-MS spectra of reaction 74. The intensity threshold is also shown.

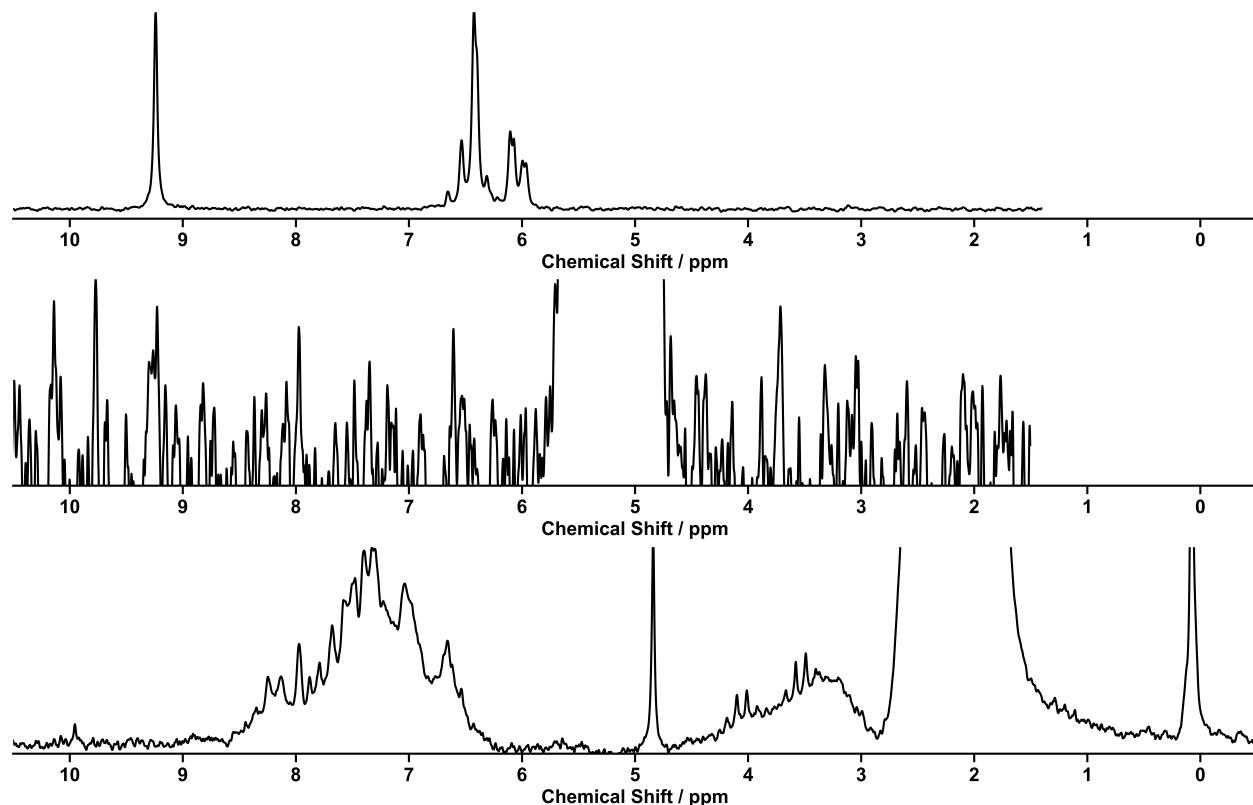
## Reaction 78



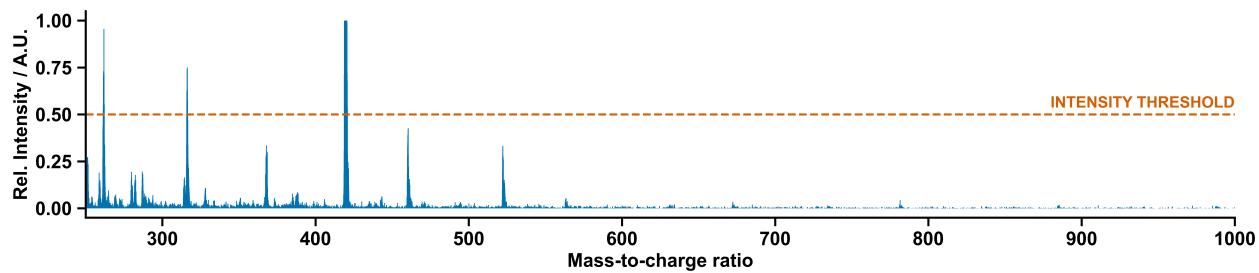
Scheme 64: Self-assembly of components 8, 20, with Yttrium(III) in a 3.0:1.5:1.0 molar ratio in  $\text{CH}_3\text{CN}$  at 60°C for 40h. These are the reagents (starting materials) for reaction 78.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: Oligomers formed.	
	Human MS Decision: Pass	MS Spectra Category: Reaction occurred, supramolecular product.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	NMR Criteria 2: N/A
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 6
		MS Criteria 3: Pass	Number of counter-ions found: 4

Decision Table 64: Human labeled and Decsision maker labeled outcomes for the  $^1\text{H}$  NMR spectroscopy and UPLC-MS spectrometry of reaction 78. Decision motivations are also given.

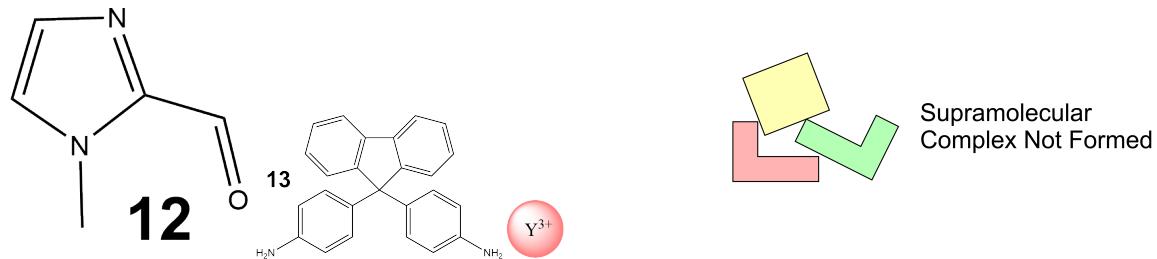


NMR Spectra 64: The stacked  $^1\text{H}$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 78.



MS Spectra 64: The ULPC-MS spectra of reaction 78. The intensity threshold is also shown.

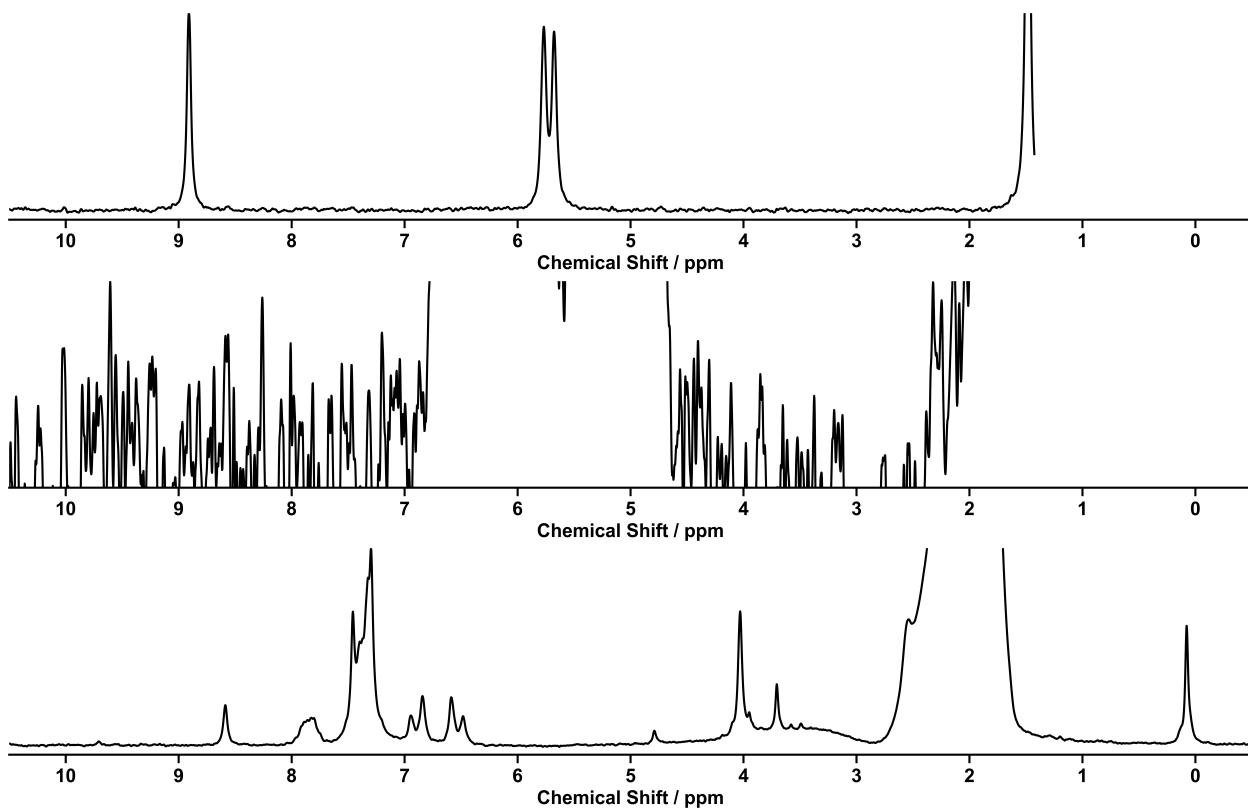
## Reaction 80



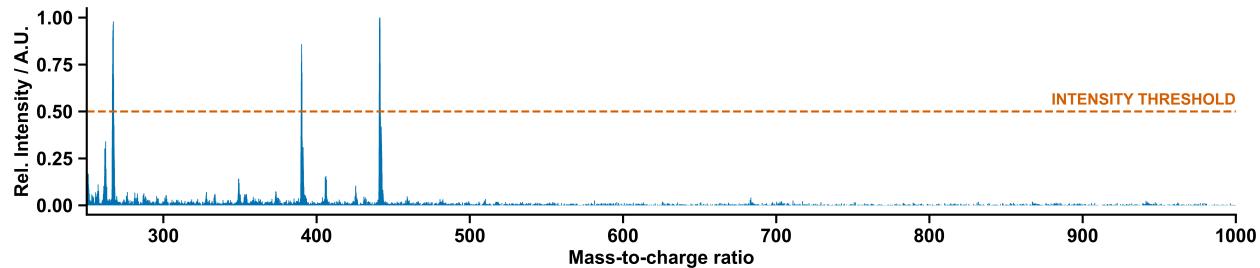
Scheme 65: Self-assembly of components 12, 13, with Yttrium(III) in a 3.0:1.5:1.0 molar ratio in  $\text{CH}_3\text{CN}$  at  $60^\circ\text{C}$  for 40h. These are the reagents (starting materials) for reaction 80.

Human Reaction Decision: Failed	Human NMR Decision: Pass	NMR Spectra Category: Single discrete species formed.	
	Human MS Decision: Failed	MS Spectra Category: Reaction occurred, unknown product.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	NMR Criteria 2: N/A
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 0
		MS Criteria 3: Pass	Number of counter-ions found: 0

Decision Table 65: Human labeled and Decision maker labeled outcomes for the  $^1\text{H}$  NMR spectroscopy and ULPC-MS spectrometry of reaction 80. Decision motivations are also given.

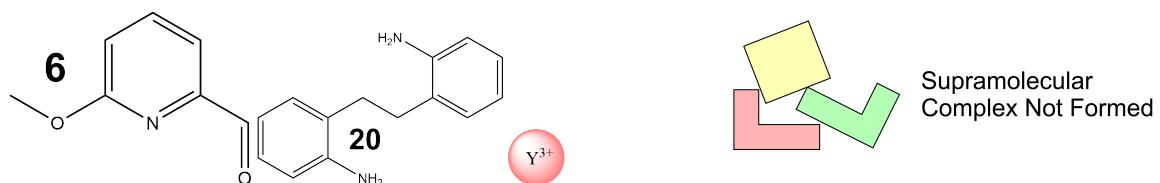


NMR Spectra 65: The stacked <sup>1</sup>H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 80.



MS Spectra 65: The ULPC-MS spectra of reaction 80. The intensity threshold is also shown.

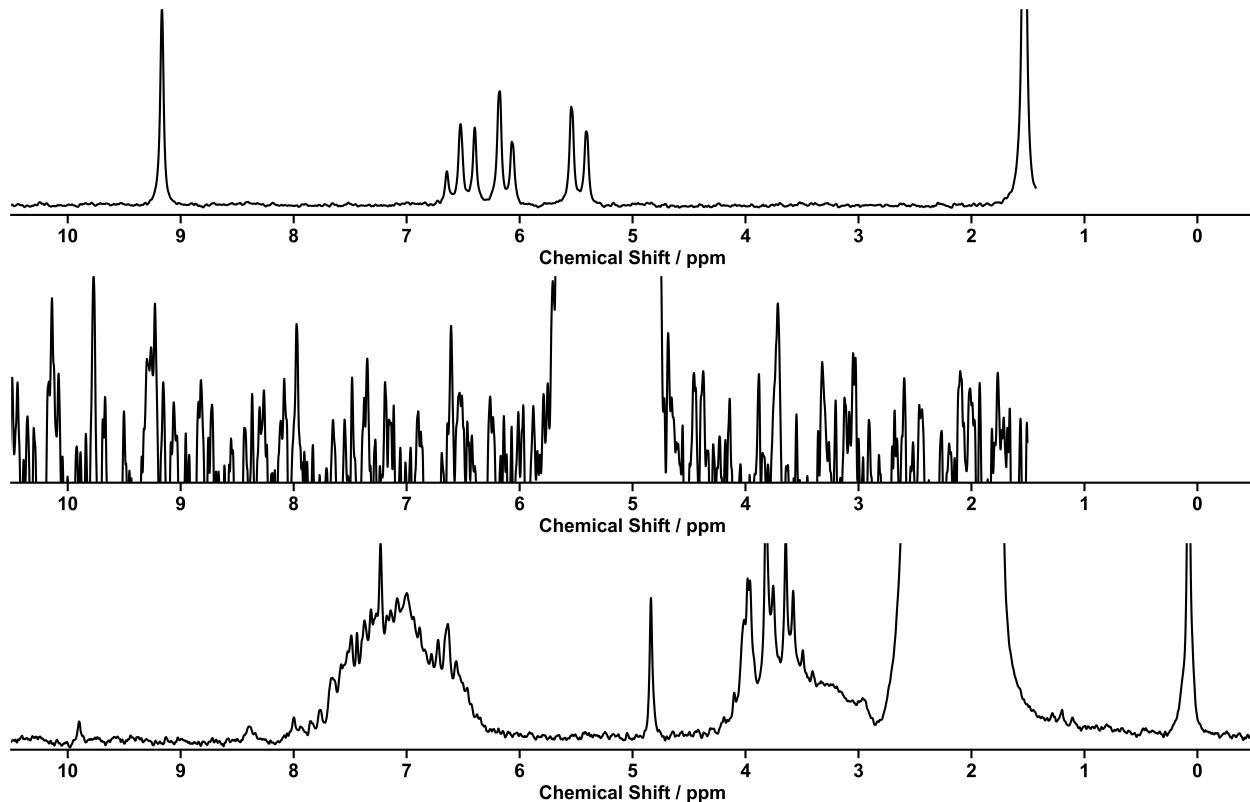
## Reaction 81



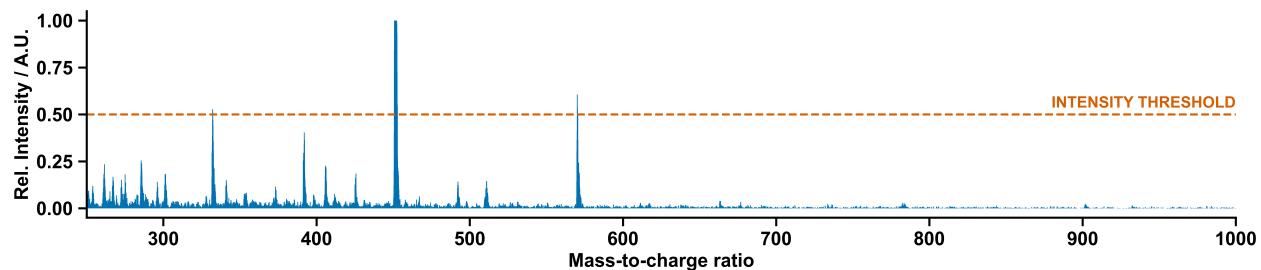
Scheme 66: Self-assembly of components 6, 20, with Yttrium(III) in a 3.0:1.5:1.0 molar ratio in CH<sub>3</sub>CN at 60°C for 40h. These are the reagents (starting materials) for reaction 81.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: Oligomers formed.	
	Human MS Decision: Failed	MS Spectra Category: Reaction occurred, unknown product.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	
		NMR Criteria 2: N/A	
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 0
		MS Criteria 3: Pass	Number of counter-ions found: 0

Decision Table 66: Human labeled and Decsision maker labeled outcomes for the  $^1\text{H}$  NMR spectroscopy and UPLC-MS spectrometry of reaction 81. Decision motivations are also given.

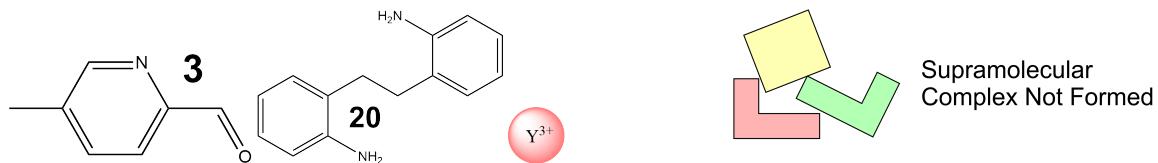


NMR Spectra 66: The stacked  $^1\text{H}$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 81.



MS Spectra 66: The UPLC-MS spectra of reaction 81. The intensity threshold is also shown.

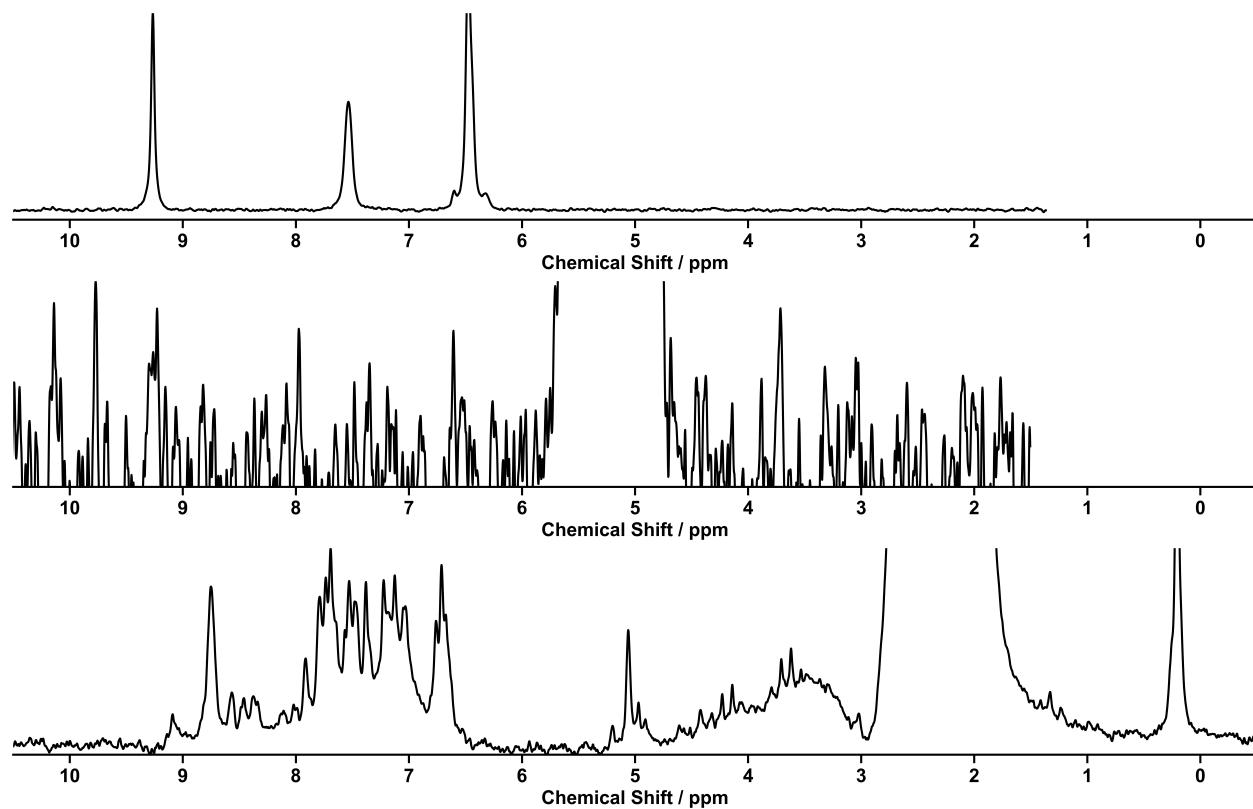
## Reaction 82



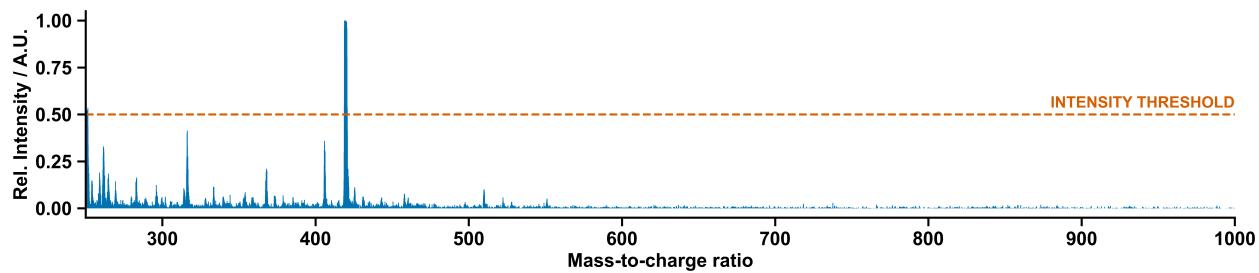
Scheme 67: Self-assembly of components **3**, **20**, with Yttrium(III) in a 3.0:1.5:1.0 molar ratio in  $\text{CH}_3\text{CN}$  at 60°C for 40h. These are the reagents (starting materials) for reaction 82.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: Oligomers formed.	
	Human MS Decision: Failed	MS Spectra Category: Reaction occurred, unknown product.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	NMR Criteria 2: N/A
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 0
		MS Criteria 3: Pass	Number of counter-ions found: 0

Decision Table 67: Human labeled and Decision maker labeled outcomes for the  $^1\text{H}$  NMR spectroscopy and UPLC-MS spectrometry of reaction 82. Decision motivations are also given.

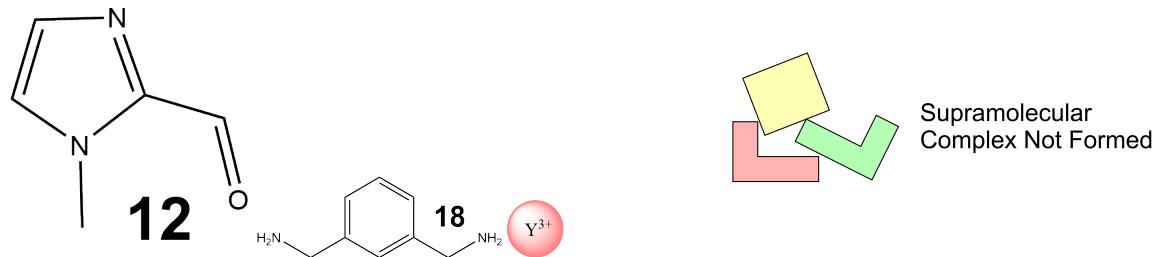


NMR Spectra 67: The stacked  $^1\text{H}$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 82.



MS Spectra 67: The ULPC-MS spectra of reaction 82. The intensity threshold is also shown.

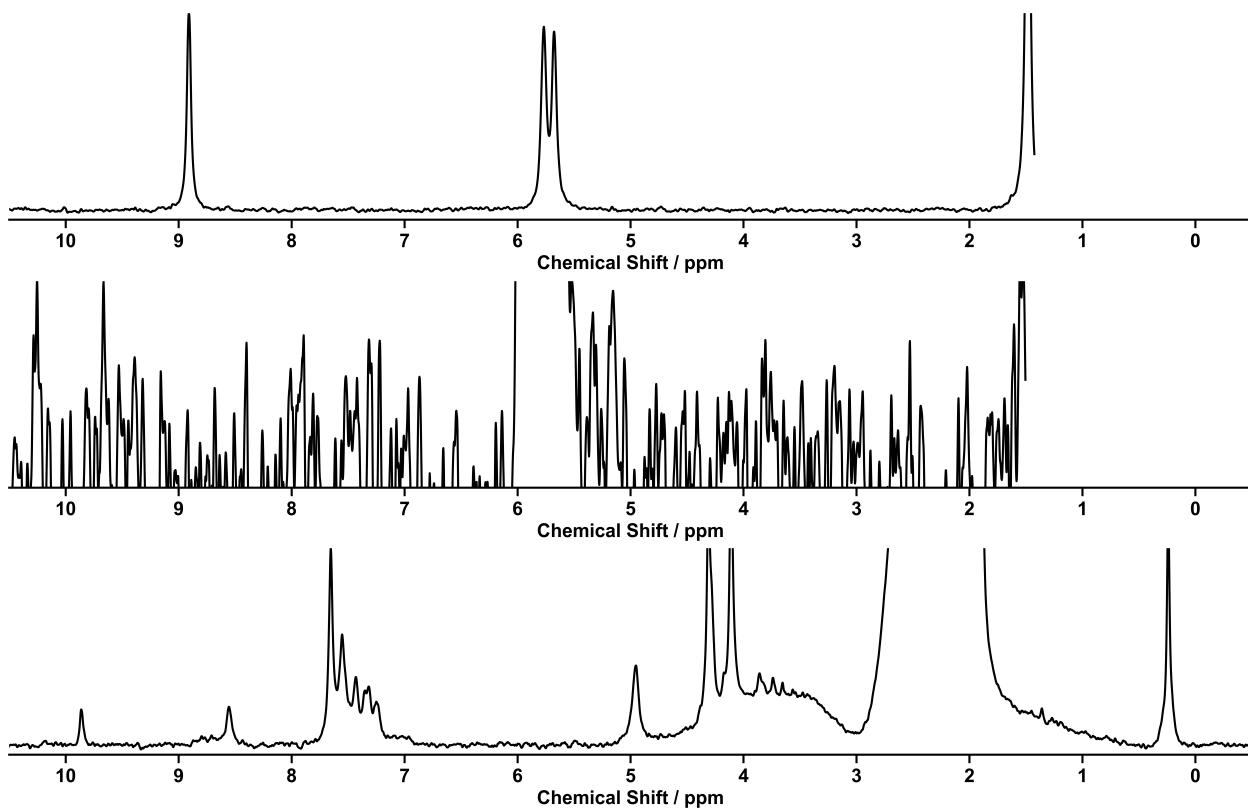
## Reaction 83



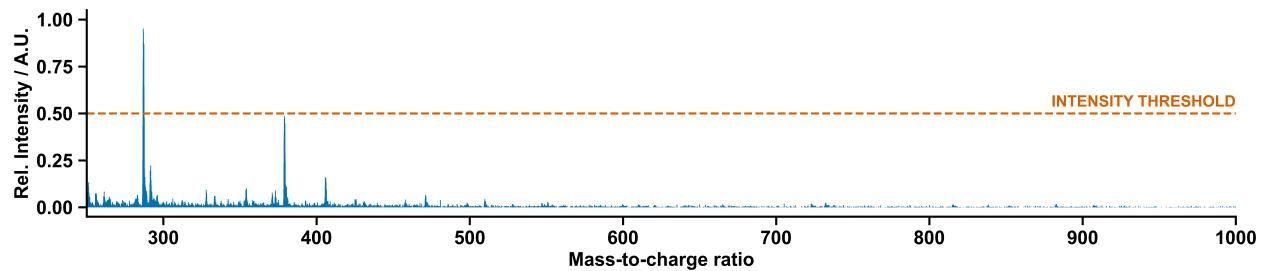
Scheme 68: Self-assembly of components 12, 18, with Yttrium(III) in a 3.0:1.5:1.0 molar ratio in CH<sub>3</sub>CN at 60°C for 40h. These are the reagents (starting materials) for reaction 83.

Human Reaction Decision: Failed	Human NMR Decision: Pass	NMR Spectra Category: Single discrete species formed.	
	Human MS Decision: Failed	MS Spectra Category: Reaction occurred, unknown product.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	NMR Criteria 2: N/A
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 2
		MS Criteria 3: Pass	Number of counter-ions found: 1

Decision Table 68: Human labeled and Decision maker labeled outcomes for the <sup>1</sup>H NMR spectroscopy and ULPC-MS spectrometry of reaction 83. Decision motivations are also given.

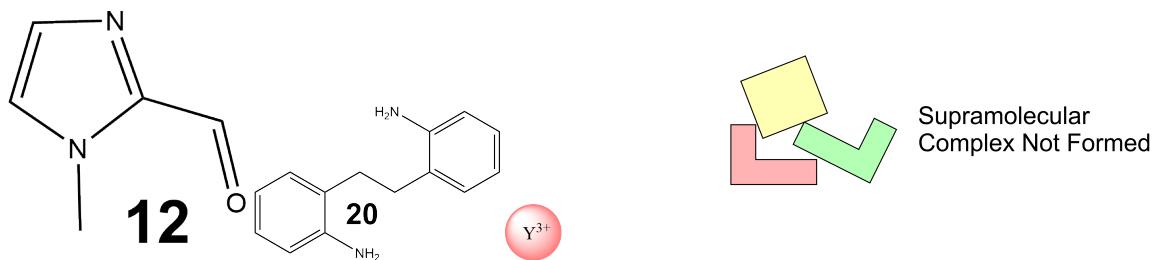


NMR Spectra 68: The stacked  $^1\text{H}$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 83.



MS Spectra 68: The ULPC-MS spectra of reaction 83. The intensity threshold is also shown.

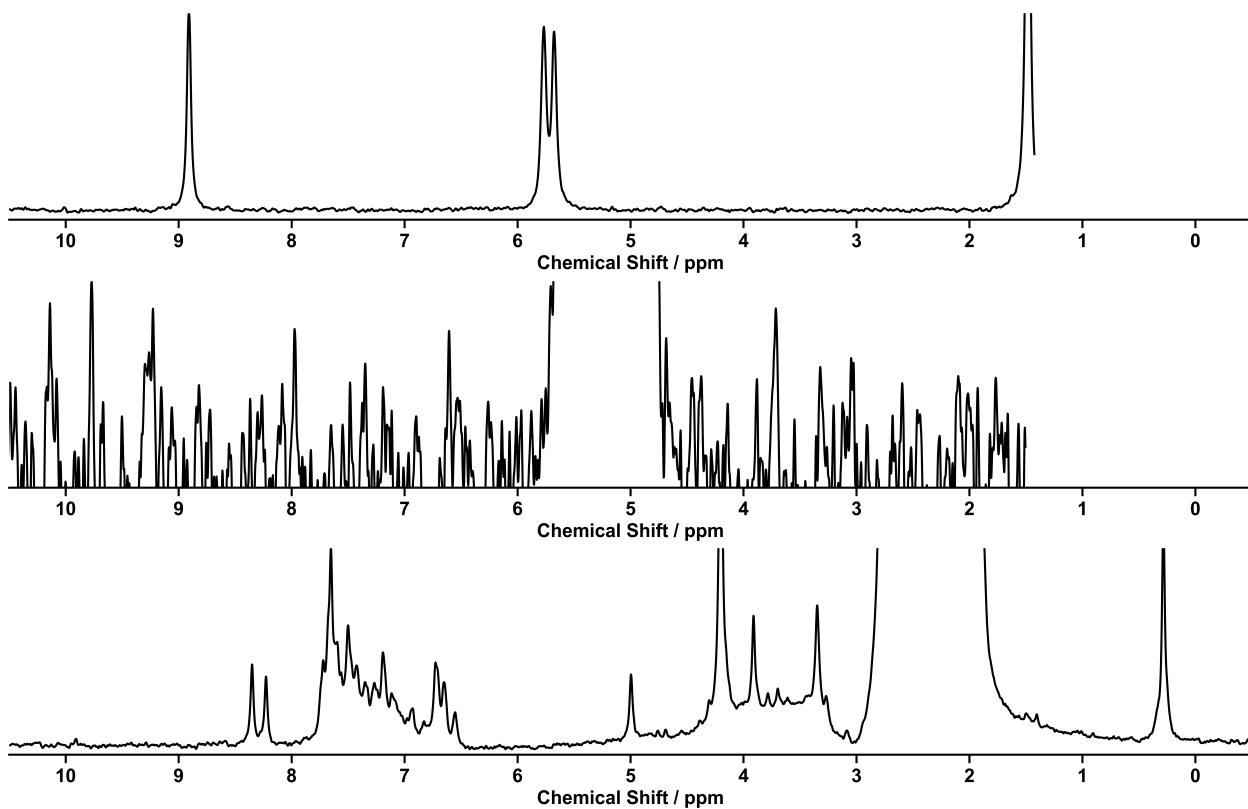
## Reaction 84



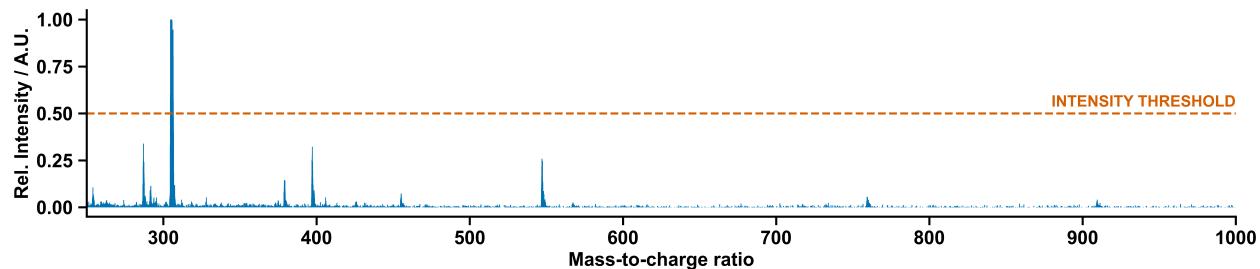
Scheme 69: Self-assembly of components 12, 20, with Yttrium(III) in a 3.0:1.5:1.0 molar ratio in  $\text{CH}_3\text{CN}$  at 60°C for 40h. These are the reagents (starting materials) for reaction 84.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: Oligomers formed.	
	Human MS Decision: Failed	MS Spectra Category: Reaction occurred, unknown product.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	
	Decision Maker MS Decision: Pass	NMR Criteria 2: N/A	Number of predicted peaks found in MS spectra with appropriate intensity: 0
	MS Criteria 1 and 2: Pass	MS Criteria 3: Pass	Number of counter-ions found: 0

Decision Table 69: Human labeled and Decsision maker labeled outcomes for the  $^1\text{H}$  NMR spectroscopy and UPLC-MS spectrometry of reaction 84. Decision motivations are also given.



NMR Spectra 69: The stacked <sup>1</sup>H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 84.



MS Spectra 69: The ULPC-MS spectra of reaction 84. The intensity threshold is also shown.

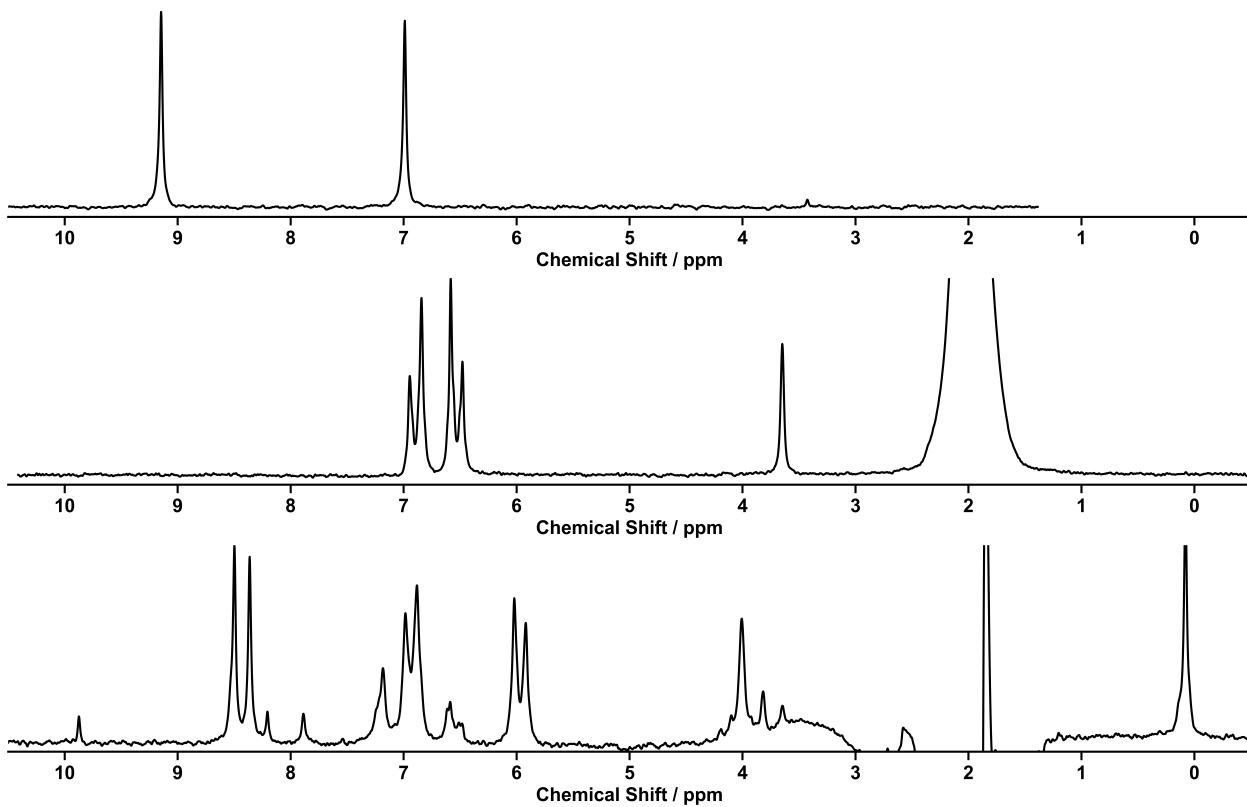
## Reaction 85



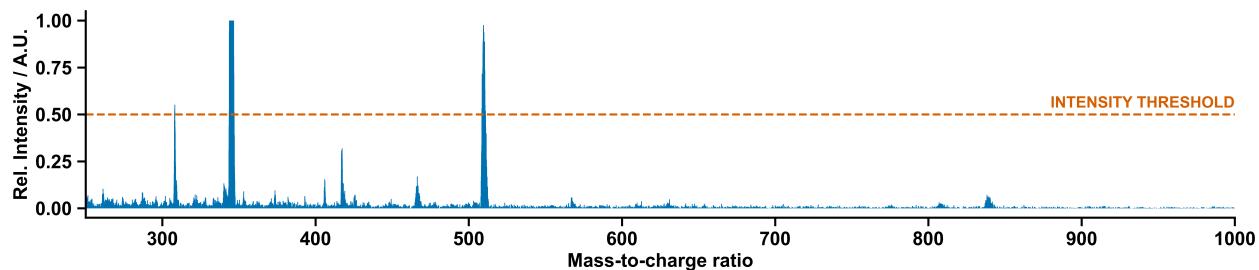
Scheme 70: Self-assembly of components 1, 17, with Zinc(II) in a 3.0:1.5:1.0 molar ratio in  $CH_3CN$  at 60°C for 40h. These are the reagents (starting materials) for reaction 85.

Human Reaction Decision: Failed	Human NMR Decision: Pass	NMR Spectra Category: Single discrete species formed.
	Human MS Decision: Failed	MS Spectra Category: Reaction occurred, unknown product.
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A
		NMR Criteria 2: N/A
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass
		Number of predicted peaks found in MS spectra with appropriate intensity: 1
	MS Criteria 3: Pass	Number of counter-ions found: 1

Decision Table 70: Human labeled and Decsision maker labeled outcomes for the  $^1\text{H}$  NMR spectroscopy and ULPC-MS spectrometry of reaction 85. Decision motivations are also given.



NMR Spectra 70: The stacked  $^1\text{H}$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 85.



MS Spectra 70: The ULPC-MS spectra of reaction 85. The intensity threshold is also shown.

