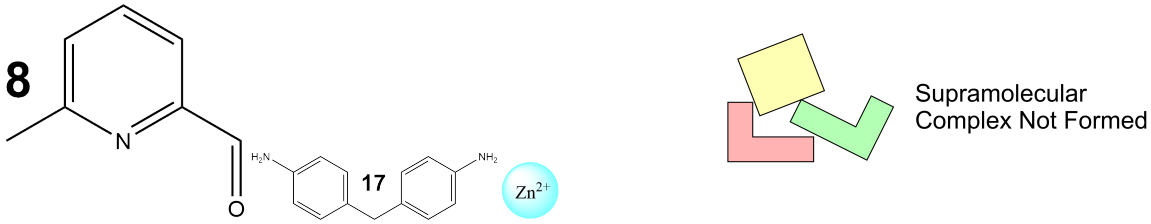
Contents

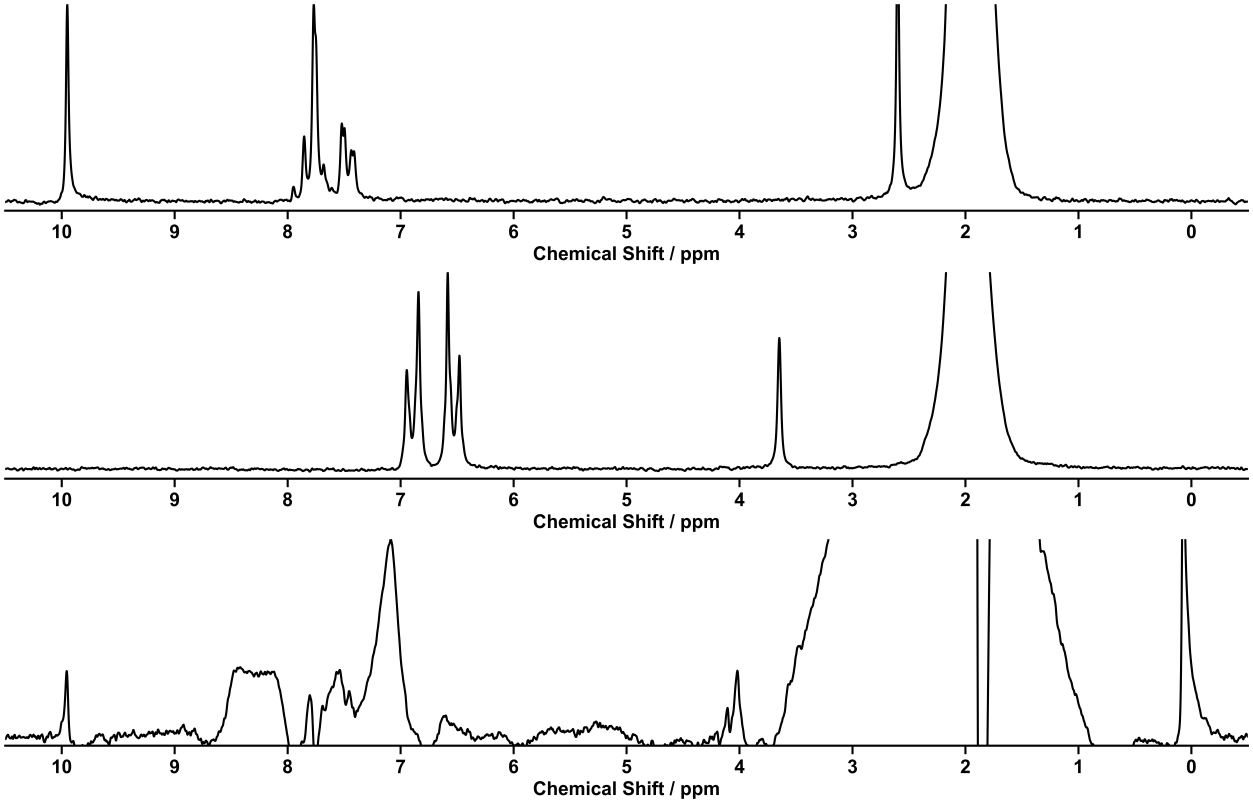
Reaction 1



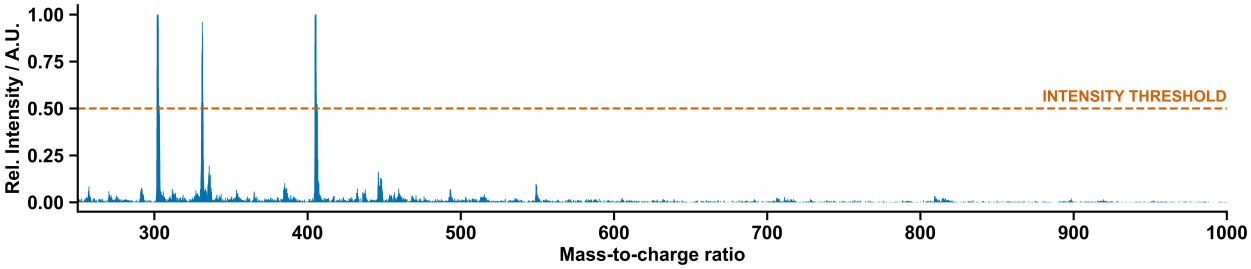
Scheme 1: Self-assembly of components 8, 17, with Zinc(II) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 1.

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



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



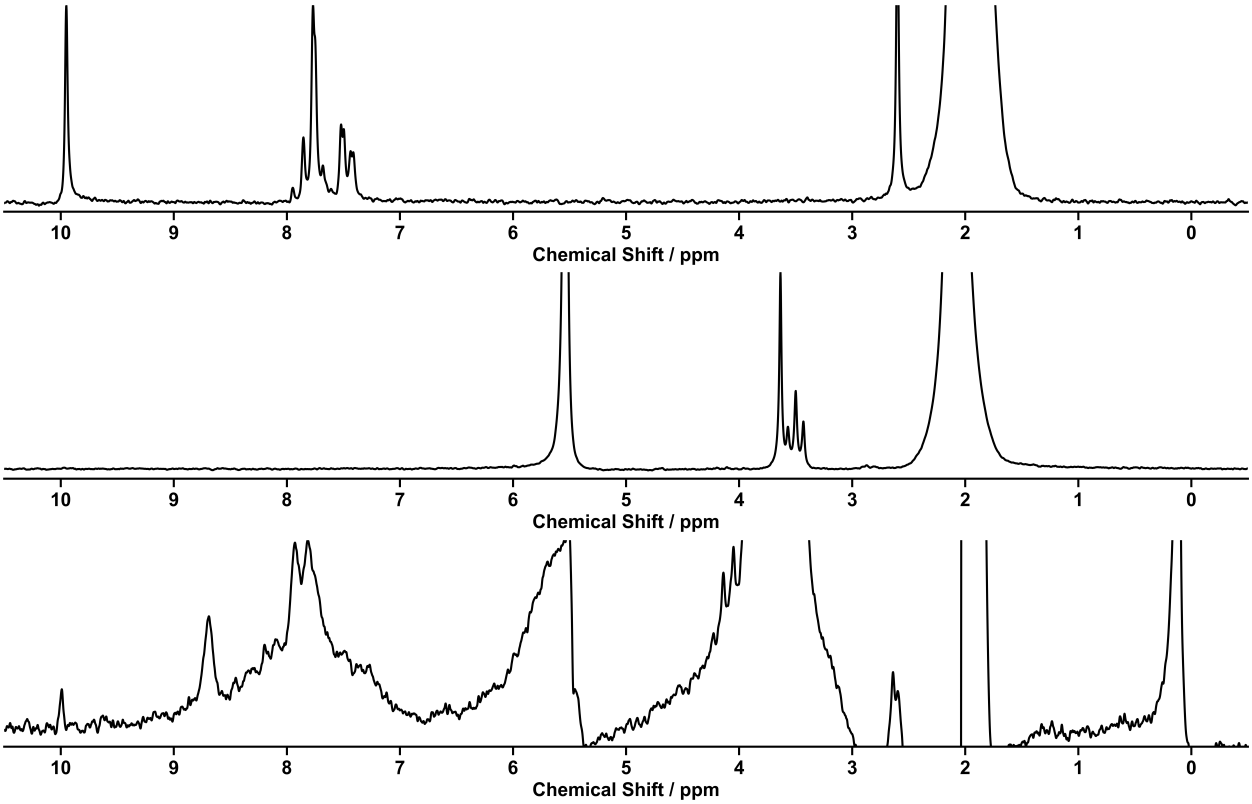
MS Spectra 1: The ULPC-MS spectra of reaction 1. The intensity threshold is also shown.

Reaction 2

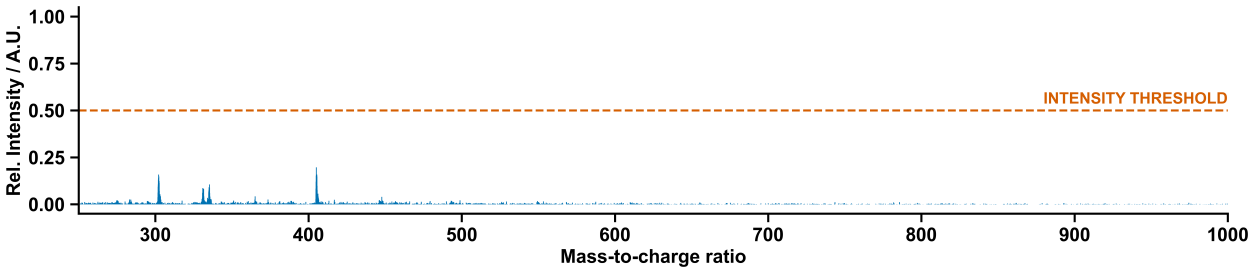
Scheme 2: Self-assembly of components 8, 19, with Zinc(II) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 2.

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 labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 2. Decision motivations are also given.

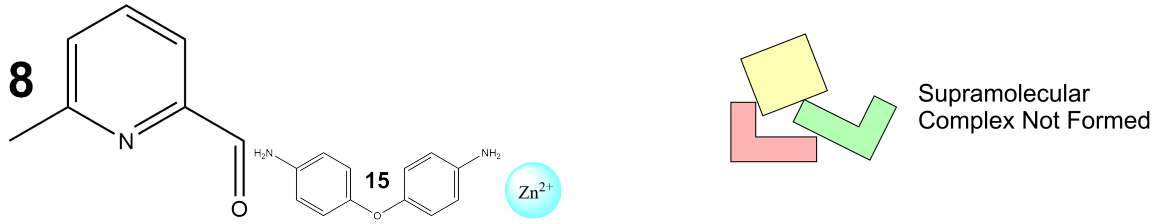


NMR Spectra 2: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 2.



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

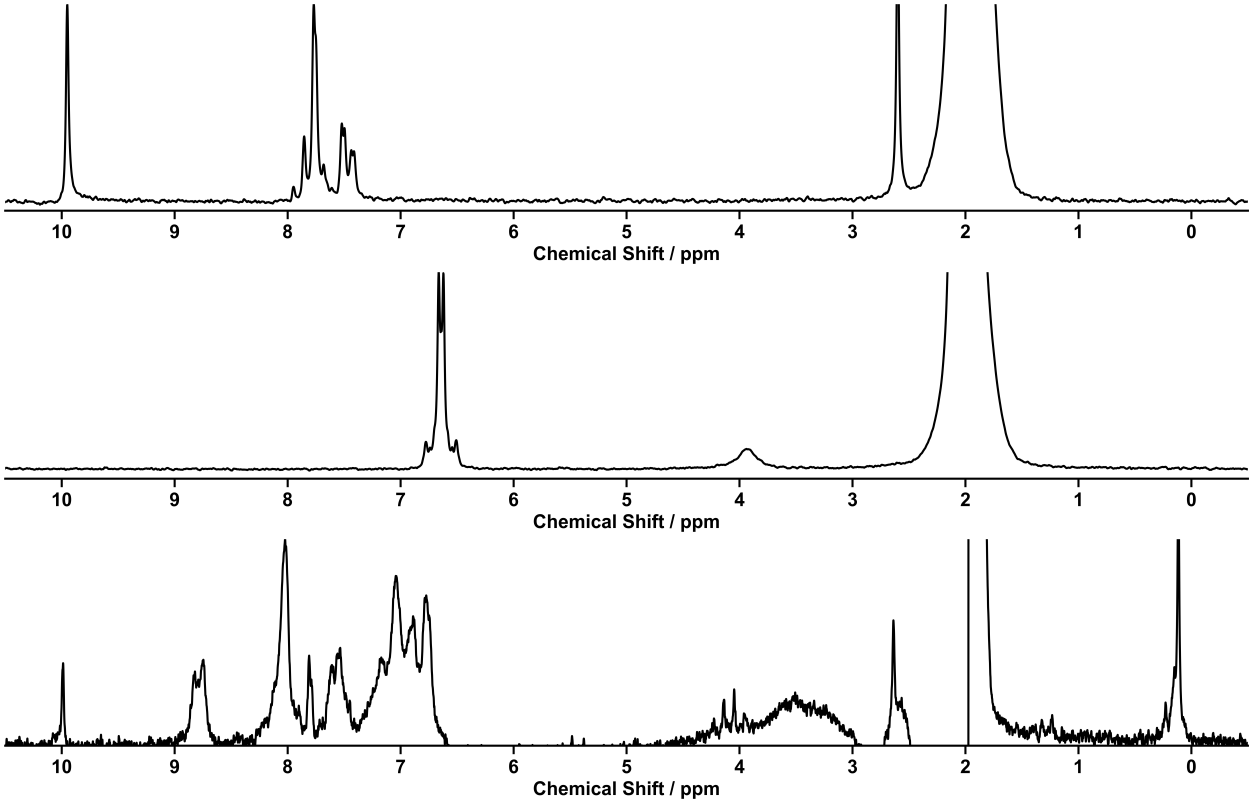
Reaction 3



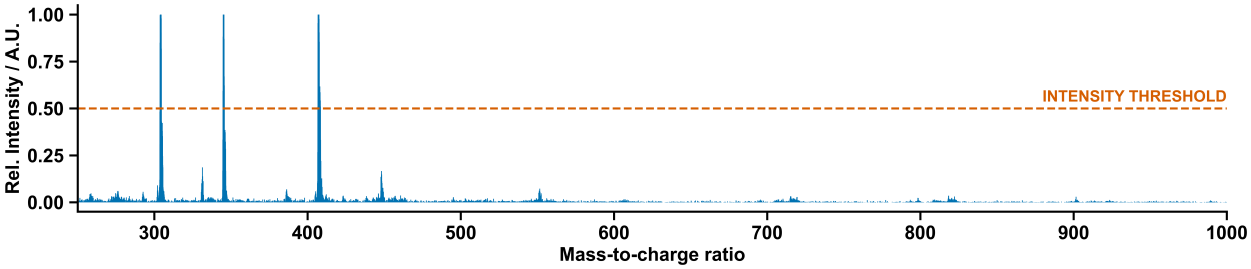
Scheme 3: Self-assembly of components 8, 15, with Zinc(II) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 3.

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 labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 3. Decision motivations are also given.

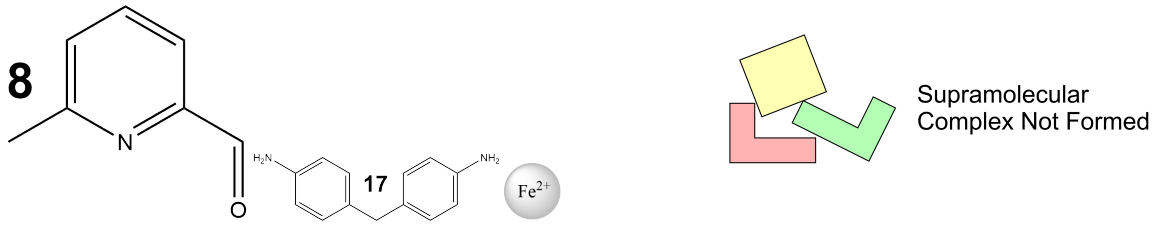


NMR Spectra 3: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 3.



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

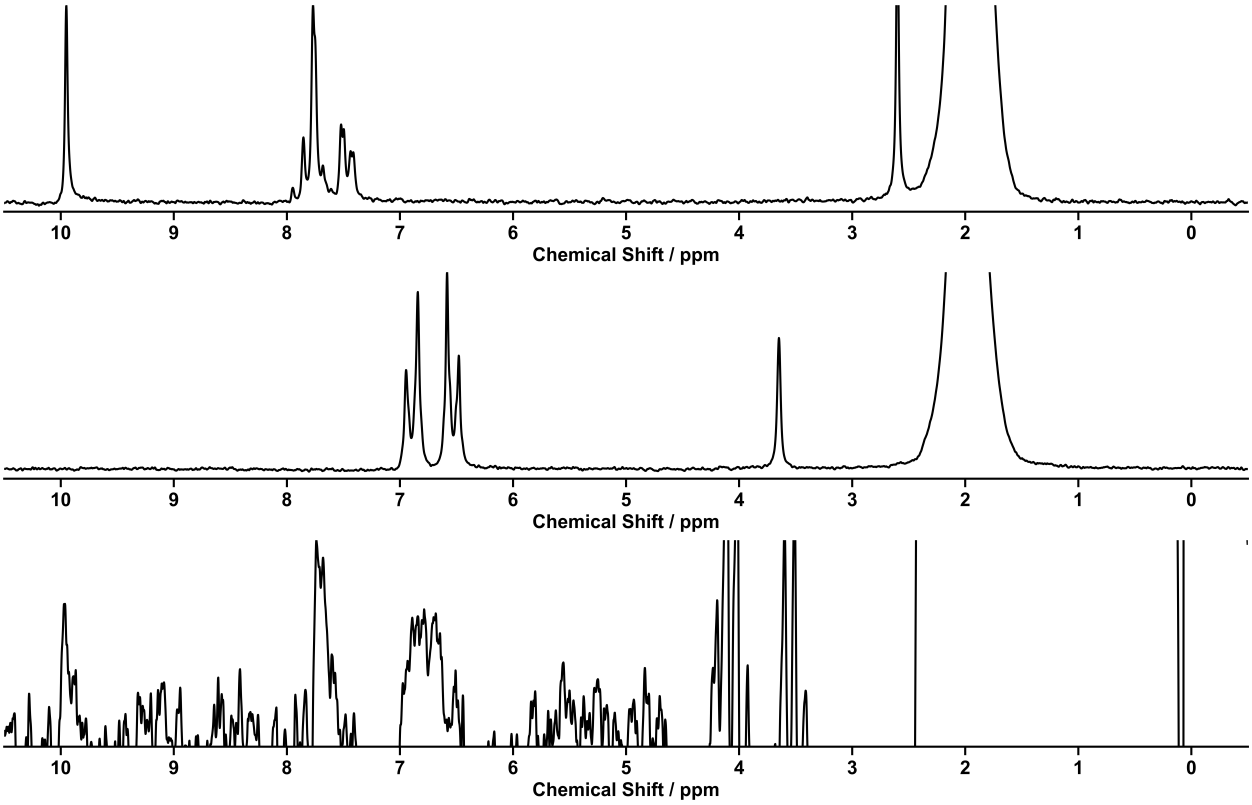
Reaction 4



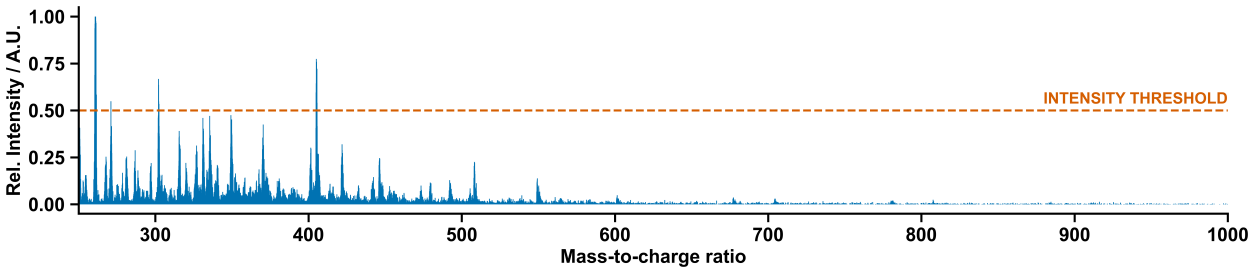
Scheme 4: Self-assembly of components 8, 17, with Iron(II) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 4.

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	
		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 4: Human labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 4. Decision motivations are also given.

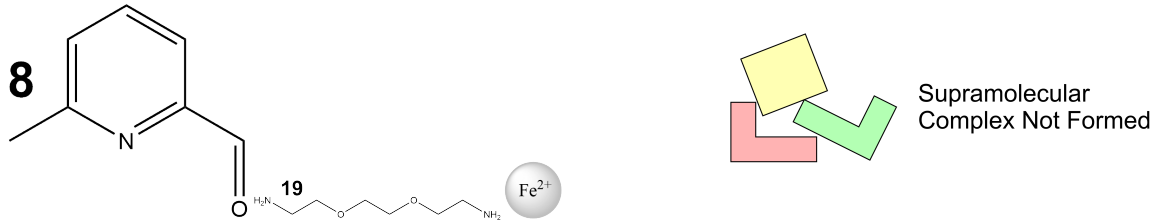


NMR Spectra 4: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 4.



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

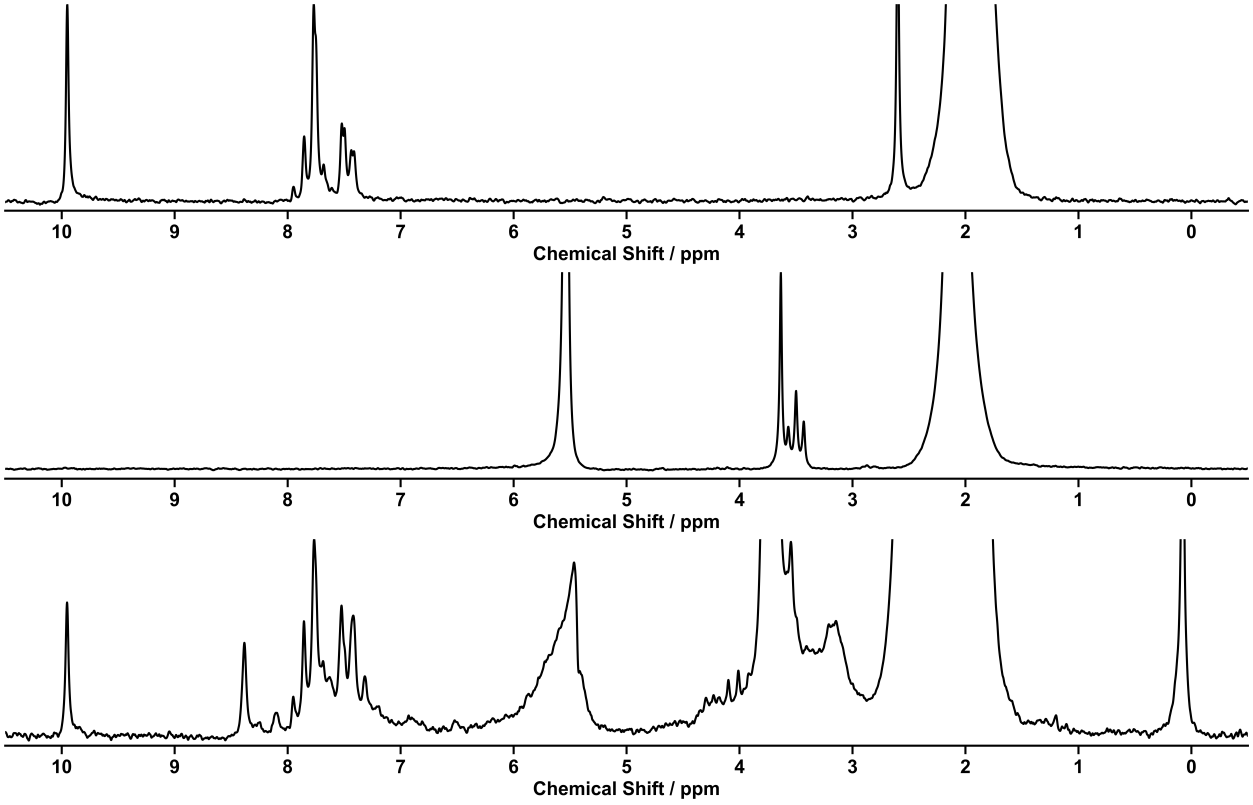
Reaction 5



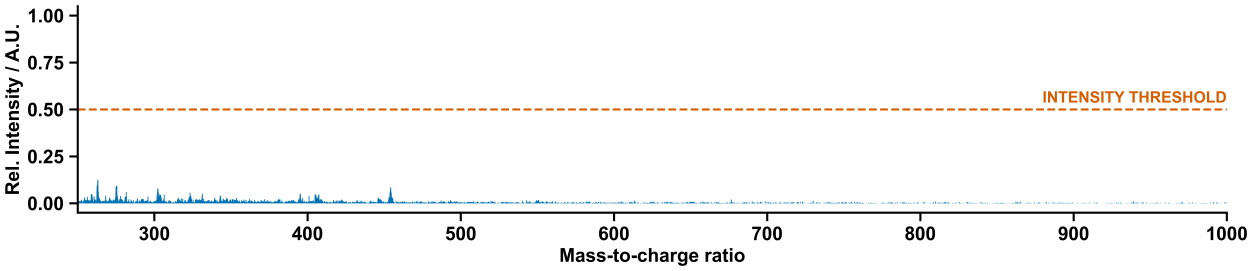
Scheme 5: Self-assembly of components 8, 19, with Iron(II) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 5.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: No reaction occured.	
	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 labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 5. Decision motivations are also given.

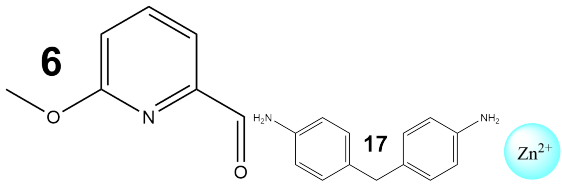


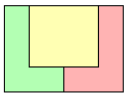
NMR Spectra 5: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 5.



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

Reaction 7



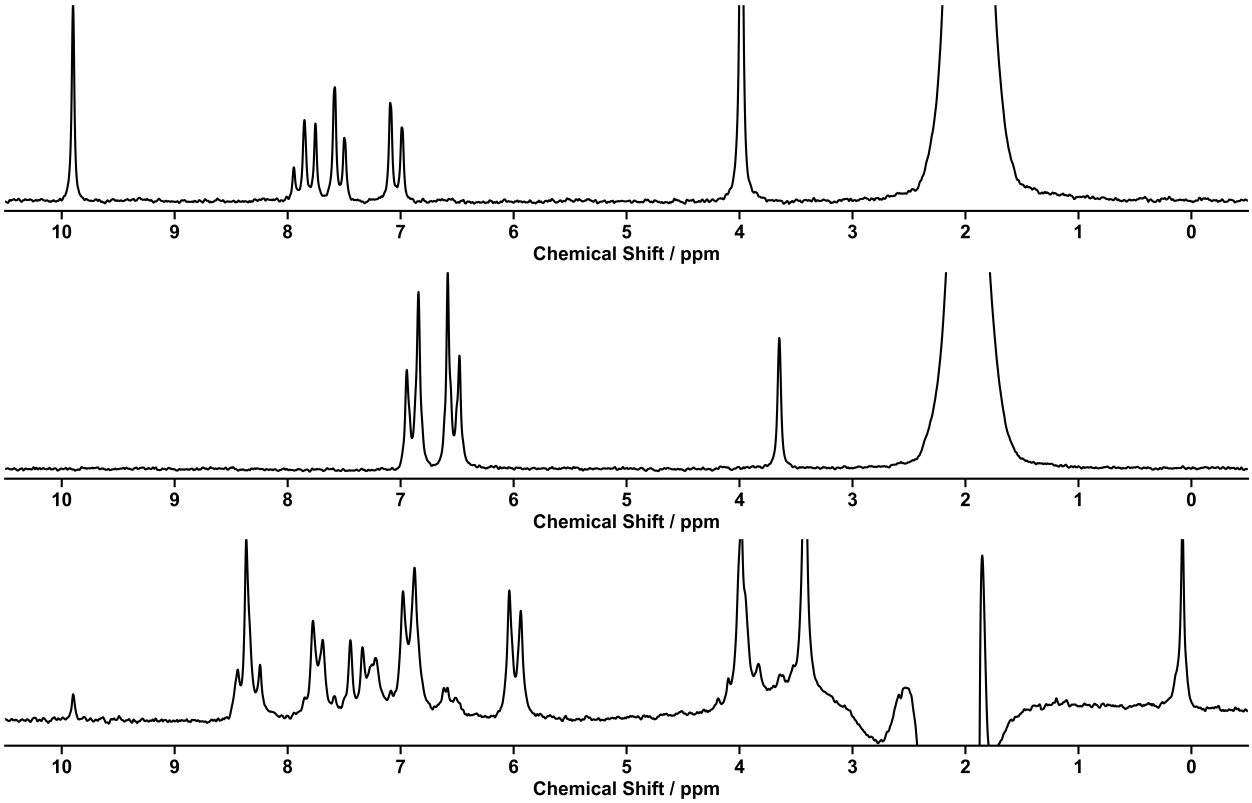


Supramolecular Complex Formed

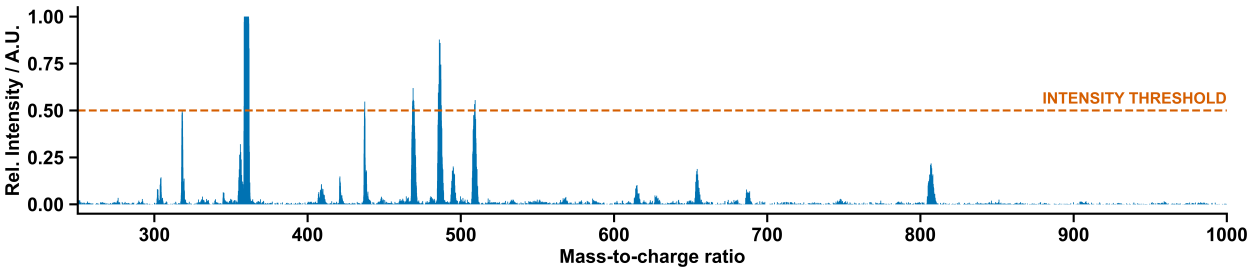
Scheme 6: Self-assembly of components 6, 17, with Zinc(II) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 7.

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

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

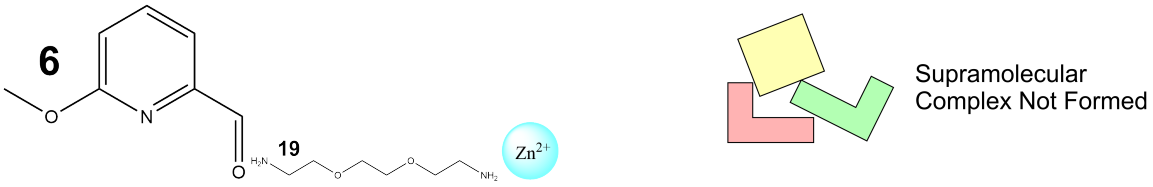


NMR Spectra 6: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 7.



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

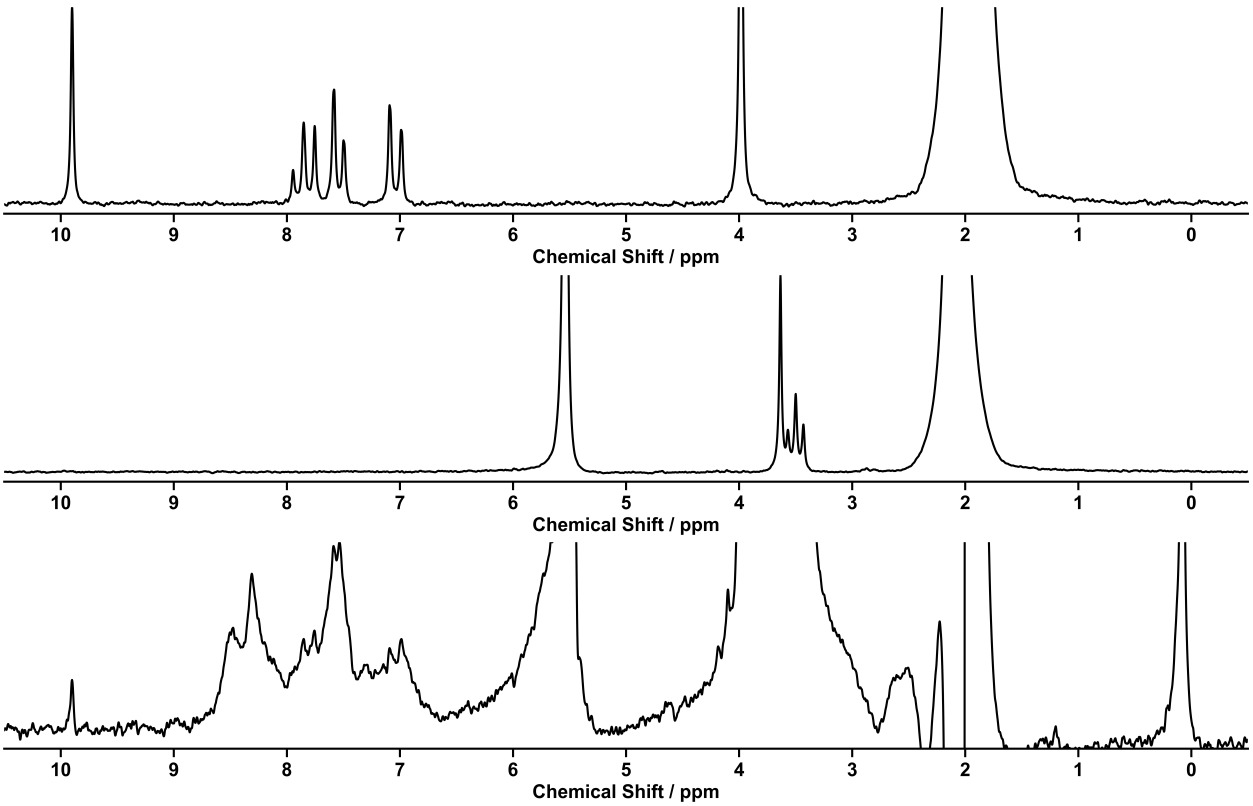
Reaction 8



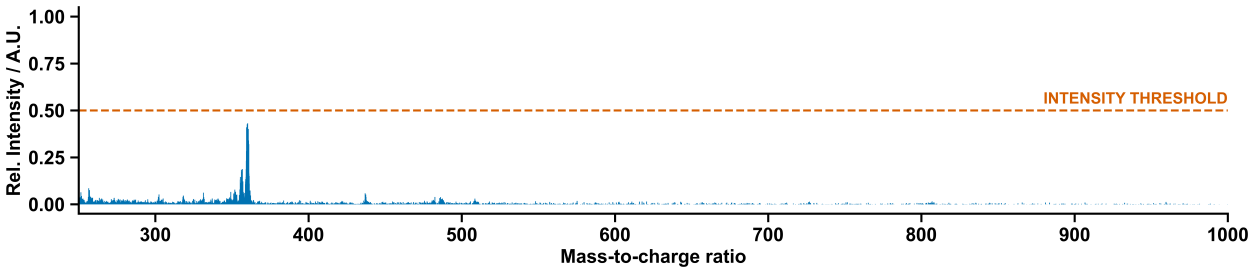
Scheme 7: Self-assembly of components 6, 19, with Zinc(II) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 8.

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 labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 8. Decision motivations are also given.

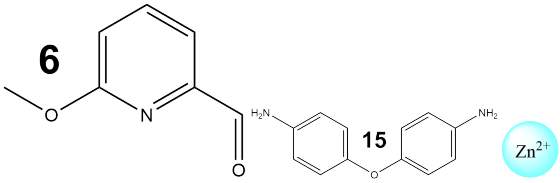


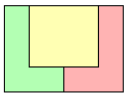
NMR Spectra 7: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 8.



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

Reaction 9



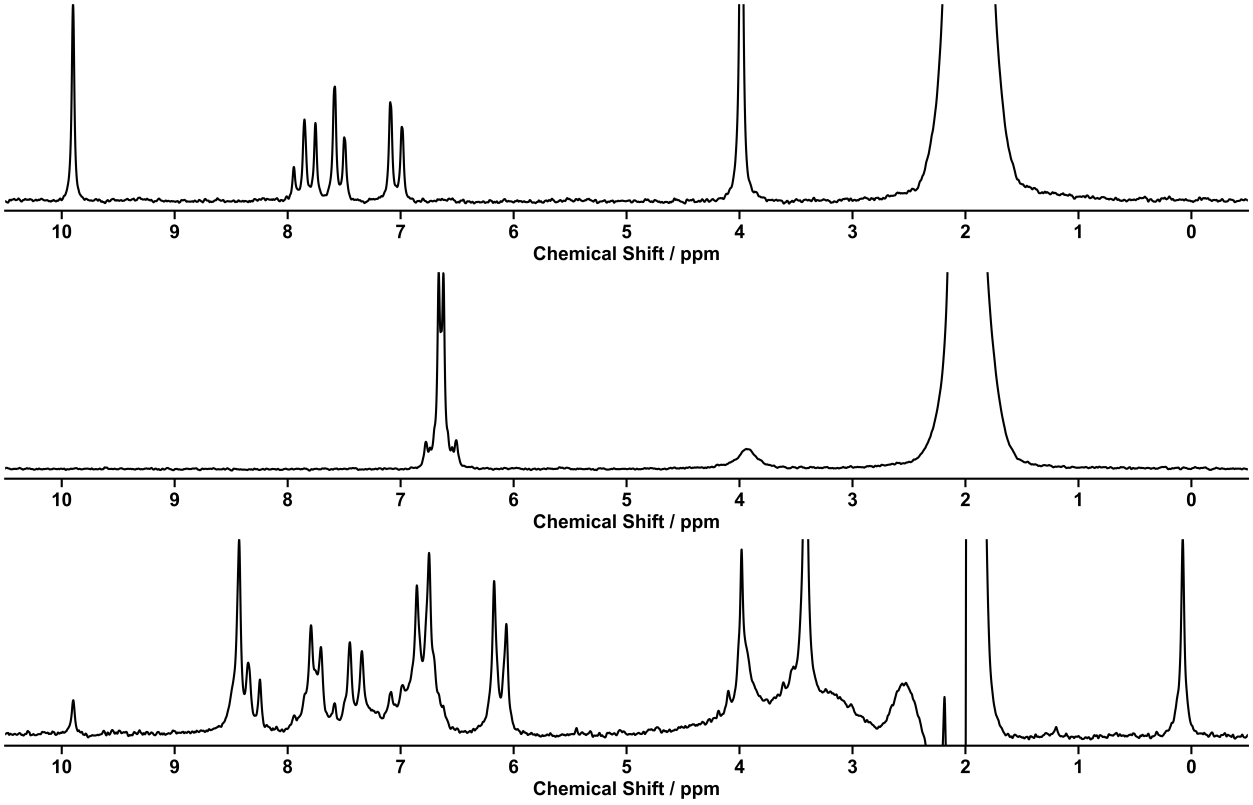


Supramolecular Complex Formed

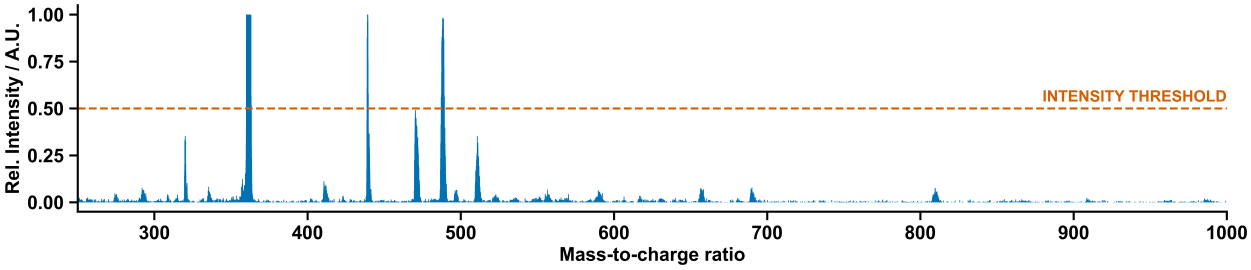
Scheme 8: Self-assembly of components 6, 15, with Zinc(II) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 9.

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 labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 9. Decision motivations are also given.

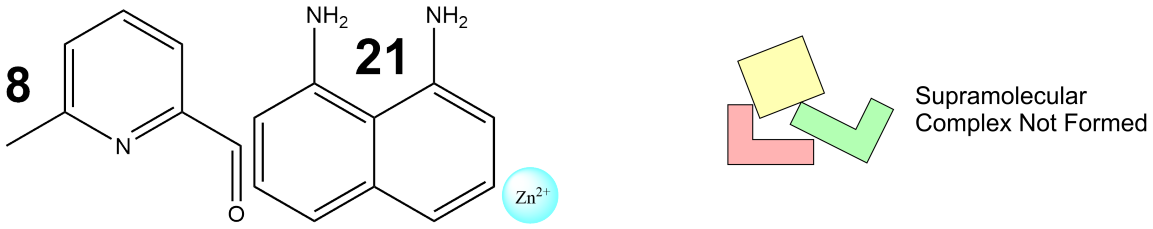


NMR Spectra 8: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 9.



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

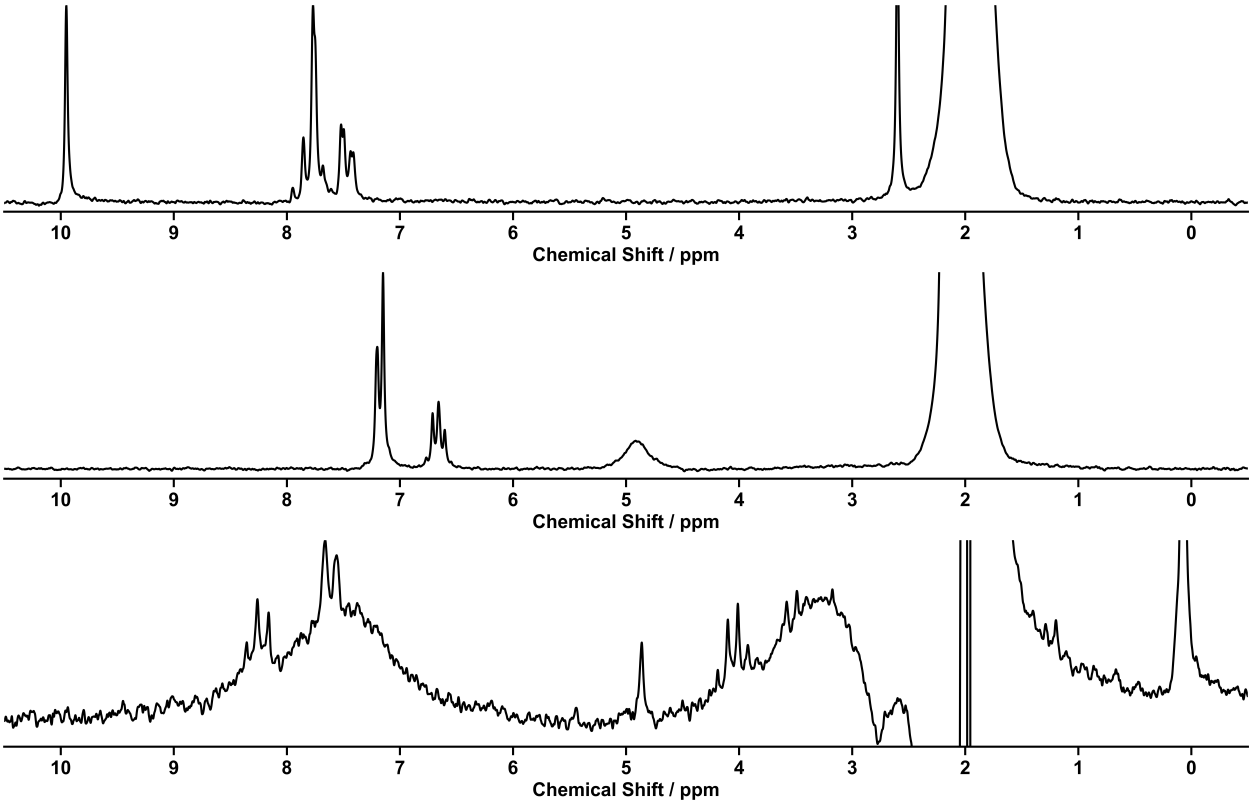
Reaction 10



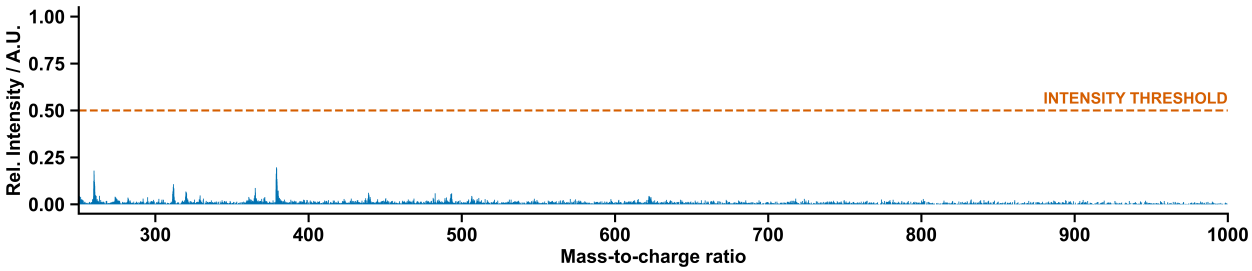
Scheme 9: Self-assembly of components 8, 21, with Zinc(II) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 10.

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 labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 10. Decision motivations are also given.

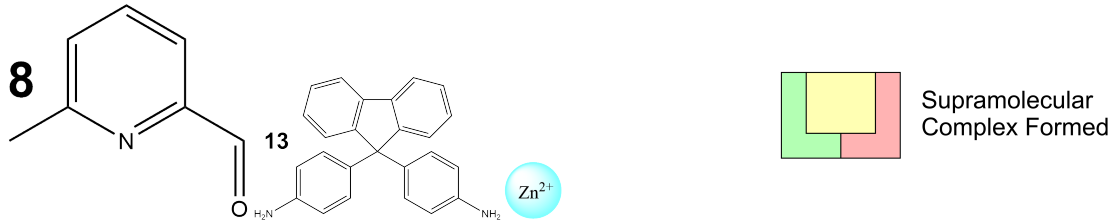


NMR Spectra 9: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 10.



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

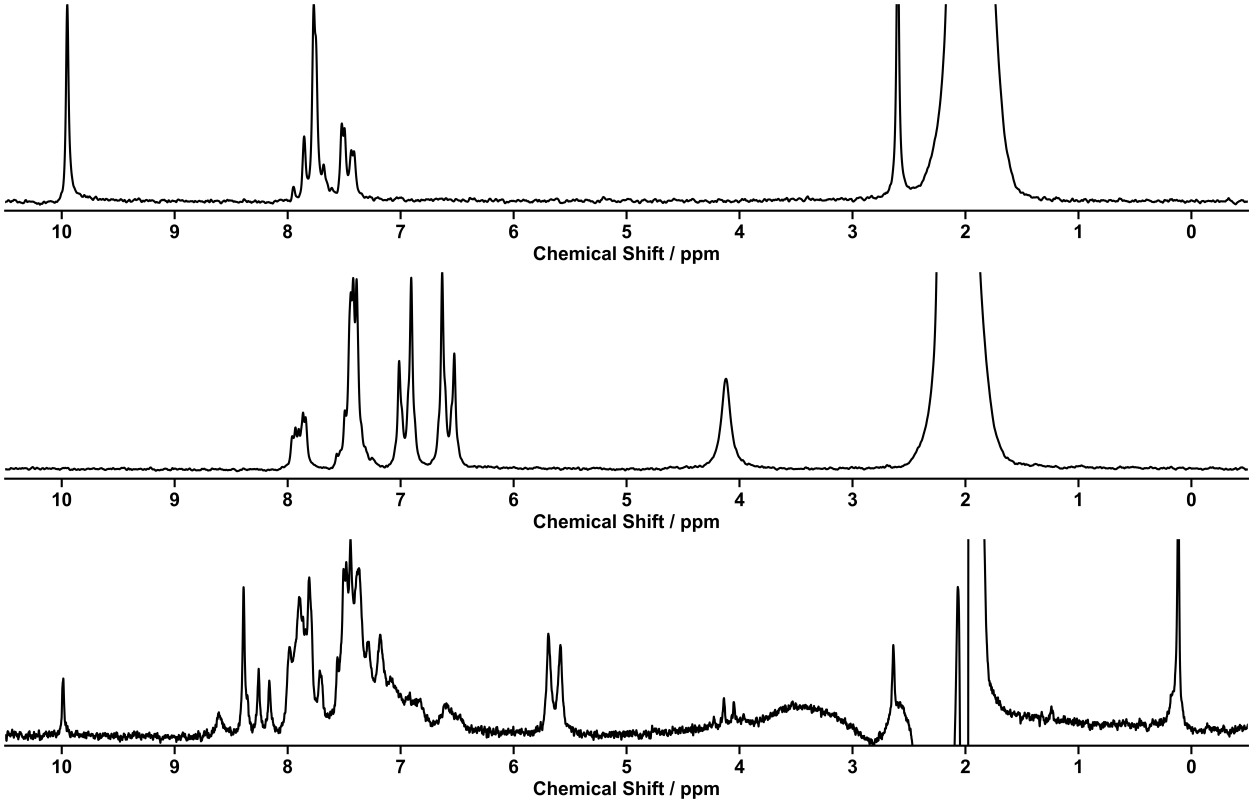
Reaction 11



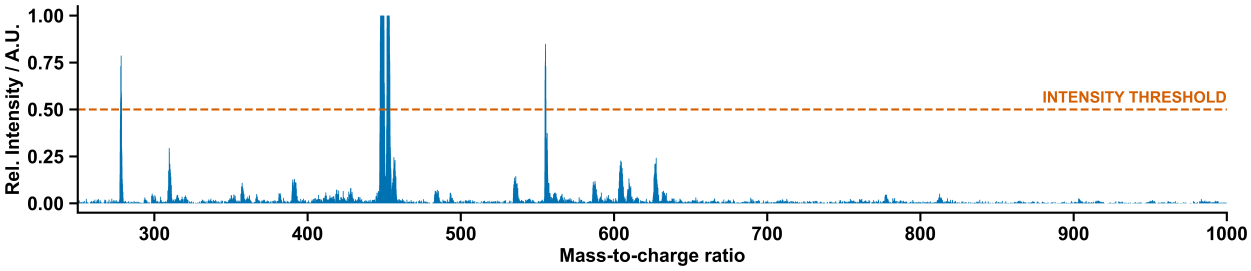
Scheme 10: Self-assembly of components 8, 13, with Zinc(II) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 11.

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 labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 11. Decision motivations are also given.

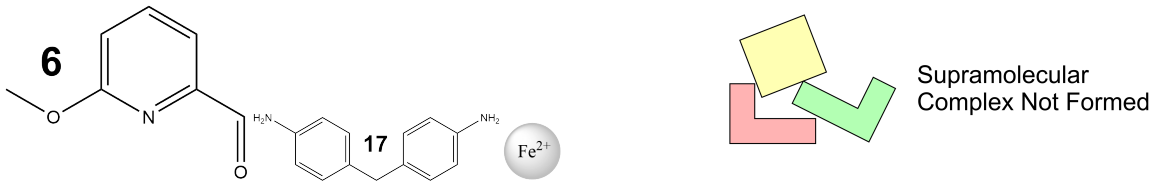


NMR Spectra 10: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 11.



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

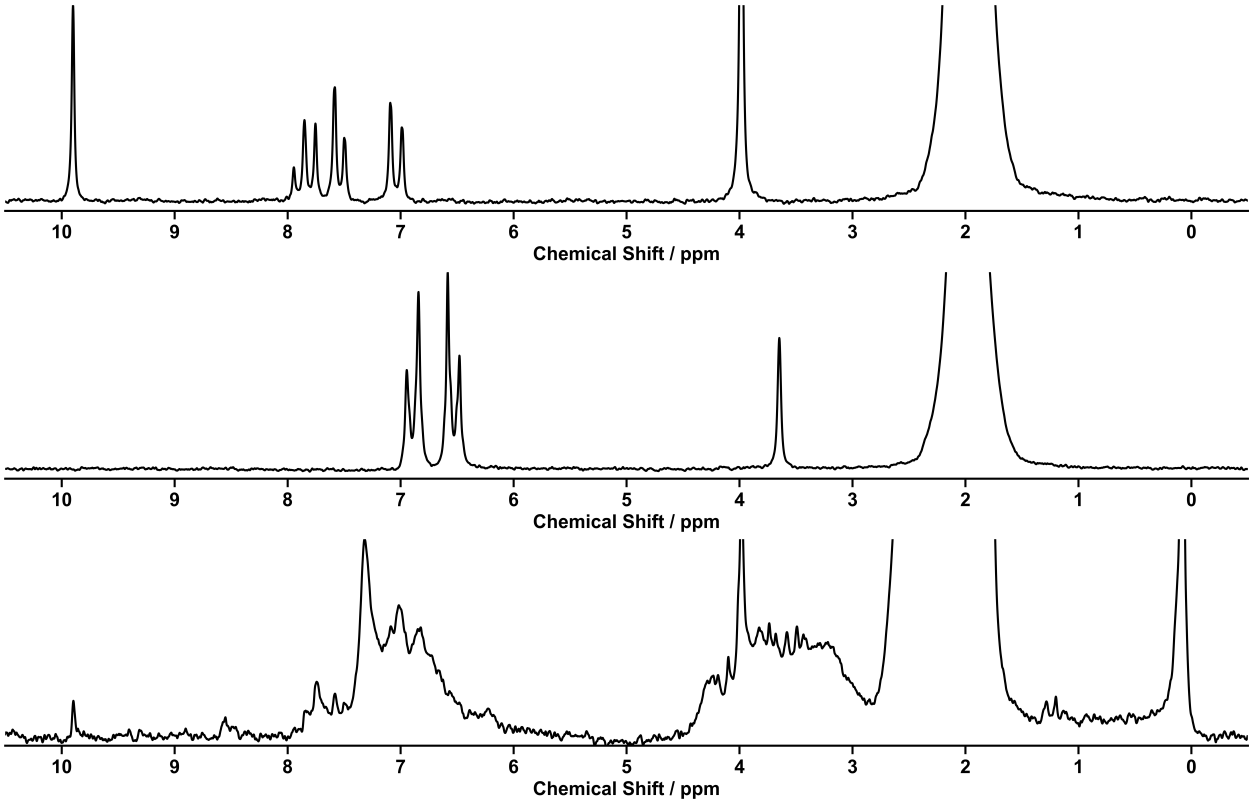
Reaction 12



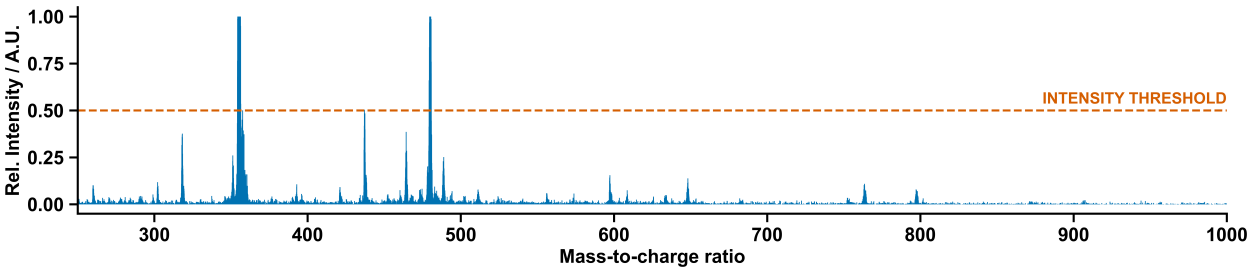
Scheme 11: Self-assembly of components 6, 17, with Iron(II) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 12.

<table>
<tr><td rowspan="2">Human Reaction Decision:
Failed</td><td>Human NMR Decision:
Failed</td><td colspan="2">NMR Spectra Category:
Paramagnetic species formed.</td></tr>
<tr><td>Human MS Decision:
Pass</td><td colspan="2">MS Spectra Category:
Reaction occurred, supramolecular product.</td></tr>
<tr><td rowspan="4">Decision Maker Reaction Decision:
N/A</td><td rowspan="2">Decision Maker NMR Decision:
N/A</td><td colspan="2">NMR Criteria 1:
N/A</td></tr>
<tr><td colspan="2">NMR Criteria 2:
N/A</td></tr>
<tr><td rowspan="2">Decision Maker MS Decision:
Pass</td><td>MS Criteria 1 and 2:
Pass</td><td>Number of predicted peaks found in MS spectra with appropriate intensity:
5</td></tr>
<tr><td>MS Criteria 3:
Pass</td><td>Number of counter-ions found:
3</td></tr>
</table>

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

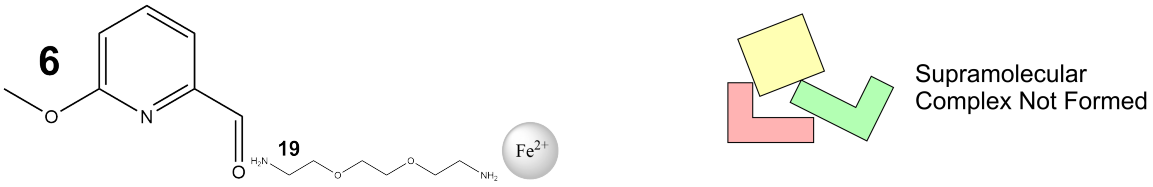


NMR Spectra 11: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 12.



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

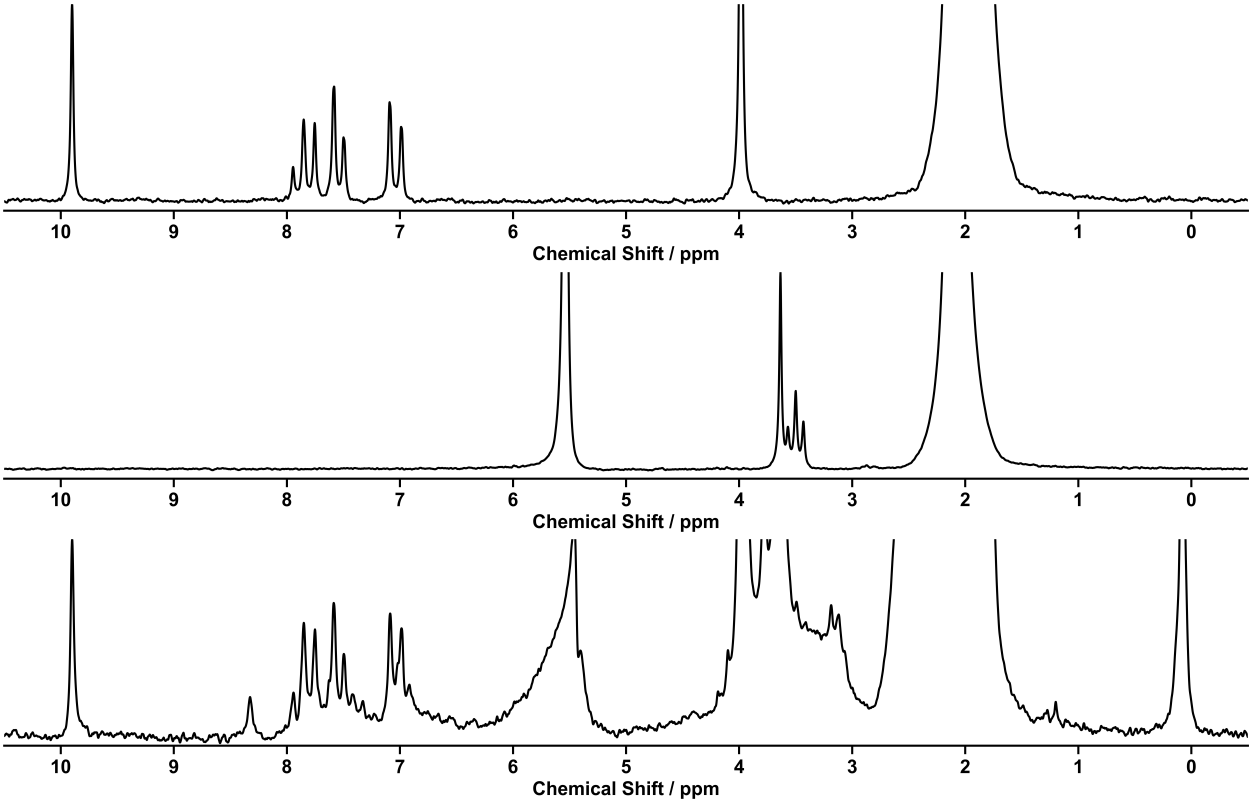
Reaction 13



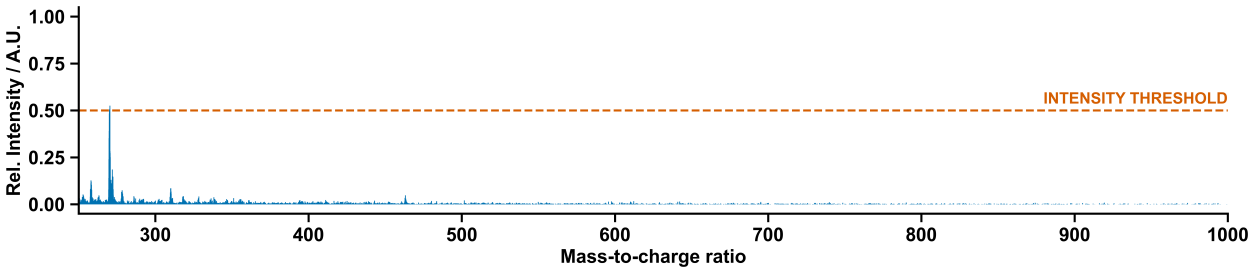
Scheme 12: Self-assembly of components 6, 19, with Iron(II) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 13.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: No reaction occured.	
	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 labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 13. Decision motivations are also given.

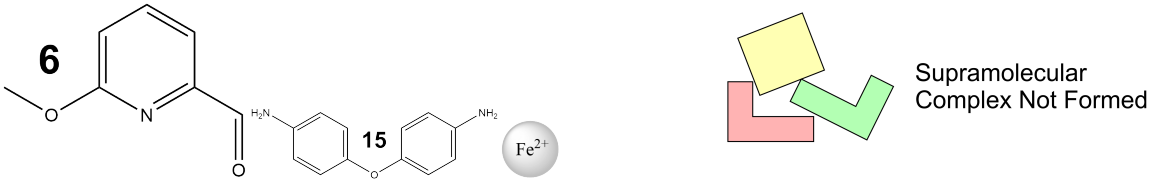


NMR Spectra 12: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 13.



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

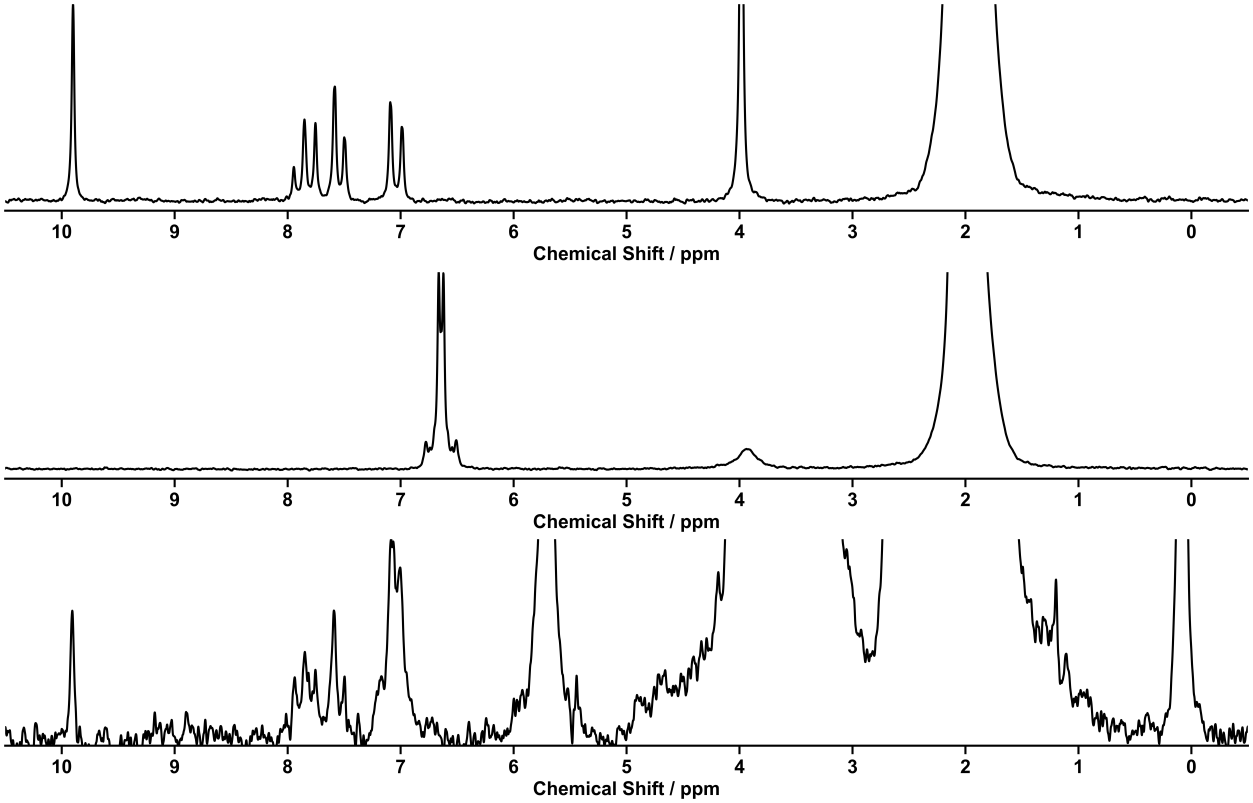
Reaction 14



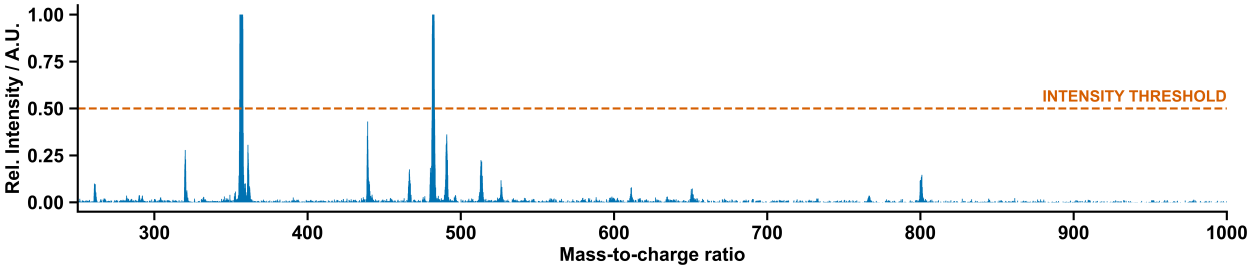
Scheme 13: Self-assembly of components 6, 15, with Iron(II) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 14.

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 labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 14. Decision motivations are also given.

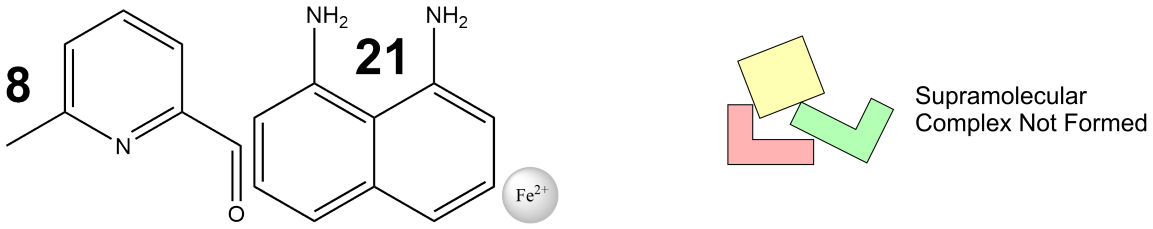


NMR Spectra 13: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 14.



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

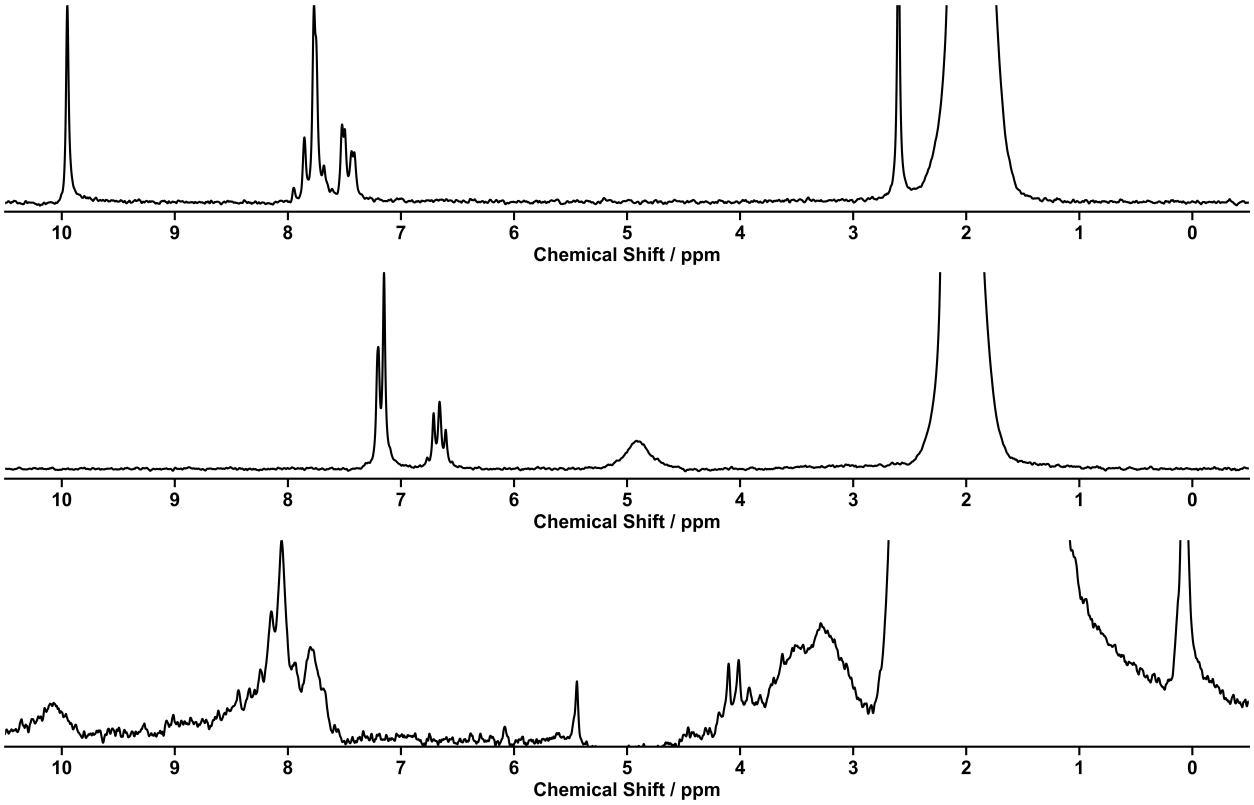
Reaction 15



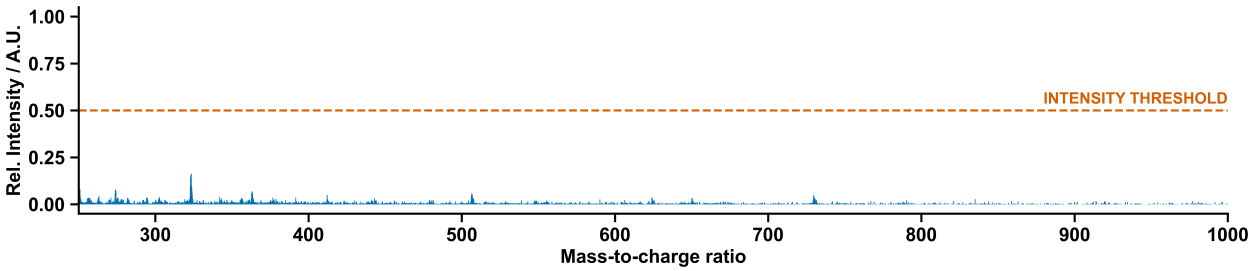
Scheme 14: Self-assembly of components 8, 21, with Iron(II) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 15.

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 labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 15. Decision motivations are also given.

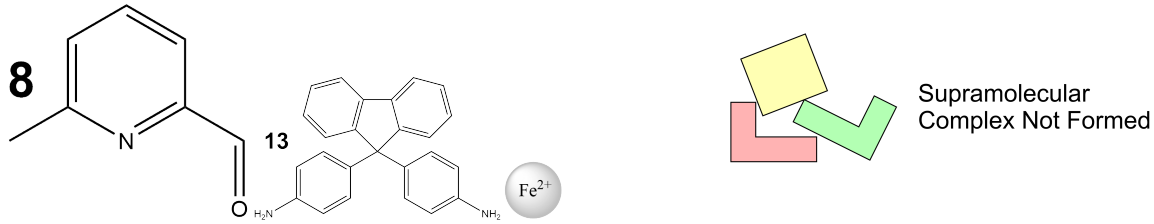


NMR Spectra 14: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 15.



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

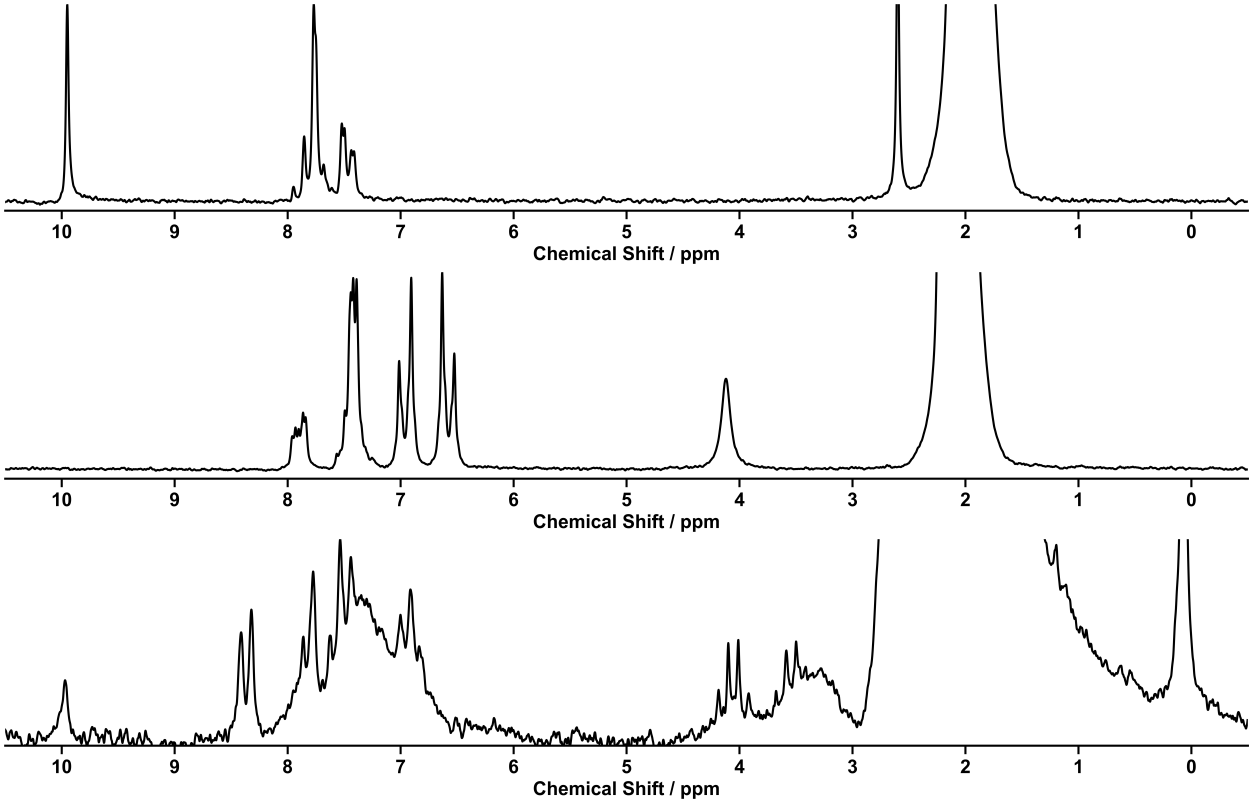
Reaction 16



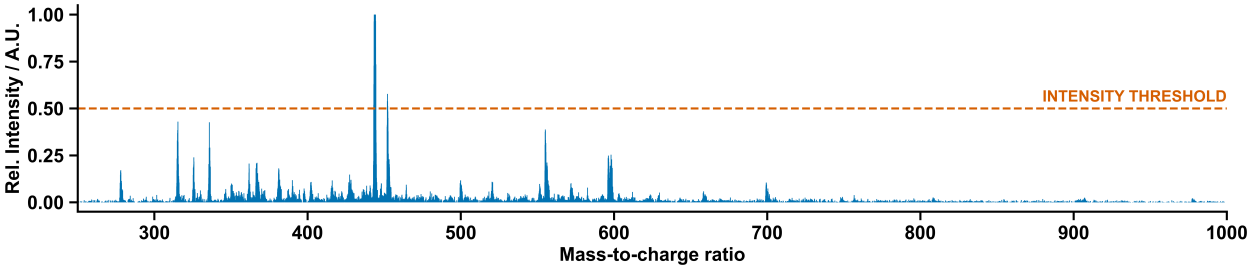
Scheme 15: Self-assembly of components 8, 13, with Iron(II) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 16.

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 labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 16. Decision motivations are also given.

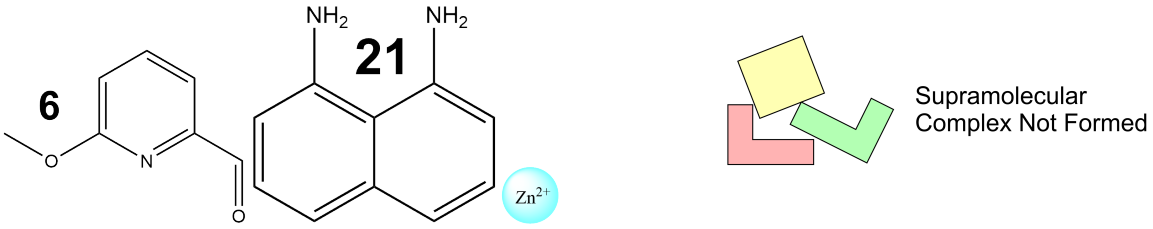


NMR Spectra 15: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 16.



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

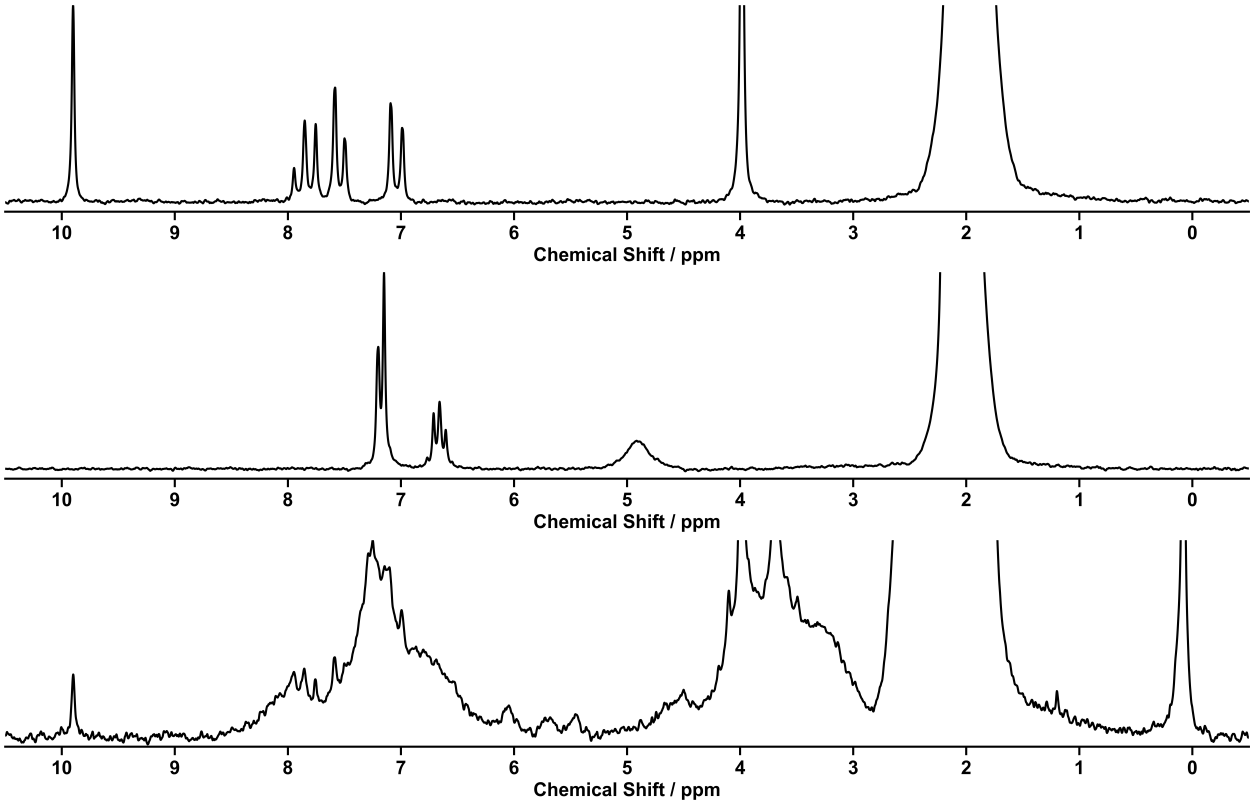
Reaction 17



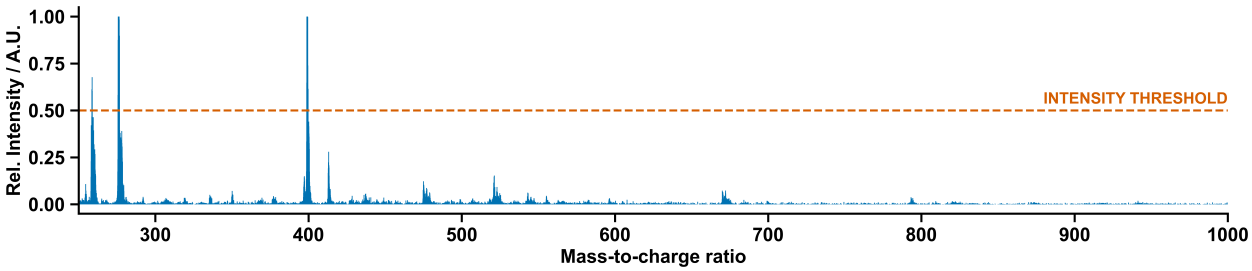
Scheme 16: Self-assembly of components 6, 21, with Zinc(II) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 17.

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 labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 17. Decision motivations are also given.

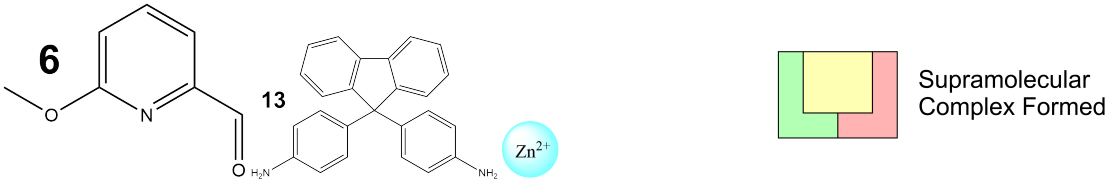


NMR Spectra 16: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 17.



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

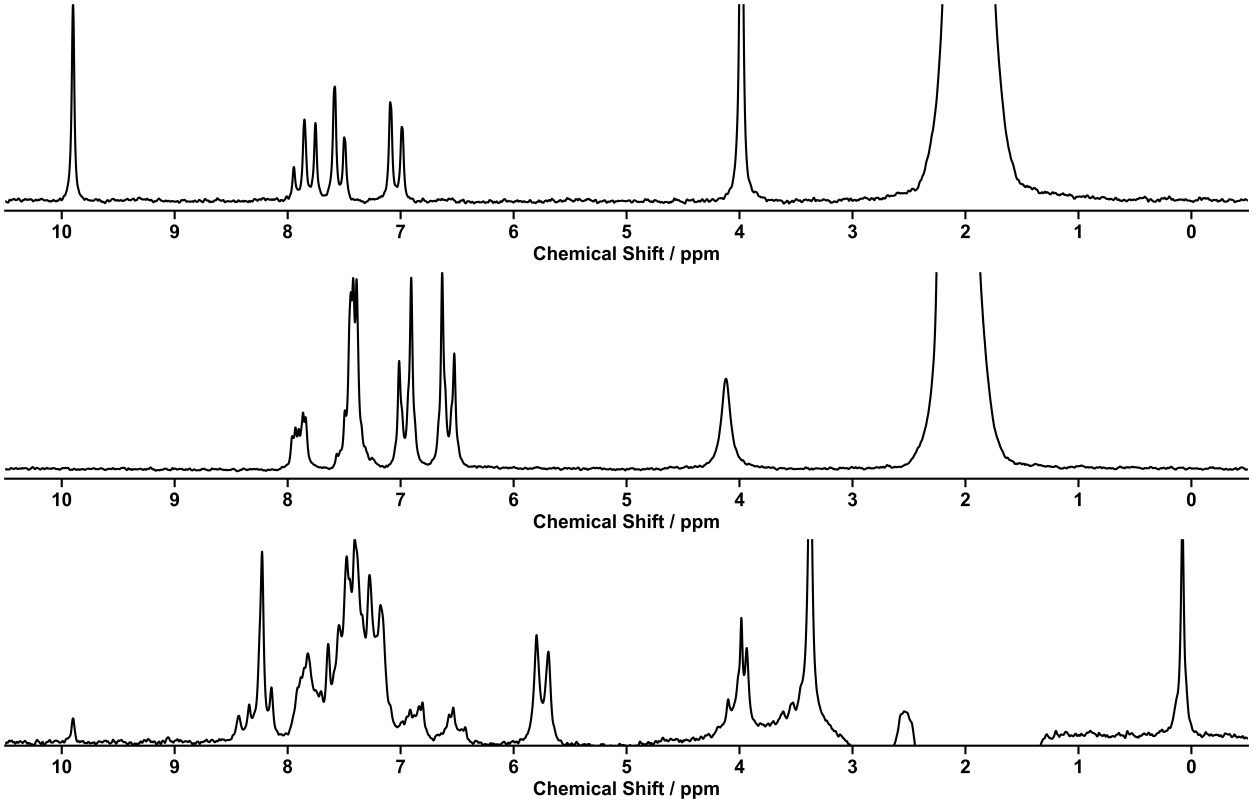
Reaction 18



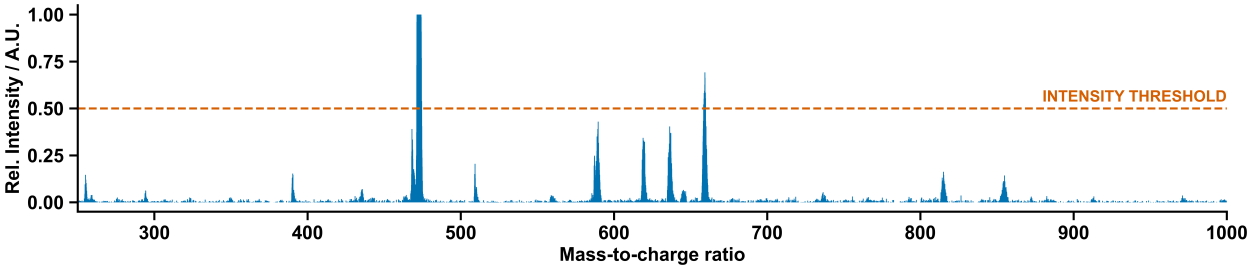
Scheme 17: Self-assembly of components 6, 13, with Zinc(II) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 18.

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 labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 18. Decision motivations are also given.

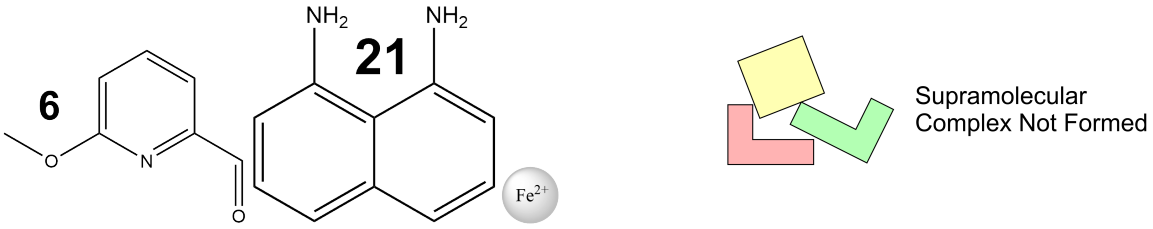


NMR Spectra 17: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 18.



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

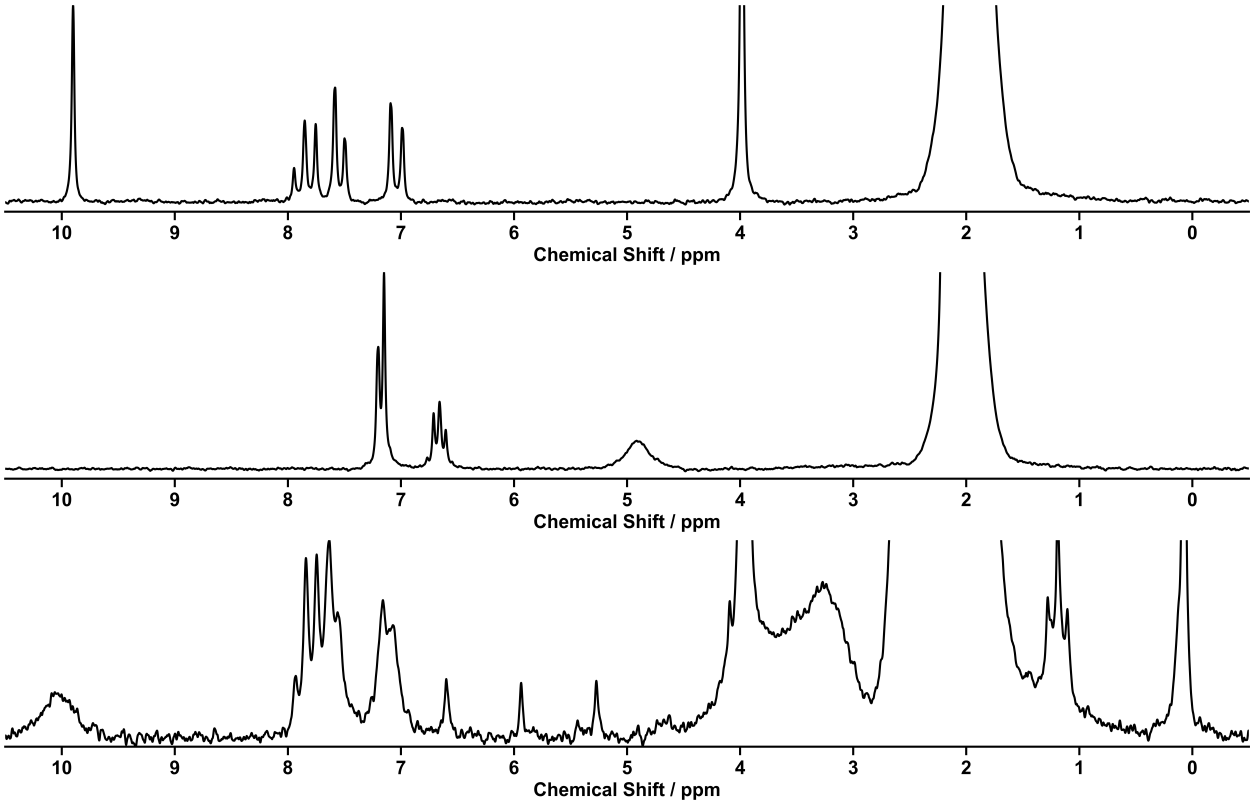
Reaction 19



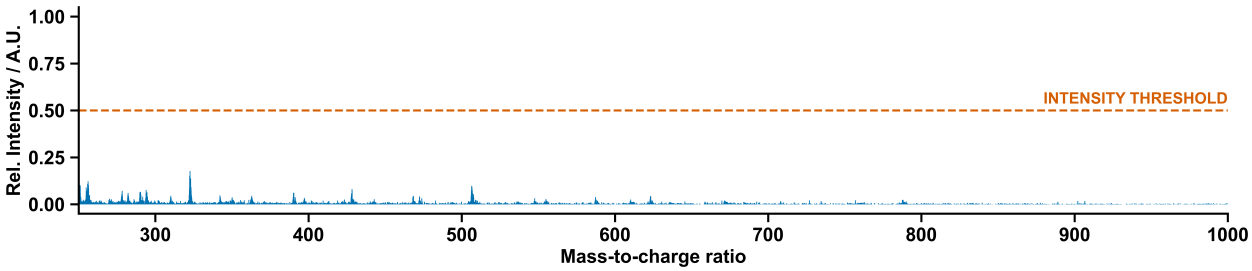
Scheme 18: Self-assembly of components 6, 21, with Iron(II) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 19.

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 labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 19. Decision motivations are also given.

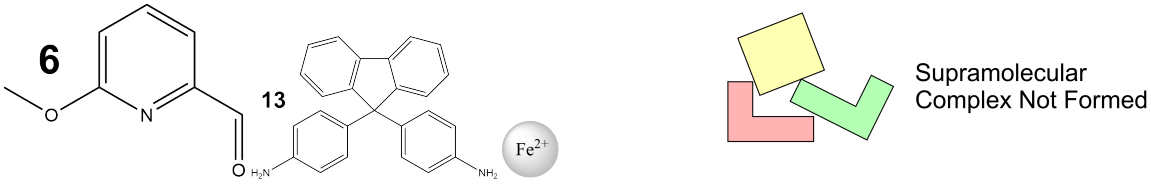


NMR Spectra 18: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 19.



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

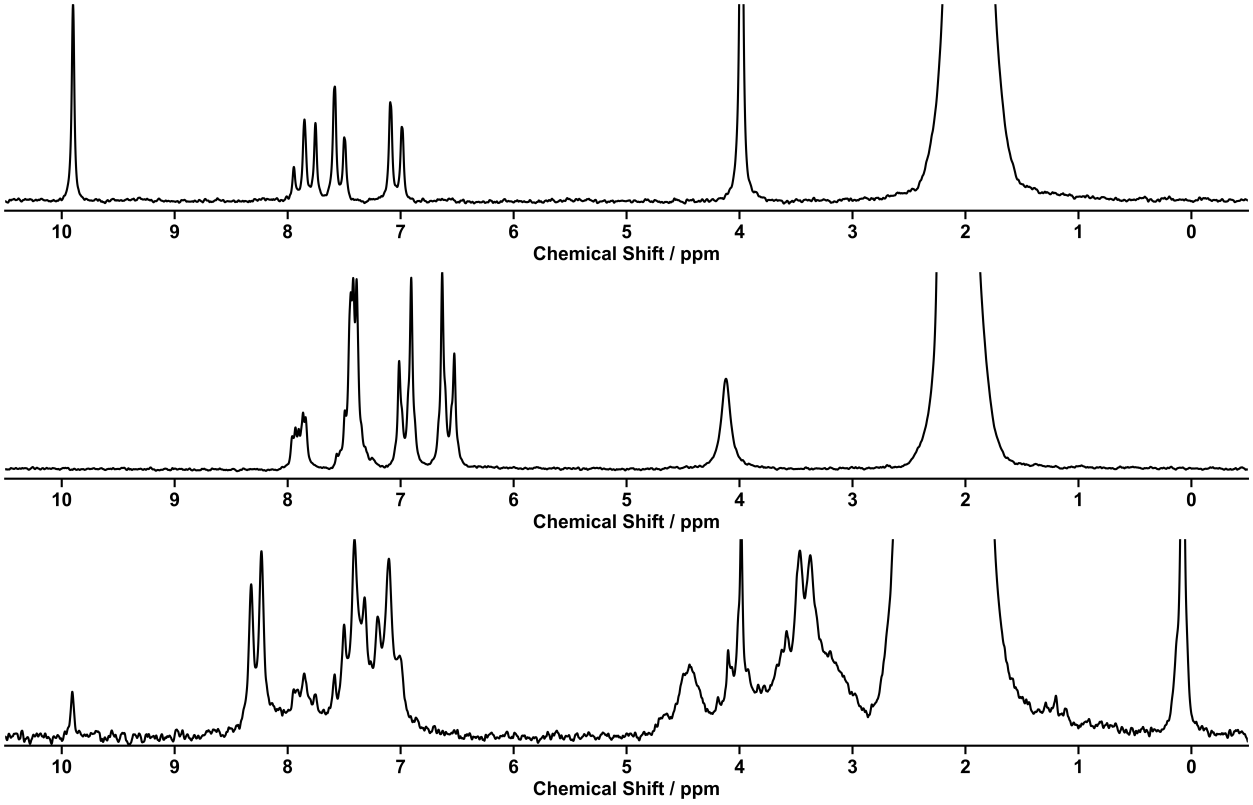
Reaction 20



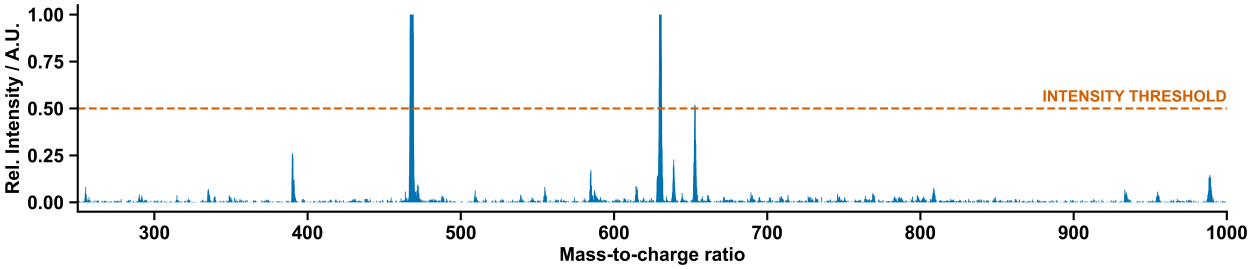
Scheme 19: Self-assembly of components 6, 13, with Iron(II) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 20.

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 labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 20. Decision motivations are also given.

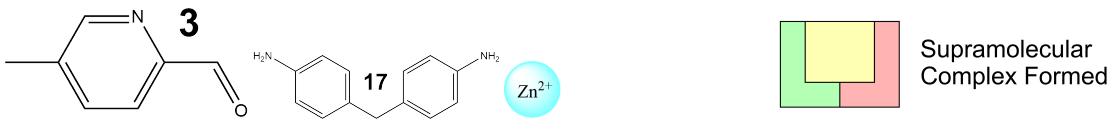


NMR Spectra 19: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 20.



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

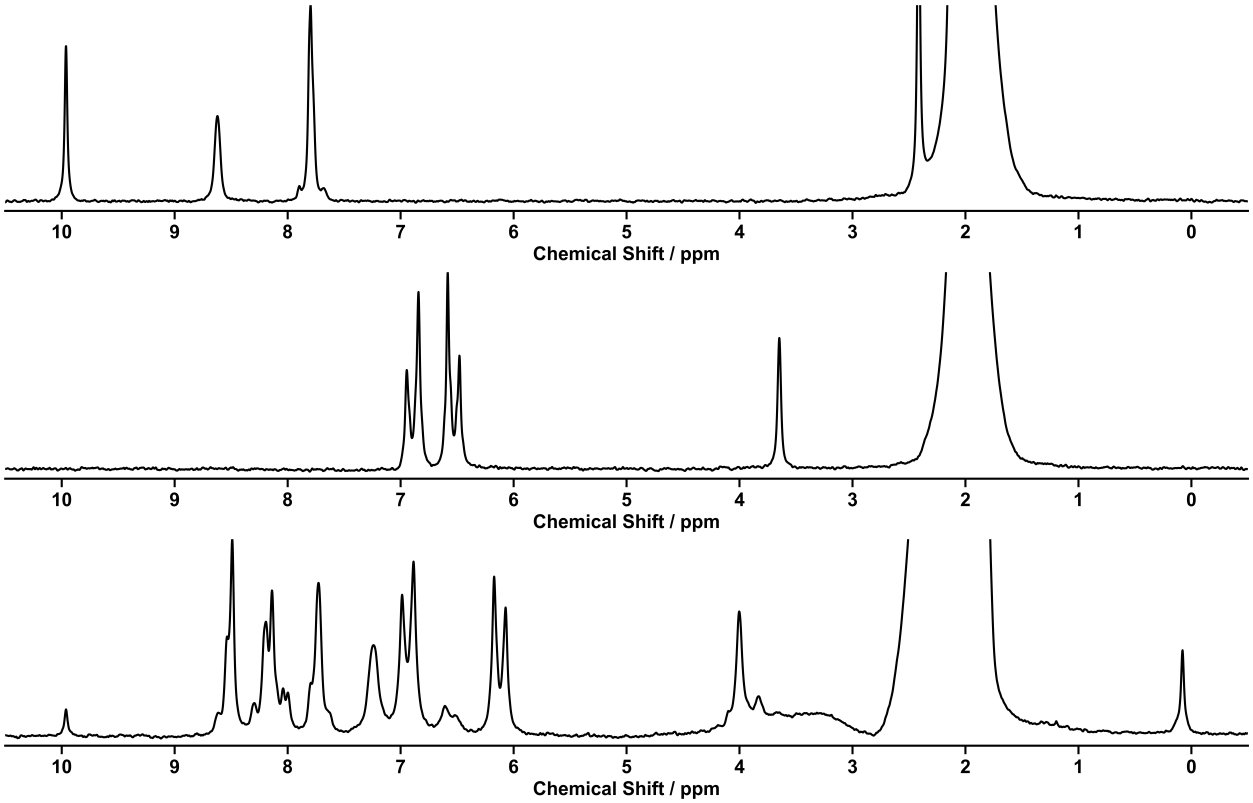
Reaction 21



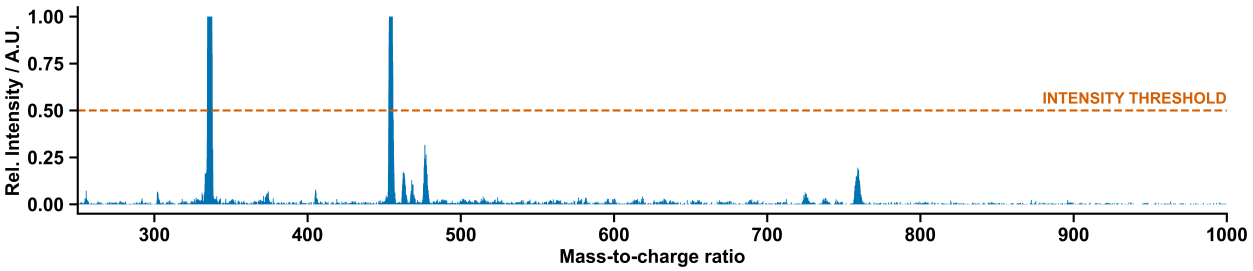
Scheme 20: Self-assembly of components 3, 17, with Zinc(II) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 21.

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

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

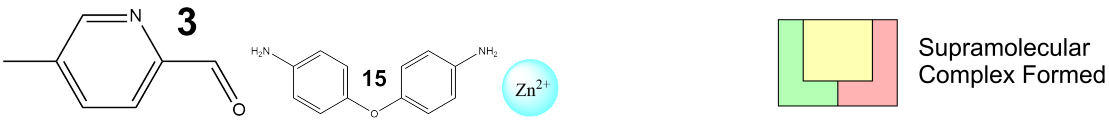


NMR Spectra 20: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 21.



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

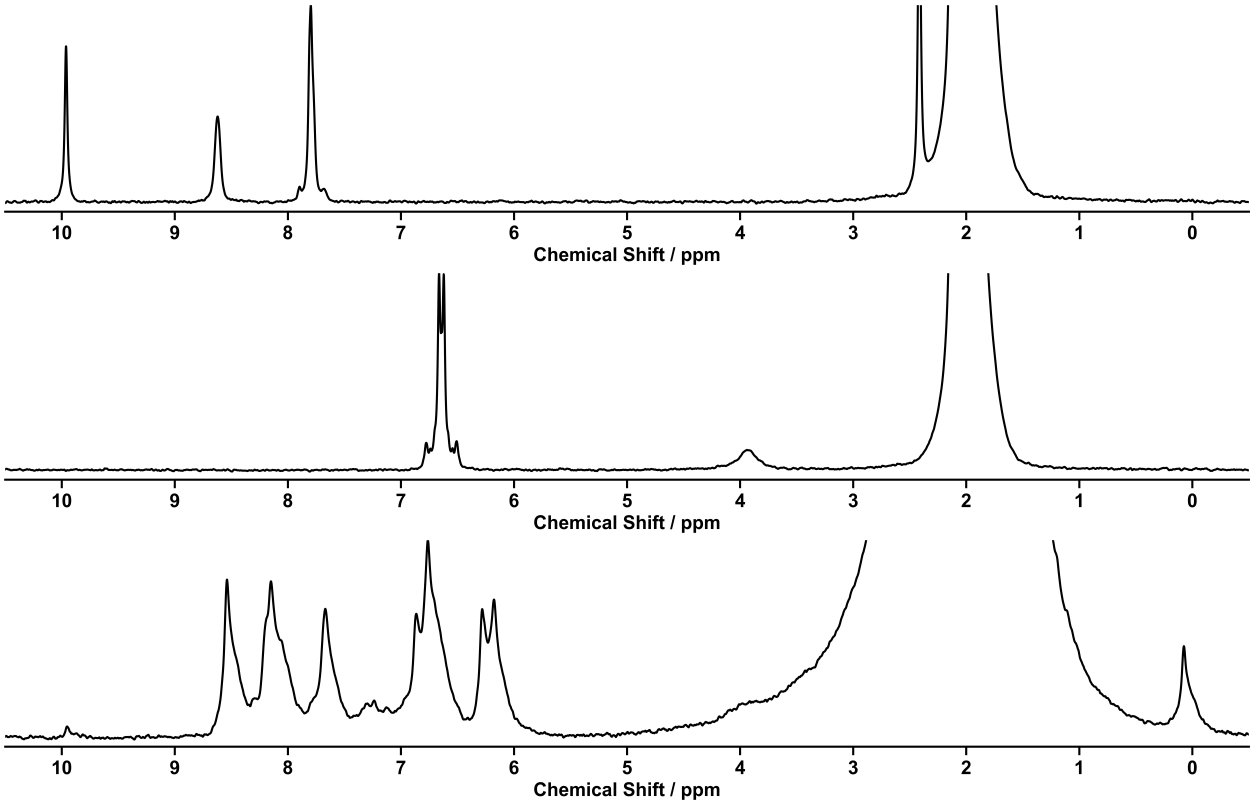
Reaction 23



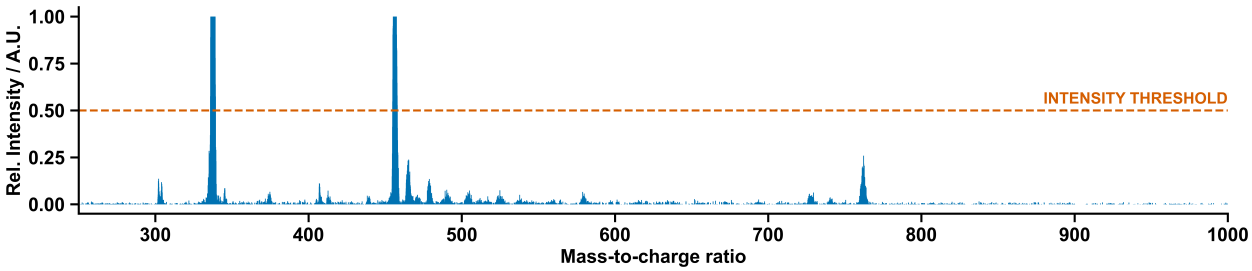
Scheme 21: Self-assembly of components 3, 15, with Zinc(II) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 23.

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	Number of counter-ions found: 1

Decision Table 21: Human labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 23. Decision motivations are also given.

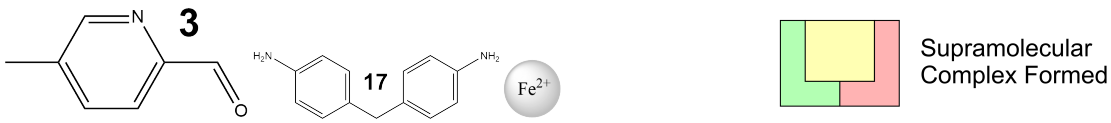


NMR Spectra 21: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 23.



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

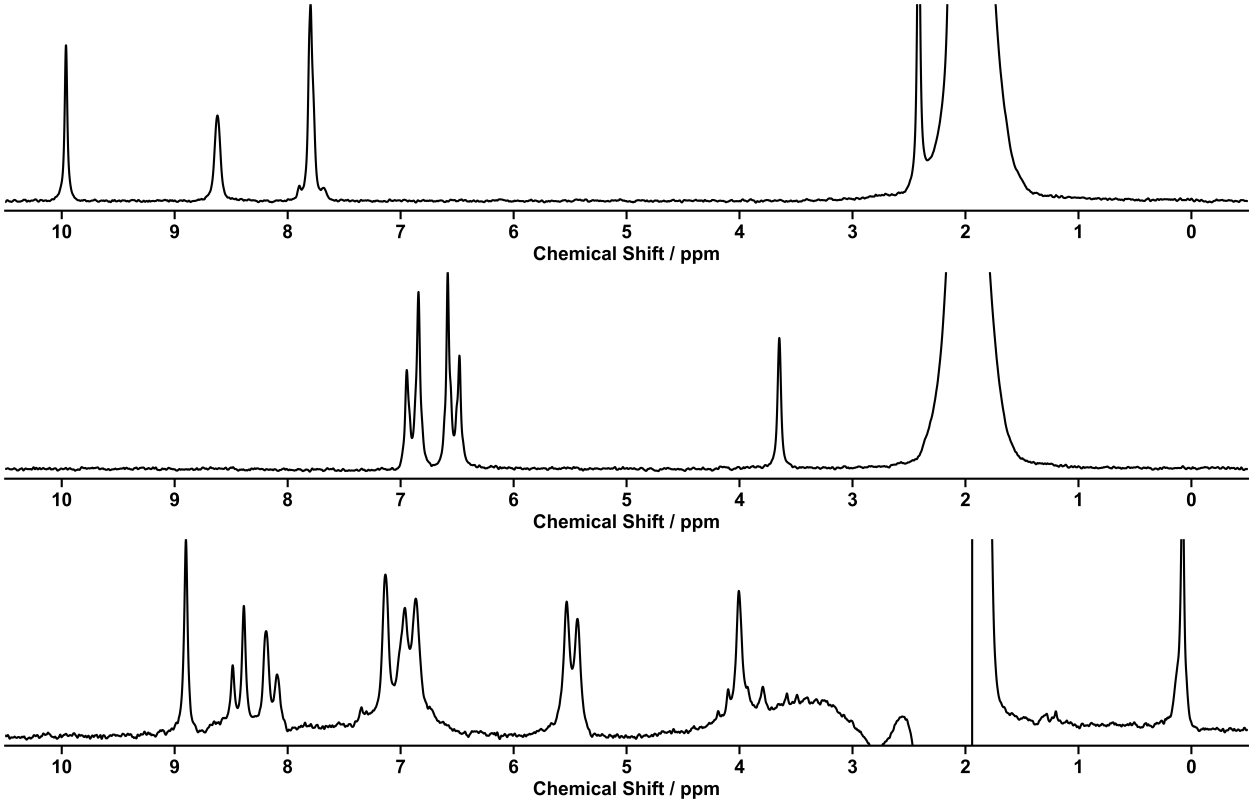
Reaction 24



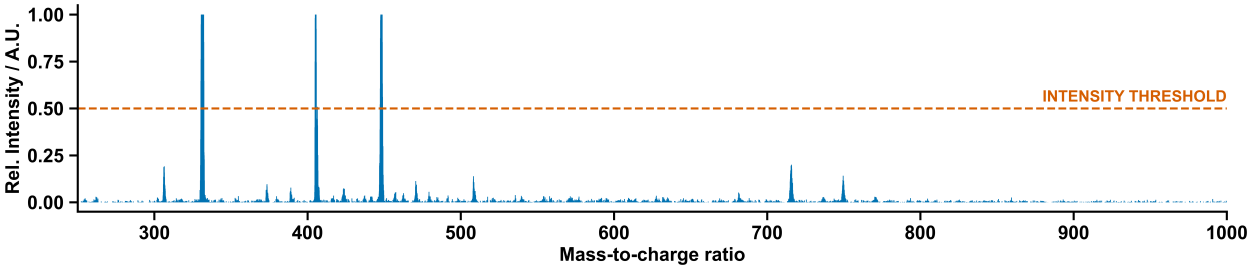
Scheme 22: Self-assembly of components 3, 17, with Iron(II) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 24.

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	
		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: 3

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

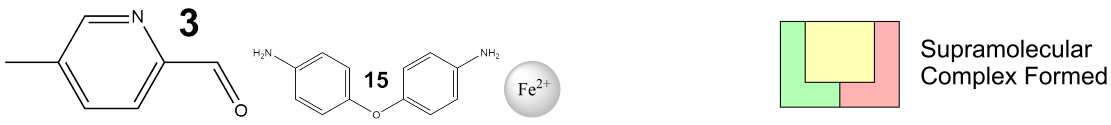


NMR Spectra 22: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 24.



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

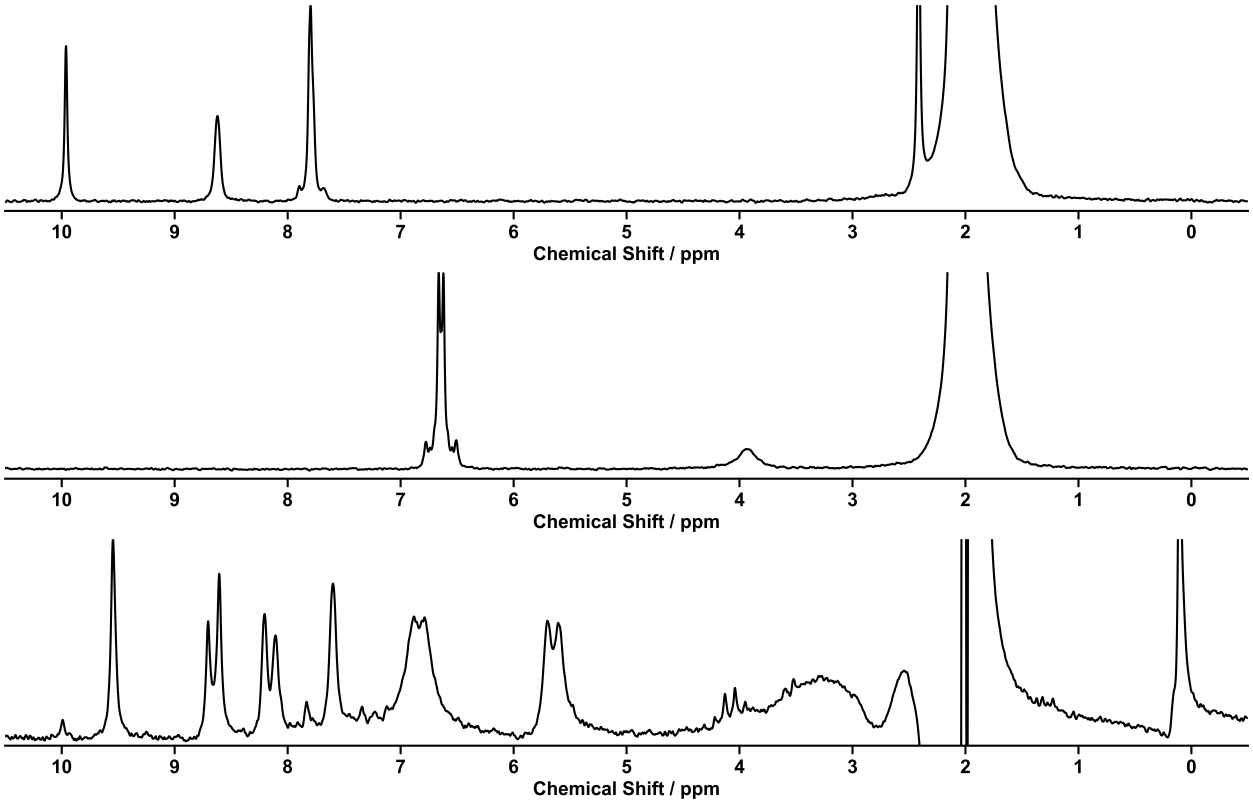
Reaction 26



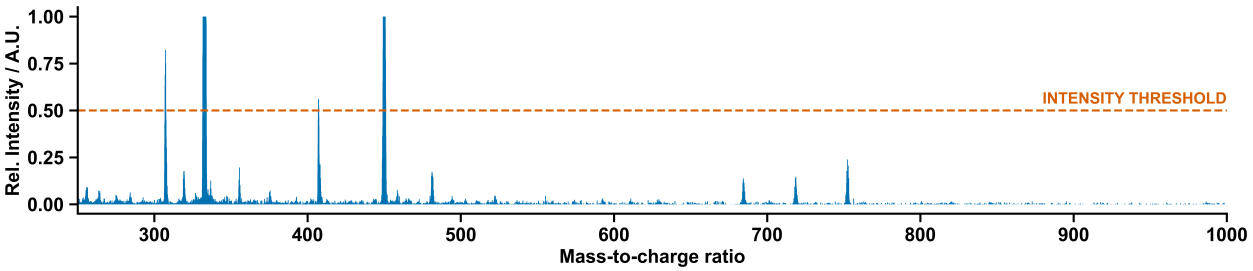
Scheme 23: Self-assembly of components 3, 15, with Iron(II) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 26.

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

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

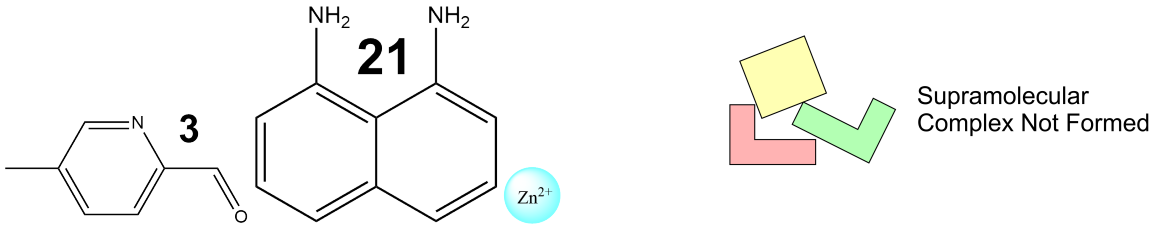


NMR Spectra 23: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 26.



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

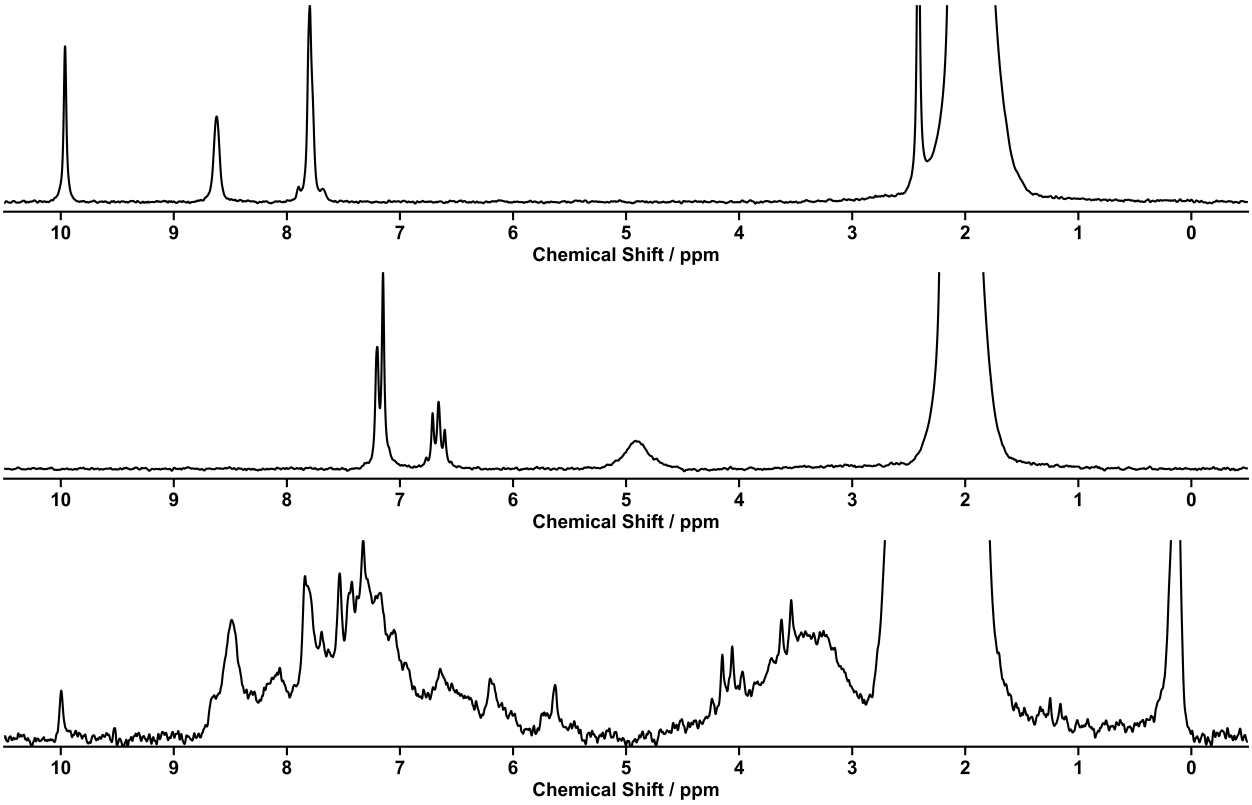
Reaction 27



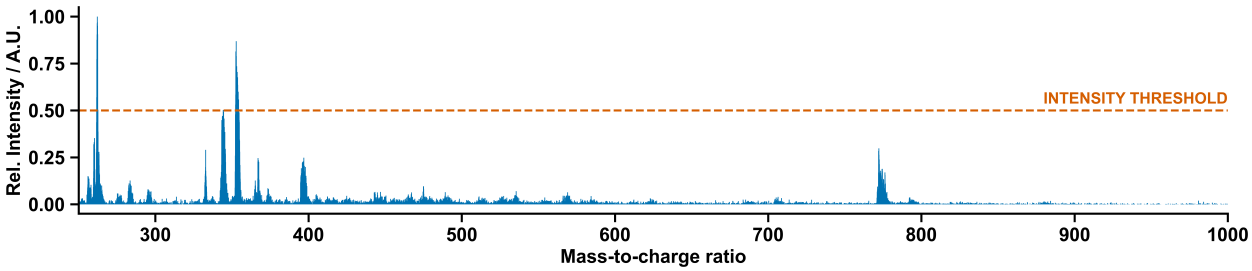
Scheme 24: Self-assembly of components 3, 21, with Zinc(II) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 27.

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 labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 27. Decision motivations are also given.

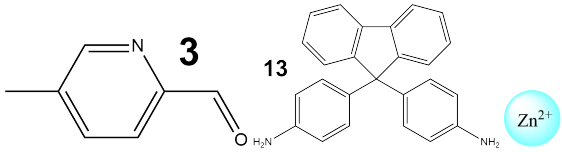


NMR Spectra 24: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 27.



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

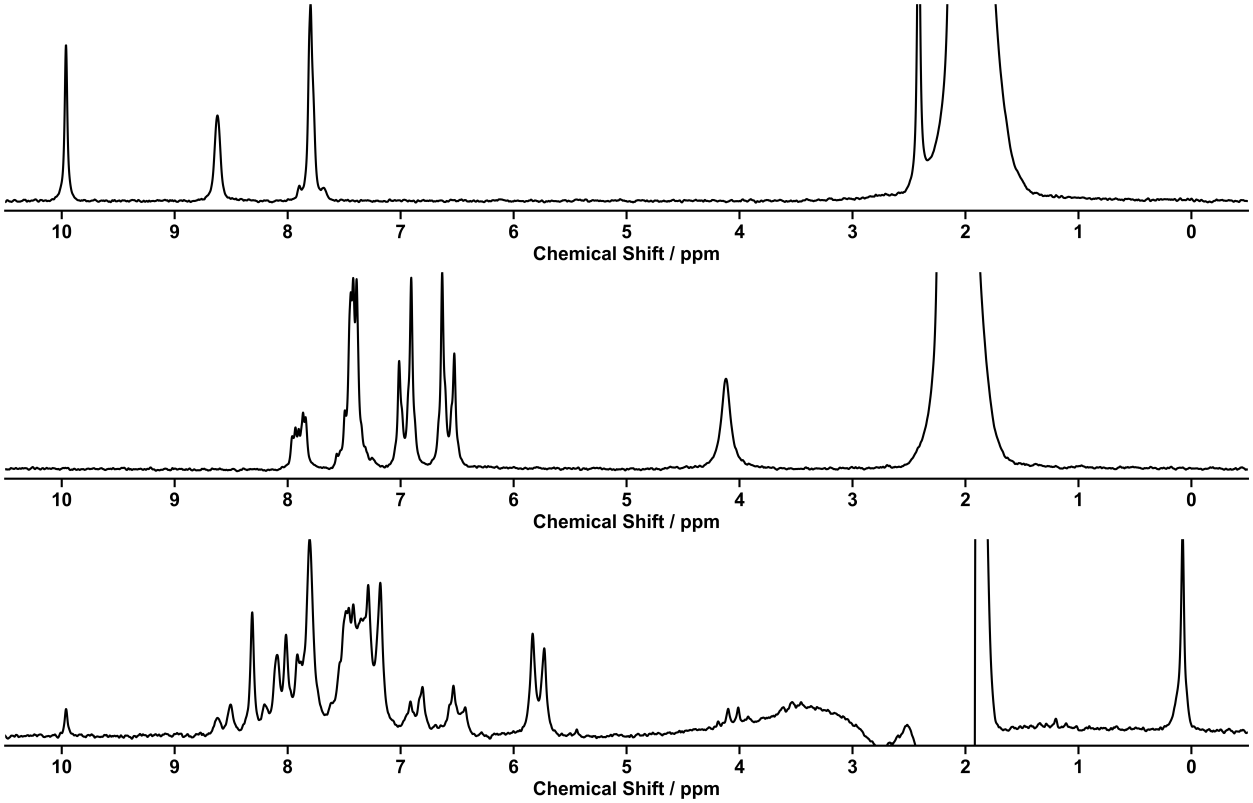
Reaction 28



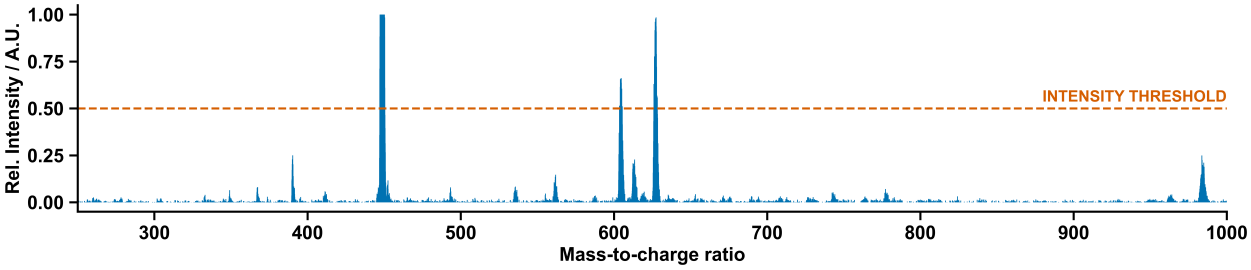
Scheme 25: Self-assembly of components 3, 13, with Zinc(II) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 28.

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

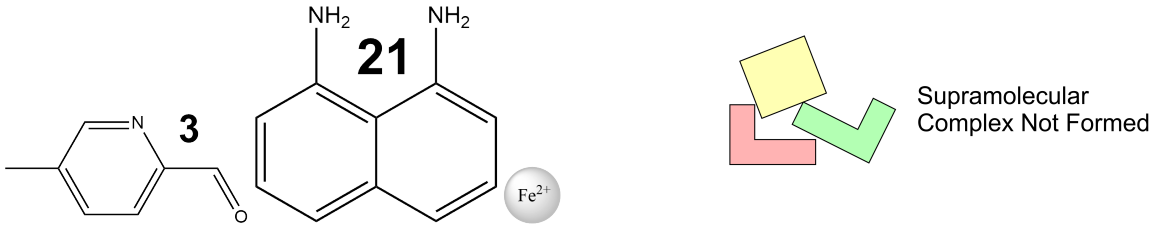


NMR Spectra 25: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 28.



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

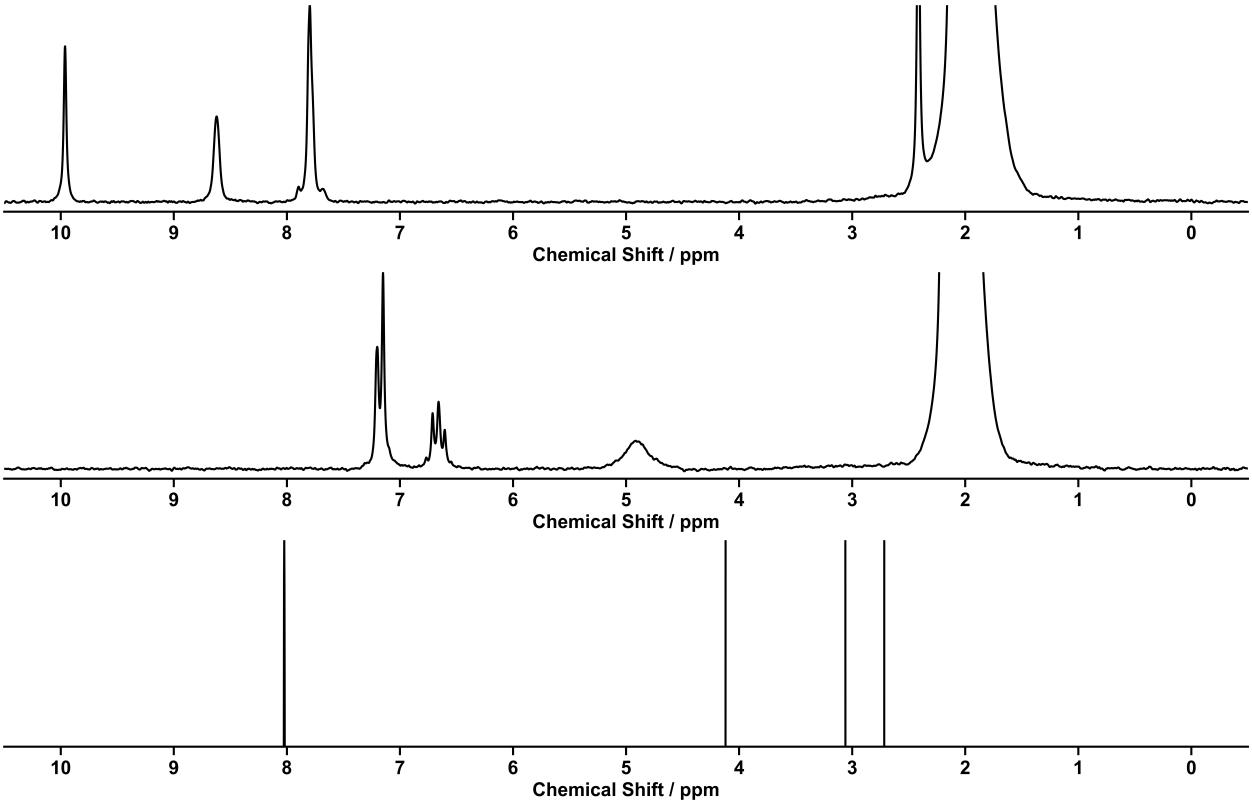
Reaction 29



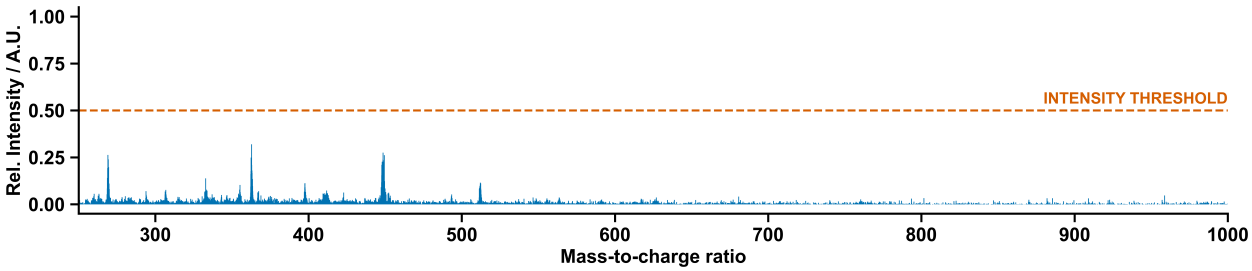
Scheme 26: Self-assembly of components 3, 21, with Iron(II) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 29.

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 labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 29. Decision motivations are also given.

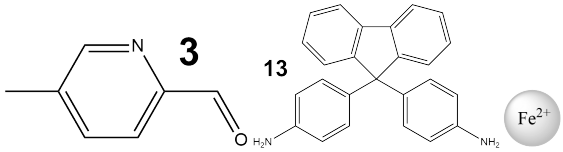


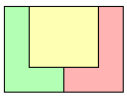
NMR Spectra 26: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 29.



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

Reaction 30



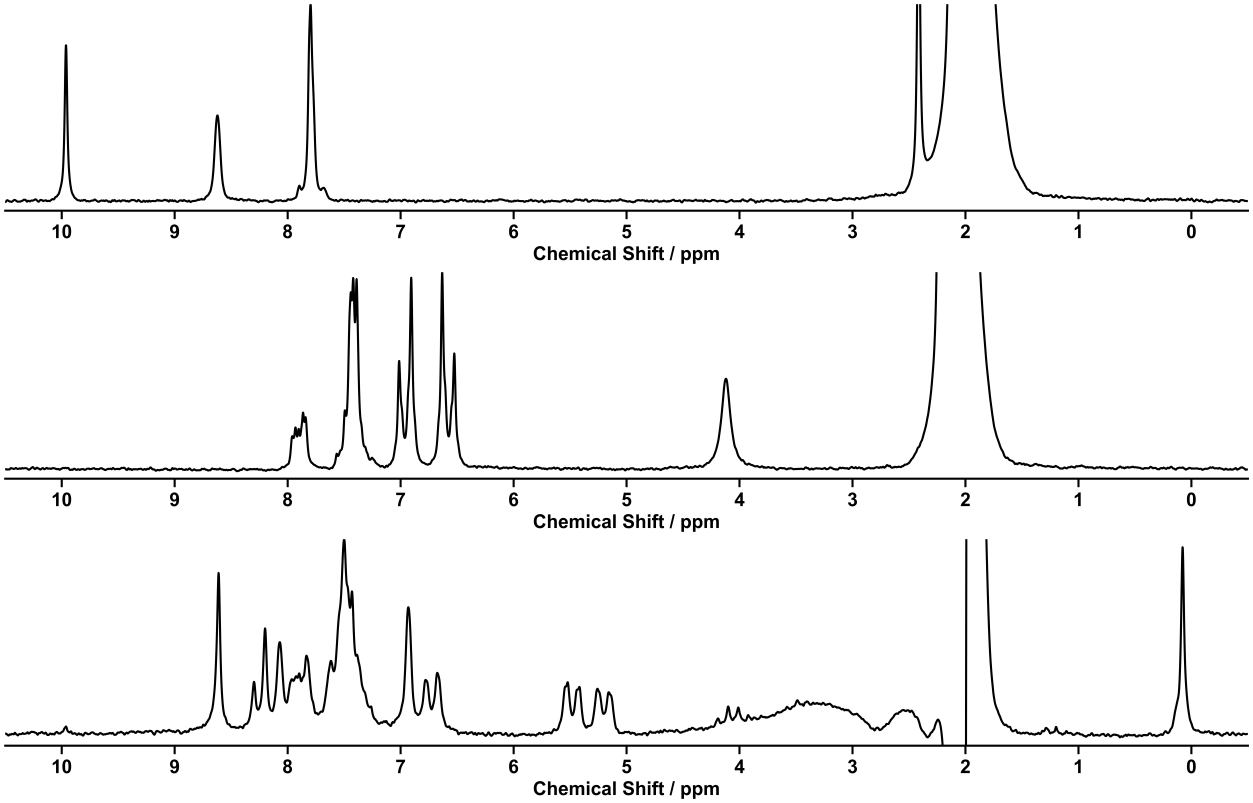


Supramolecular Complex Formed

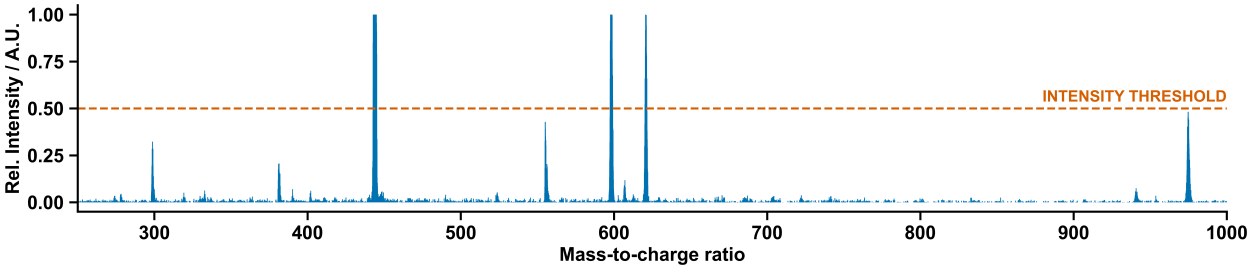
Scheme 27: Self-assembly of components 3, 13, with Iron(II) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 30.