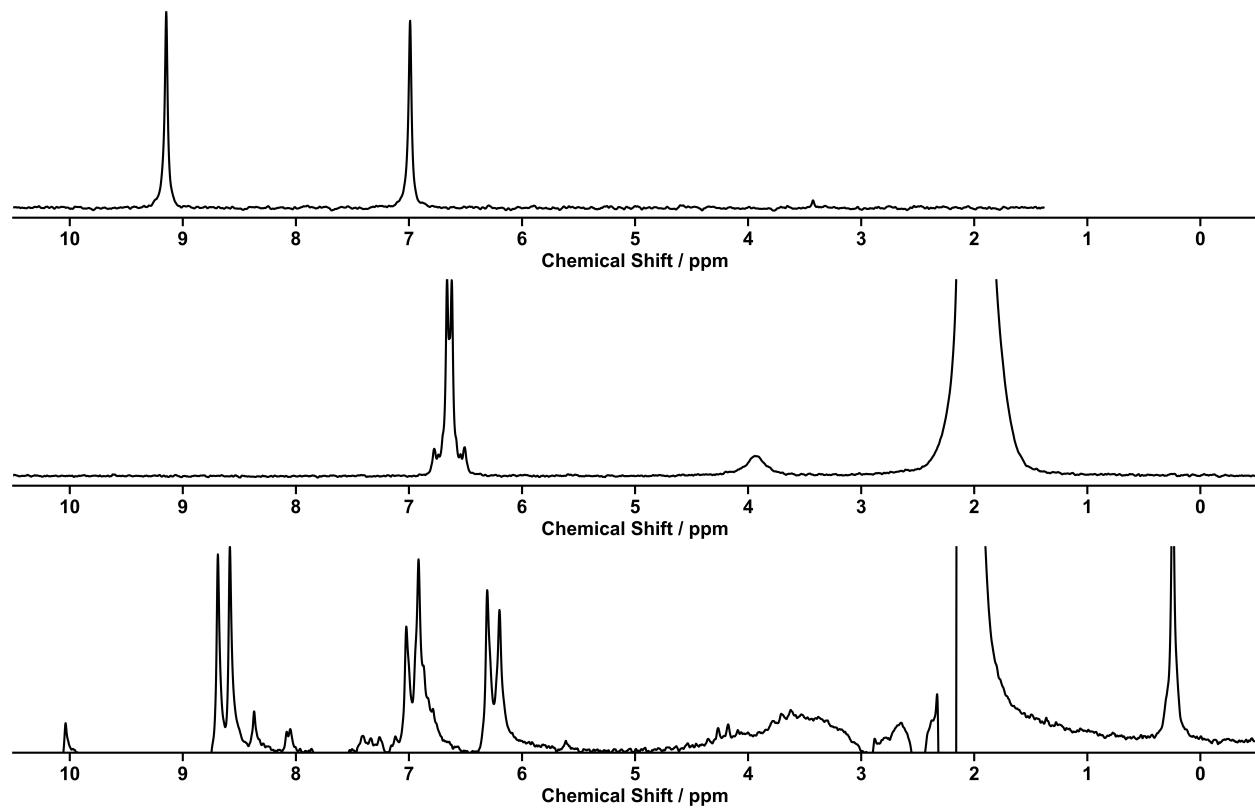
## Reaction 87



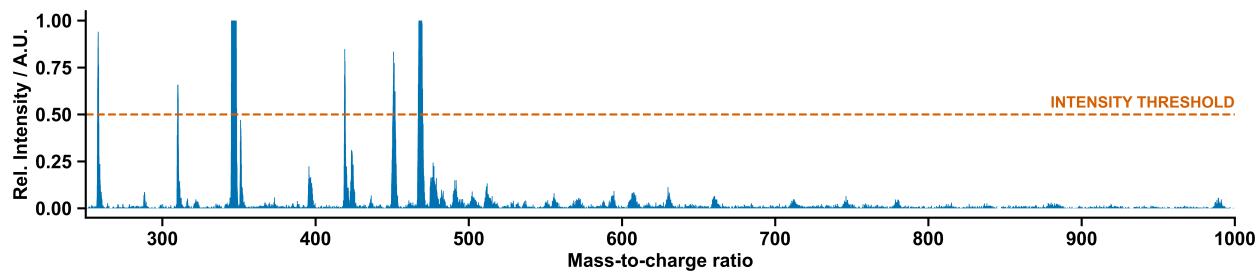
Scheme 71: Self-assembly of components 1, 15, with Zinc(II) in a 3.0:1.5:1.0 molar ratio in  $CH_3CN$  at  $60^\circ C$  for 40h. These are the reagents (starting materials) for reaction 87.

Human Reaction Decision: Failed	Human NMR Decision: Pass	NMR Spectra Category: Single discrete species formed.	
	Human MS Decision: Failed	MS Spectra Category: Reaction occurred, unknown product.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	NMR Criteria 2: N/A
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 2
		MS Criteria 3: Pass	Number of counter-ions found: 2

Decision Table 71: Human labeled and Decision maker labeled outcomes for the  $^1H$  NMR spectroscopy and UPLC-MS spectrometry of reaction 87. Decision motivations are also given.

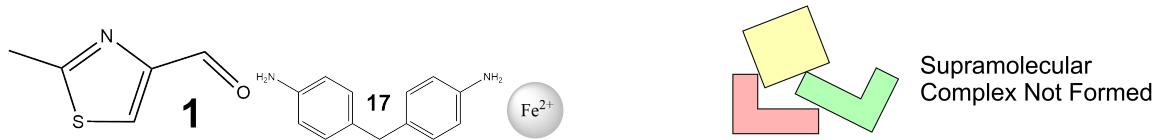


NMR Spectra 71: The stacked  $^1H$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 87.



MS Spectra 71: The ULPC-MS spectra of reaction 87. The intensity threshold is also shown.

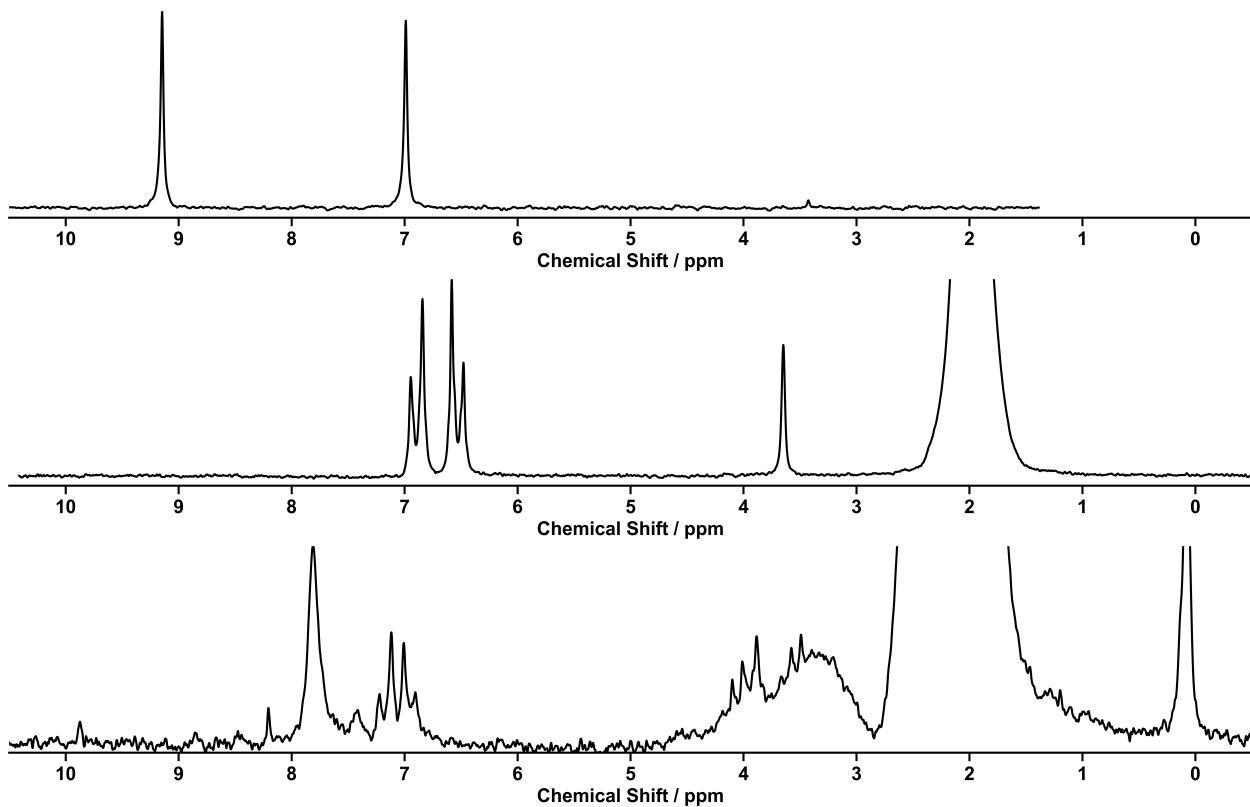
## Reaction 88



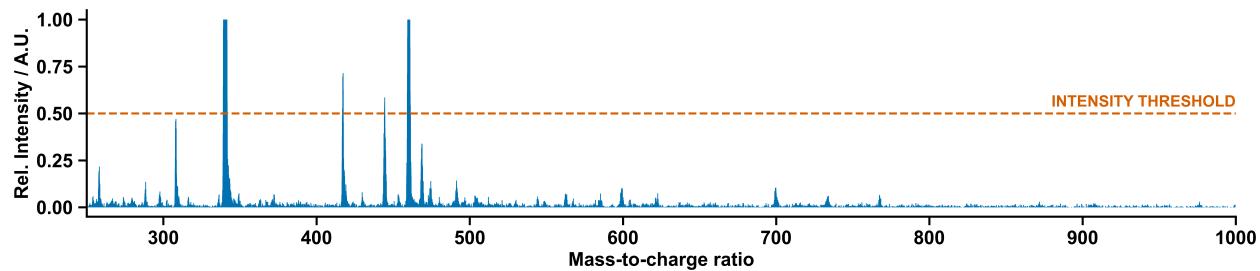
Scheme 72: Self-assembly of components **1**, **17**, with Iron(II) in a 3.0:1.5:1.0 molar ratio in  $\text{CH}_3\text{CN}$  at  $60^\circ\text{C}$  for 40h. These are the reagents (starting materials) for reaction 88.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: Paramagnetic species formed.	
	Human MS Decision: Pass	MS Spectra Category: Reaction occurred, supramolecular product.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	NMR Criteria 2: N/A
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 5
		MS Criteria 3: Pass	Number of counter-ions found: 3

Decision Table 72: Human labeled and Decision maker labeled outcomes for the  $^1\text{H}$  NMR spectroscopy and ULPC-MS spectrometry of reaction 88. Decision motivations are also given.

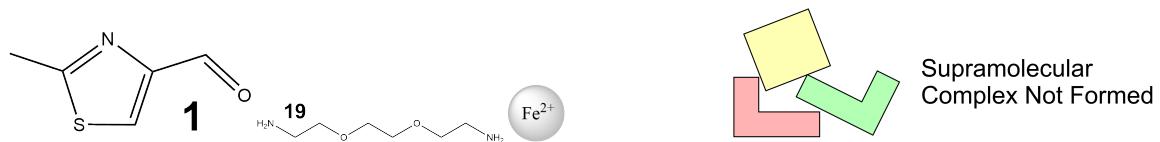


NMR Spectra 72: The stacked <sup>1</sup>H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 88.



MS Spectra 72: The ULPC-MS spectra of reaction 88. The intensity threshold is also shown.

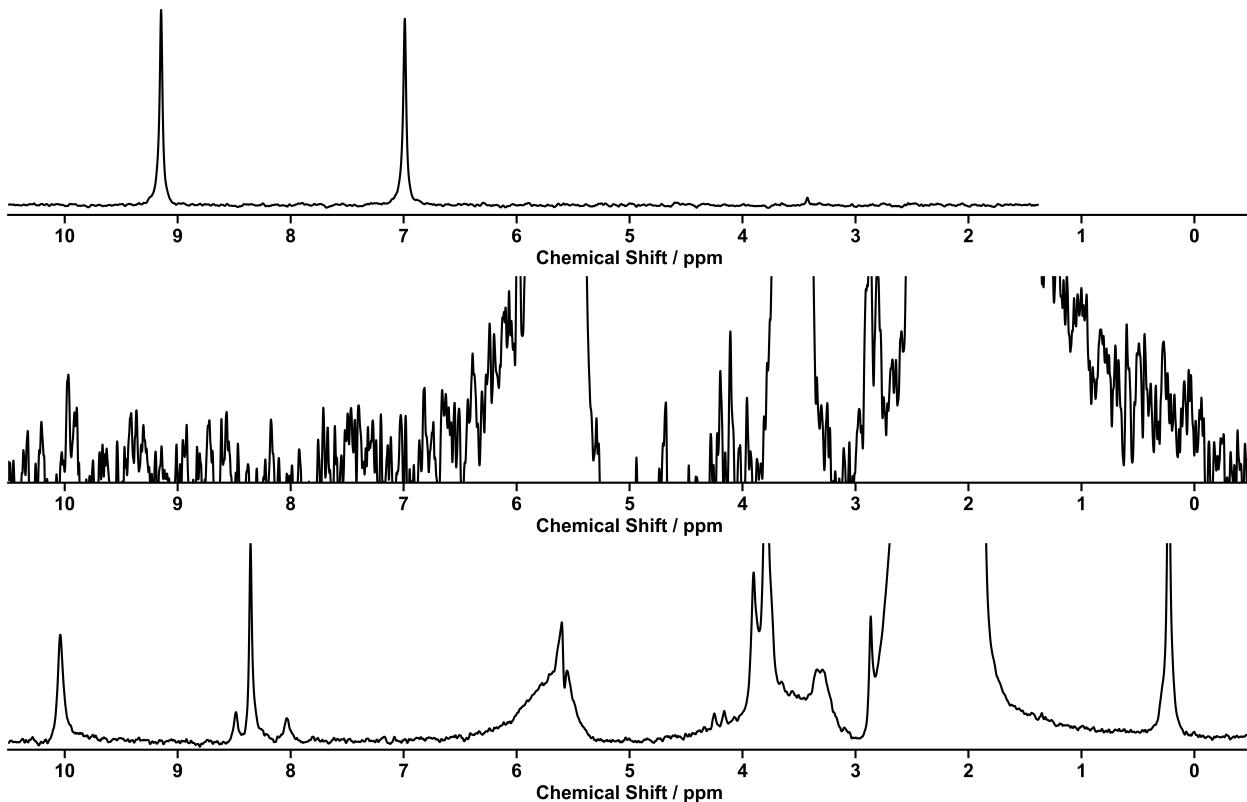
## Reaction 89



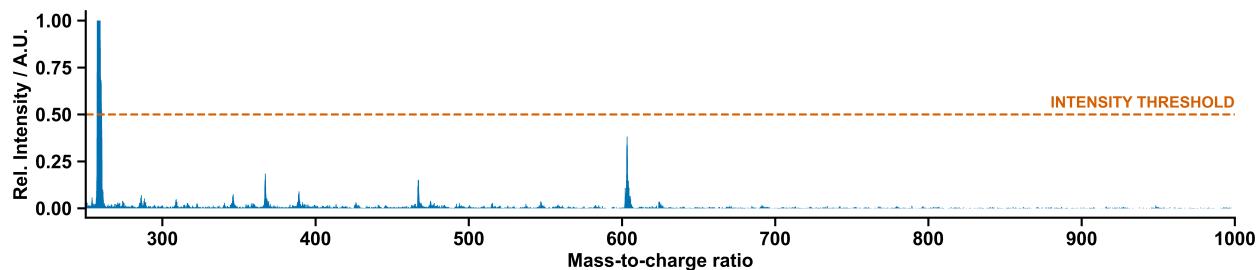
Scheme 73: Self-assembly of components 1, 19, with Iron(II) in a 3.0:1.5:1.0 molar ratio in  $\text{CH}_3\text{CN}$  at 60°C for 40h. These are the reagents (starting materials) for reaction 89.

Human Reaction Decision: Failed	Human NMR Decision: Pass	NMR Spectra Category: Single discrete species formed.
	Human MS Decision: Failed	MS Spectra Category: Reaction occurred, unknown product.
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A
		NMR Criteria 2: N/A
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass
		Number of predicted peaks found in MS spectra with appropriate intensity: 0
	MS Criteria 3: Pass	Number of counter-ions found: 0

Decision Table 73: Human labeled and Decsision maker labeled outcomes for the  $^1\text{H}$  NMR spectroscopy and ULPC-MS spectrometry of reaction 89. Decision motivations are also given.

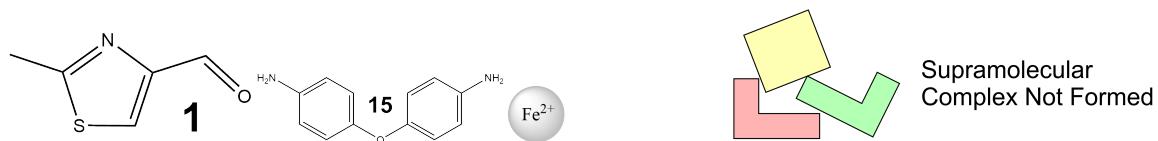


NMR Spectra 73: The stacked  $^1\text{H}$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 89.



MS Spectra 73: The ULPC-MS spectra of reaction 89. The intensity threshold is also shown.

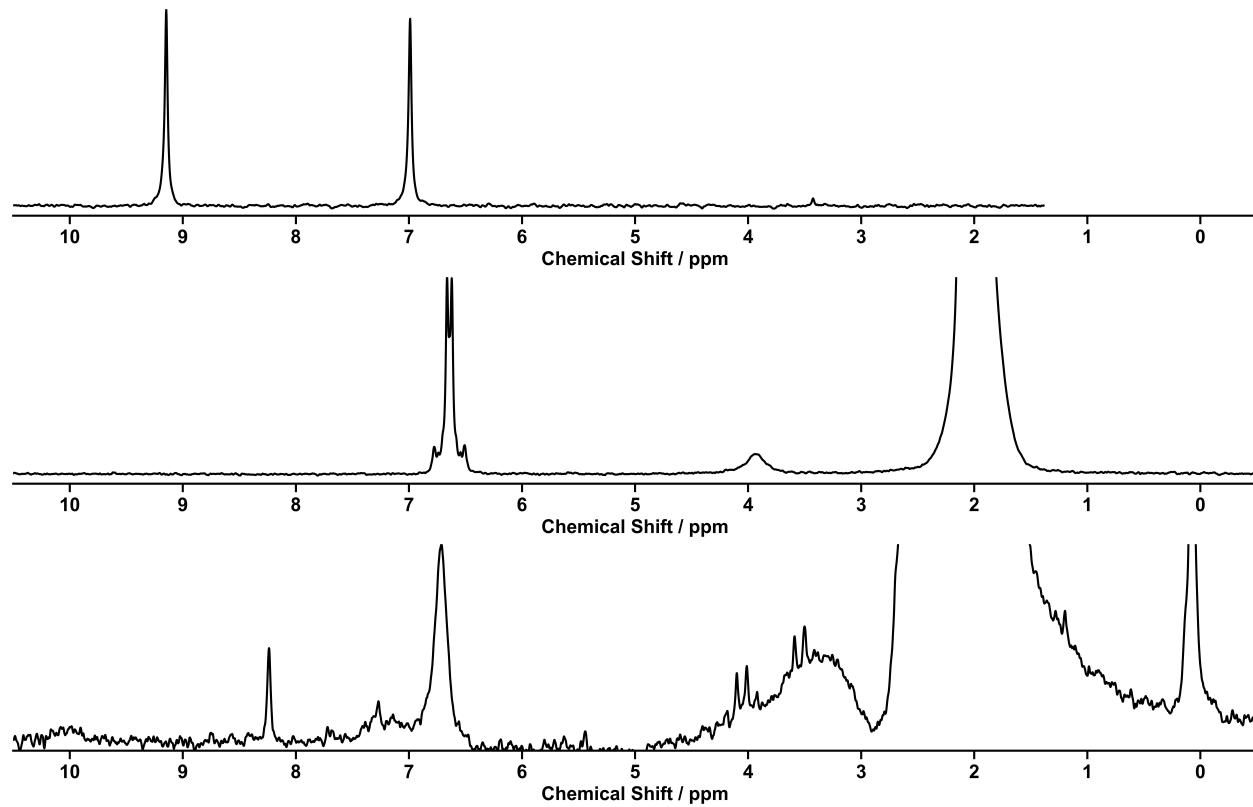
## Reaction 90



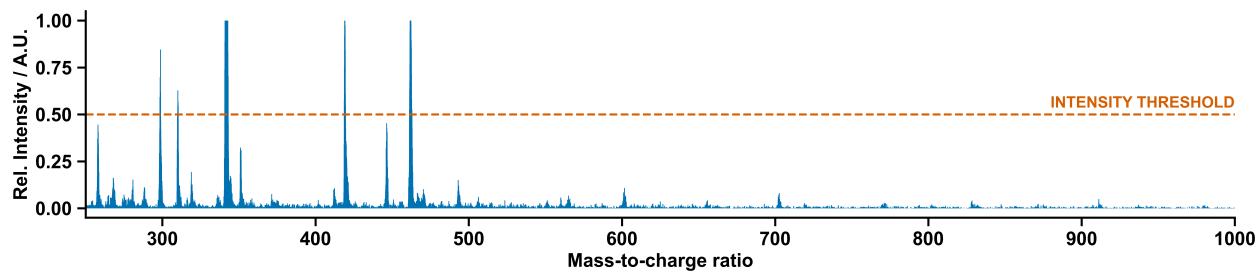
Scheme 74: Self-assembly of components 1, 15, with Iron(II) in a 3.0:1.5:1.0 molar ratio in  $\text{CH}_3\text{CN}$  at 60°C for 40h. These are the reagents (starting materials) for reaction 90.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: Paramagnetic species formed.	
	Human MS Decision: Pass	MS Spectra Category: Reaction occurred, supramolecular product.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	NMR Criteria 2: N/A
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 5
	MS Criteria 3: Pass	Number of counter-ions found: 3	

Decision Table 74: Human labeled and Decision maker labeled outcomes for the  $^1\text{H}$  NMR spectroscopy and UPLC-MS spectrometry of reaction 90. Decision motivations are also given.

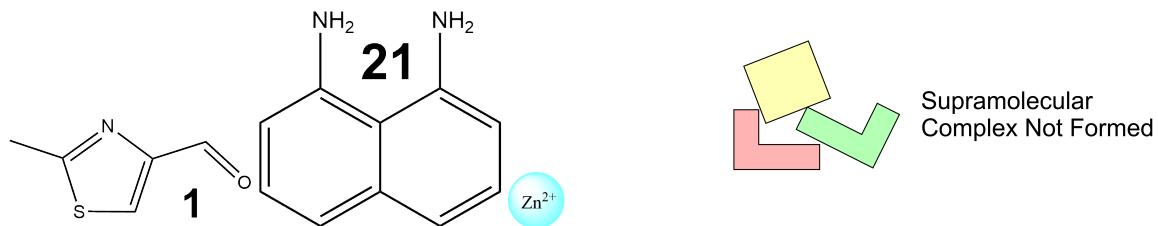


NMR Spectra 74: The stacked  $^1\text{H}$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 90.



MS Spectra 74: The ULPC-MS spectra of reaction 90. The intensity threshold is also shown.

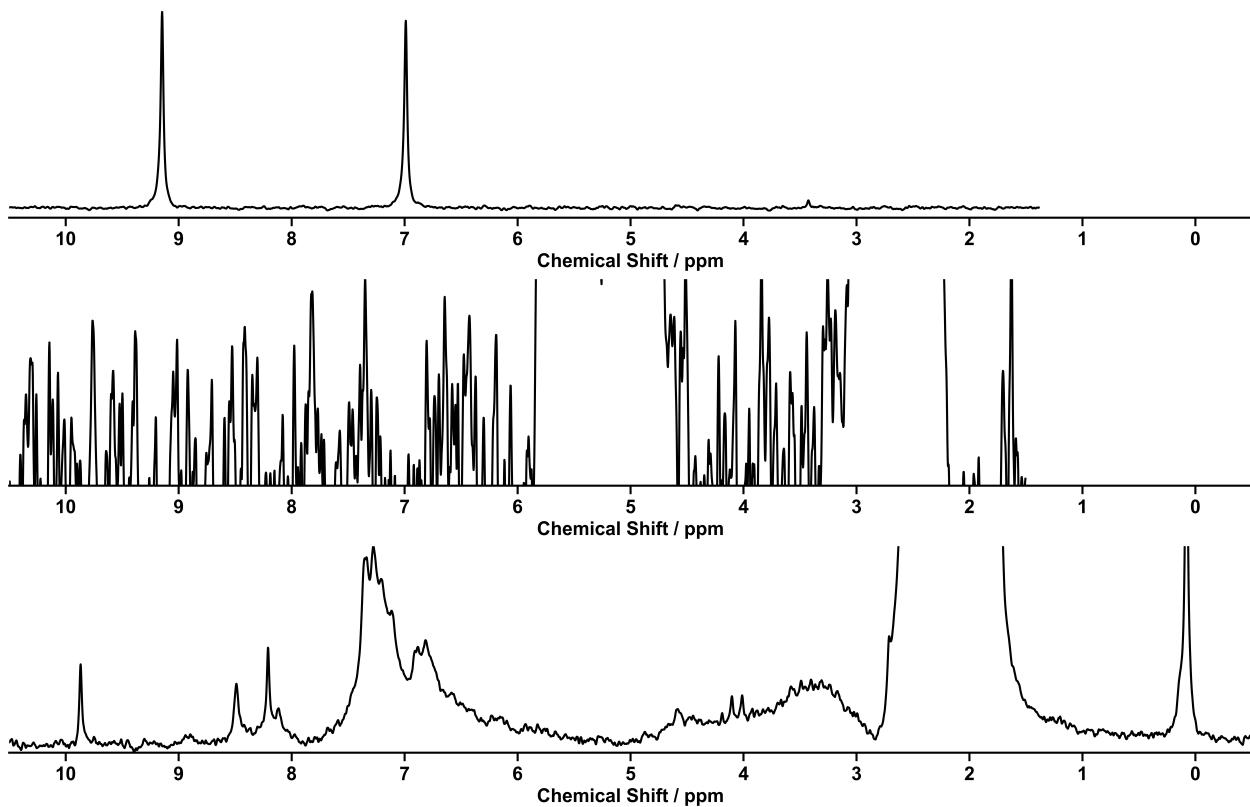
## Reaction 91



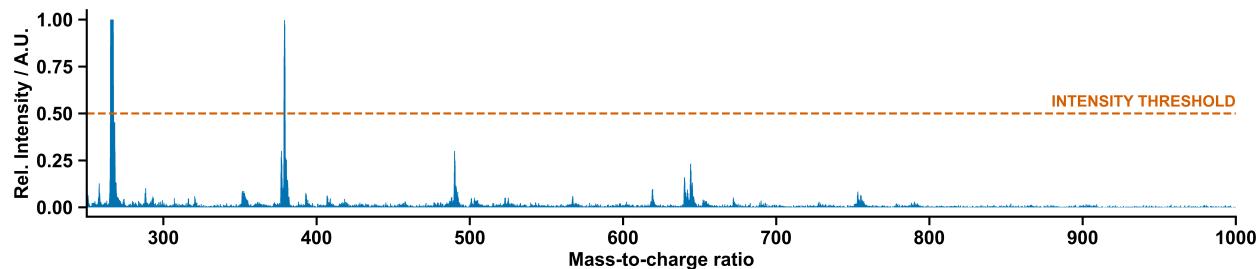
Scheme 75: Self-assembly of components 1, 21, with Zinc(II) in a 3.0:1.5:1.0 molar ratio in CH<sub>3</sub>CN at 60°C for 40h. These are the reagents (starting materials) for reaction 91.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: Oligomers formed.	
	Human MS Decision: Failed	MS Spectra Category: Reaction occurred, unknown product.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	NMR Criteria 2: N/A
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 0
		MS Criteria 3: Pass	Number of counter-ions found: 0

Decision Table 75: Human labeled and Decsision maker labeled outcomes for the <sup>1</sup>H NMR spectroscopy and ULPC-MS spectrometry of reaction 91. Decision motivations are also given.



NMR Spectra 75: The stacked <sup>1</sup>H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 91.



MS Spectra 75: The ULPC-MS spectra of reaction 91. The intensity threshold is also shown.

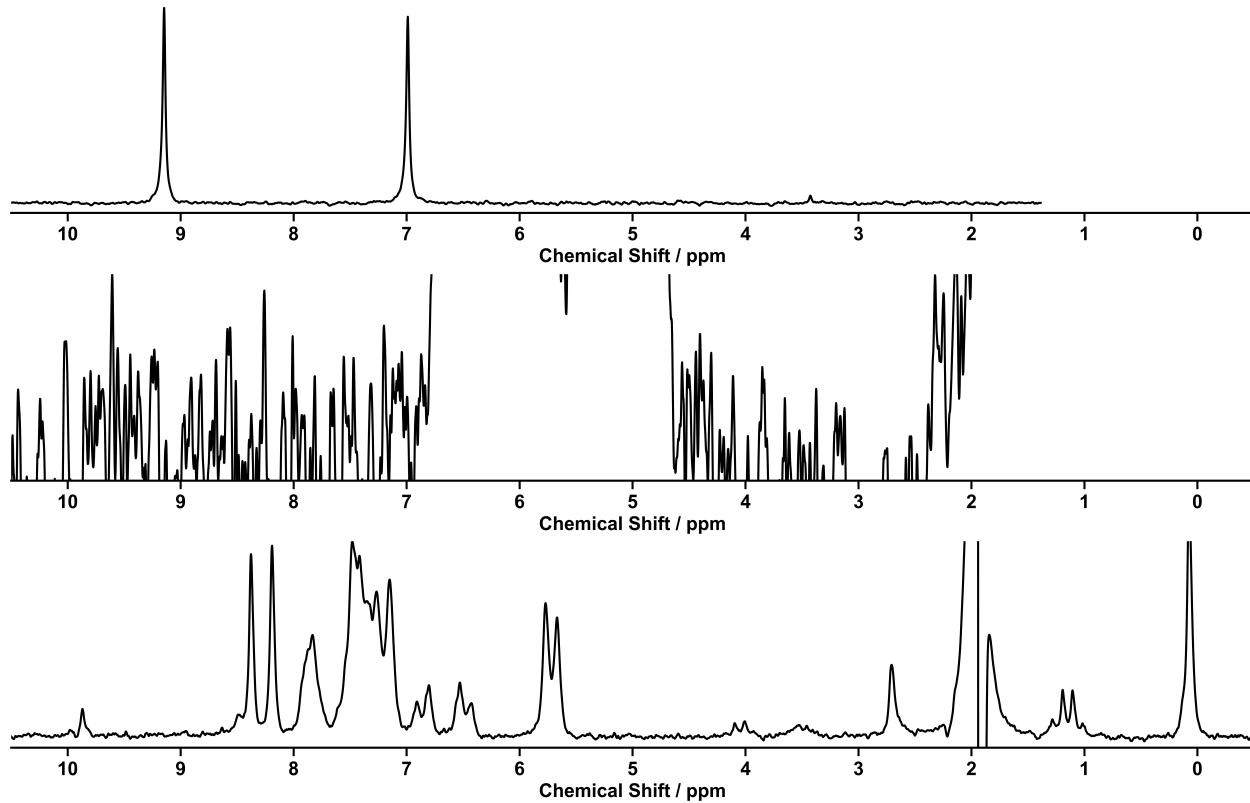
## Reaction 92



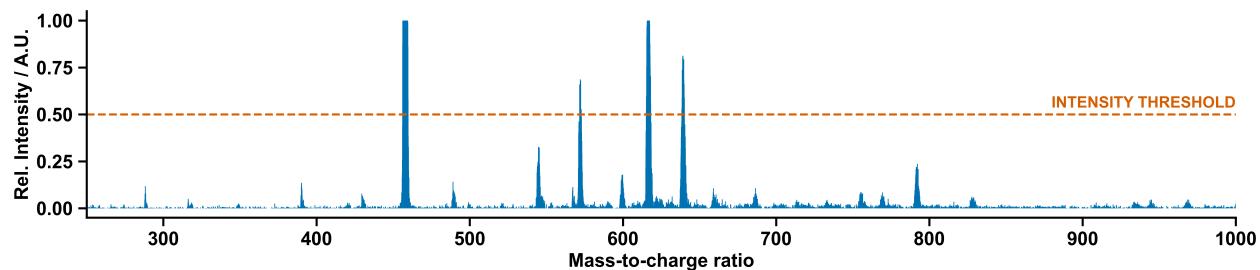
Scheme 76: Self-assembly of components 1, 13, with Zinc(II) in a 3.0:1.5:1.0 molar ratio in  $CH_3CN$  at 60°C for 40h. These are the reagents (starting materials) for reaction 92.

Human Reaction Decision: Pass	Human NMR Decision: Pass	NMR Spectra Category: Single discrete species formed.	
	Human MS Decision: Pass	MS Spectra Category: Reaction occurred, supramolecular product.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	
		NMR Criteria 2: N/A	
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 4
	MS Criteria 3: Pass	Number of counter-ions found: 2	

Decision Table 76: Human labeled and Decsision maker labeled outcomes for the  $^1\text{H}$  NMR spectroscopy and ULPC-MS spectrometry of reaction 92. Decision motivations are also given.

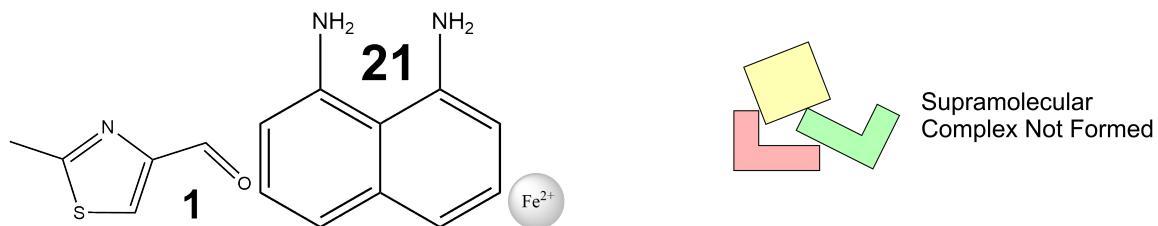


NMR Spectra 76: The stacked  $^1\text{H}$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 92.



MS Spectra 76: The ULPC-MS spectra of reaction 92. The intensity threshold is also shown.

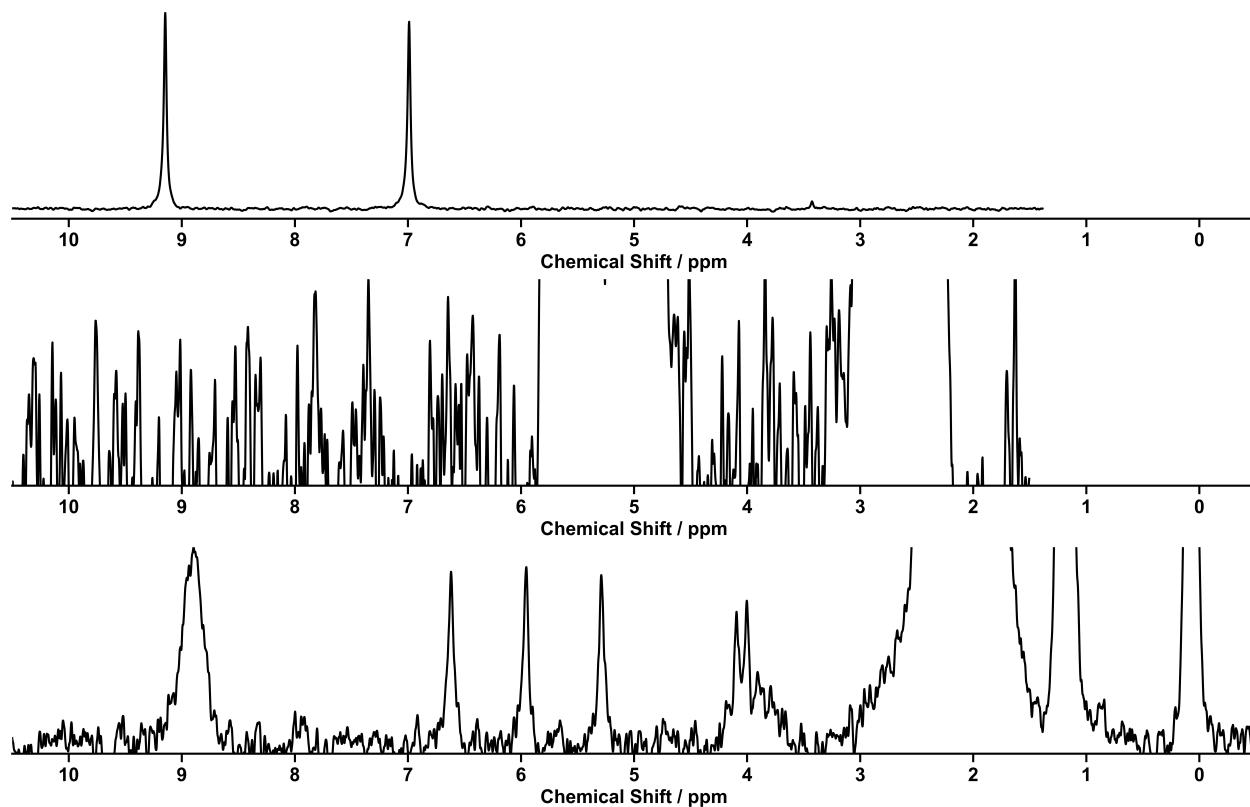
## Reaction 93



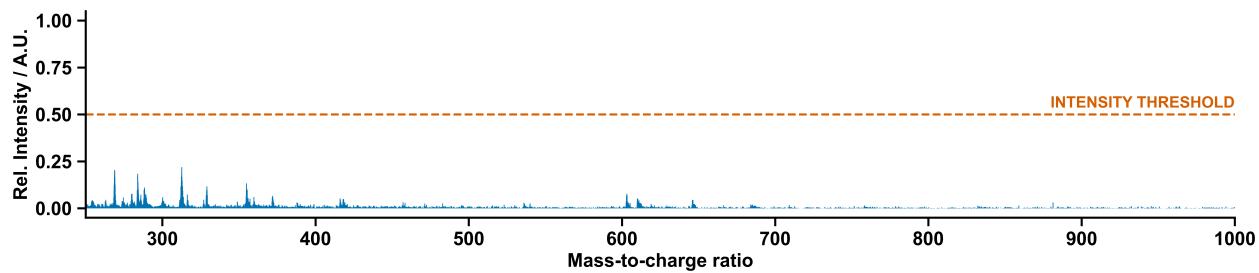
Scheme 77: Self-assembly of components 1, 21, with Iron(II) in a 3.0:1.5:1.0 molar ratio in CH<sub>3</sub>CN at 60°C for 40h. These are the reagents (starting materials) for reaction 93.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: No reaction occurred.	
	Human MS Decision: Failed	MS Spectra Category: Reaction failed.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	NMR Criteria 2: N/A
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 0
		MS Criteria 3: Pass	Number of counter-ions found: 0

Decision Table 77: Human labeled and Decsision maker labeled outcomes for the <sup>1</sup>H NMR spectroscopy and ULP-MS spectrometry of reaction 93. Decision motivations are also given.

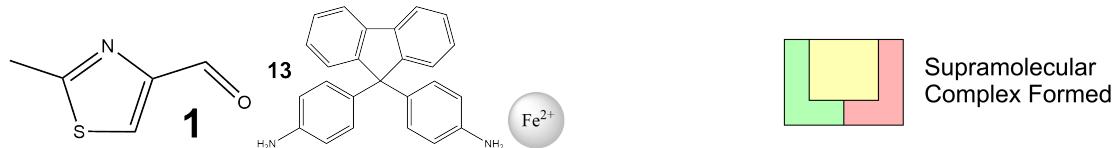


NMR Spectra 77: The stacked <sup>1</sup>H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 93.



MS Spectra 77: The ULPC-MS spectra of reaction 93. The intensity threshold is also shown.

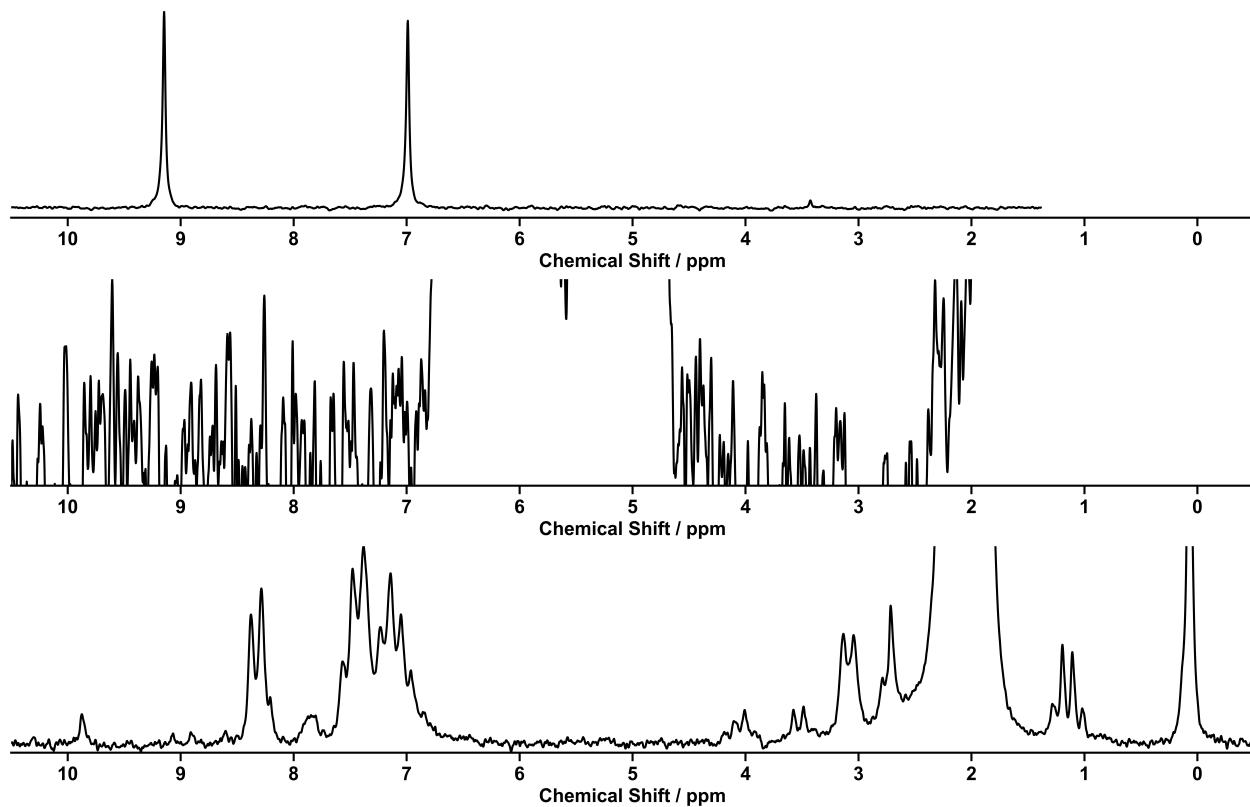
## Reaction 94



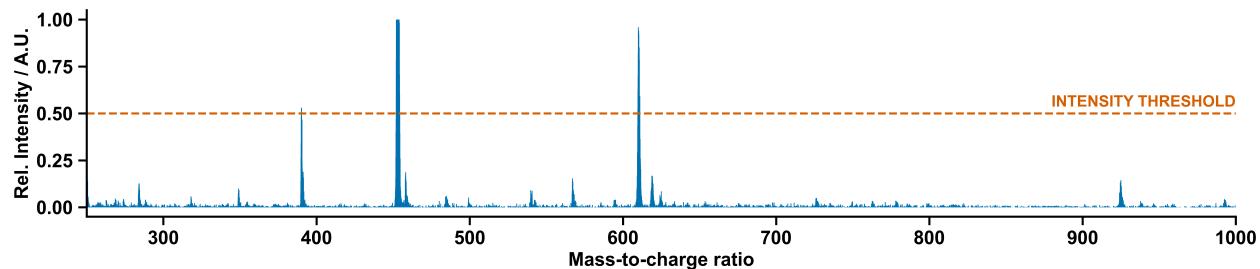
Scheme 78: Self-assembly of components 1, 13, with Iron(II) in a 3.0:1.5:1.0 molar ratio in CH<sub>3</sub>CN at 60°C for 40h. These are the reagents (starting materials) for reaction 94.

Human Reaction Decision: Pass	Human NMR Decision: Pass	NMR Spectra Category: Single discrete species formed.	
	Human MS Decision: Pass	MS Spectra Category: Reaction occurred, supramolecular product.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	
	Decision Maker MS Decision: Pass	NMR Criteria 2: N/A	MS Criteria 1 and 2: Pass
		Number of predicted peaks found in MS spectra with appropriate intensity: 5	Number of counter-ions found: 3
		MS Criteria 3: Pass	

Decision Table 78: Human labeled and Decision maker labeled outcomes for the <sup>1</sup>H NMR spectroscopy and ULPC-MS spectrometry of reaction 94. Decision motivations are also given.

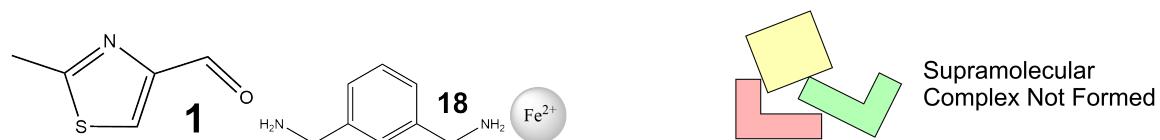


NMR Spectra 78: The stacked <sup>1</sup>H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 94.



MS Spectra 78: The ULPC-MS spectra of reaction 94. The intensity threshold is also shown.

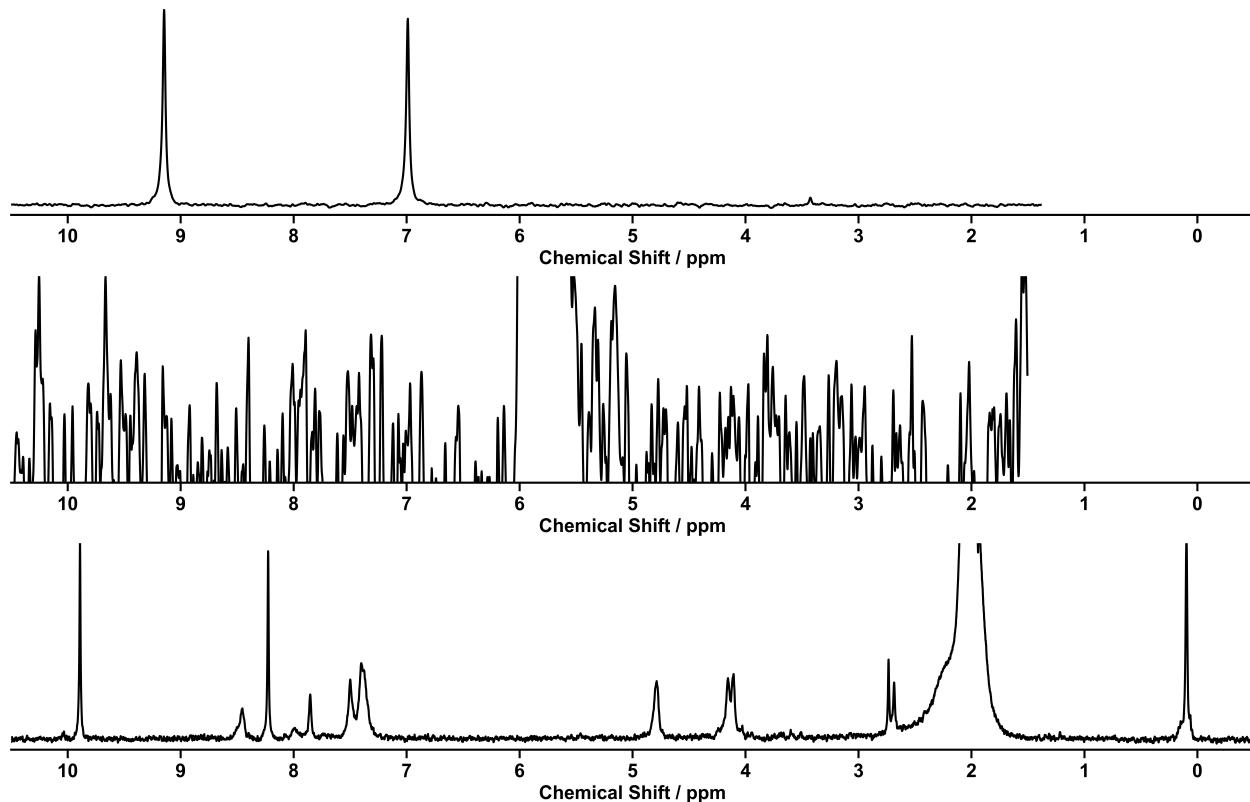
## Reaction 96



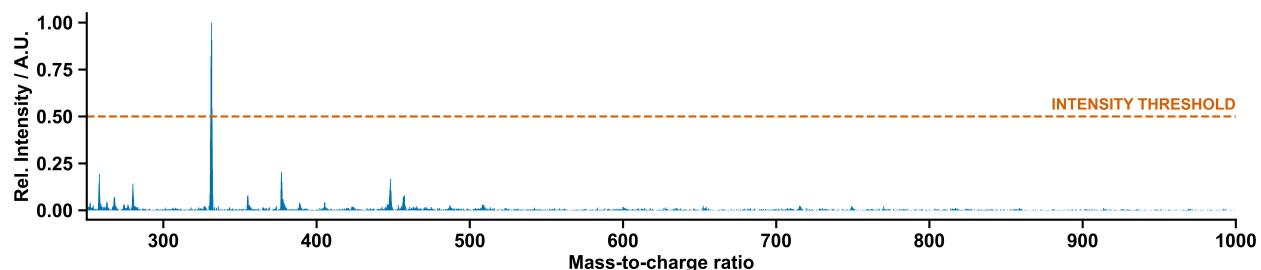
Scheme 79: Self-assembly of components **1**, **18**, with Iron(II) in a 3.0:1.5:1.0 molar ratio in  $\text{CH}_3\text{CN}$  at 60°C for 40h. These are the reagents (starting materials) for reaction 96.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: No reaction occurred.	
	Human MS Decision: Failed	MS Spectra Category: Reaction occurred, unknown product.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	
		NMR Criteria 2: N/A	
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 0
		MS Criteria 3: Pass	Number of counter-ions found: 0

Decision Table 79: Human labeled and Decsision maker labeled outcomes for the  $^1\text{H}$  NMR spectroscopy and UPLC-MS spectrometry of reaction 96. Decision motivations are also given.

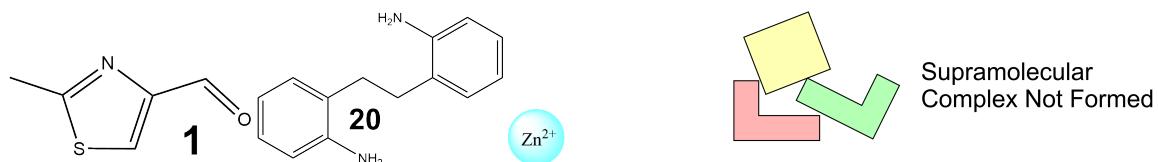


NMR Spectra 79: The stacked  $^1\text{H}$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 96.



MS Spectra 79: The ULPC-MS spectra of reaction 96. The intensity threshold is also shown.

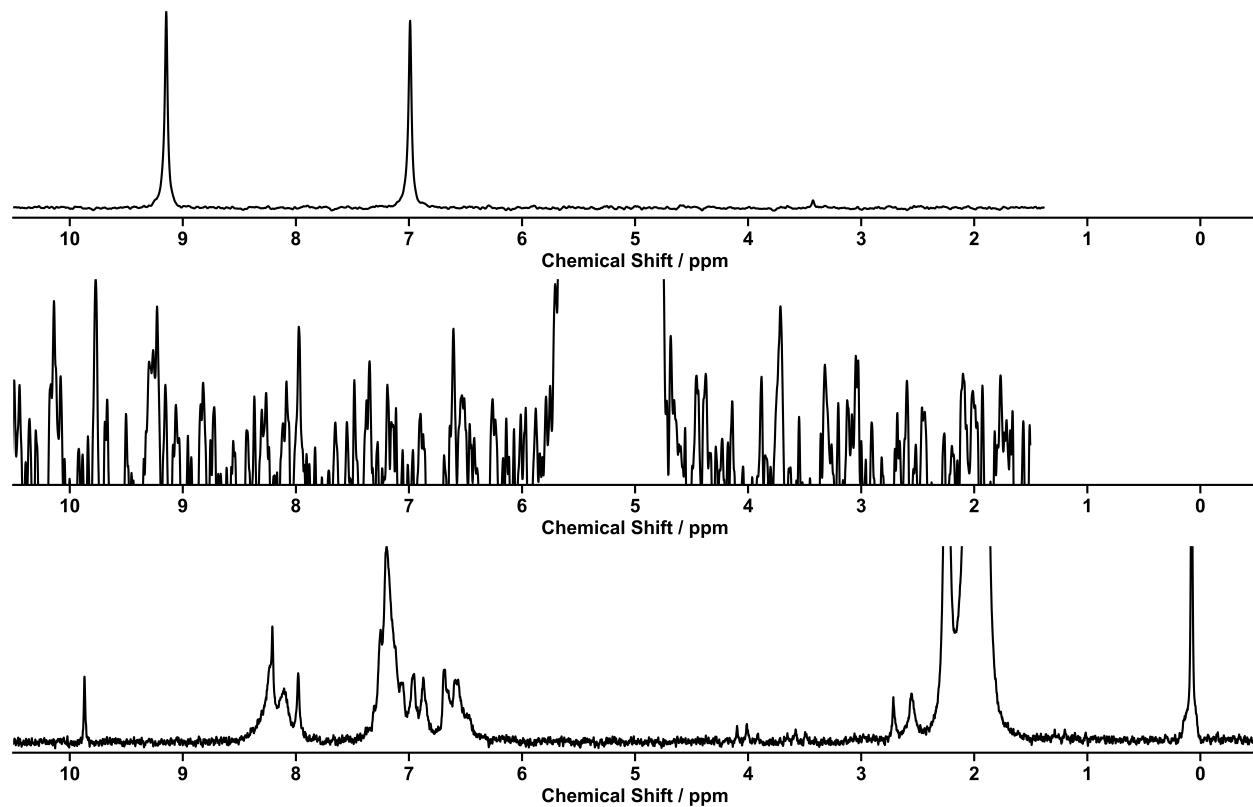
## Reaction 97



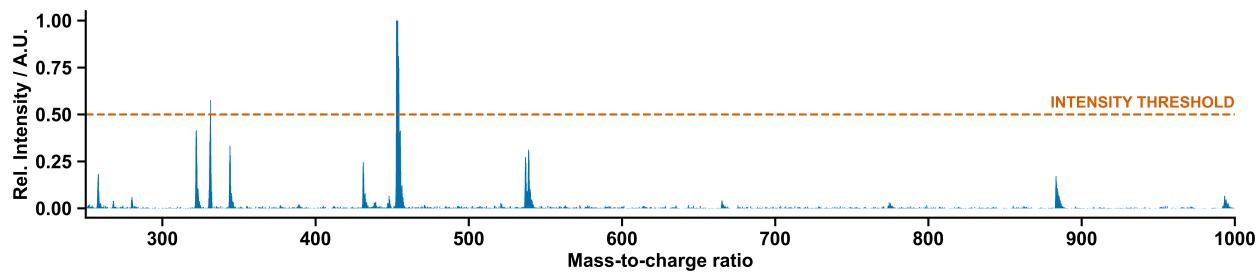
Scheme 80: Self-assembly of components **1**, **20**, with Zinc(II) in a 3.0:1.5:1.0 molar ratio in  $\text{CH}_3\text{CN}$  at  $60^\circ\text{C}$  for 40h. These are the reagents (starting materials) for reaction 97.

Human Reaction Decision: Failed	Human NMR Decision: Pass	NMR Spectra Category: Single discrete species formed.	
	Human MS Decision: Failed	MS Spectra Category: Reaction occurred, unknown product.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	NMR Criteria 2: N/A
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 0
		MS Criteria 3: Pass	Number of counter-ions found: 0

Decision Table 80: Human labeled and Decsision maker labeled outcomes for the  $^1\text{H}$  NMR spectroscopy and ULPC-MS spectrometry of reaction 97. Decision motivations are also given.

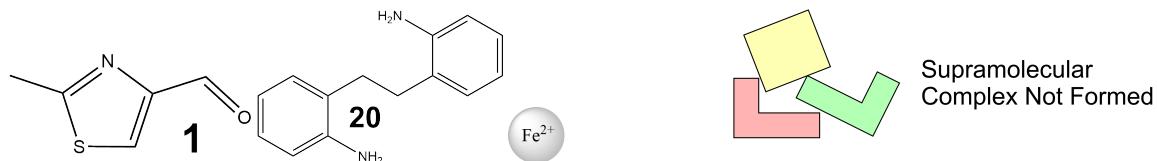


NMR Spectra 80: The stacked  $^1\text{H}$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 97.



MS Spectra 80: The ULPC-MS spectra of reaction 97. The intensity threshold is also shown.

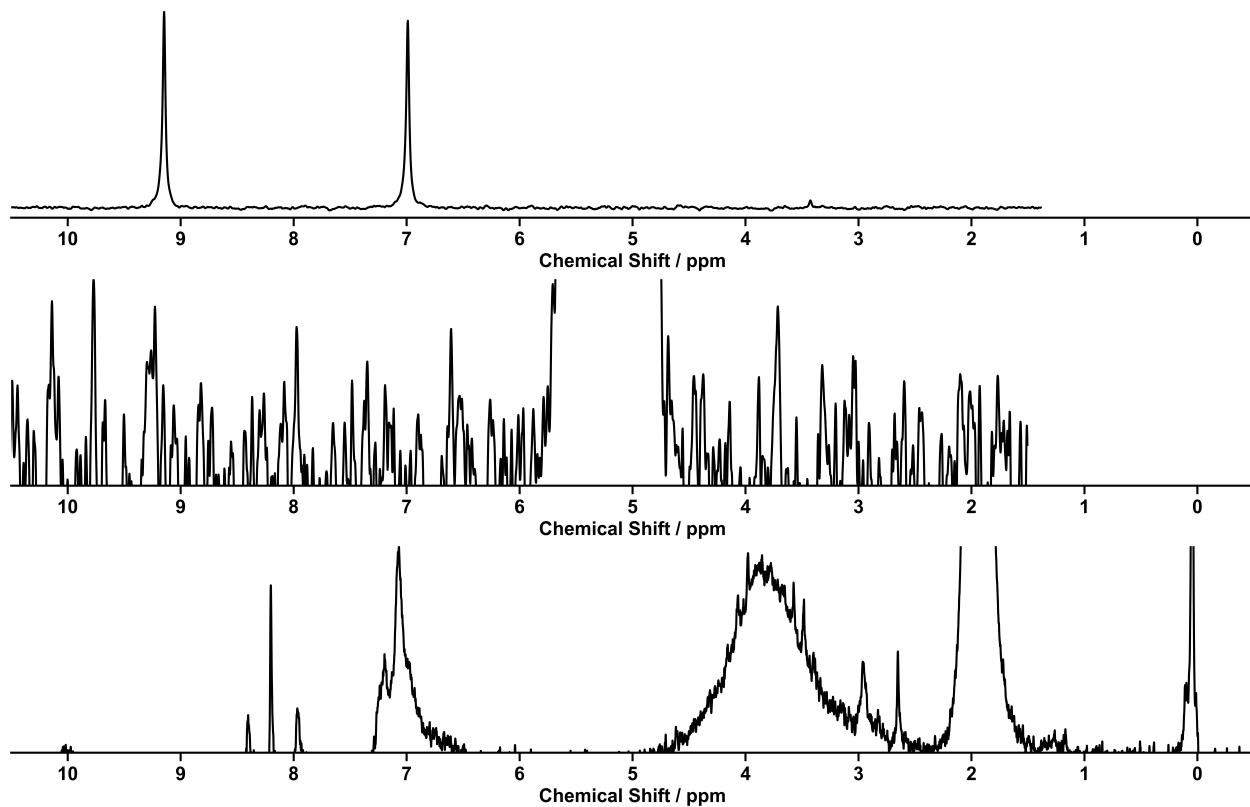
## Reaction 98



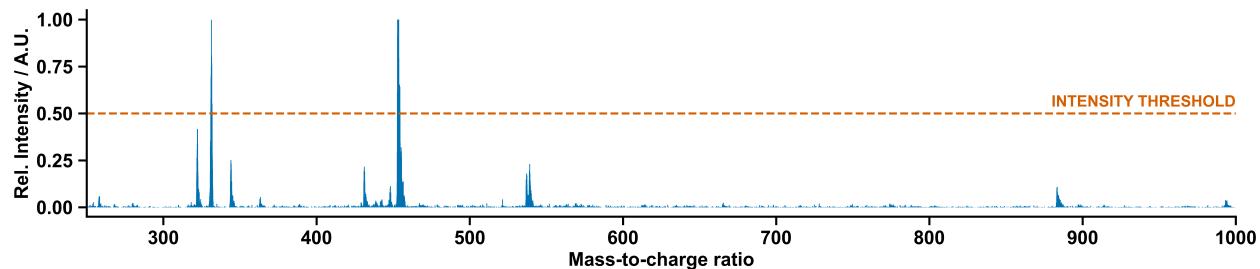
Scheme 81: Self-assembly of components 1, 20, with Iron(II) in a 3.0:1.5:1.0 molar ratio in CH<sub>3</sub>CN at 60°C for 40h. These are the reagents (starting materials) for reaction 98.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: Paramagnetic species formed.	
	Human MS Decision: Failed	MS Spectra Category: Reaction occurred, unknown product.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	NMR Criteria 2: N/A
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 0
		MS Criteria 3: Pass	Number of counter-ions found: 0

Decision Table 81: Human labeled and Decsision maker labeled outcomes for the <sup>1</sup>H NMR spectroscopy and ULPC-MS spectrometry of reaction 98. Decision motivations are also given.

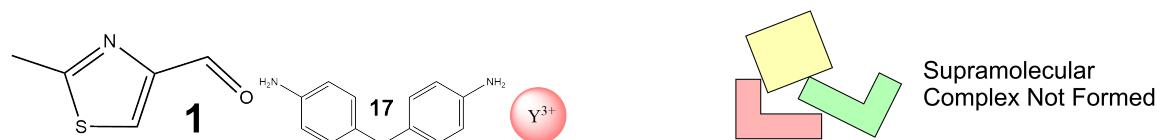


NMR Spectra 81: The stacked <sup>1</sup>H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 98.



MS Spectra 81: The ULPC-MS spectra of reaction 98. The intensity threshold is also shown.

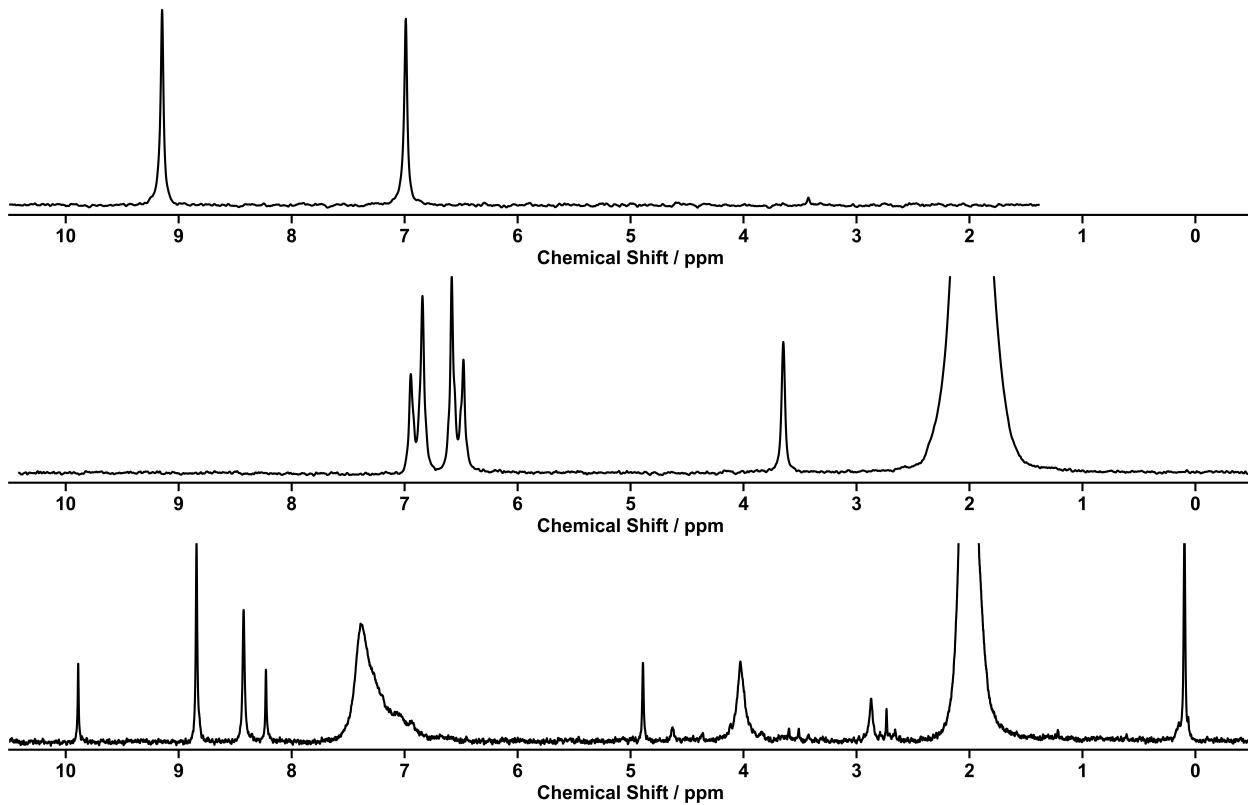
## Reaction 99



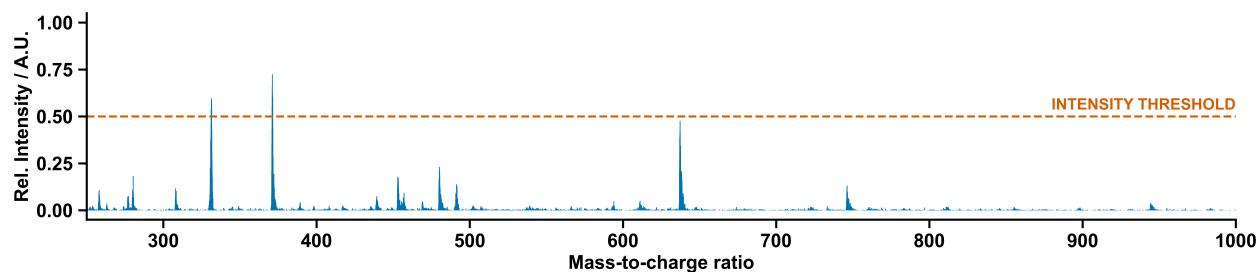
Scheme 82: Self-assembly of components 1, 17, with Yttrium(III) in a 3.0:1.5:1.0 molar ratio in CH<sub>3</sub>CN at 60°C for 40h. These are the reagents (starting materials) for reaction 99.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: No reaction occurred.	
	Human MS Decision: Failed	MS Spectra Category: Reaction failed.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	
		NMR Criteria 2: N/A	
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 0
	MS Criteria 3: Pass	Number of counter-ions found: 0	

Decision Table 82: Human labeled and Decsision maker labeled outcomes for the  $^1\text{H}$  NMR spectroscopy and ULPC-MS spectrometry of reaction 99. Decision motivations are also given.

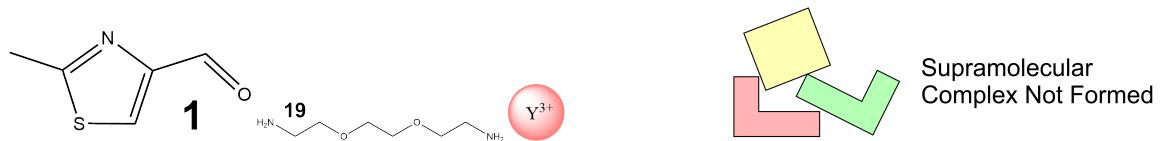


NMR Spectra 82: The stacked  $^1\text{H}$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 99.



MS Spectra 82: The ULPC-MS spectra of reaction 99. The intensity threshold is also shown.

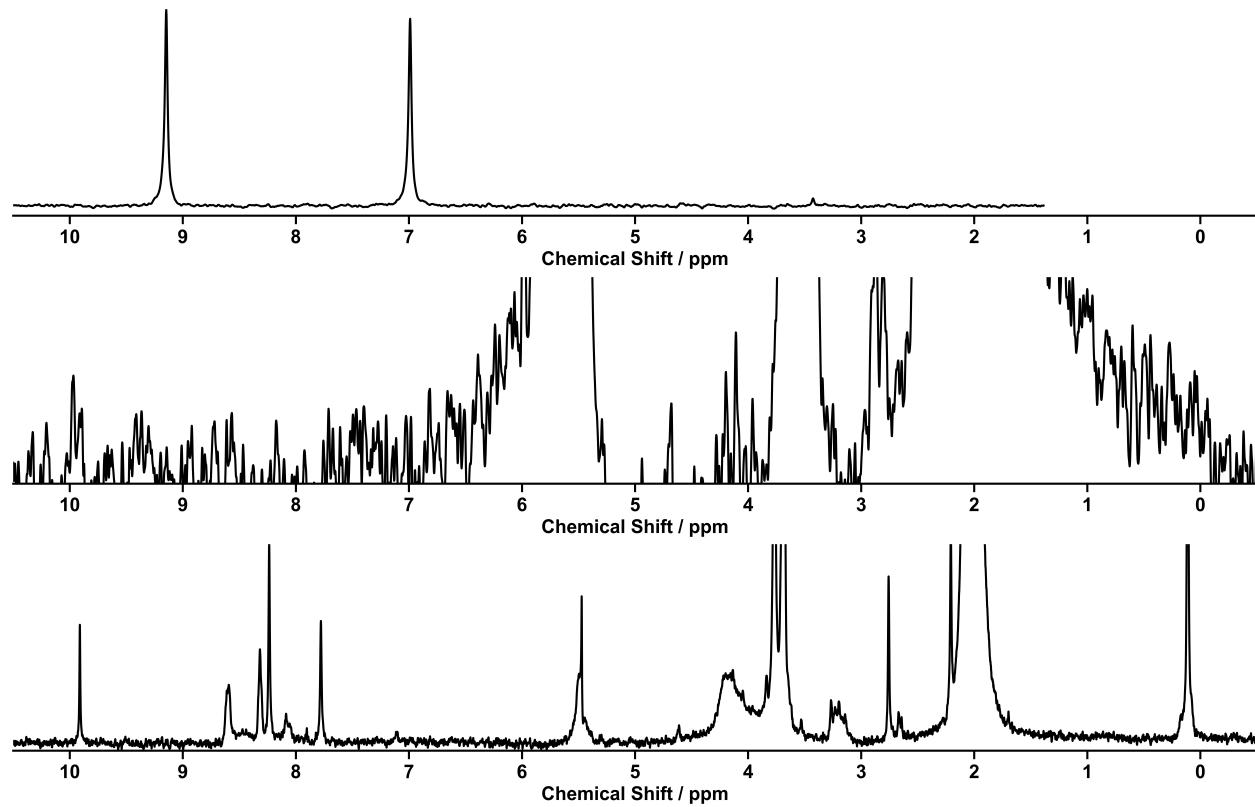
## Reaction 100



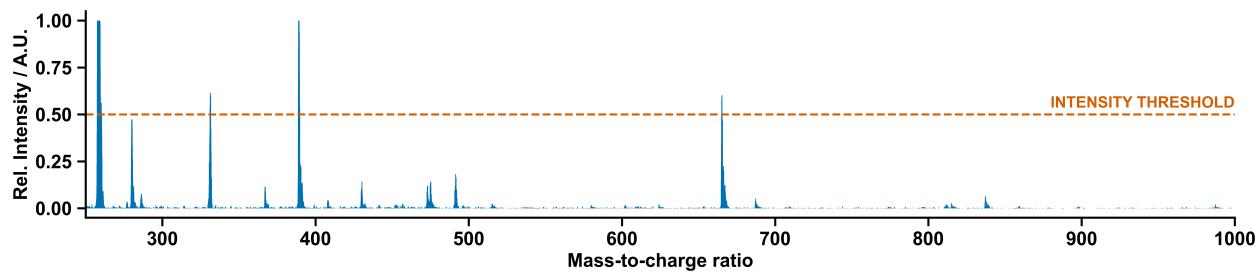
Scheme 83: Self-assembly of components 1, 19, with Yttrium(III) in a 3.0:1.5:1.0 molar ratio in  $\text{CH}_3\text{CN}$  at 60°C for 40h. These are the reagents (starting materials) for reaction 100.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: No reaction occurred.	
	Human MS Decision: Failed	MS Spectra Category: Reaction occurred, unknown product.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	NMR Criteria 2: N/A
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 2
		MS Criteria 3: Pass	Number of counter-ions found: 2

Decision Table 83: Human labeled and Decision maker labeled outcomes for the  $^1\text{H}$  NMR spectroscopy and UPLC-MS spectrometry of reaction 100. Decision motivations are also given.

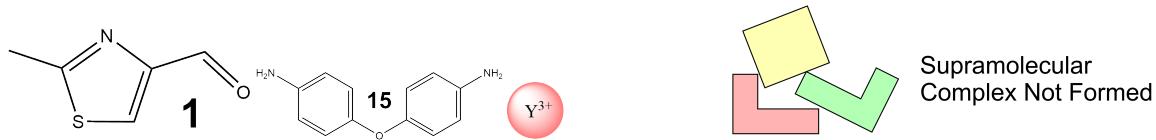


NMR Spectra 83: The stacked  $^1\text{H}$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 100.



MS Spectra 83: The ULPC-MS spectra of reaction 100. The intensity threshold is also shown.

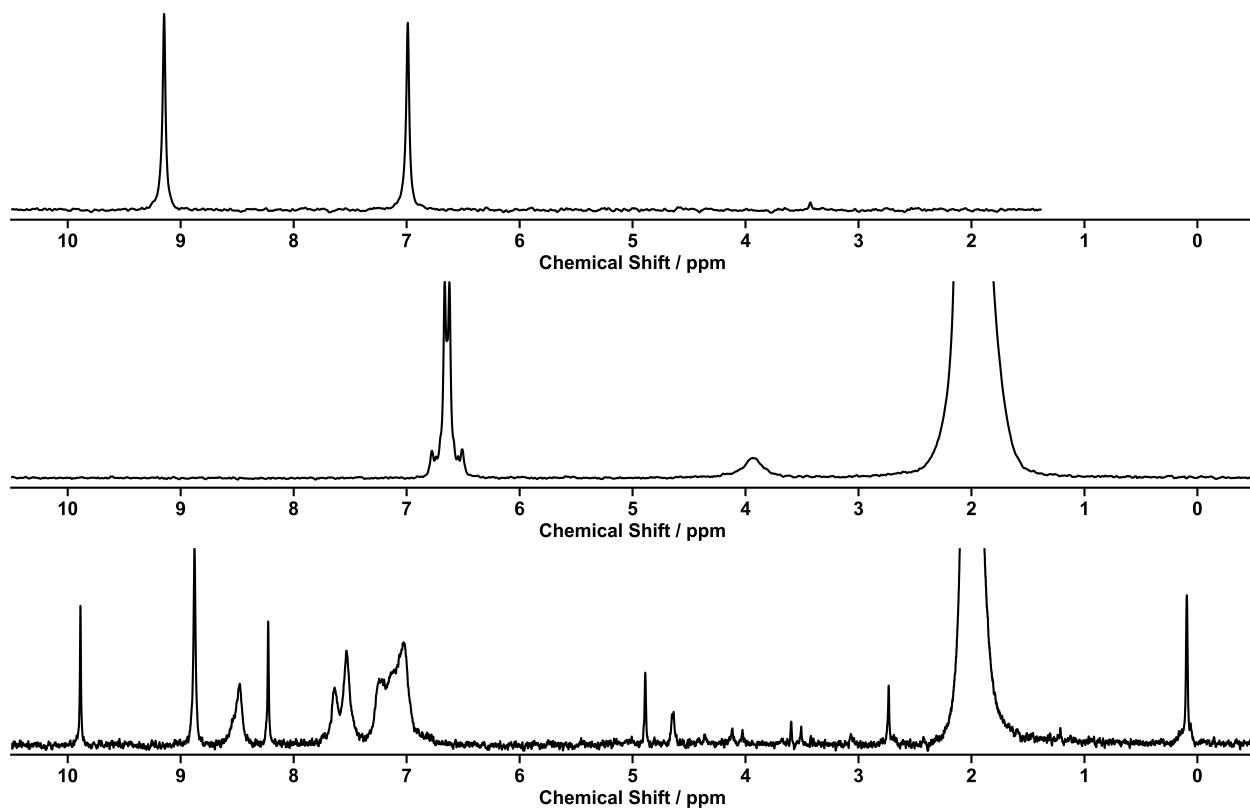
## Reaction 101



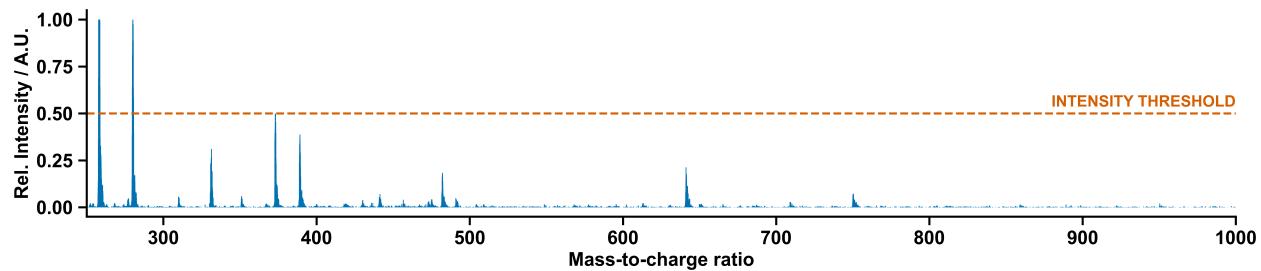
Scheme 84: Self-assembly of components 1, 15, with Yttrium(III) in a 3.0:1.5:1.0 molar ratio in CH<sub>3</sub>CN at 60°C for 40h. These are the reagents (starting materials) for reaction 101.

Human Reaction Decision: Failed	Human NMR Decision: Pass	NMR Spectra Category: Single discrete species formed.	
	Human MS Decision: Failed	MS Spectra Category: Reaction occurred, unknown product.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	NMR Criteria 2: N/A
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 0
		MS Criteria 3: Pass	Number of counter-ions found: 0

Decision Table 84: Human labeled and Decision maker labeled outcomes for the <sup>1</sup>H NMR spectroscopy and ULPC-MS spectrometry of reaction 101. Decision motivations are also given.

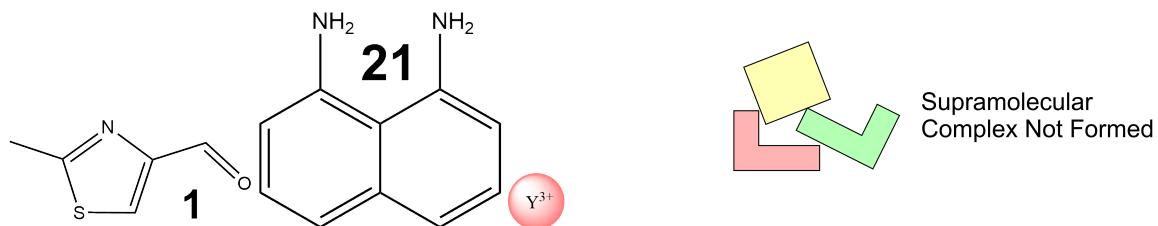


NMR Spectra 84: The stacked  $^1\text{H}$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 101.



MS Spectra 84: The ULPC-MS spectra of reaction 101. The intensity threshold is also shown.

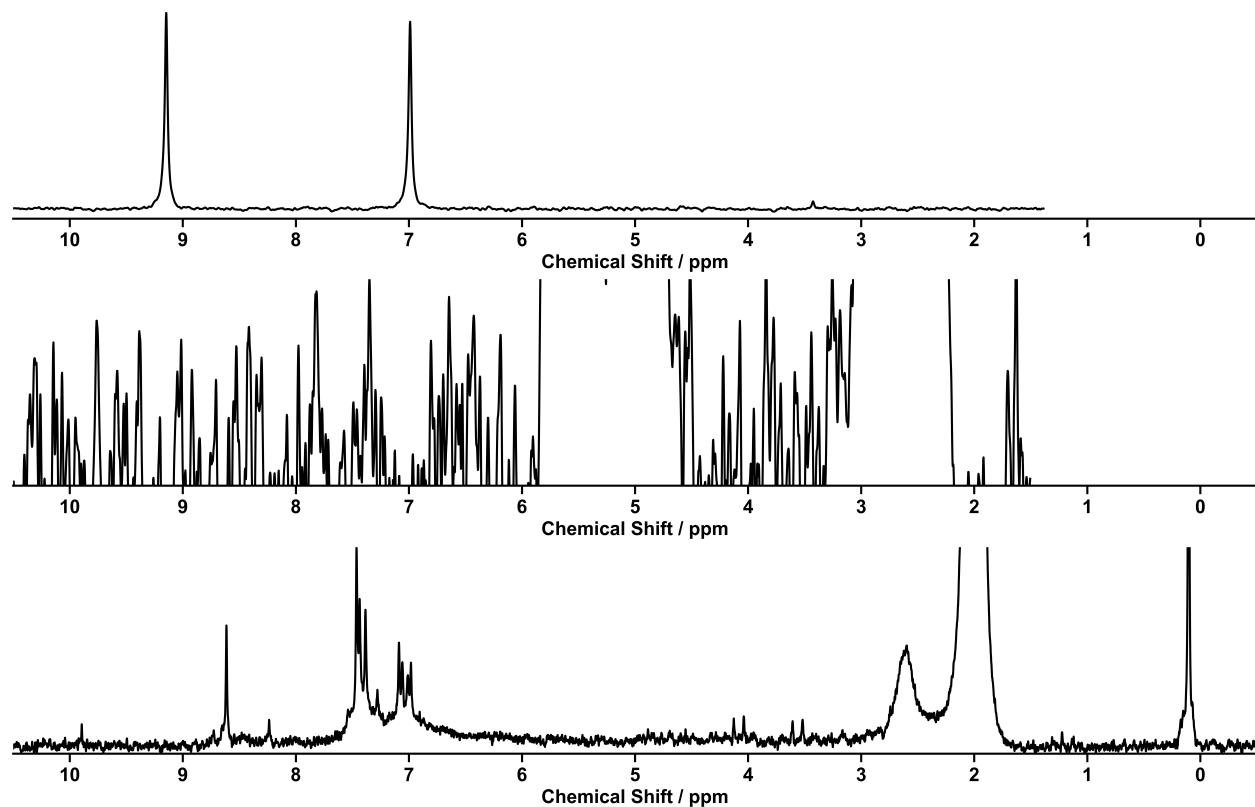
## Reaction 102



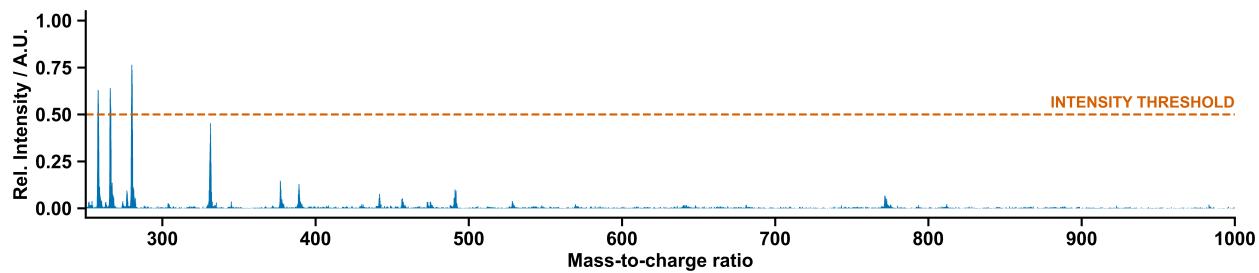
Scheme 85: Self-assembly of components 1, 21, with Yttrium(III) in a 3.0:1.5:1.0 molar ratio in  $\text{CH}_3\text{CN}$  at  $60^\circ\text{C}$  for 40h. These are the reagents (starting materials) for reaction 102.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: No reaction occurred.	
	Human MS Decision: Failed	MS Spectra Category: Reaction failed.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	NMR Criteria 2: N/A
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 0
		MS Criteria 3: Pass	Number of counter-ions found: 0

Decision Table 85: Human labeled and Decision maker labeled outcomes for the  $^1\text{H}$  NMR spectroscopy and UPLC-MS spectrometry of reaction 102. Decision motivations are also given.