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	
		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: 10
		MS Criteria 3: Pass	Number of counter-ions found: 6

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

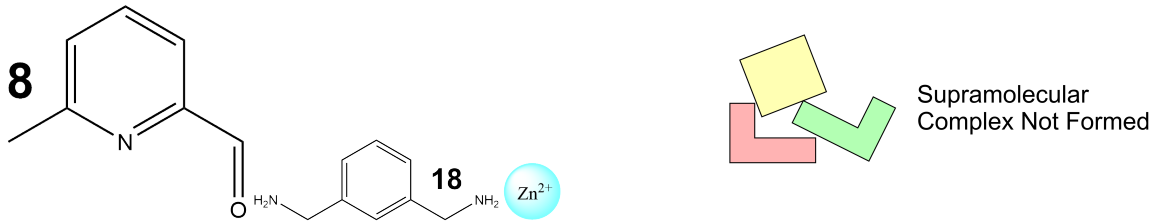


NMR Spectra 27: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 30.



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

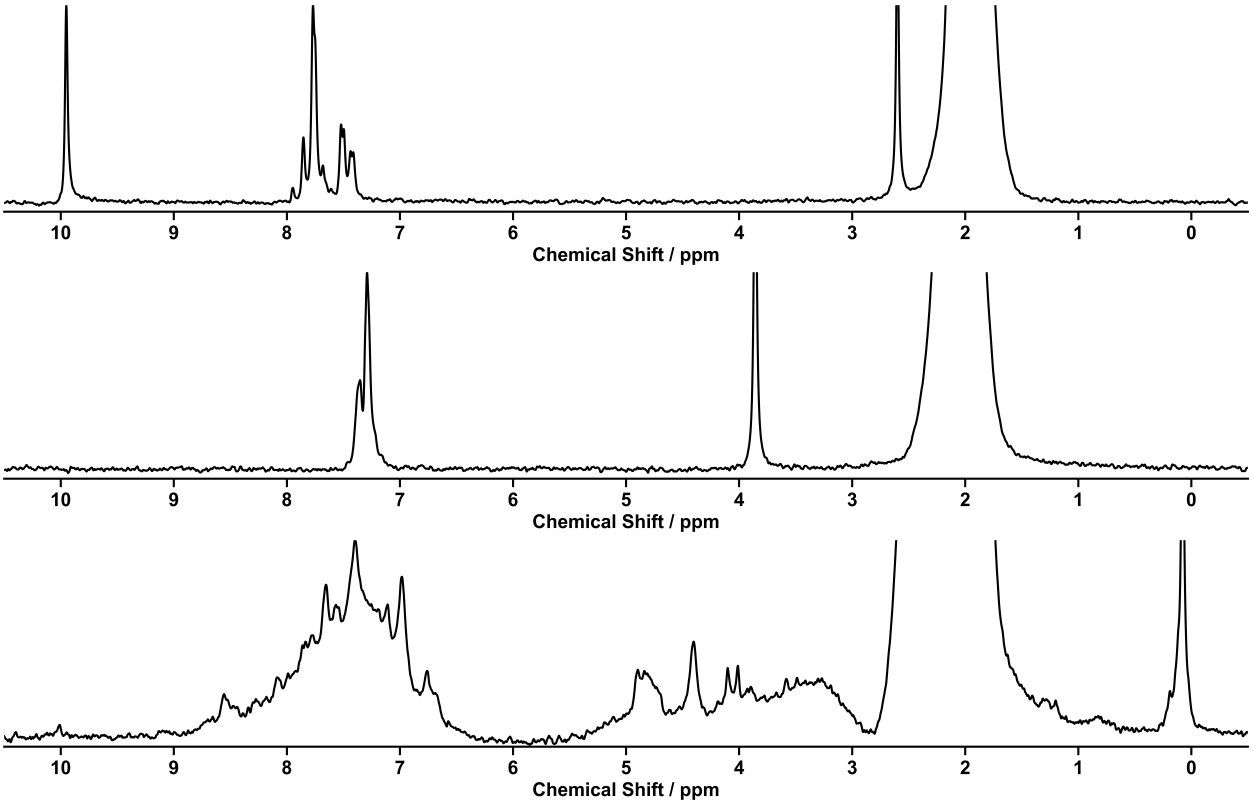
Reaction 31



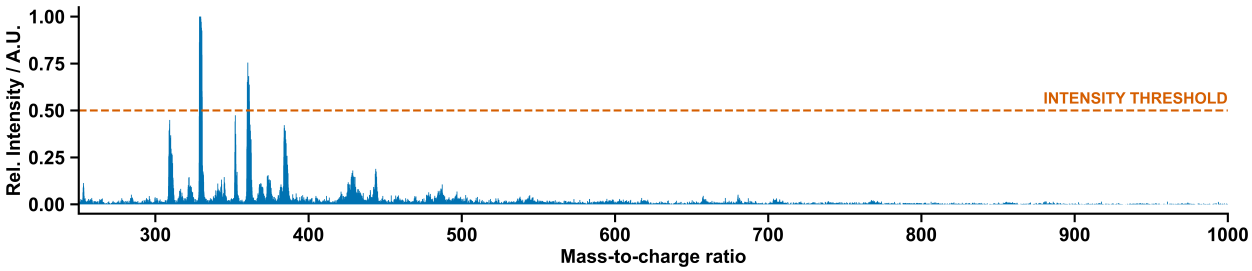
Scheme 28: Self-assembly of components 8, 18, with Zinc(II) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 31.

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 labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 31. Decision motivations are also given.

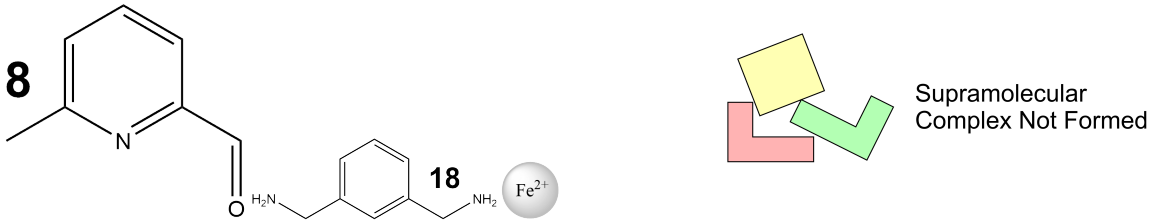


NMR Spectra 28: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 31.



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

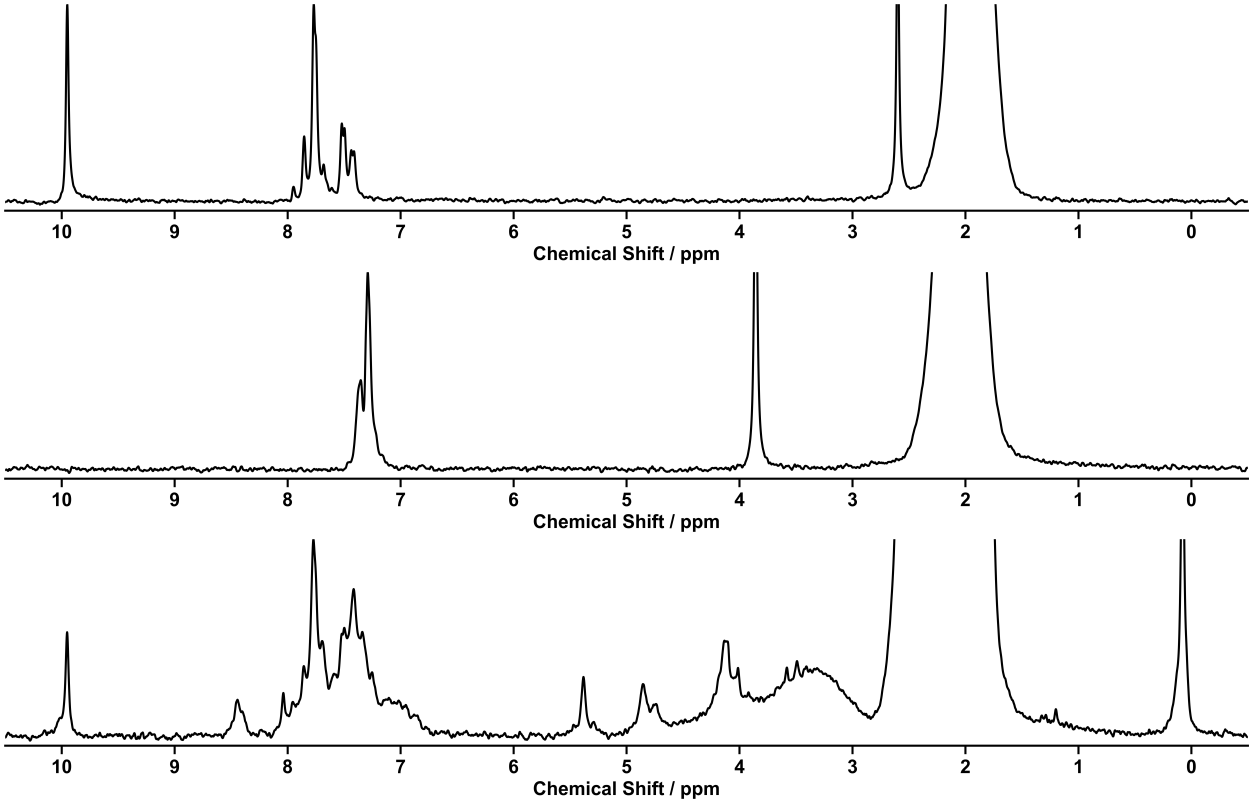
Reaction 32



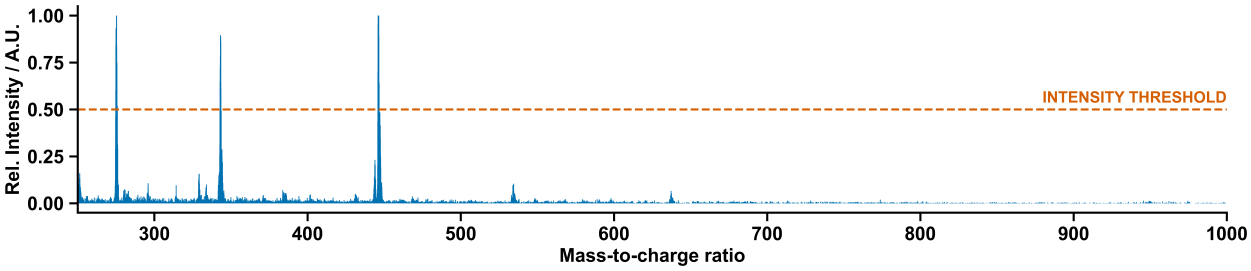
Scheme 29: Self-assembly of components 8, 18, with Iron(II) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 32.

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 labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 32. Decision motivations are also given.

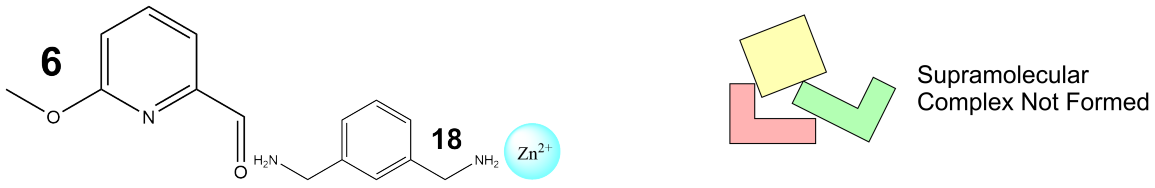


NMR Spectra 29: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 32.



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

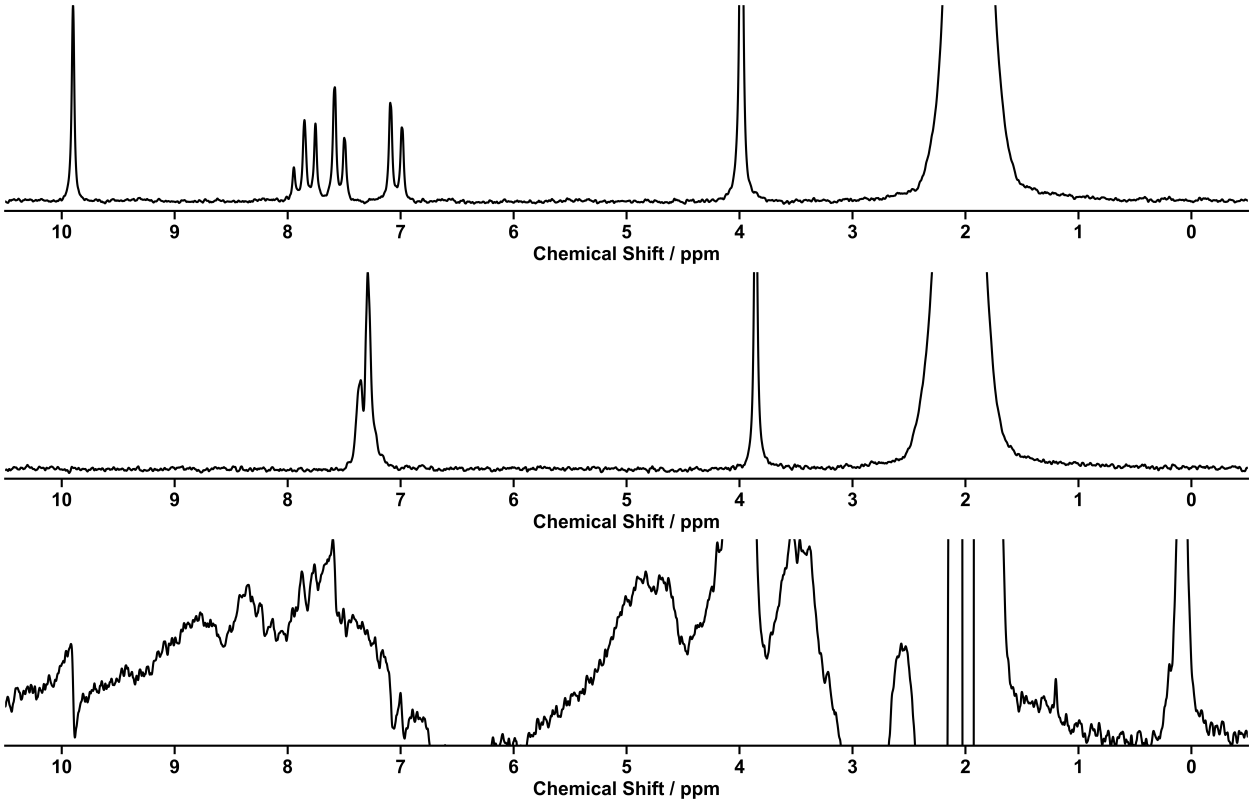
Reaction 33



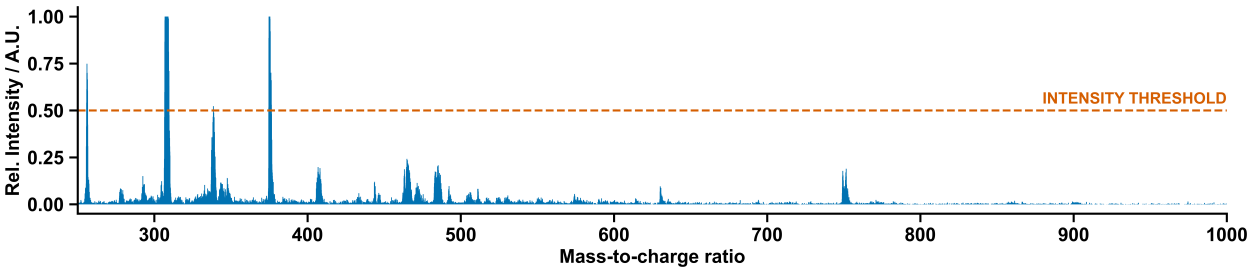
Scheme 30: Self-assembly of components 6, 18, with Zinc(II) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 33.

<table>
<tr><td rowspan="2">Human Reaction Decision:
Failed</td><td>Human NMR Decision:
Failed</td><td colspan="2">NMR Spectra Category:
Oligomers formed.</td></tr>
<tr><td>Human MS Decision:
Pass</td><td colspan="2">MS Spectra Category:
Reaction occurred, supramolecular product.</td></tr>
<tr><td rowspan="4">Decision Maker Reaction Decision:
N/A</td><td rowspan="2">Decision Maker NMR Decision:
N/A</td><td colspan="2">NMR Criteria 1:
N/A</td></tr>
<tr><td colspan="2">NMR Criteria 2:
N/A</td></tr>
<tr><td rowspan="2">Decision Maker MS Decision:
Pass</td><td>MS Criteria 1 and 2:
Pass</td><td>Number of predicted peaks found in MS spectra with appropriate intensity:
0</td></tr>
<tr><td>MS Criteria 3:
Pass</td><td>Number of counter-ions found:
0</td></tr>
</table>

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

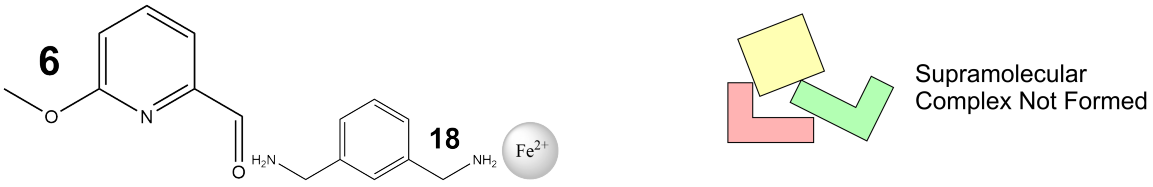


NMR Spectra 30: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 33.



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

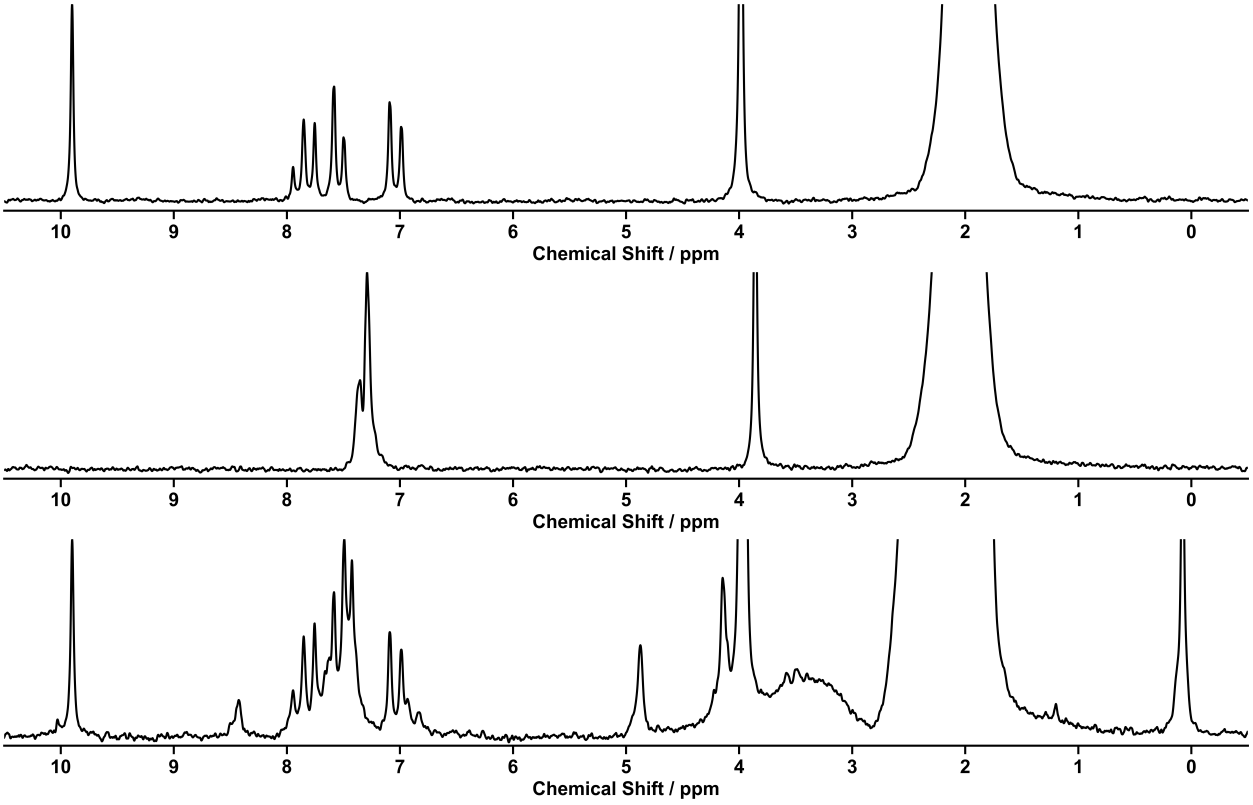
Reaction 34



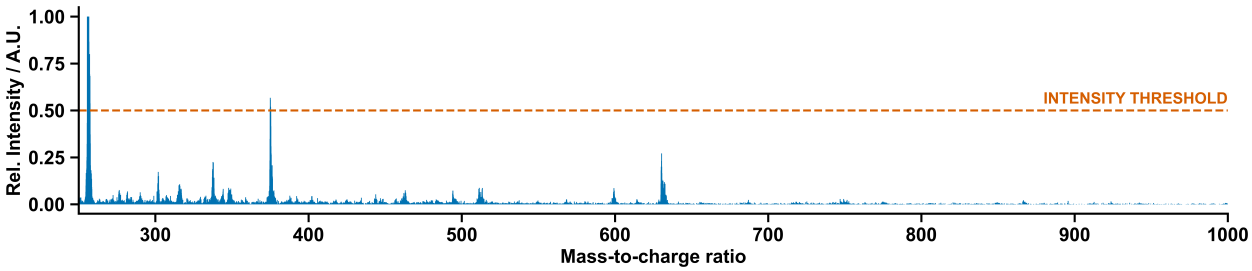
Scheme 31: Self-assembly of components 6, 18, with Iron(II) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 34.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: No reaction occured.	
	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 labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 34. Decision motivations are also given.

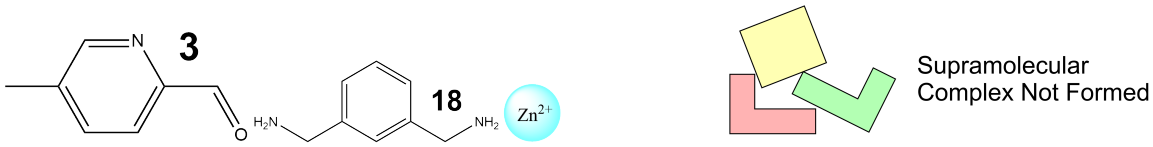


NMR Spectra 31: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 34.



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

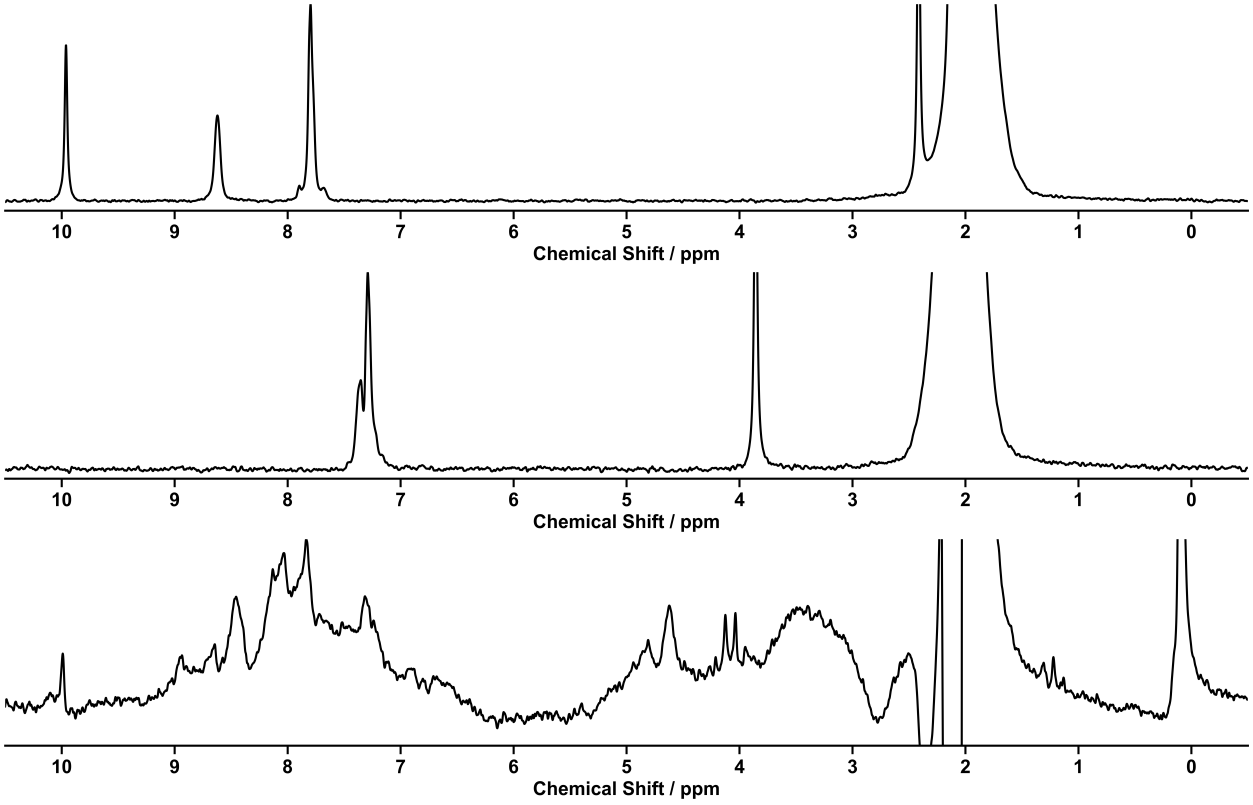
Reaction 35



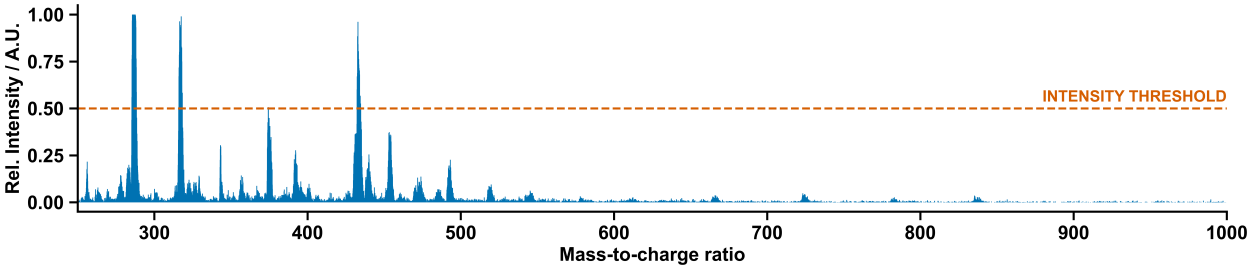
Scheme 32: Self-assembly of components 3, 18, with Zinc(II) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 35.

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 labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 35. Decision motivations are also given.

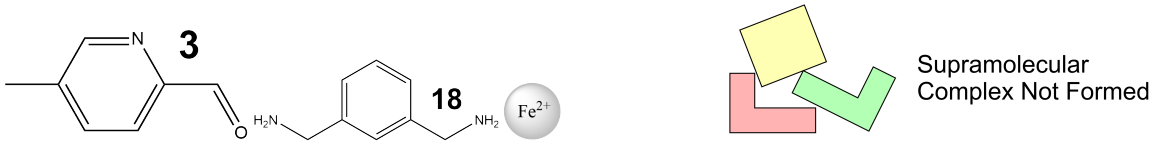


NMR Spectra 32: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 35.



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

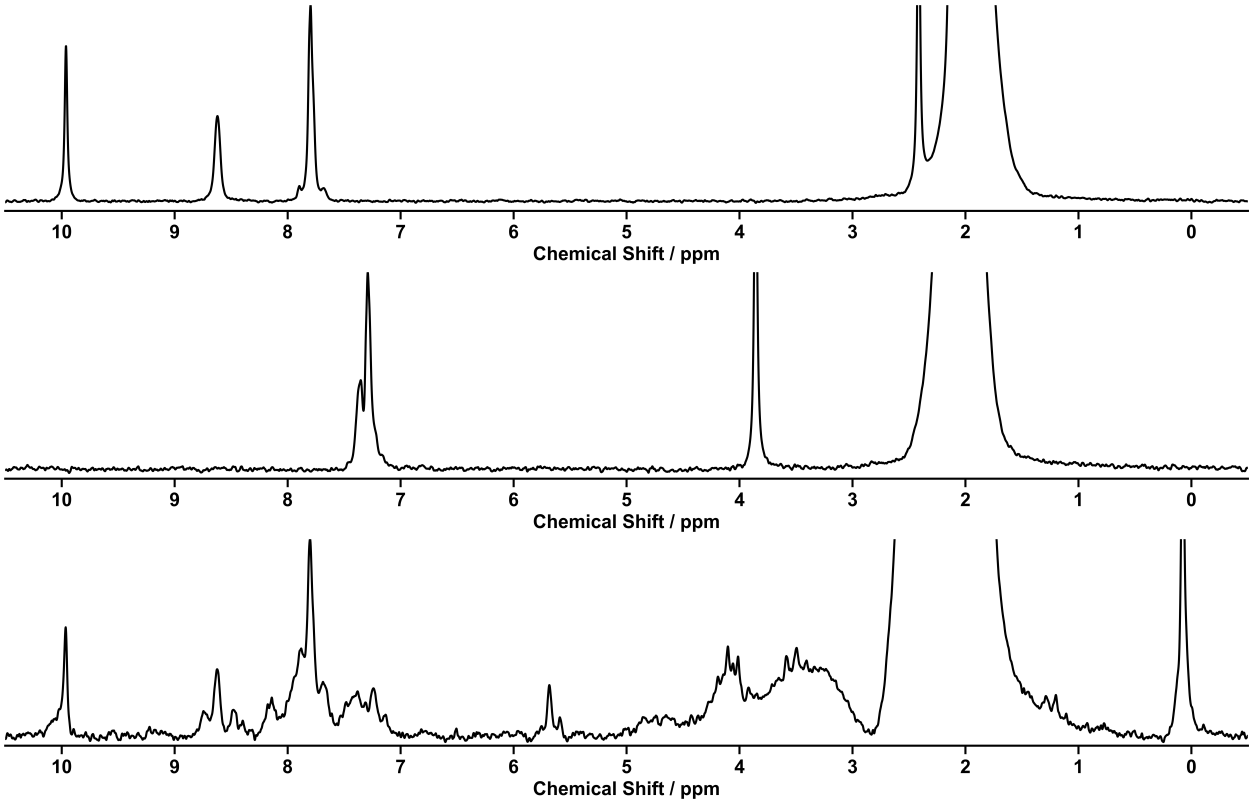
Reaction 36



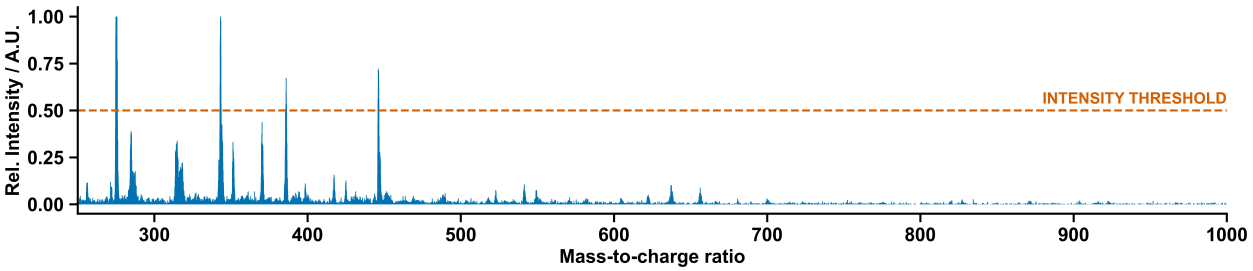
Scheme 33: Self-assembly of components 3, 18, with Iron(II) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 36.

<table>
<tr><td rowspan="2">Human Reaction Decision:
Failed</td><td>Human NMR Decision:
Failed</td><td colspan="2">NMR Spectra Category:
Paramagnetic species formed.</td></tr>
<tr><td>Human MS Decision:
Failed</td><td colspan="2">MS Spectra Category:
Reaction occurred, unknown product.</td></tr>
<tr><td rowspan="4">Decision Maker Reaction Decision:
N/A</td><td rowspan="2">Decision Maker NMR Decision:
N/A</td><td colspan="2">NMR Criteria 1:
N/A</td></tr>
<tr><td colspan="2">NMR Criteria 2:
N/A</td></tr>
<tr><td rowspan="2">Decision Maker MS Decision:
Pass</td><td>MS Criteria 1 and 2:
Pass</td><td>Number of predicted peaks found in MS spectra with appropriate intensity:
0</td></tr>
<tr><td>MS Criteria 3:
Pass</td><td>Number of counter-ions found:
0</td></tr>
</table>

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

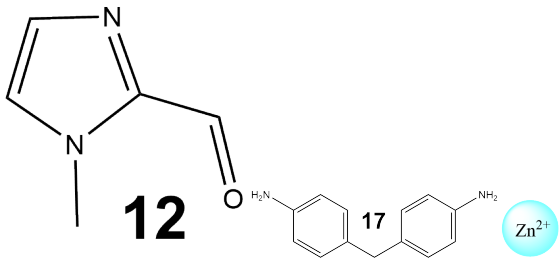


NMR Spectra 33: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 36.



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

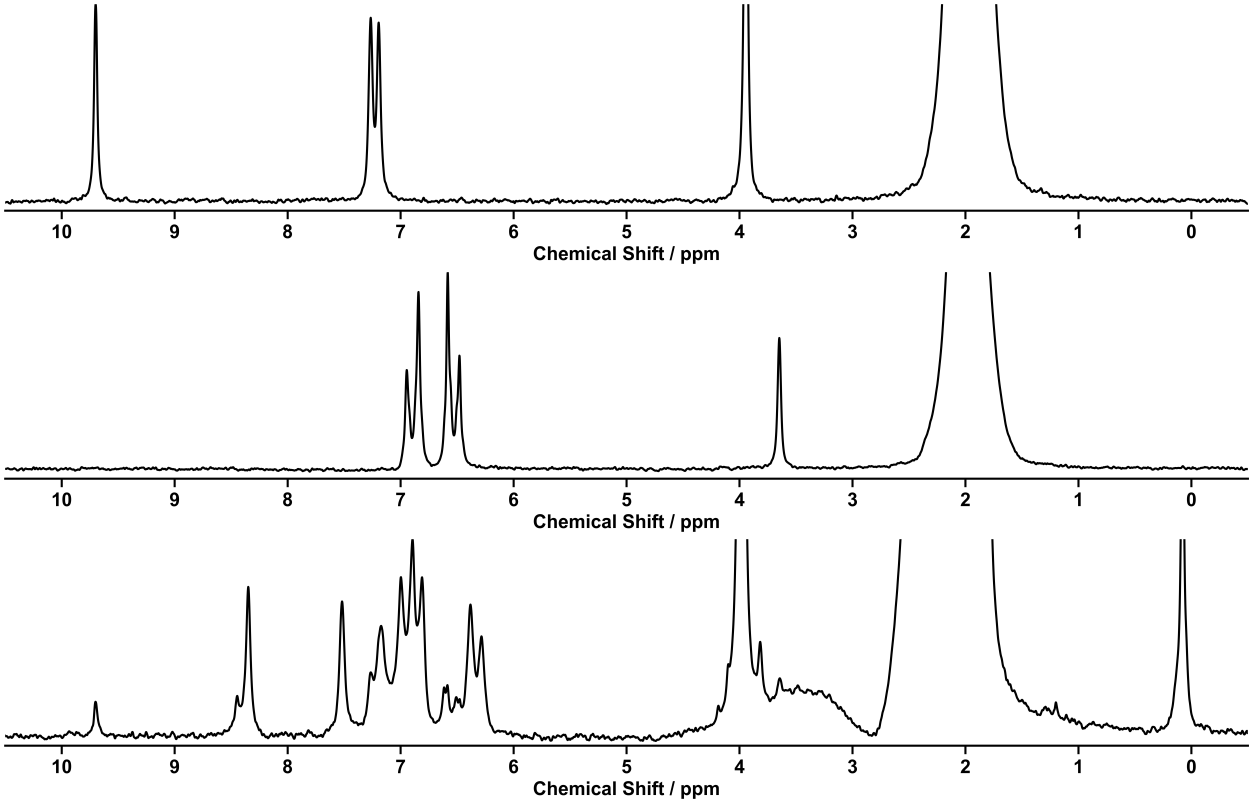
Reaction 37



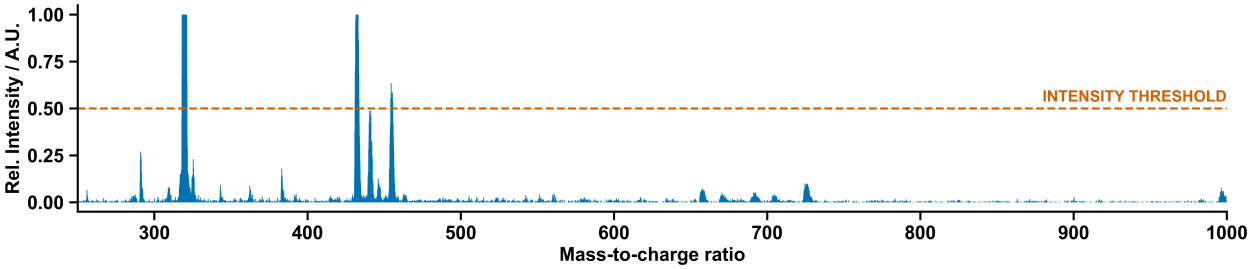
Scheme 34: Self-assembly of components 12, 17, with Zinc(II) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 37.

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 labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 37. Decision motivations are also given.

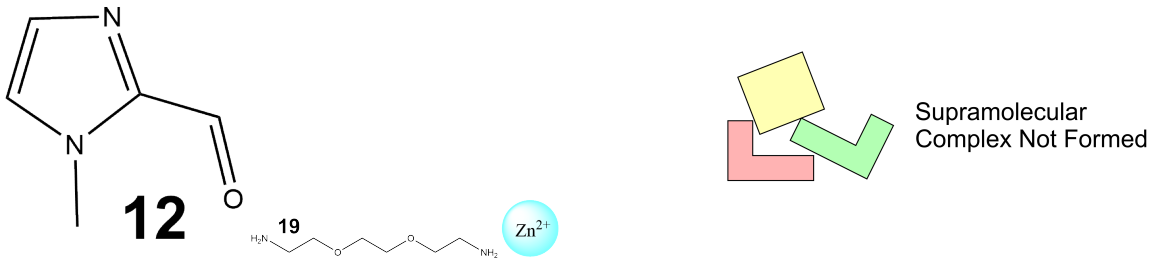


NMR Spectra 34: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 37.



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

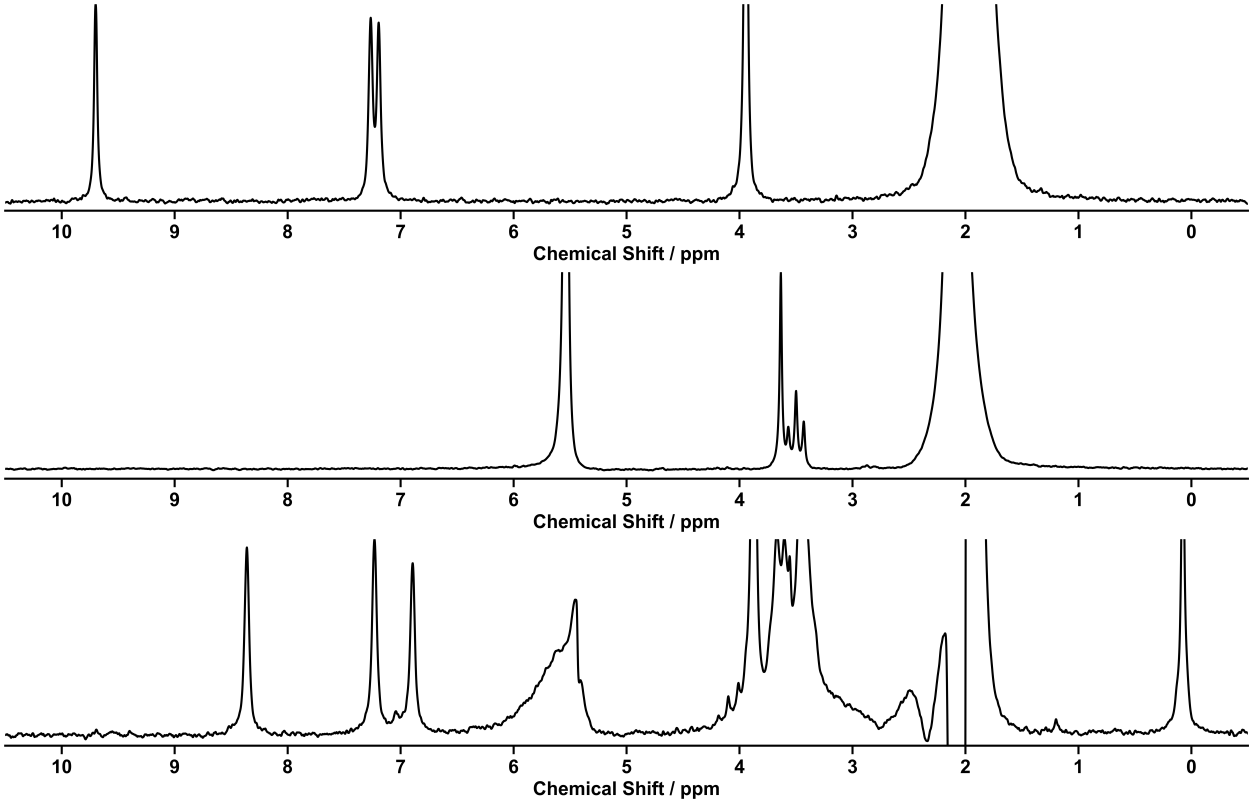
Reaction 38



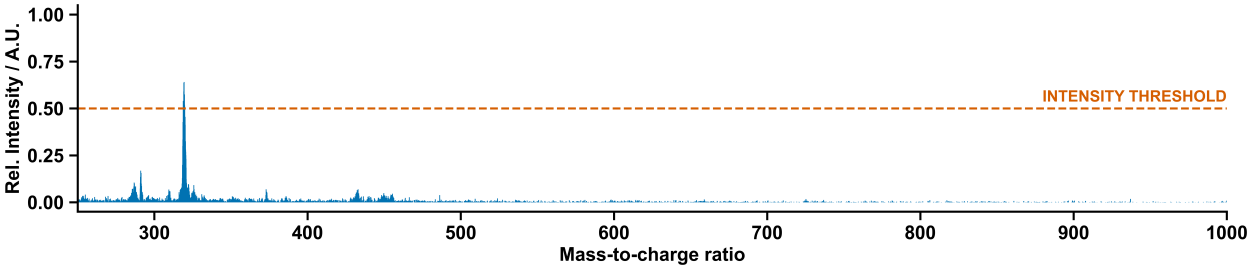
Scheme 35: Self-assembly of components 12, 19, with Zinc(II) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 38.

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	
		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 35: Human labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 38. Decision motivations are also given.

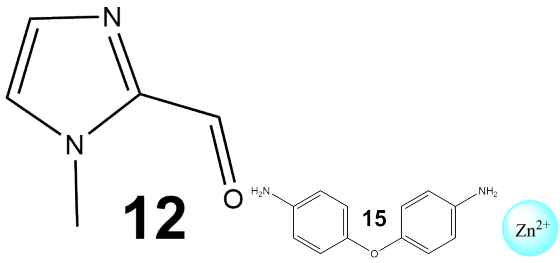


NMR Spectra 35: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 38.



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

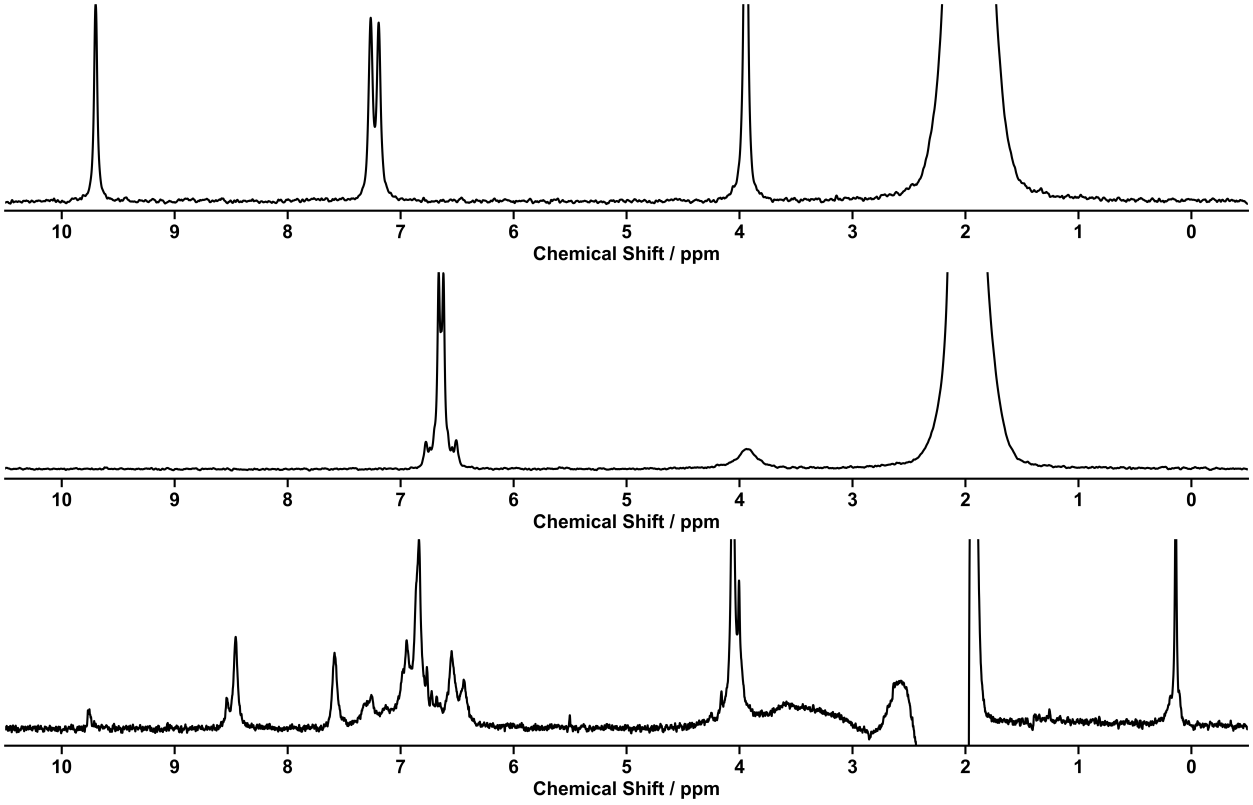
Reaction 39



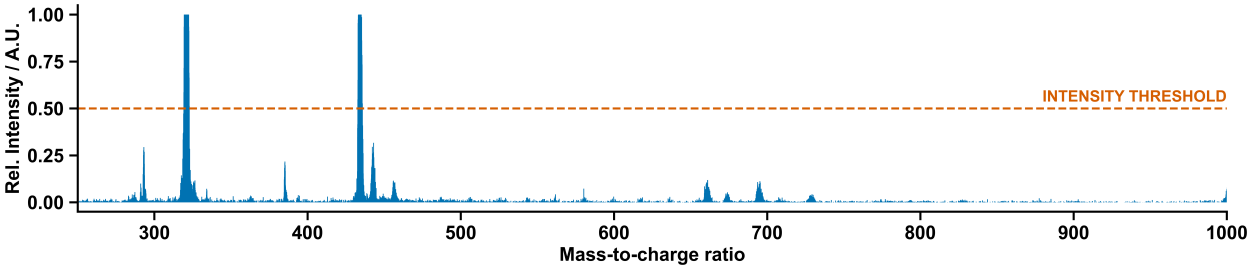
Scheme 36: Self-assembly of components 12, 15, with Zinc(II) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 39.

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 labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 39. Decision motivations are also given.

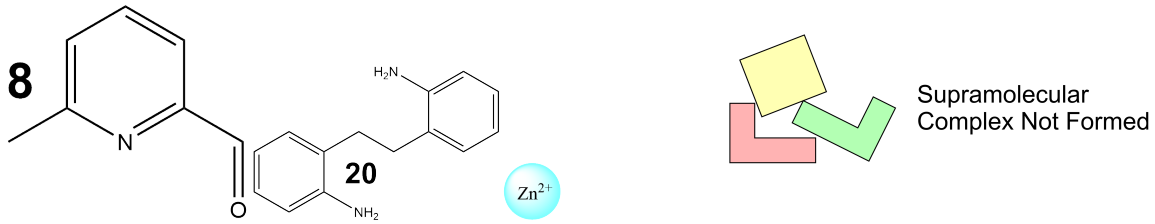


NMR Spectra 36: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 39.



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

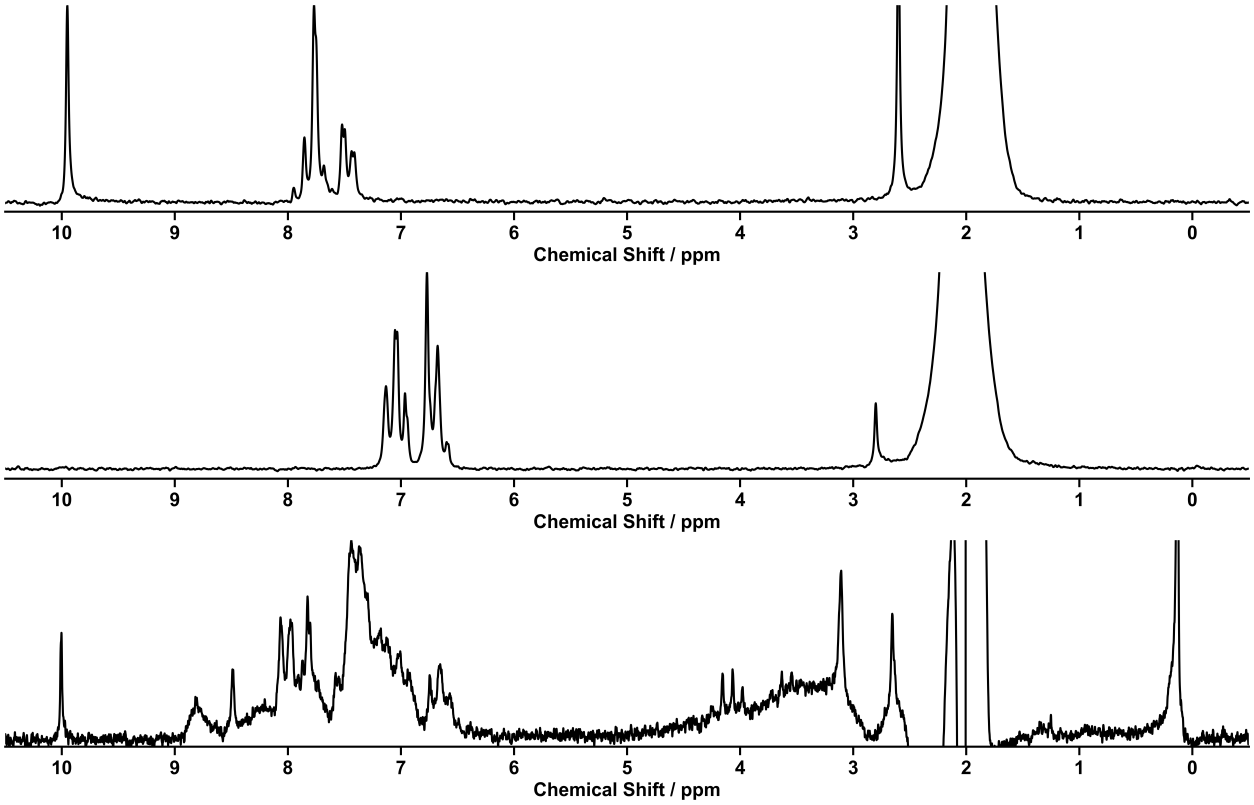
Reaction 40



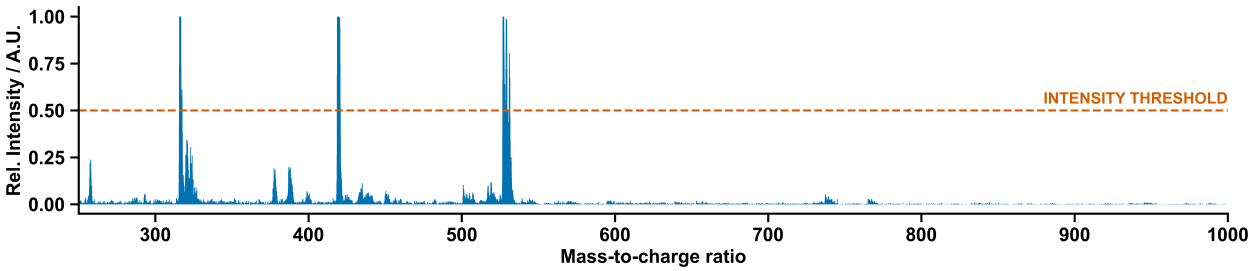
Scheme 37: Self-assembly of components 8, 20, with Zinc(II) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 40.

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 labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 40. Decision motivations are also given.

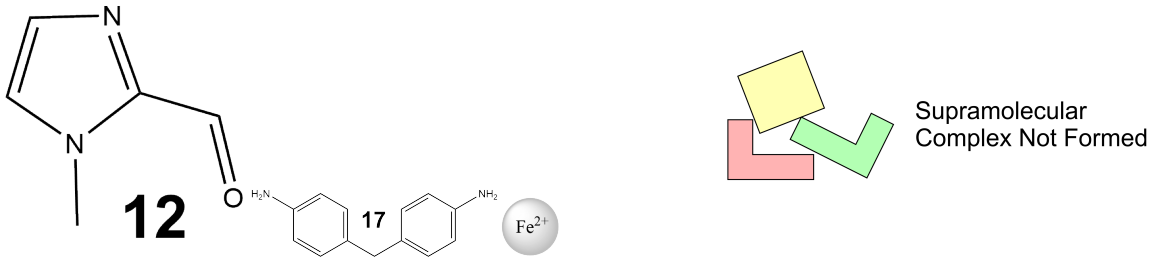


NMR Spectra 37: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 40.



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

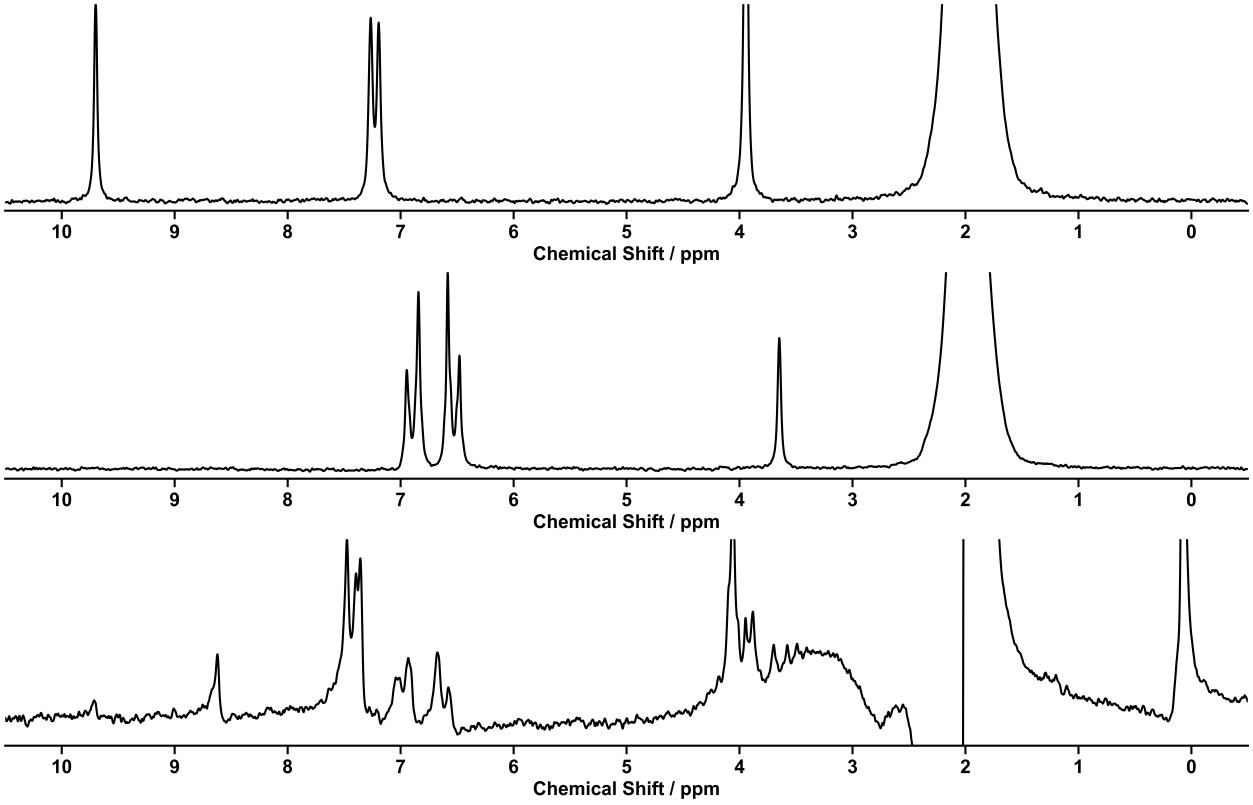
Reaction 41



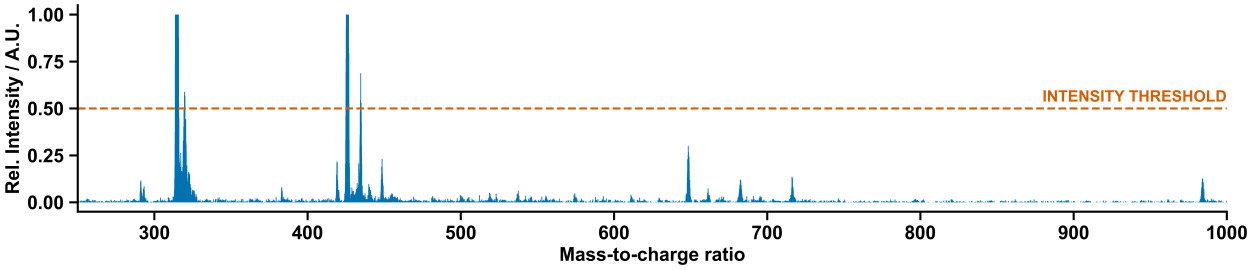
Scheme 38: Self-assembly of components 12, 17, with Iron(II) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 41.

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 labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 41. Decision motivations are also given.

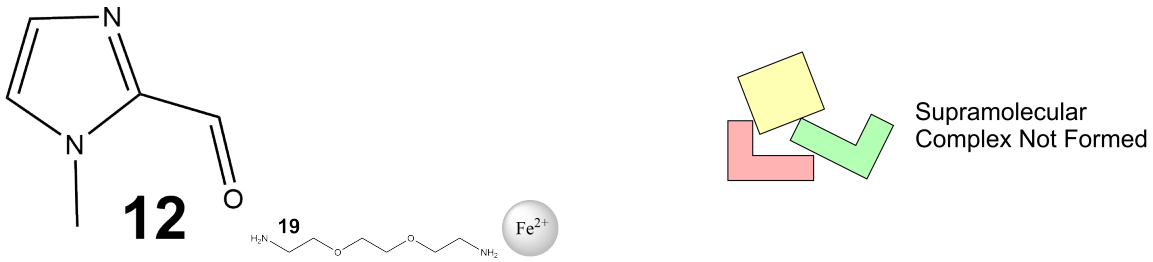


NMR Spectra 38: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 41.



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

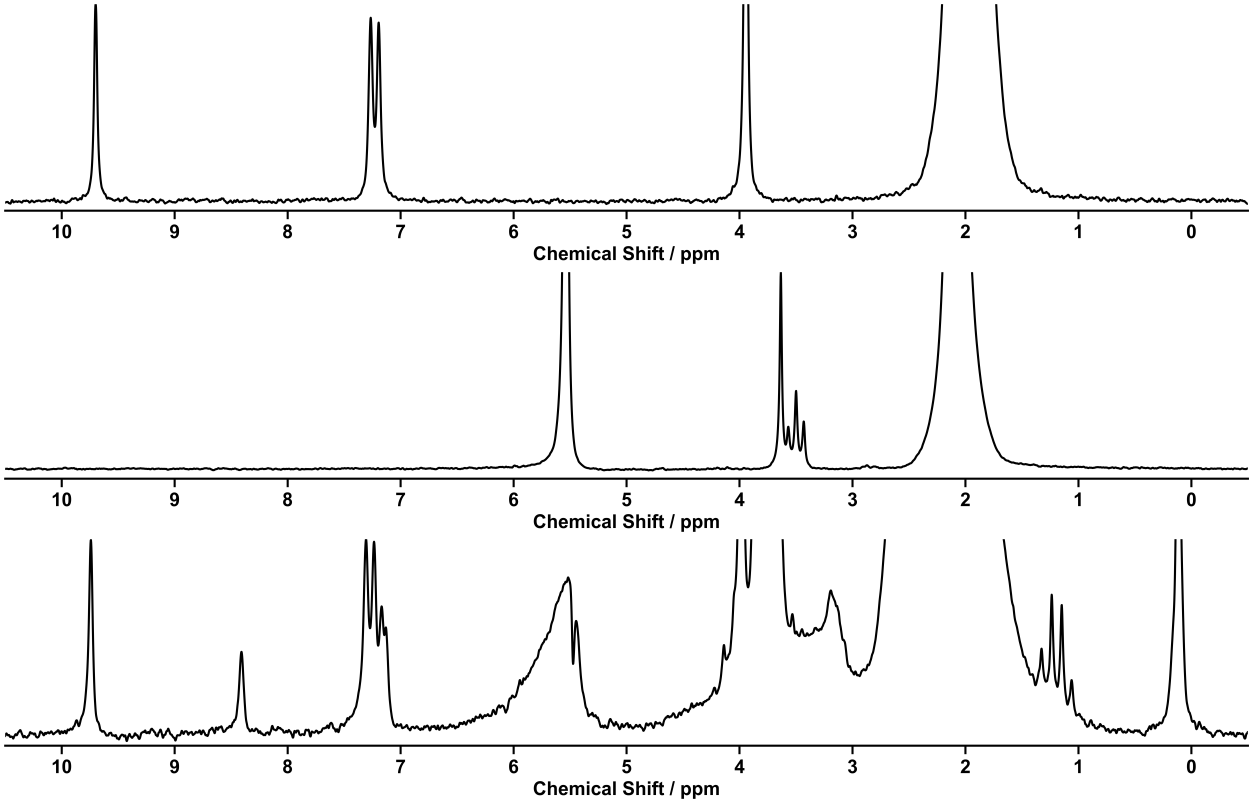
Reaction 42



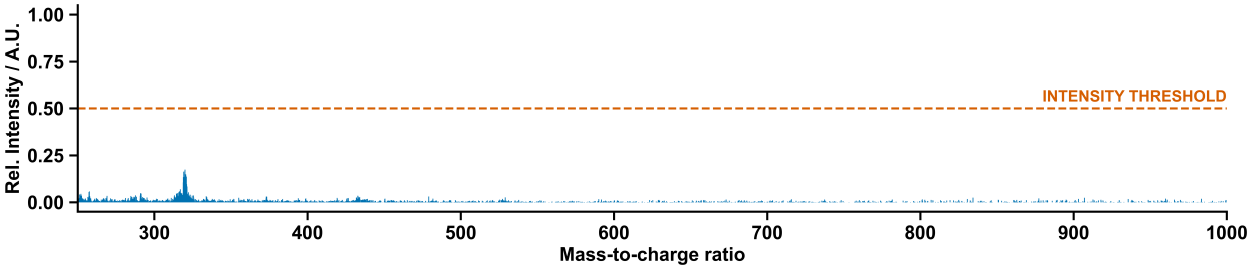
Scheme 39: Self-assembly of components 12, 19, with Iron(II) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 42.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: No reaction occured.	
	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 39: Human labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 42. Decision motivations are also given.

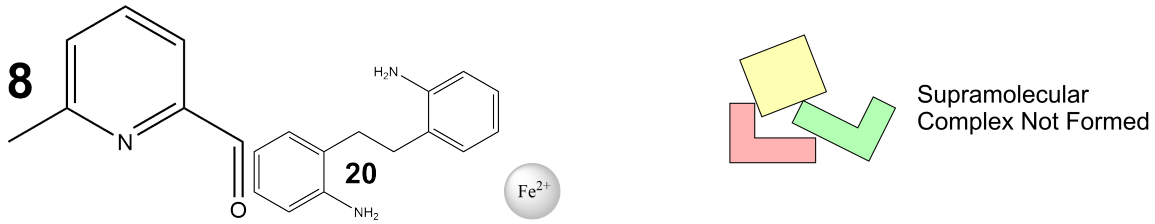


NMR Spectra 39: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 42.



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

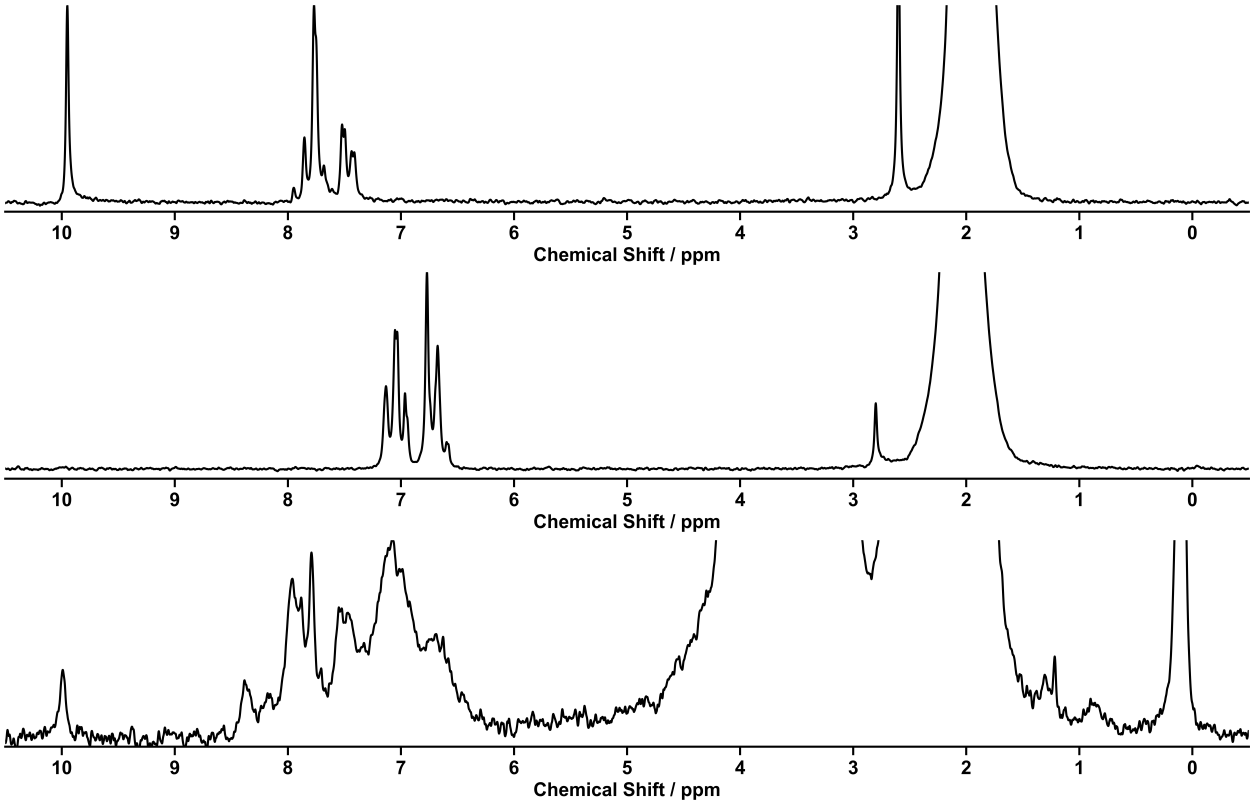
Reaction 44



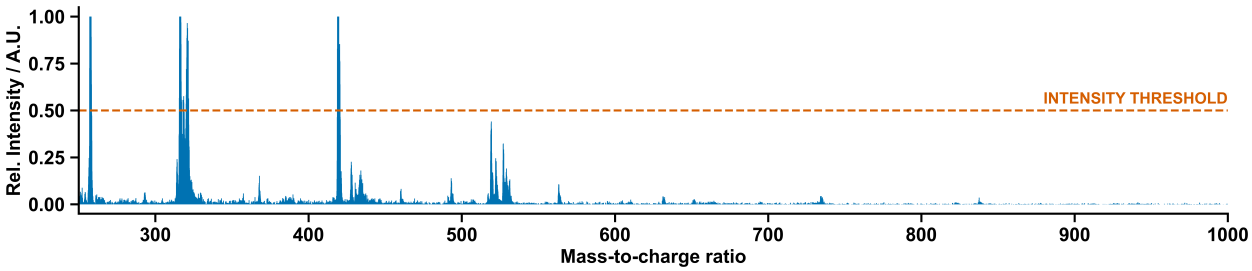
Scheme 40: Self-assembly of components 8, 20, with Iron(II) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 44.

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 labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 44. Decision motivations are also given.

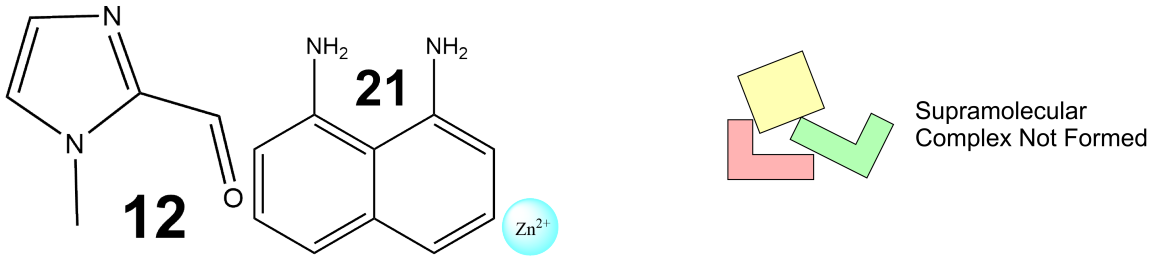


NMR Spectra 40: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 44.



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

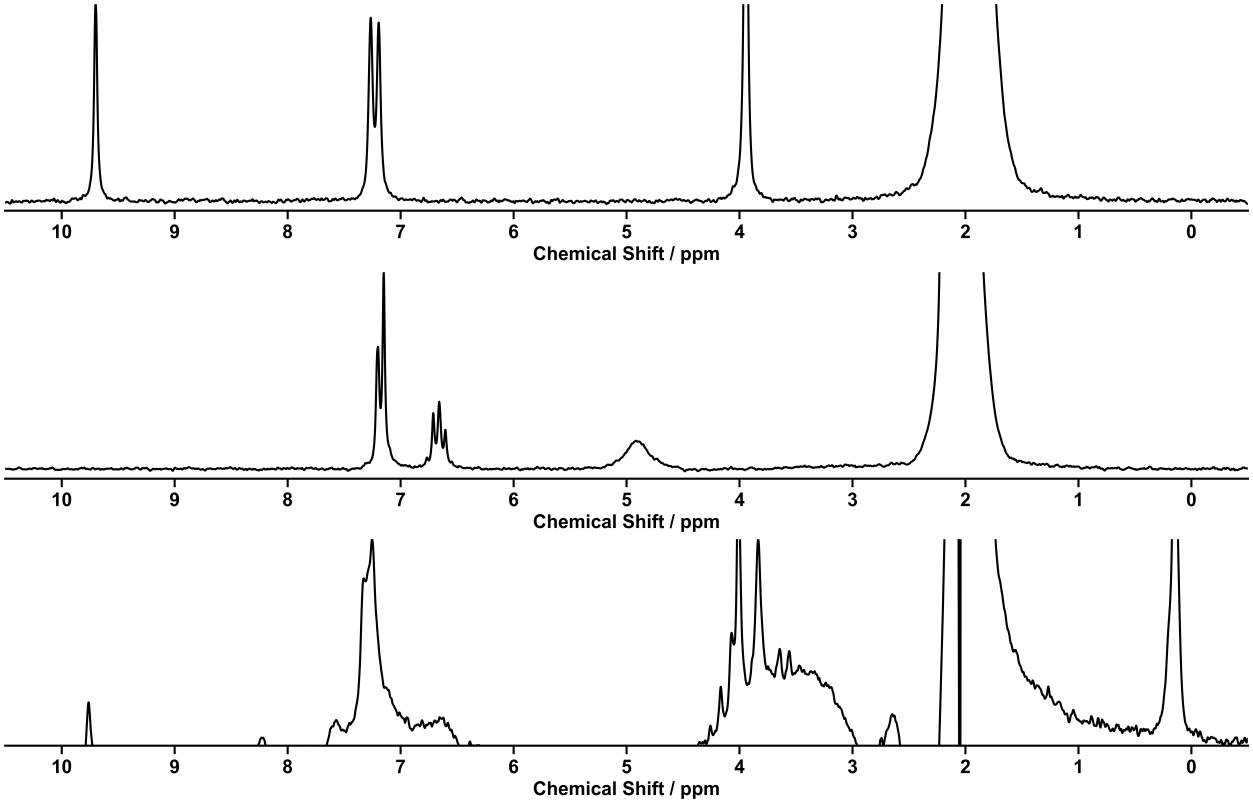
Reaction 45



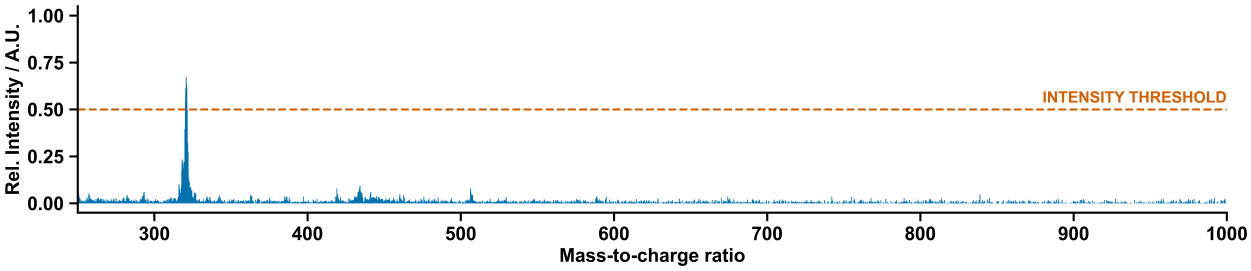
Scheme 41: Self-assembly of components 12, 21, with Zinc(II) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 45.

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 labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 45. Decision motivations are also given.

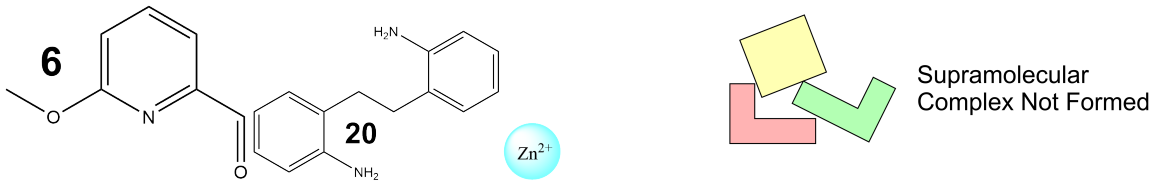


NMR Spectra 41: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 45.



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

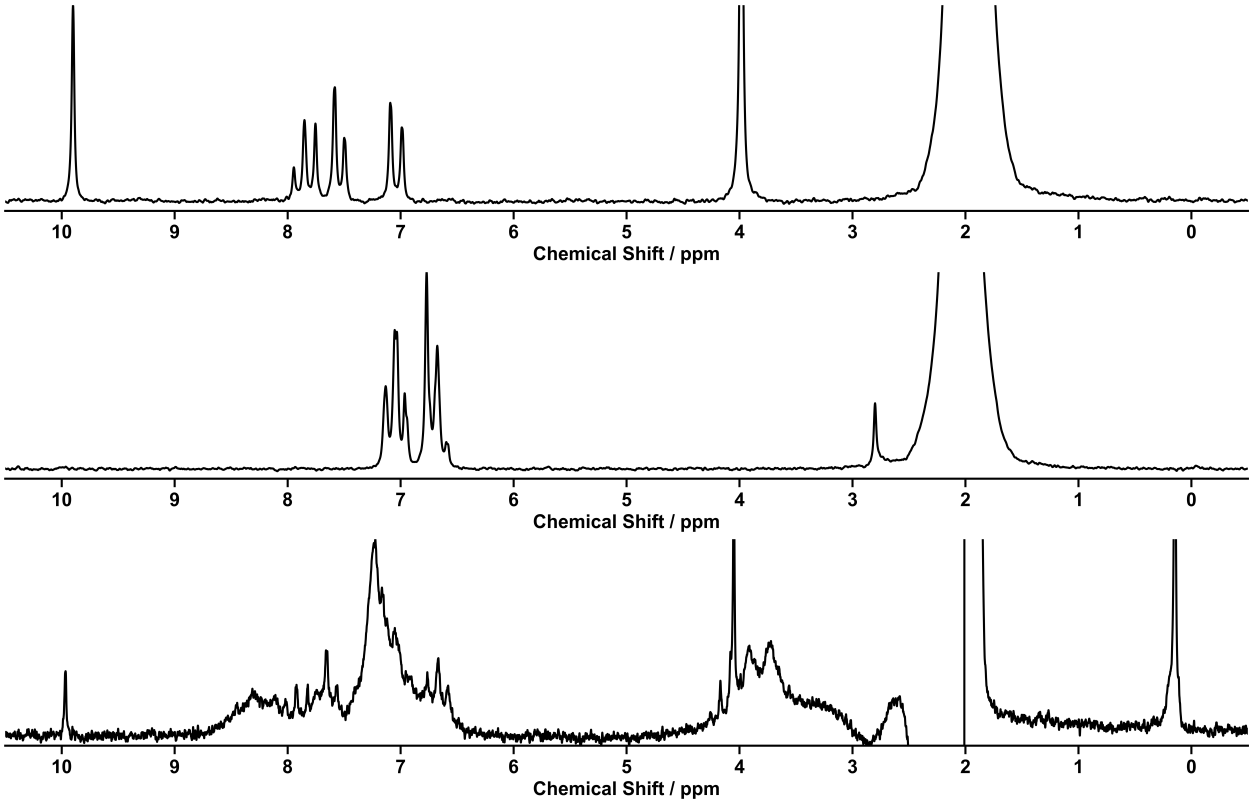
Reaction 47



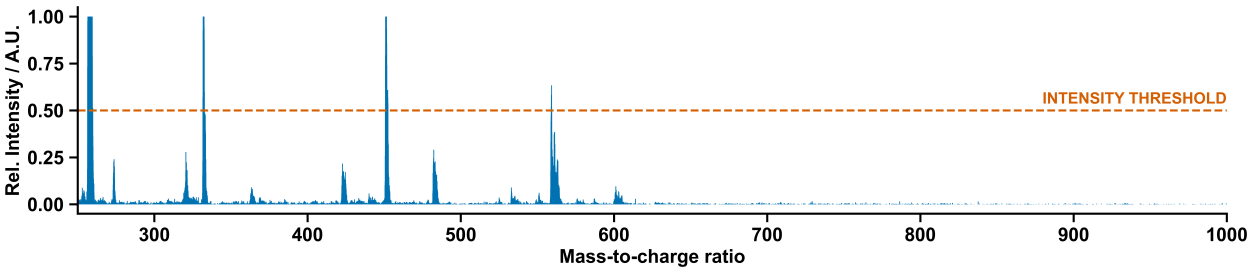
Scheme 42: Self-assembly of components 6, 20, with Zinc(II) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 47.

<table>
<tr><td rowspan="2">Human Reaction Decision:
Failed</td><td>Human NMR Decision:
Failed</td><td colspan="2">NMR Spectra Category:
Oligomers formed.</td></tr>
<tr><td>Human MS Decision:
Failed</td><td colspan="2">MS Spectra Category:
Reaction occurred, unknown product.</td></tr>
<tr><td rowspan="4">Decision Maker Reaction Decision:
N/A</td><td rowspan="2">Decision Maker NMR Decision:
N/A</td><td colspan="2">NMR Criteria 1:
N/A</td></tr>
<tr><td colspan="2">NMR Criteria 2:
N/A</td></tr>
<tr><td rowspan="2">Decision Maker MS Decision:
Pass</td><td>MS Criteria 1 and 2:
Pass</td><td>Number of predicted peaks found in MS spectra with appropriate intensity:
1</td></tr>
<tr><td>MS Criteria 3:
Pass</td><td>Number of counter-ions found:
0</td></tr>
</table>

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

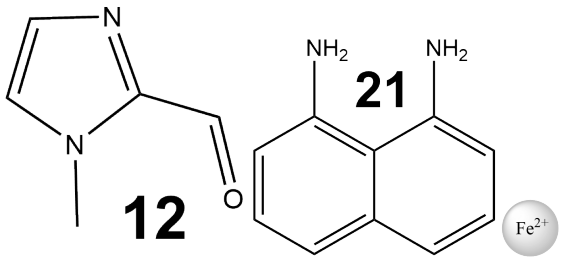


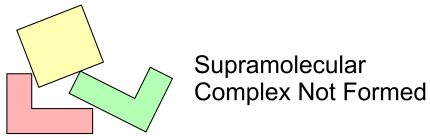
NMR Spectra 42: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 47.



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

Reaction 48

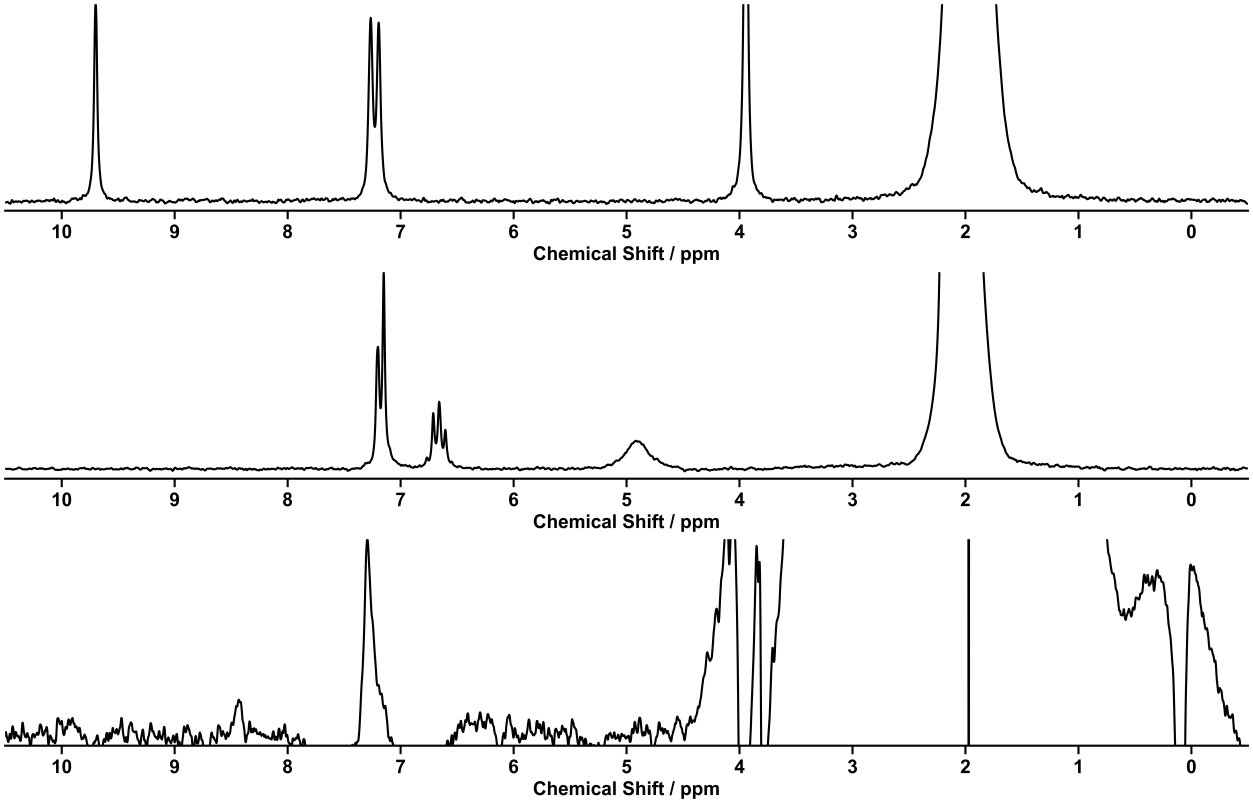




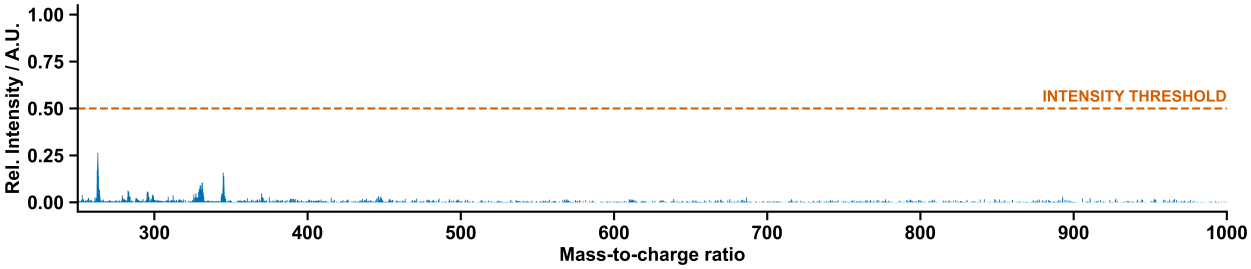
Scheme 43: Self-assembly of components 12, 21, with Iron(II) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 48.

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 labled and Decsision maker labled outcomes for the ^1H NMR spectroscopy and ULPC-MS spectrometry of reaction 48. Decision motivations are also given.

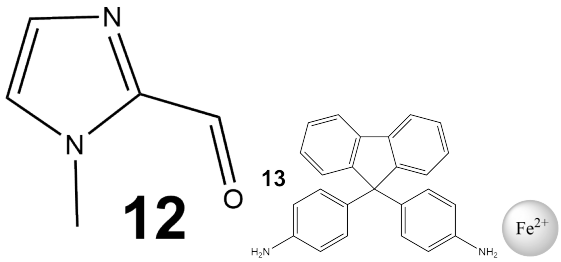


NMR Spectra 43: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 48.



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

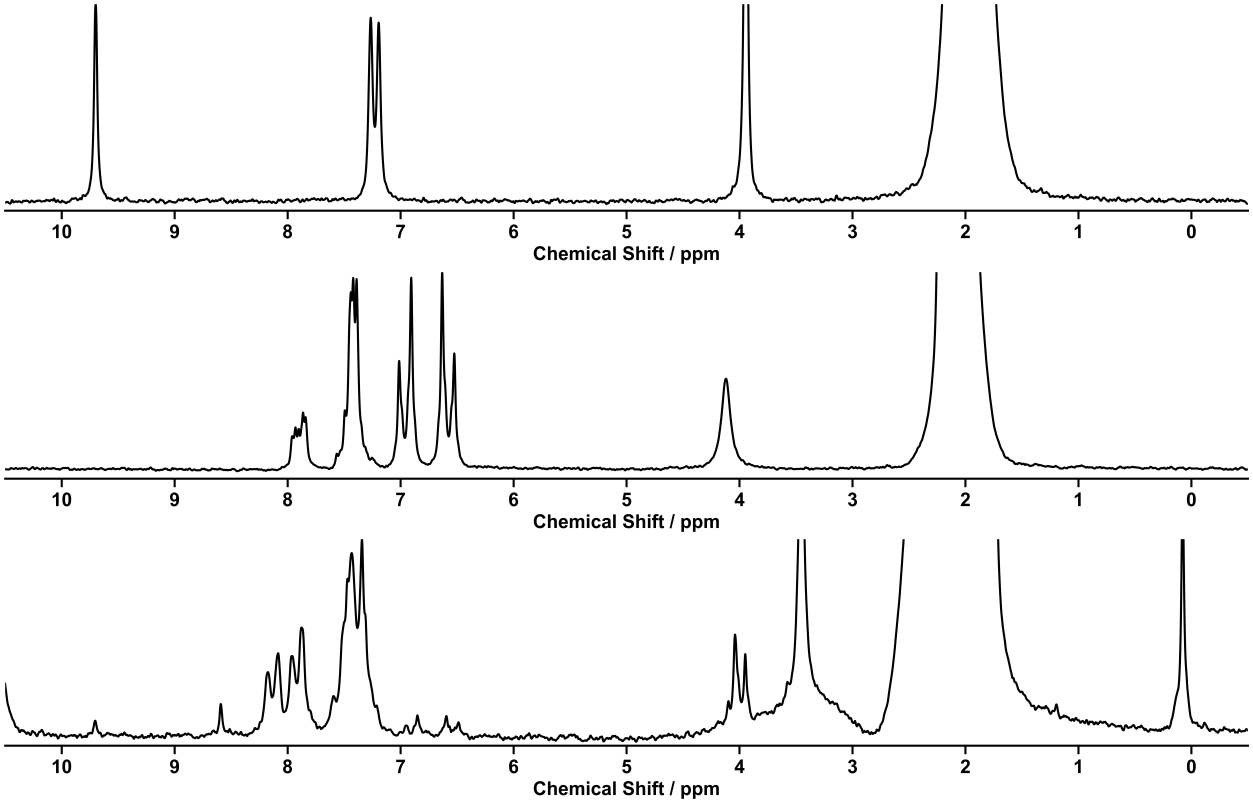
Reaction 49



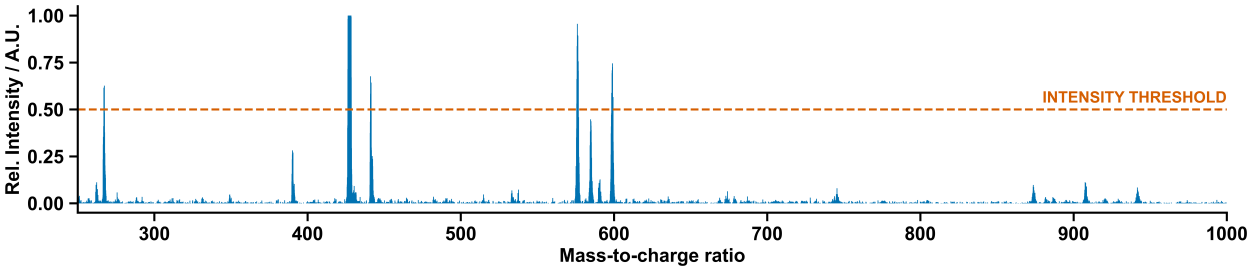
Scheme 44: Self-assembly of components 12, 13, with Iron(II) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 49.

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 labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 49. Decision motivations are also given.

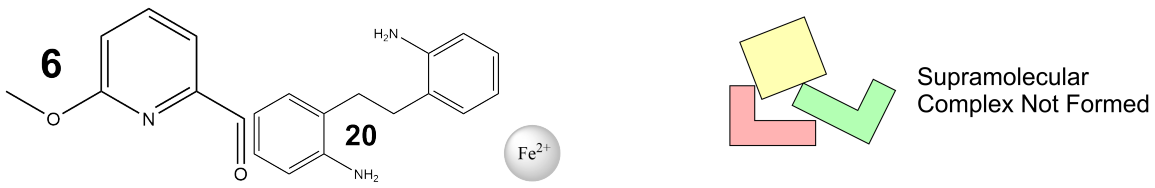


NMR Spectra 44: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 49.



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

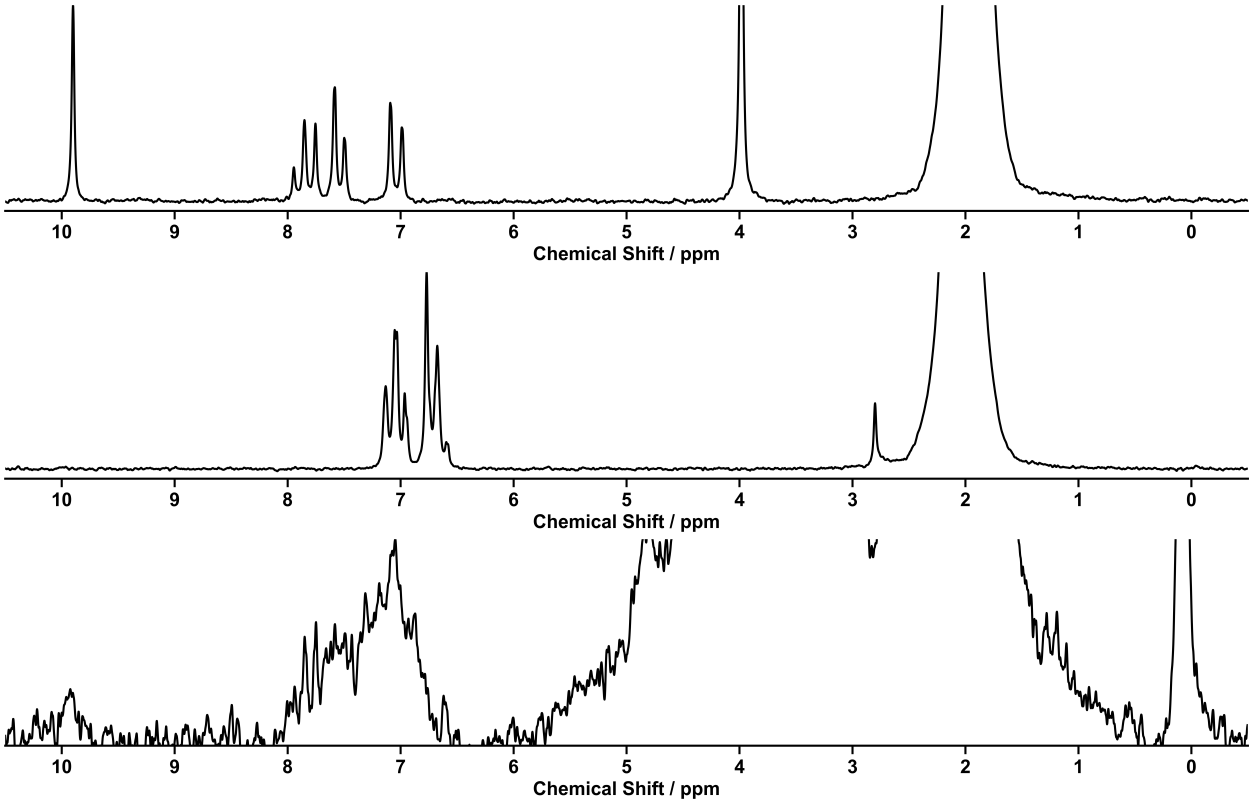
Reaction 50



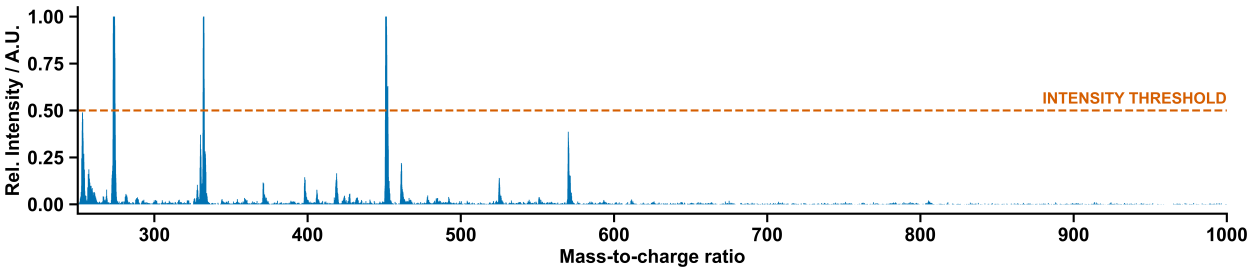
Scheme 45: Self-assembly of components 6, 20, with Iron(II) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 50.

<table>
<tr><td rowspan="2">Human Reaction Decision:
Failed</td><td>Human NMR Decision:
Failed</td><td colspan="2">NMR Spectra Category:
Paramagnetic species formed.</td></tr>
<tr><td>Human MS Decision:
Failed</td><td colspan="2">MS Spectra Category:
Reaction occurred, unknown product.</td></tr>
<tr><td rowspan="4">Decision Maker Reaction Decision:
N/A</td><td rowspan="2">Decision Maker NMR Decision:
N/A</td><td colspan="2">NMR Criteria 1:
N/A</td></tr>
<tr><td colspan="2">NMR Criteria 2:
N/A</td></tr>
<tr><td rowspan="2">Decision Maker MS Decision:
Pass</td><td>MS Criteria 1 and 2:
Pass</td><td>Number of predicted peaks found in MS spectra with appropriate intensity:
0</td></tr>
<tr><td>MS Criteria 3:
Pass</td><td>Number of counter-ions found:
0</td></tr>
</table>

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

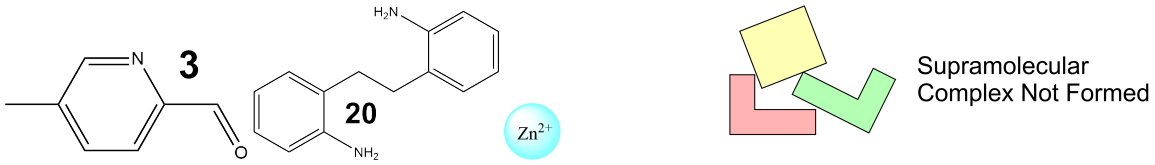


NMR Spectra 45: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 50.



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

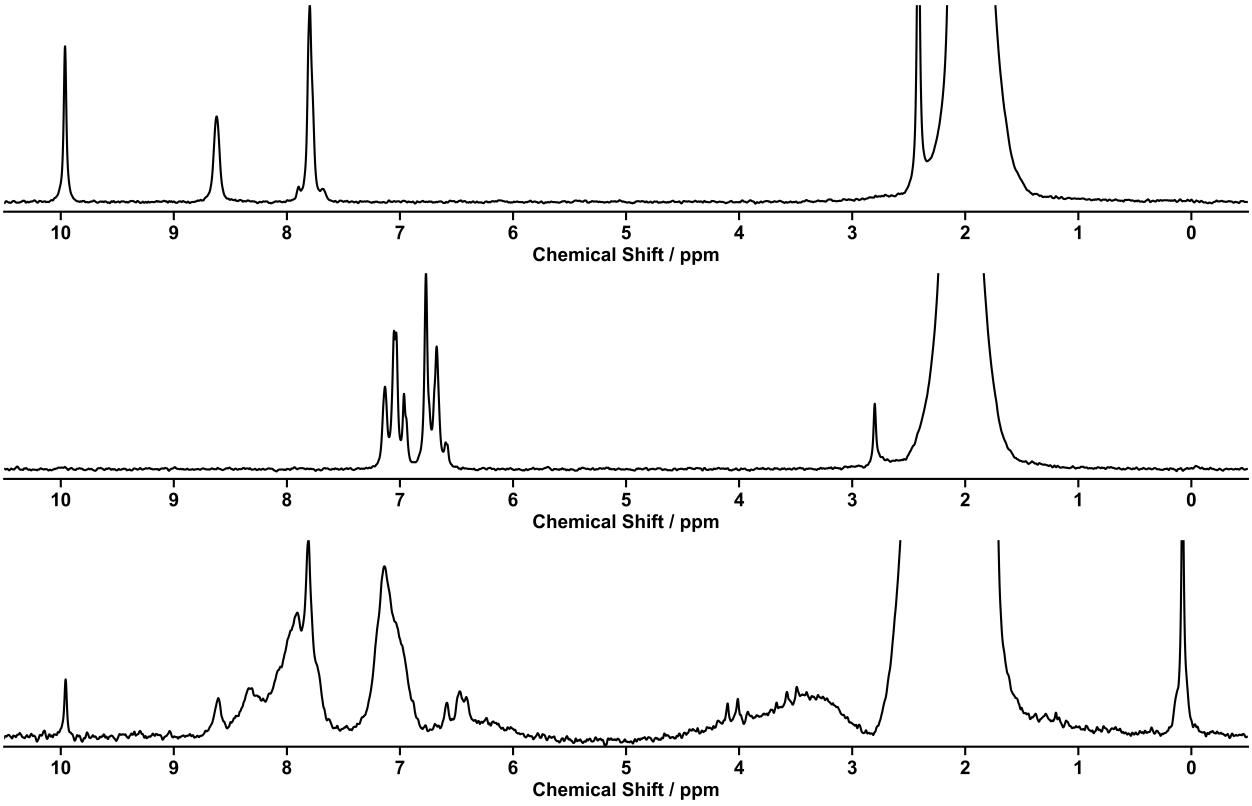
Reaction 51



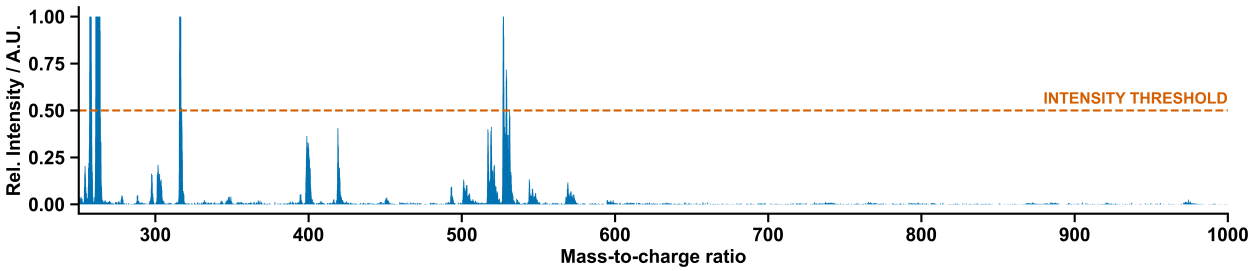
Scheme 46: Self-assembly of components 3, 20, with Zinc(II) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 51.

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 labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 51. Decision motivations are also given.

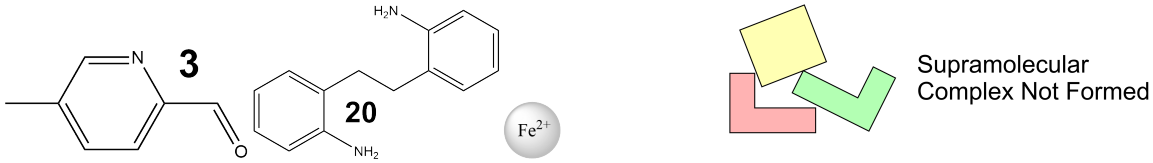


NMR Spectra 46: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 51.



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

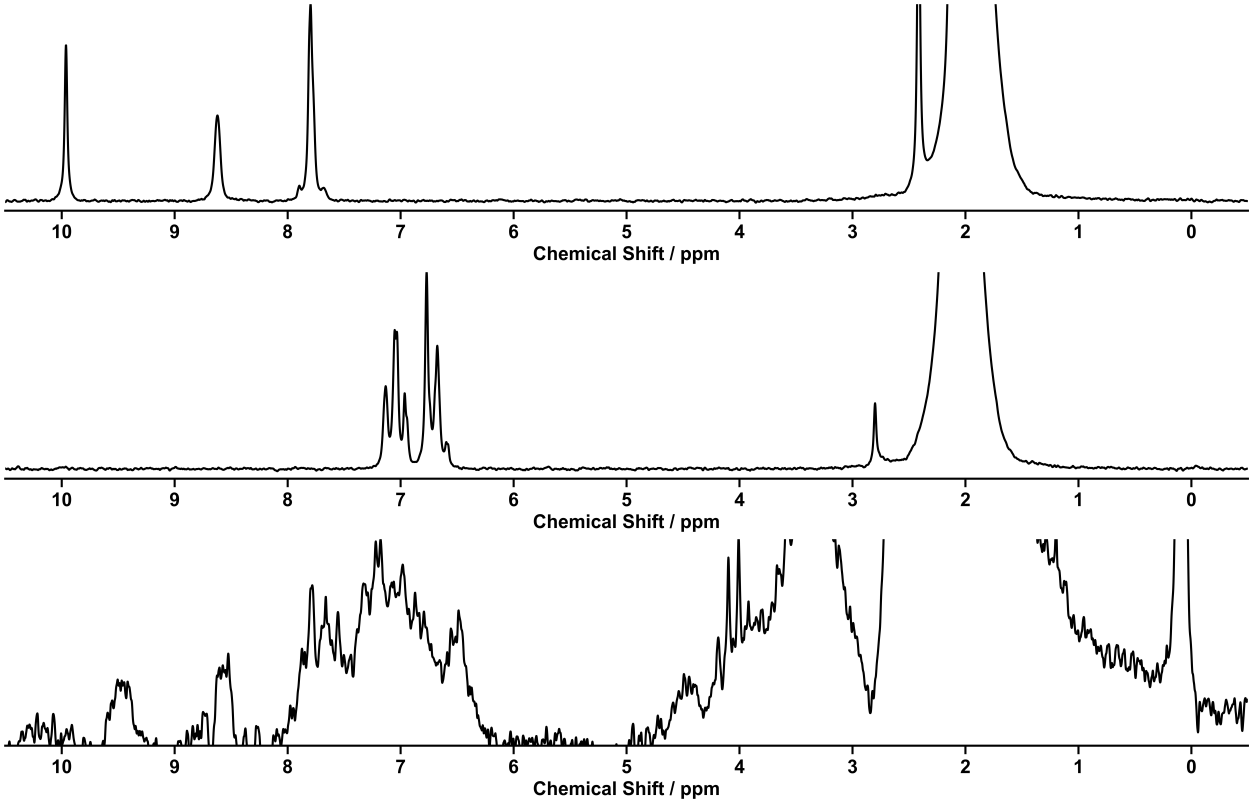
Reaction 52



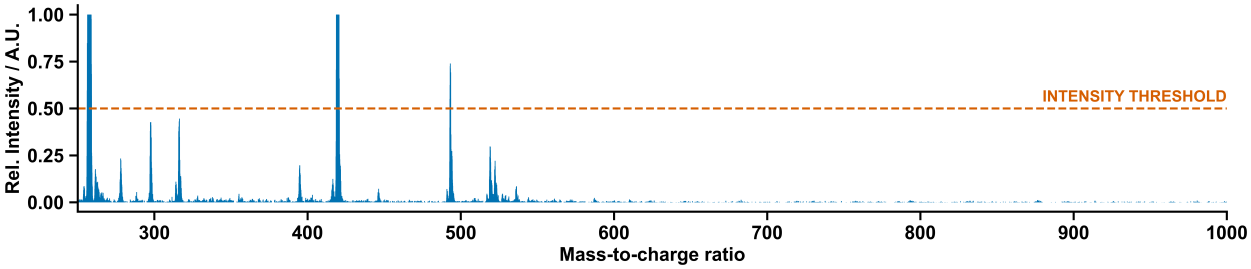
Scheme 47: Self-assembly of components 3, 20, with Iron(II) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 52.

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 labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 52. Decision motivations are also given.

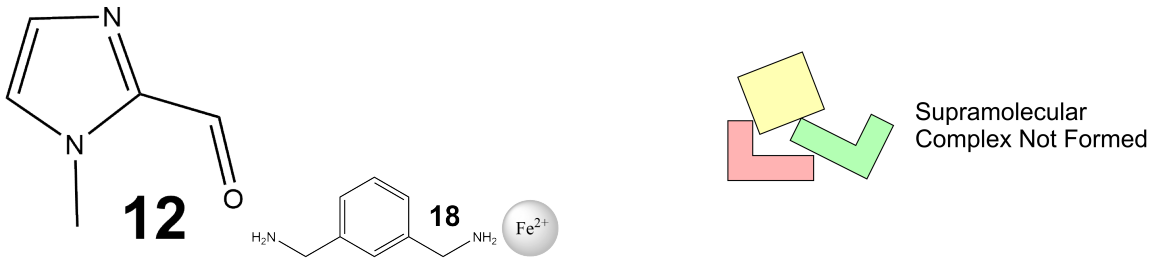


NMR Spectra 47: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 52.



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

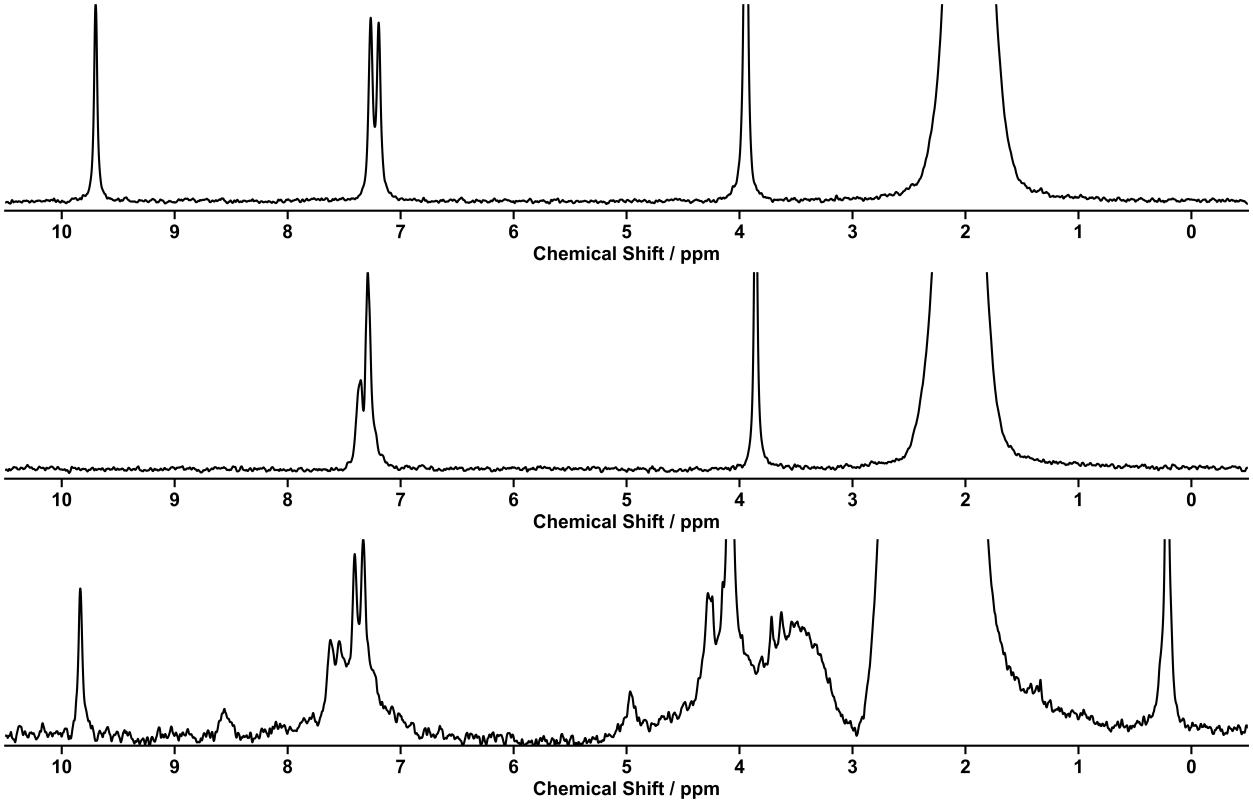
Reaction 54



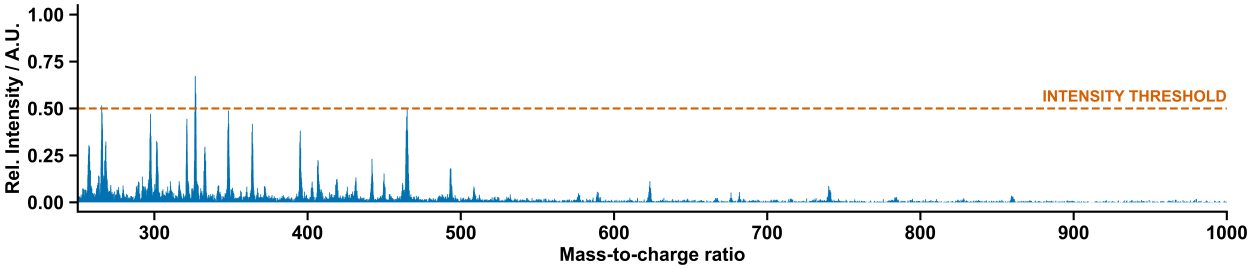
Scheme 48: Self-assembly of components 12, 18, with Iron(II) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 54.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: No reaction occured.	
	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 48: Human labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 54. Decision motivations are also given.

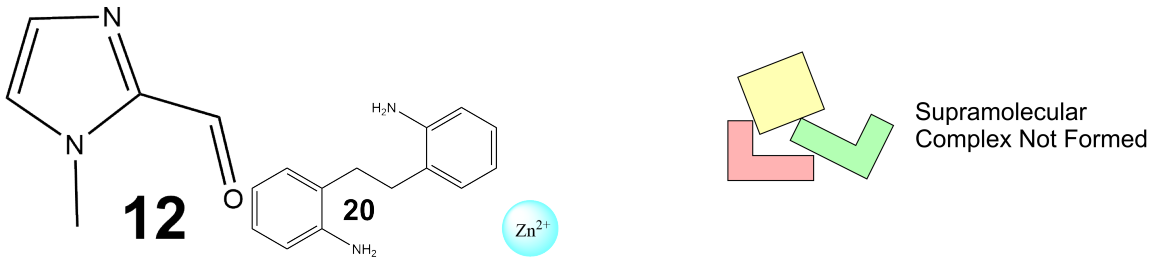


NMR Spectra 48: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 54.



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

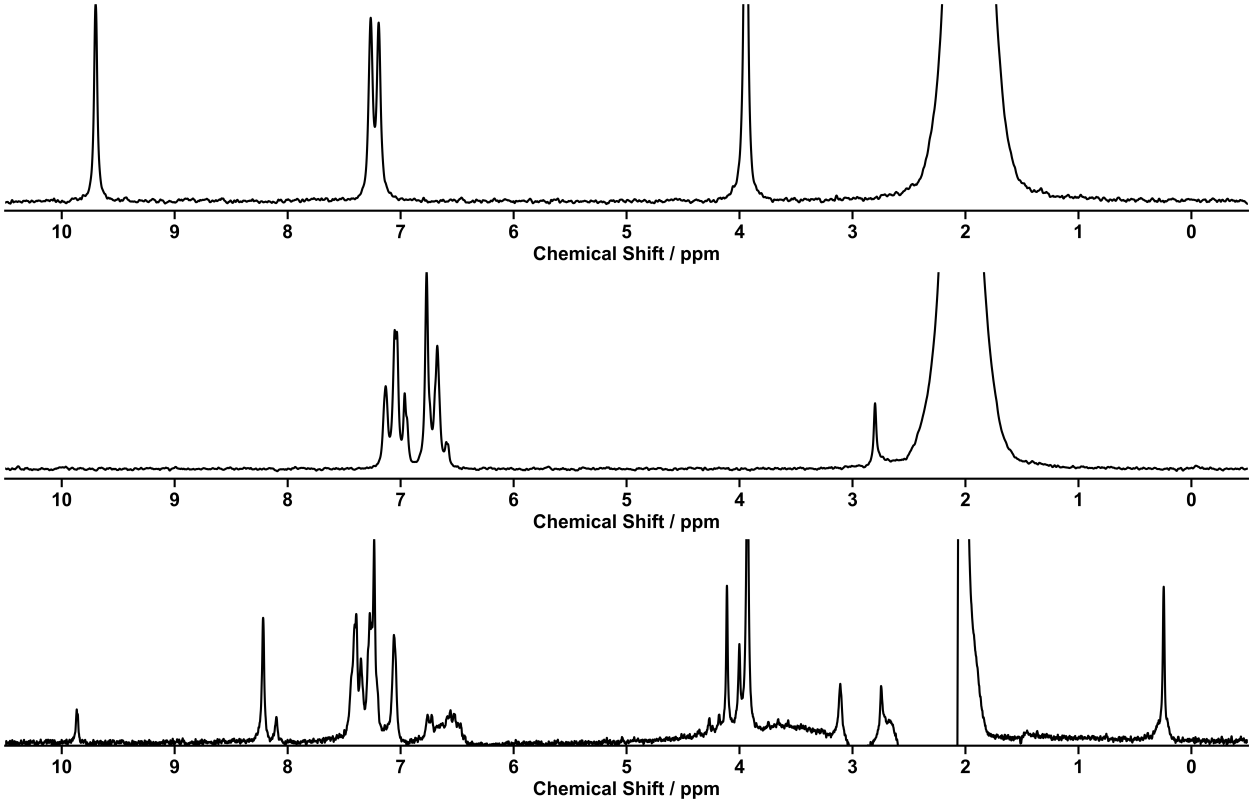
Reaction 55



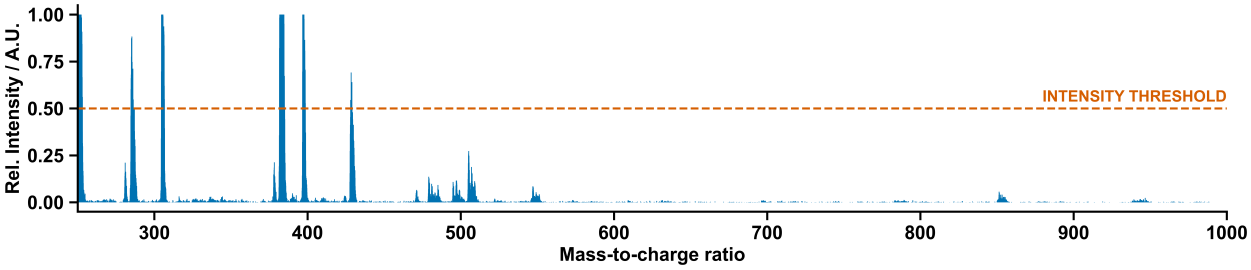
Scheme 49: Self-assembly of components 12, 20, with Zinc(II) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 55.

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	
		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 49: Human labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 55. Decision motivations are also given.

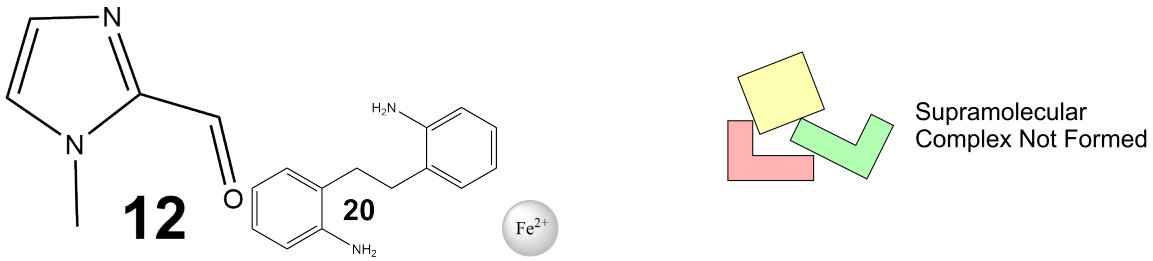


NMR Spectra 49: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 55.



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

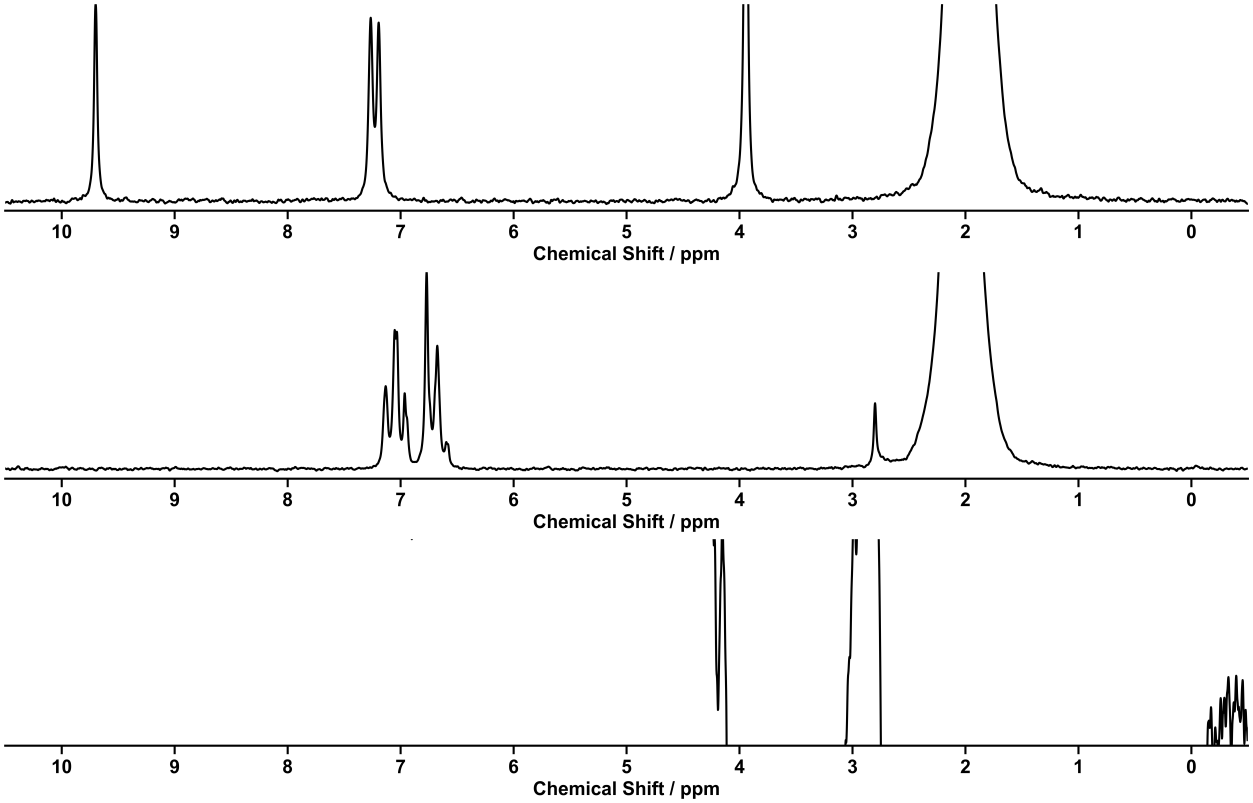
Reaction 56



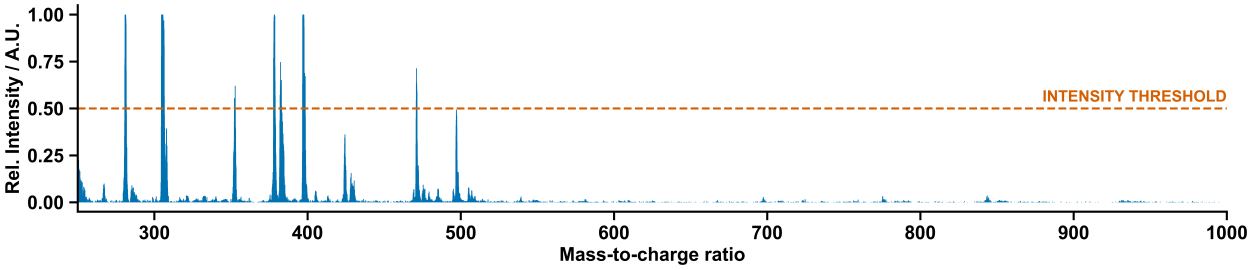
Scheme 50: Self-assembly of components 12, 20, with Iron(II) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 56.

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	
		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 50: Human labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 56. Decision motivations are also given.

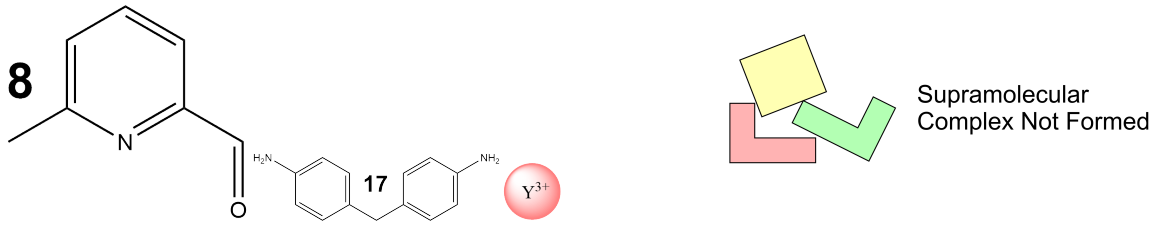


NMR Spectra 50: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 56.



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

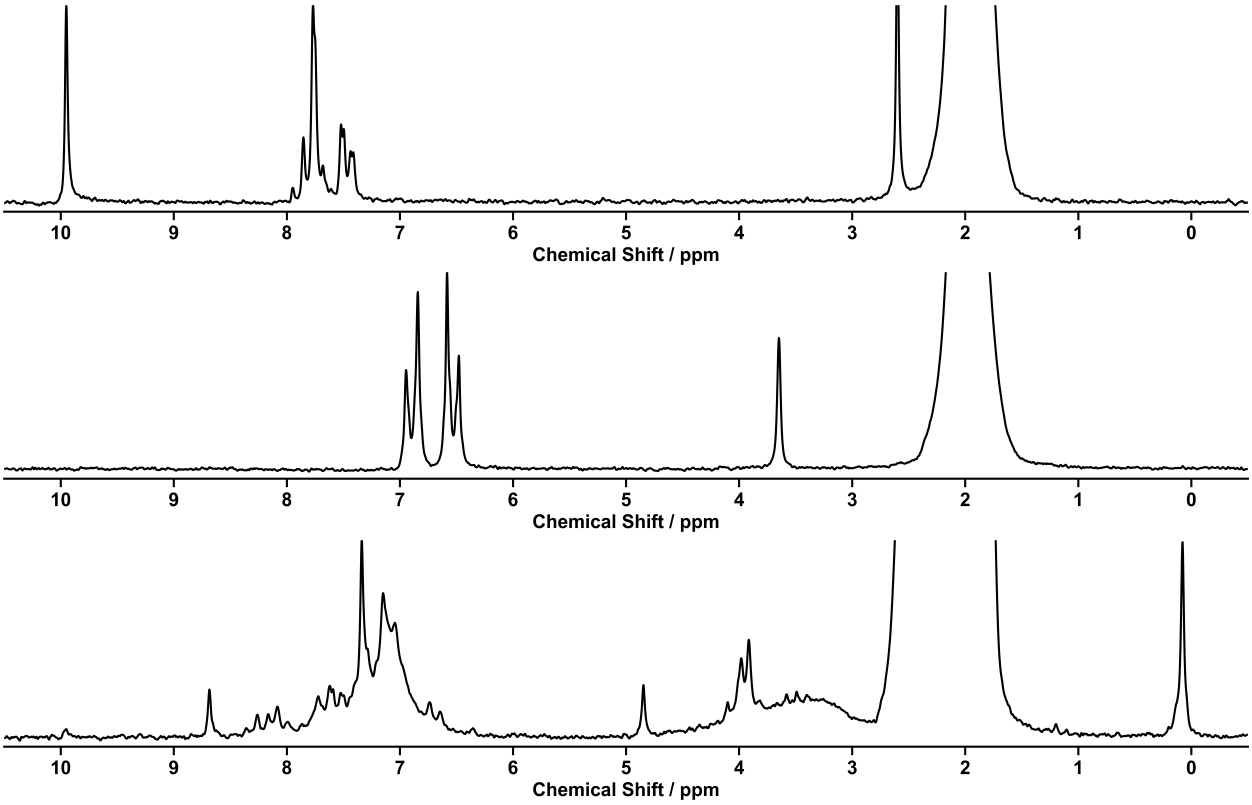
Reaction 57



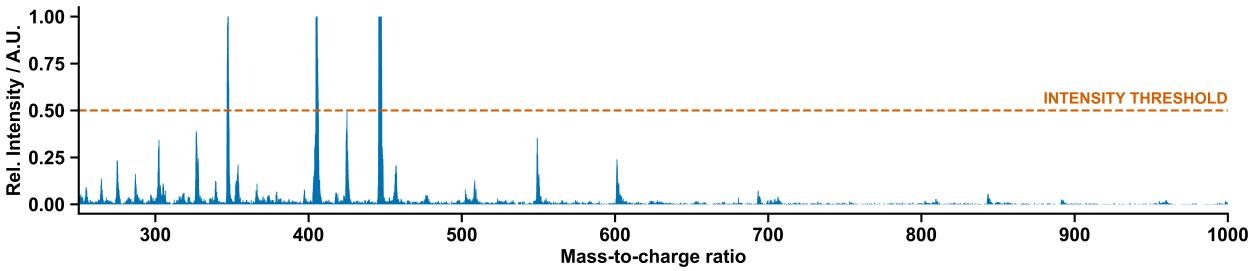
Scheme 51: Self-assembly of components 8, 17, with Yittrium(III) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 57.

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 labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 57. Decision motivations are also given.

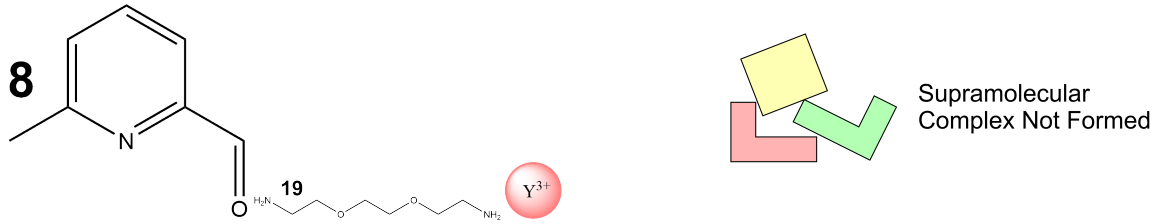


NMR Spectra 51: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 57.



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

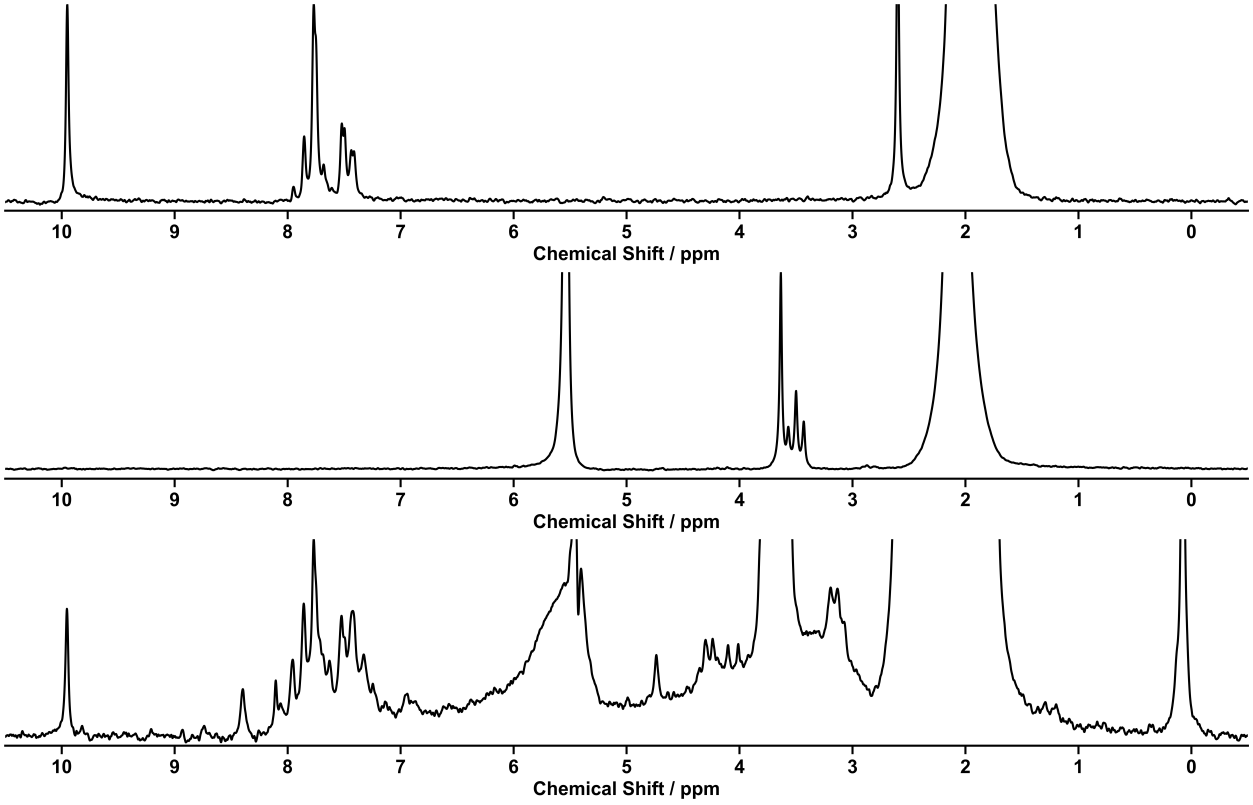
Reaction 58



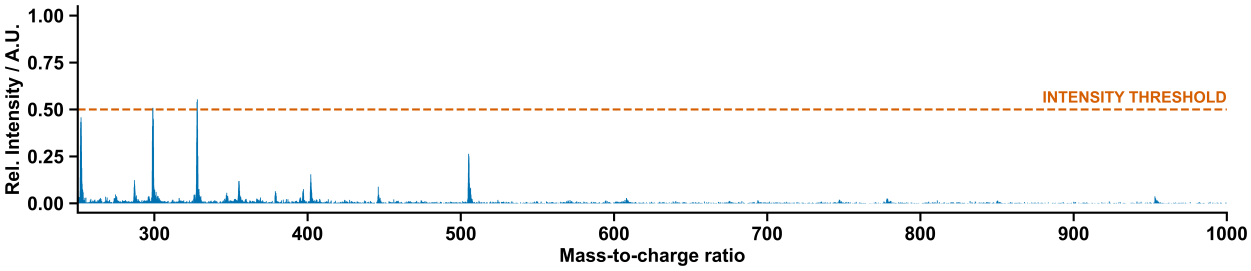
Scheme 52: Self-assembly of components 8, 19, with Yittrium(III) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 58.

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 labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 58. Decision motivations are also given.

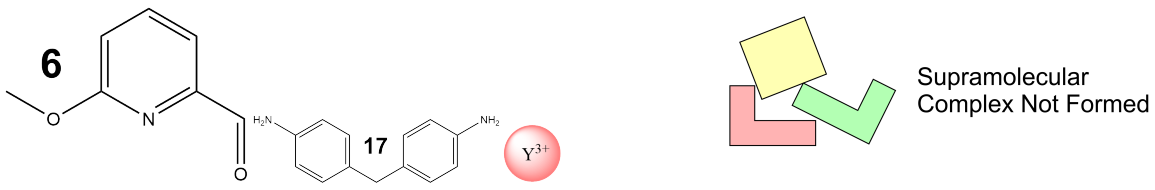


NMR Spectra 52: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 58.