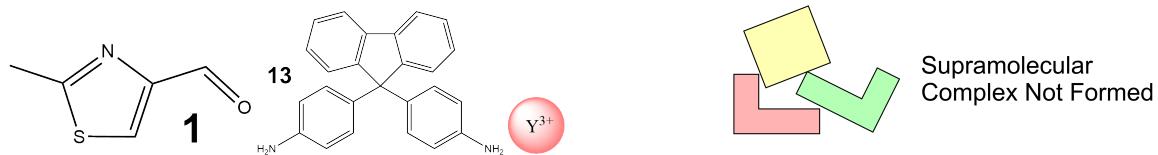


NMR Spectra 85: The stacked  $^1\text{H}$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 102.



MS Spectra 85: The ULPC-MS spectra of reaction 102. The intensity threshold is also shown.

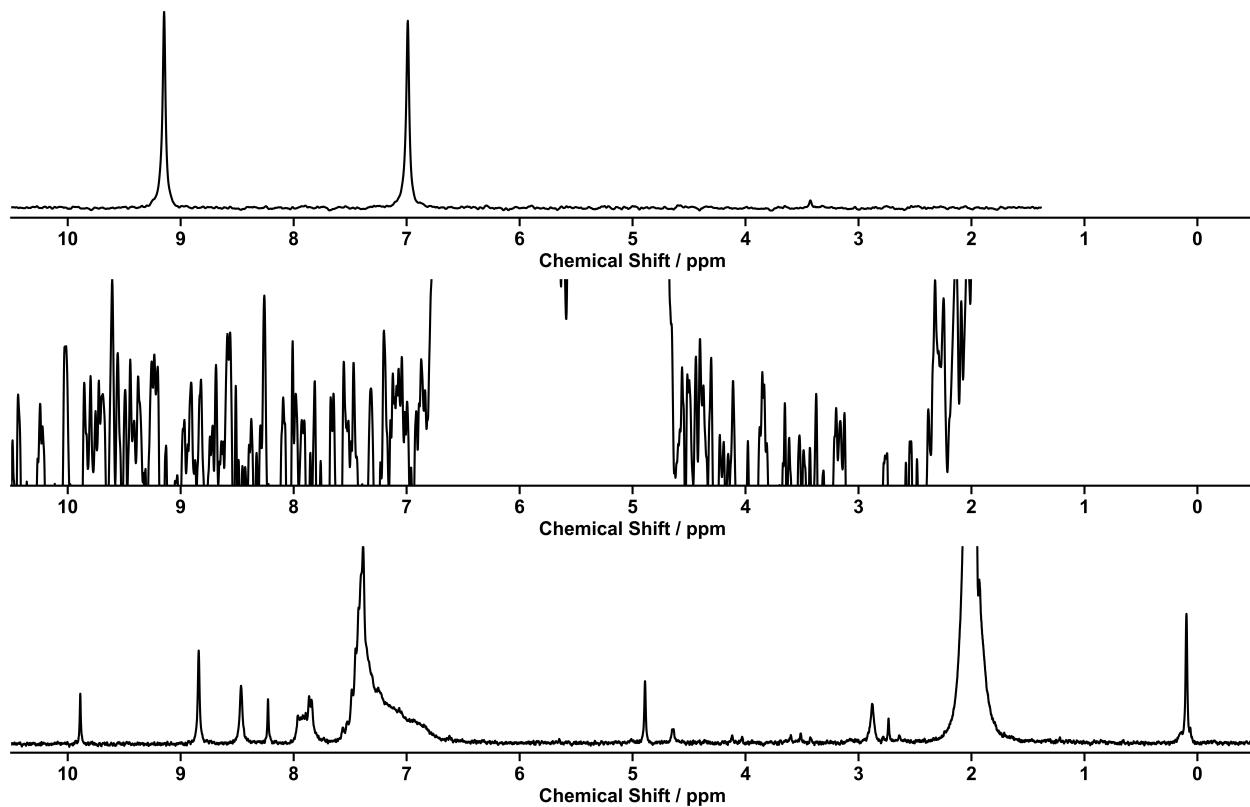
## Reaction 103



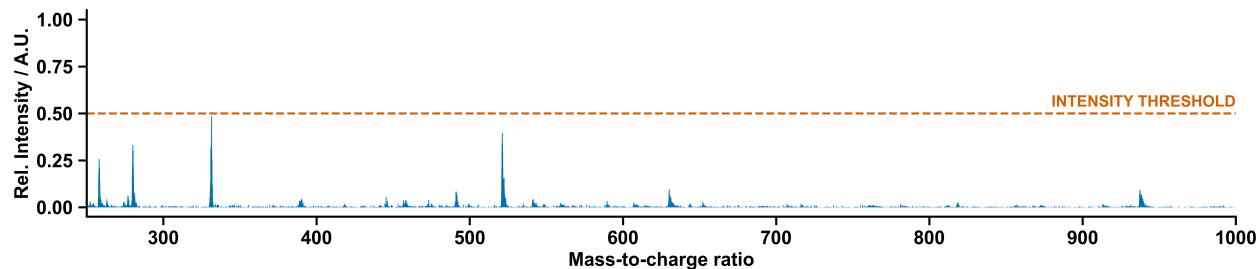
Scheme 86: Self-assembly of components 1, 13, with Yttrium(III) in a 3.0:1.5:1.0 molar ratio in  $\text{CH}_3\text{CN}$  at  $60^\circ\text{C}$  for 40h. These are the reagents (starting materials) for reaction 103.

Human Reaction Decision: Failed	Human NMR Decision: Pass	NMR Spectra Category: Single discrete species formed.	
	Human MS Decision: Failed	MS Spectra Category: Reaction failed.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	NMR Criteria 2: N/A
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 0
		MS Criteria 3: Pass	Number of counter-ions found: 0

Decision Table 86: Human labeled and Decision maker labeled outcomes for the  $^1\text{H}$  NMR spectroscopy and ULPC-MS spectrometry of reaction 103. Decision motivations are also given.

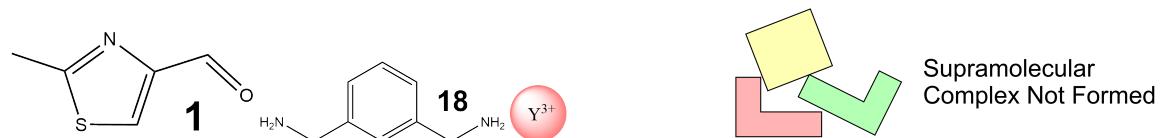


NMR Spectra 86: The stacked <sup>1</sup>H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 103.



MS Spectra 86: The ULPC-MS spectra of reaction 103. The intensity threshold is also shown.

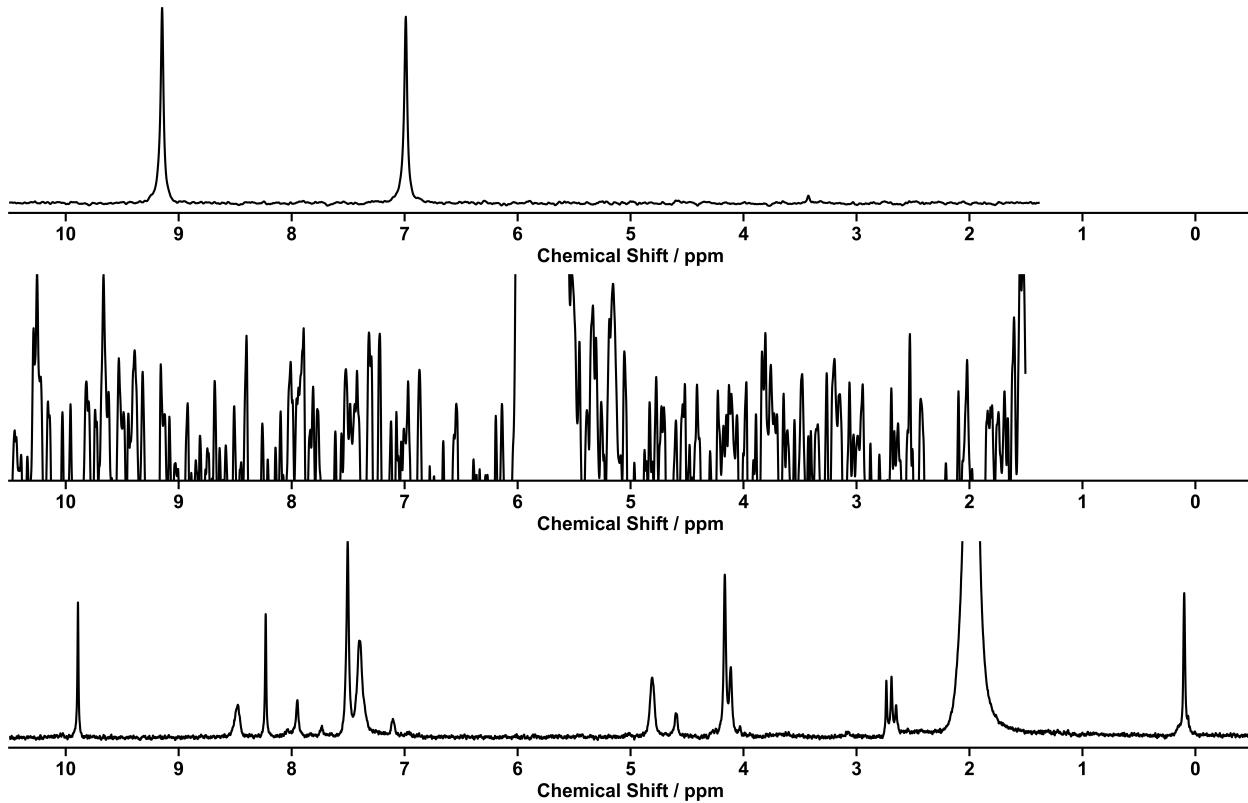
## Reaction 104



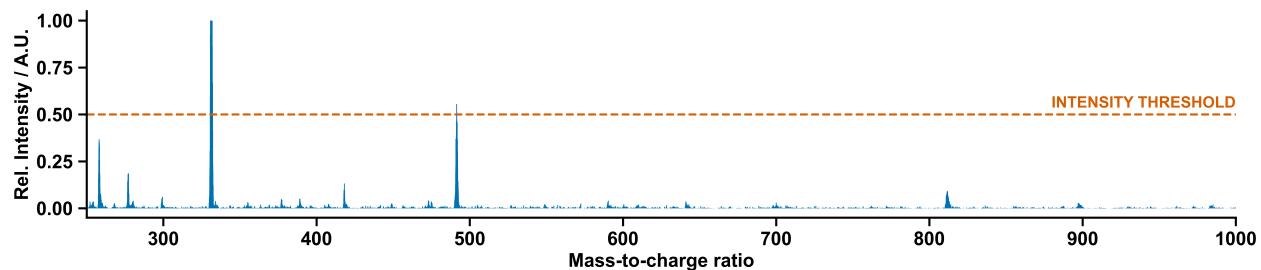
Scheme 87: Self-assembly of components **1**, **18**, with Yttrium(III) in a 3.0:1.5:1.0 molar ratio in  $\text{CH}_3\text{CN}$  at 60°C for 40h. These are the reagents (starting materials) for reaction 104.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: No reaction occurred.	
	Human MS Decision: Failed	MS Spectra Category: Reaction occurred, unknown product.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A		NMR Criteria 1: N/A
	Decision Maker MS Decision: Pass		NMR Criteria 2: N/A
	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 1	MS Criteria 3: Pass
			Number of counter-ions found: 1

Decision Table 87: Human labeled and Decsision maker labeled outcomes for the  $^1\text{H}$  NMR spectroscopy and ULPC-MS spectrometry of reaction 104. Decision motivations are also given.

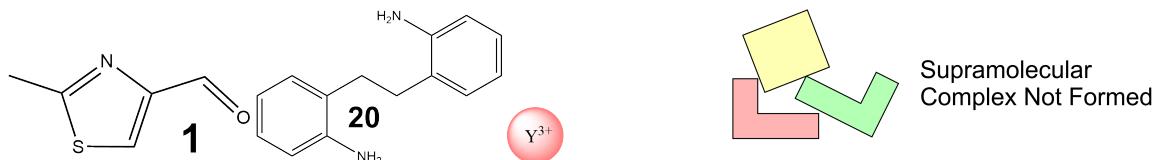


NMR Spectra 87: The stacked  $^1\text{H}$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 104.



MS Spectra 87: The ULPC-MS spectra of reaction 104. The intensity threshold is also shown.

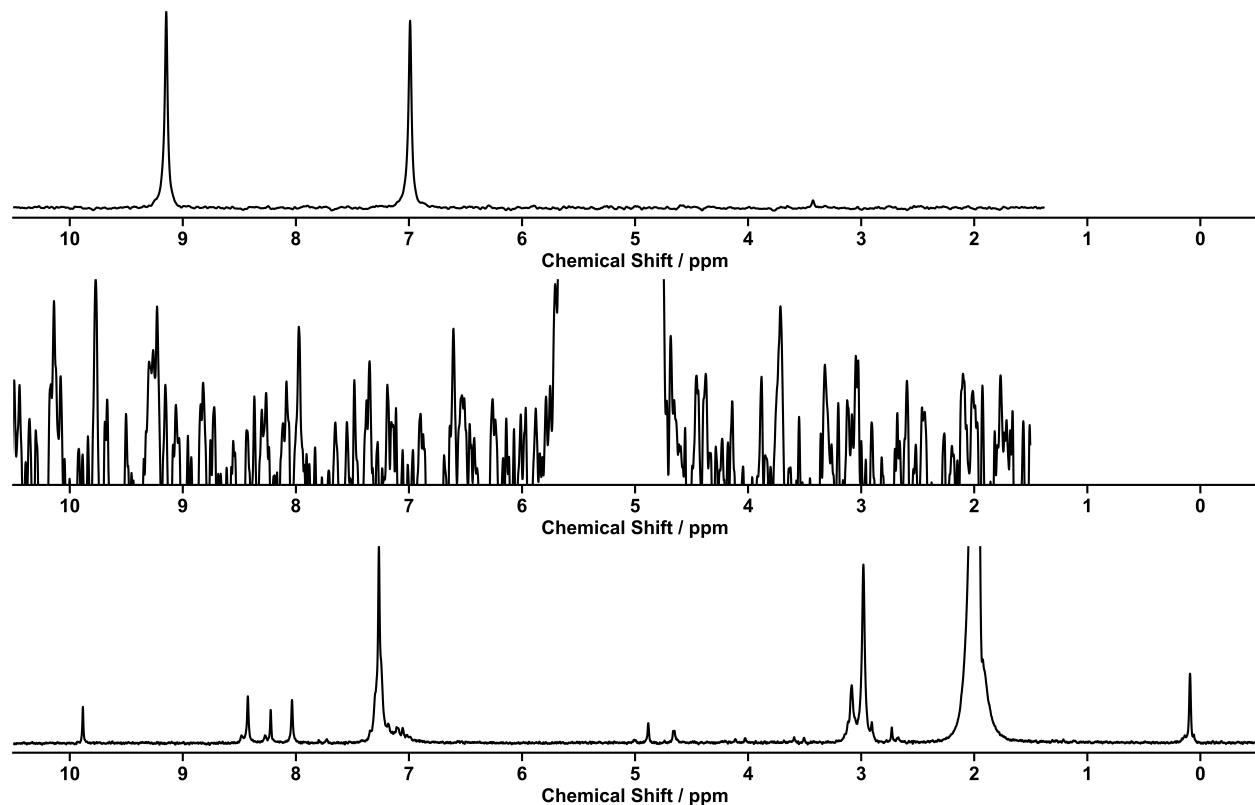
## Reaction 105



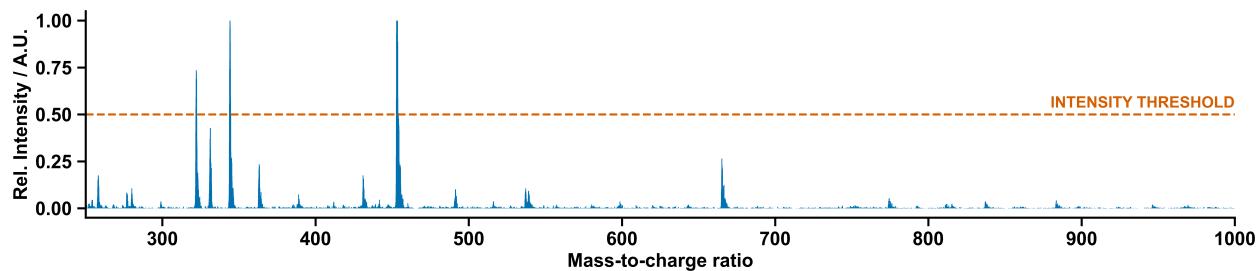
Scheme 88: Self-assembly of components 1, 20, with Yttrium(III) in a 3.0:1.5:1.0 molar ratio in CH<sub>3</sub>CN at 60°C for 40h. These are the reagents (starting materials) for reaction 105.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: No reaction occurred.	
	Human MS Decision: Failed	MS Spectra Category: Reaction occurred, unknown product.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	NMR Criteria 2: N/A
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 0
		MS Criteria 3: Pass	Number of counter-ions found: 0

Decision Table 88: Human labeled and Decision maker labeled outcomes for the <sup>1</sup>H NMR spectroscopy and ULPC-MS spectrometry of reaction 105. Decision motivations are also given.

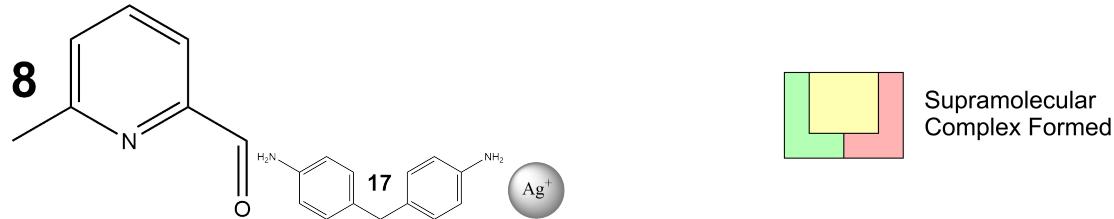


NMR Spectra 88: The stacked <sup>1</sup>H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 105.



MS Spectra 88: The ULPC-MS spectra of reaction 105. The intensity threshold is also shown.

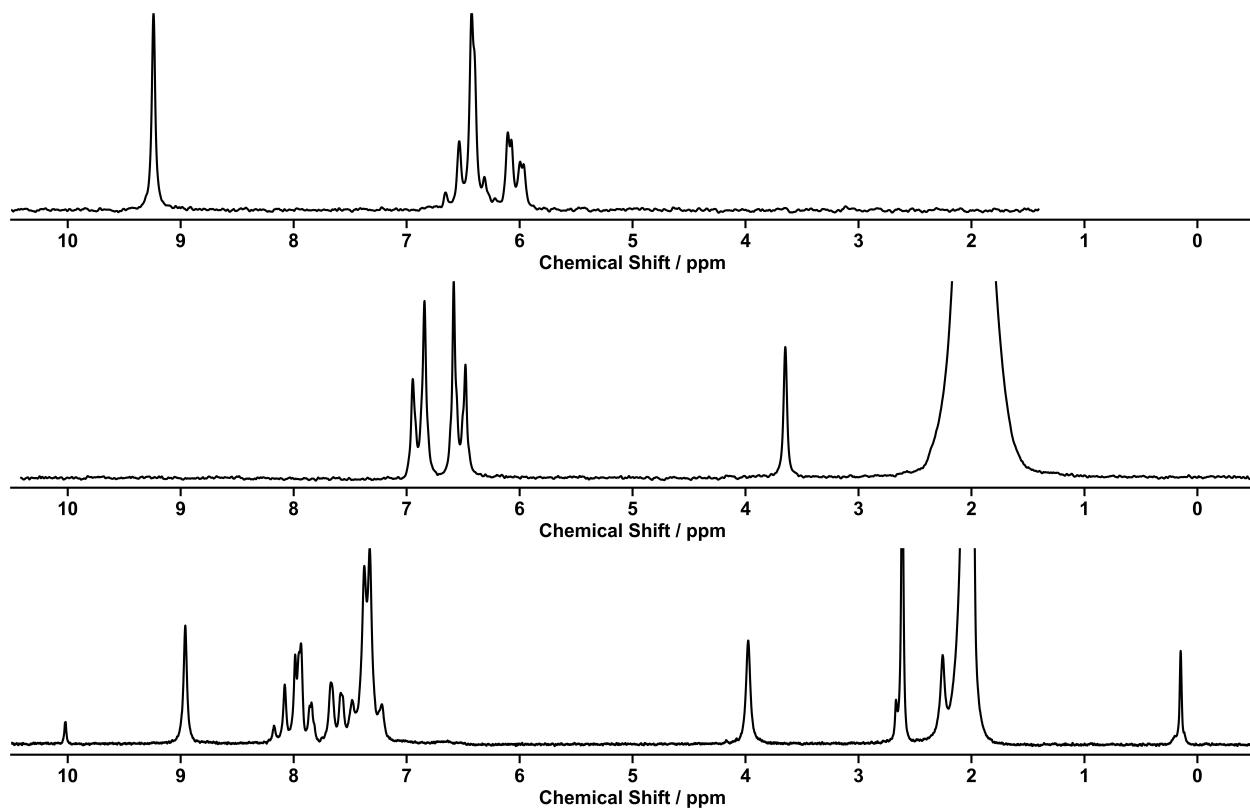
## Reaction 106



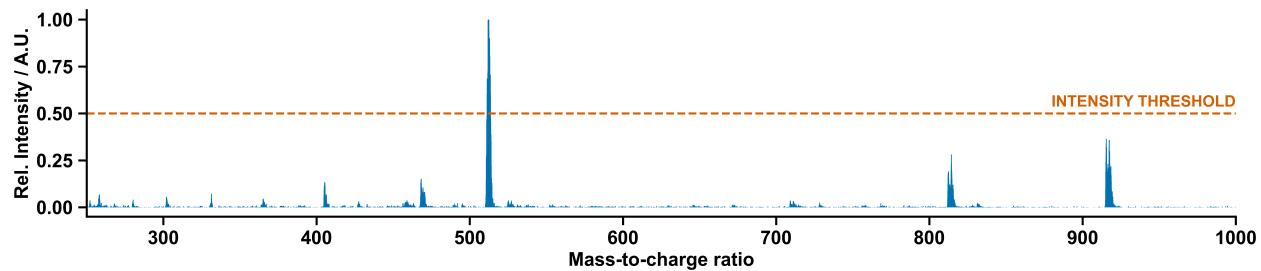
Scheme 89: Self-assembly of components 8, 17, with Silver(I) in a 3.0:1.5:1.0 molar ratio in CH<sub>3</sub>CN at 60°C for 40h. These are the reagents (starting materials) for reaction 106.

Human Reaction Decision: Pass	Human NMR Decision: Pass	NMR Spectra Category: Single discrete species formed.
	Human MS Decision: Pass	MS Spectra Category: Reaction occurred, supramolecular product.
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A
		NMR Criteria 2: N/A
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass
		Number of predicted peaks found in MS spectra with appropriate intensity: 3
	MS Criteria 3: Pass	Number of counter-ions found: 2

Decision Table 89: Human labeled and Decsision maker labeled outcomes for the  $^1\text{H}$  NMR spectroscopy and ULPC-MS spectrometry of reaction 106. Decision motivations are also given.

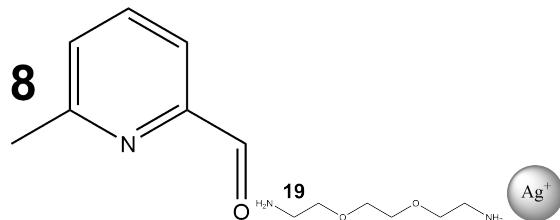


NMR Spectra 89: The stacked  $^1\text{H}$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 106.



MS Spectra 89: The ULPC-MS spectra of reaction 106. The intensity threshold is also shown.

## Reaction 107

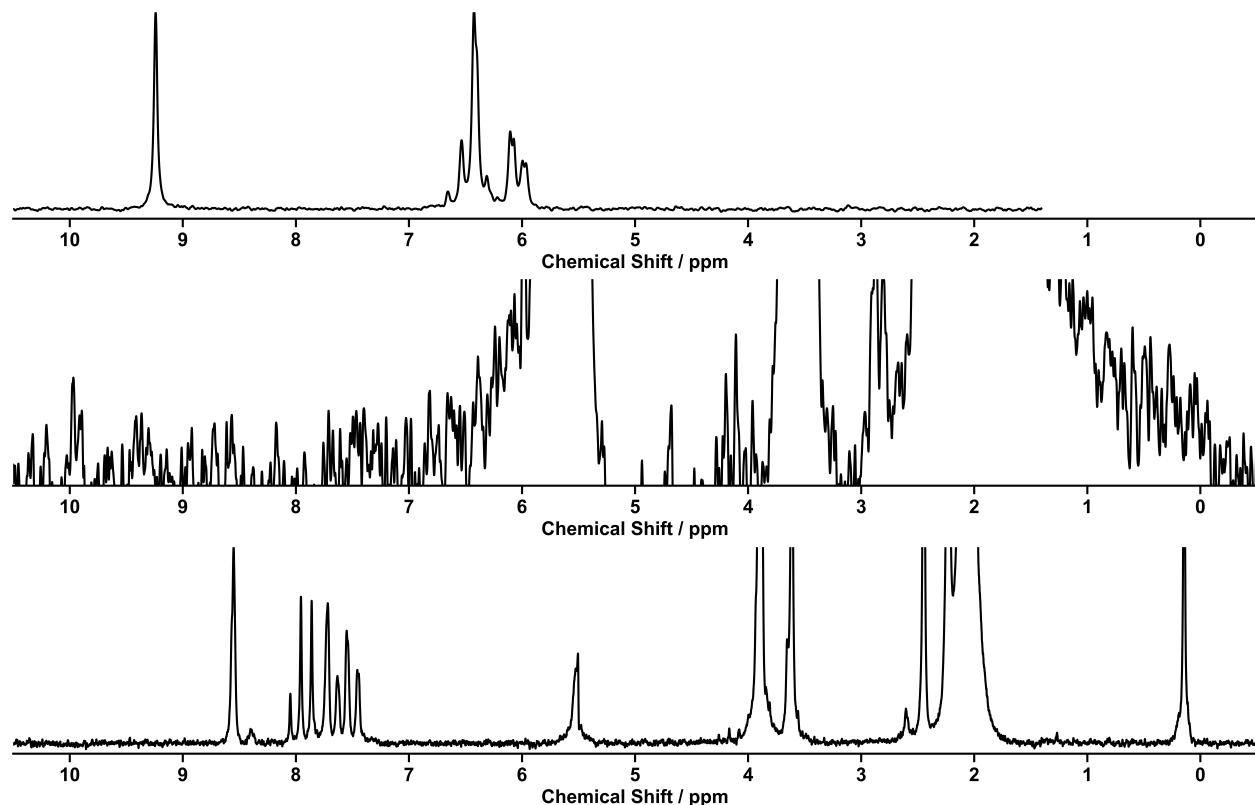


Supramolecular Complex Formed

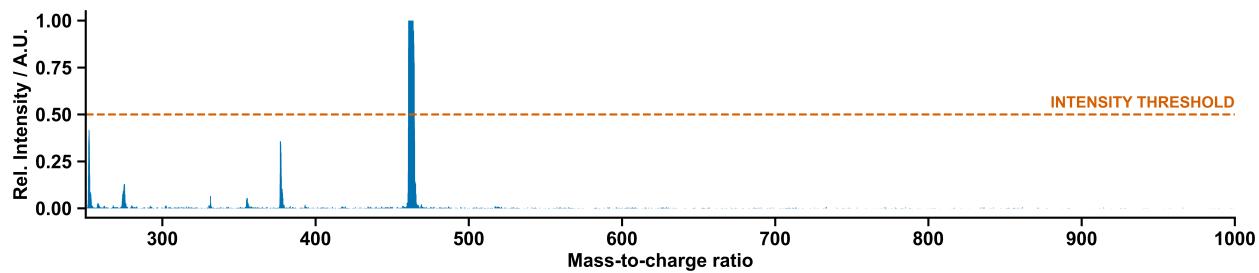
Scheme 90: Self-assembly of components 8, 19, with Silver(I) in a 3.0:1.5:1.0 molar ratio in  $\text{CH}_3\text{CN}$  at 60°C for 40h. These are the reagents (starting materials) for reaction 107.

Human Reaction Decision: Pass	Human NMR Decision: Pass	NMR Spectra Category: Single discrete species formed.	
	Human MS Decision: Pass	MS Spectra Category: Reaction occurred, supramolecular product.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	NMR Criteria 2: N/A
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 3
		MS Criteria 3: Pass	Number of counter-ions found: 2

Decision Table 90: Human labeled and Decsision maker labeled outcomes for the  $^1\text{H}$  NMR spectroscopy and UPLC-MS spectrometry of reaction 107. Decision motivations are also given.

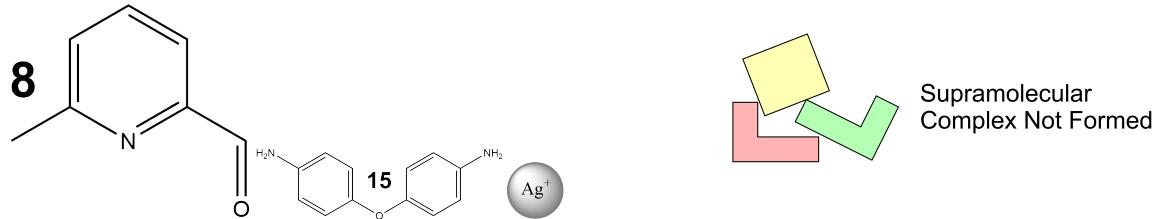


NMR Spectra 90: The stacked  $^1\text{H}$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 107.



MS Spectra 90: The ULPC-MS spectra of reaction 107. The intensity threshold is also shown.

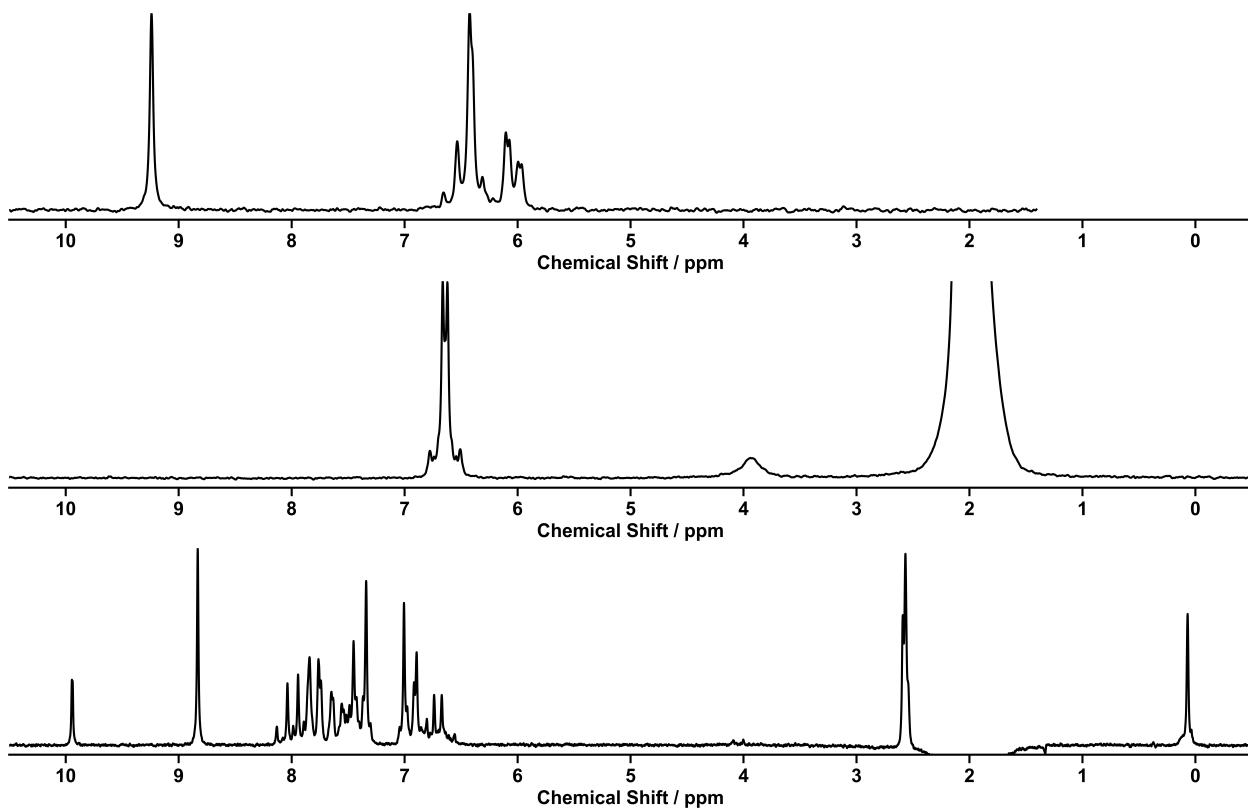
## Reaction 108



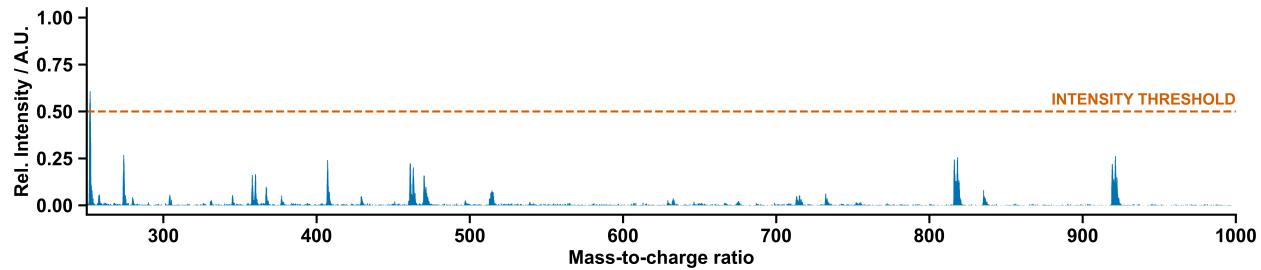
Scheme 91: Self-assembly of components 8, 15, with Silver(I) in a 3.0:1.5:1.0 molar ratio in CH<sub>3</sub>CN at 60°C for 40h. These are the reagents (starting materials) for reaction 108.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: No reaction occurred.	
	Human MS Decision: Failed	MS Spectra Category: Reaction failed.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	NMR Criteria 2: N/A
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 0
		MS Criteria 3: Pass	Number of counter-ions found: 0

Decision Table 91: Human labeled and Decsision maker labeled outcomes for the <sup>1</sup>H NMR spectroscopy and ULPC-MS spectrometry of reaction 108. Decision motivations are also given.

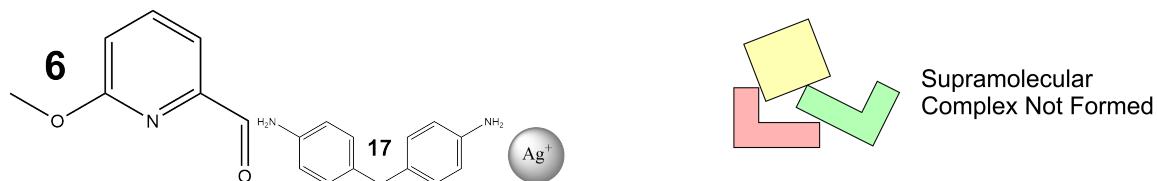


NMR Spectra 91: The stacked <sup>1</sup>H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 108.



MS Spectra 91: The ULPC-MS spectra of reaction 108. The intensity threshold is also shown.

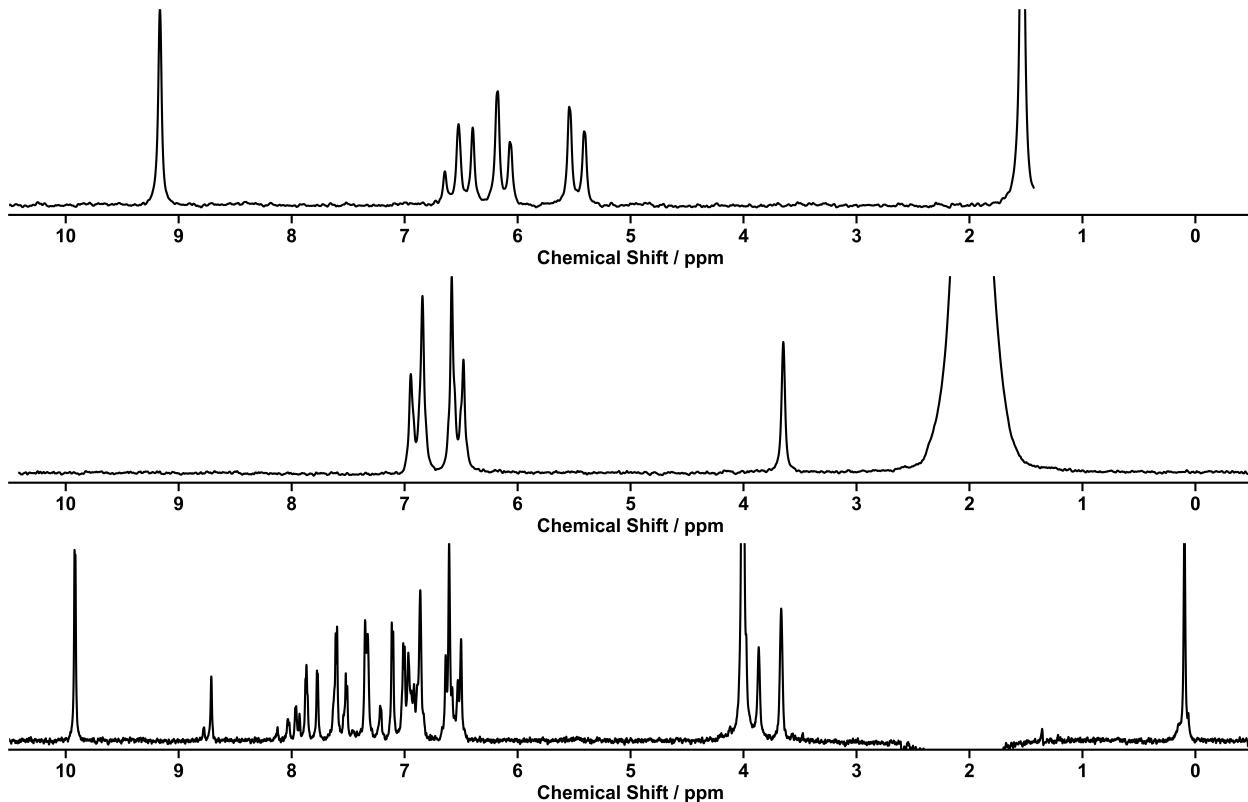
## Reaction 109



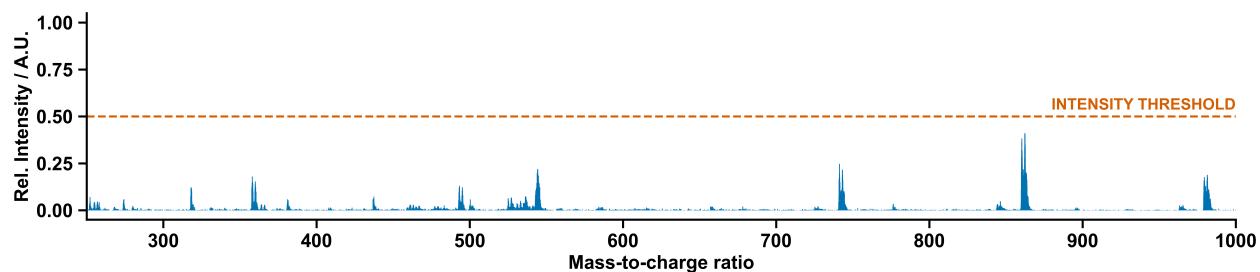
Scheme 92: Self-assembly of components 6, 17, with Silver(I) in a 3.0:1.5:1.0 molar ratio in  $\text{CH}_3\text{CN}$  at 60°C for 40h. These are the reagents (starting materials) for reaction 109.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: No reaction occurred.	
	Human MS Decision: Failed	MS Spectra Category: Reaction failed.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A		NMR Criteria 1: N/A
	Decision Maker MS Decision: Pass		NMR Criteria 2: N/A
	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 0	MS Criteria 3: Pass
			Number of counter-ions found: 0

Decision Table 92: Human labeled and Decsision maker labeled outcomes for the  $^1\text{H}$  NMR spectroscopy and ULPC-MS spectrometry of reaction 109. Decision motivations are also given.