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

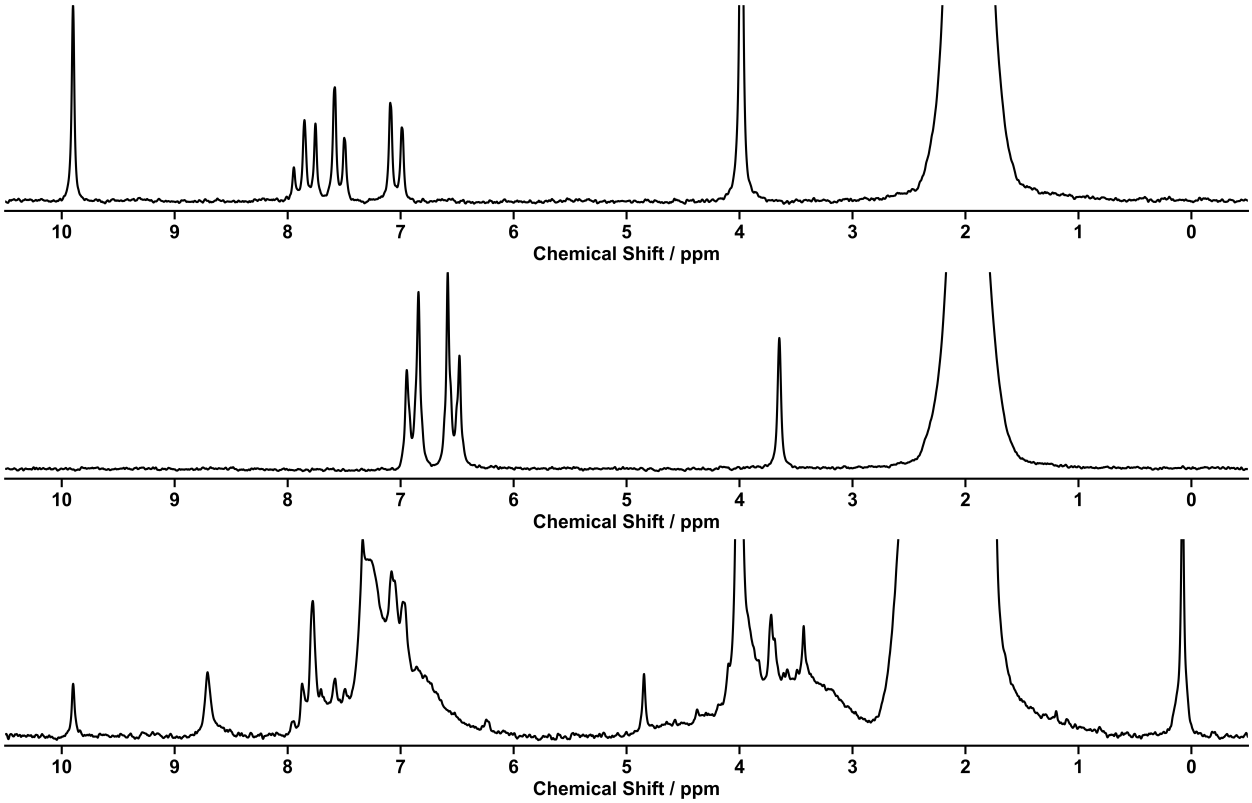
Reaction 60



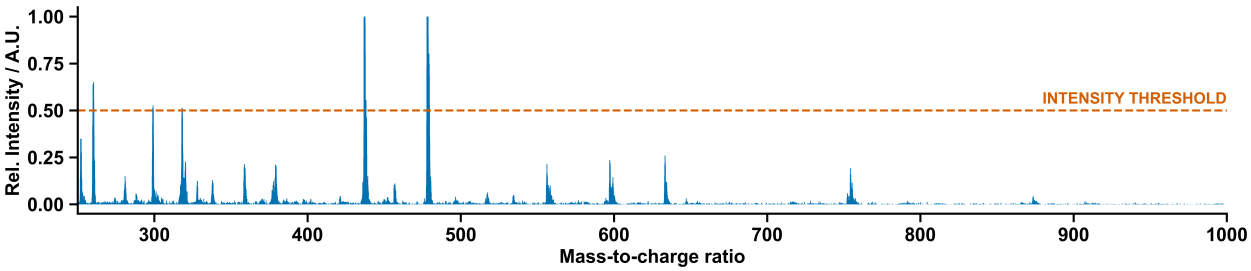
Scheme 53: Self-assembly of components 6, 17, with Yittrium(III) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 60.

<table>
<tr><td rowspan="2">Human Reaction Decision:
Failed</td><td>Human NMR Decision:
Pass</td><td colspan="2">NMR Spectra Category:
Single discrete species formed.</td></tr>
<tr><td>Human MS Decision:
Failed</td><td colspan="2">MS Spectra Category:
Reaction occurred, unknown product.</td></tr>
<tr><td rowspan="4">Decision Maker Reaction Decision:
N/A</td><td rowspan="2">Decision Maker NMR Decision:
N/A</td><td colspan="2">NMR Criteria 1:
N/A</td></tr>
<tr><td colspan="2">NMR Criteria 2:
N/A</td></tr>
<tr><td rowspan="2">Decision Maker MS Decision:
Pass</td><td>MS Criteria 1 and 2:
Pass</td><td>Number of predicted peaks found in MS spectra with appropriate intensity:
0</td></tr>
<tr><td>MS Criteria 3:
Pass</td><td>Number of counter-ions found:
0</td></tr>
</table>

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

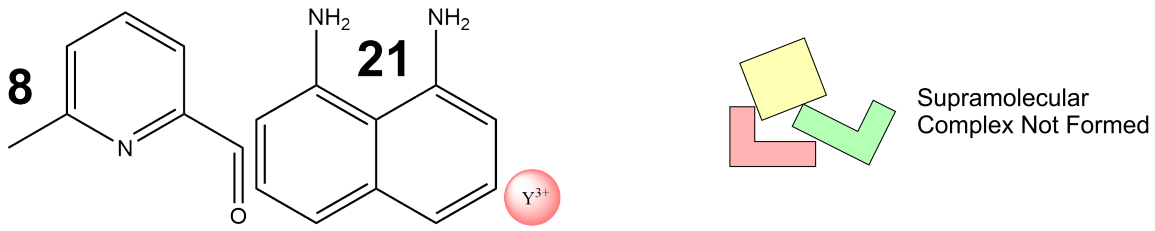


NMR Spectra 53: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 60.



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

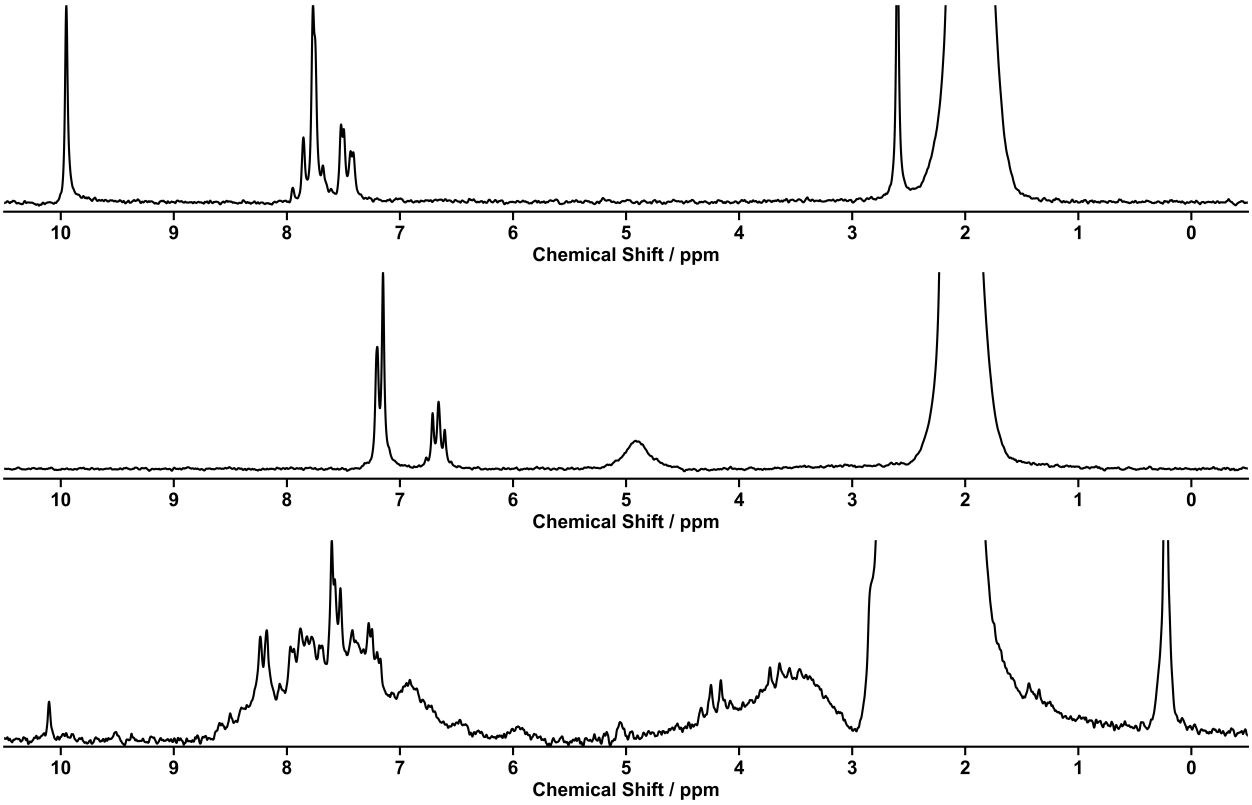
Reaction 63



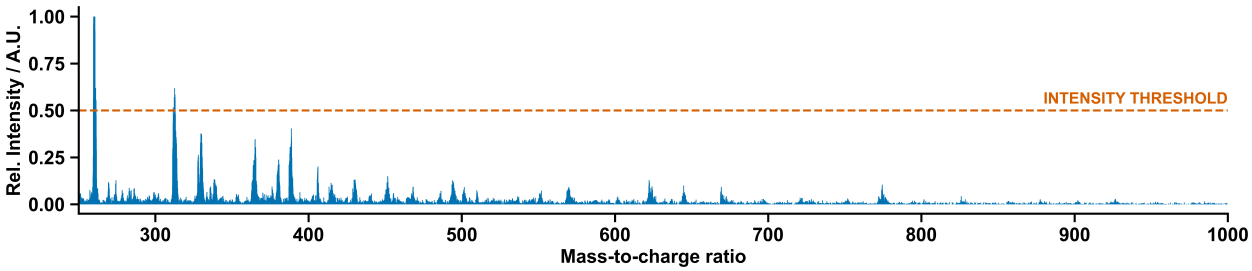
Scheme 54: Self-assembly of components 8, 21, with Yittrium(III) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 63.

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 labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 63. Decision motivations are also given.

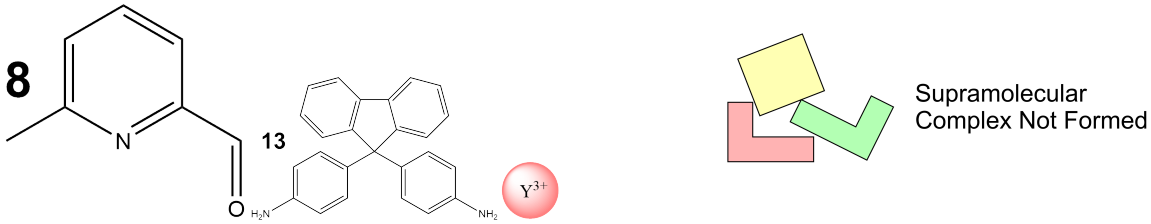


NMR Spectra 54: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 63.



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

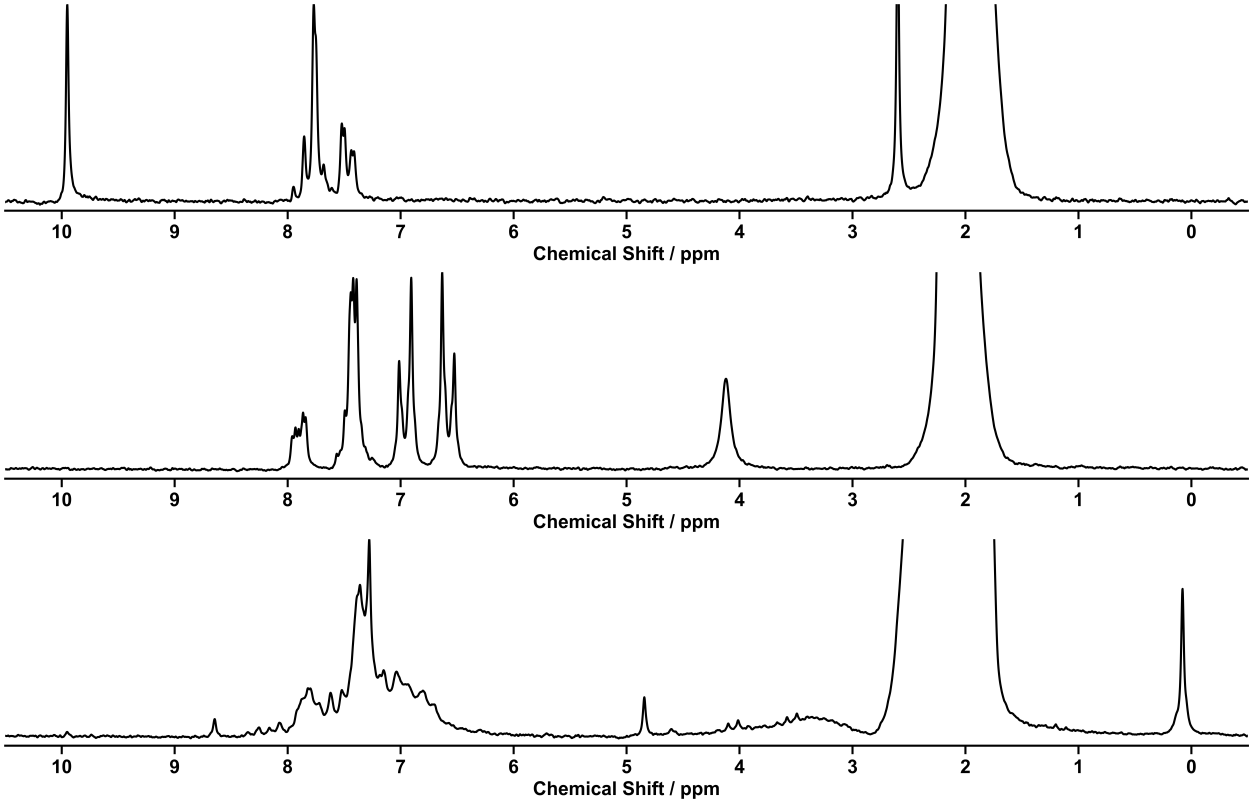
Reaction 64



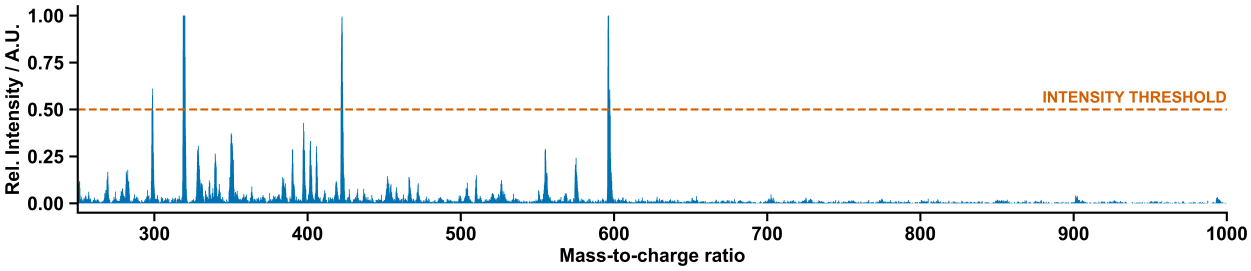
Scheme 55: Self-assembly of components 8, 13, with Yittrium(III) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 64.

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 labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 64. Decision motivations are also given.

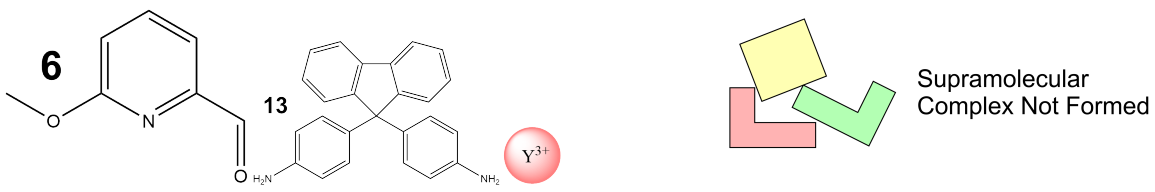


NMR Spectra 55: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 64.



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

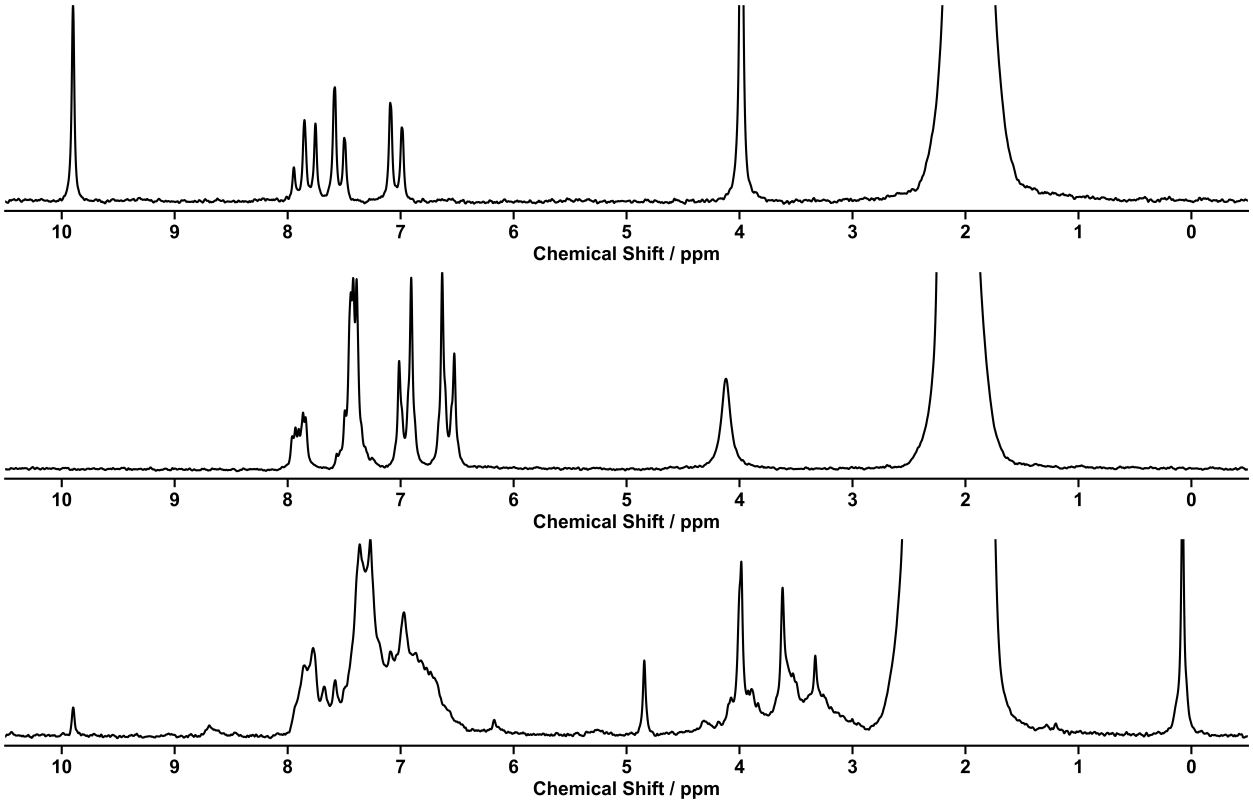
Reaction 66



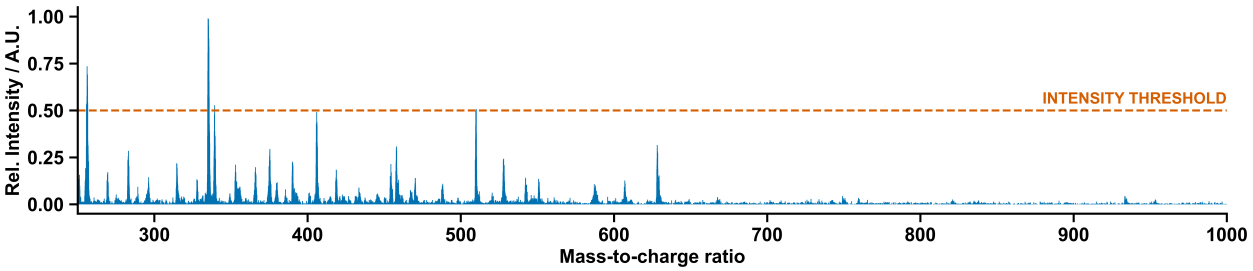
Scheme 56: Self-assembly of components 6, 13, with Yittrium(III) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 66.

<table>
<tr><td rowspan="2">Human Reaction Decision:
Failed</td><td>Human NMR Decision:
Pass</td><td colspan="2">NMR Spectra Category:
Single discrete species formed.</td></tr>
<tr><td>Human MS Decision:
Failed</td><td colspan="2">MS Spectra Category:
Reaction occurred, unknown product.</td></tr>
<tr><td rowspan="4">Decision Maker Reaction Decision:
N/A</td><td rowspan="2">Decision Maker NMR Decision:
N/A</td><td colspan="2">NMR Criteria 1:
N/A</td></tr>
<tr><td colspan="2">NMR Criteria 2:
N/A</td></tr>
<tr><td rowspan="2">Decision Maker MS Decision:
Pass</td><td>MS Criteria 1 and 2:
Pass</td><td>Number of predicted peaks found in MS spectra with appropriate intensity:
1</td></tr>
<tr><td>MS Criteria 3:
Pass</td><td>Number of counter-ions found:
0</td></tr>
</table>

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

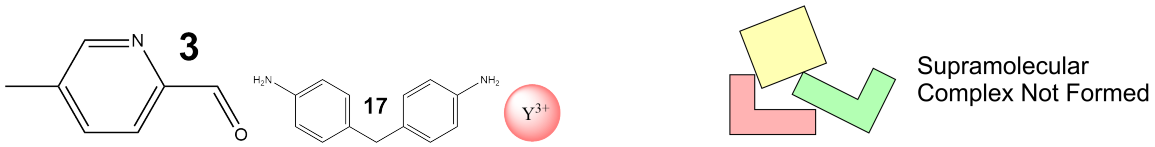


NMR Spectra 56: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 66.



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

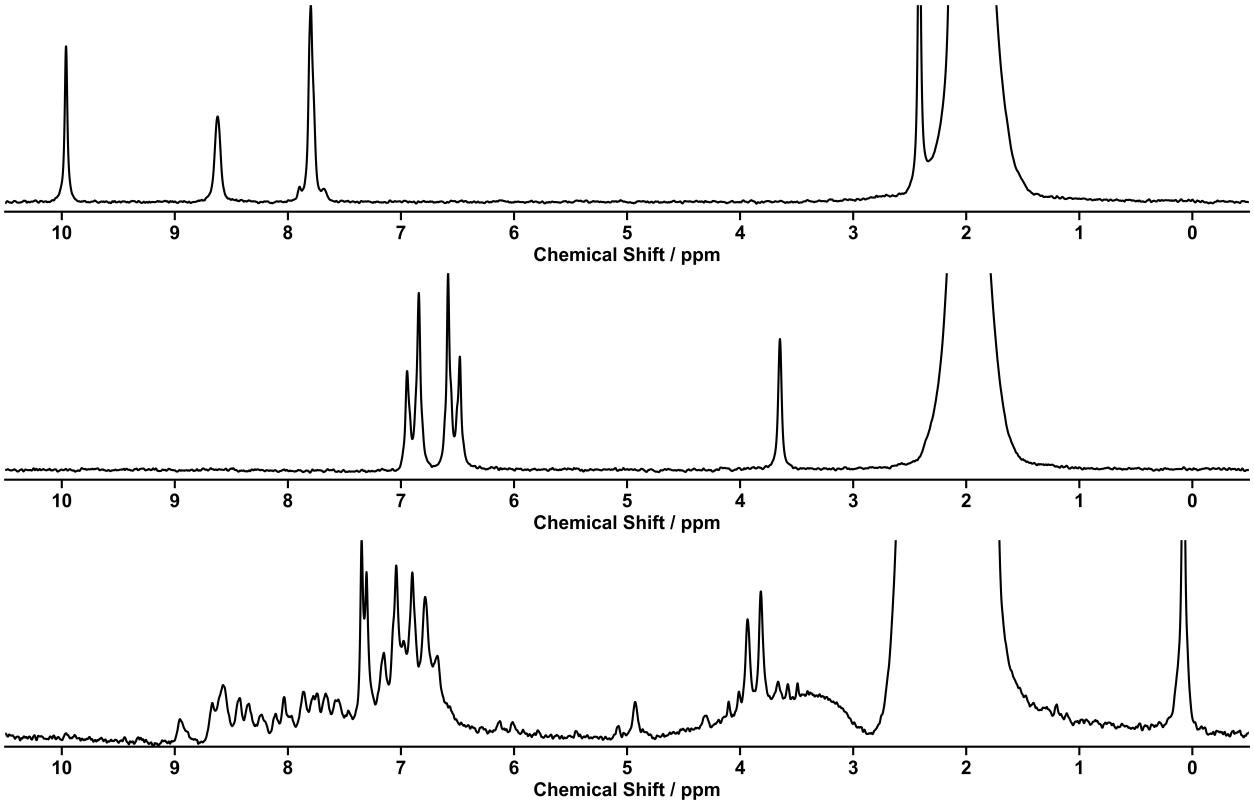
Reaction 67



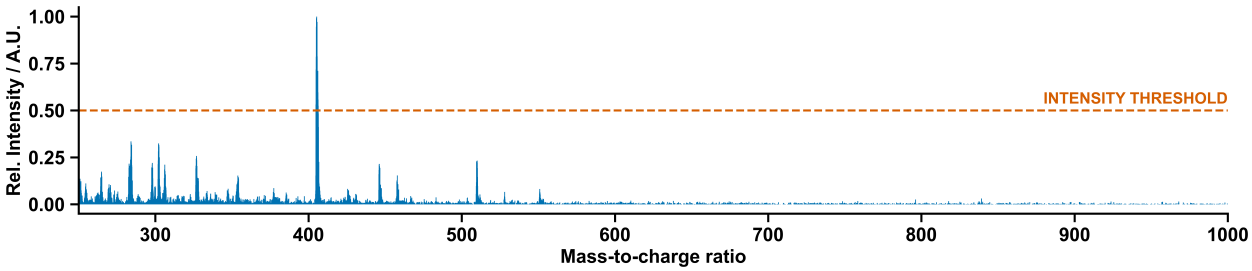
Scheme 57: Self-assembly of components 3, 17, with Yittrium(III) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 67.

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 labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 67. Decision motivations are also given.

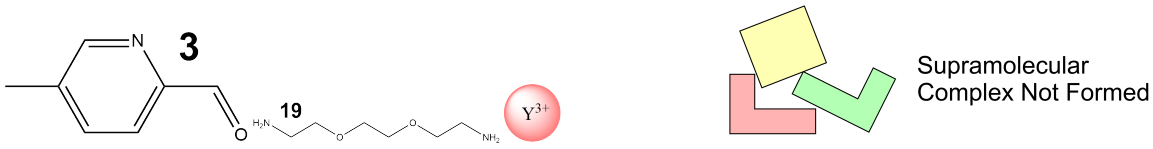


NMR Spectra 57: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 67.



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

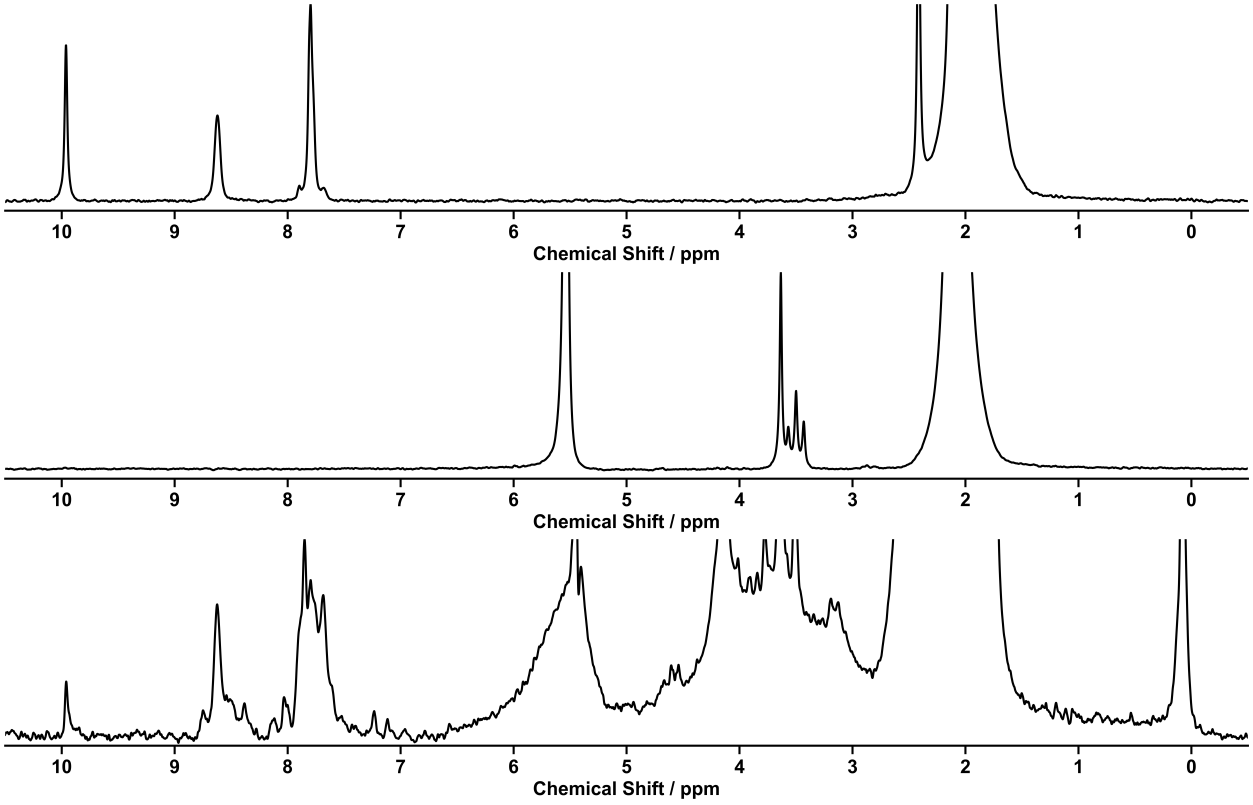
Reaction 68



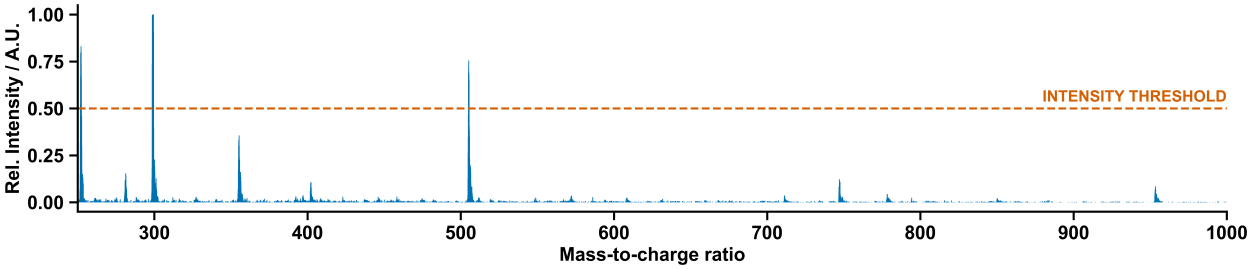
Scheme 58: Self-assembly of components 3, 19, with Yittrium(III) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 68.

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 labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 68. Decision motivations are also given.

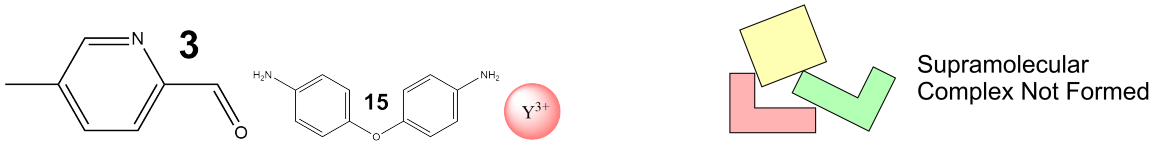


NMR Spectra 58: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 68.



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

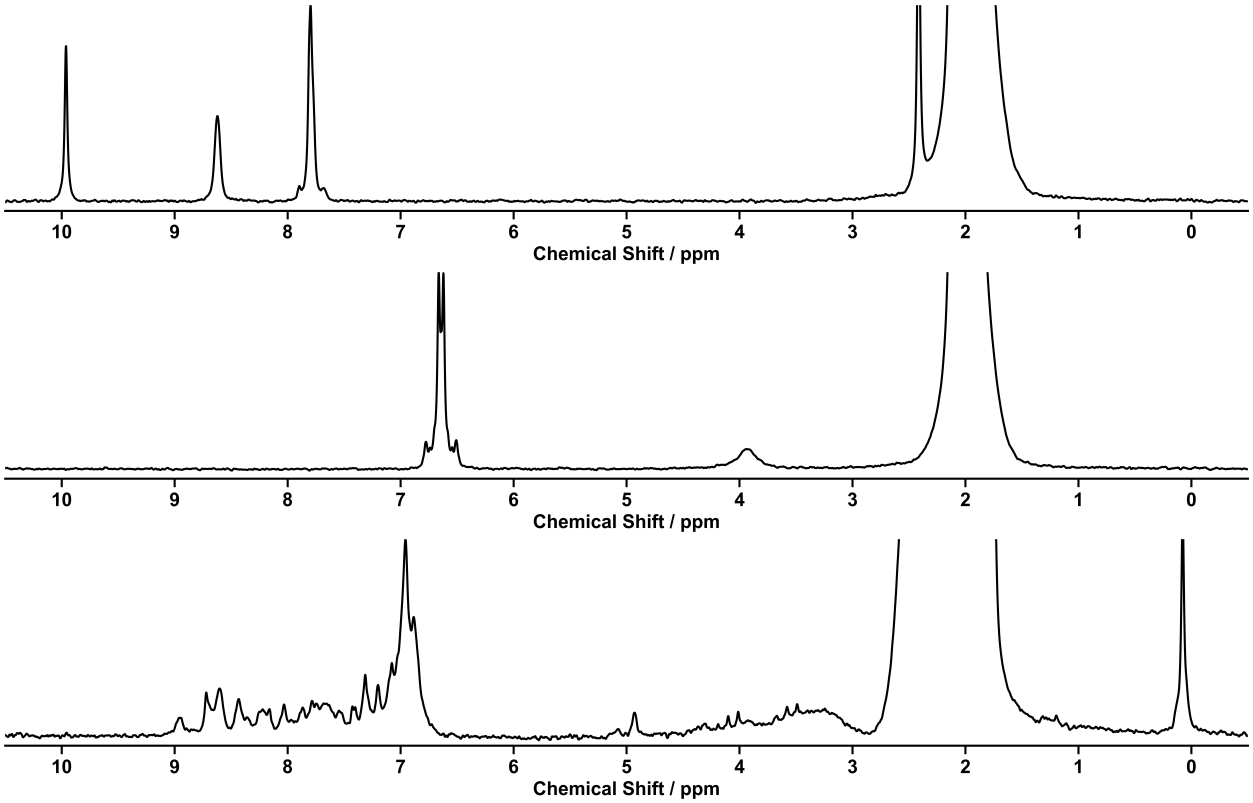
Reaction 69



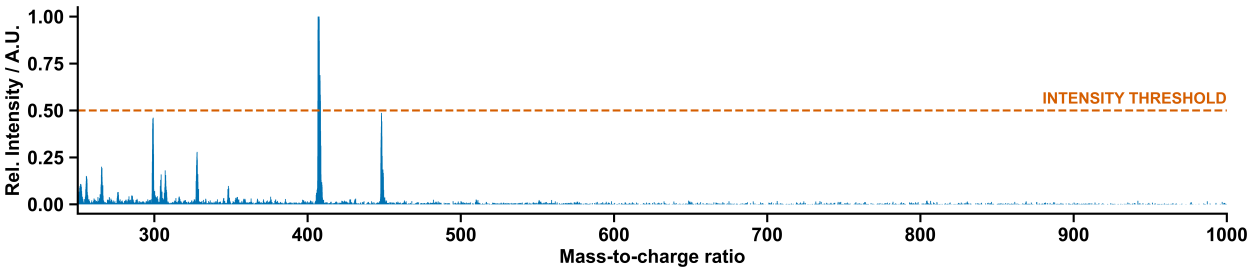
Scheme 59: Self-assembly of components 3, 15, with Yittrium(III) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 69.

<table>
<tr><td rowspan="2">Human Reaction Decision:
Failed</td><td>Human NMR Decision:
Failed</td><td colspan="2">NMR Spectra Category:
Oligomers formed.</td></tr>
<tr><td>Human MS Decision:
Failed</td><td colspan="2">MS Spectra Category:
Reaction occurred, unknown product.</td></tr>
<tr><td rowspan="4">Decision Maker Reaction Decision:
N/A</td><td rowspan="2">Decision Maker NMR Decision:
N/A</td><td colspan="2">NMR Criteria 1:
N/A</td></tr>
<tr><td colspan="2">NMR Criteria 2:
N/A</td></tr>
<tr><td rowspan="2">Decision Maker MS Decision:
Pass</td><td>MS Criteria 1 and 2:
Pass</td><td>Number of predicted peaks found in MS spectra with appropriate intensity:
0</td></tr>
<tr><td>MS Criteria 3:
Pass</td><td>Number of counter-ions found:
0</td></tr>
</table>

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

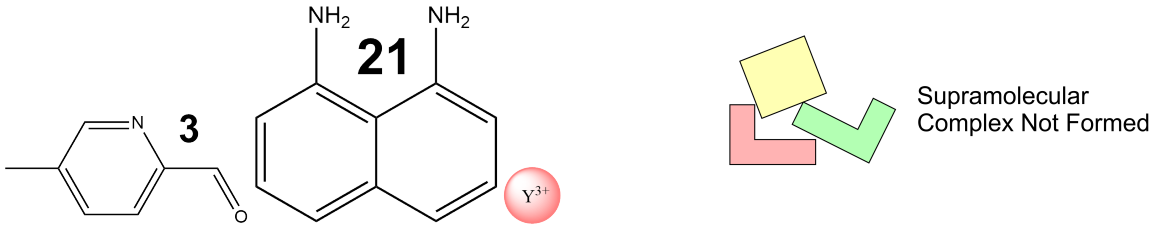


NMR Spectra 59: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 69.



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

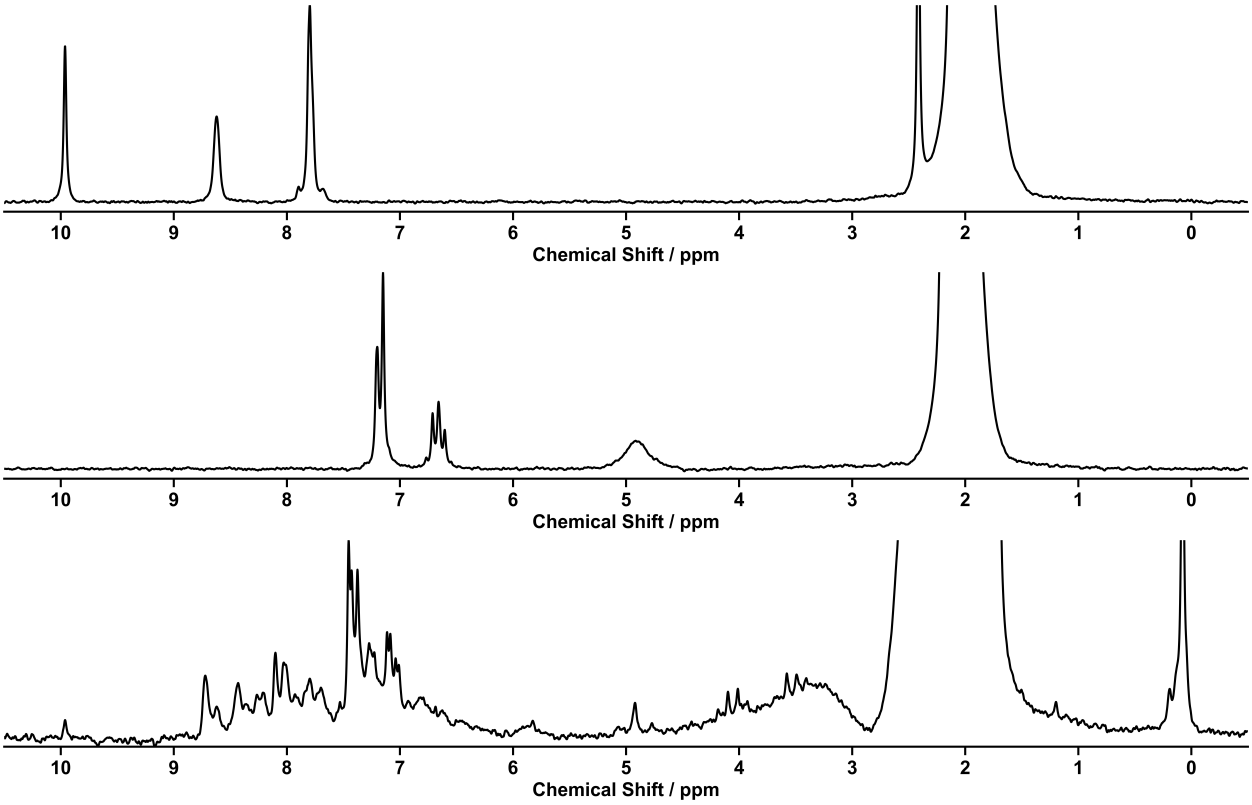
Reaction 70



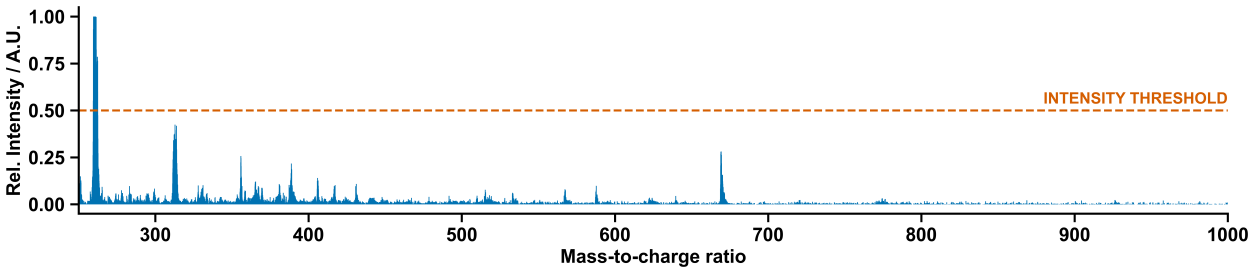
Scheme 60: Self-assembly of components 3, 21, with Yittrium(III) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 70.

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 labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 70. Decision motivations are also given.

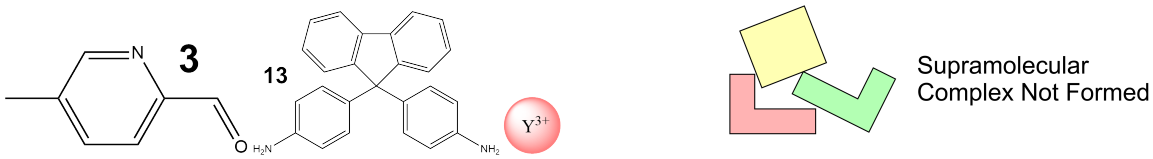


NMR Spectra 60: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 70.



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

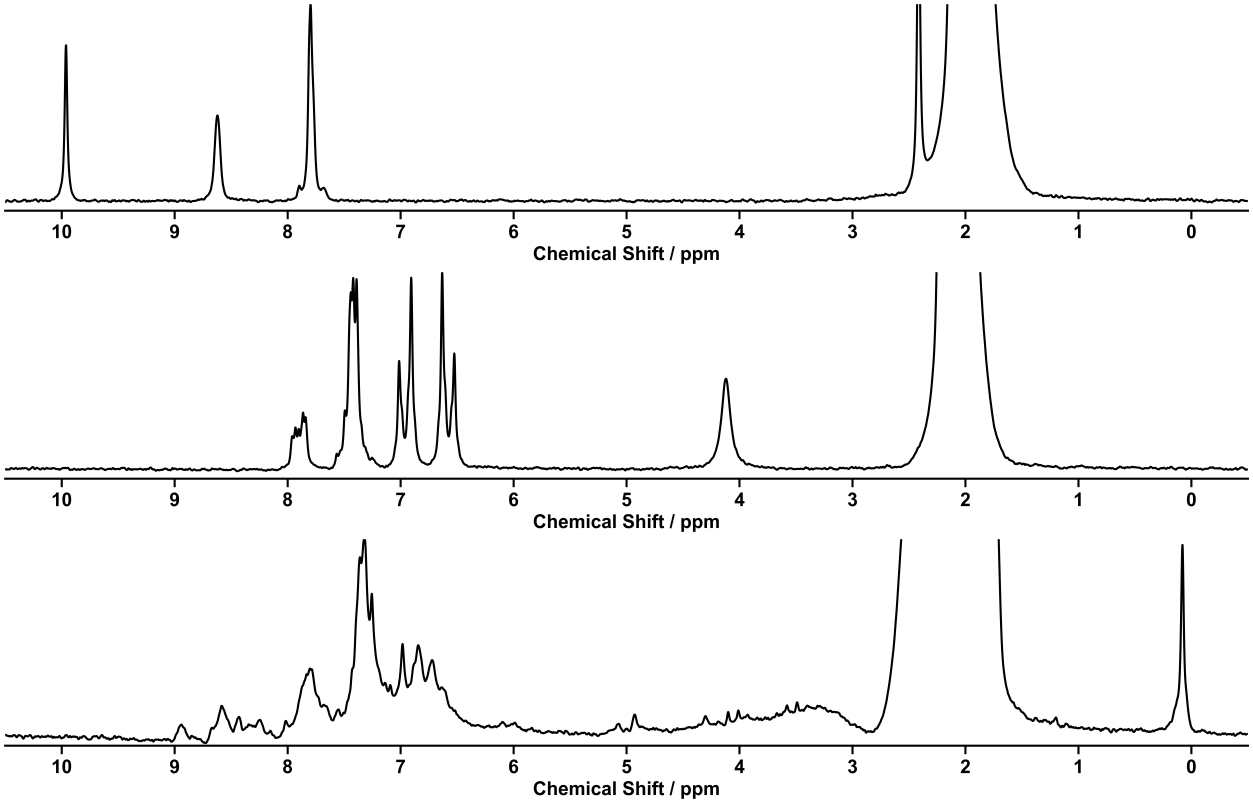
Reaction 71



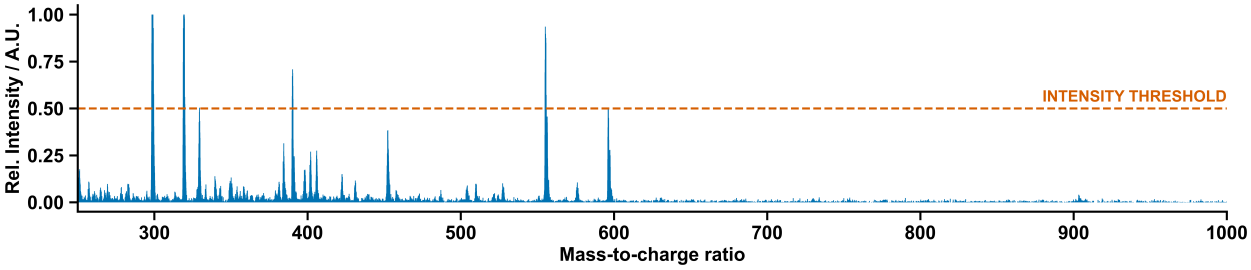
Scheme 61: Self-assembly of components 3, 13, with Yittrium(III) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 71.

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 labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 71. Decision motivations are also given.

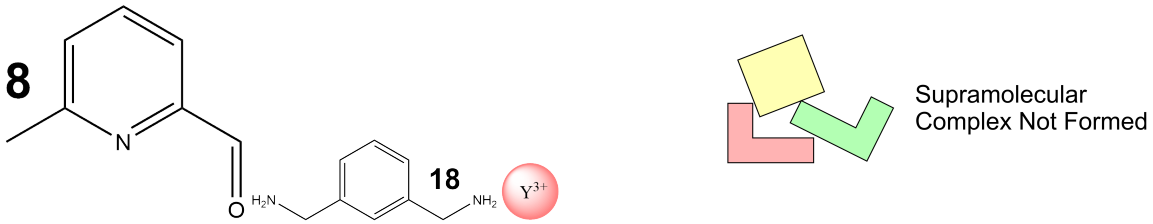


NMR Spectra 61: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 71.



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

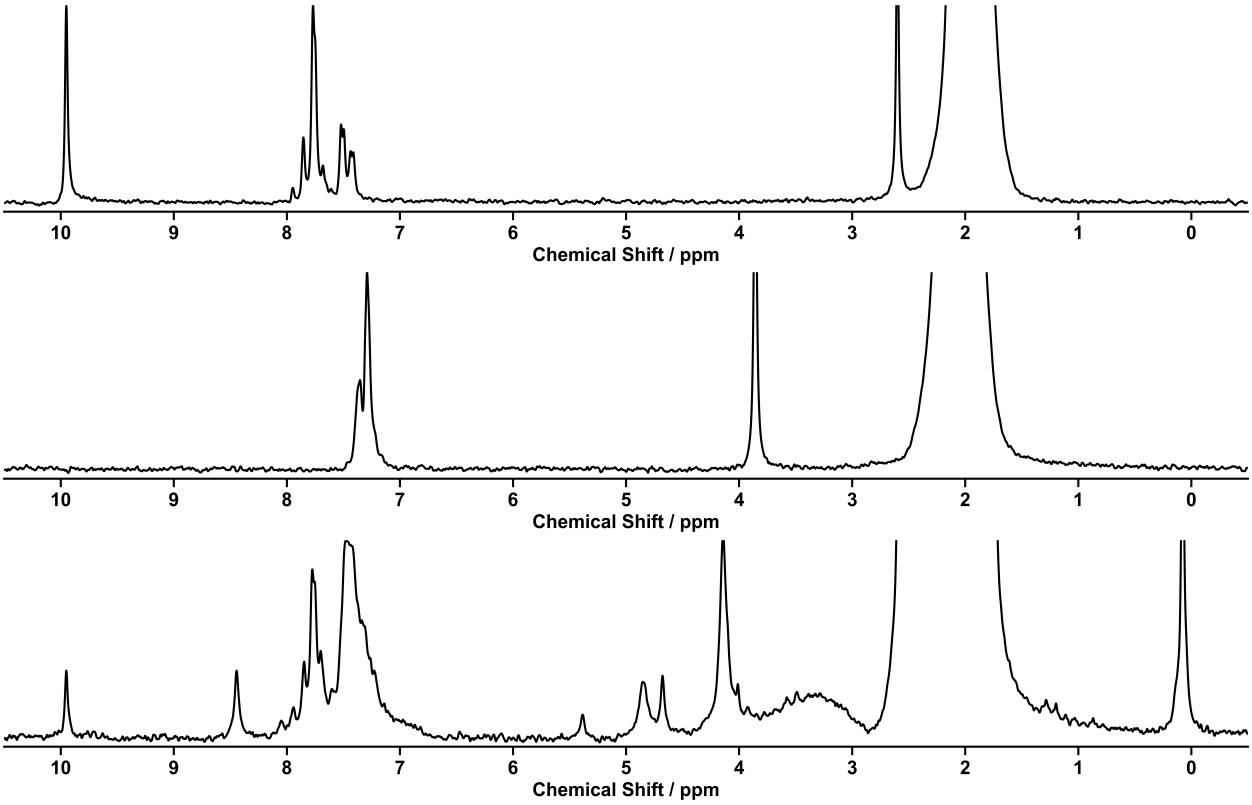
Reaction 72



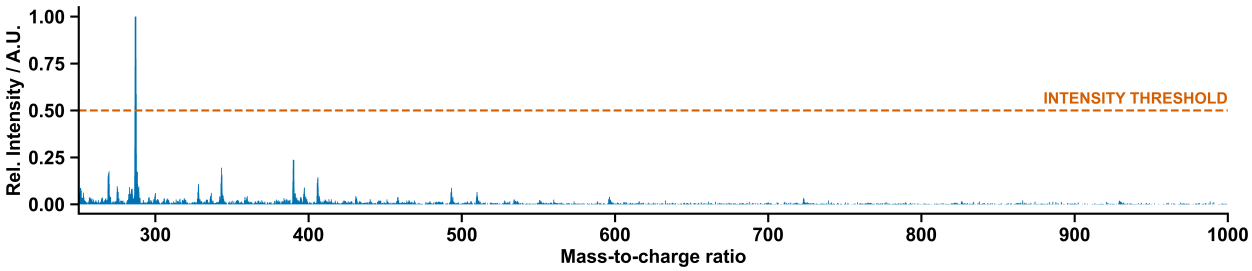
Scheme 62: Self-assembly of components 8, 18, with Yittrium(III) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 72.

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 labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 72. Decision motivations are also given.

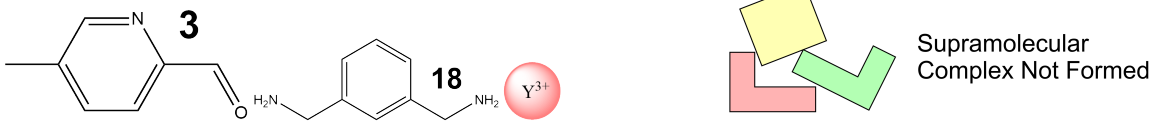


NMR Spectra 62: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 72.



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

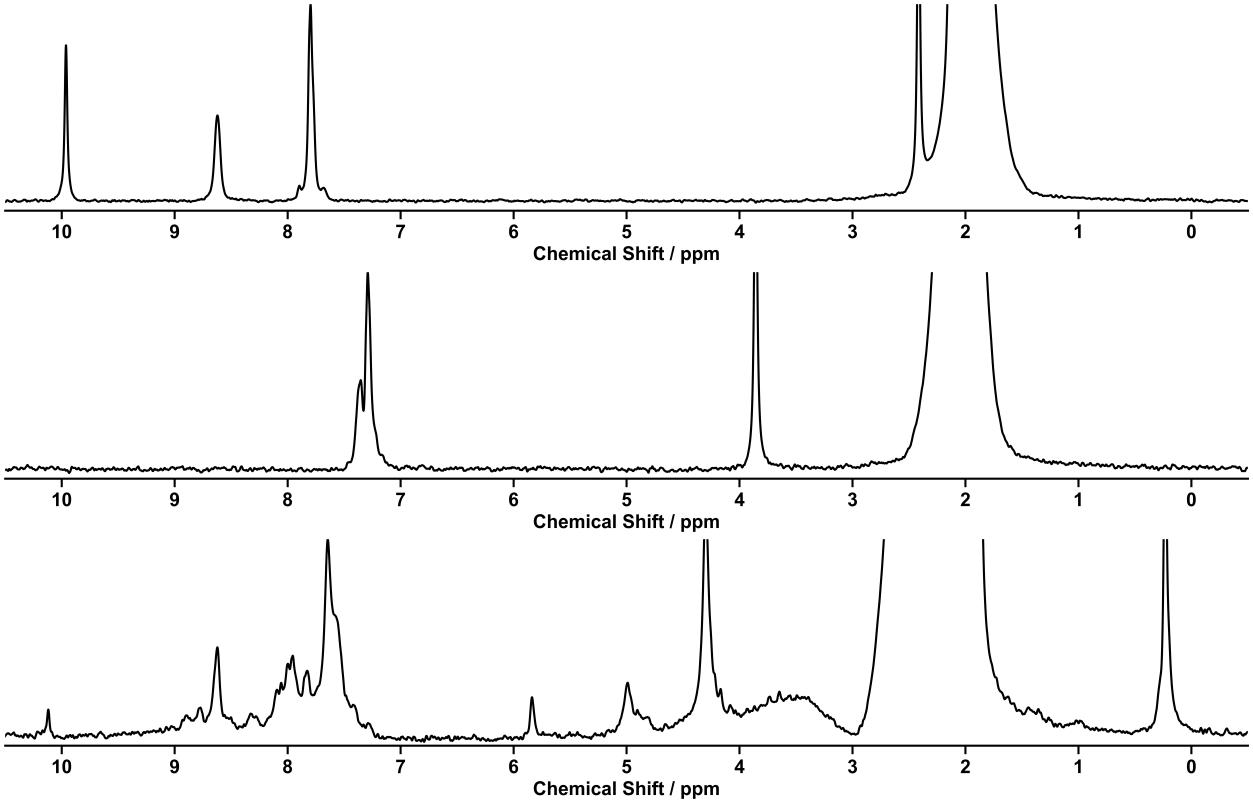
Reaction 74



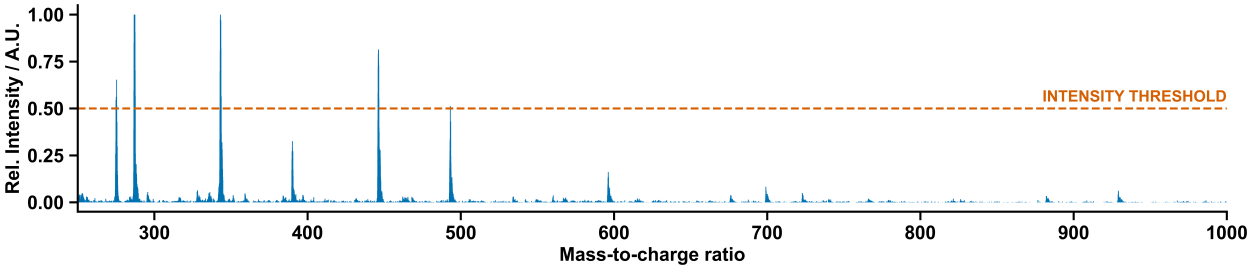
Scheme 63: Self-assembly of components 3, 18, with Yittrium(III) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 74.

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 labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 74. Decision motivations are also given.

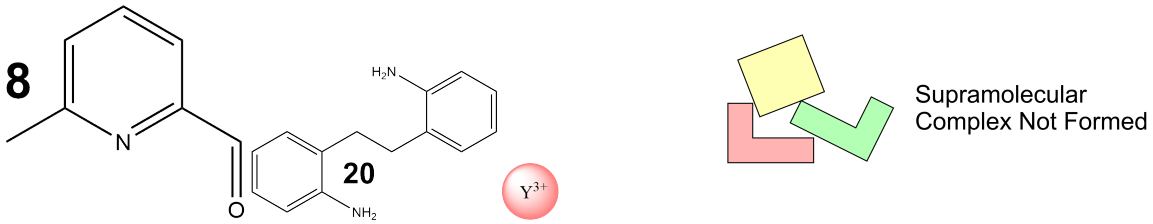


NMR Spectra 63: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 74.



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

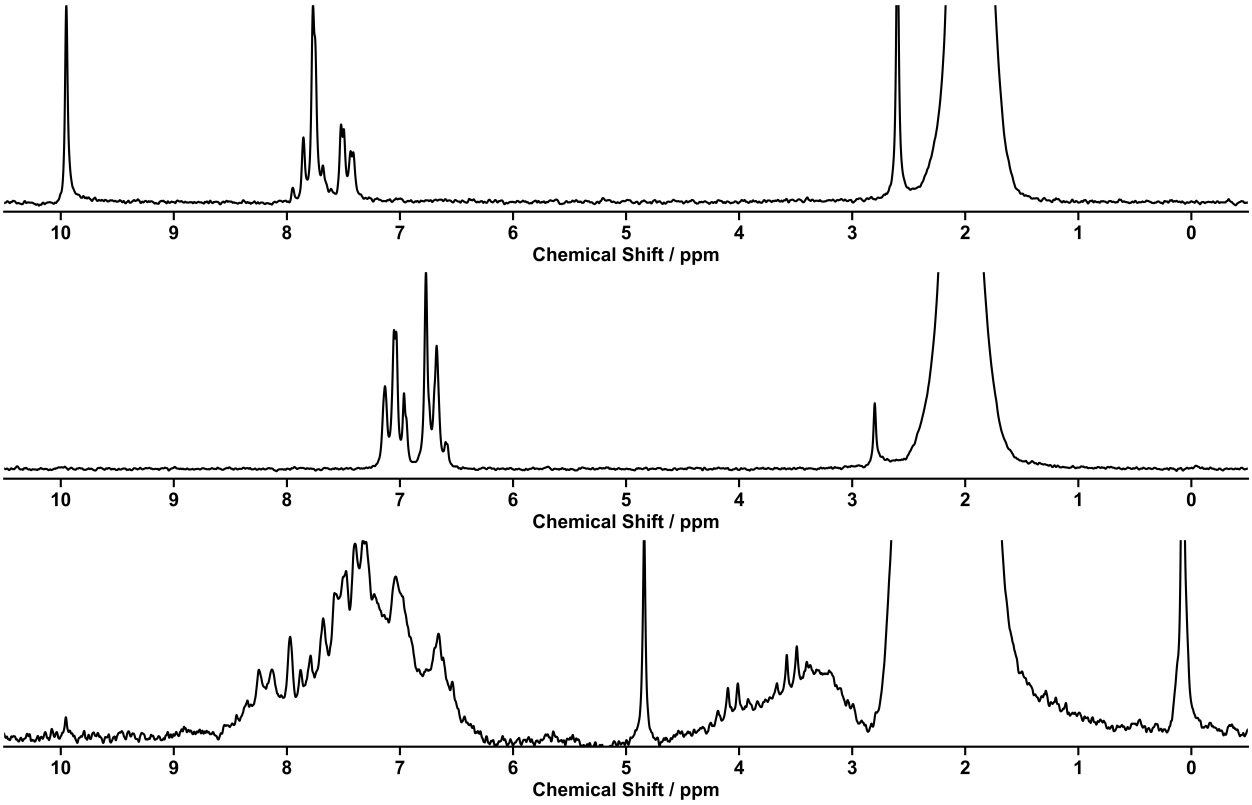
Reaction 78



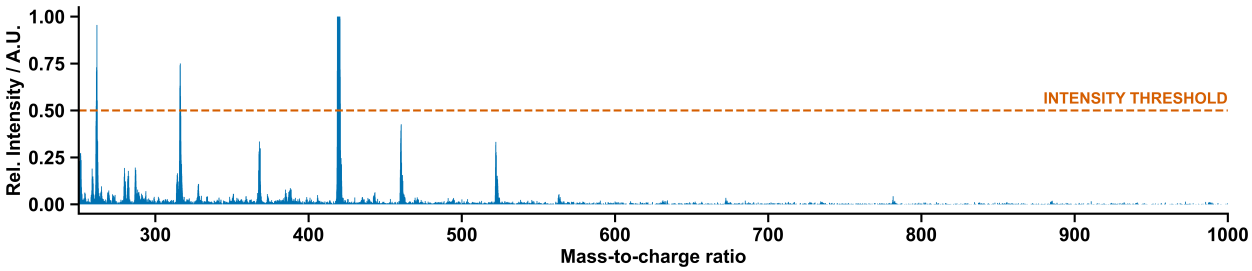
Scheme 64: Self-assembly of components 8, 20, with Yittrium(III) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 78.

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 labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 78. Decision motivations are also given.

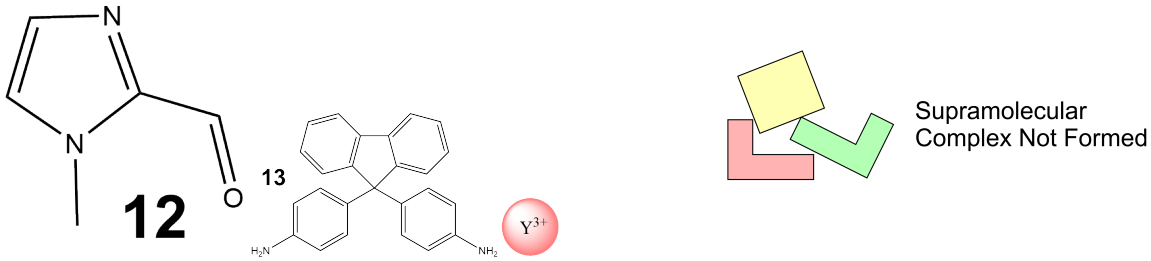


NMR Spectra 64: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 78.



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

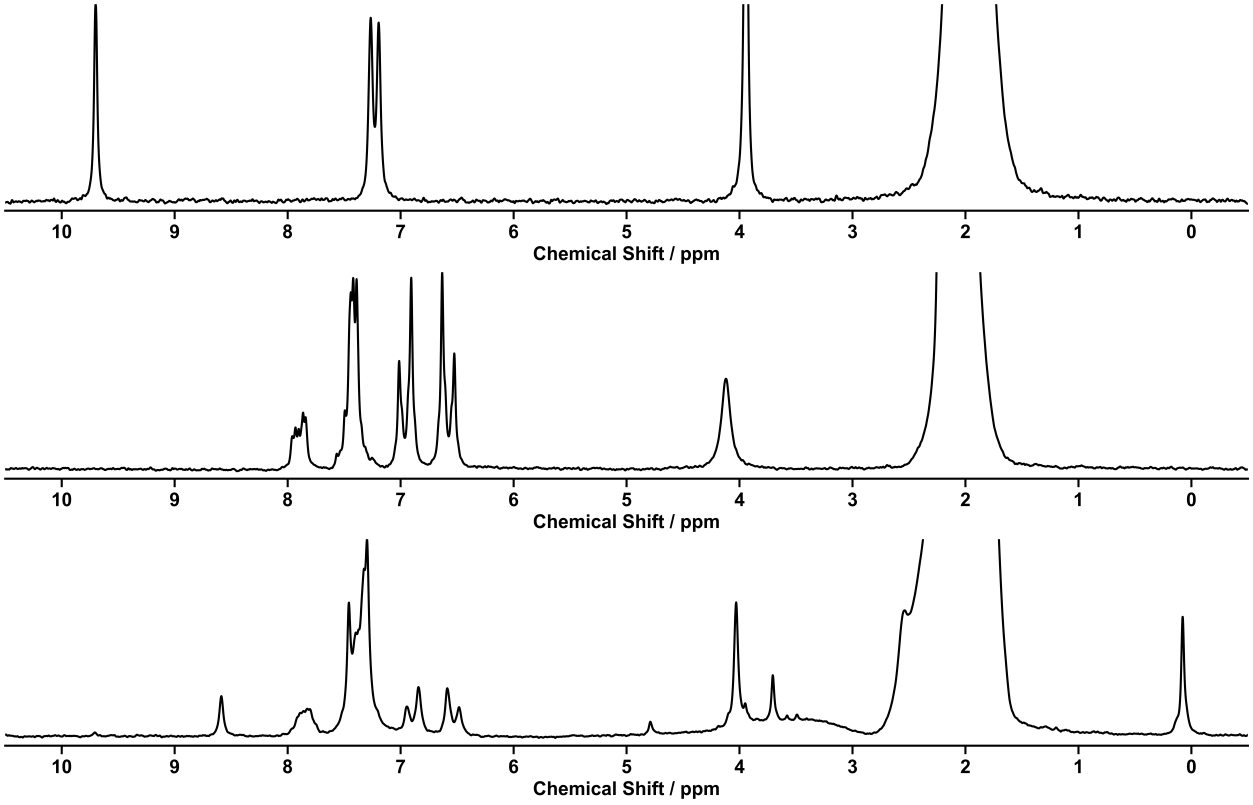
Reaction 80



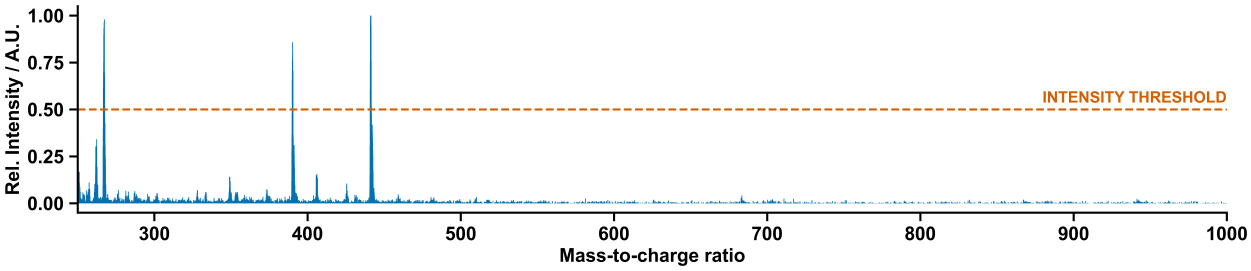
Scheme 65: Self-assembly of components 12, 13, with Yittrium(III) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 80.

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 labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 80. Decision motivations are also given.

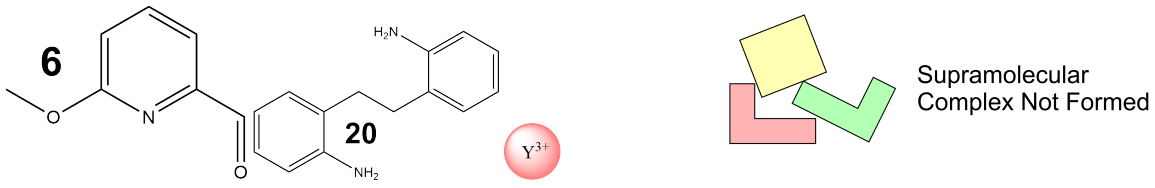


NMR Spectra 65: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 80.