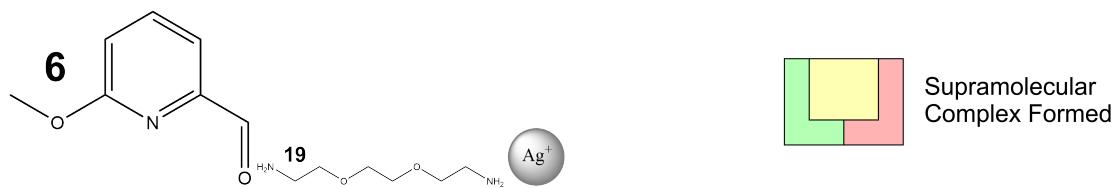


NMR Spectra 92: The stacked  $^1\text{H}$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 109.



MS Spectra 92: The ULPC-MS spectra of reaction 109. The intensity threshold is also shown.

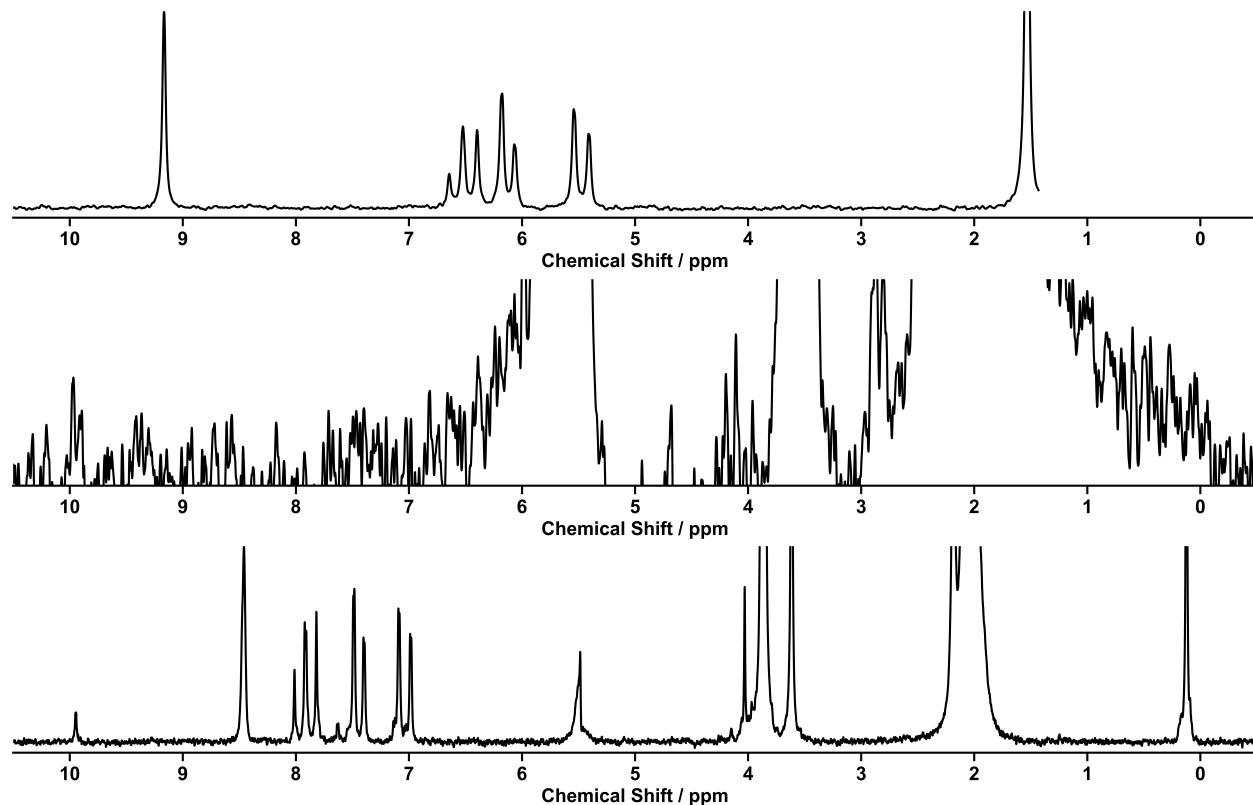
## Reaction 110



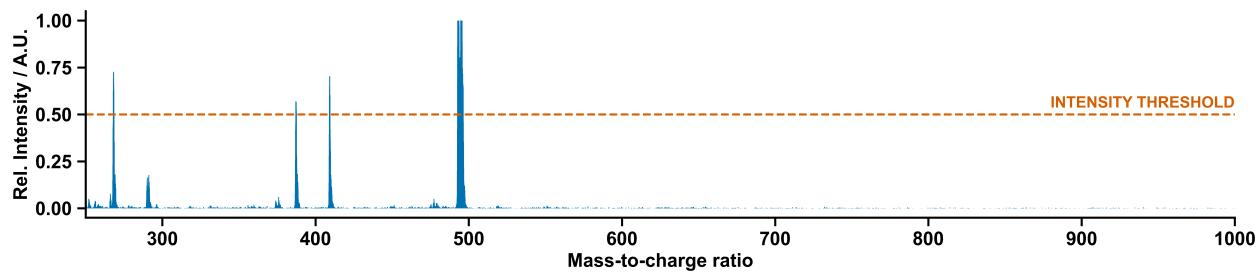
Scheme 93: Self-assembly of components 6, 19, with Silver(I) in a 3.0:1.5:1.0 molar ratio in  $\text{CH}_3\text{CN}$  at  $60^\circ\text{C}$  for 40h. These are the reagents (starting materials) for reaction 110.

Human Reaction Decision: Pass	Human NMR Decision: Pass	NMR Spectra Category: Single discrete species formed.	
	Human MS Decision: Pass	MS Spectra Category: Reaction occurred, supramolecular product.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	NMR Criteria 2: N/A
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 3
		MS Criteria 3: Pass	Number of counter-ions found: 2

Decision Table 93: Human labeled and Decision maker labeled outcomes for the  $^1\text{H}$  NMR spectroscopy and UPLC-MS spectrometry of reaction 110. Decision motivations are also given.

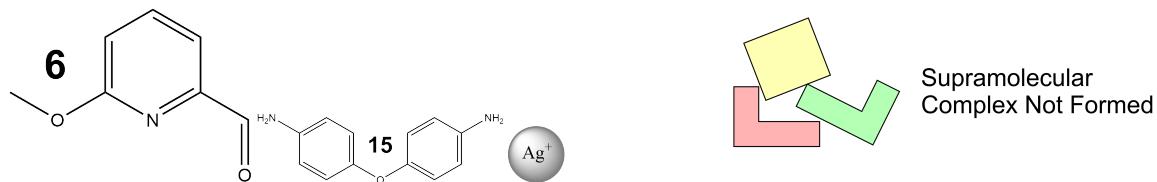


NMR Spectra 93: The stacked  $^1\text{H}$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 110.



MS Spectra 93: The ULPC-MS spectra of reaction 110. The intensity threshold is also shown.

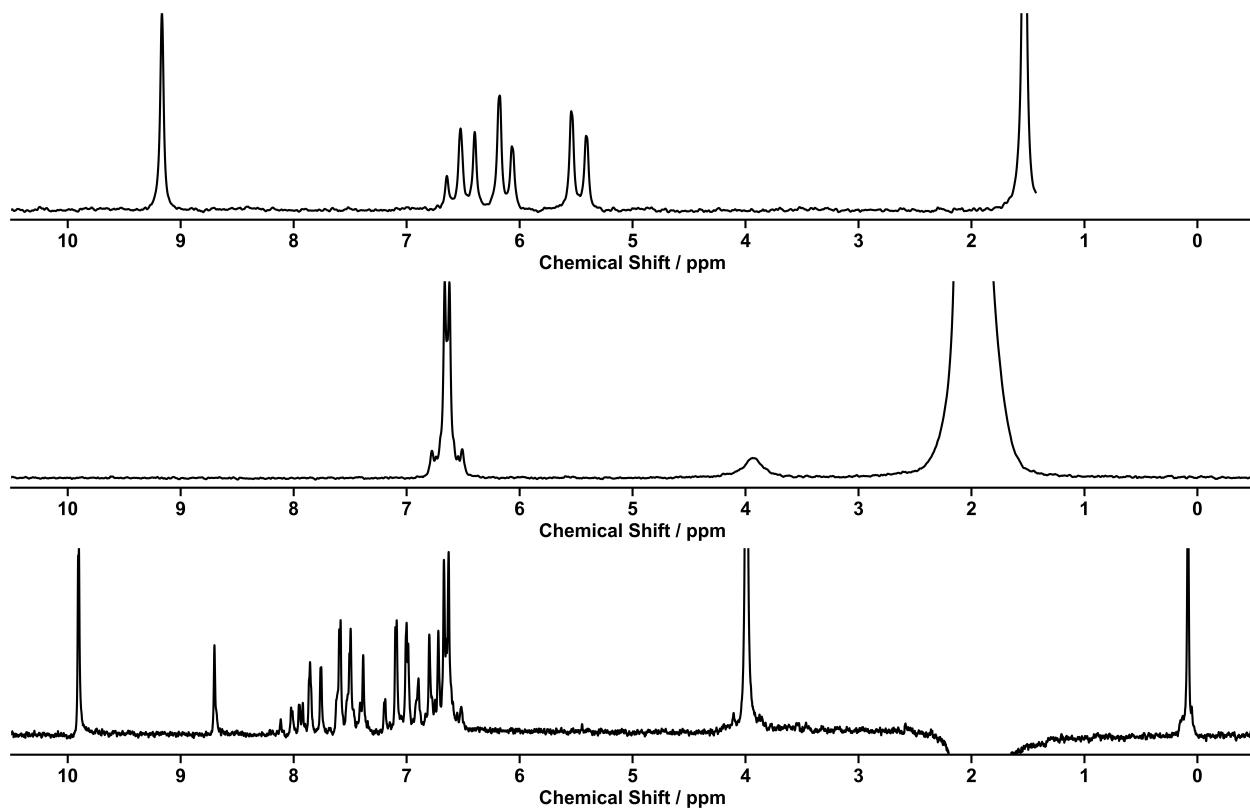
## Reaction 111



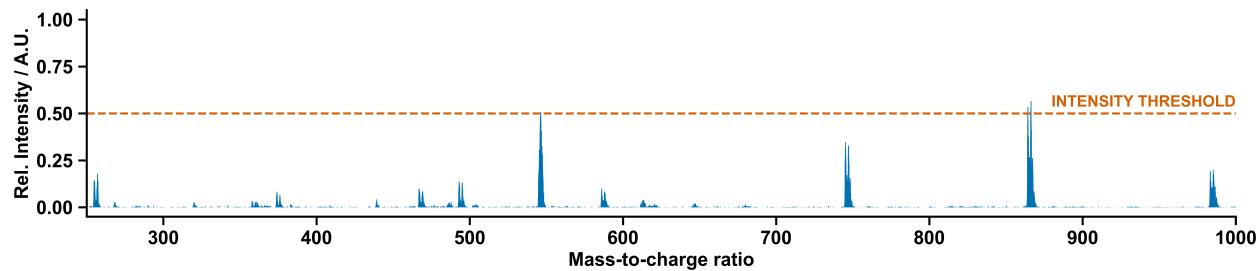
Scheme 94: Self-assembly of components 6, 15, with Silver(I) in a 3.0:1.5:1.0 molar ratio in  $\text{CH}_3\text{CN}$  at  $60^\circ\text{C}$  for 40h. These are the reagents (starting materials) for reaction 111.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: No reaction occurred.	
	Human MS Decision: Failed	MS Spectra Category: Reaction failed.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	NMR Criteria 2: N/A
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 3
		MS Criteria 3: Pass	Number of counter-ions found: 2

Decision Table 94: Human labeled and Decision maker labeled outcomes for the  $^1\text{H}$  NMR spectroscopy and ULPC-MS spectrometry of reaction 111. Decision motivations are also given.

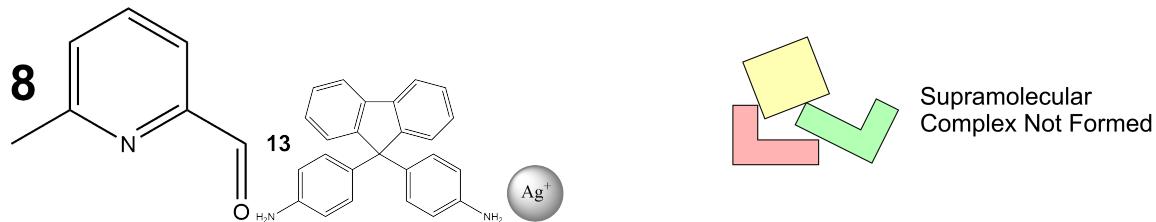


NMR Spectra 94: The stacked  $^1\text{H}$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 111.



MS Spectra 94: The ULPC-MS spectra of reaction 111. The intensity threshold is also shown.

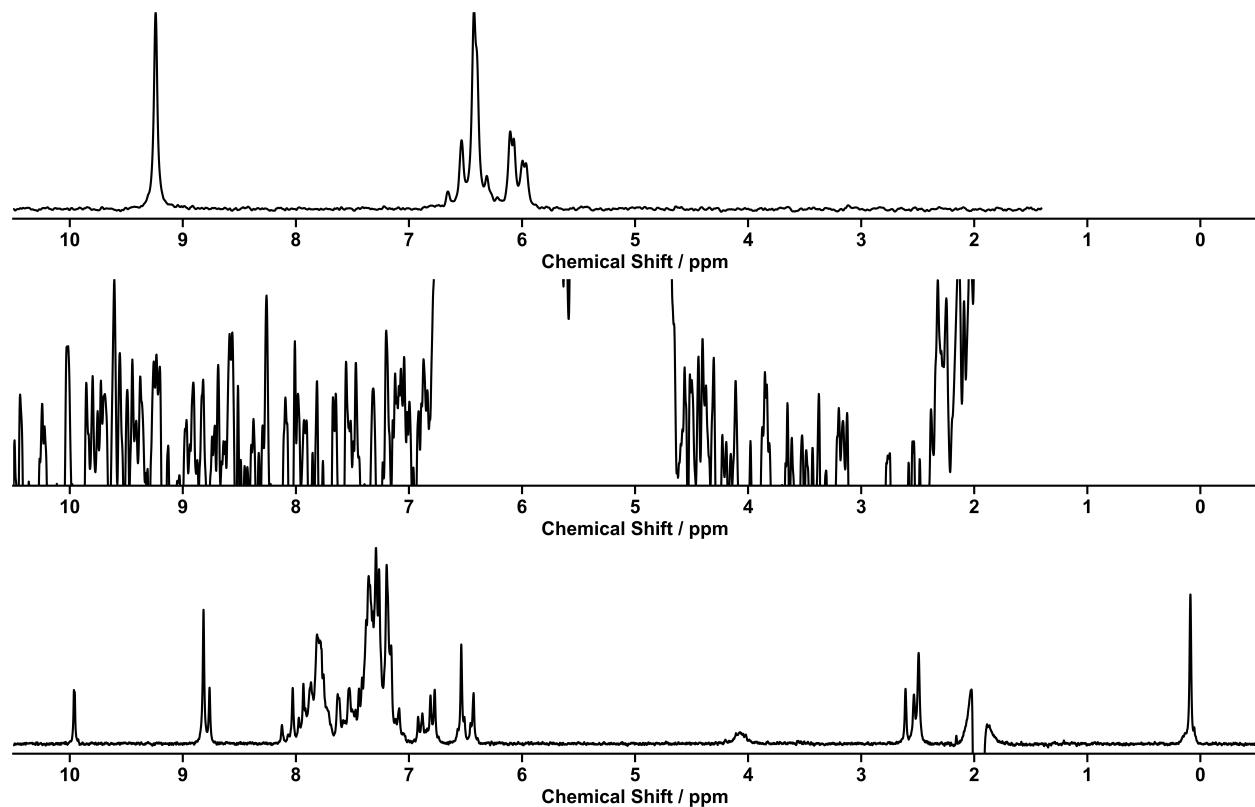
## Reaction 113



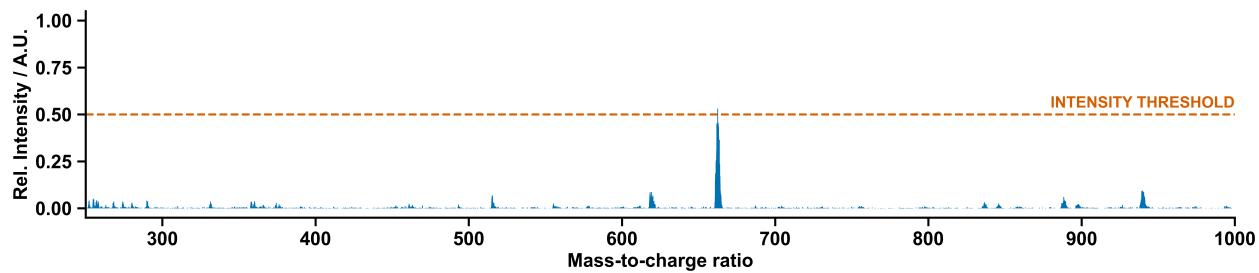
Scheme 95: Self-assembly of components 8, 13, with Silver(I) in a 3.0:1.5:1.0 molar ratio in  $\text{CH}_3\text{CN}$  at  $60^\circ\text{C}$  for 40h. These are the reagents (starting materials) for reaction 113.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: No reaction occurred.	
	Human MS Decision: Failed	MS Spectra Category: Reaction failed.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	NMR Criteria 2: N/A
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 3
		MS Criteria 3: Pass	Number of counter-ions found: 2

Decision Table 95: Human labeled and Decsision maker labeled outcomes for the  $^1\text{H}$  NMR spectroscopy and UPLC-MS spectrometry of reaction 113. Decision motivations are also given.

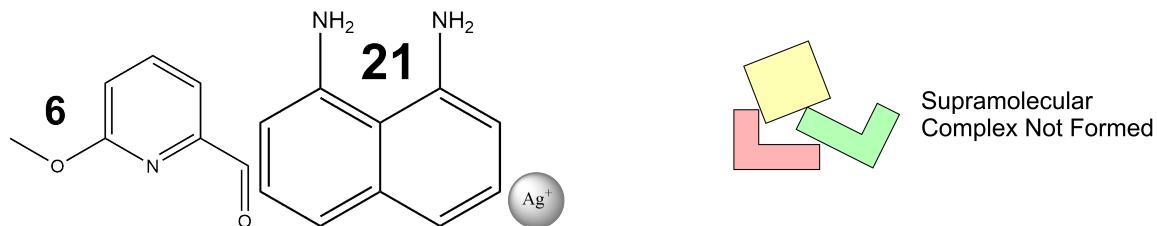


NMR Spectra 95: The stacked  $^1\text{H}$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 113.



MS Spectra 95: The ULPC-MS spectra of reaction 113. The intensity threshold is also shown.

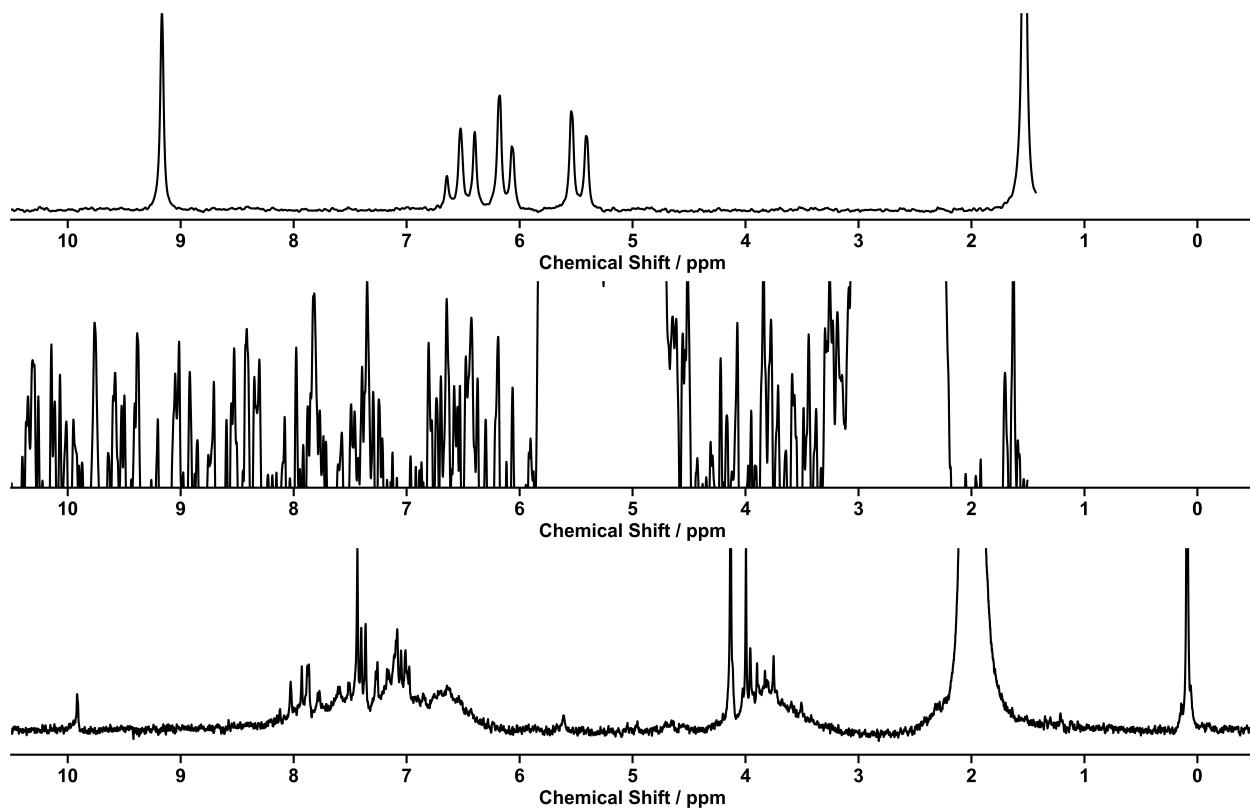
## Reaction 114



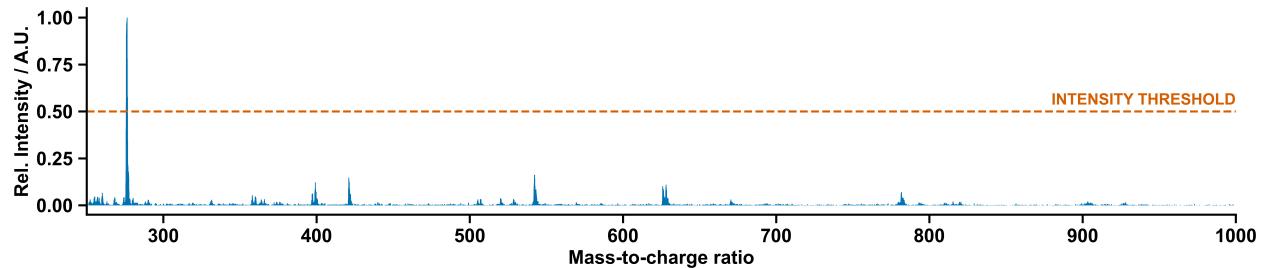
Scheme 96: Self-assembly of components 6, 21, with Silver(I) in a 3.0:1.5:1.0 molar ratio in  $\text{CH}_3\text{CN}$  at  $60^\circ\text{C}$  for 40h. These are the reagents (starting materials) for reaction 114.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: Oligomers formed.	
	Human MS Decision: Failed	MS Spectra Category: Reaction failed.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	
	Decision Maker MS Decision: Pass	NMR Criteria 2: N/A	MS Criteria 1 and 2: Pass
		Number of predicted peaks found in MS spectra with appropriate intensity: 0	Number of counter-ions found: 0
		MS Criteria 3: Pass	Number of counter-ions found: 0

Decision Table 96: Human labeled and Decsision maker labeled outcomes for the  $^1\text{H}$  NMR spectroscopy and ULPC-MS spectrometry of reaction 114. Decision motivations are also given.

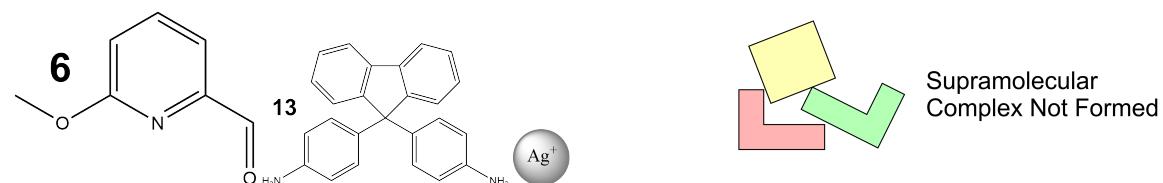


NMR Spectra 96: The stacked <sup>1</sup>H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 114.



MS Spectra 96: The ULPC-MS spectra of reaction 114. The intensity threshold is also shown.

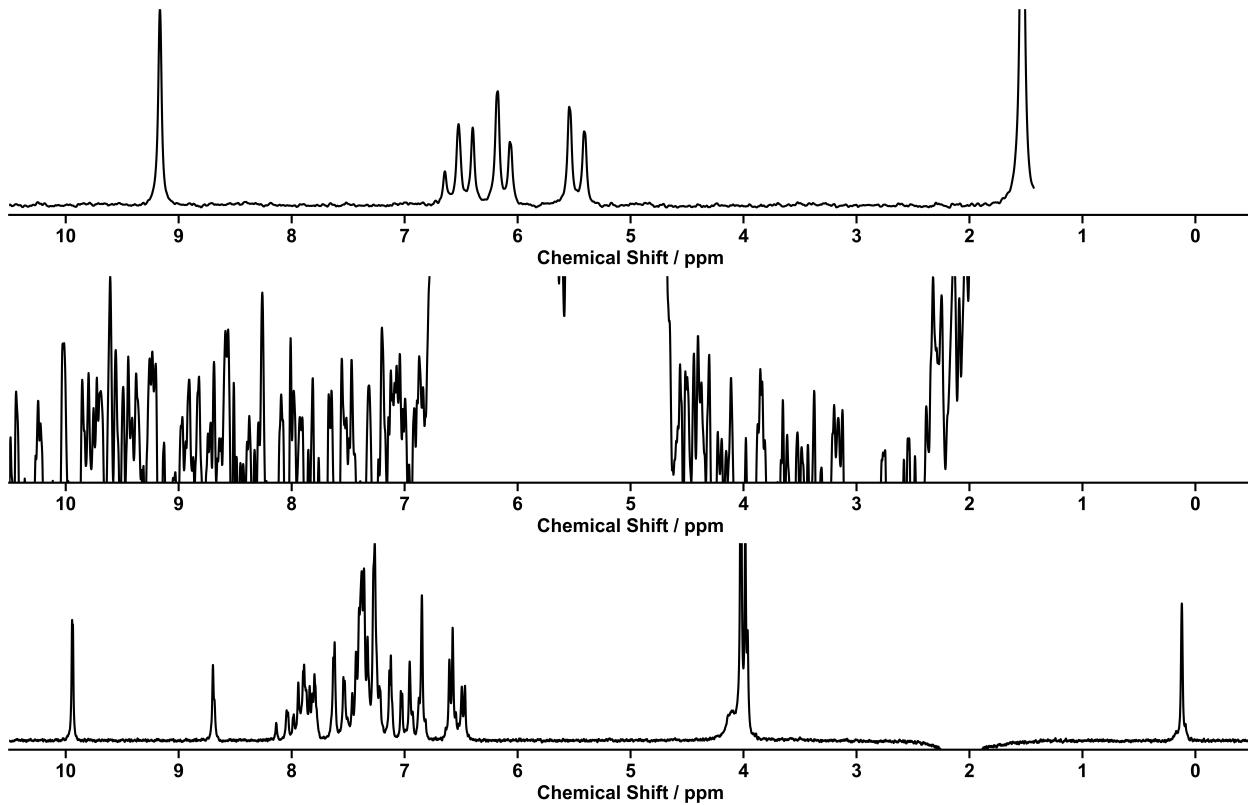
## Reaction 115



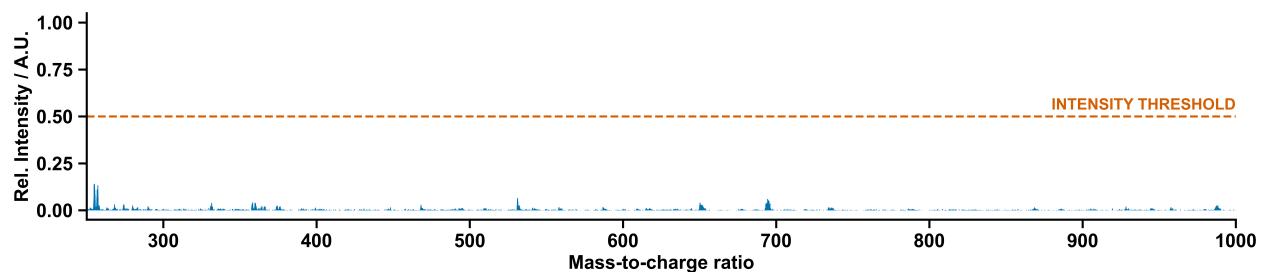
Scheme 97: Self-assembly of components 6, 13, with Silver(I) in a 3.0:1.5:1.0 molar ratio in  $\text{CH}_3\text{CN}$  at 60°C for 40h. These are the reagents (starting materials) for reaction 115.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: No reaction occurred.	
	Human MS Decision: Failed	MS Spectra Category: Reaction failed.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 0
		MS Criteria 3: Pass	Number of counter-ions found: 0

Decision Table 97: Human labeled and Decsision maker labeled outcomes for the  $^1\text{H}$  NMR spectroscopy and ULPC-MS spectrometry of reaction 115. Decision motivations are also given.

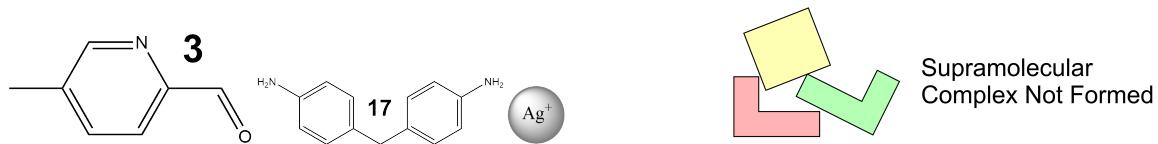


NMR Spectra 97: The stacked  $^1\text{H}$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 115.



MS Spectra 97: The ULPC-MS spectra of reaction 115. The intensity threshold is also shown.

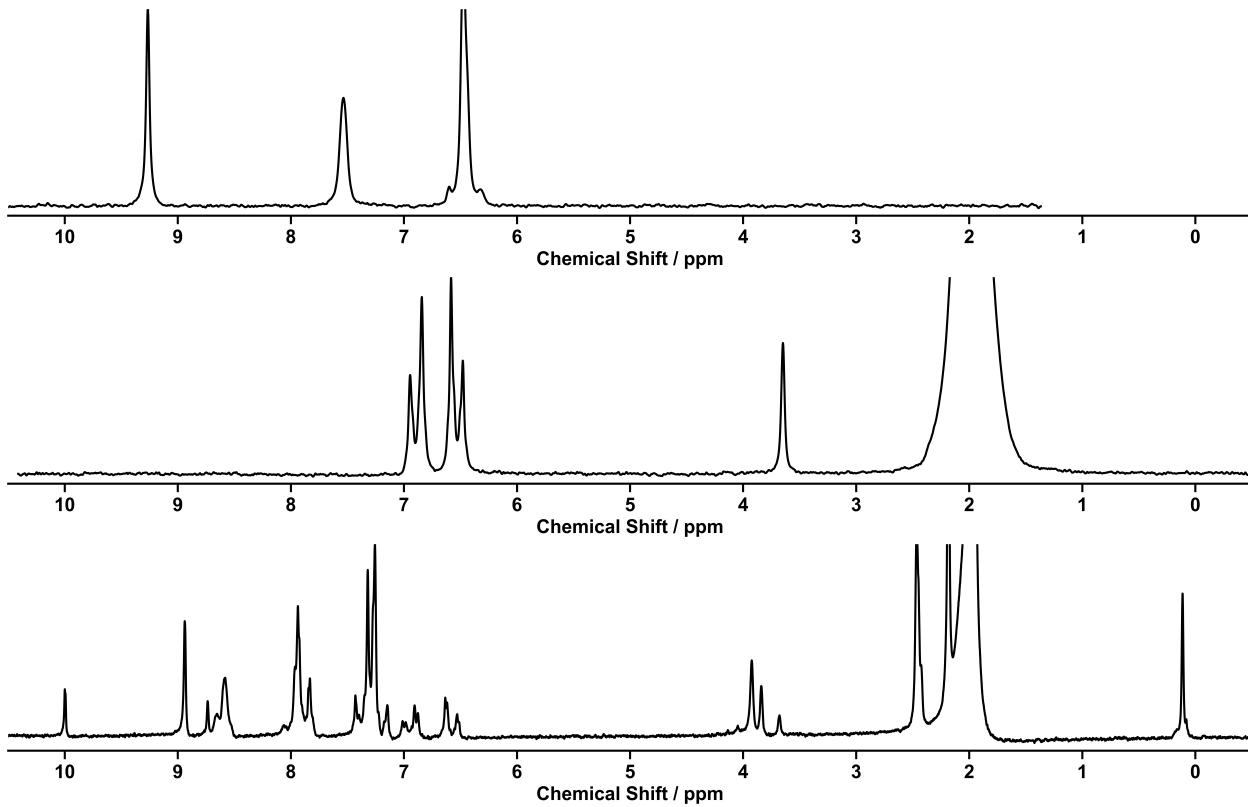
## Reaction 116



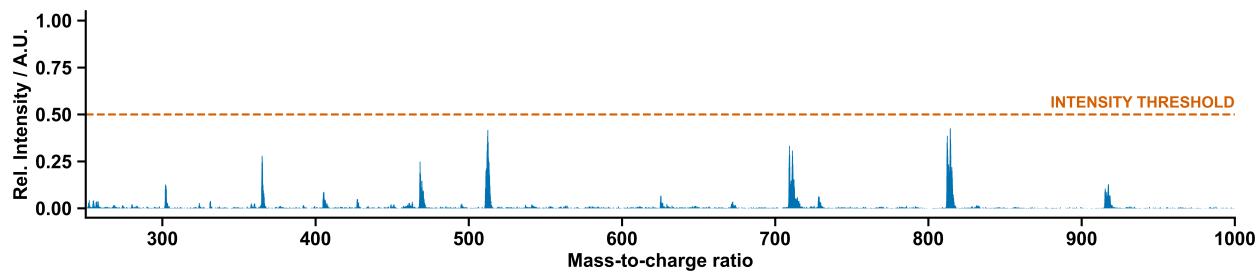
Scheme 98: Self-assembly of components 3, 17, with Silver(I) in a 3.0:1.5:1.0 molar ratio in  $\text{CH}_3\text{CN}$  at 60°C for 40h. These are the reagents (starting materials) for reaction 116.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: No reaction occurred.	
	Human MS Decision: Failed	MS Spectra Category: Reaction failed.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	NMR Criteria 2: N/A
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 0
		MS Criteria 3: Pass	Number of counter-ions found: 0

Decision Table 98: Human labeled and Decision maker labeled outcomes for the  $^1\text{H}$  NMR spectroscopy and UPLC-MS spectrometry of reaction 116. Decision motivations are also given.

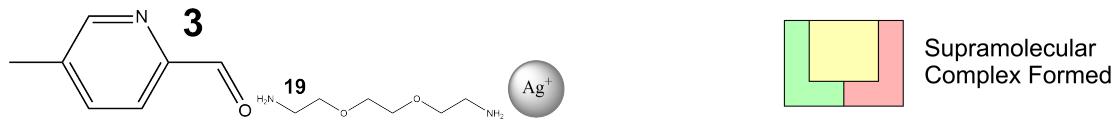


NMR Spectra 98: The stacked  $^1\text{H}$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 116.



MS Spectra 98: The ULPC-MS spectra of reaction 116. The intensity threshold is also shown.

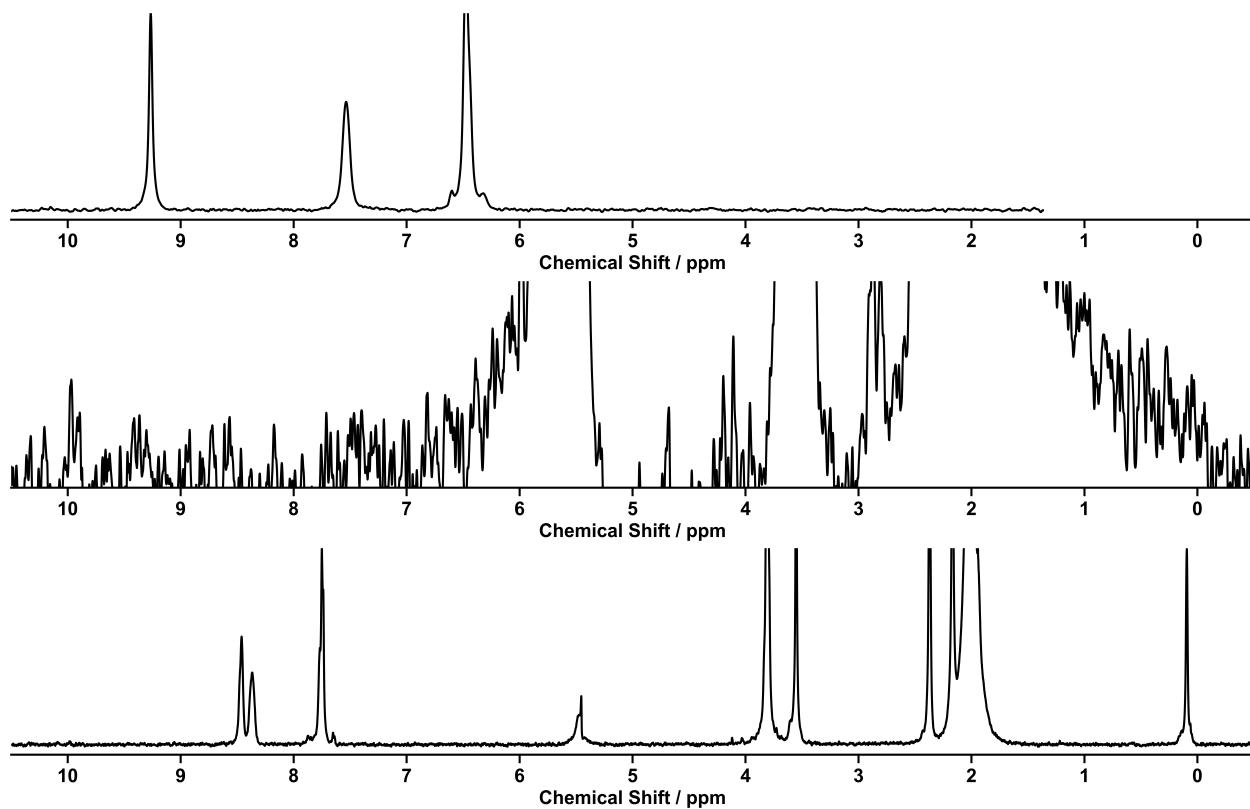
## Reaction 117



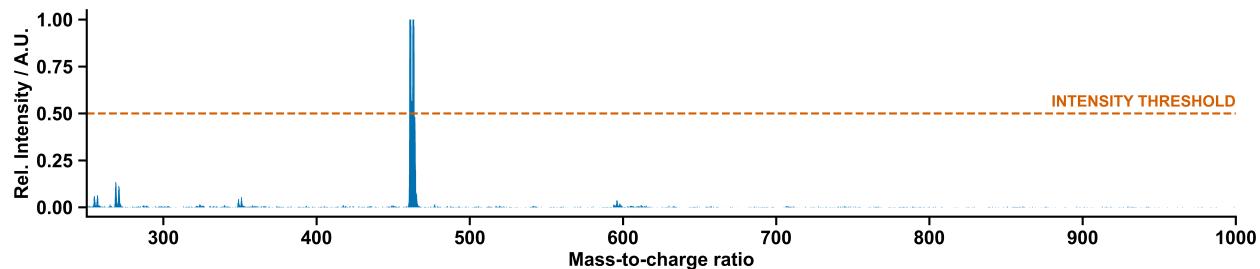
Scheme 99: Self-assembly of components 3, 19, with Silver(I) in a 3.0:1.5:1.0 molar ratio in CH<sub>3</sub>CN at 60°C for 40h. These are the reagents (starting materials) for reaction 117.