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

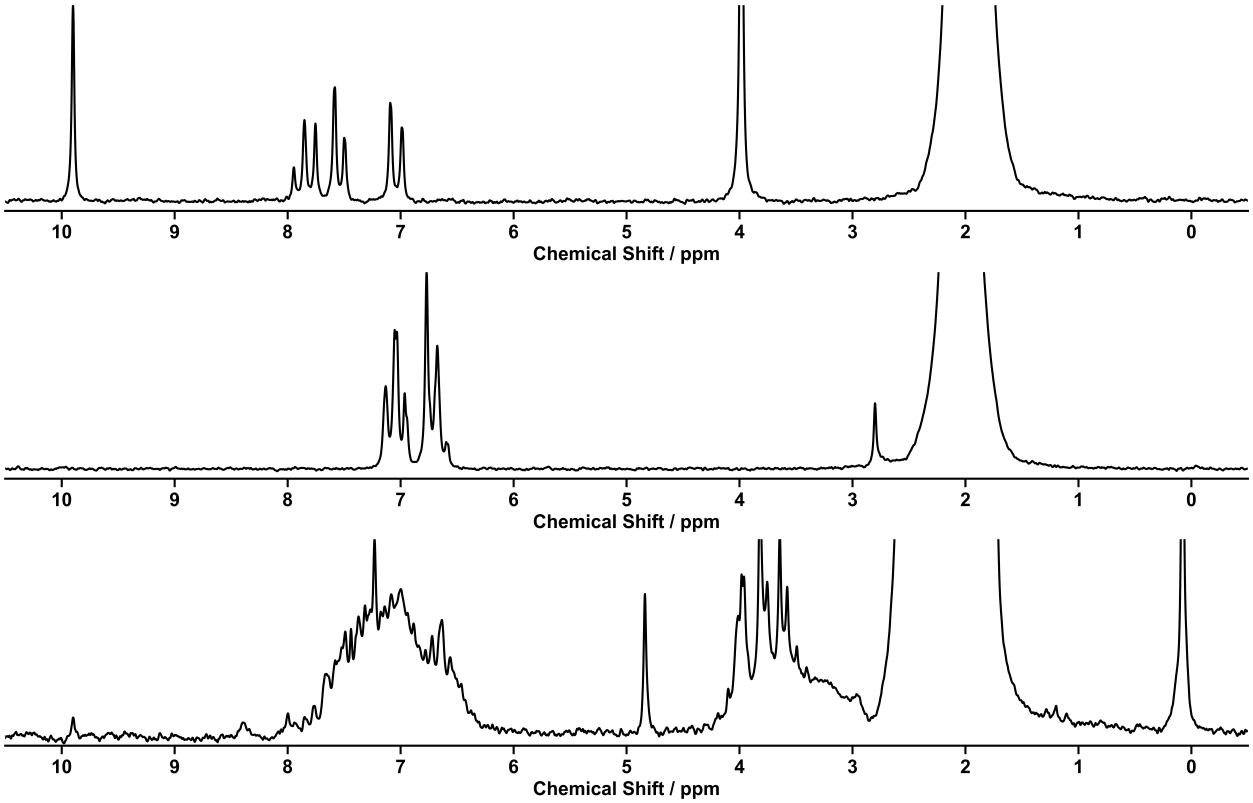
Reaction 81



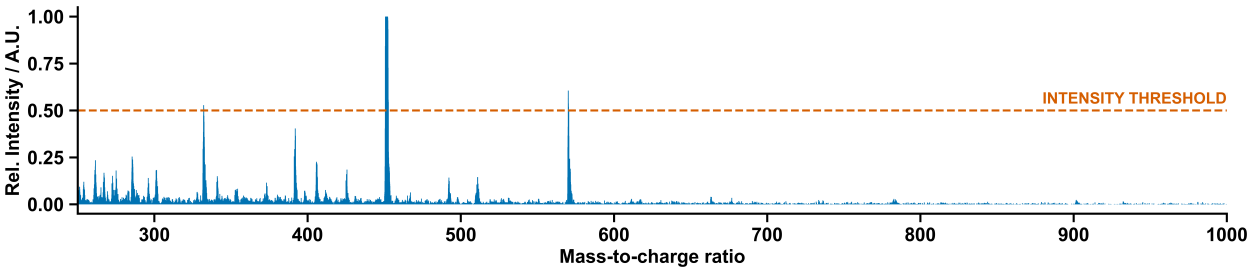
Scheme 66: Self-assembly of components 6, 20, with Yittrium(III) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 81.

<table>
<tr><td rowspan="2">Human Reaction Decision:
Failed</td><td>Human NMR Decision:
Failed</td><td colspan="2">NMR Spectra Category:
Oligomers formed.</td></tr>
<tr><td>Human MS Decision:
Failed</td><td colspan="2">MS Spectra Category:
Reaction occurred, unknown product.</td></tr>
<tr><td rowspan="4">Decision Maker Reaction Decision:
N/A</td><td rowspan="2">Decision Maker NMR Decision:
N/A</td><td colspan="2">NMR Criteria 1:
N/A</td></tr>
<tr><td colspan="2">NMR Criteria 2:
N/A</td></tr>
<tr><td rowspan="2">Decision Maker MS Decision:
Pass</td><td>MS Criteria 1 and 2:
Pass</td><td>Number of predicted peaks found in MS spectra with appropriate intensity:
0</td></tr>
<tr><td>MS Criteria 3:
Pass</td><td>Number of counter-ions found:
0</td></tr>
</table>

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

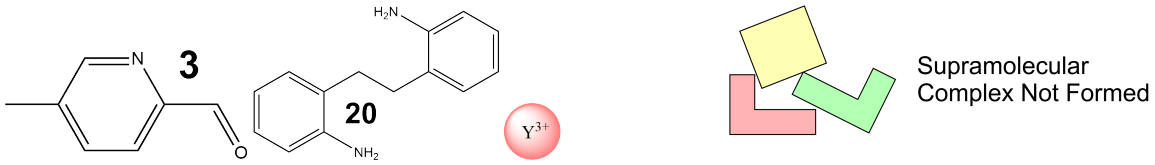


NMR Spectra 66: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 81.



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

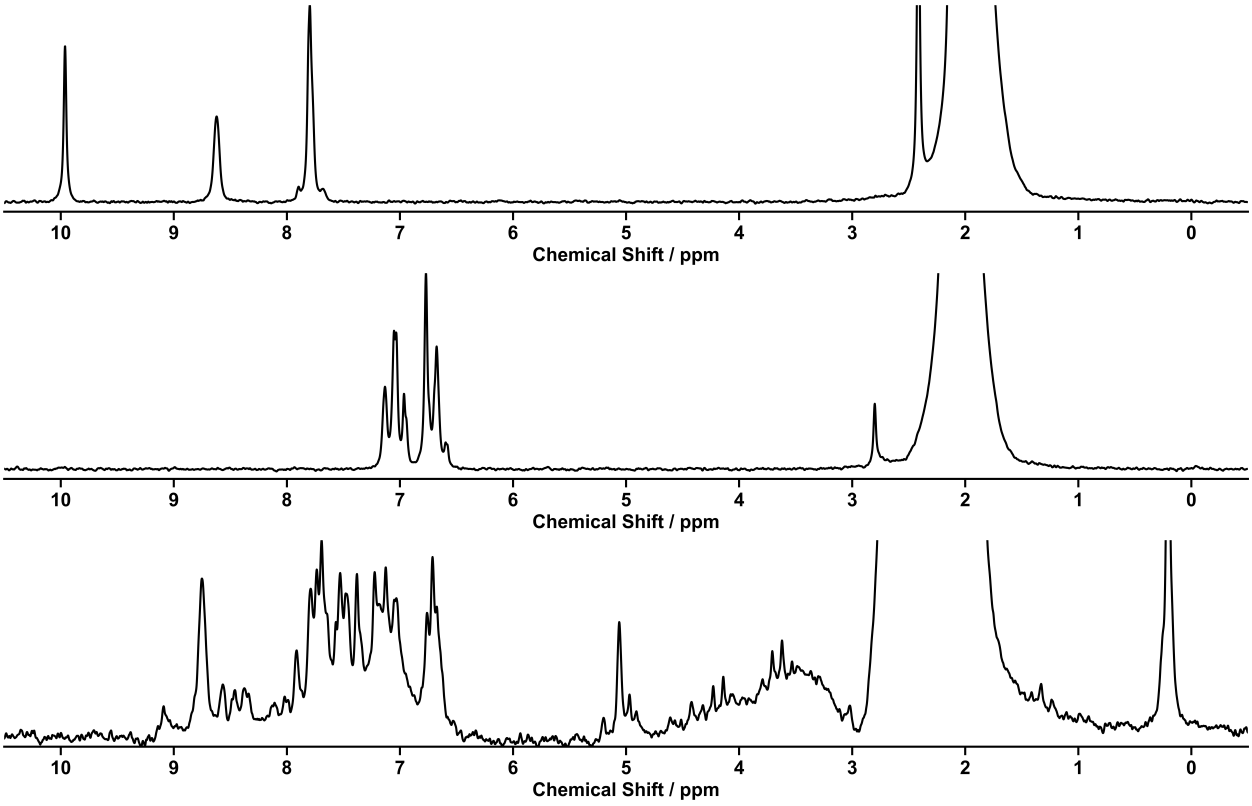
Reaction 82



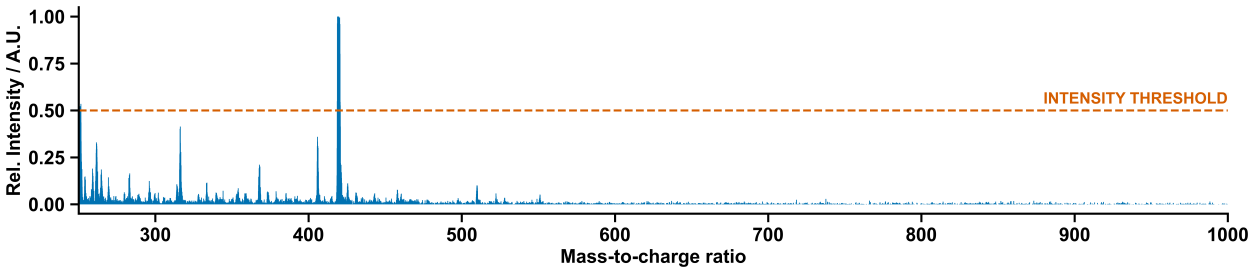
Scheme 67: Self-assembly of components 3, 20, with Yittrium(III) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 82.

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 labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 82. Decision motivations are also given.

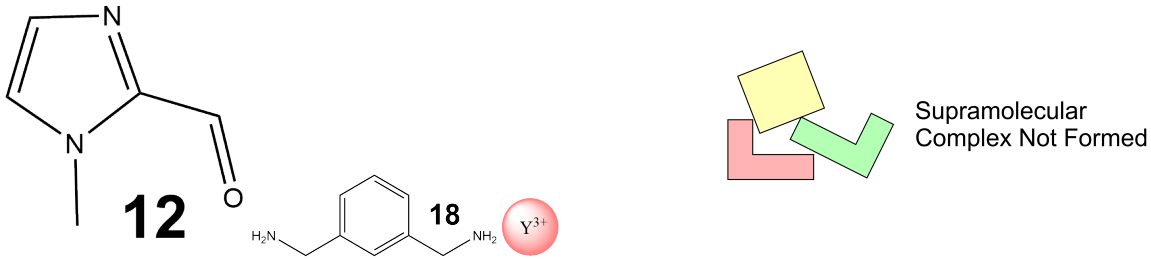


NMR Spectra 67: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 82.



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

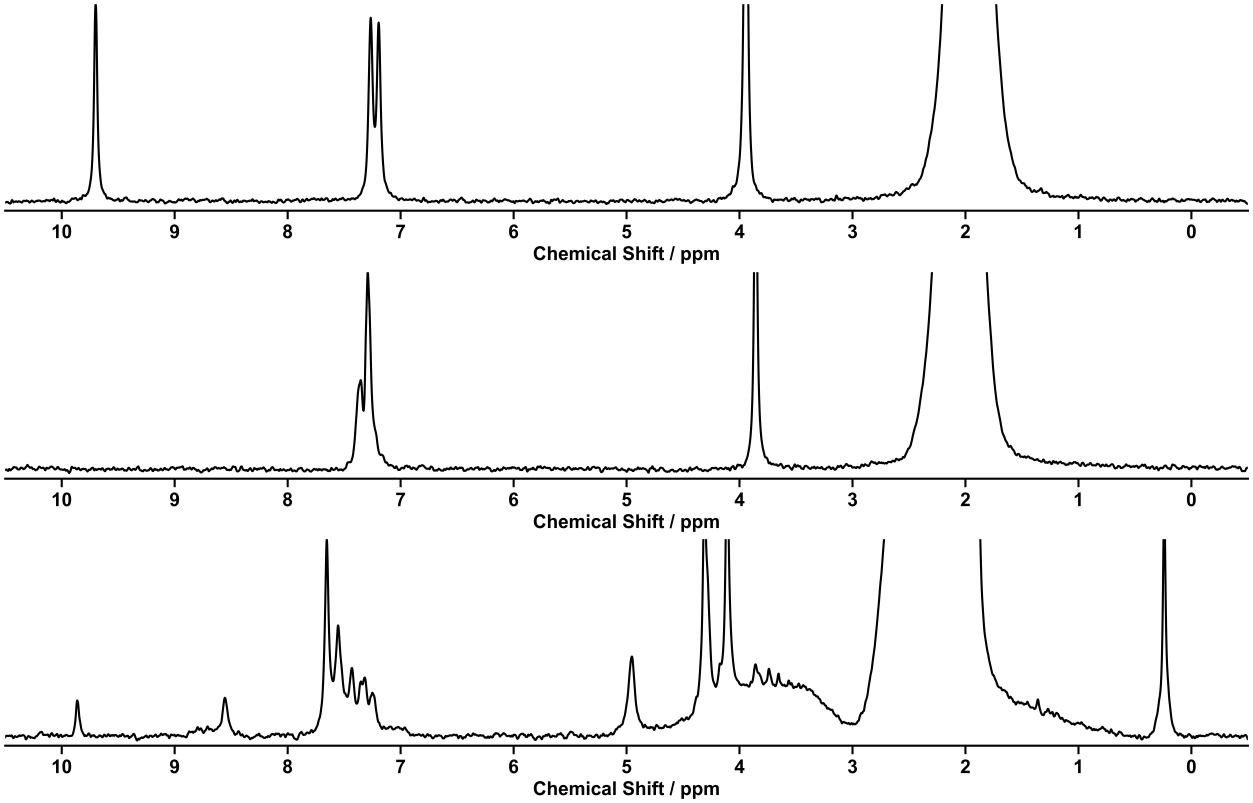
Reaction 83



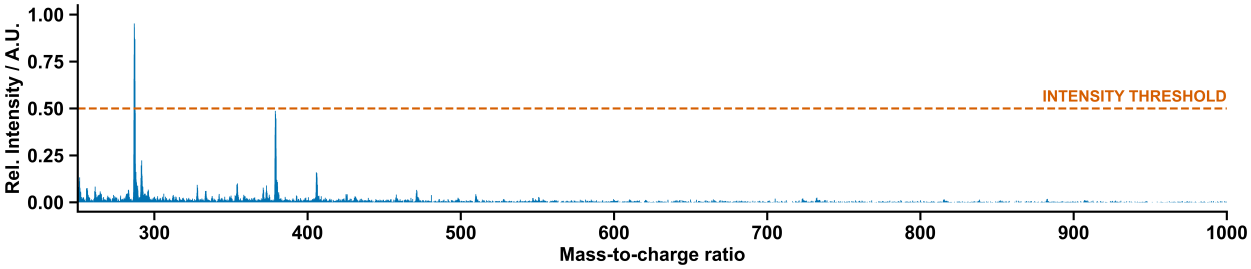
Scheme 68: Self-assembly of components 12, 18, with Yittrium(III) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 83.

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 labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 83. Decision motivations are also given.

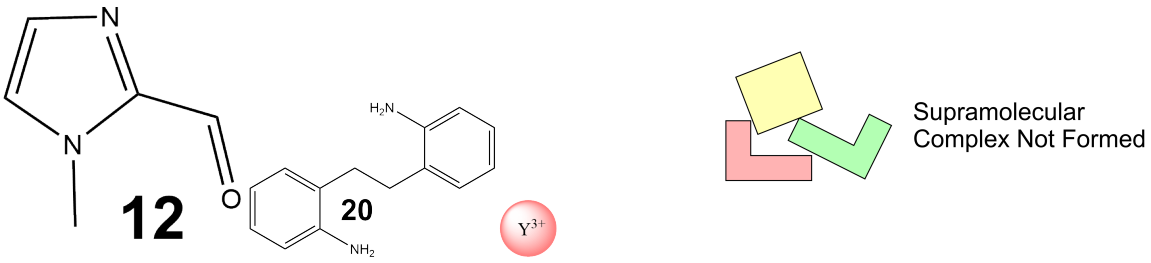


NMR Spectra 68: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 83.



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

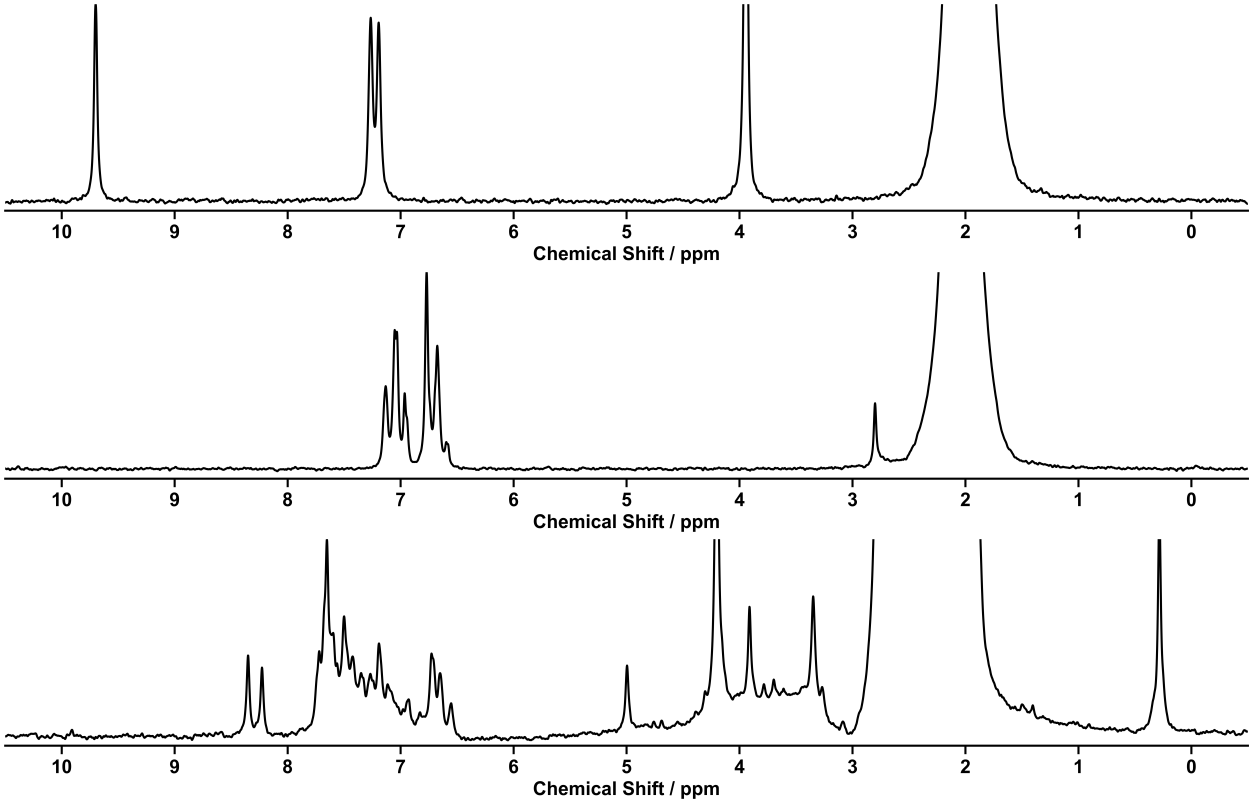
Reaction 84



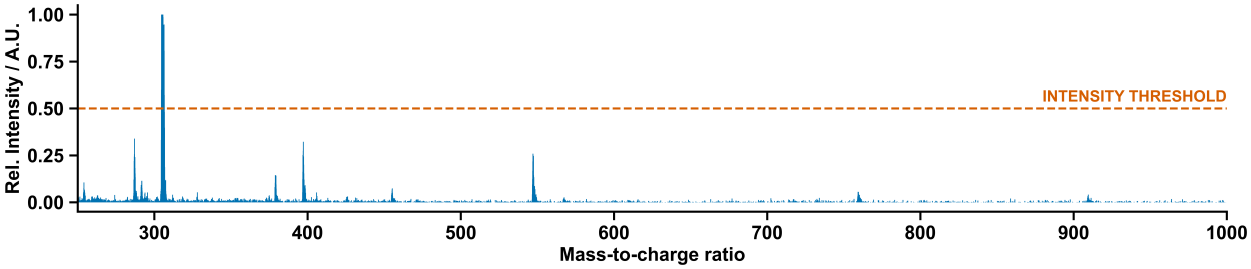
Scheme 69: Self-assembly of components 12, 20, with Yittrium(III) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 84.

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	
		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 69: Human labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 84. Decision motivations are also given.

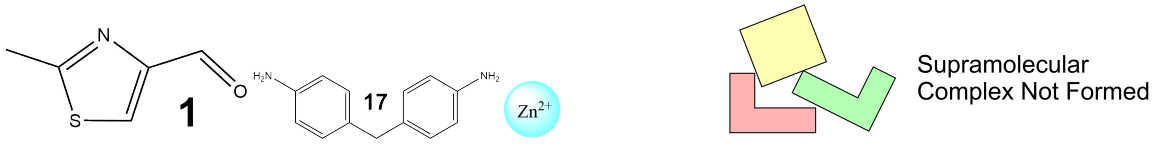


NMR Spectra 69: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 84.



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

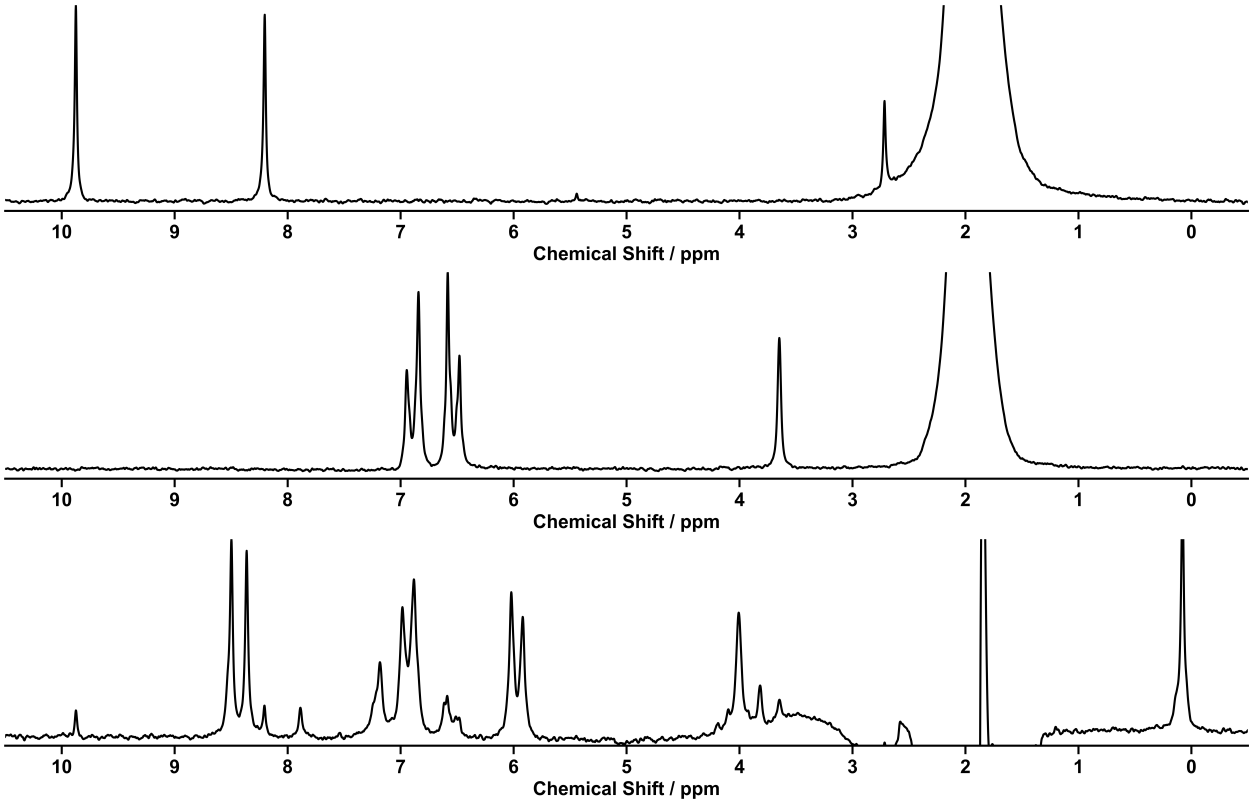
Reaction 85



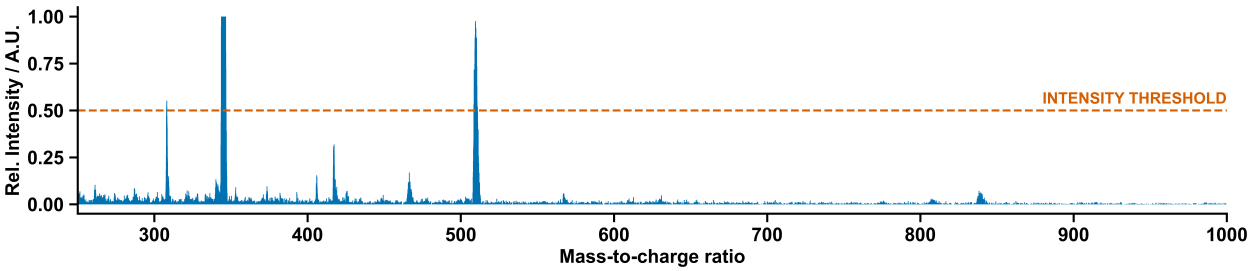
Scheme 70: Self-assembly of components 1, 17, with Zinc(II) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 85.

<table>
<tr><td rowspan="2">Human Reaction Decision:
Failed</td><td>Human NMR Decision:
Pass</td><td colspan="2">NMR Spectra Category:
Single discrete species formed.</td></tr>
<tr><td>Human MS Decision:
Failed</td><td colspan="2">MS Spectra Category:
Reaction occurred, unknown product.</td></tr>
<tr><td rowspan="4">Decision Maker Reaction Decision:
N/A</td><td rowspan="2">Decision Maker NMR Decision:
N/A</td><td colspan="2">NMR Criteria 1:
N/A</td></tr>
<tr><td colspan="2">NMR Criteria 2:
N/A</td></tr>
<tr><td rowspan="2">Decision Maker MS Decision:
Pass</td><td>MS Criteria 1 and 2:
Pass</td><td>Number of predicted peaks found in MS spectra with appropriate intensity:
1</td></tr>
<tr><td>MS Criteria 3:
Pass</td><td>Number of counter-ions found:
1</td></tr>
</table>

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

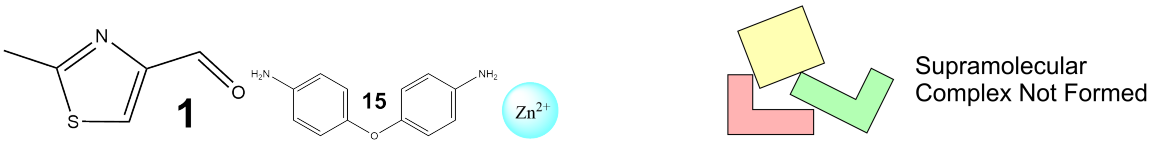


NMR Spectra 70: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 85.



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

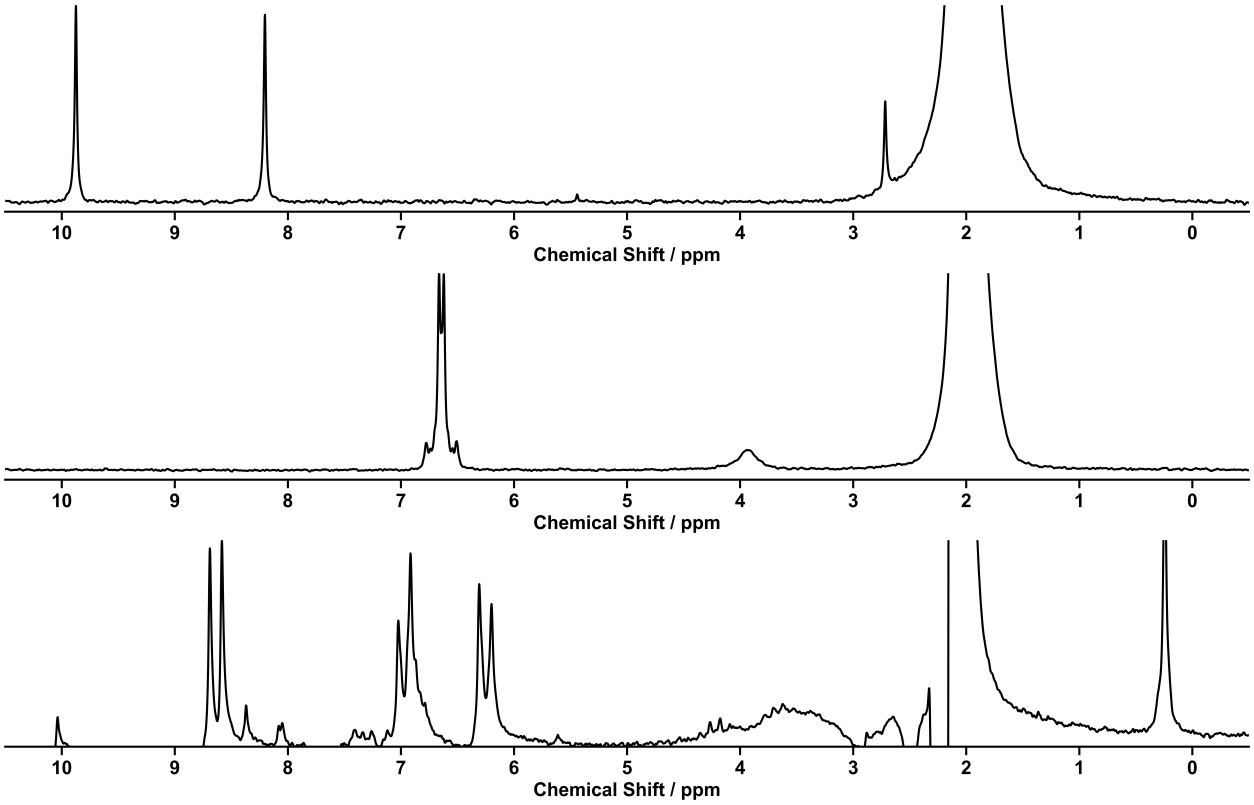
Reaction 87



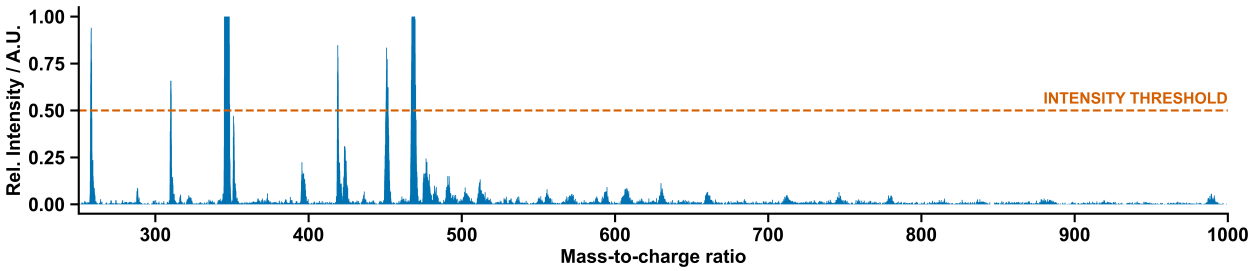
Scheme 71: Self-assembly of components 1, 15, with Zinc(II) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 87.

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 labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 87. Decision motivations are also given.

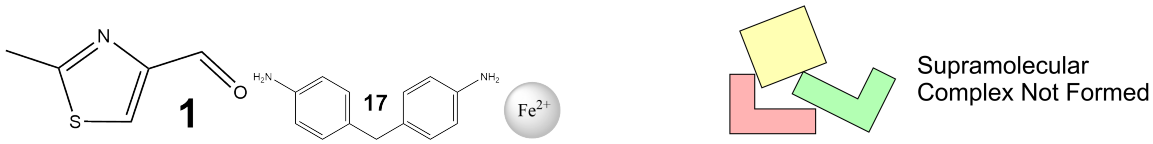


NMR Spectra 71: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 87.



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

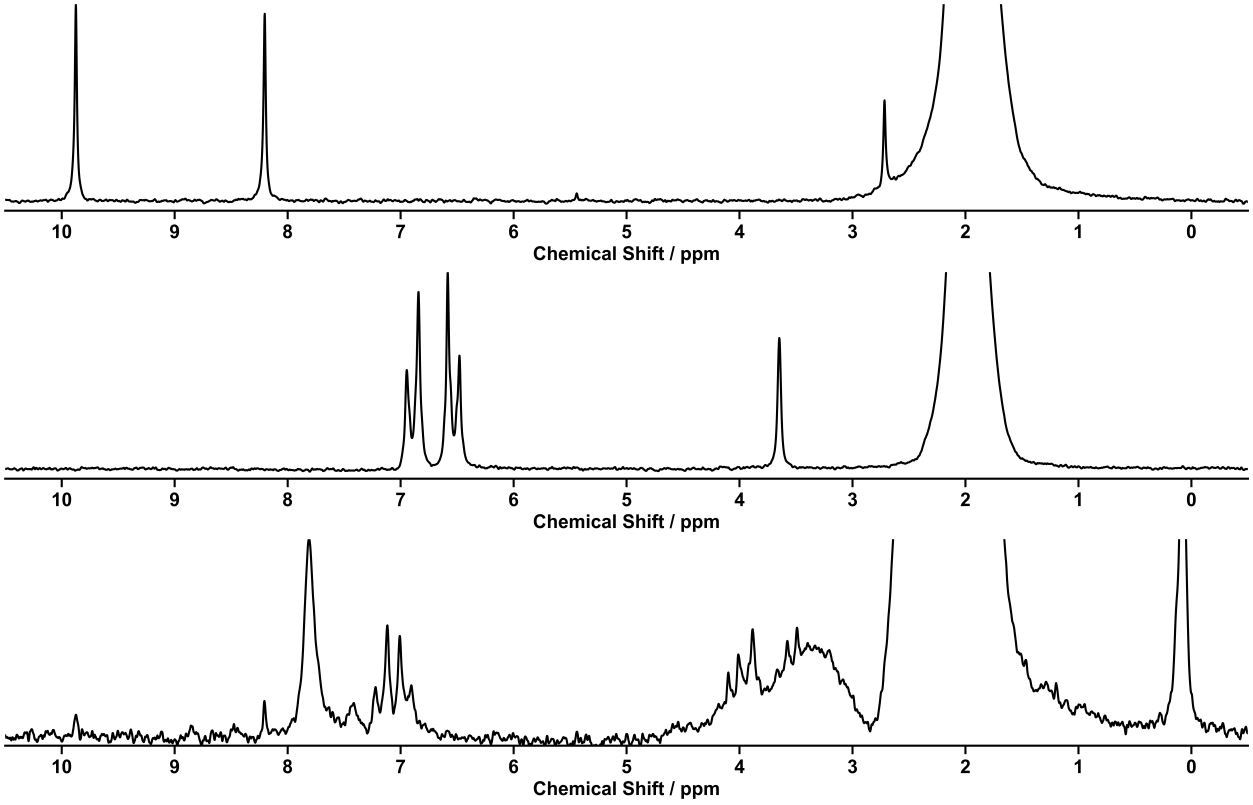
Reaction 88



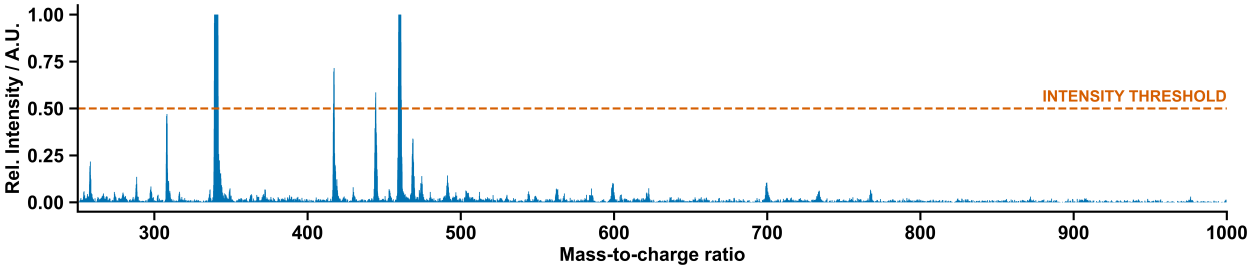
Scheme 72: Self-assembly of components 1, 17, with Iron(II) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 88.

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 labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 88. Decision motivations are also given.

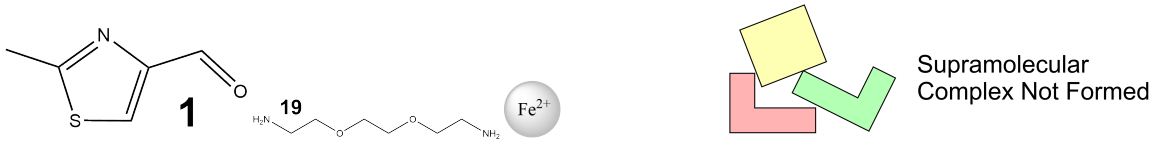


NMR Spectra 72: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 88.



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

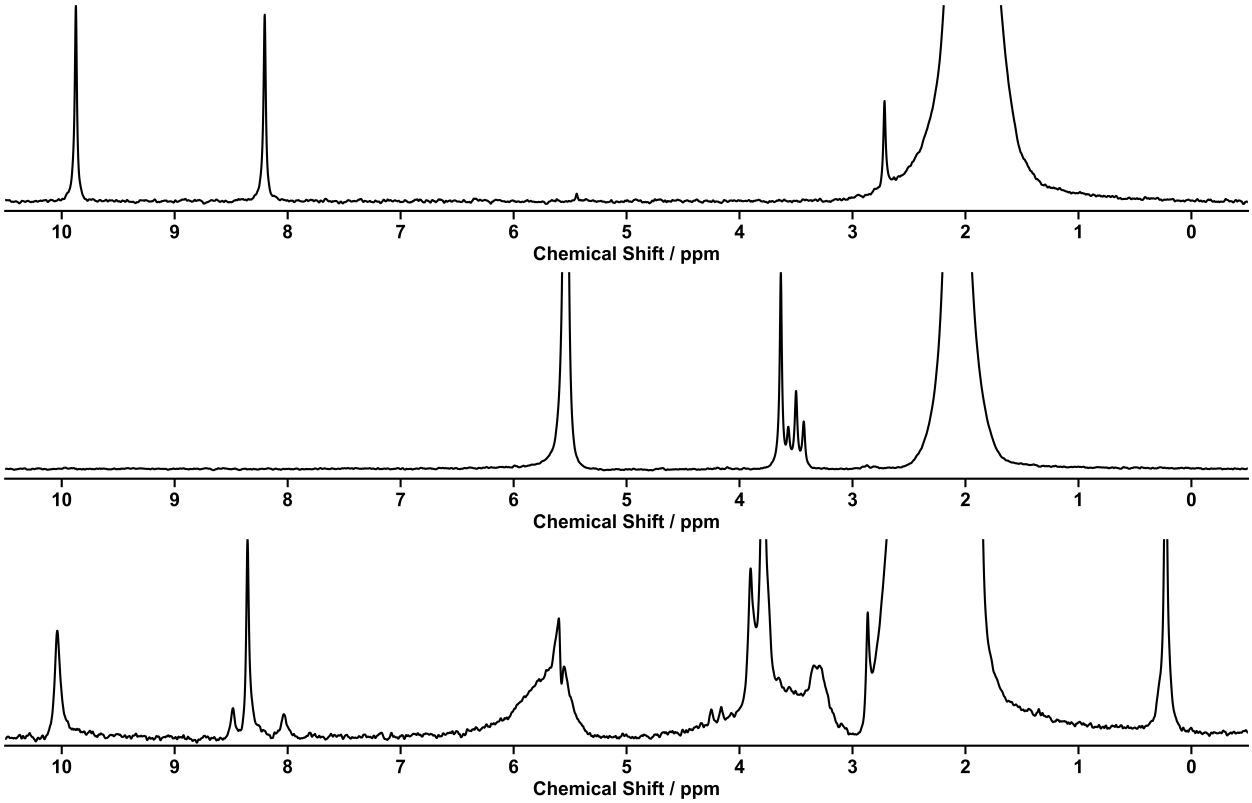
Reaction 89



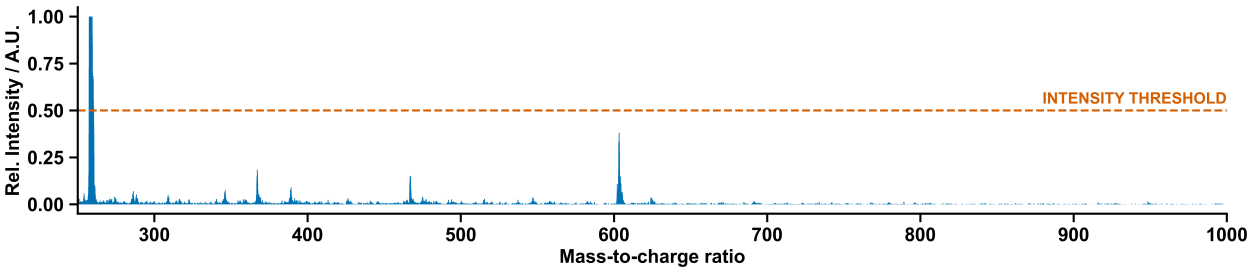
Scheme 73: Self-assembly of components 1, 19, with Iron(II) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 89.

<table>
<tr><td rowspan="2">Human Reaction Decision:
Failed</td><td>Human NMR Decision:
Pass</td><td colspan="2">NMR Spectra Category:
Single discrete species formed.</td></tr>
<tr><td>Human MS Decision:
Failed</td><td colspan="2">MS Spectra Category:
Reaction occurred, unknown product.</td></tr>
<tr><td rowspan="4">Decision Maker Reaction Decision:
N/A</td><td rowspan="2">Decision Maker NMR Decision:
N/A</td><td colspan="2">NMR Criteria 1:
N/A</td></tr>
<tr><td colspan="2">NMR Criteria 2:
N/A</td></tr>
<tr><td rowspan="2">Decision Maker MS Decision:
Pass</td><td>MS Criteria 1 and 2:
Pass</td><td>Number of predicted peaks found in MS spectra with appropriate intensity:
0</td></tr>
<tr><td>MS Criteria 3:
Pass</td><td>Number of counter-ions found:
0</td></tr>
</table>

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

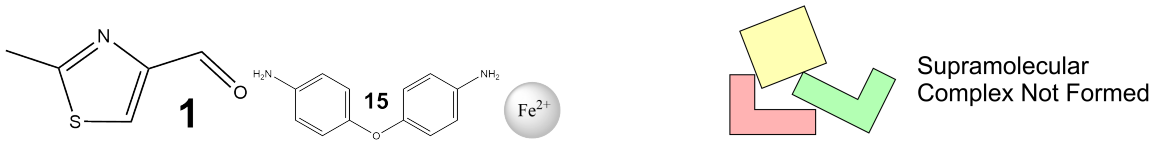


NMR Spectra 73: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 89.



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

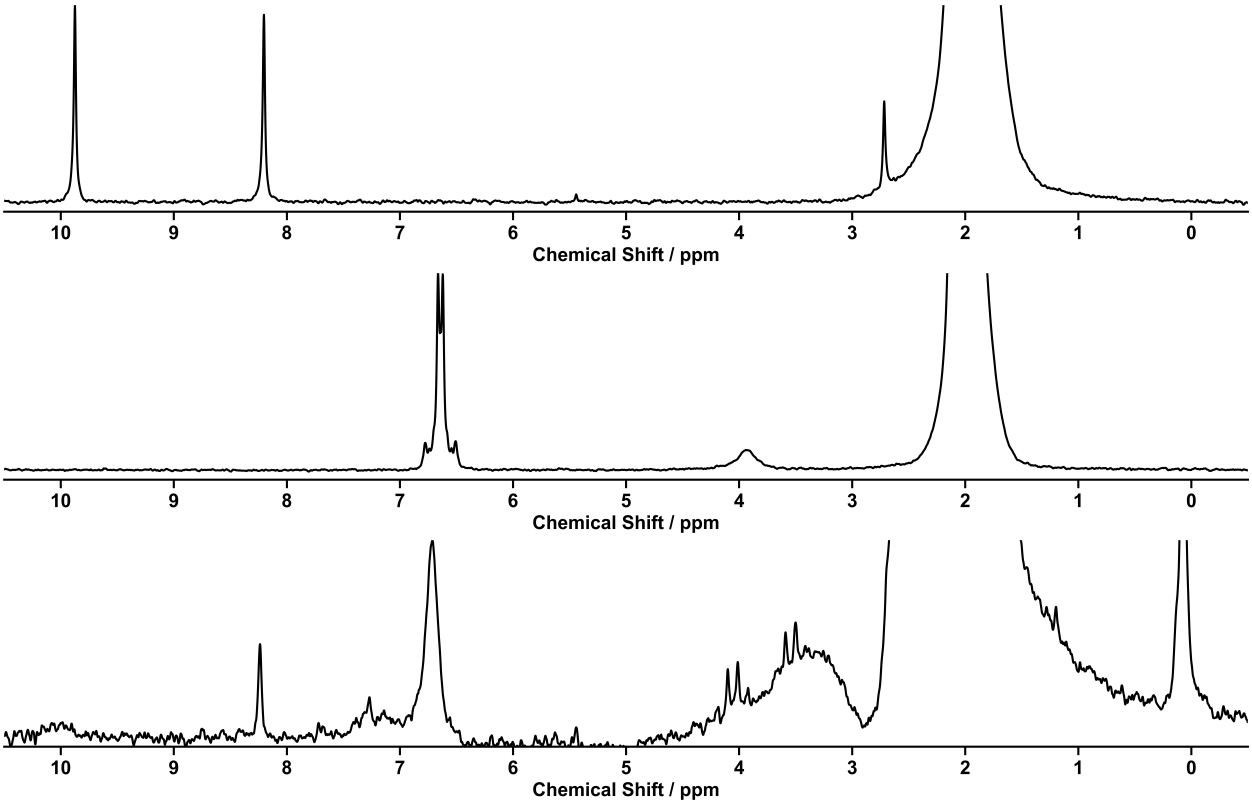
Reaction 90



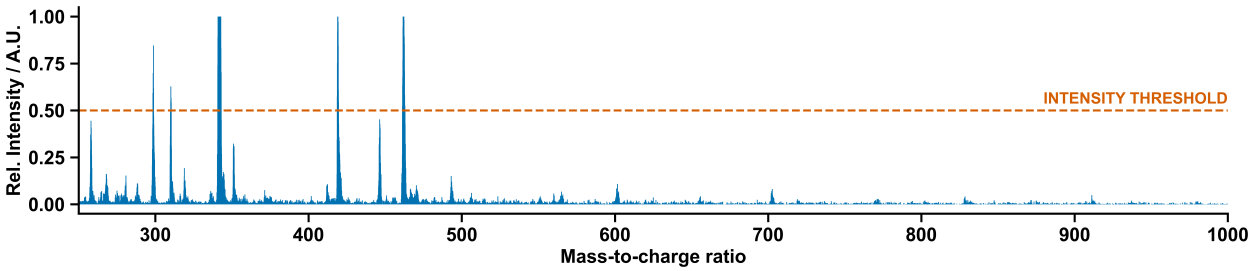
Scheme 74: Self-assembly of components 1, 15, with Iron(II) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 90.

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 labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 90. Decision motivations are also given.

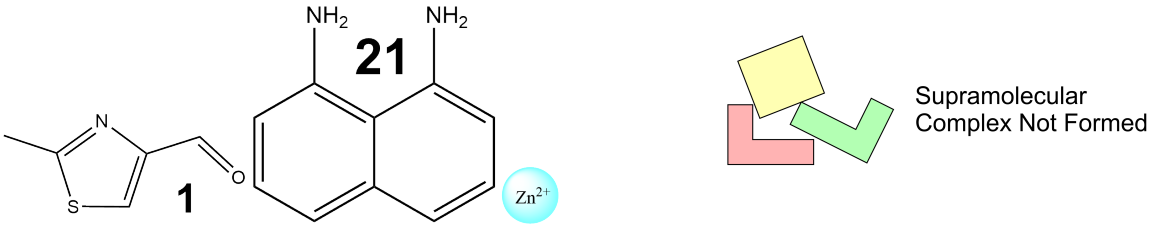


NMR Spectra 74: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 90.



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

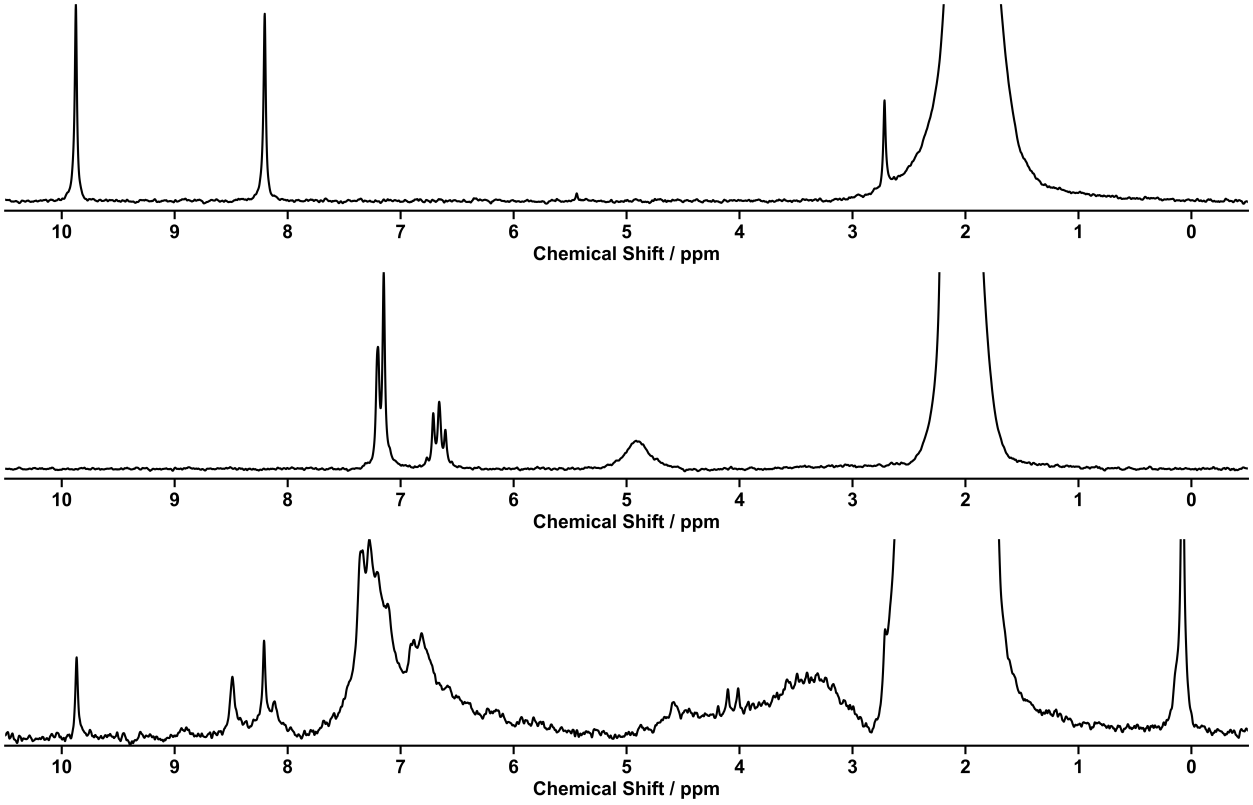
Reaction 91



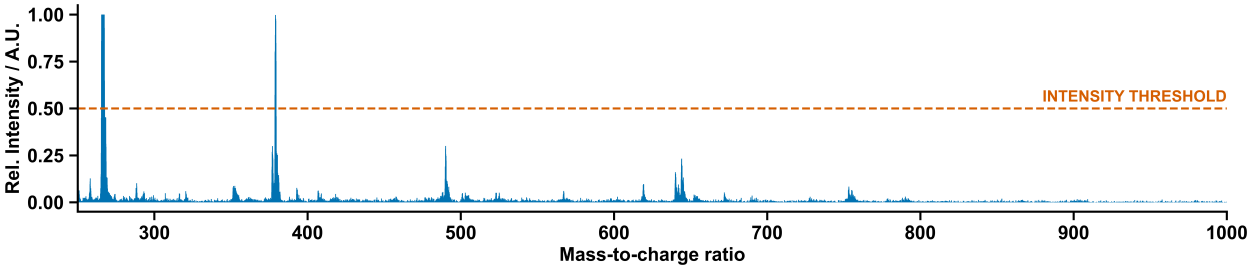
Scheme 75: Self-assembly of components 1, 21, with Zinc(II) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 91.

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 labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 91. Decision motivations are also given.

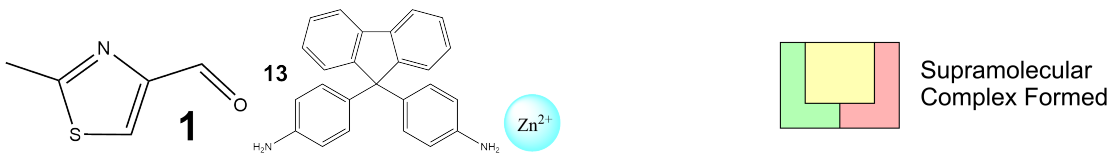


NMR Spectra 75: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 91.



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

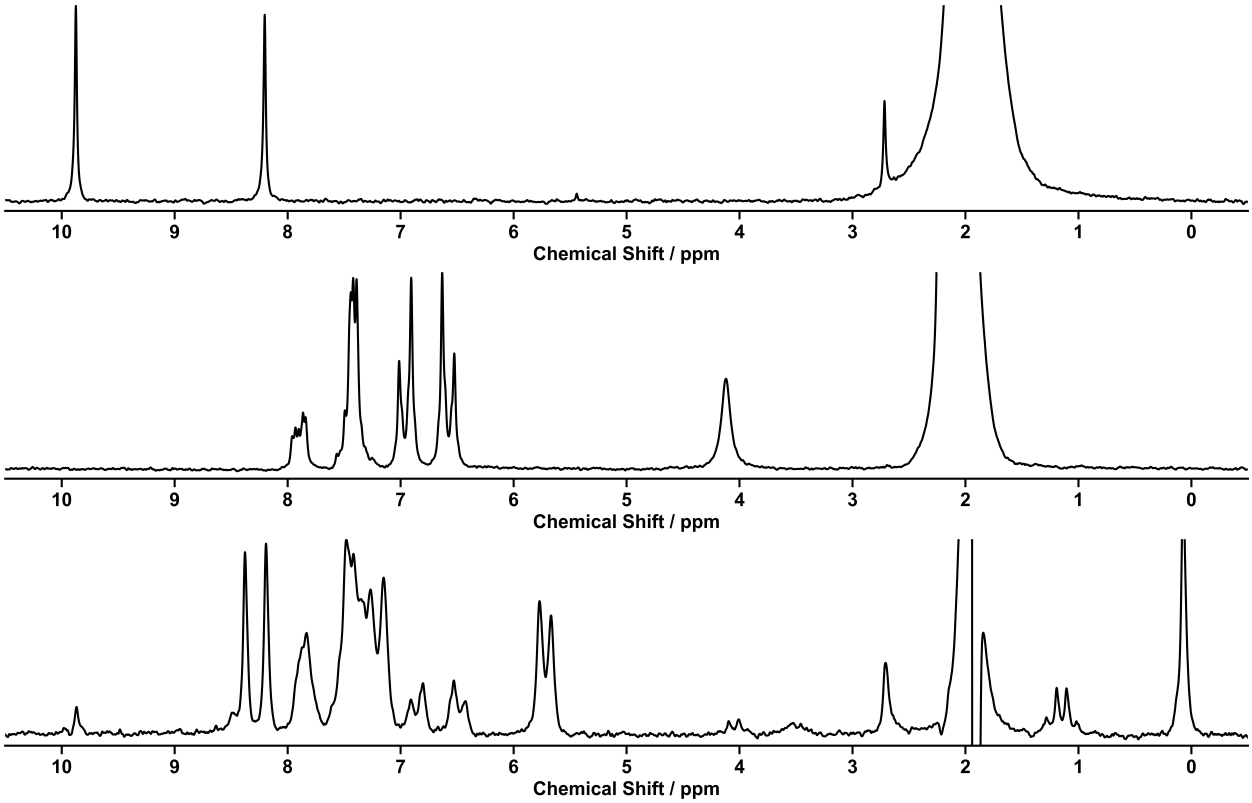
Reaction 92



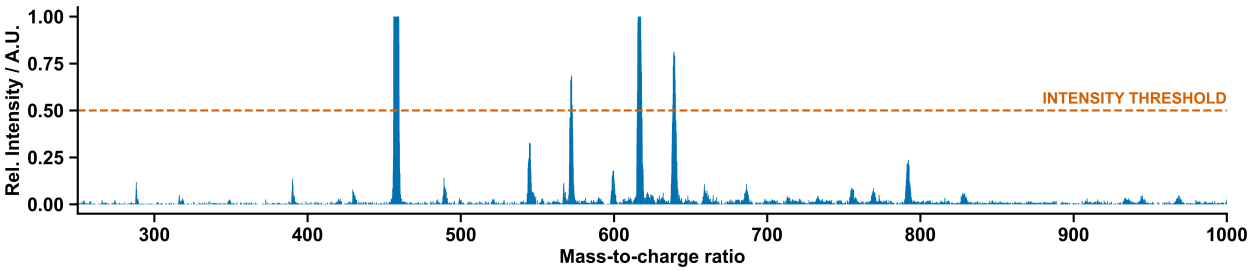
Scheme 76: Self-assembly of components 1, 13, with Zinc(II) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 92.

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

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

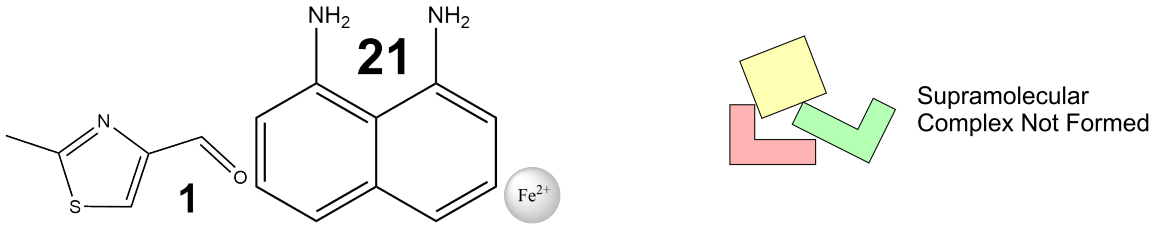


NMR Spectra 76: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 92.



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

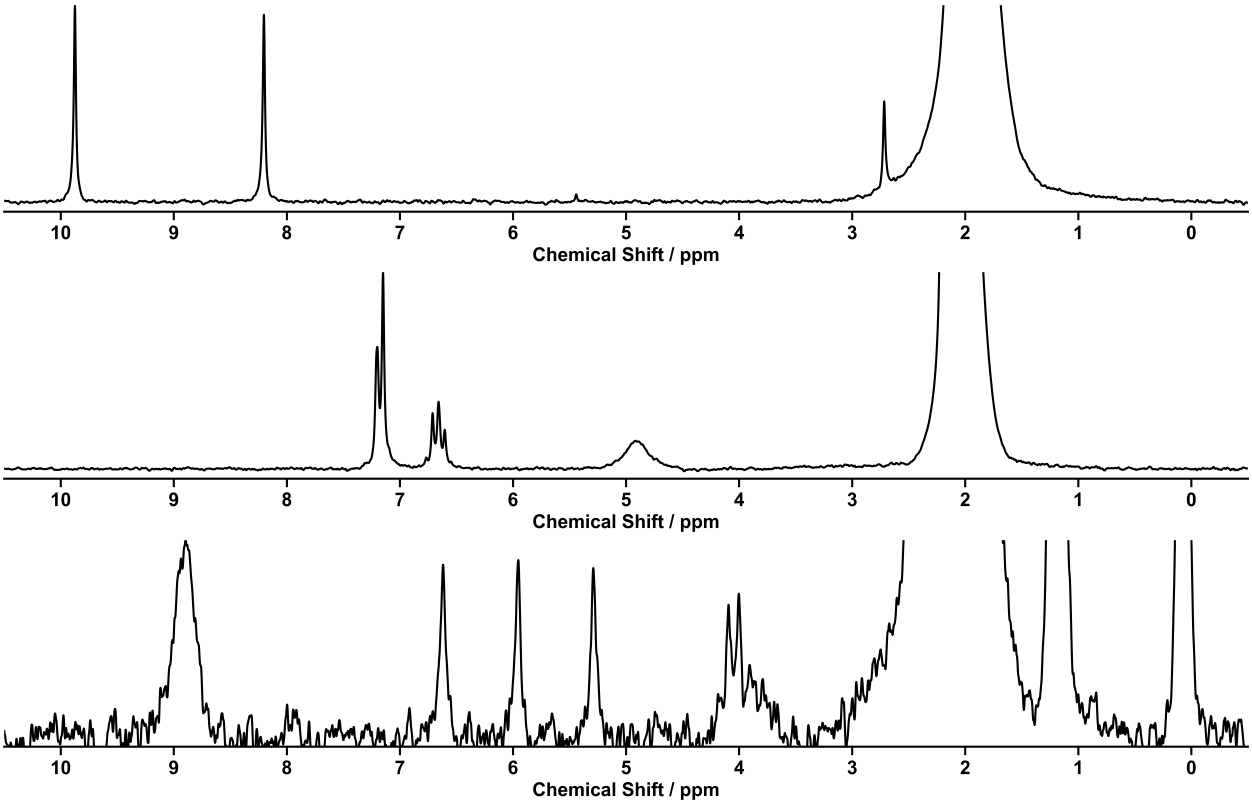
Reaction 93



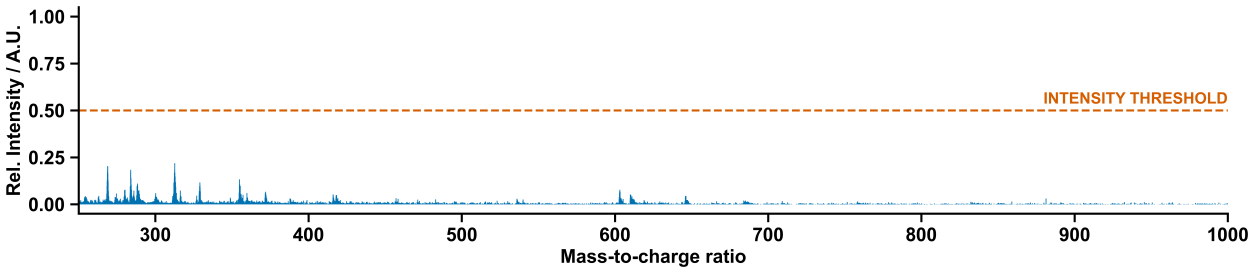
Scheme 77: Self-assembly of components 1, 21, with Iron(II) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 93.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: No reaction occured.	
	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 labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 93. Decision motivations are also given.

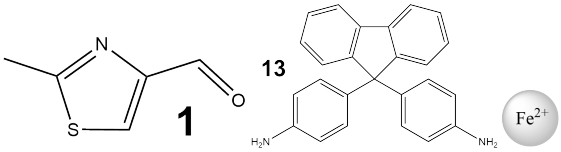


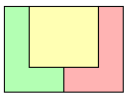
NMR Spectra 77: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 93.



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

Reaction 94



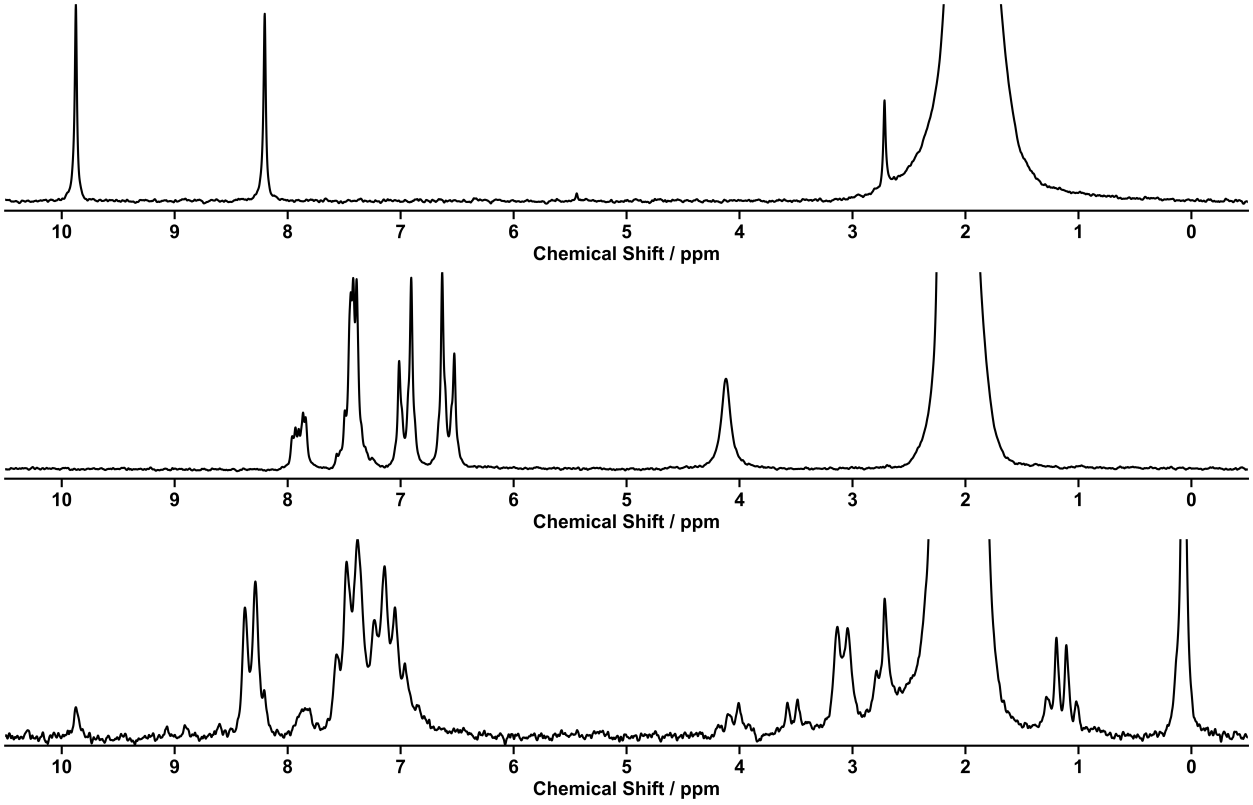


Supramolecular Complex Formed

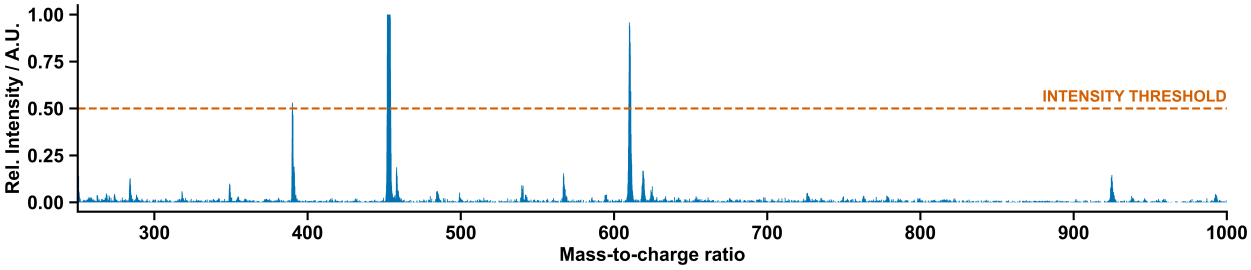
Scheme 78: Self-assembly of components 1, 13, with Iron(II) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 94.

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	
		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 78: Human labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 94. Decision motivations are also given.

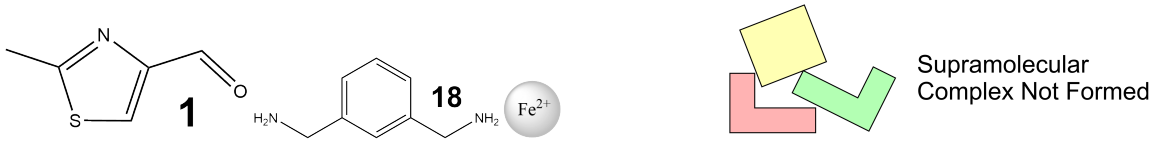


NMR Spectra 78: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 94.