Human Reaction Decision: Pass	Human NMR Decision: Pass	NMR Spectra Category: Single discrete species formed.	
	Human MS Decision: Pass	MS Spectra Category: Reaction occurred, supramolecular product.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	
	Decision Maker MS Decision: Pass	NMR Criteria 2: N/A	MS Criteria 1 and 2: Pass
		Number of predicted peaks found in MS spectra with appropriate intensity: 3	Number of counter-ions found: 2
		MS Criteria 3: Pass	

Decision Table 99: Human labeled and Decision maker labeled outcomes for the <sup>1</sup>H NMR spectroscopy and ULPC-MS spectrometry of reaction 117. Decision motivations are also given.

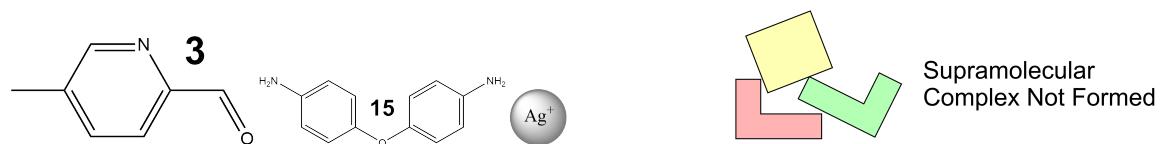


NMR Spectra 99: The stacked <sup>1</sup>H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 117.



MS Spectra 99: The ULPC-MS spectra of reaction 117. The intensity threshold is also shown.

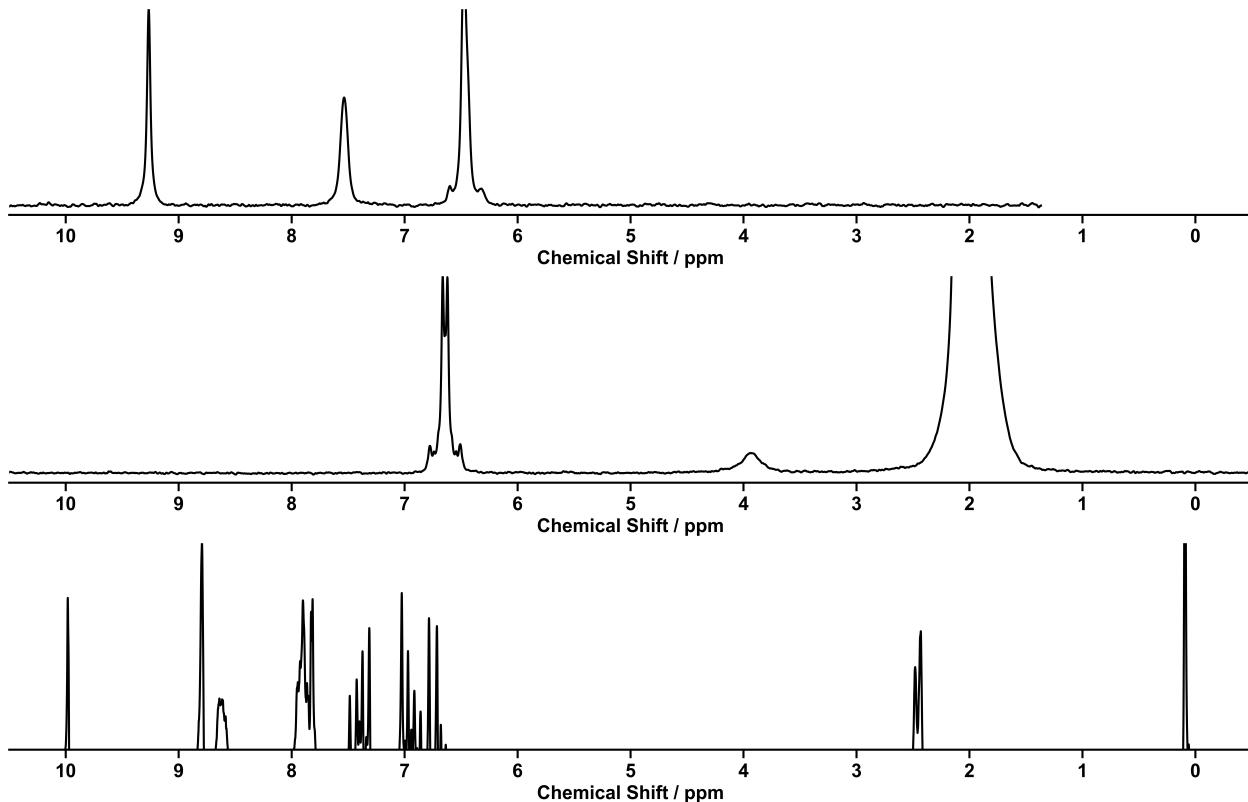
## Reaction 118



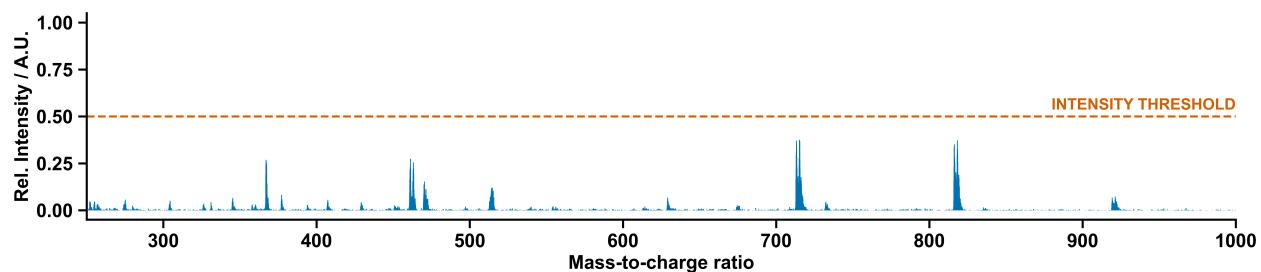
Scheme 100: Self-assembly of components 3, 15, with Silver(I) in a 3.0:1.5:1.0 molar ratio in  $\text{CH}_3\text{CN}$  at 60°C for 40h. These are the reagents (starting materials) for reaction 118.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: No reaction occurred.	
	Human MS Decision: Failed	MS Spectra Category: Reaction failed.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A		NMR Criteria 1: N/A
	Decision Maker MS Decision: Pass		NMR Criteria 2: N/A
	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 0	MS Criteria 3: Pass
			Number of counter-ions found: 0

Decision Table 100: Human labeled and Decsision maker labeled outcomes for the  $^1\text{H}$  NMR spectroscopy and ULPC-MS spectrometry of reaction 118. Decision motivations are also given.

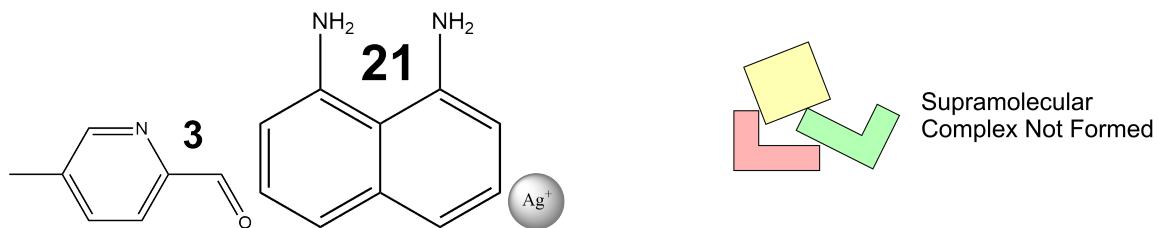


NMR Spectra 100: The stacked  $^1\text{H}$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 118.



MS Spectra 100: The ULPC-MS spectra of reaction 118. The intensity threshold is also shown.

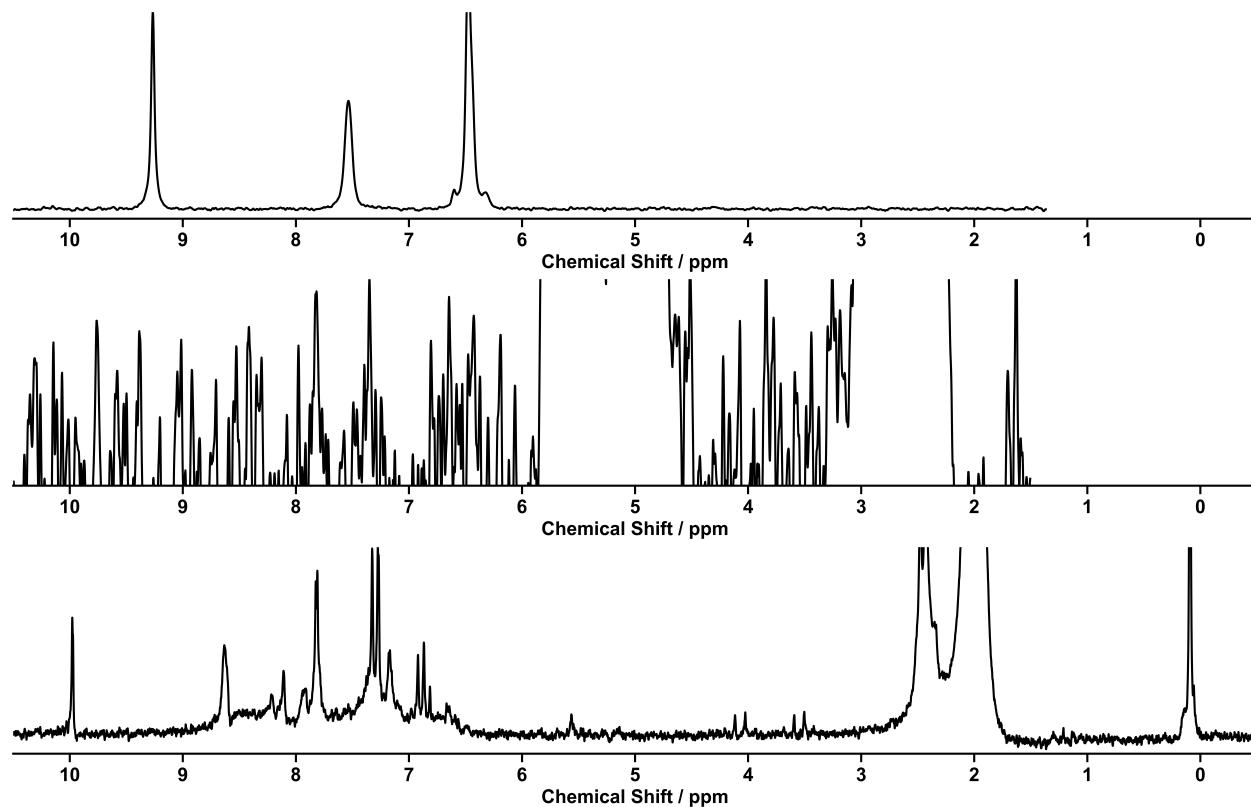
## Reaction 119



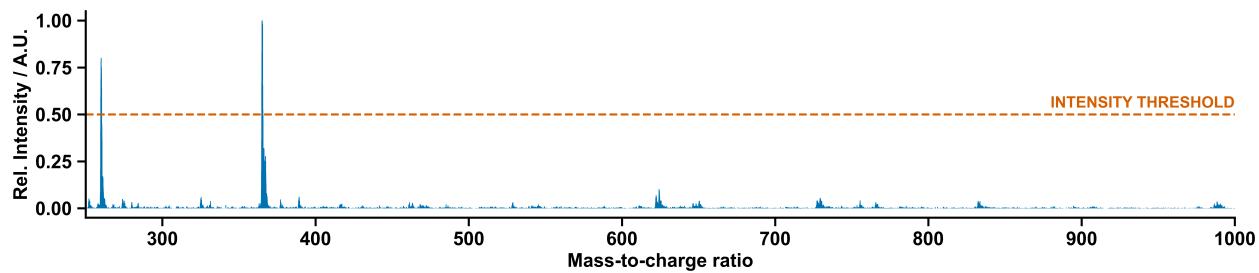
Scheme 101: Self-assembly of components 3, 21, with Silver(I) in a 3.0:1.5:1.0 molar ratio in  $\text{CH}_3\text{CN}$  at  $60^\circ\text{C}$  for 40h. These are the reagents (starting materials) for reaction 119.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: No reaction occurred.	
	Human MS Decision: Failed	MS Spectra Category: Reaction occurred, unknown product.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	NMR Criteria 2: N/A
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 0
		MS Criteria 3: Pass	Number of counter-ions found: 0

Decision Table 101: Human labeled and Decision maker labeled outcomes for the  $^1\text{H}$  NMR spectroscopy and UPLC-MS spectrometry of reaction 119. Decision motivations are also given.

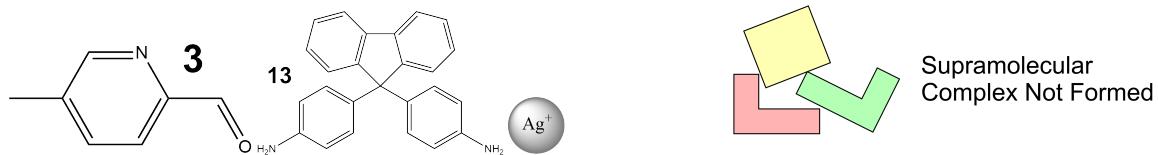


NMR Spectra 101: The stacked  $^1\text{H}$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 119.



MS Spectra 101: The ULPC-MS spectra of reaction 119. The intensity threshold is also shown.

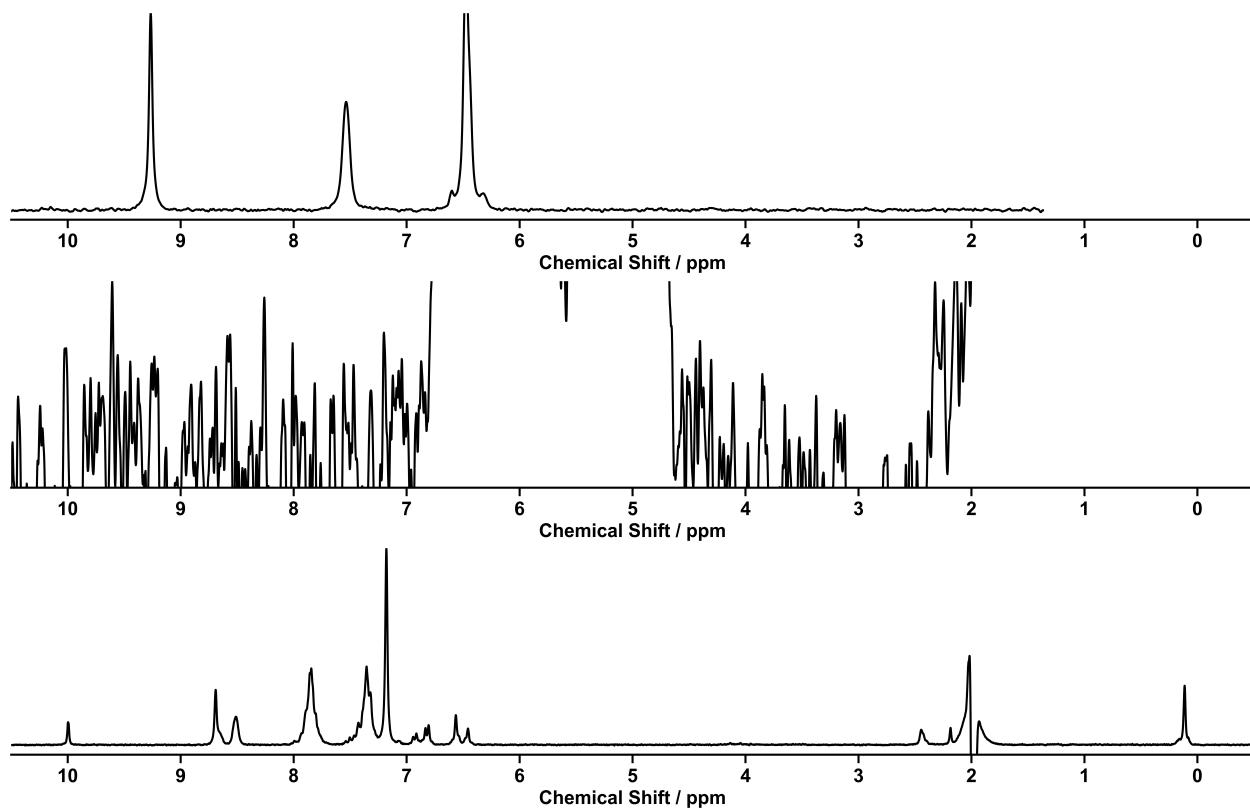
## Reaction 120



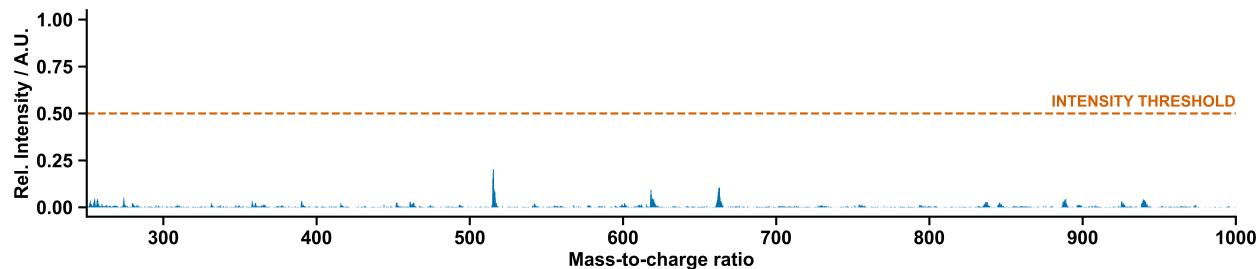
Scheme 102: Self-assembly of components 3, 13, with Silver(I) in a 3.0:1.5:1.0 molar ratio in  $\text{CH}_3\text{CN}$  at  $60^\circ\text{C}$  for 40h. These are the reagents (starting materials) for reaction 120.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: No reaction occurred.	
	Human MS Decision: Failed	MS Spectra Category: Reaction failed.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	NMR Criteria 2: N/A
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 0
		MS Criteria 3: Pass	Number of counter-ions found: 0

Decision Table 102: Human labeled and Decsision maker labeled outcomes for the  $^1\text{H}$  NMR spectroscopy and ULPC-MS spectrometry of reaction 120. Decision motivations are also given.

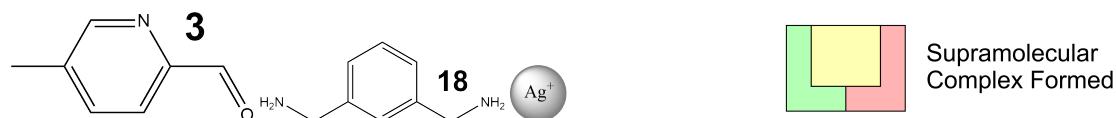


NMR Spectra 102: The stacked <sup>1</sup>H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 120.



MS Spectra 102: The ULPC-MS spectra of reaction 120. The intensity threshold is also shown.

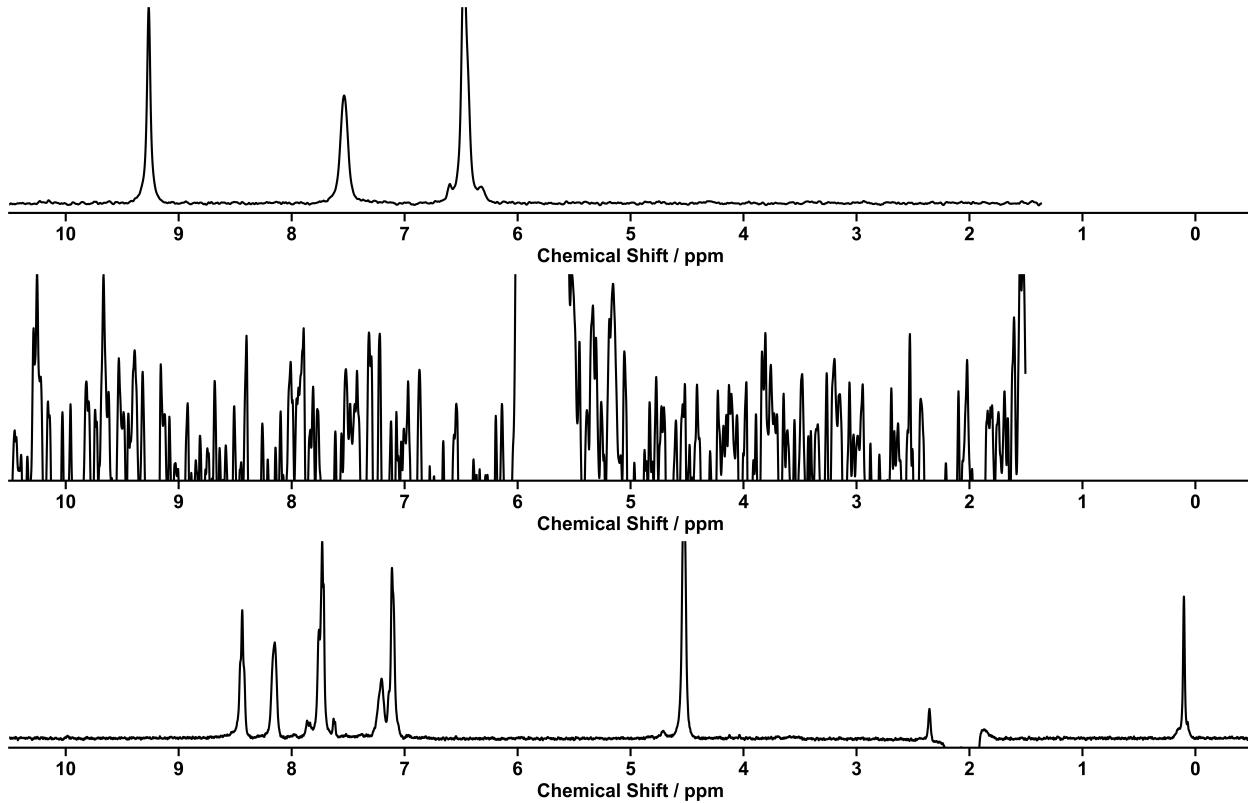
## Reaction 123



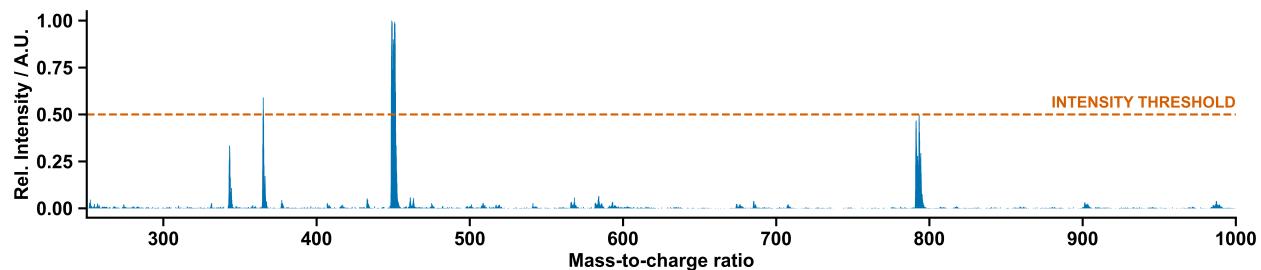
Scheme 103: Self-assembly of components 3, 18, with Silver(I) in a 3.0:1.5:1.0 molar ratio in CH<sub>3</sub>CN at 60°C for 40h. These are the reagents (starting materials) for reaction 123.

Human Reaction Decision: Pass	Human NMR Decision: Pass	NMR Spectra Category: Single discrete species formed.	
	Human MS Decision: Pass	MS Spectra Category: Reaction occurred, supramolecular product.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	
		NMR Criteria 2: N/A	
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 3
		MS Criteria 3: Pass	Number of counter-ions found: 2

Decision Table 103: Human labeled and Decsision maker labeled outcomes for the  $^1\text{H}$  NMR spectroscopy and ULPC-MS spectrometry of reaction 123. Decision motivations are also given.

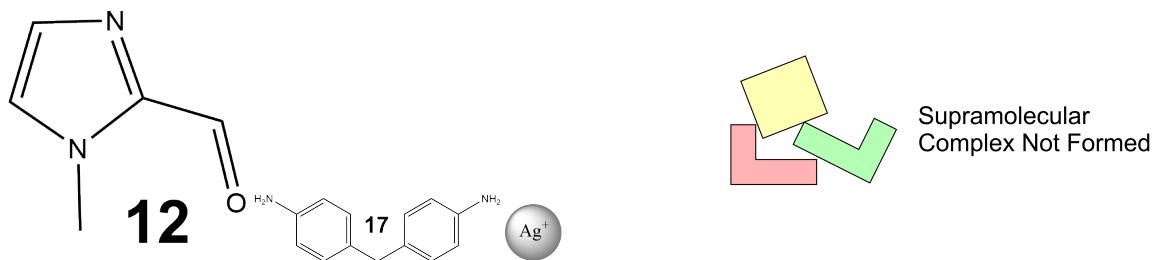


NMR Spectra 103: The stacked  $^1\text{H}$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 123.



MS Spectra 103: The ULPC-MS spectra of reaction 123. The intensity threshold is also shown.

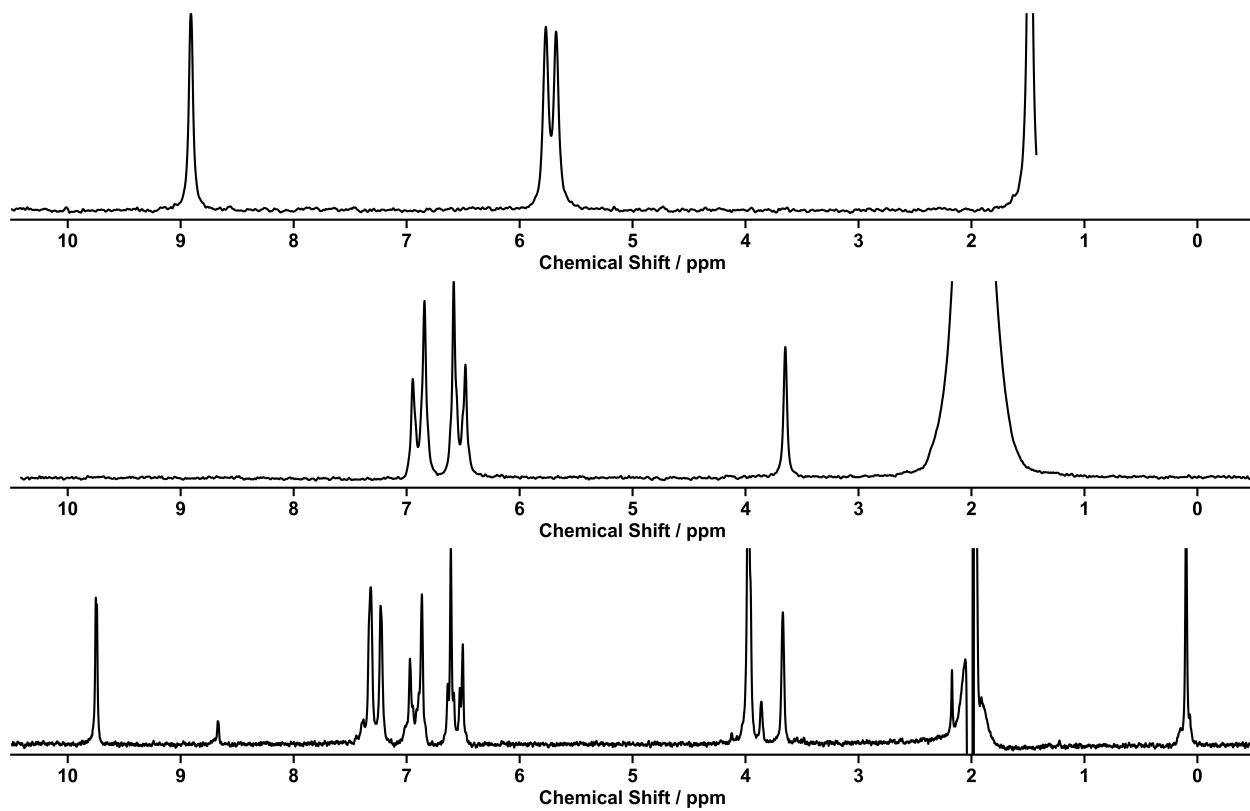
## Reaction 124



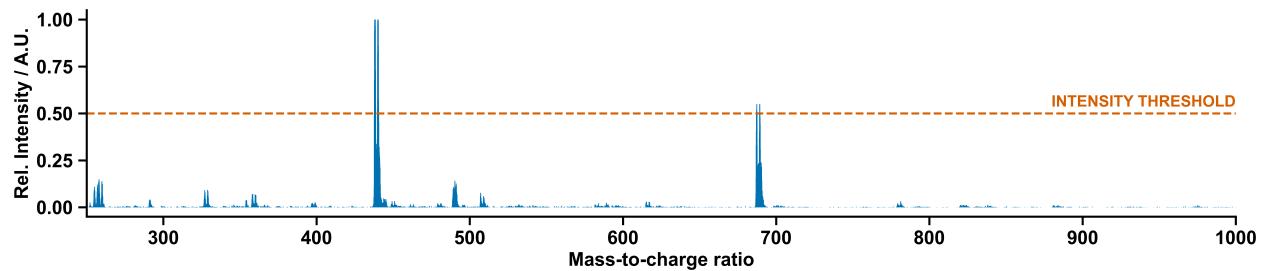
Scheme 104: Self-assembly of components 12, 17, with Silver(I) in a 3.0:1.5:1.0 molar ratio in  $\text{CH}_3\text{CN}$  at 60°C for 40h. These are the reagents (starting materials) for reaction 124.

Human Reaction Decision: Failed	Human NMR Decision: Pass	NMR Spectra Category: Single discrete species formed.	
	Human MS Decision: Failed	MS Spectra Category: Reaction occurred, unknown product.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	
	Decision Maker MS Decision: Pass	NMR Criteria 2: N/A	MS Criteria 1 and 2: Pass
		Number of predicted peaks found in MS spectra with appropriate intensity: 0	Number of counter-ions found: 0
	MS Criteria 3: Pass		

Decision Table 104: Human labeled and Decsision maker labeled outcomes for the  $^1\text{H}$  NMR spectroscopy and UPLC-MS spectrometry of reaction 124. Decision motivations are also given.

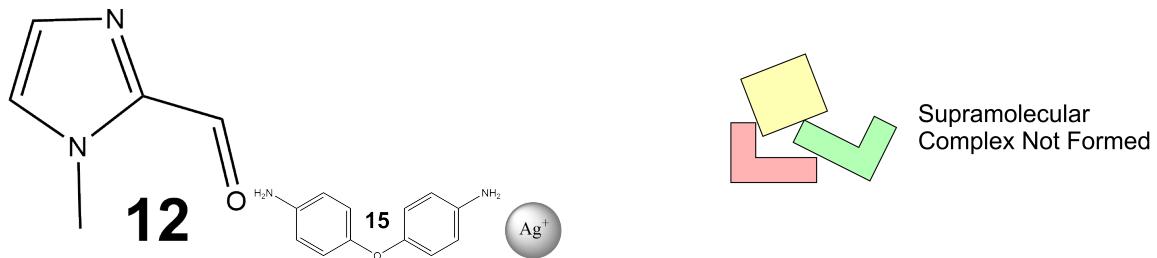


NMR Spectra 104: The stacked  $^1\text{H}$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 124.



MS Spectra 104: The ULPC-MS spectra of reaction 124. The intensity threshold is also shown.

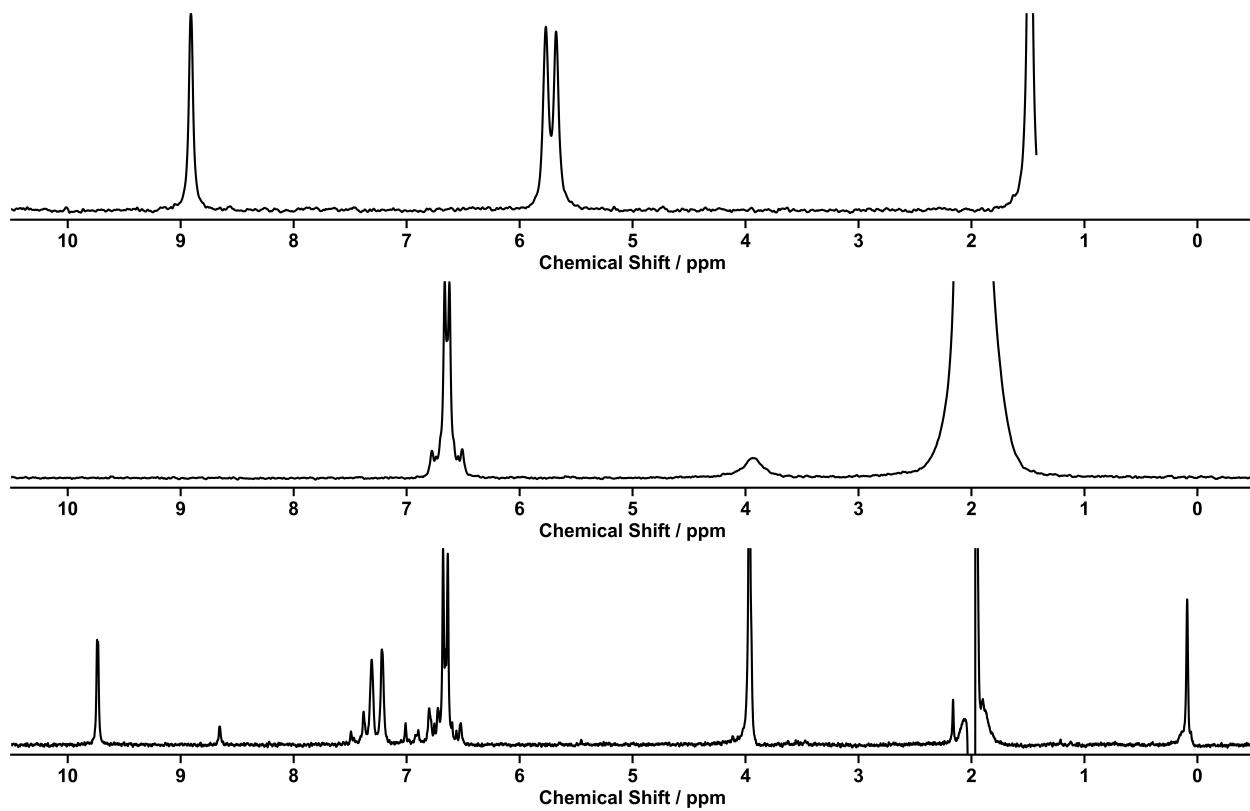
## Reaction 126



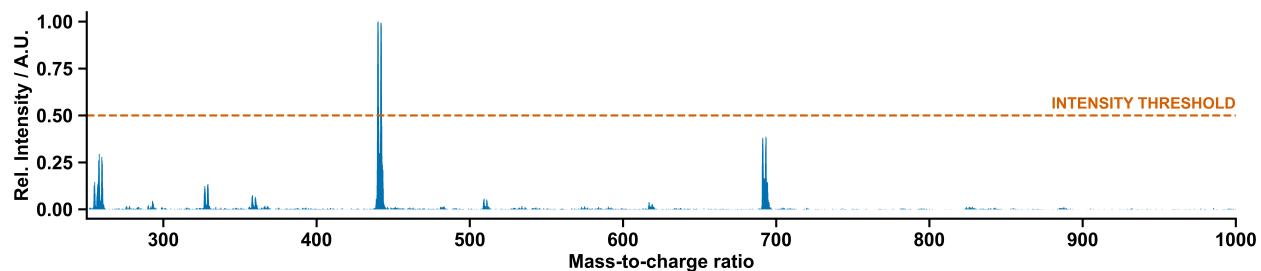
Scheme 105: Self-assembly of components 12, 15, with Silver(I) in a 3.0:1.5:1.0 molar ratio in  $\text{CH}_3\text{CN}$  at 60°C for 40h. These are the reagents (starting materials) for reaction 126.

Human Reaction Decision: Failed	Human NMR Decision: Pass	NMR Spectra Category: Single discrete species formed.
	Human MS Decision: Failed	MS Spectra Category: Reaction occurred, unknown product.
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A
	Decision Maker MS Decision: Pass	NMR Criteria 2: N/A
	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 0
	MS Criteria 3: Pass	Number of counter-ions found: 0

Decision Table 105: Human labeled and Decision maker labeled outcomes for the  $^1\text{H}$  NMR spectroscopy and UPLC-MS spectrometry of reaction 126. Decision motivations are also given.

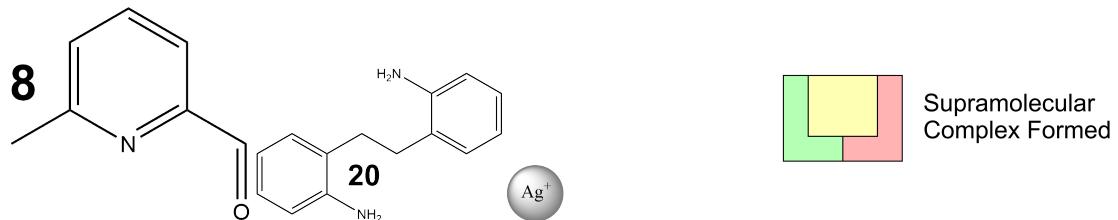


NMR Spectra 105: The stacked  $^1\text{H}$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 126.



MS Spectra 105: The ULPC-MS spectra of reaction 126. The intensity threshold is also shown.

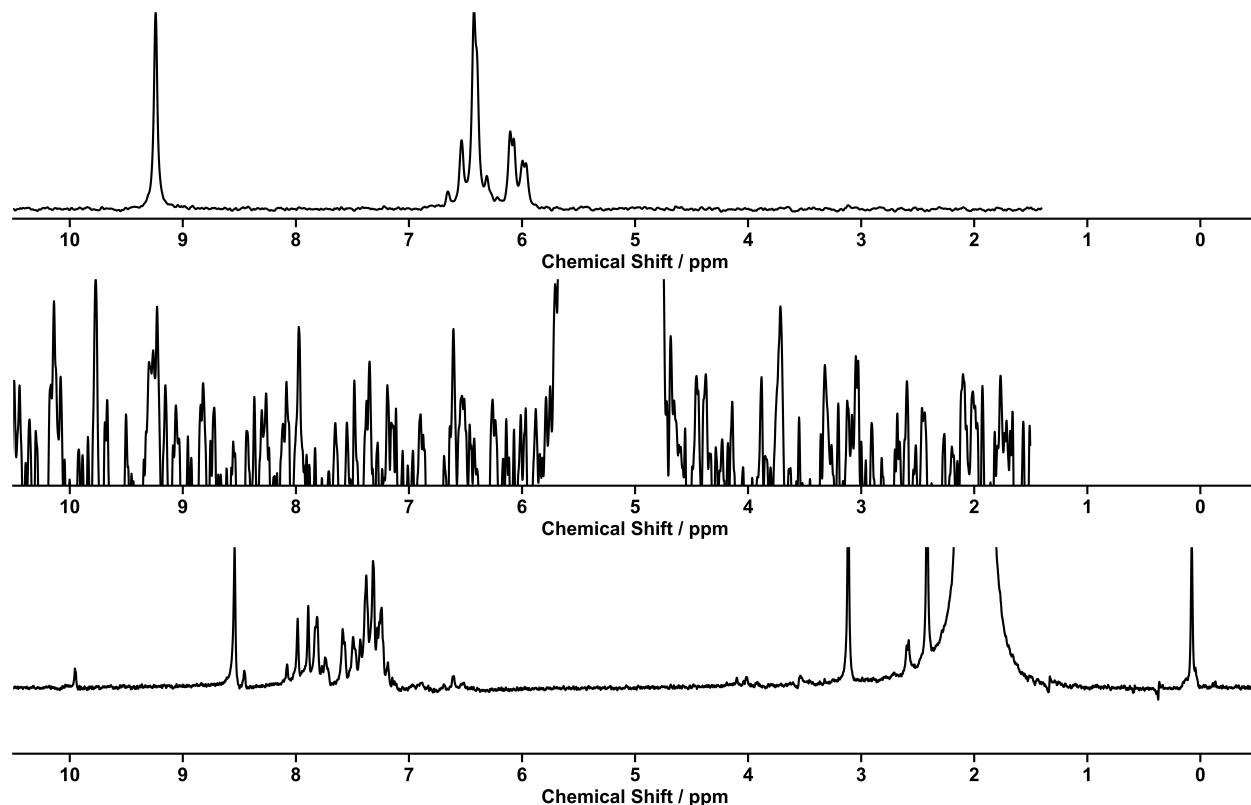
## Reaction 127



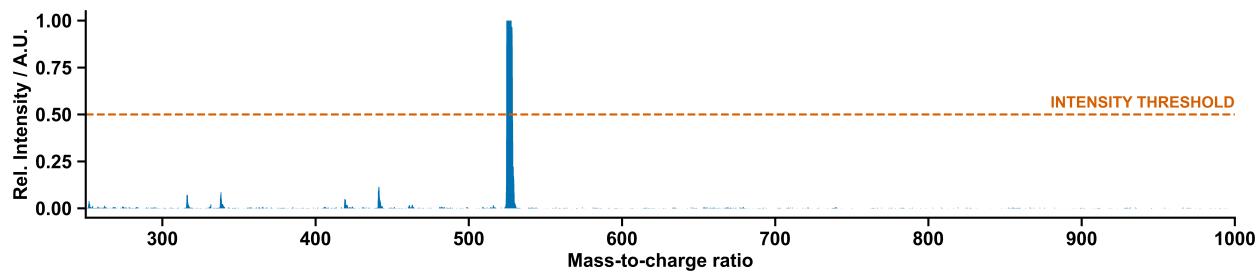
Scheme 106: Self-assembly of components 8, 20, with Silver(I) in a 3.0:1.5:1.0 molar ratio in  $\text{CH}_3\text{CN}$  at 60°C for 40h. These are the reagents (starting materials) for reaction 127.

Human Reaction Decision: Pass	Human NMR Decision: Pass	NMR Spectra Category: Single discrete species formed.	
	Human MS Decision: Pass	MS Spectra Category: Reaction occurred, supramolecular product.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	NMR Criteria 2: N/A
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 3
		MS Criteria 3: Pass	Number of counter-ions found: 2

Decision Table 106: Human labeled and Decision maker labeled outcomes for the  $^1\text{H}$  NMR spectroscopy and UPLC-MS spectrometry of reaction 127. Decision motivations are also given.

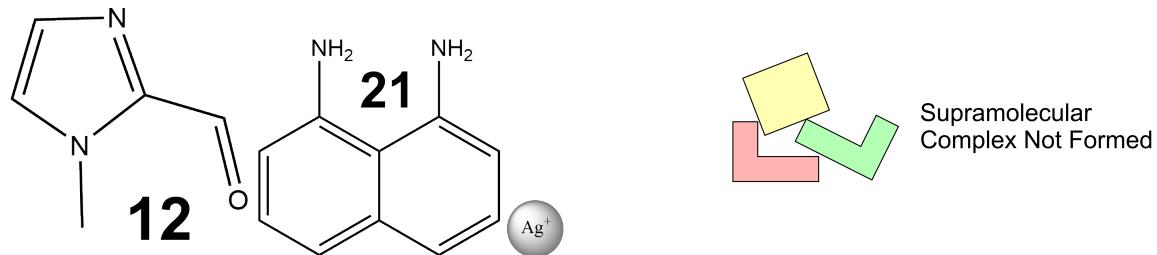


NMR Spectra 106: The stacked  $^1\text{H}$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 127.



MS Spectra 106: The ULPC-MS spectra of reaction 127. The intensity threshold is also shown.

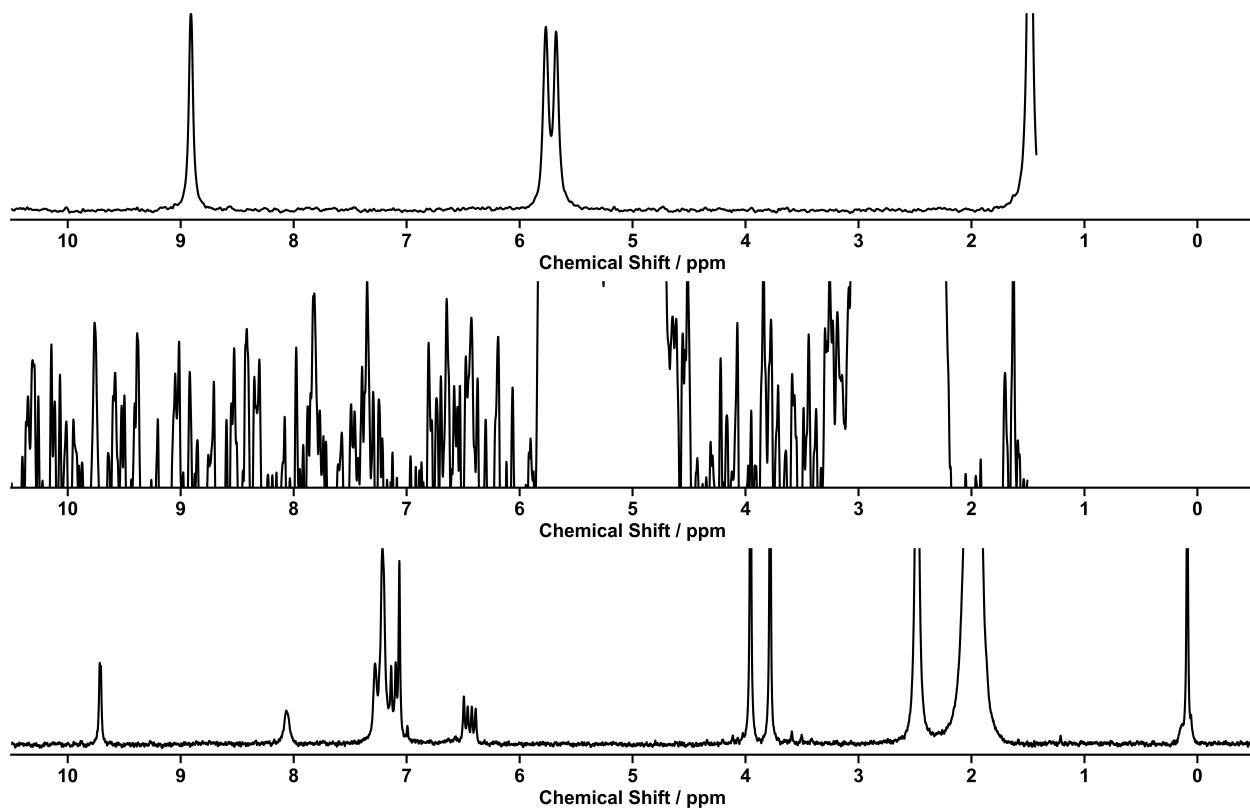
## Reaction 128



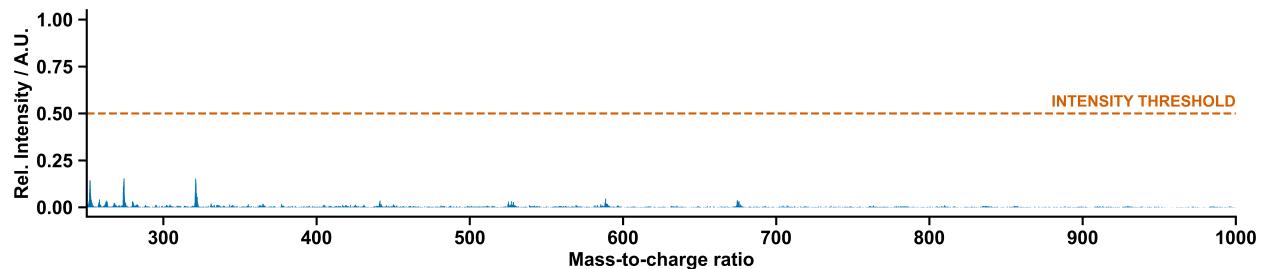
Scheme 107: Self-assembly of components 12, 21, with Silver(I) in a 3.0:1.5:1.0 molar ratio in  $\text{CH}_3\text{CN}$  at 60°C for 40h. These are the reagents (starting materials) for reaction 128.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: No reaction occurred.	
	Human MS Decision: Failed	MS Spectra Category: Reaction failed.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	NMR Criteria 2: N/A
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 0
		MS Criteria 3: Pass	Number of counter-ions found: 0

Decision Table 107: Human labeled and Decision maker labeled outcomes for the  $^1\text{H}$  NMR spectroscopy and ULPC-MS spectrometry of reaction 128. Decision motivations are also given.

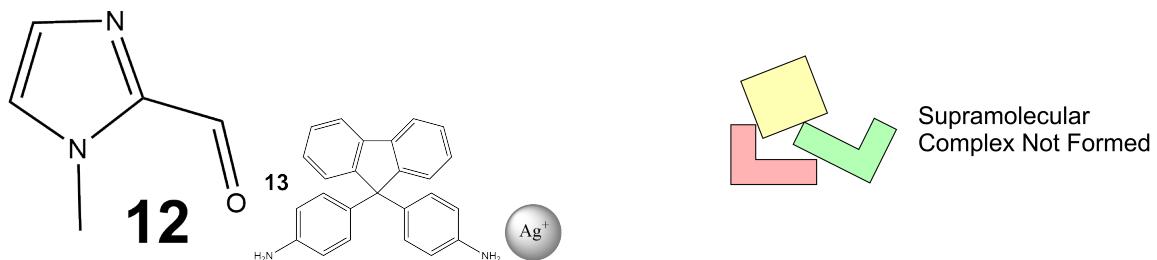


NMR Spectra 107: The stacked  $^1\text{H}$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 128.



MS Spectra 107: The ULPC-MS spectra of reaction 128. The intensity threshold is also shown.

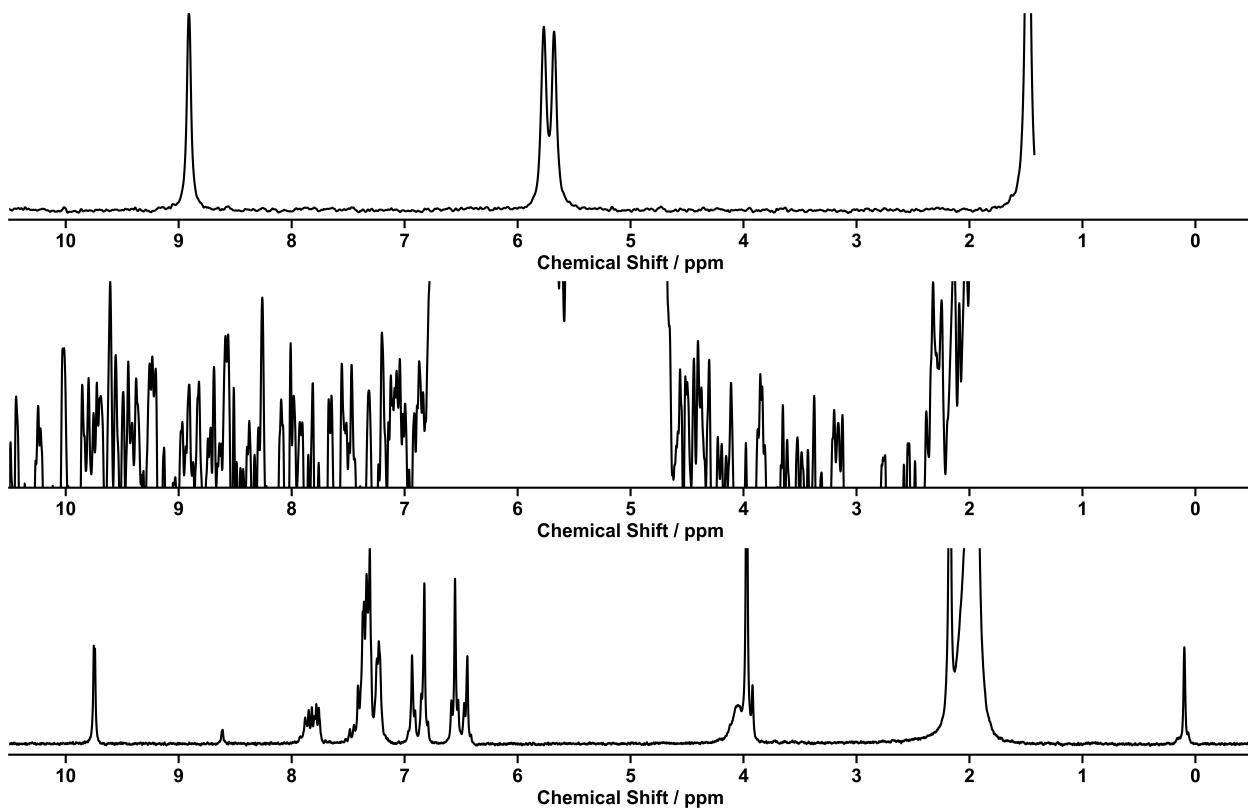
## Reaction 129



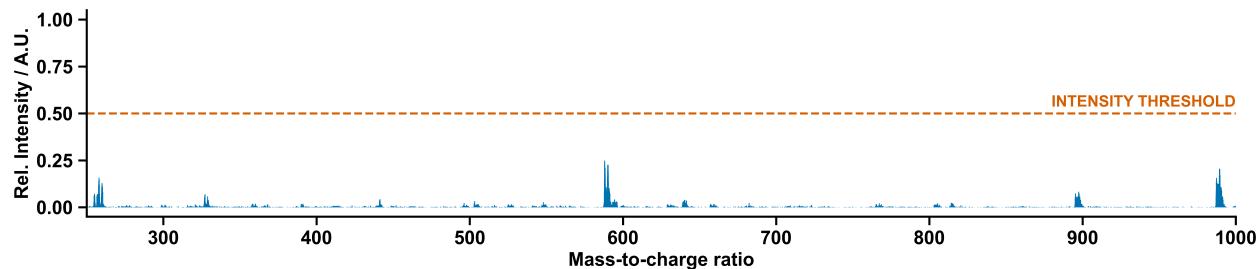
Scheme 108: Self-assembly of components 12, 13, with Silver(I) in a 3.0:1.5:1.0 molar ratio in CH<sub>3</sub>CN at 60°C for 40h. These are the reagents (starting materials) for reaction 129.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: No reaction occurred.	
	Human MS Decision: Failed	MS Spectra Category: Reaction failed.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	
	Decision Maker MS Decision: Pass	NMR Criteria 2: N/A	MS Criteria 1 and 2: Pass
		Number of predicted peaks found in MS spectra with appropriate intensity: 0	
		MS Criteria 3: Pass	Number of counter-ions found: 0

Decision Table 108: Human labeled and Decsision maker labeled outcomes for the <sup>1</sup>H NMR spectroscopy and UPLC-MS spectrometry of reaction 129. Decision motivations are also given.

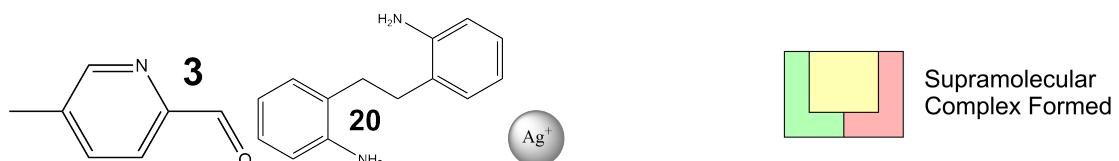


NMR Spectra 108: The stacked <sup>1</sup>H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 129.



MS Spectra 108: The ULPC-MS spectra of reaction 129. The intensity threshold is also shown.

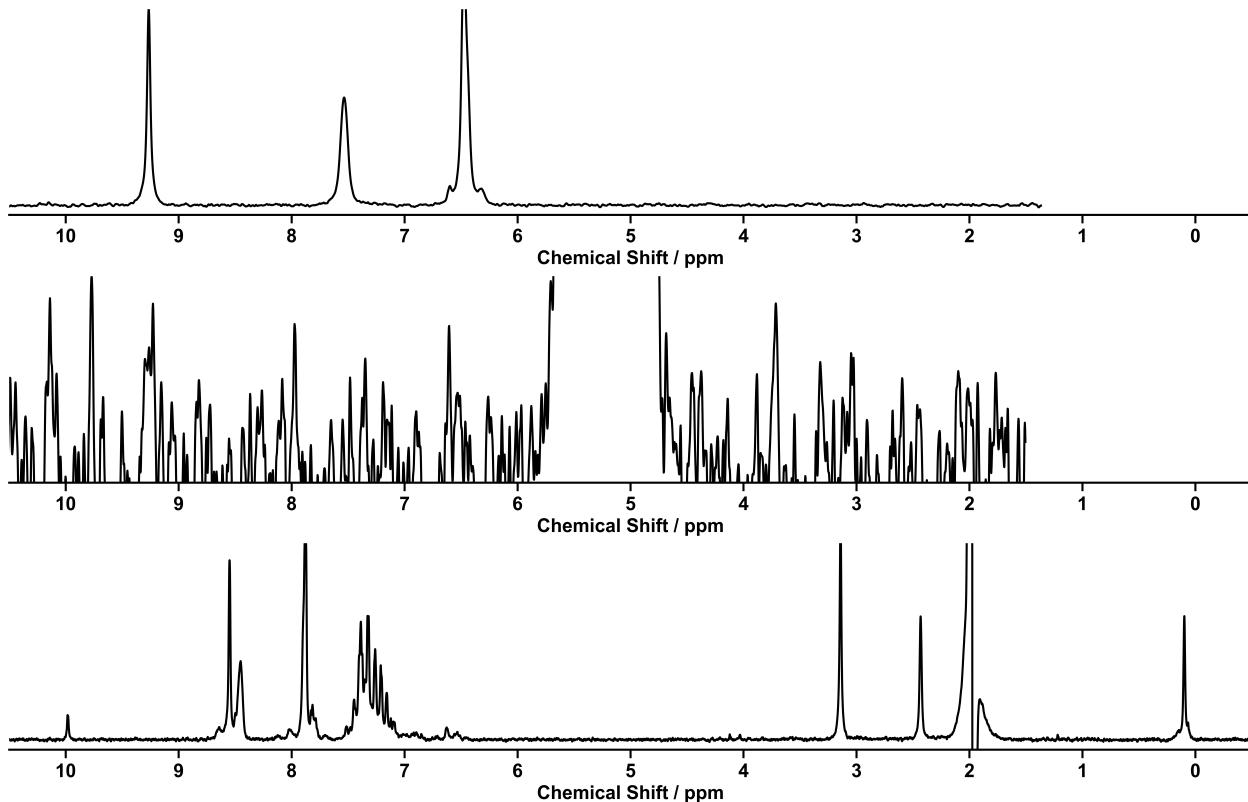
## Reaction 131



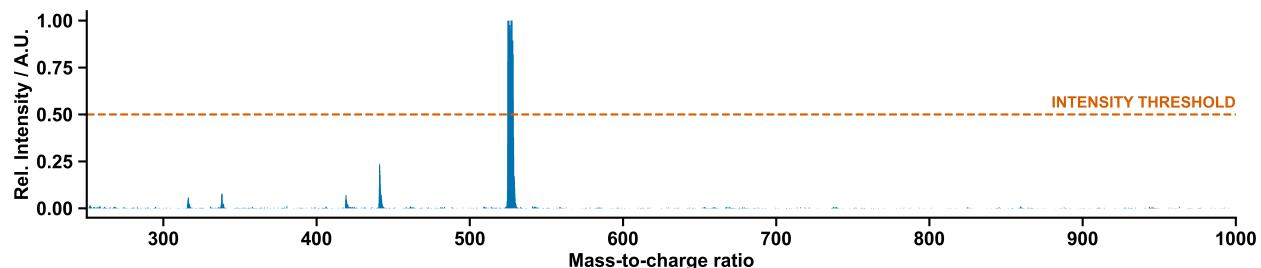
Scheme 109: Self-assembly of components 3, 20, with Silver(I) in a 3.0:1.5:1.0 molar ratio in  $\text{CH}_3\text{CN}$  at 60°C for 40h. These are the reagents (starting materials) for reaction 131.

Human Reaction Decision: Pass	Human NMR Decision: Pass	NMR Spectra Category: Single discrete species formed.	
	Human MS Decision: Pass	MS Spectra Category: Reaction occurred, supramolecular product.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	
		NMR Criteria 2: N/A	
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 3
		MS Criteria 3: Pass	Number of counter-ions found: 2

Decision Table 109: Human labeled and Decsision maker labeled outcomes for the  $^1\text{H}$  NMR spectroscopy and ULPC-MS spectrometry of reaction 131. Decision motivations are also given.

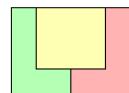
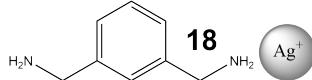
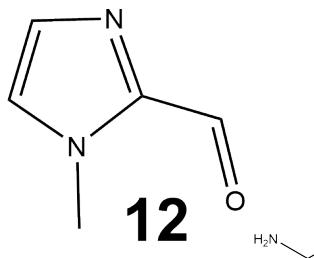


NMR Spectra 109: The stacked  $^1\text{H}$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 131.



MS Spectra 109: The ULPC-MS spectra of reaction 131. The intensity threshold is also shown.

## Reaction 132

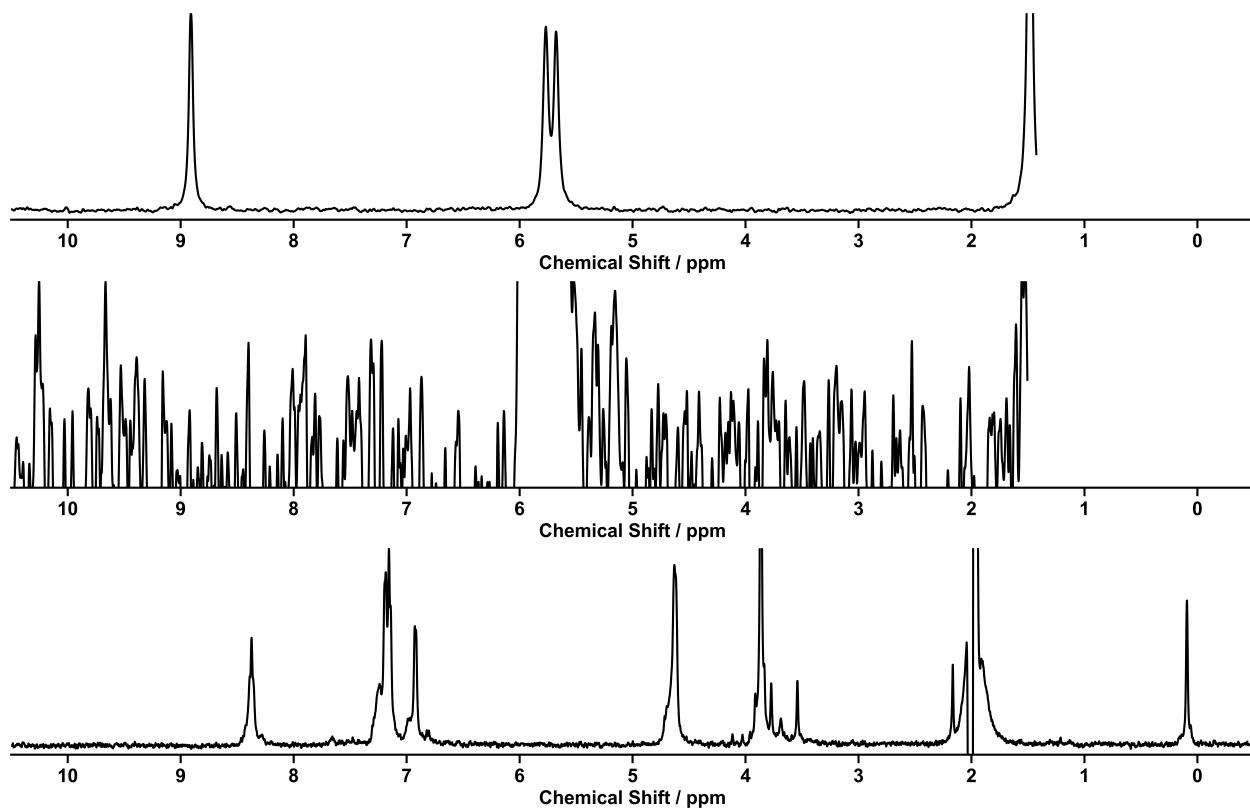


Supramolecular  
Complex Formed

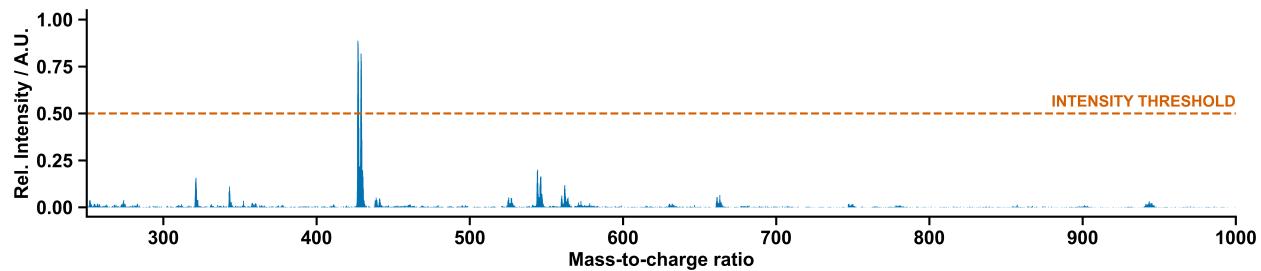
Scheme 110: Self-assembly of components 12, 18, with Silver(I) in a 3.0:1.5:1.0 molar ratio in CH<sub>3</sub>CN at 60°C for 40h. These are the reagents (starting materials) for reaction 132.

Human Reaction Decision: Pass	Human NMR Decision: Pass	NMR Spectra Category: Single discrete species formed.	
	Human MS Decision: Pass	MS Spectra Category: Reaction occurred, supramolecular product.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	NMR Criteria 2: N/A
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 0
		MS Criteria 3: Pass	Number of counter-ions found: 0

Decision Table 110: Human labeled and Decsision maker labeled outcomes for the <sup>1</sup>H NMR spectroscopy and UPLC-MS spectrometry of reaction 132. Decision motivations are also given.

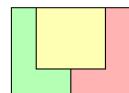
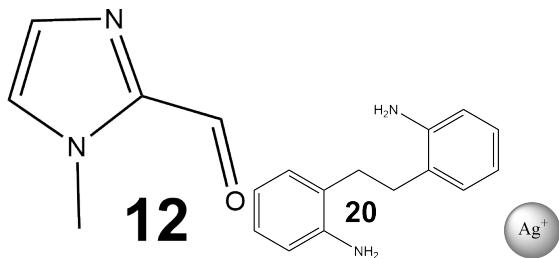


NMR Spectra 110: The stacked  $^1\text{H}$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 132.



MS Spectra 110: The ULPC-MS spectra of reaction 132. The intensity threshold is also shown.

## Reaction 133

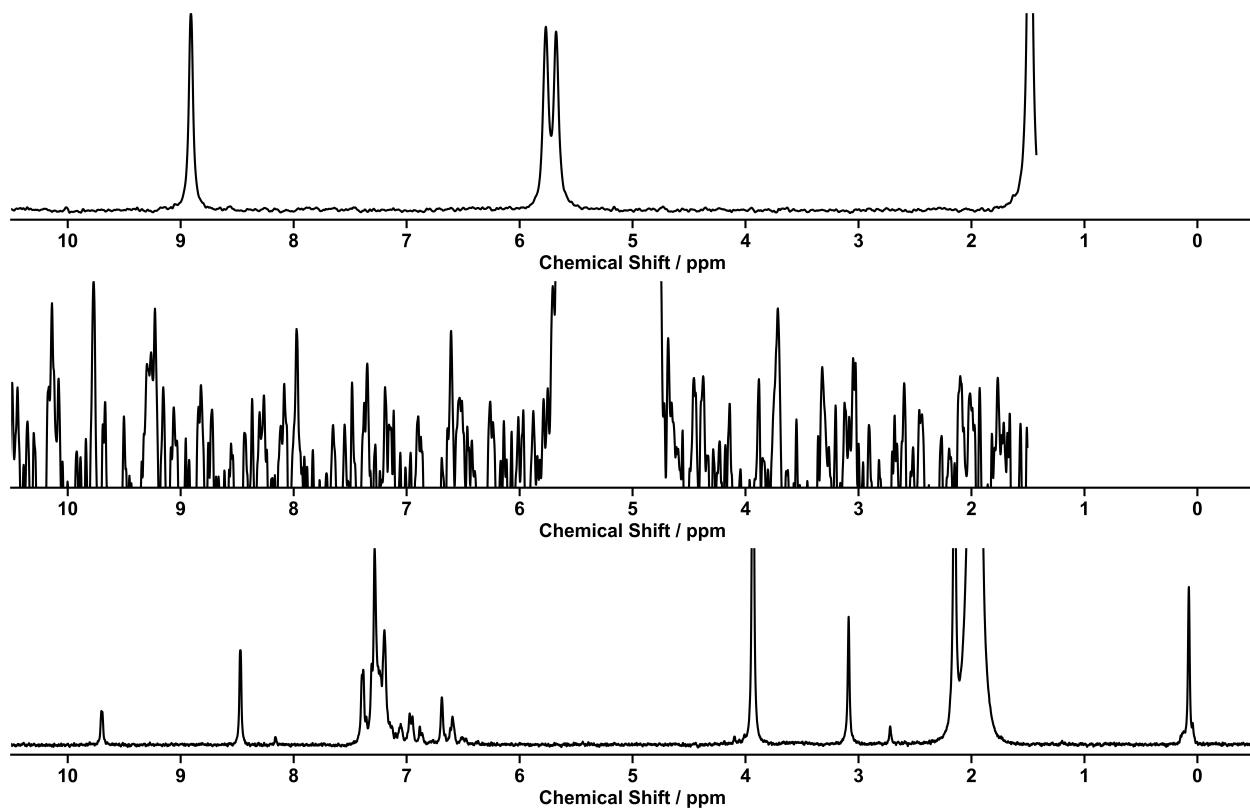


Supramolecular  
Complex Formed

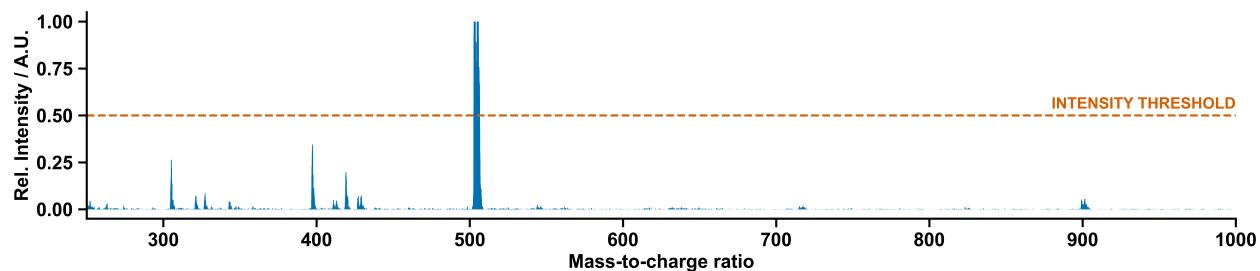
Scheme 111: Self-assembly of components 12, 20, with Silver(I) in a 3.0:1.5:1.0 molar ratio in  $\text{CH}_3\text{CN}$  at 60°C for 40h. These are the reagents (starting materials) for reaction 133.

Human Reaction Decision: Pass	Human NMR Decision: Pass	NMR Spectra Category: Single discrete species formed.	
	Human MS Decision: Pass	MS Spectra Category: Reaction occurred, supramolecular product.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	
		NMR Criteria 2: N/A	
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 3
		MS Criteria 3: Pass	Number of counter-ions found: 2

Decision Table 111: Human labeled and Decsision maker labeled outcomes for the  $^1\text{H}$  NMR spectroscopy and UPLC-MS spectrometry of reaction 133. Decision motivations are also given.

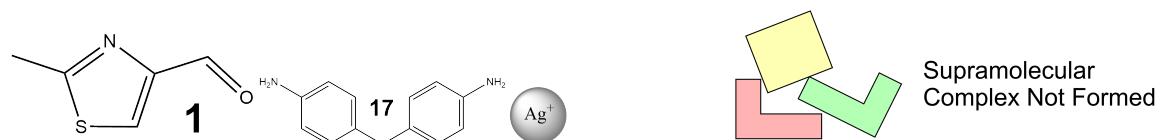


NMR Spectra 111: The stacked <sup>1</sup>H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 133.



MS Spectra 111: The ULPC-MS spectra of reaction 133. The intensity threshold is also shown.

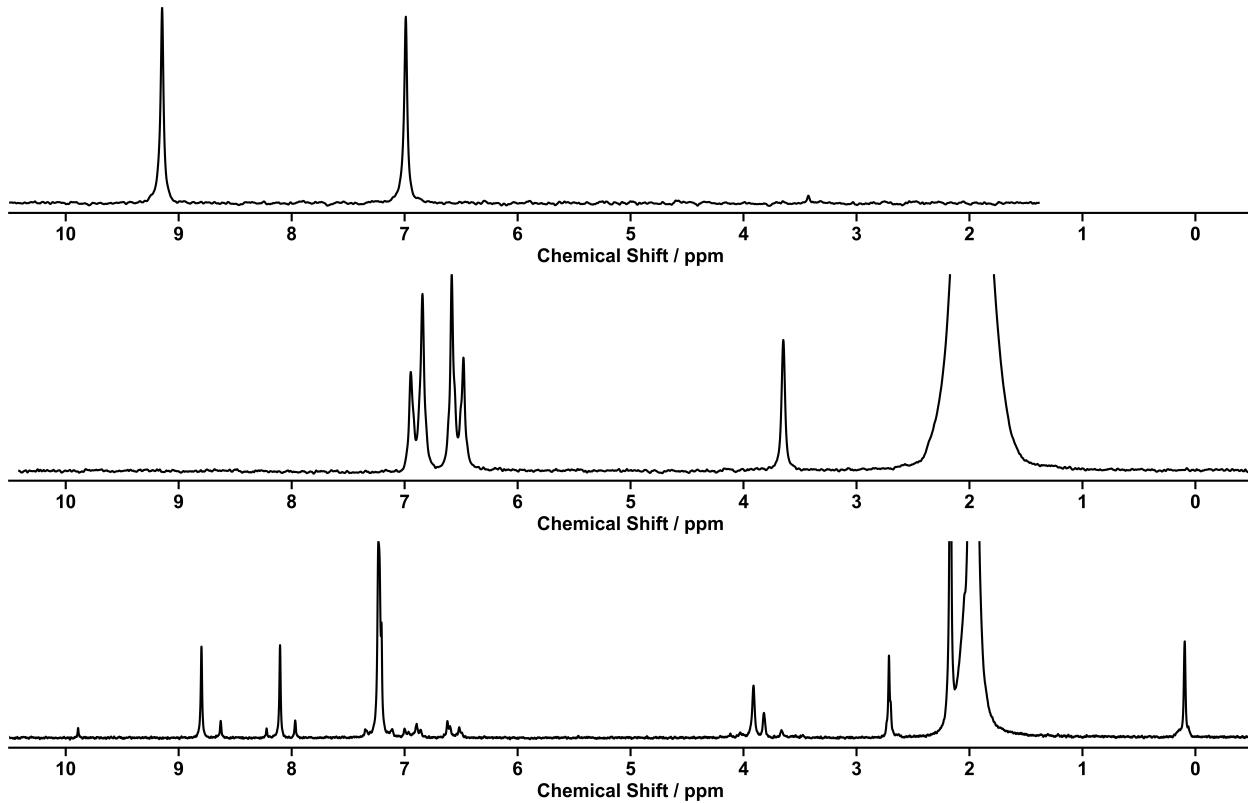
## Reaction 134



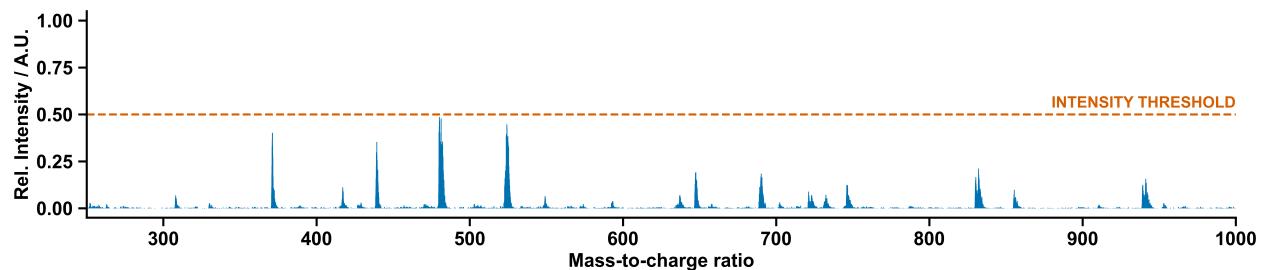
Scheme 112: Self-assembly of components 1, 17, with Silver(I) in a 3.0:1.5:1.0 molar ratio in  $\text{CH}_3\text{CN}$  at 60°C for 40h. These are the reagents (starting materials) for reaction 134.

Human Reaction Decision: Failed	Human NMR Decision: Pass	NMR Spectra Category: Single discrete species formed.	
	Human MS Decision: Failed	MS Spectra Category: Reaction failed.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	
	Decision Maker MS Decision: Pass	NMR Criteria 2: N/A	MS Criteria 1 and 2: Pass Number of predicted peaks found in MS spectra with appropriate intensity: 0
	MS Criteria 3: Pass	Number of counter-ions found: 0	

Decision Table 112: Human labeled and Decsision maker labeled outcomes for the  $^1\text{H}$  NMR spectroscopy and ULPC-MS spectrometry of reaction 134. Decision motivations are also given.

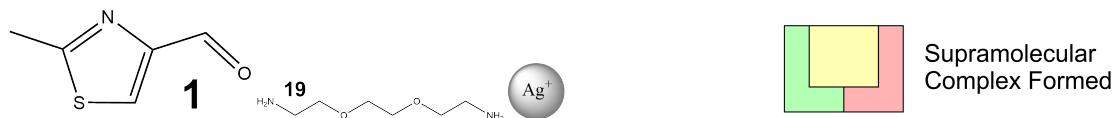


NMR Spectra 112: The stacked  $^1\text{H}$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 134.



MS Spectra 112: The ULPC-MS spectra of reaction 134. The intensity threshold is also shown.

## Reaction 135

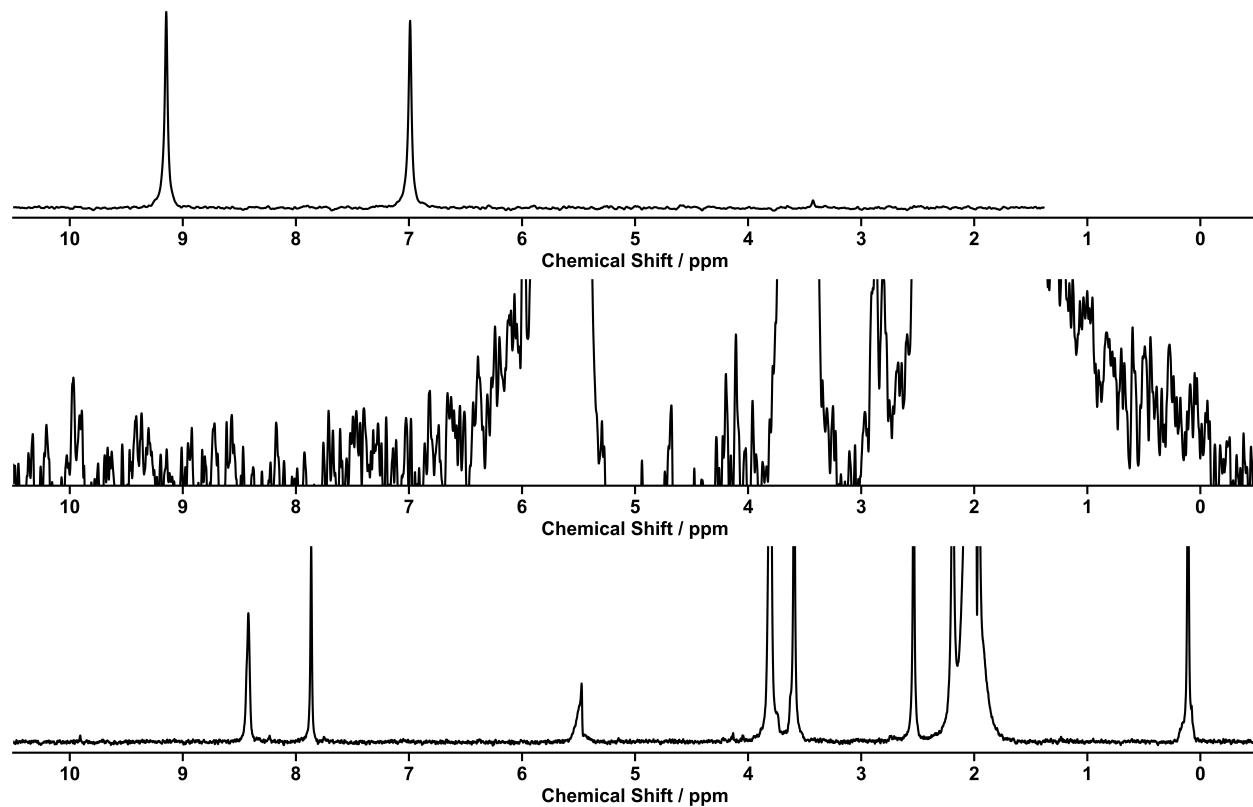


Supramolecular  
Complex Formed

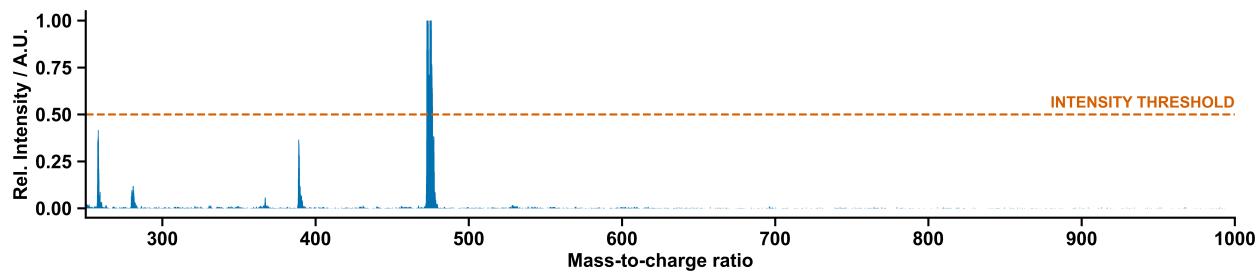
Scheme 113: Self-assembly of components **1**, **19**, with Silver(I) in a 3.0:1.5:1.0 molar ratio in  $\text{CH}_3\text{CN}$  at 60°C for 40h. These are the reagents (starting materials) for reaction 135.