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

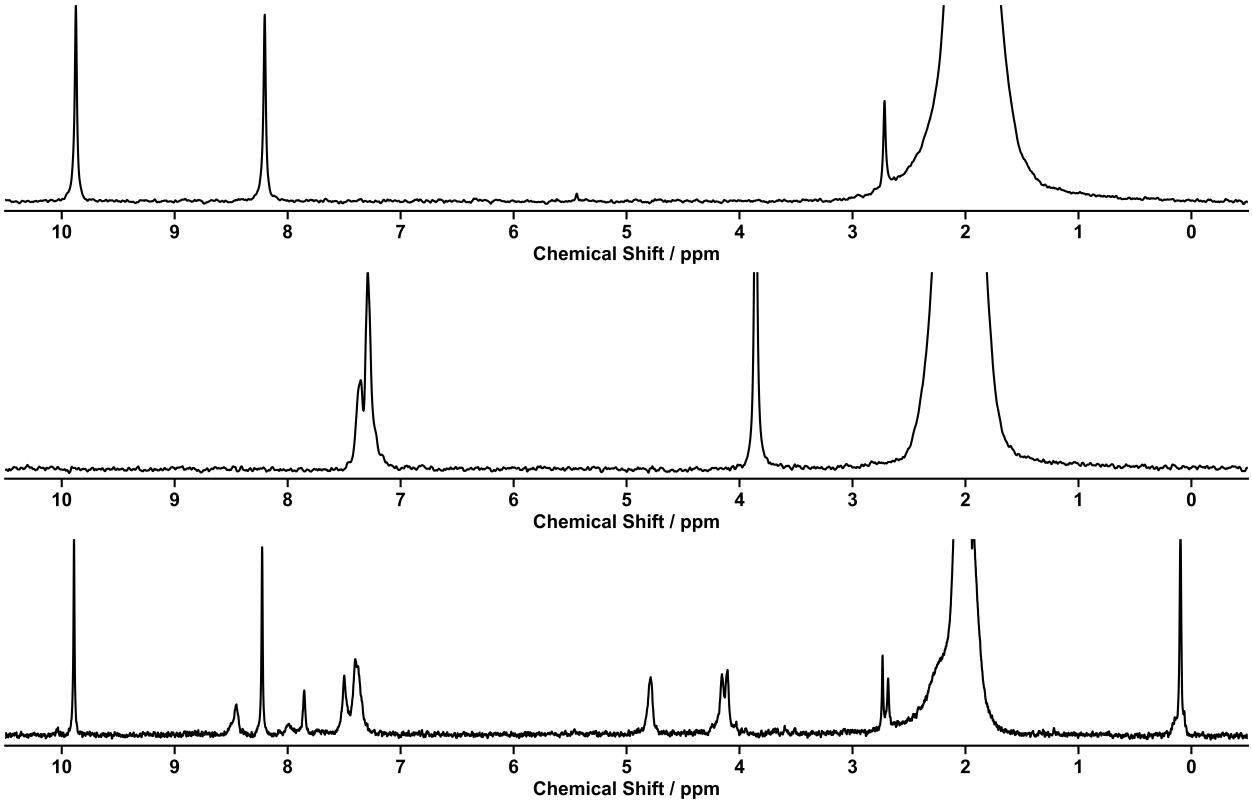
Reaction 96



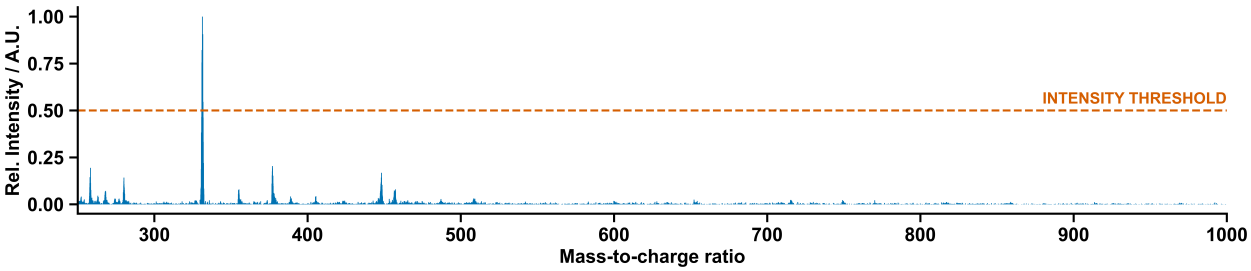
Scheme 79: Self-assembly of components 1, 18, with Iron(II) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 96.

<table>
<tr><td rowspan="2">Human Reaction Decision:
Failed</td><td>Human NMR Decision:
Failed</td><td colspan="2">NMR Spectra Category:
No reaction occured.</td></tr>
<tr><td>Human MS Decision:
Failed</td><td colspan="2">MS Spectra Category:
Reaction occurred, unknown product.</td></tr>
<tr><td rowspan="4">Decision Maker Reaction Decision:
N/A</td><td rowspan="2">Decision Maker NMR Decision:
N/A</td><td colspan="2">NMR Criteria 1:
N/A</td></tr>
<tr><td colspan="2">NMR Criteria 2:
N/A</td></tr>
<tr><td rowspan="2">Decision Maker MS Decision:
Pass</td><td>MS Criteria 1 and 2:
Pass</td><td>Number of predicted peaks found in MS spectra with appropriate intensity:
0</td></tr>
<tr><td>MS Criteria 3:
Pass</td><td>Number of counter-ions found:
0</td></tr>
</table>

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

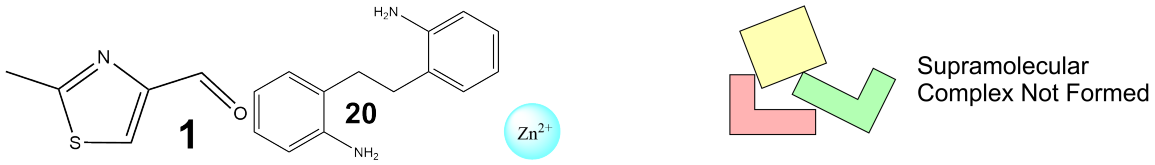


NMR Spectra 79: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 96.



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

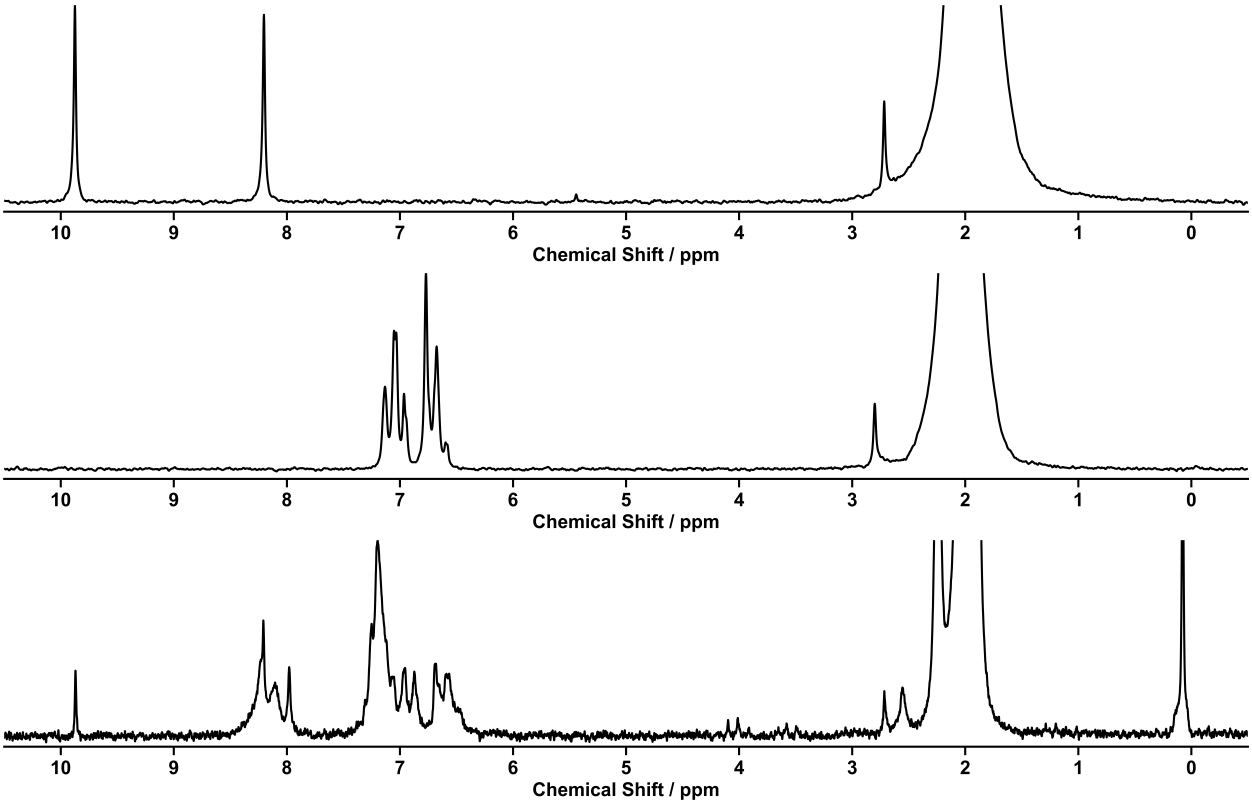
Reaction 97



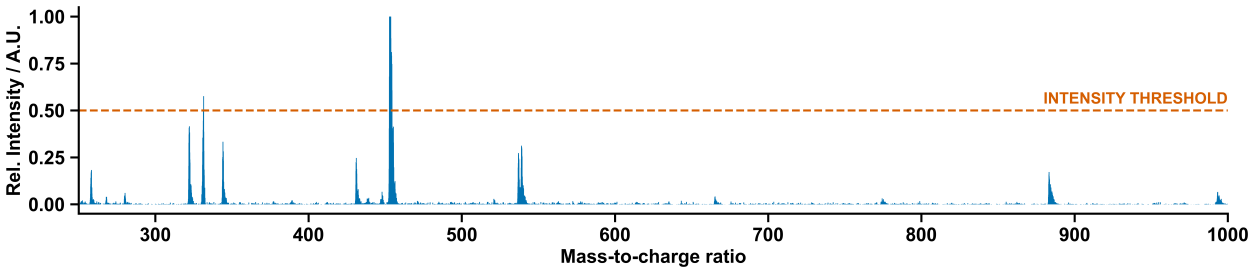
Scheme 80: Self-assembly of components 1, 20, with Zinc(II) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 97.

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 labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 97. Decision motivations are also given.

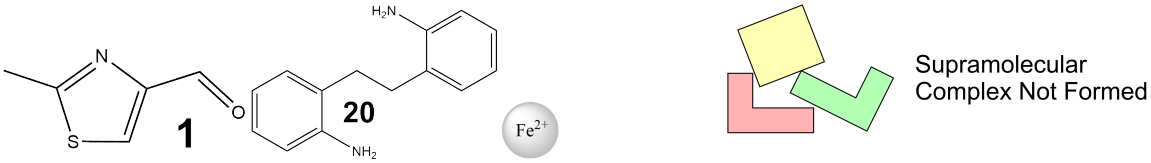


NMR Spectra 80: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 97.



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

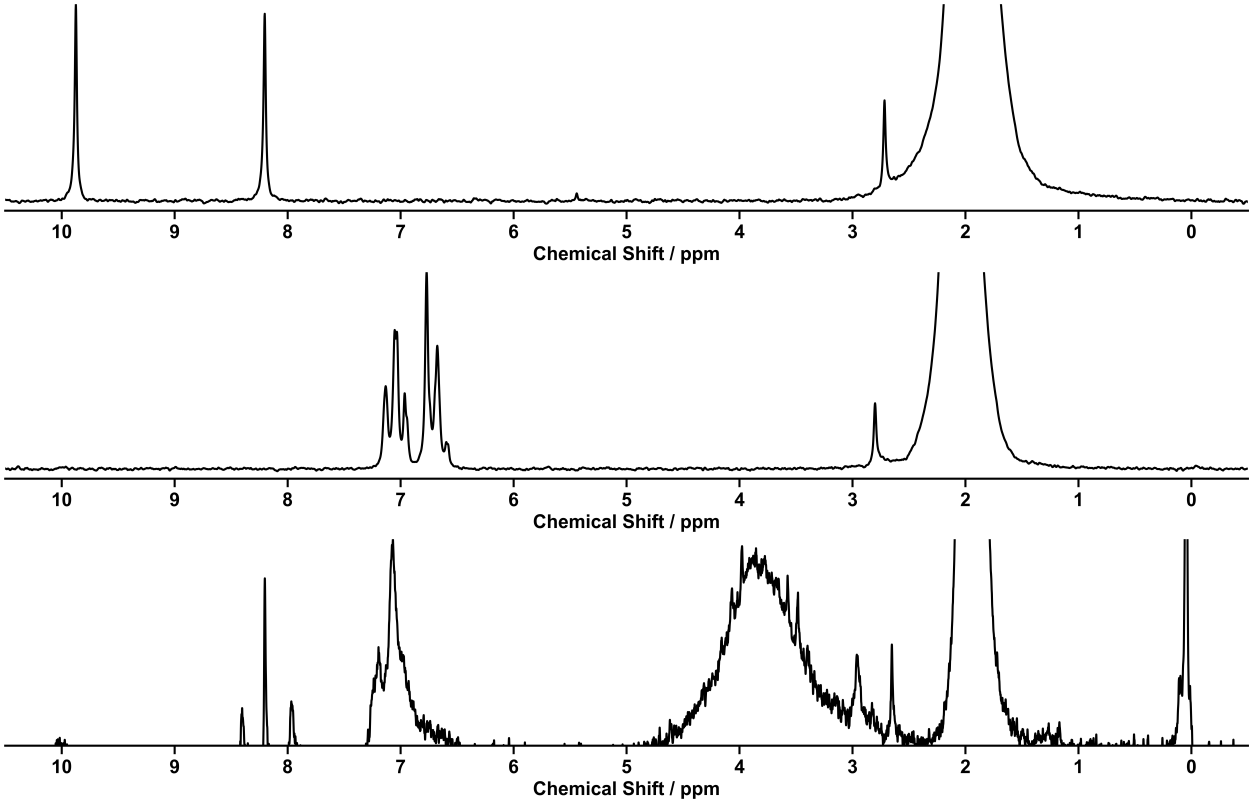
Reaction 98



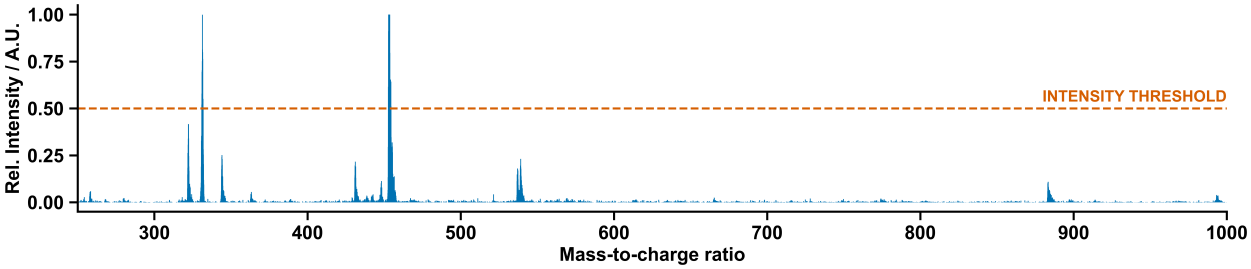
Scheme 81: Self-assembly of components 1, 20, with Iron(II) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 98.

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 labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 98. Decision motivations are also given.

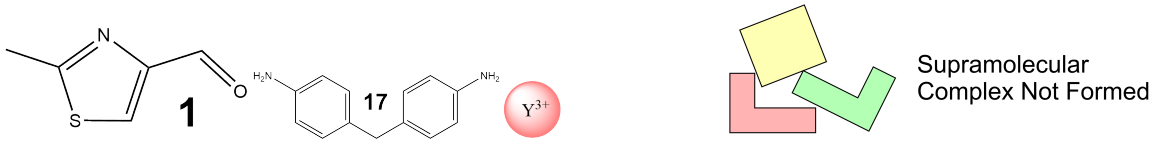


NMR Spectra 81: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 98.



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

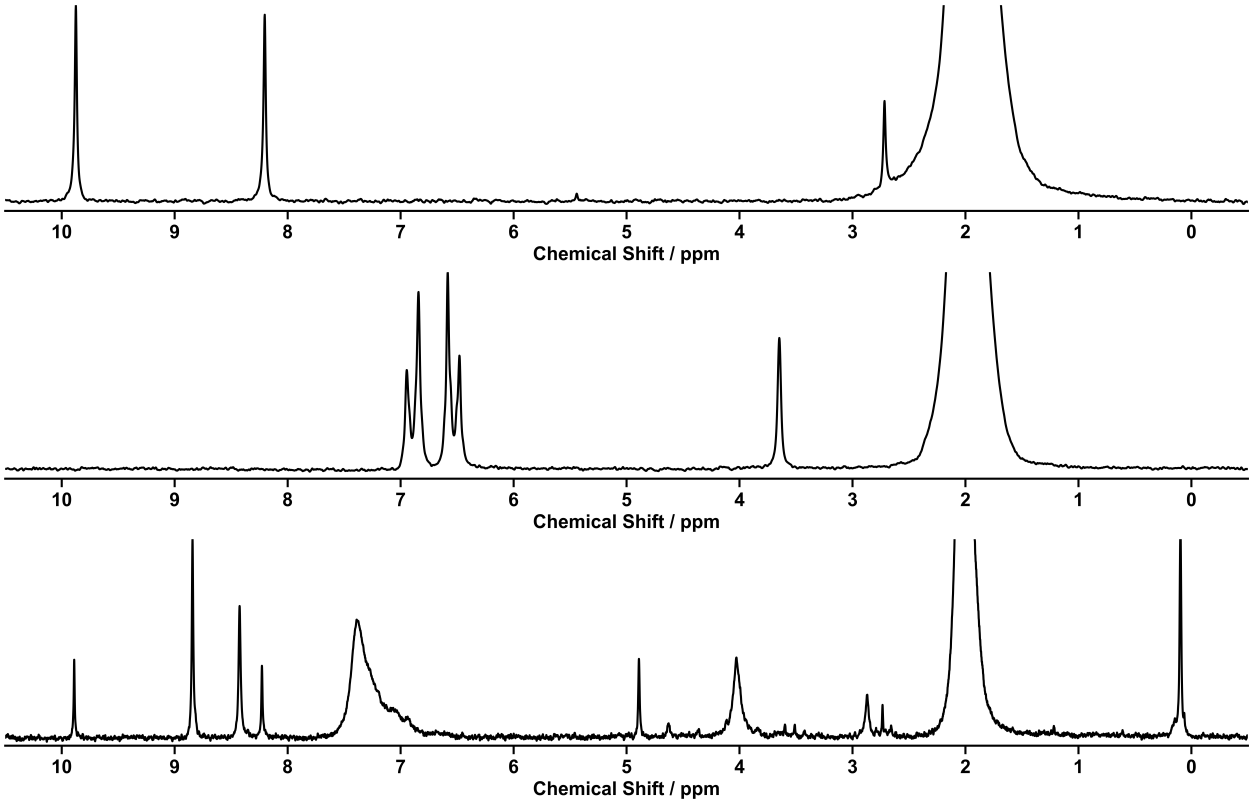
Reaction 99



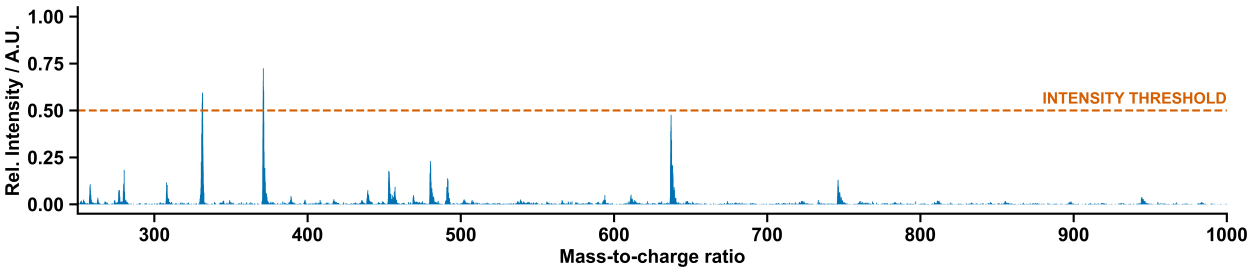
Scheme 82: Self-assembly of components 1, 17, with Yittrium(III) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 99.

<table>
<tr><td rowspan="2">Human Reaction Decision:
Failed</td><td>Human NMR Decision:
Failed</td><td colspan="2">NMR Spectra Category:
No reaction occured.</td></tr>
<tr><td>Human MS Decision:
Failed</td><td colspan="2">MS Spectra Category:
Reaction failed.</td></tr>
<tr><td rowspan="4">Decision Maker Reaction Decision:
N/A</td><td rowspan="2">Decision Maker NMR Decision:
N/A</td><td colspan="2">NMR Criteria 1:
N/A</td></tr>
<tr><td colspan="2">NMR Criteria 2:
N/A</td></tr>
<tr><td rowspan="2">Decision Maker MS Decision:
Pass</td><td>MS Criteria 1 and 2:
Pass</td><td>Number of predicted peaks found in MS spectra with appropriate intensity:
0</td></tr>
<tr><td>MS Criteria 3:
Pass</td><td>Number of counter-ions found:
0</td></tr>
</table>

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

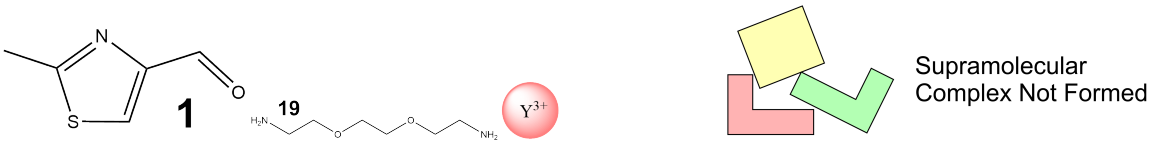


NMR Spectra 82: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 99.



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

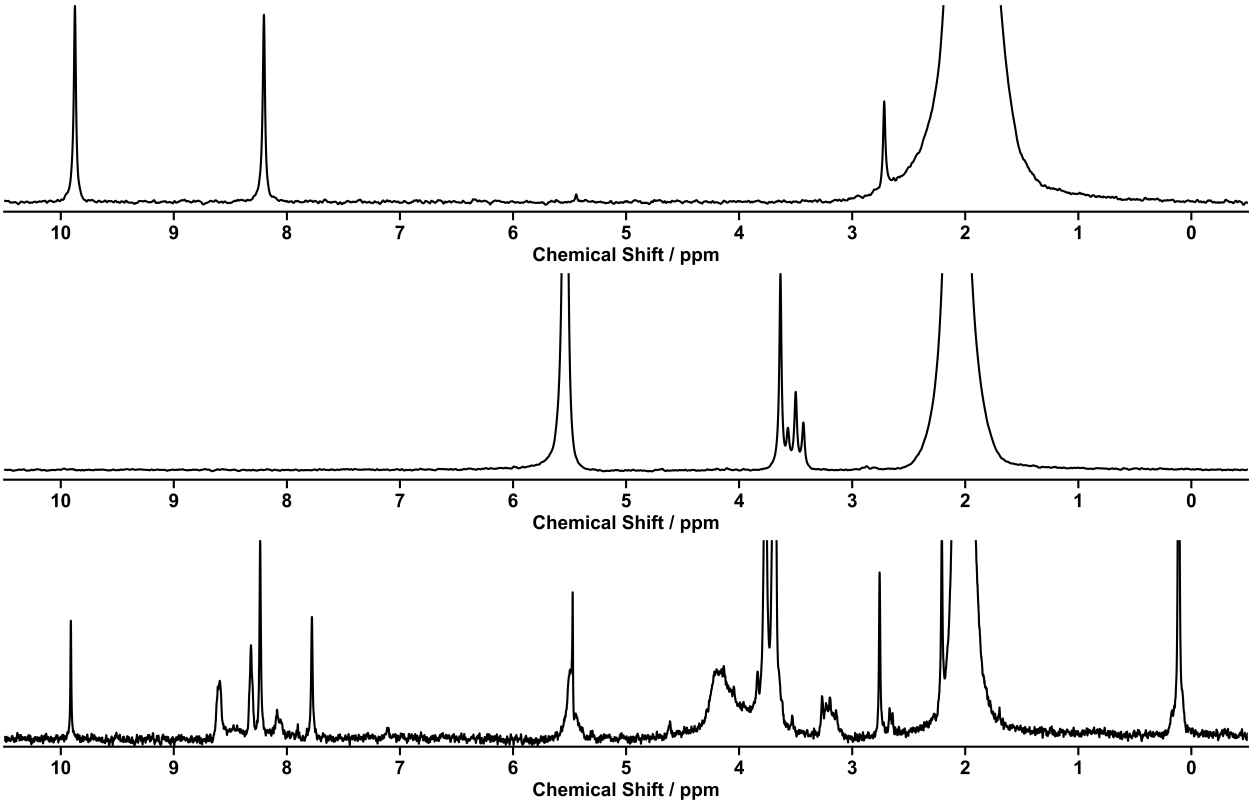
Reaction 100



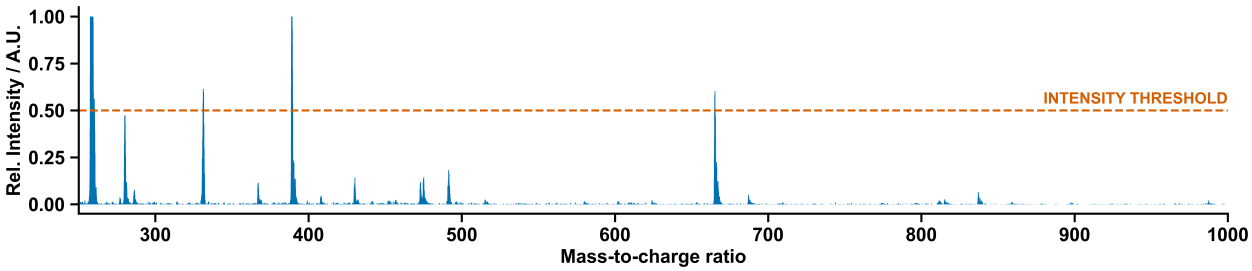
Scheme 83: Self-assembly of components 1, 19, with Yittrium(III) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 100.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: No reaction occured.	
	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 labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 100. Decision motivations are also given.

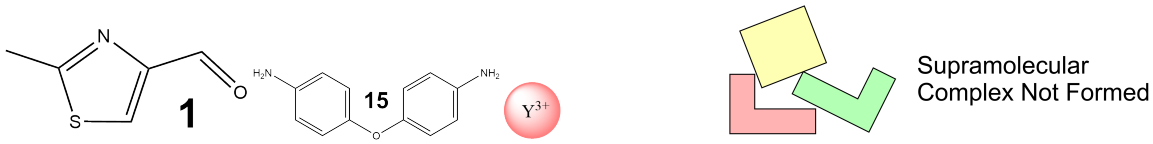


NMR Spectra 83: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 100.



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

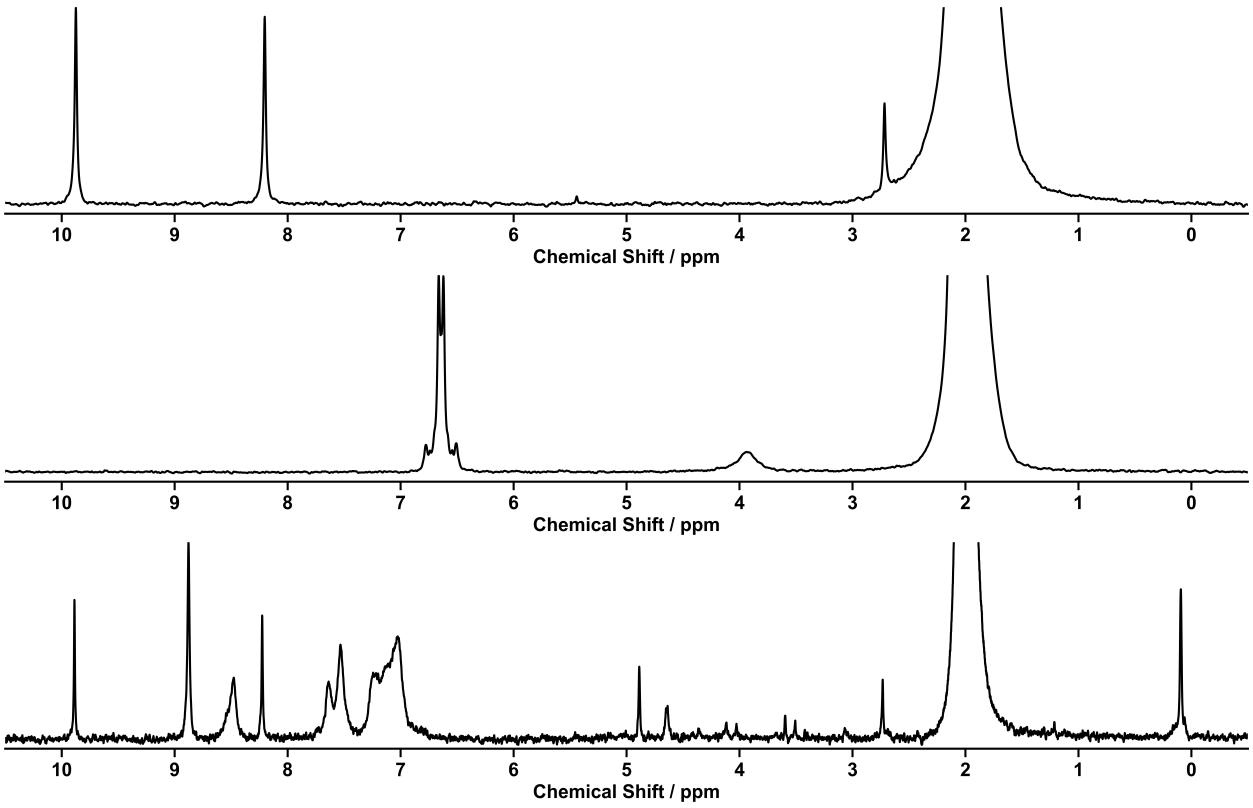
Reaction 101



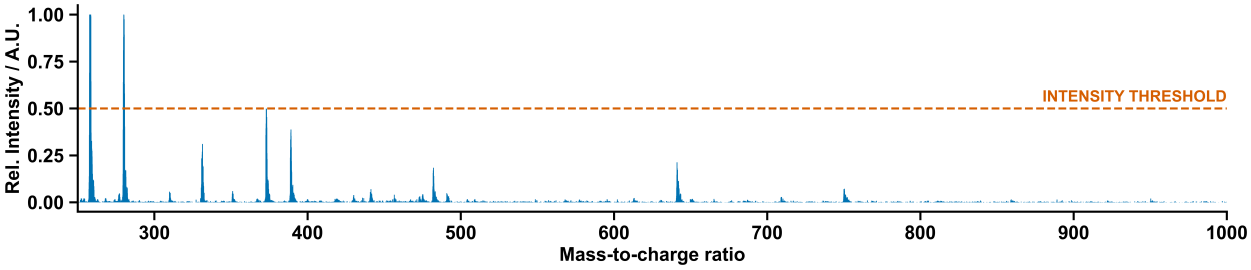
Scheme 84: Self-assembly of components 1, 15, with Yittrium(III) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 101.

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 labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 101. Decision motivations are also given.

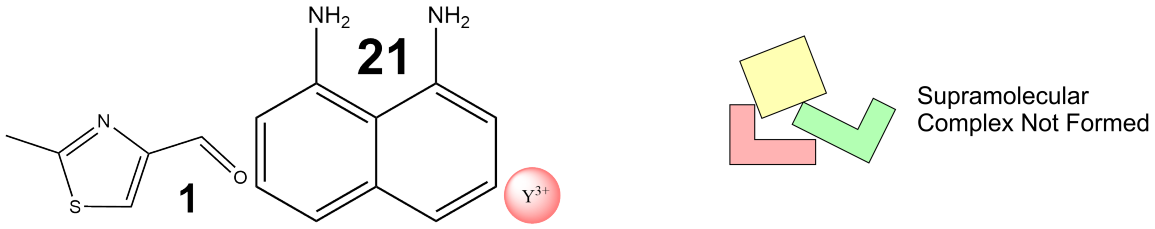


NMR Spectra 84: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 101.



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

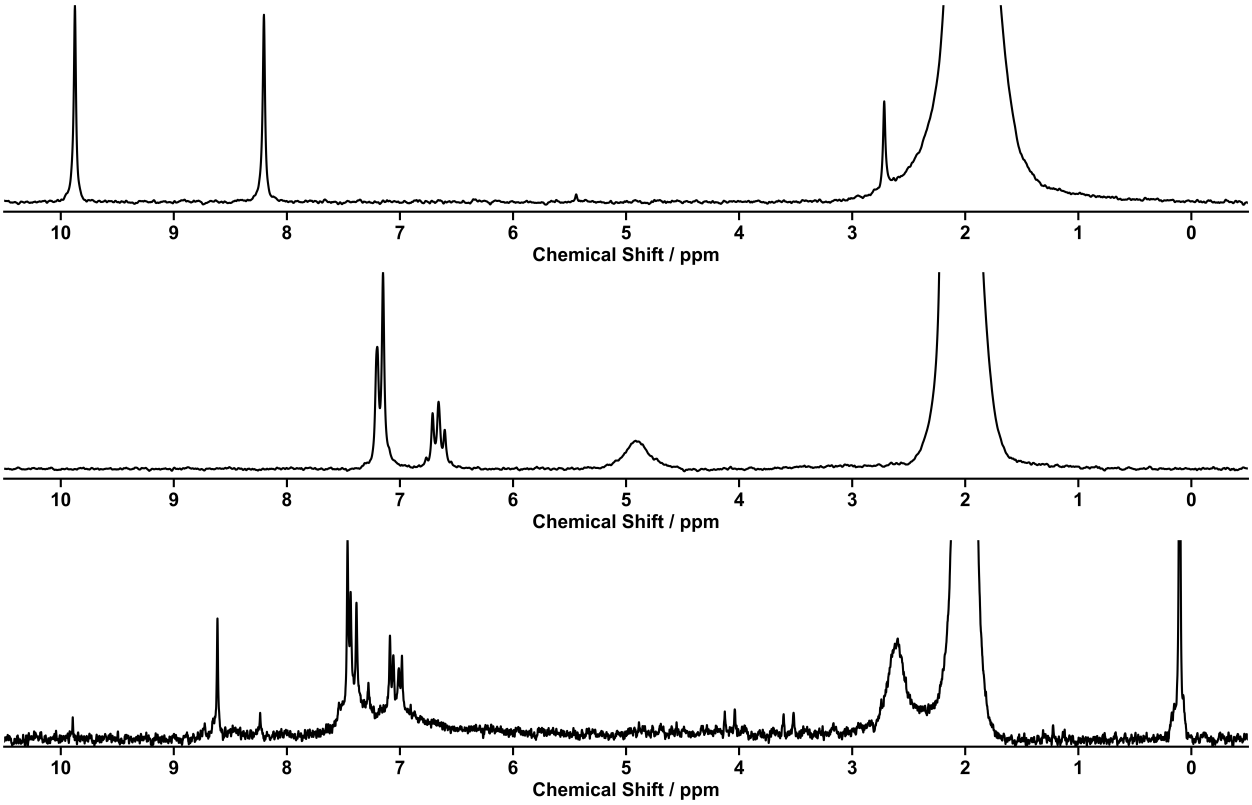
Reaction 102



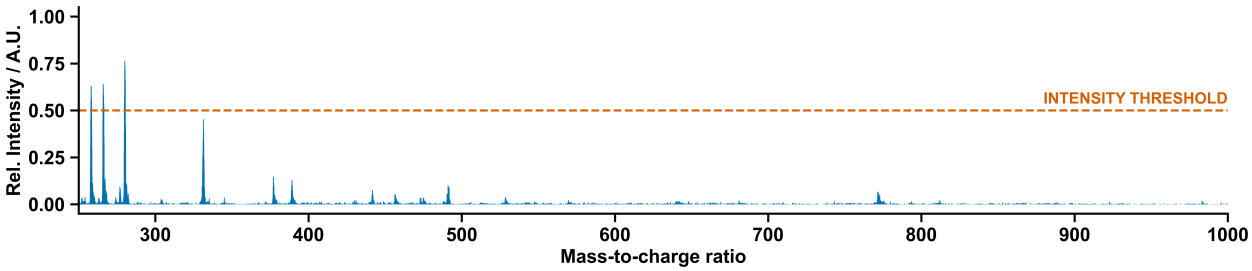
Scheme 85: Self-assembly of components 1, 21, with Yittrium(III) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 102.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: No reaction occured.	
	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 labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 102. Decision motivations are also given.

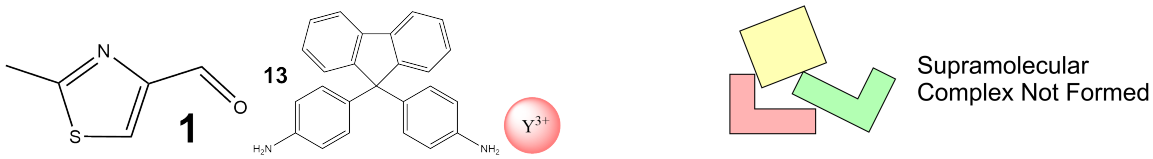


NMR Spectra 85: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 102.



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

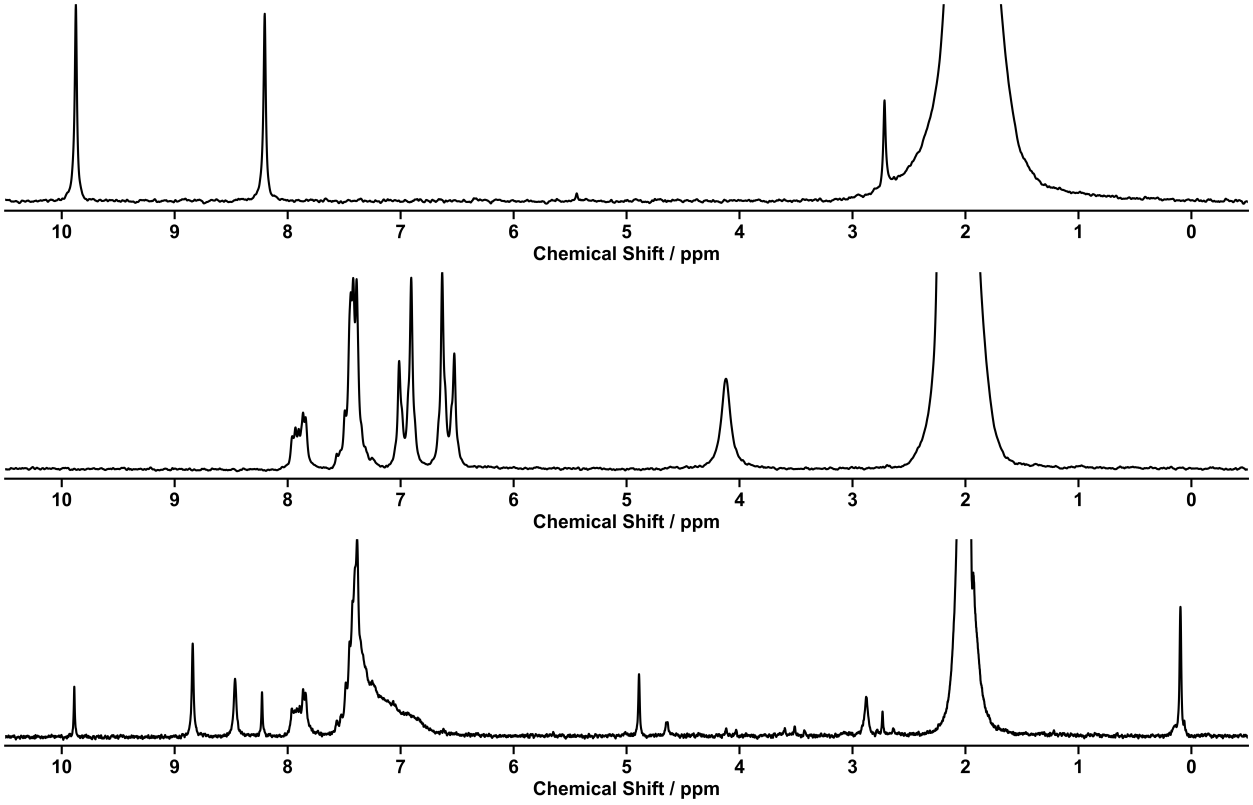
Reaction 103



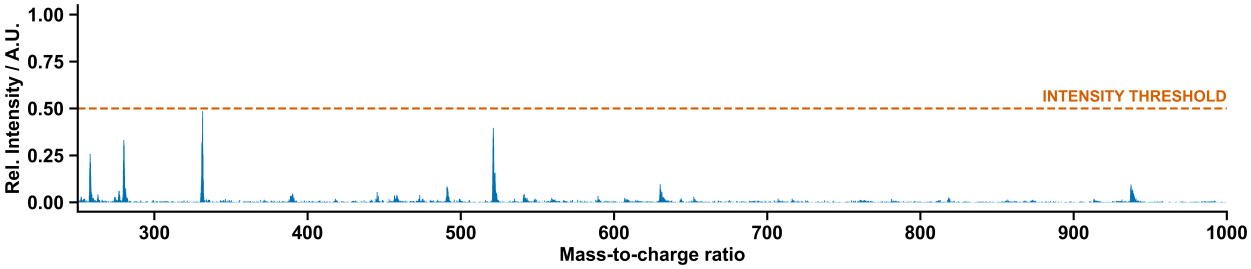
Scheme 86: Self-assembly of components 1, 13, with Yittrium(III) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 103.

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 labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 103. Decision motivations are also given.

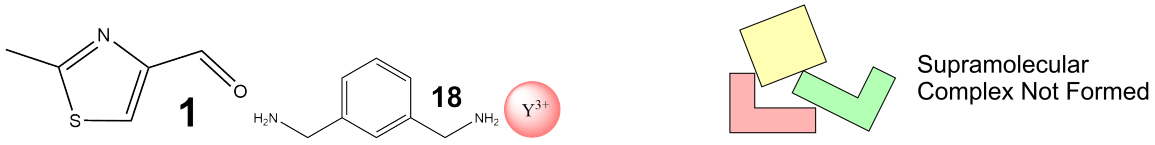


NMR Spectra 86: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 103.



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

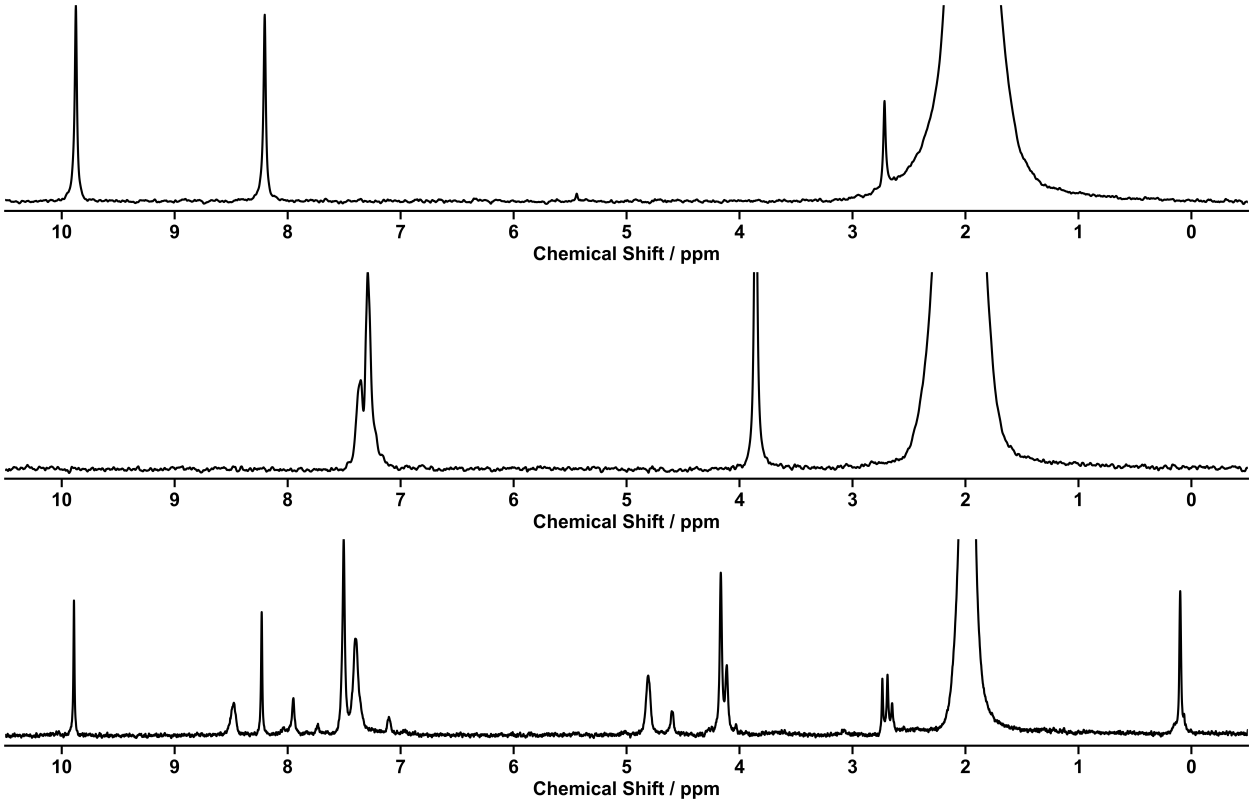
Reaction 104



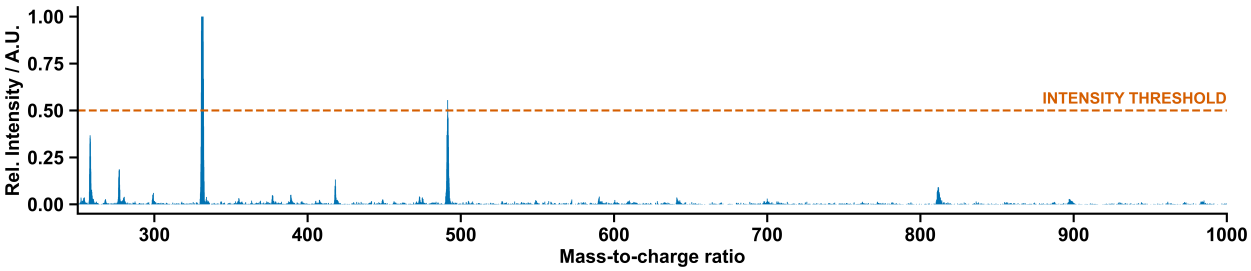
Scheme 87: Self-assembly of components 1, 18, with Yittrium(III) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 104.

<table>
<tr><td rowspan="2">Human Reaction Decision:
Failed</td><td>Human NMR Decision:
Failed</td><td colspan="2">NMR Spectra Category:
No reaction occured.</td></tr>
<tr><td>Human MS Decision:
Failed</td><td colspan="2">MS Spectra Category:
Reaction occurred, unknown product.</td></tr>
<tr><td rowspan="4">Decision Maker Reaction Decision:
N/A</td><td rowspan="2">Decision Maker NMR Decision:
N/A</td><td colspan="2">NMR Criteria 1:
N/A</td></tr>
<tr><td colspan="2">NMR Criteria 2:
N/A</td></tr>
<tr><td rowspan="2">Decision Maker MS Decision:
Pass</td><td>MS Criteria 1 and 2:
Pass</td><td>Number of predicted peaks found in MS spectra with appropriate intensity:
1</td></tr>
<tr><td>MS Criteria 3:
Pass</td><td>Number of counter-ions found:
1</td></tr>
</table>

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

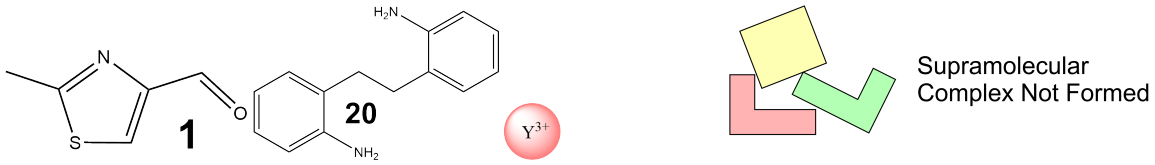


NMR Spectra 87: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 104.



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

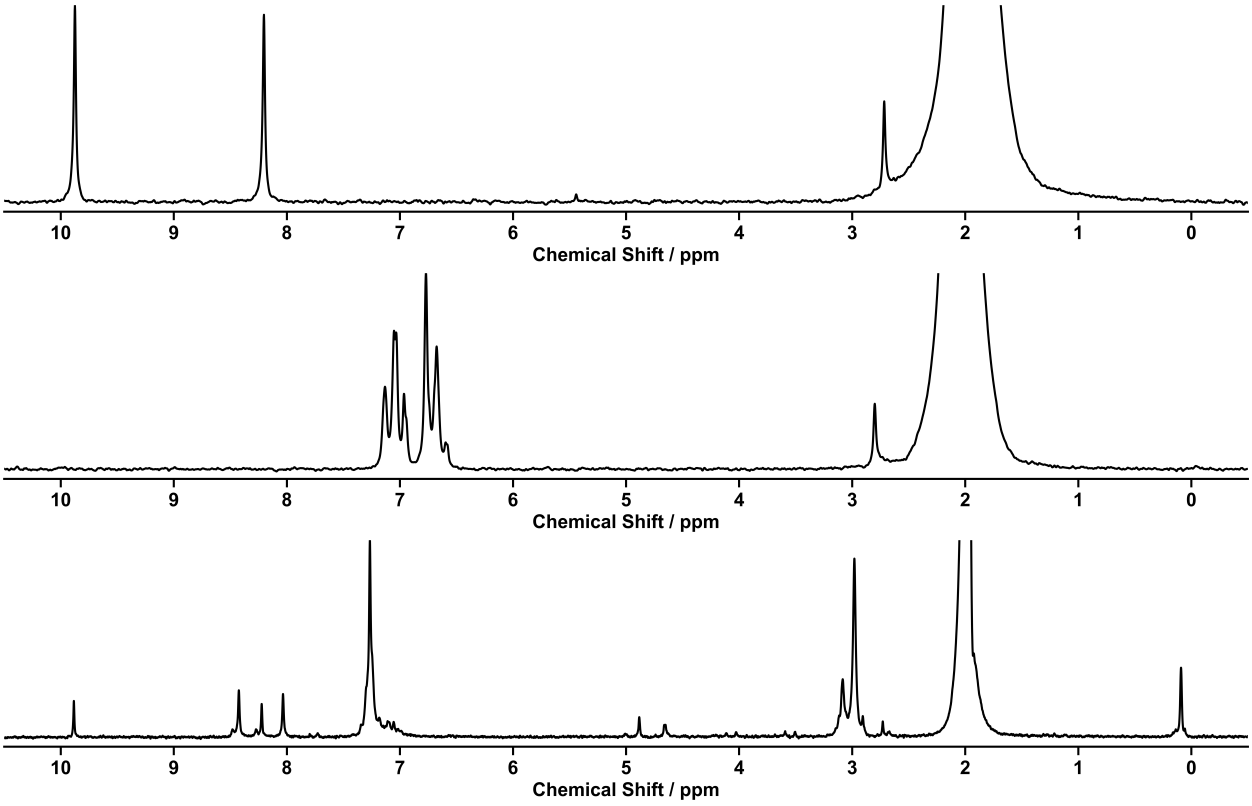
Reaction 105



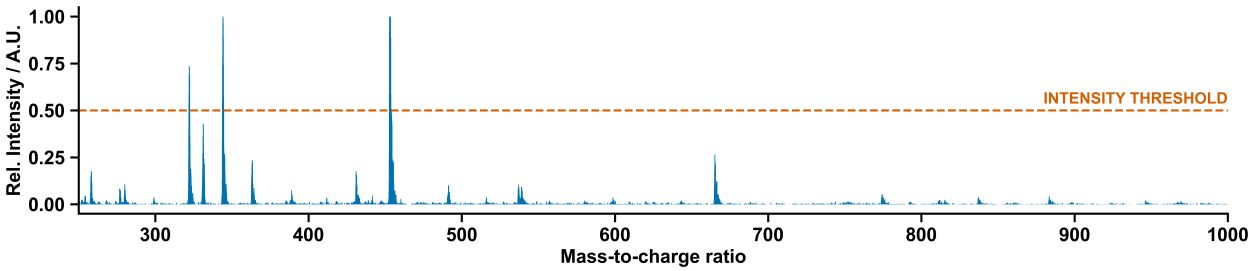
Scheme 88: Self-assembly of components 1, 20, with Yittrium(III) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 105.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: No reaction occured.	
	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 labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 105. Decision motivations are also given.

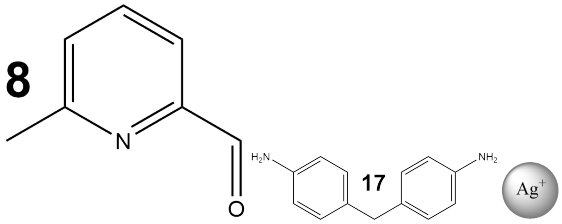


NMR Spectra 88: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 105.



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

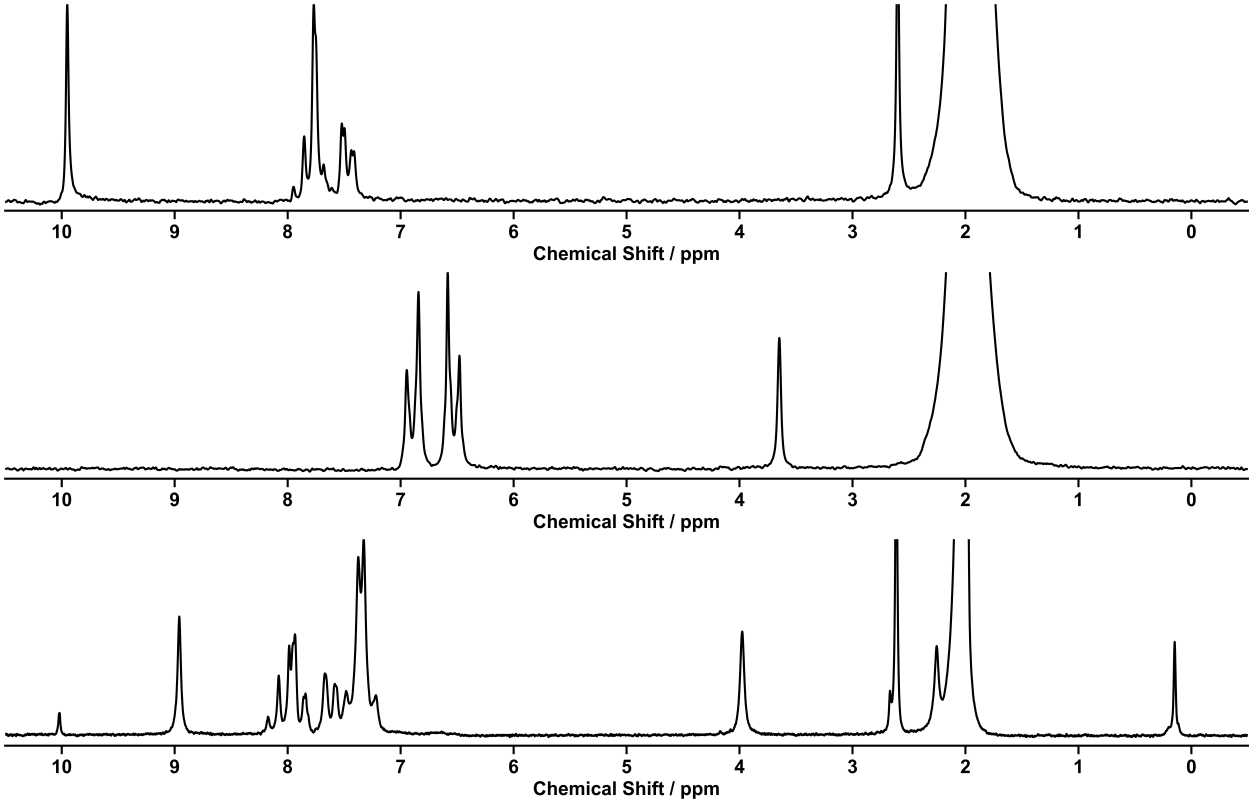
Reaction 106



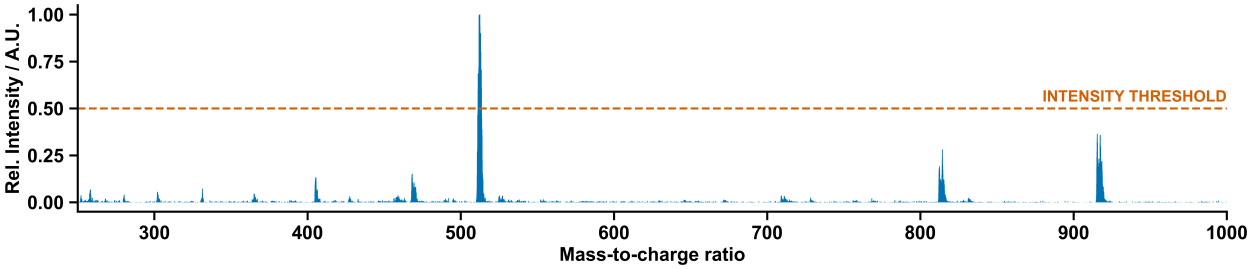
Scheme 89: Self-assembly of components 8, 17, with Silver(I) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 106.

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 labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 106. Decision motivations are also given.

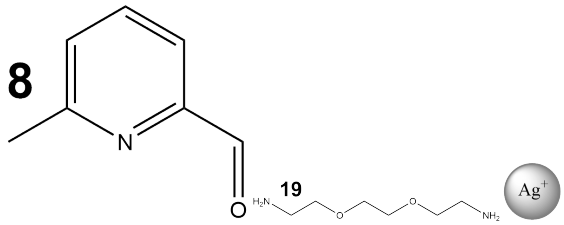


NMR Spectra 89: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 106.



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

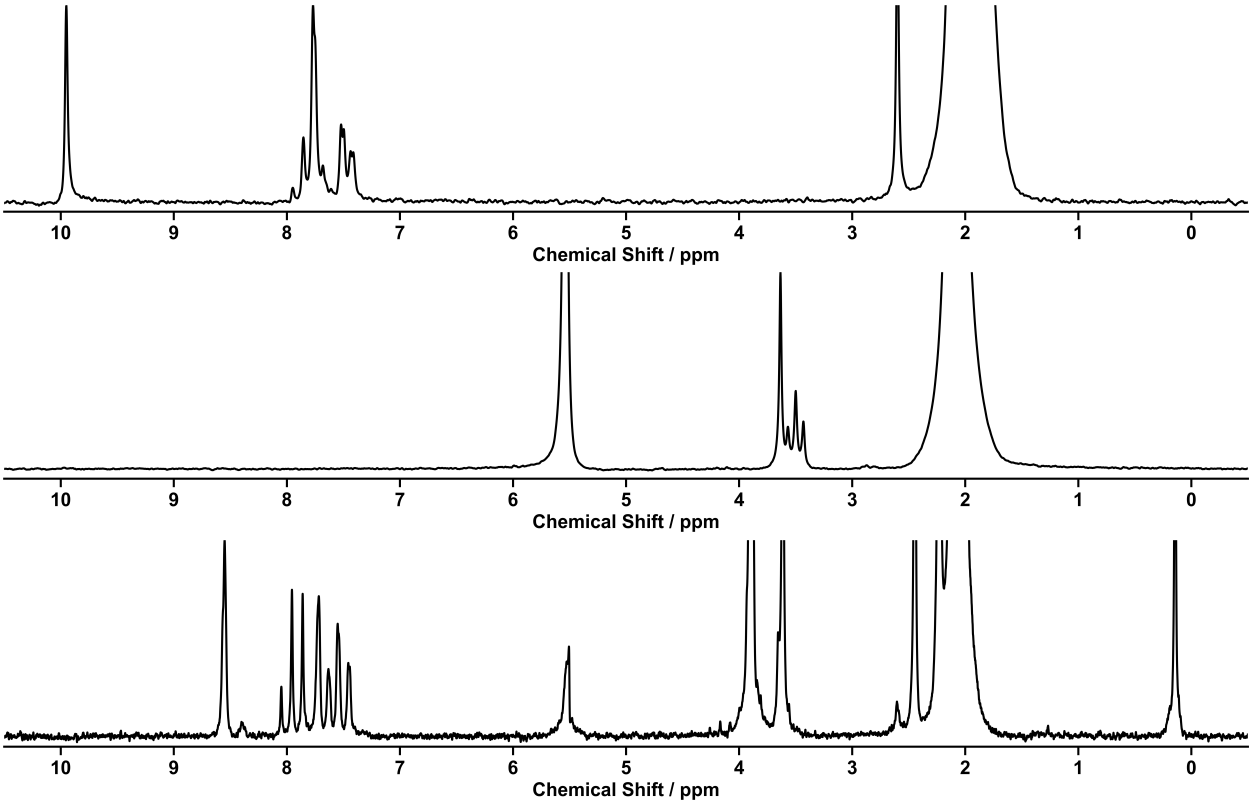
Reaction 107



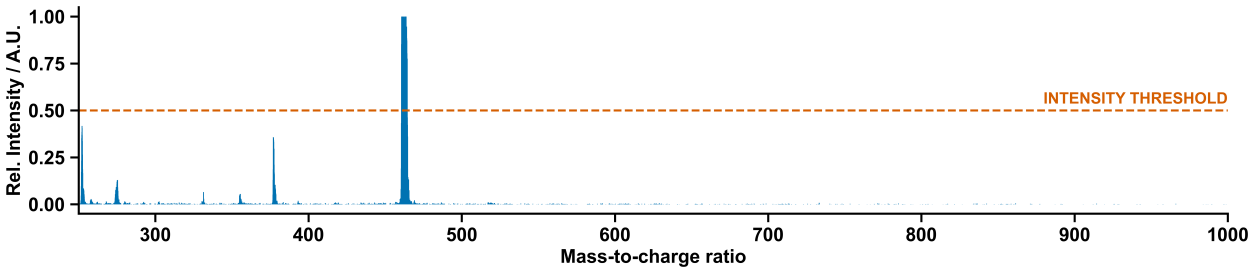
Scheme 90: Self-assembly of components 8, 19, with Silver(I) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 107.

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 labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 107. Decision motivations are also given.

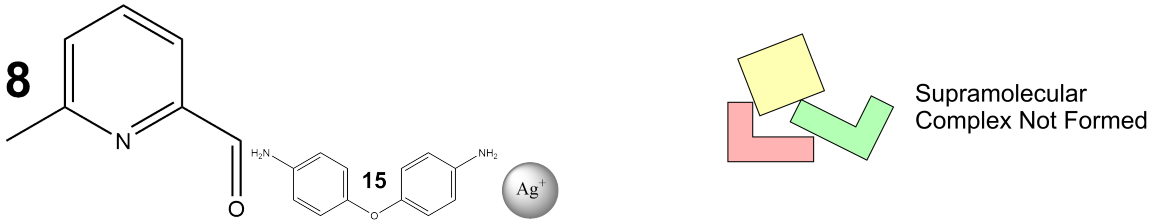


NMR Spectra 90: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 107.



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

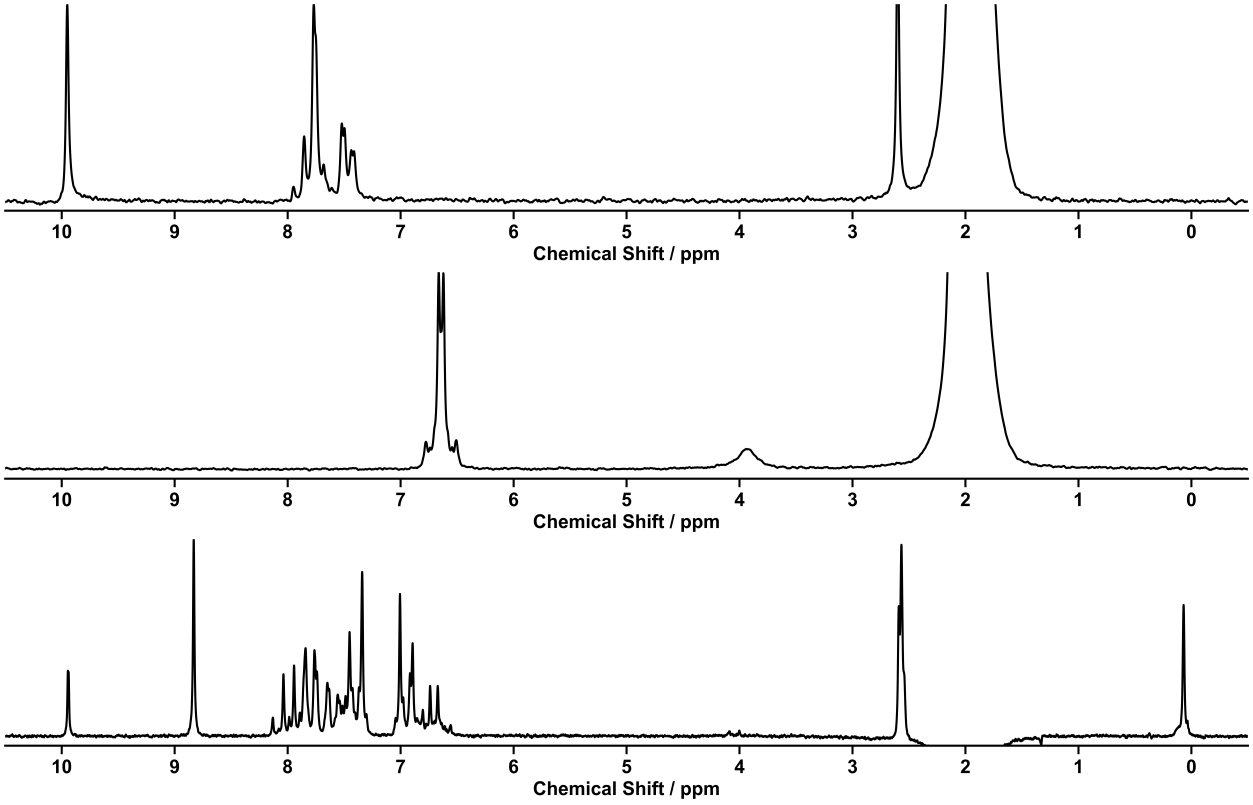
Reaction 108



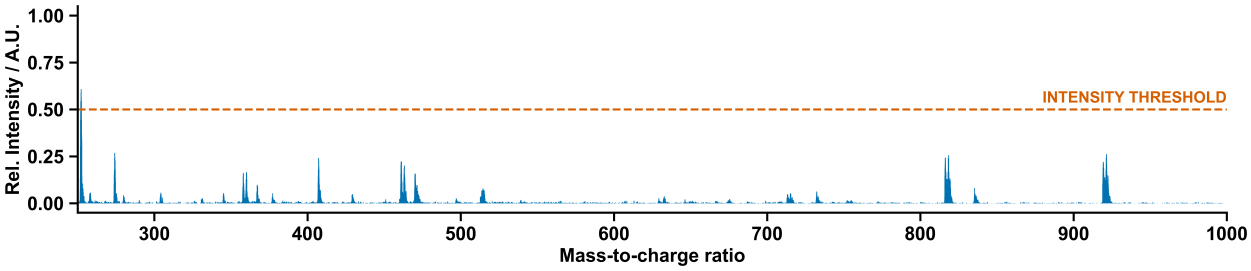
Scheme 91: Self-assembly of components 8, 15, with Silver(I) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 108.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: No reaction occured.	
	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 labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 108. Decision motivations are also given.

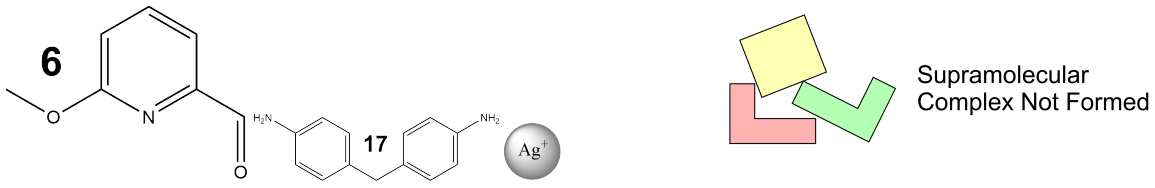


NMR Spectra 91: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 108.