Human Reaction Decision: Pass	Human NMR Decision: Pass	NMR Spectra Category: Single discrete species formed.	
	Human MS Decision: Pass	MS Spectra Category: Reaction occurred, supramolecular product.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	NMR Criteria 2: N/A
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 3
		MS Criteria 3: Pass	Number of counter-ions found: 2

Decision Table 113: Human labeled and Decision maker labeled outcomes for the  $^1\text{H}$  NMR spectroscopy and UPLC-MS spectrometry of reaction 135. Decision motivations are also given.

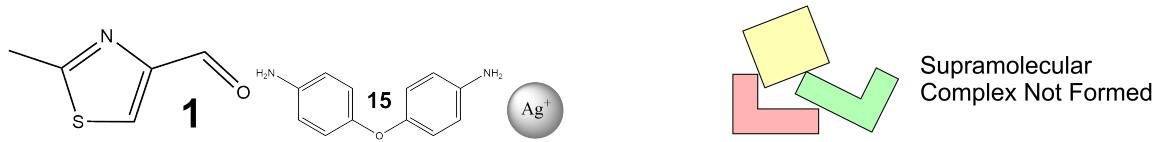


NMR Spectra 113: The stacked  $^1\text{H}$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 135.



MS Spectra 113: The ULPC-MS spectra of reaction 135. The intensity threshold is also shown.

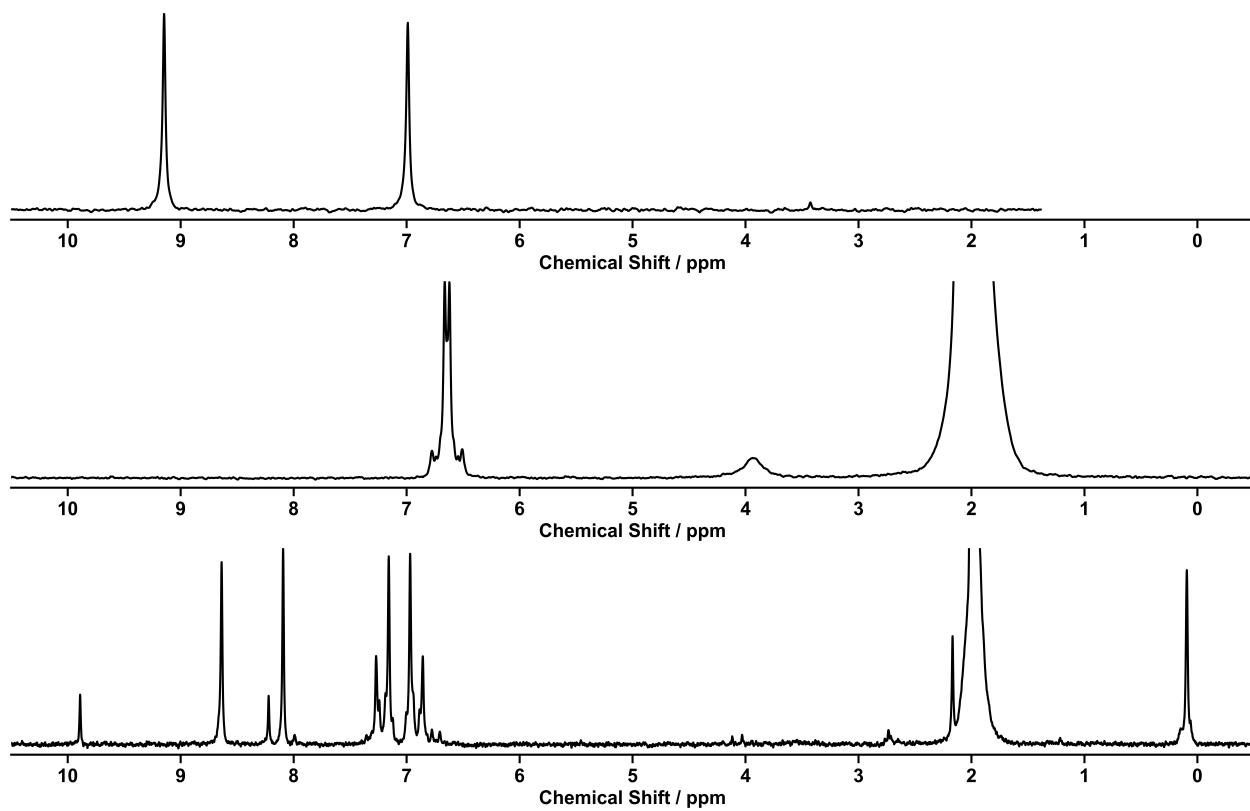
## Reaction 136



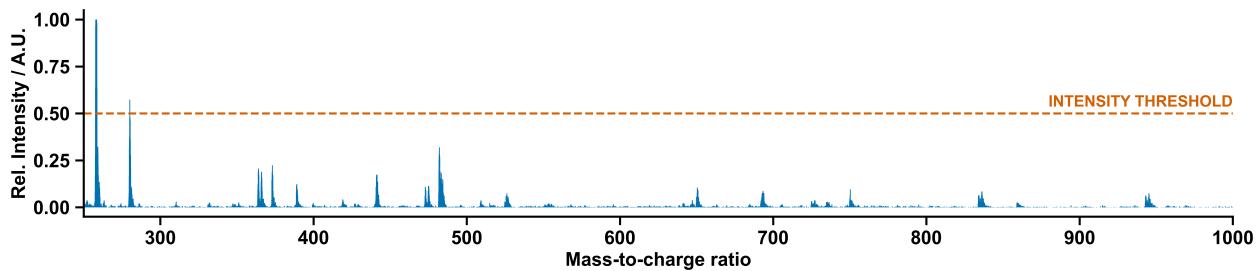
Scheme 114: Self-assembly of components 1, 15, with Silver(I) in a 3.0:1.5:1.0 molar ratio in  $\text{CH}_3\text{CN}$  at  $60^\circ\text{C}$  for 40h. These are the reagents (starting materials) for reaction 136.

Human Reaction Decision: Failed	Human NMR Decision: Pass	NMR Spectra Category: Single discrete species formed.	
	Human MS Decision: Failed	MS Spectra Category: Reaction occurred, unknown product.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	
	Decision Maker MS Decision: Pass	NMR Criteria 2: N/A	MS Criteria 1 and 2: Pass
		Number of predicted peaks found in MS spectra with appropriate intensity: 0	MS Criteria 3: Pass
		Number of counter-ions found: 0	

Decision Table 114: Human labeled and Decsision maker labeled outcomes for the  $^1\text{H}$  NMR spectroscopy and ULPC-MS spectrometry of reaction 136. Decision motivations are also given.

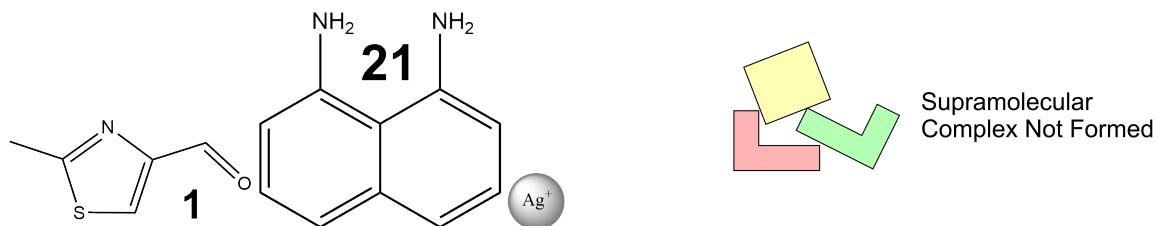


NMR Spectra 114: The stacked  $^1\text{H}$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 136.



MS Spectra 114: The ULPC-MS spectra of reaction 136. The intensity threshold is also shown.

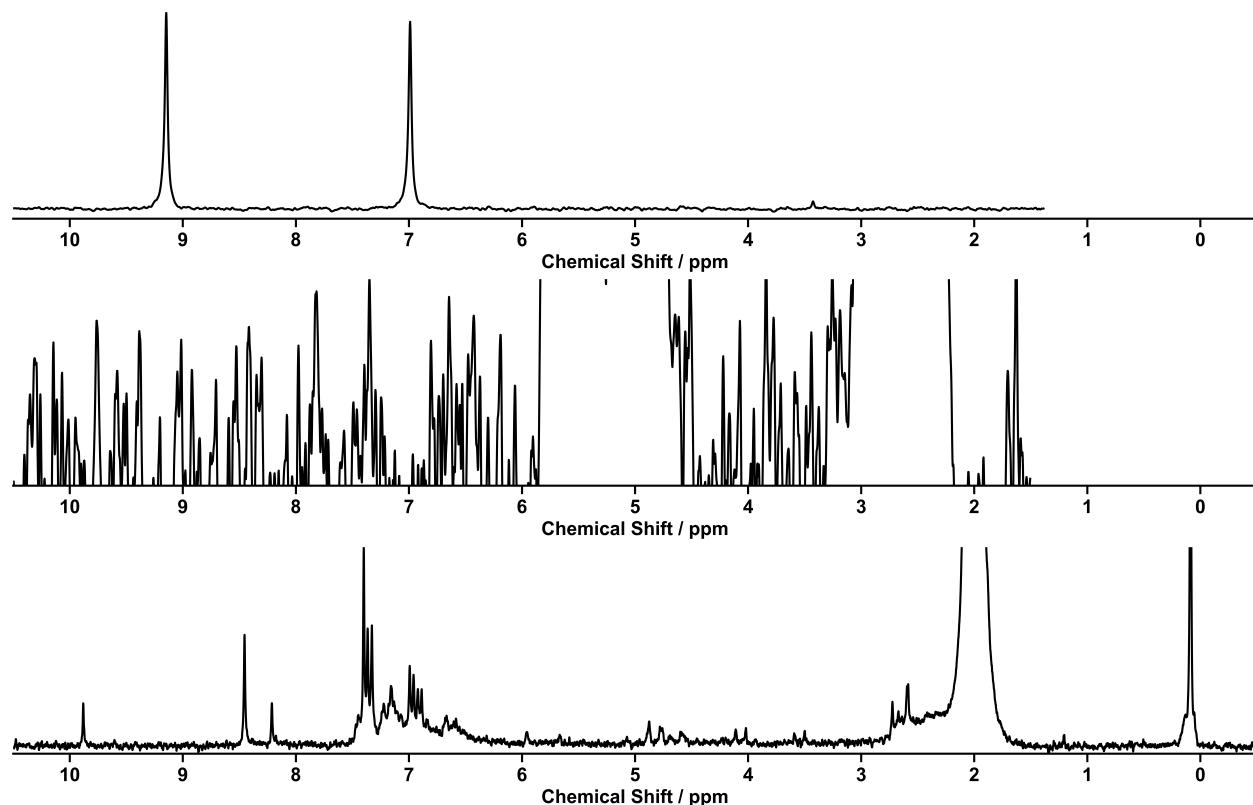
## Reaction 137



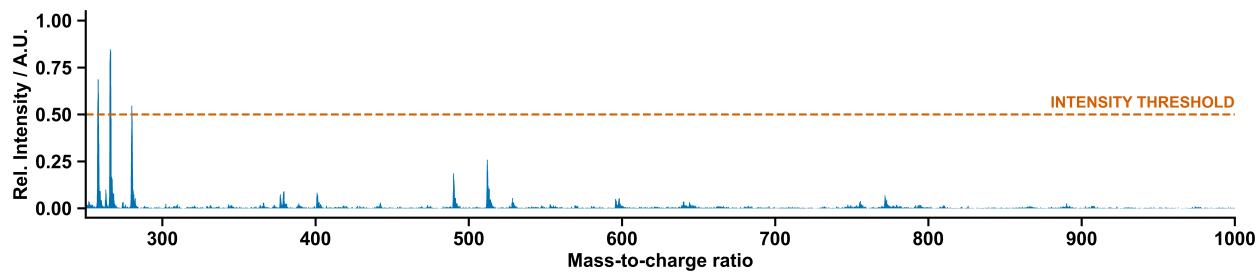
Scheme 115: Self-assembly of components 1, 21, with Silver(I) in a 3.0:1.5:1.0 molar ratio in CH<sub>3</sub>CN at 60°C for 40h. These are the reagents (starting materials) for reaction 137.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: No reaction occurred.	
	Human MS Decision: Failed	MS Spectra Category: Reaction failed.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	NMR Criteria 2: N/A
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 0
		MS Criteria 3: Pass	Number of counter-ions found: 0

Decision Table 115: Human labeled and Decision maker labeled outcomes for the <sup>1</sup>H NMR spectroscopy and UPLC-MS spectrometry of reaction 137. Decision motivations are also given.

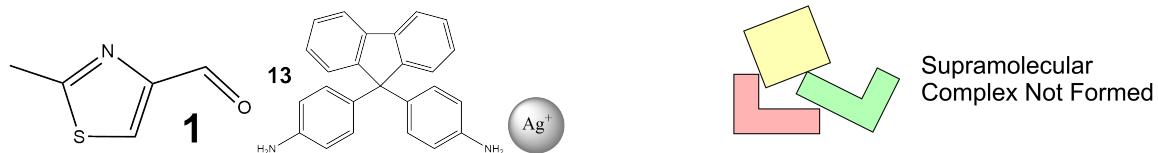


NMR Spectra 115: The stacked <sup>1</sup>H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 137.



MS Spectra 115: The ULPC-MS spectra of reaction 137. The intensity threshold is also shown.

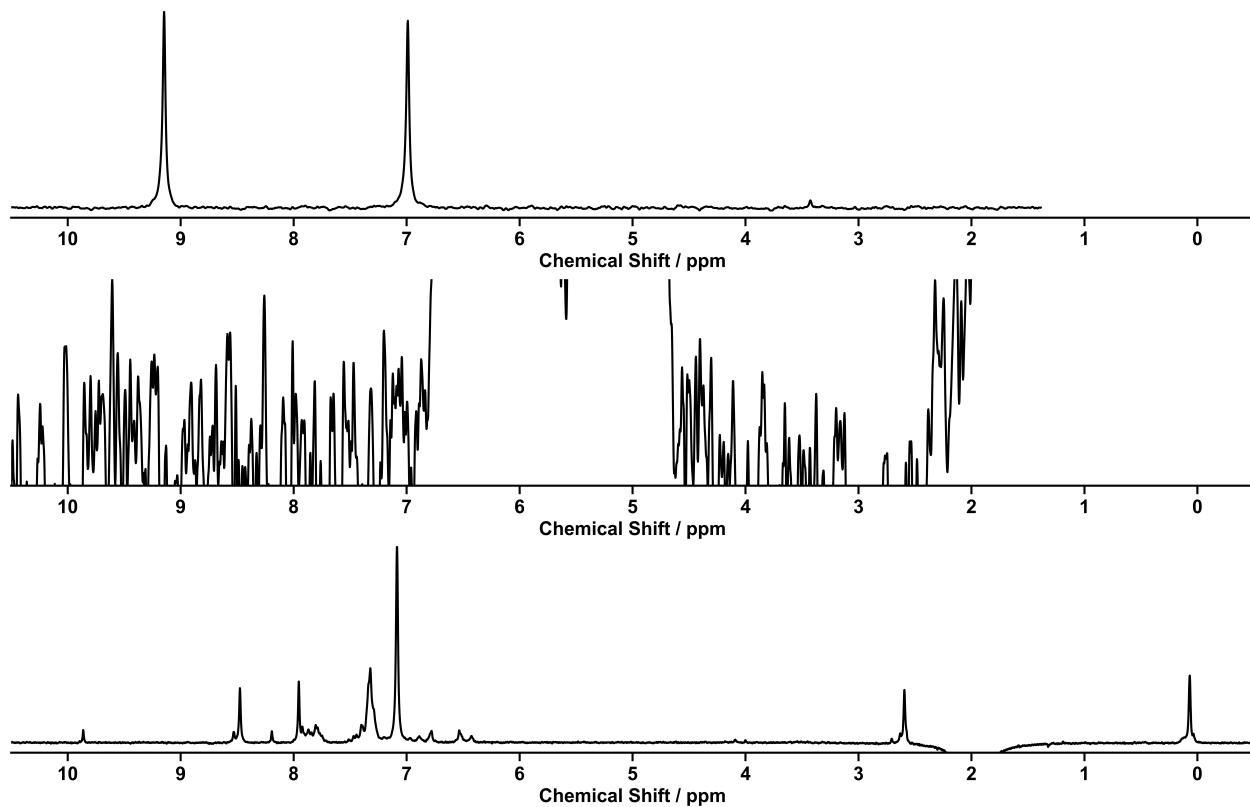
## Reaction 138



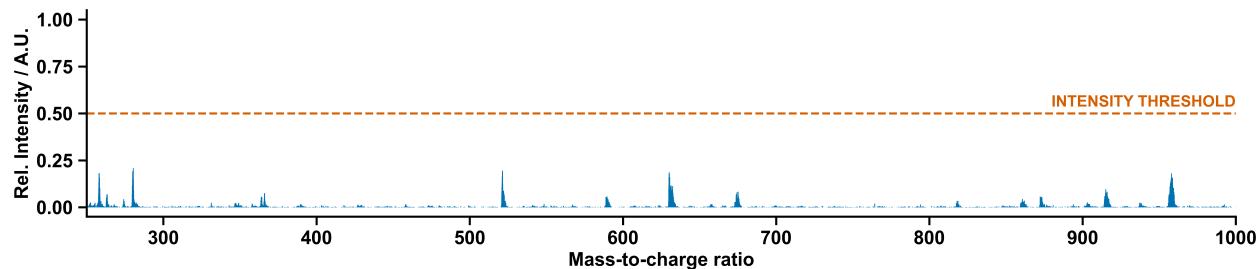
Scheme 116: Self-assembly of components 1, 13, with Silver(I) in a 3.0:1.5:1.0 molar ratio in CH<sub>3</sub>CN at 60°C for 40h. These are the reagents (starting materials) for reaction 138.

Human Reaction Decision: Failed	Human NMR Decision: Pass	NMR Spectra Category: Single discrete species formed.	
	Human MS Decision: Failed	MS Spectra Category: Reaction failed.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	NMR Criteria 2: N/A
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 0
		MS Criteria 3: Pass	Number of counter-ions found: 0

Decision Table 116: Human labeled and Decsision maker labeled outcomes for the <sup>1</sup>H NMR spectroscopy and ULPC-MS spectrometry of reaction 138. Decision motivations are also given.

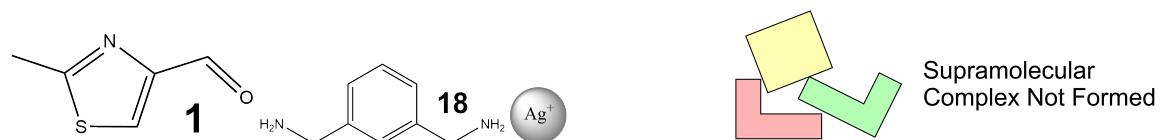


NMR Spectra 116: The stacked <sup>1</sup>H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 138.



MS Spectra 116: The ULPC-MS spectra of reaction 138. The intensity threshold is also shown.

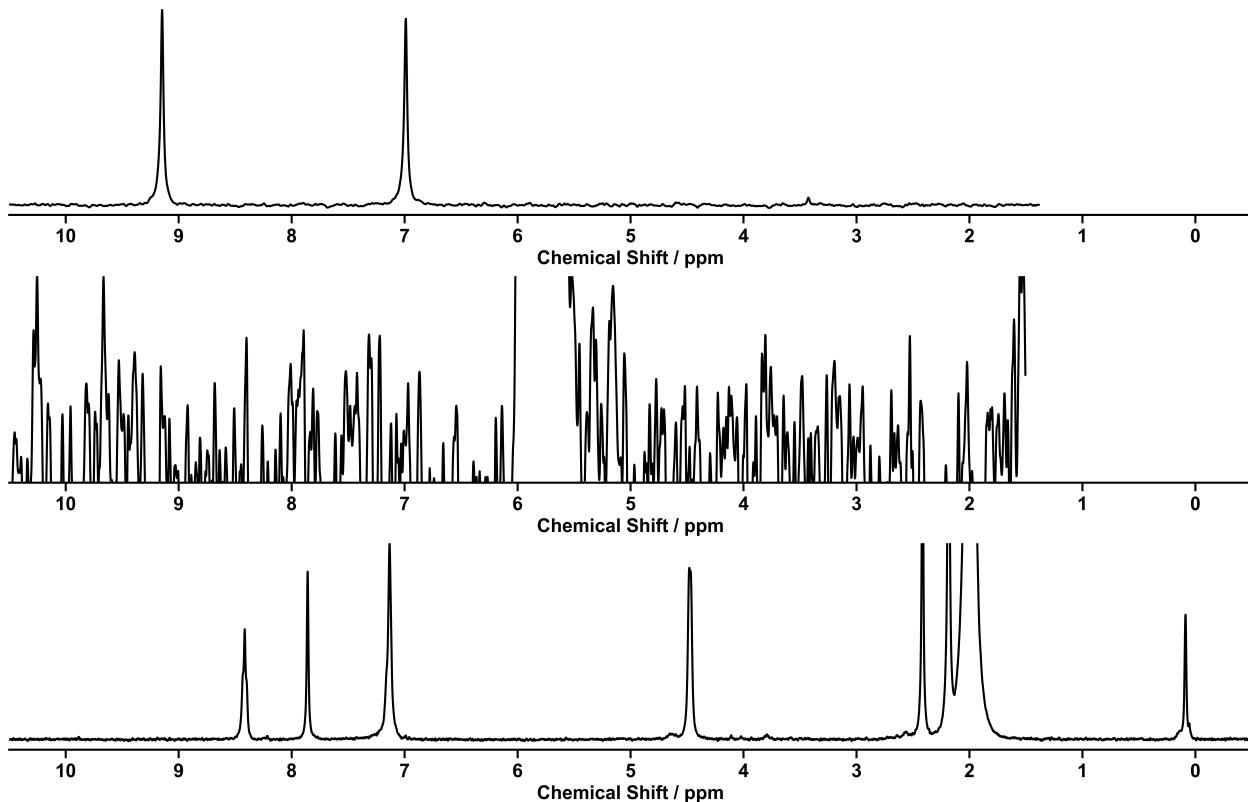
## Reaction 139



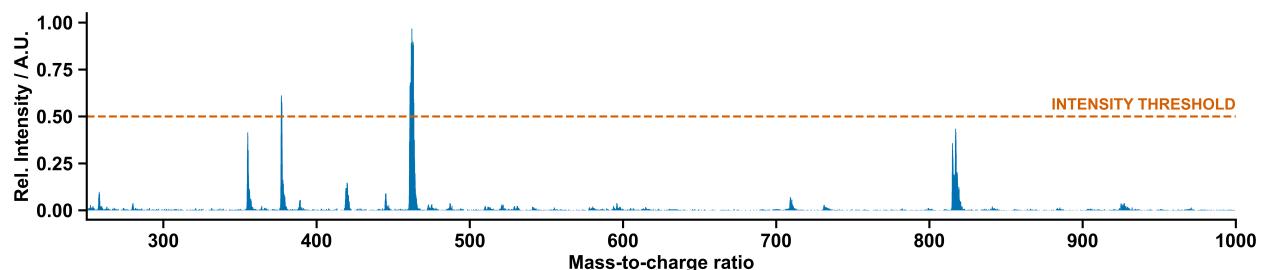
Scheme 117: Self-assembly of components 1, 18, with Silver(I) in a 3.0:1.5:1.0 molar ratio in CH<sub>3</sub>CN at 60°C for 40h. These are the reagents (starting materials) for reaction 139.

Human Reaction Decision: Failed	Human NMR Decision: Pass	NMR Spectra Category: Single discrete species formed.	
	Human MS Decision: Failed	MS Spectra Category: Reaction occurred, unknown product.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	
	Decision Maker MS Decision: Pass	NMR Criteria 2: N/A	MS Criteria 1 and 2: Pass
		Number of predicted peaks found in MS spectra with appropriate intensity: 3	MS Criteria 3: Pass
		Number of counter-ions found: 2	

Decision Table 117: Human labeled and Decsision maker labeled outcomes for the  $^1\text{H}$  NMR spectroscopy and ULPC-MS spectrometry of reaction 139. Decision motivations are also given.

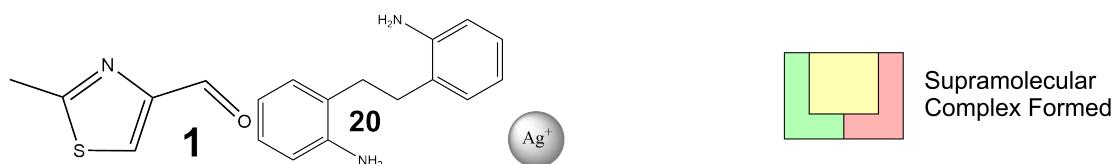


NMR Spectra 117: The stacked  $^1\text{H}$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 139.



MS Spectra 117: The ULPC-MS spectra of reaction 139. The intensity threshold is also shown.

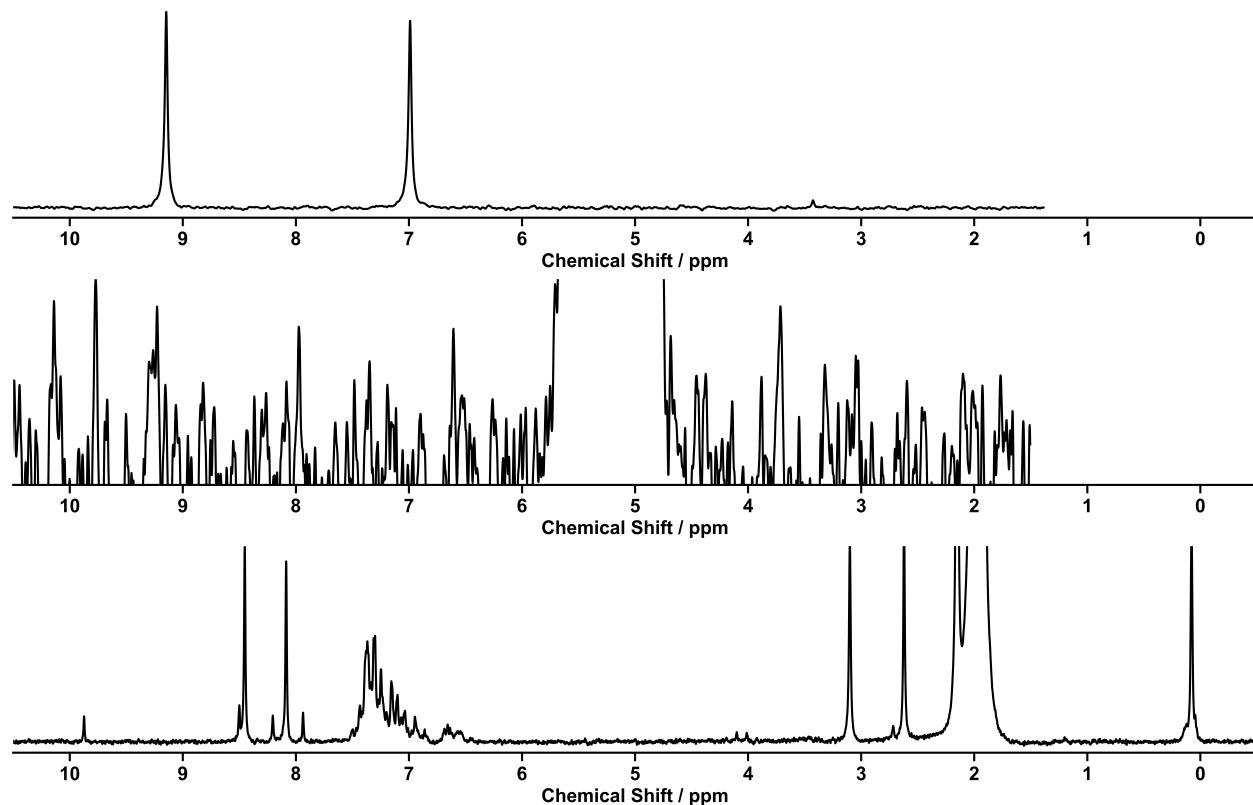
## Reaction 140



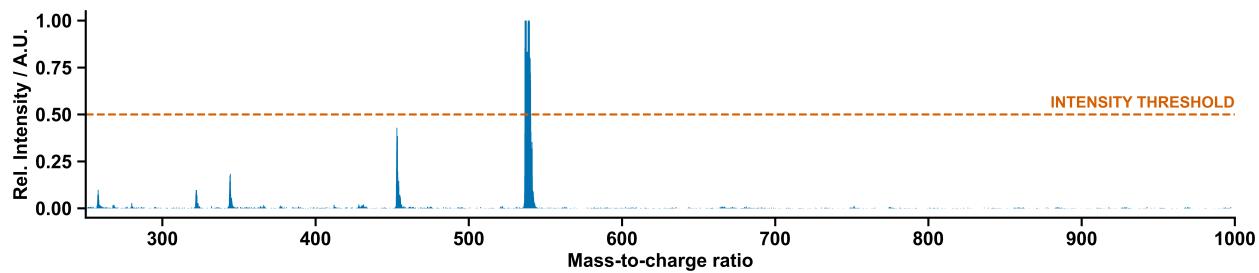
Scheme 118: Self-assembly of components 1, 20, with Silver(I) in a 3.0:1.5:1.0 molar ratio in  $\text{CH}_3\text{CN}$  at 60°C for 40h. These are the reagents (starting materials) for reaction 140.

Human Reaction Decision: Pass	Human NMR Decision: Pass	NMR Spectra Category: Single discrete species formed.	
	Human MS Decision: Pass	MS Spectra Category: Reaction occurred, supramolecular product.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	NMR Criteria 2: N/A
	Decision Maker MS Decision: Pass	MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 4
		MS Criteria 3: Pass	Number of counter-ions found: 2

Decision Table 118: Human labeled and Decsision maker labeled outcomes for the  $^1\text{H}$  NMR spectroscopy and ULPC-MS spectrometry of reaction 140. Decision motivations are also given.



NMR Spectra 118: The stacked  $^1\text{H}$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 140.



MS Spectra 118: The ULPC-MS spectra of reaction 140. The intensity threshold is also shown.

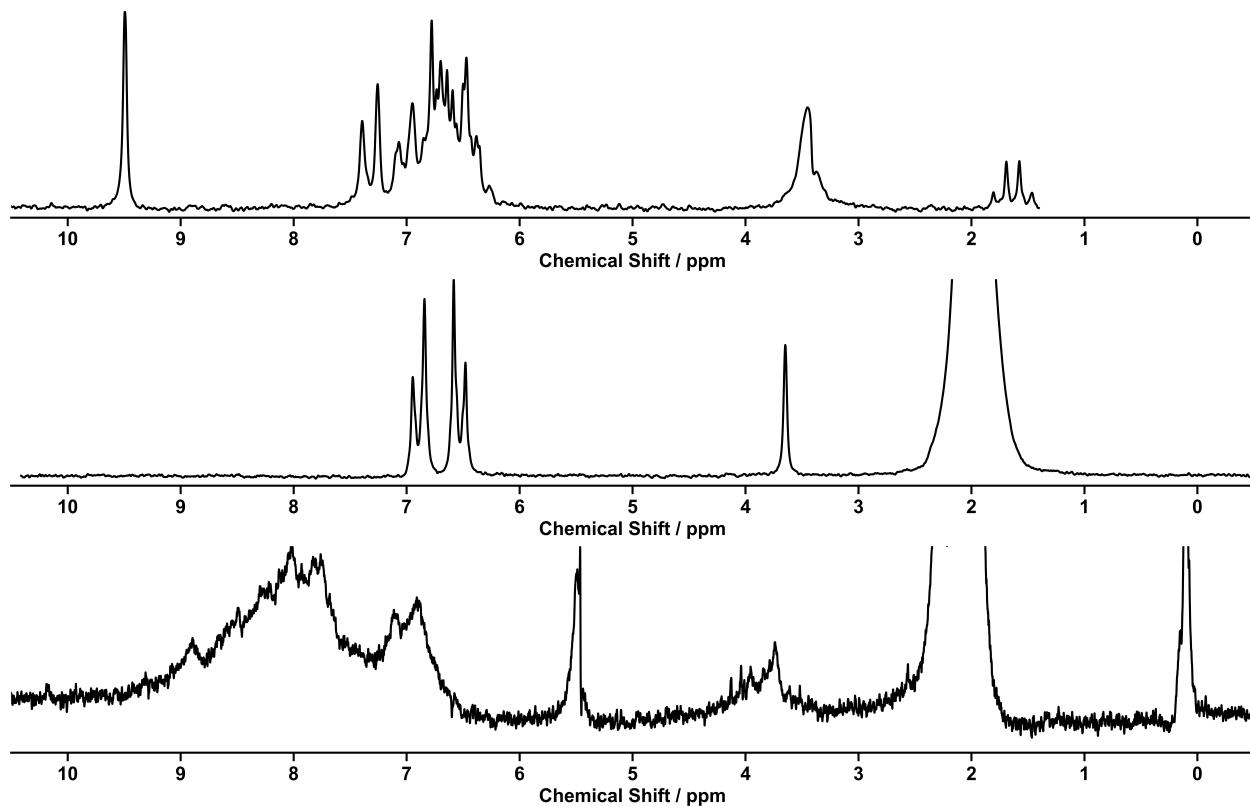
## Reaction 141



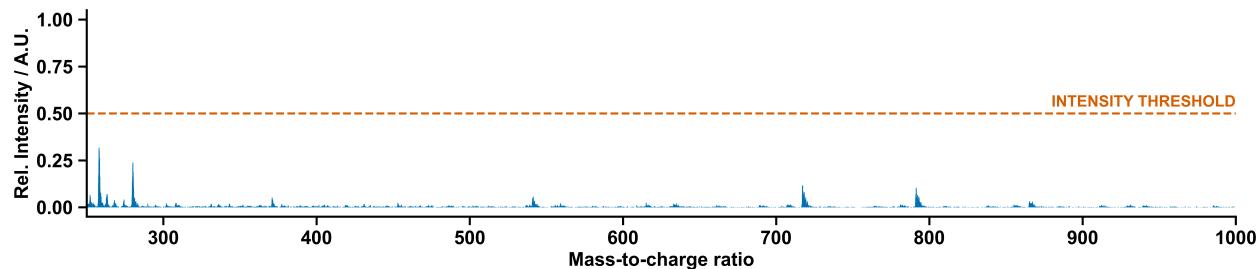
Scheme 119: Self-assembly of components 4, 17, with Zinc(II) in a 3.0:1.5:1.0 molar ratio in CH<sub>3</sub>CN at 60°C for 40h. These are the reagents (starting materials) for reaction 141.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: Oligomers formed.	
	Human MS Decision: Failed	MS Spectra Category: Reaction failed.	NMR Criteria 1: N/A
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 2: N/A	MS Criteria 1 and 2: Pass
	Decision Maker MS Decision: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 0	MS Criteria 3: Pass

Decision Table 119: Human labeled and Decsision maker labled outcomes for the <sup>1</sup>H NMR spectroscopy and ULPC-MS spectrometry of reaction 141. Decision motivations are also given.



NMR Spectra 119: The stacked <sup>1</sup>H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 141.



MS Spectra 119: The ULPC-MS spectra of reaction 141. The intensity threshold is also shown.

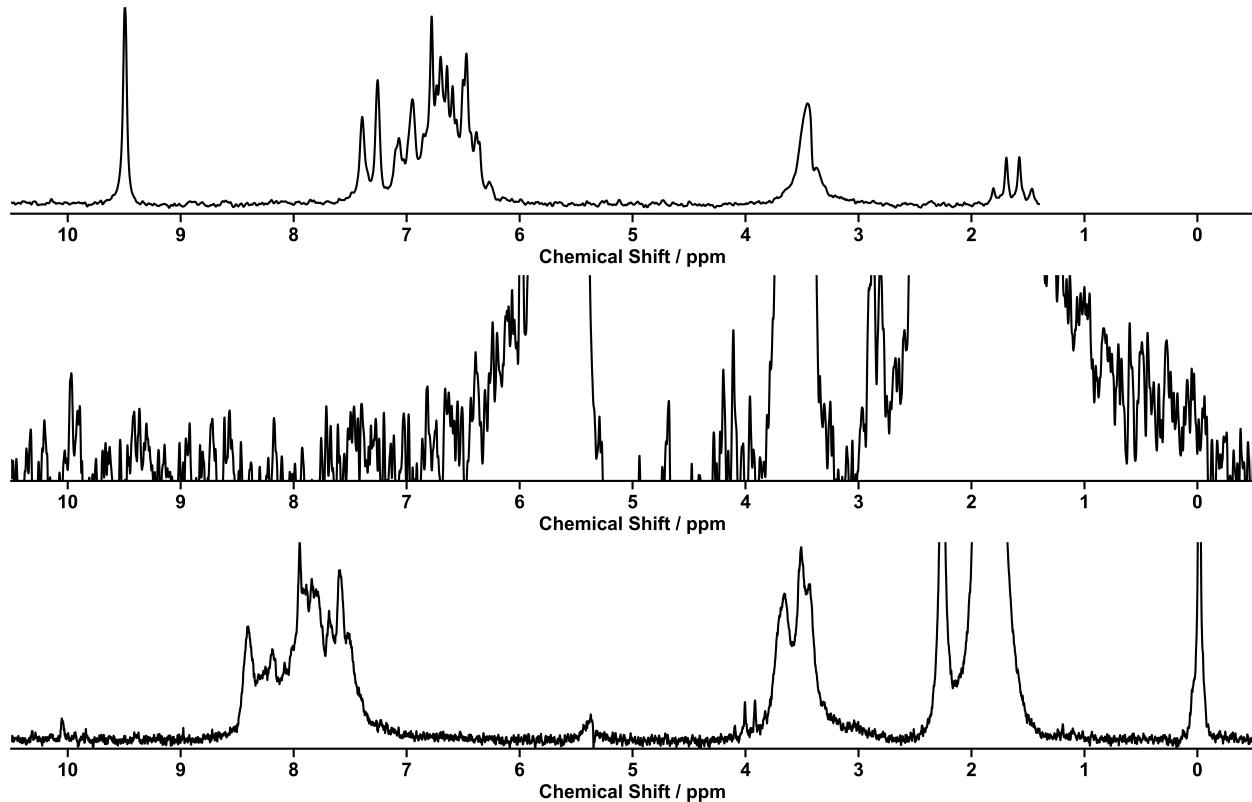
## Reaction 142



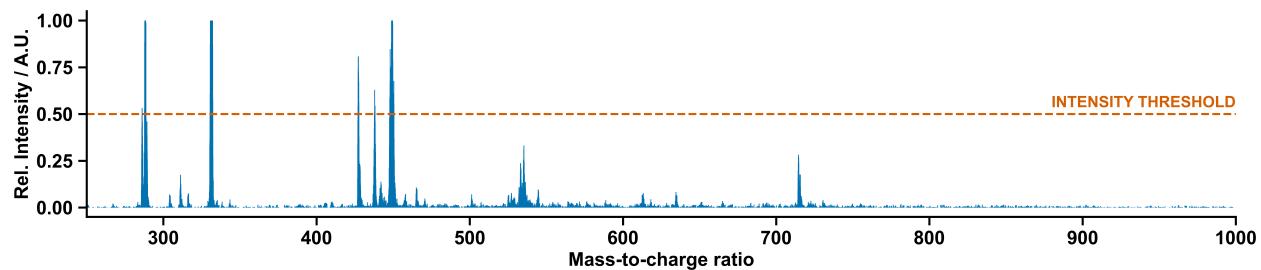
Scheme 120: Self-assembly of components 4, 19, with Zinc(II) in a 3.0:1.5:1.0 molar ratio in  $\text{CH}_3\text{CN}$  at 60°C for 40h. These are the reagents (starting materials) for reaction 142.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: Oligomers formed.	
	Human MS Decision: Failed	MS Spectra Category: Reaction occurred, unknown product.	
Decision Maker Reaction Decision: N/A	Decision Maker NMR Decision: N/A	NMR Criteria 1: N/A	
	Decision Maker MS Decision: Pass	NMR Criteria 2: N/A	
		MS Criteria 1 and 2: Pass	Number of predicted peaks found in MS spectra with appropriate intensity: 1
	MS Criteria 3: Pass	Number of counter-ions found: 1	

Decision Table 120: Human labeled and Decsision maker labeled outcomes for the  $^1\text{H}$  NMR spectroscopy and ULPC-MS spectrometry of reaction 142. Decision motivations are also given.



NMR Spectra 120: The stacked  $^1\text{H}$  NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 142.



MS Spectra 120: The ULPC-MS spectra of reaction 142. The intensity threshold is also shown.