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

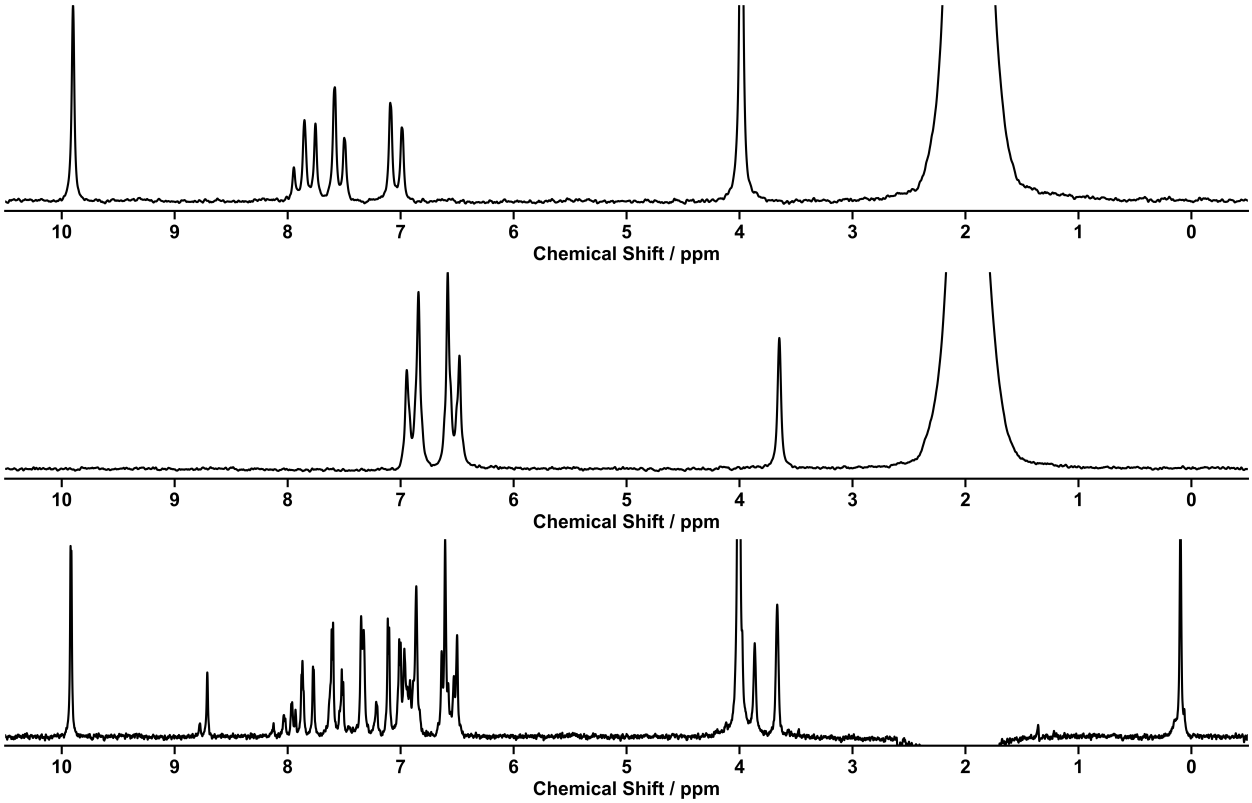
Reaction 109



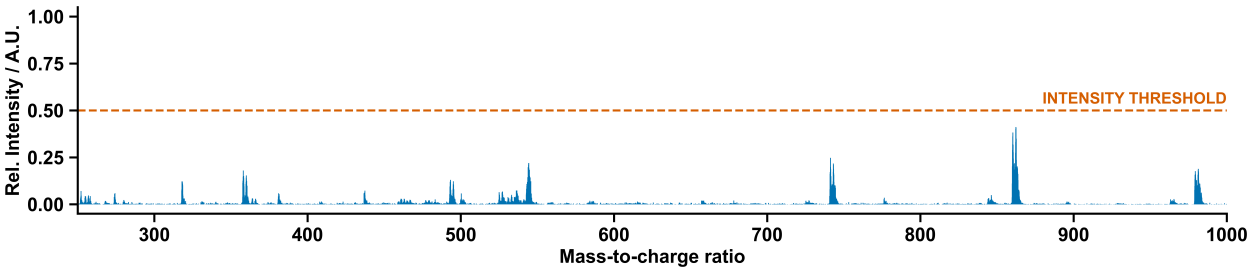
Scheme 92: Self-assembly of components 6, 17, with Silver(I) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 109.

<table>
<tr><td rowspan="2">Human Reaction Decision:
Failed</td><td>Human NMR Decision:
Failed</td><td colspan="2">NMR Spectra Category:
No reaction occured.</td></tr>
<tr><td>Human MS Decision:
Failed</td><td colspan="2">MS Spectra Category:
Reaction failed.</td></tr>
<tr><td rowspan="4">Decision Maker Reaction Decision:
N/A</td><td rowspan="2">Decision Maker NMR Decision:
N/A</td><td colspan="2">NMR Criteria 1:
N/A</td></tr>
<tr><td colspan="2">NMR Criteria 2:
N/A</td></tr>
<tr><td rowspan="2">Decision Maker MS Decision:
Pass</td><td>MS Criteria 1 and 2:
Pass</td><td>Number of predicted peaks found in MS spectra with appropriate intensity:
0</td></tr>
<tr><td>MS Criteria 3:
Pass</td><td>Number of counter-ions found:
0</td></tr>
</table>

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

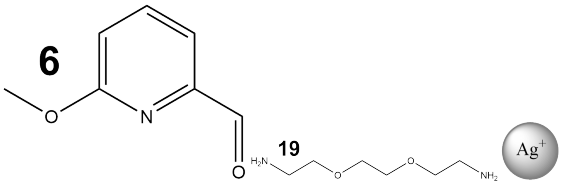


NMR Spectra 92: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 109.



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

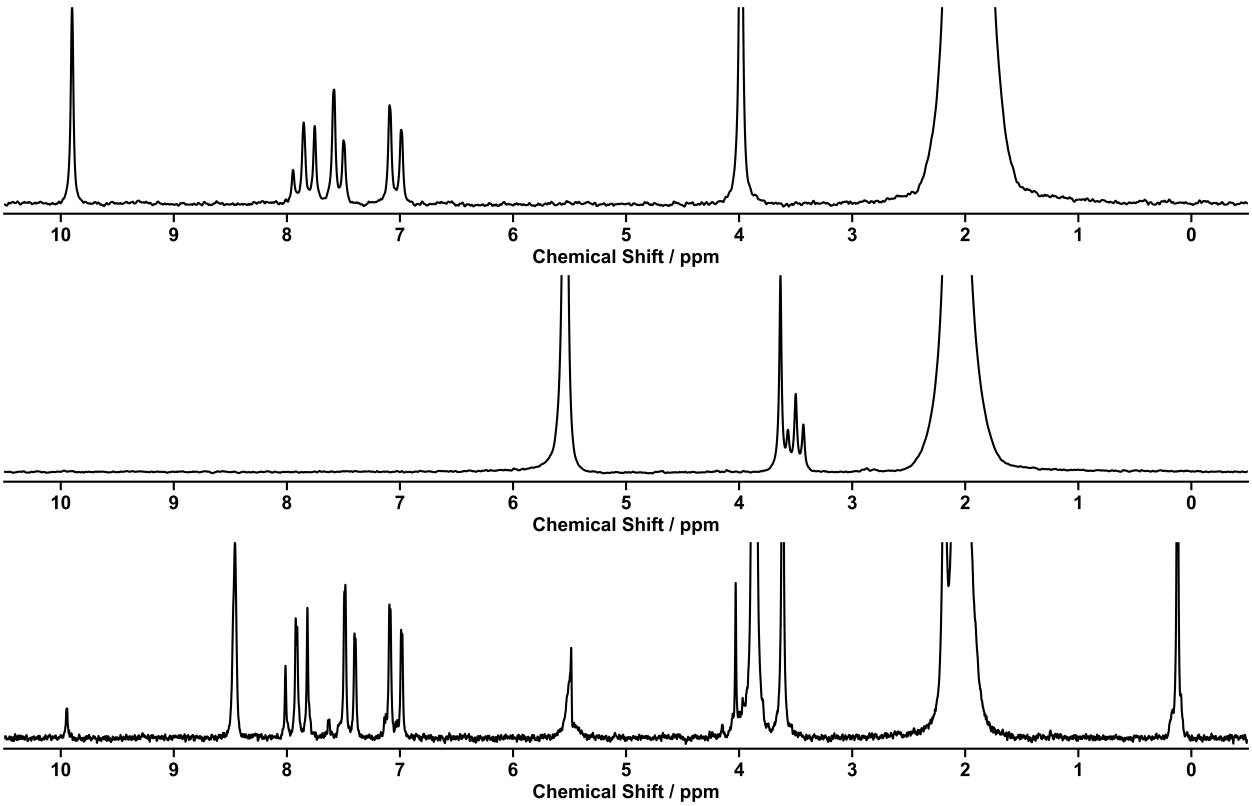
Reaction 110



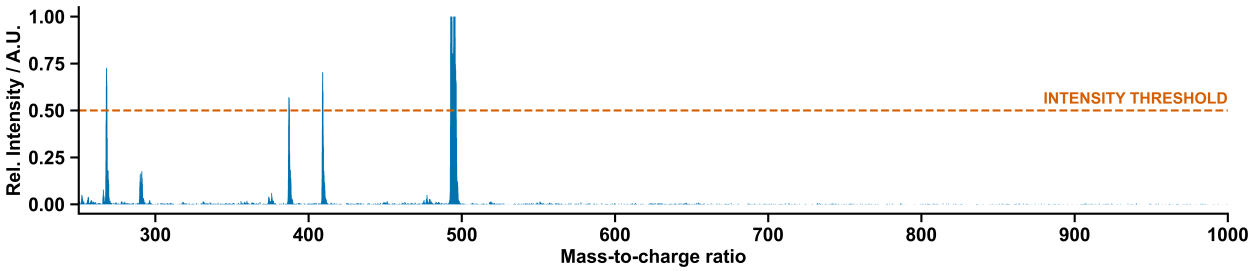
Scheme 93: Self-assembly of components 6, 19, with Silver(I) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 110.

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 labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 110. Decision motivations are also given.

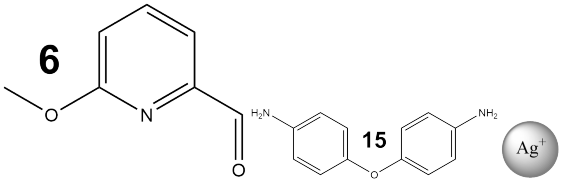


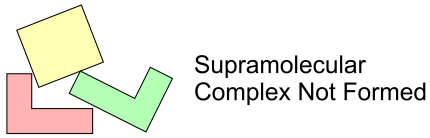
NMR Spectra 93: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 110.



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

Reaction 111

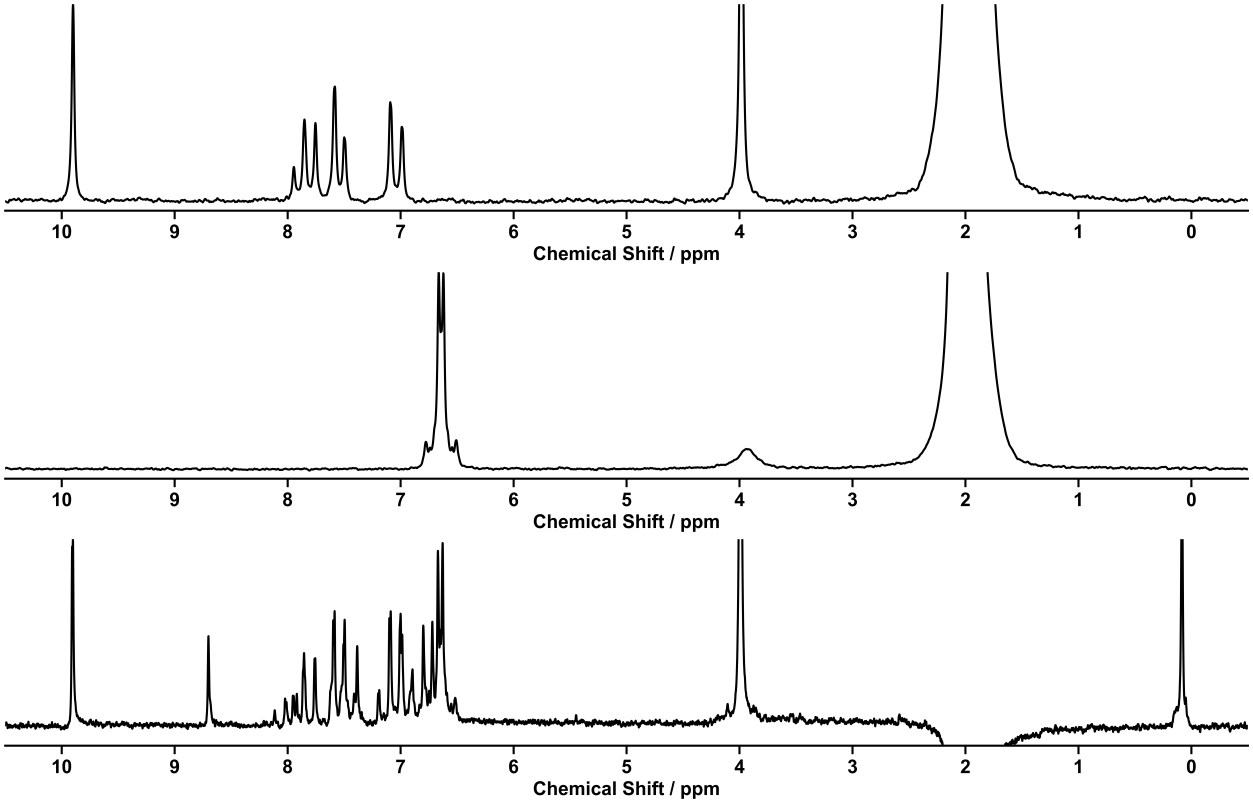




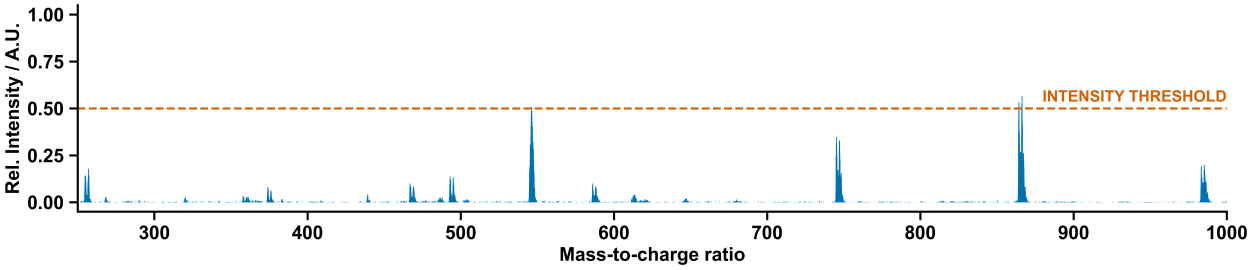
Scheme 94: Self-assembly of components 6, 15, with Silver(I) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 111.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: No reaction occured.	
	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 labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 111. Decision motivations are also given.

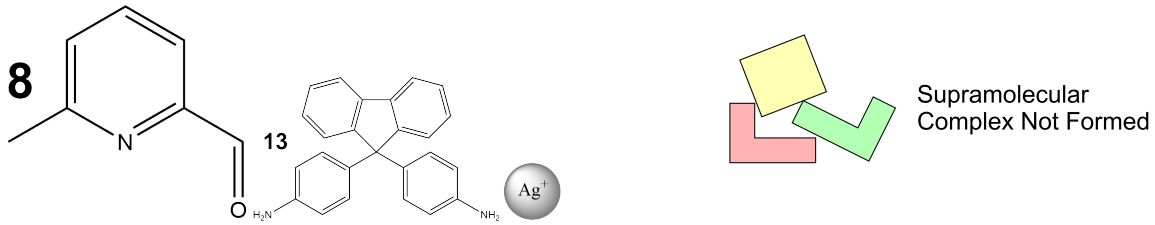


NMR Spectra 94: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 111.



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

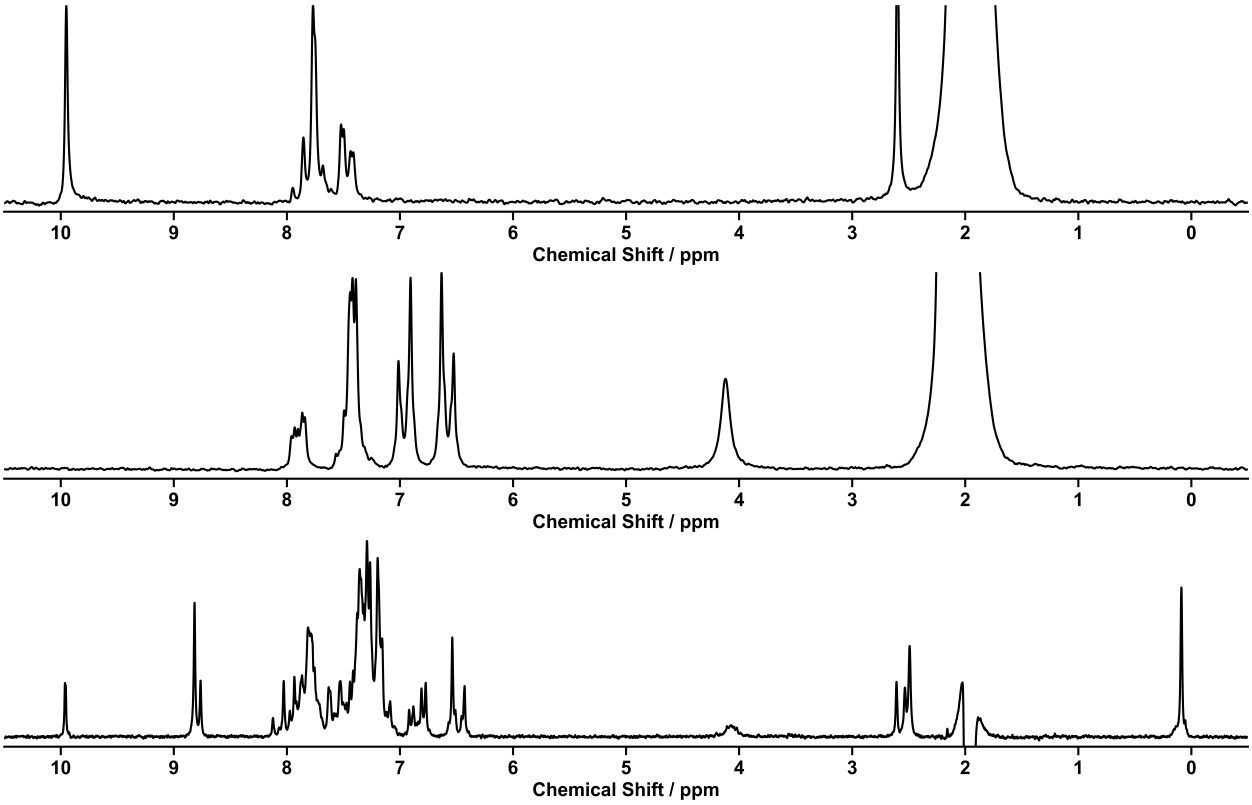
Reaction 113



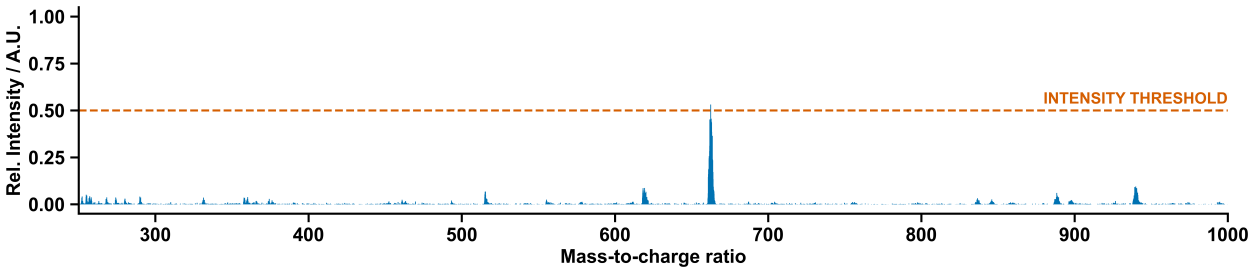
Scheme 95: Self-assembly of components 8, 13, with Silver(I) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 113.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: No reaction occured.	
	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 labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 113. Decision motivations are also given.

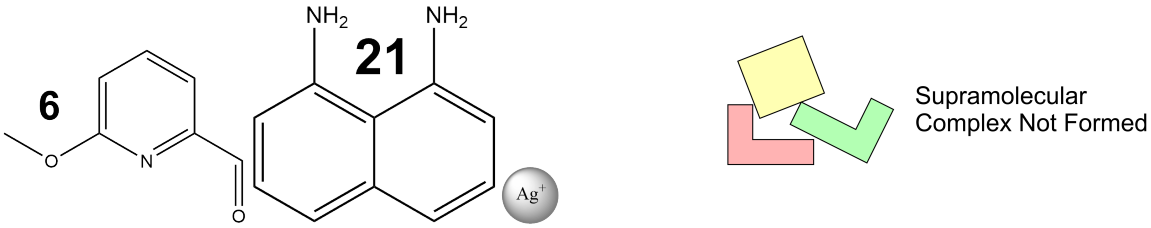


NMR Spectra 95: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 113.



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

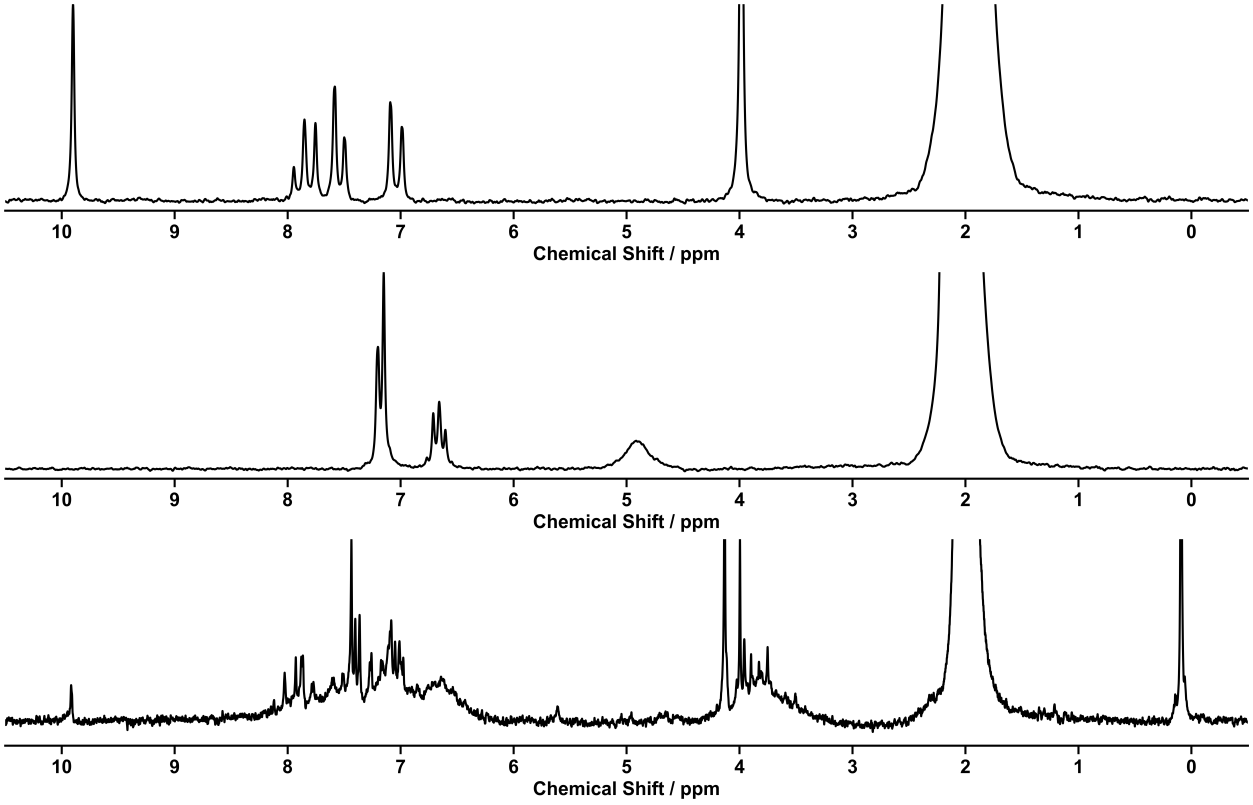
Reaction 114



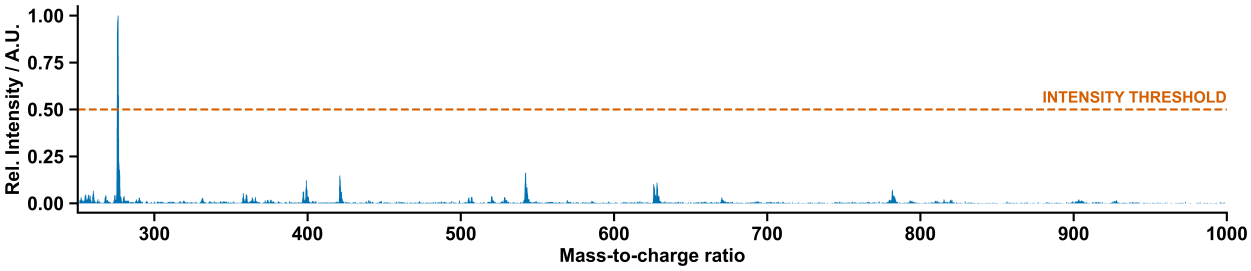
Scheme 96: Self-assembly of components 6, 21, with Silver(I) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 114.

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

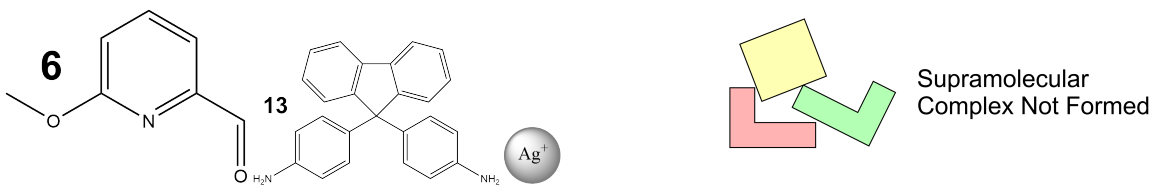


NMR Spectra 96: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 114.



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

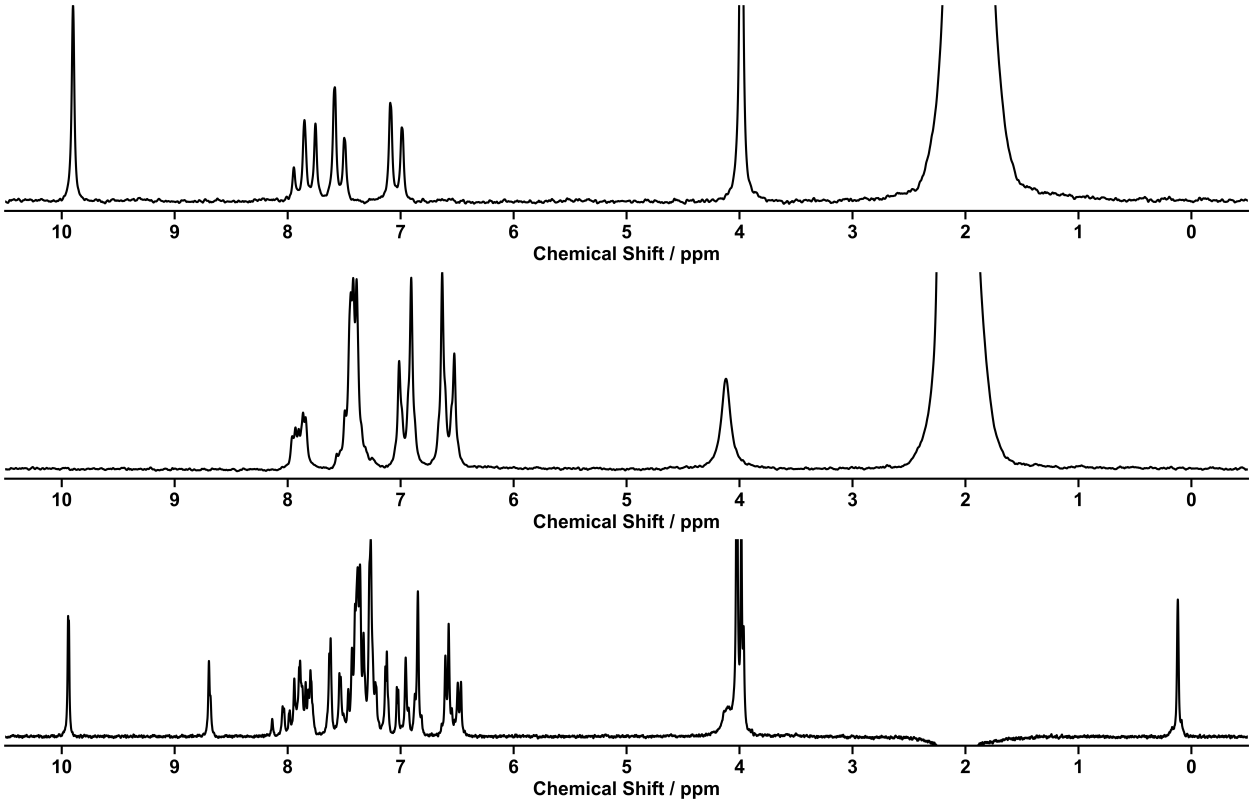
Reaction 115



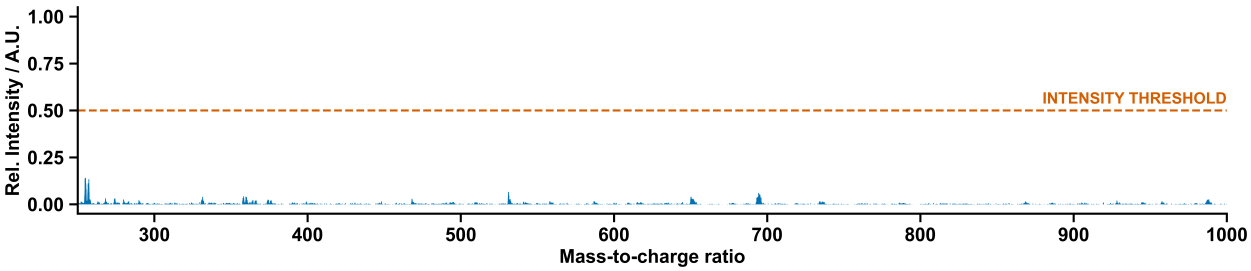
Scheme 97: Self-assembly of components 6, 13, with Silver(I) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 115.

<table>
<tr><td rowspan="2">Human Reaction Decision:
Failed</td><td>Human NMR Decision:
Failed</td><td colspan="2">NMR Spectra Category:
No reaction occured.</td></tr>
<tr><td>Human MS Decision:
Failed</td><td colspan="2">MS Spectra Category:
Reaction failed.</td></tr>
<tr><td rowspan="4">Decision Maker Reaction Decision:
N/A</td><td rowspan="2">Decision Maker NMR Decision:
N/A</td><td colspan="2">NMR Criteria 1:
N/A</td></tr>
<tr><td colspan="2">NMR Criteria 2:
N/A</td></tr>
<tr><td rowspan="2">Decision Maker MS Decision:
Pass</td><td>MS Criteria 1 and 2:
Pass</td><td>Number of predicted peaks found in MS spectra with appropriate intensity:
0</td></tr>
<tr><td>MS Criteria 3:
Pass</td><td>Number of counter-ions found:
0</td></tr>
</table>

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

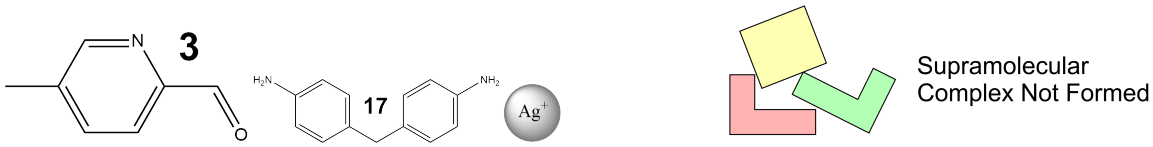


NMR Spectra 97: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 115.



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

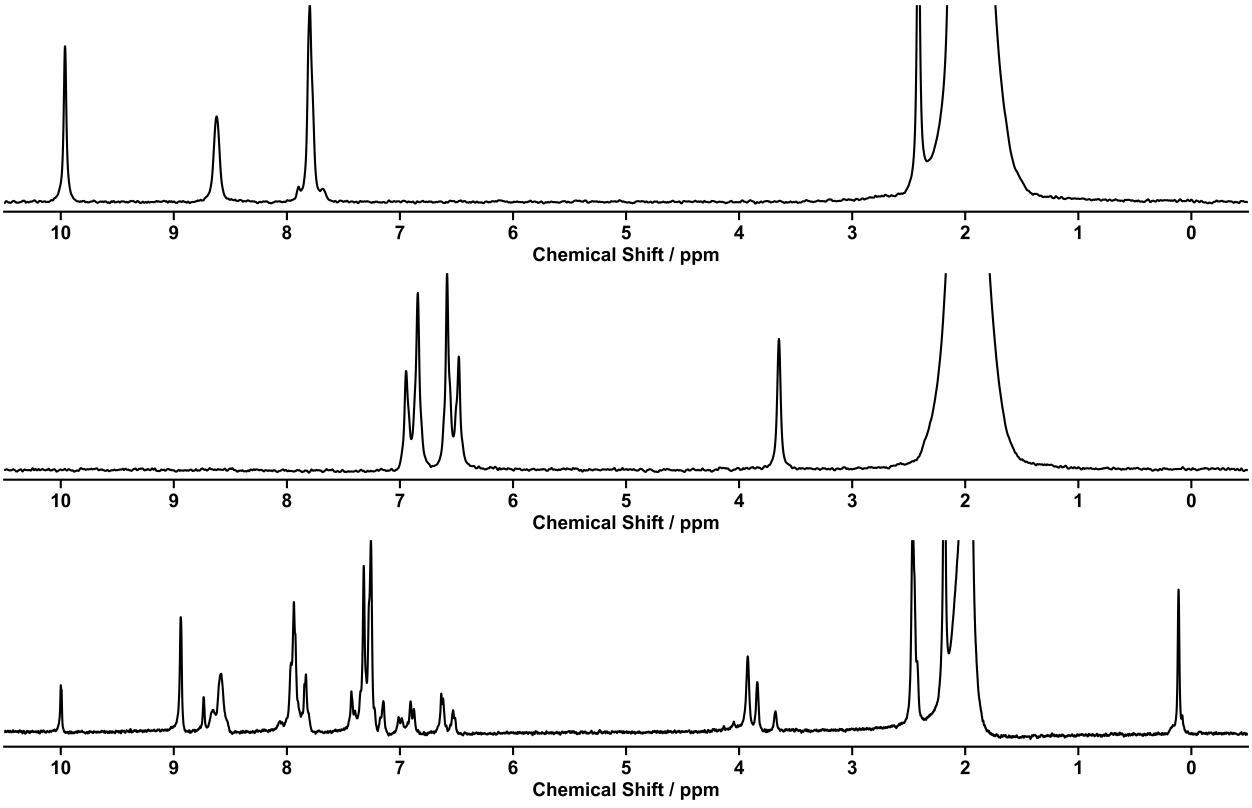
Reaction 116



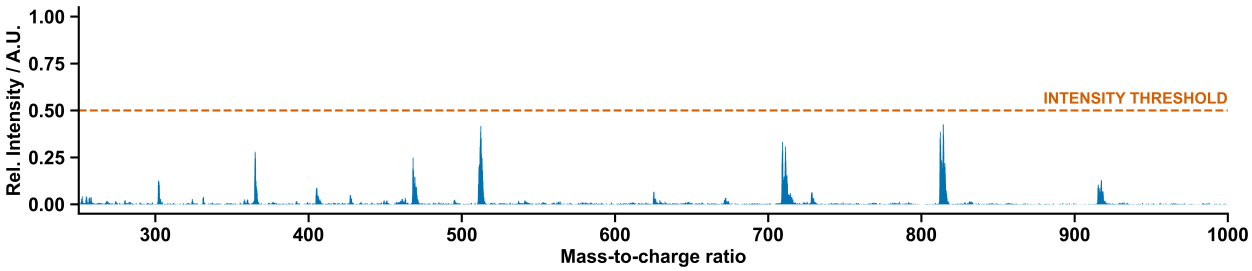
Scheme 98: Self-assembly of components 3, 17, with Silver(I) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 116.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: No reaction occured.	
	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 labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 116. Decision motivations are also given.

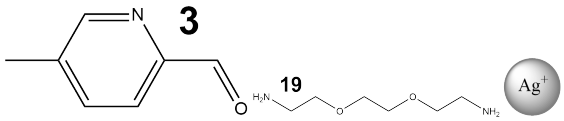


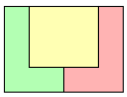
NMR Spectra 98: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 116.



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

Reaction 117



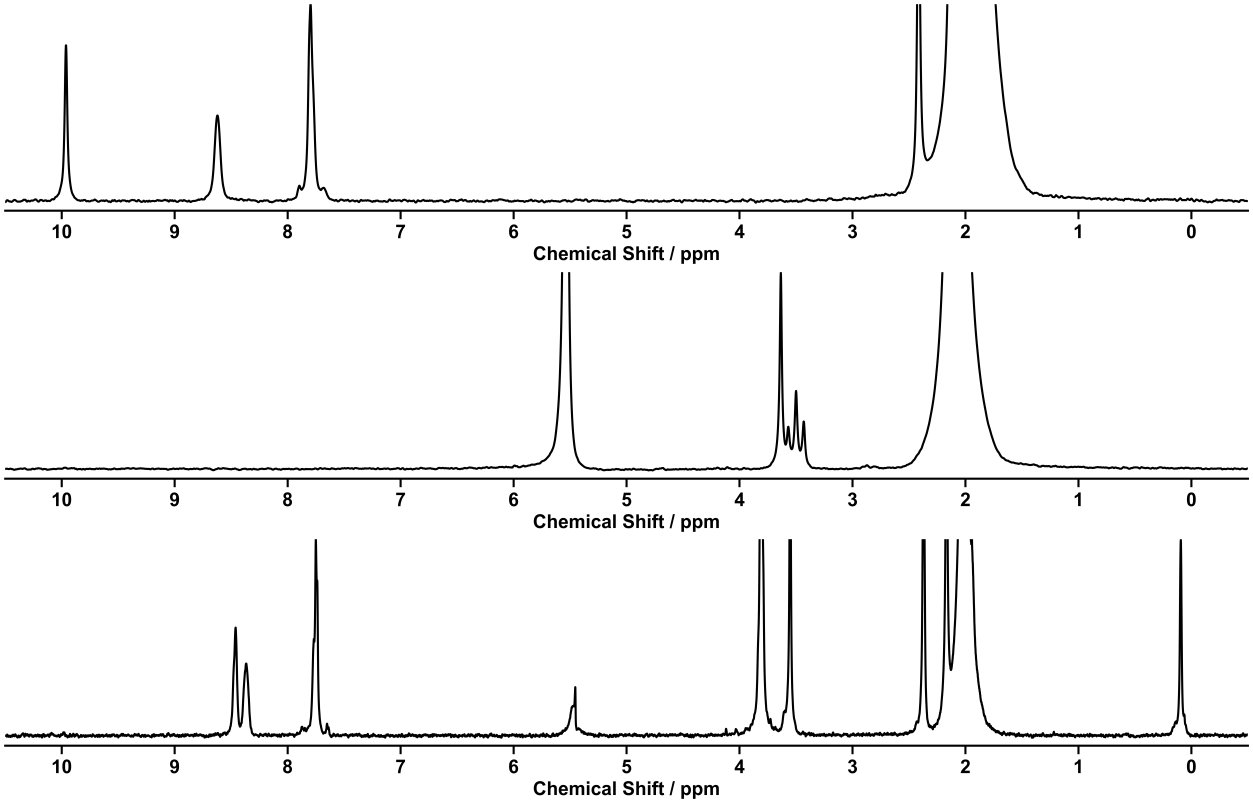


Supramolecular
Complex Formed

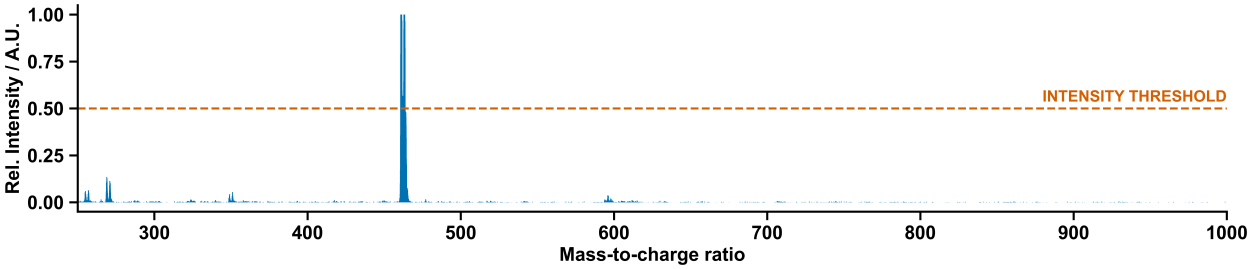
Scheme 99: Self-assembly of components 3, 19, with Silver(I) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 117.

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	
		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 99: Human labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 117. Decision motivations are also given.

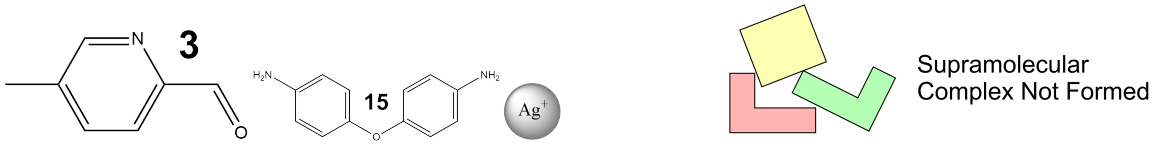


NMR Spectra 99: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 117.



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

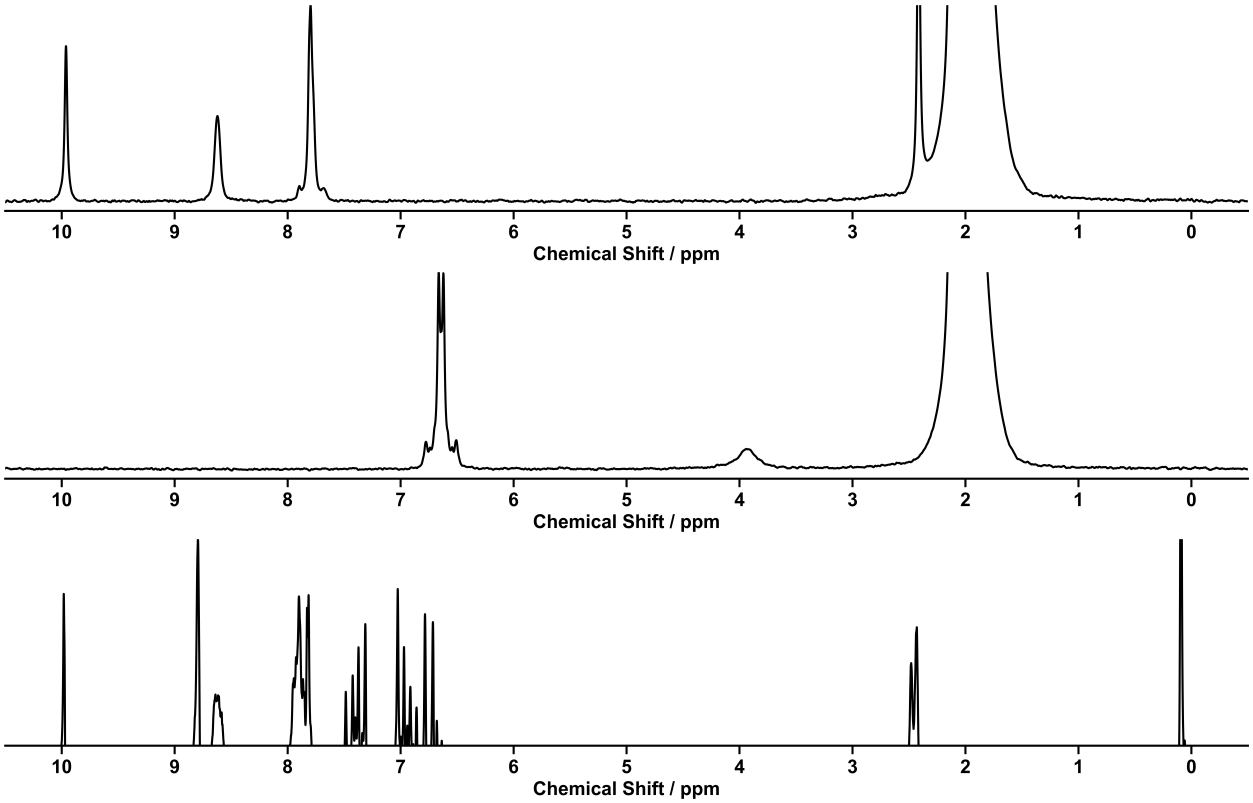
Reaction 118



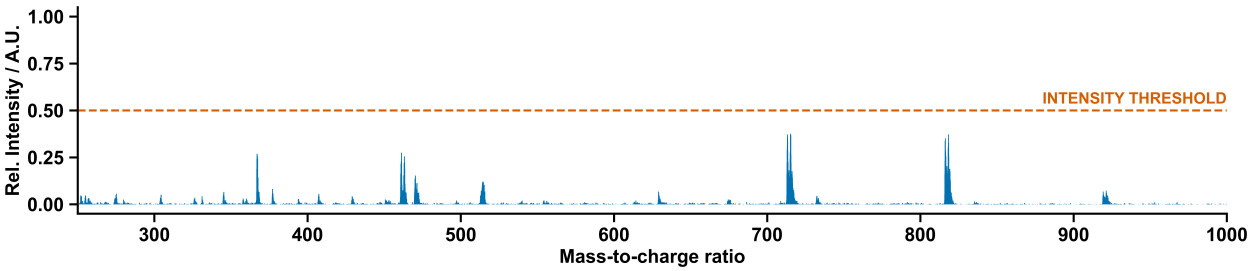
Scheme 100: Self-assembly of components 3, 15, with Silver(I) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 118.

<table>
<tr><td rowspan="2">Human Reaction Decision:
Failed</td><td>Human NMR Decision:
Failed</td><td colspan="2">NMR Spectra Category:
No reaction occured.</td></tr>
<tr><td>Human MS Decision:
Failed</td><td colspan="2">MS Spectra Category:
Reaction failed.</td></tr>
<tr><td rowspan="4">Decision Maker Reaction Decision:
N/A</td><td rowspan="2">Decision Maker NMR Decision:
N/A</td><td colspan="2">NMR Criteria 1:
N/A</td></tr>
<tr><td colspan="2">NMR Criteria 2:
N/A</td></tr>
<tr><td rowspan="2">Decision Maker MS Decision:
Pass</td><td>MS Criteria 1 and 2:
Pass</td><td>Number of predicted peaks found in MS spectra with appropriate intensity:
0</td></tr>
<tr><td>MS Criteria 3:
Pass</td><td>Number of counter-ions found:
0</td></tr>
</table>

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

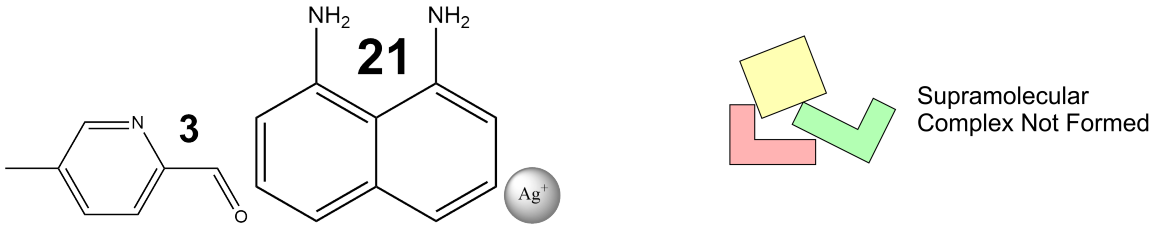


NMR Spectra 100: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 118.



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

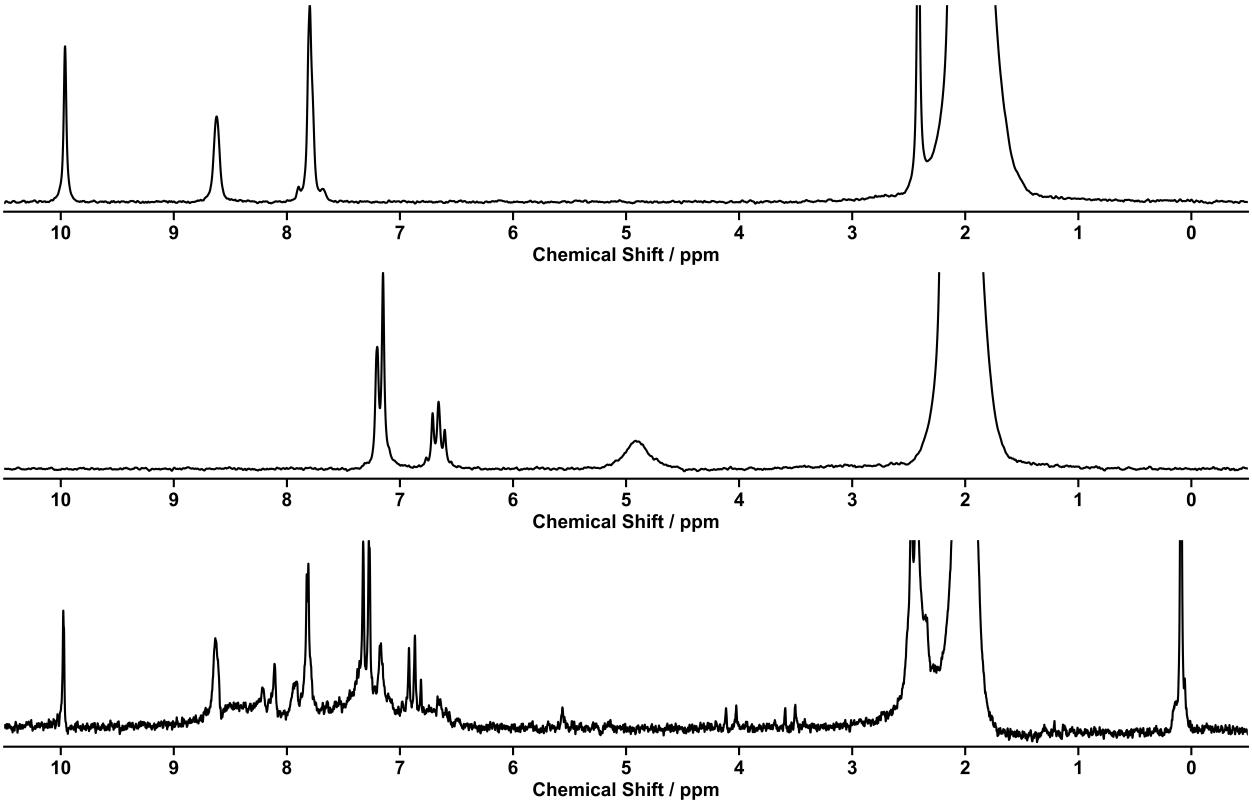
Reaction 119



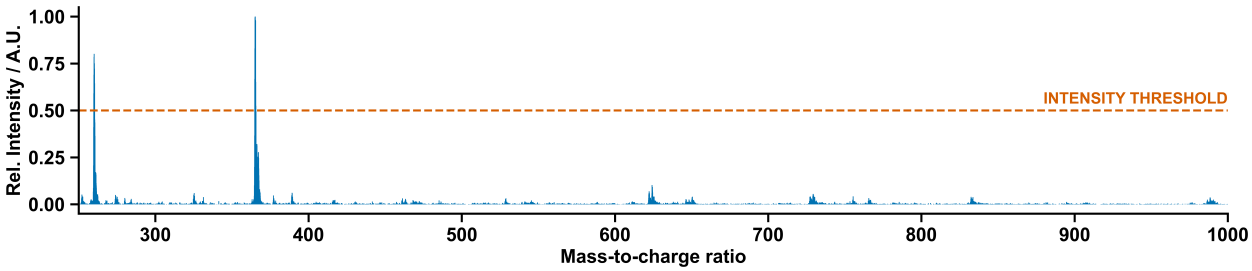
Scheme 101: Self-assembly of components 3, 21, with Silver(I) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 119.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: No reaction occured.	
	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 labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 119. Decision motivations are also given.

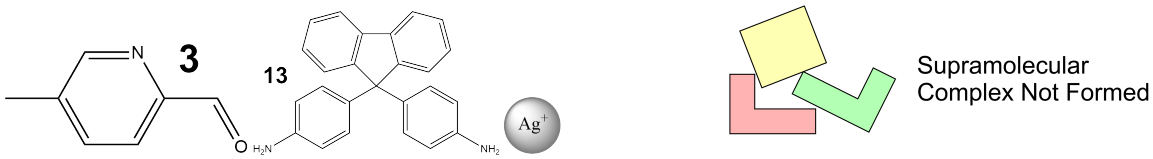


NMR Spectra 101: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 119.



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

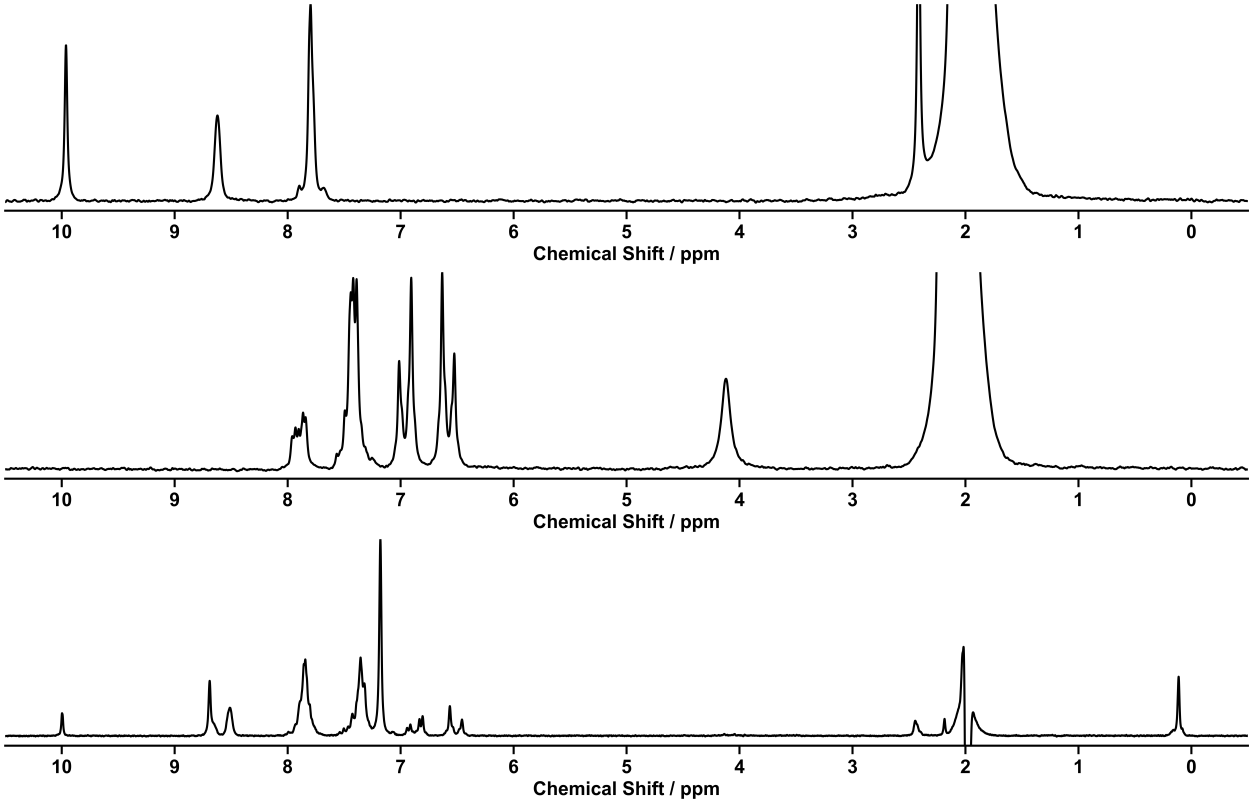
Reaction 120



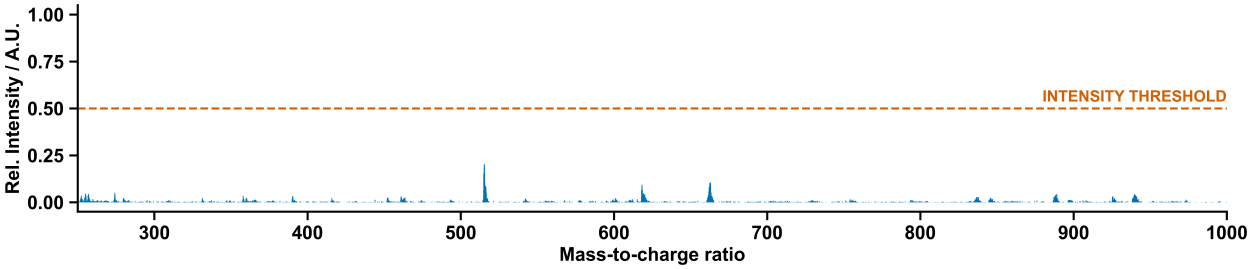
Scheme 102: Self-assembly of components 3, 13, with Silver(I) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 120.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: No reaction occured.	
	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 labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 120. Decision motivations are also given.

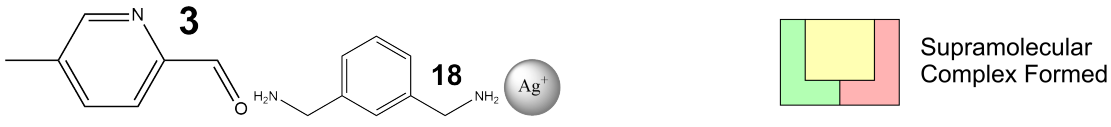


NMR Spectra 102: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 120.



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

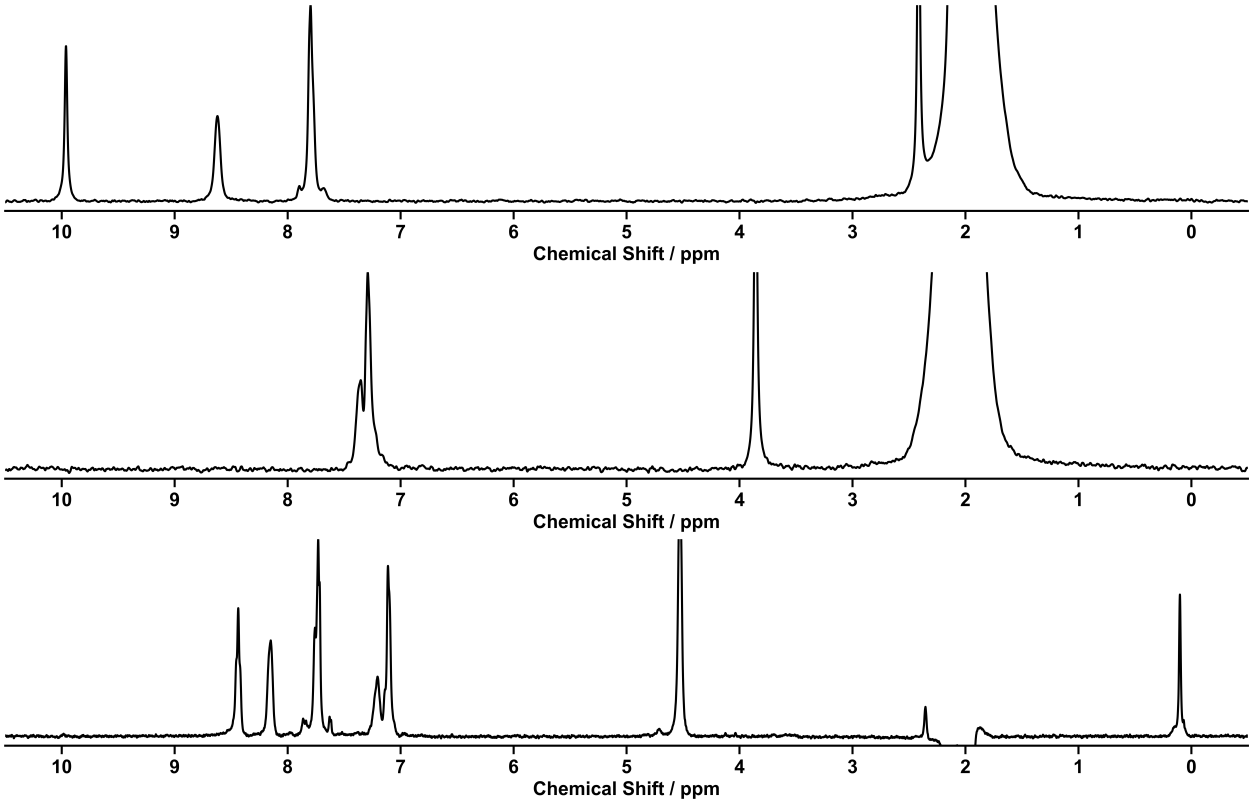
Reaction 123



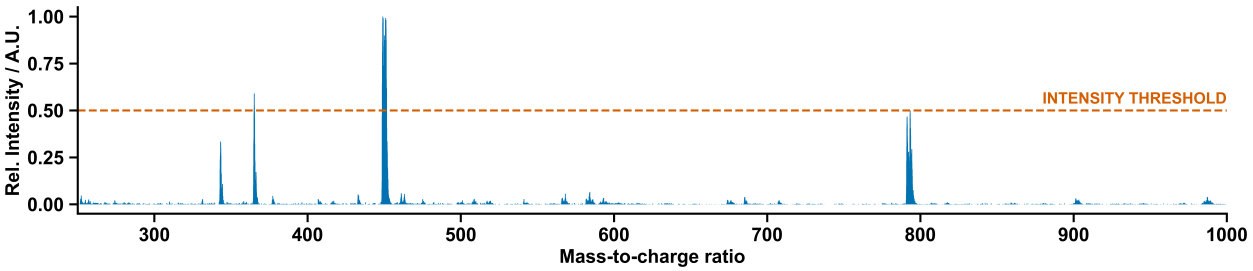
Scheme 103: Self-assembly of components 3, 18, with Silver(I) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 123.

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

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

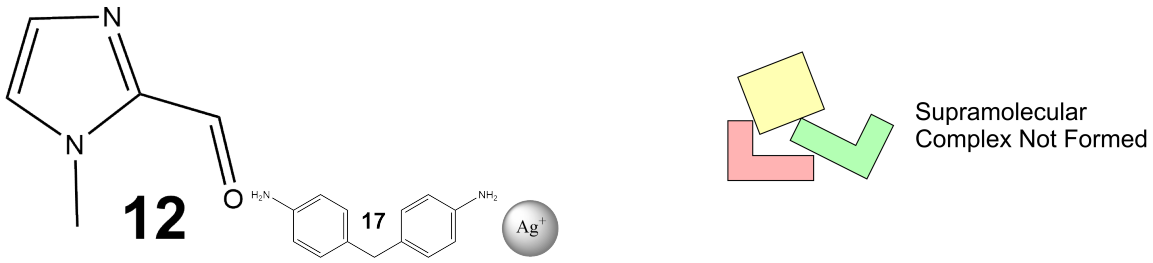


NMR Spectra 103: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 123.



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

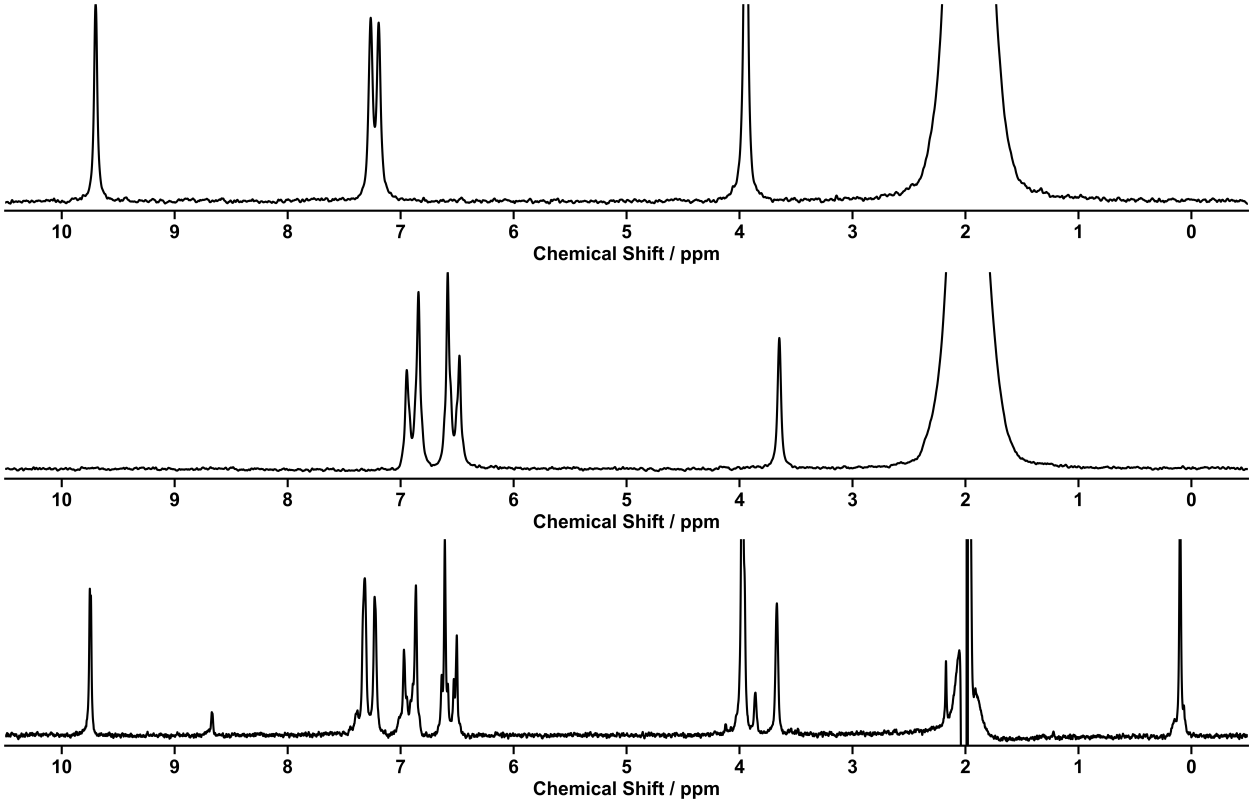
Reaction 124



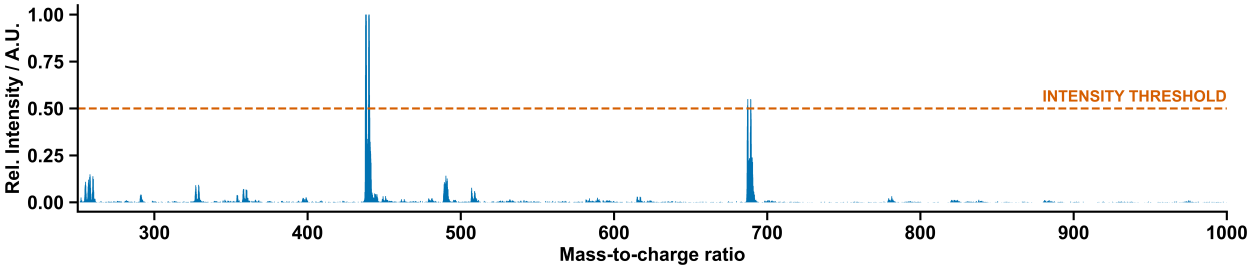
Scheme 104: Self-assembly of components 12, 17, with Silver(I) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 124.

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	
		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 104: Human labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 124. Decision motivations are also given.

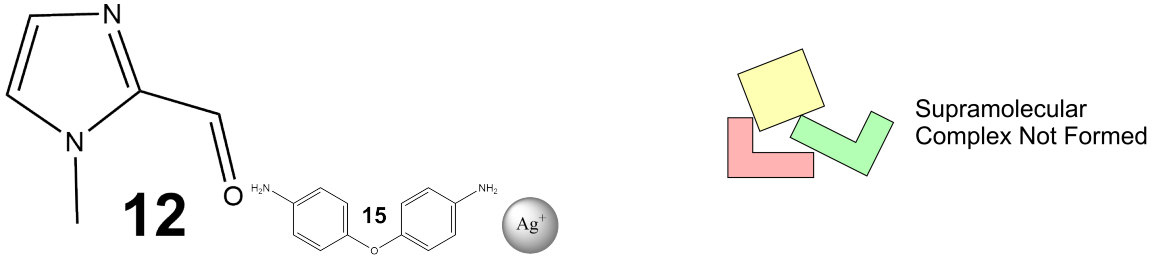


NMR Spectra 104: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 124.



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

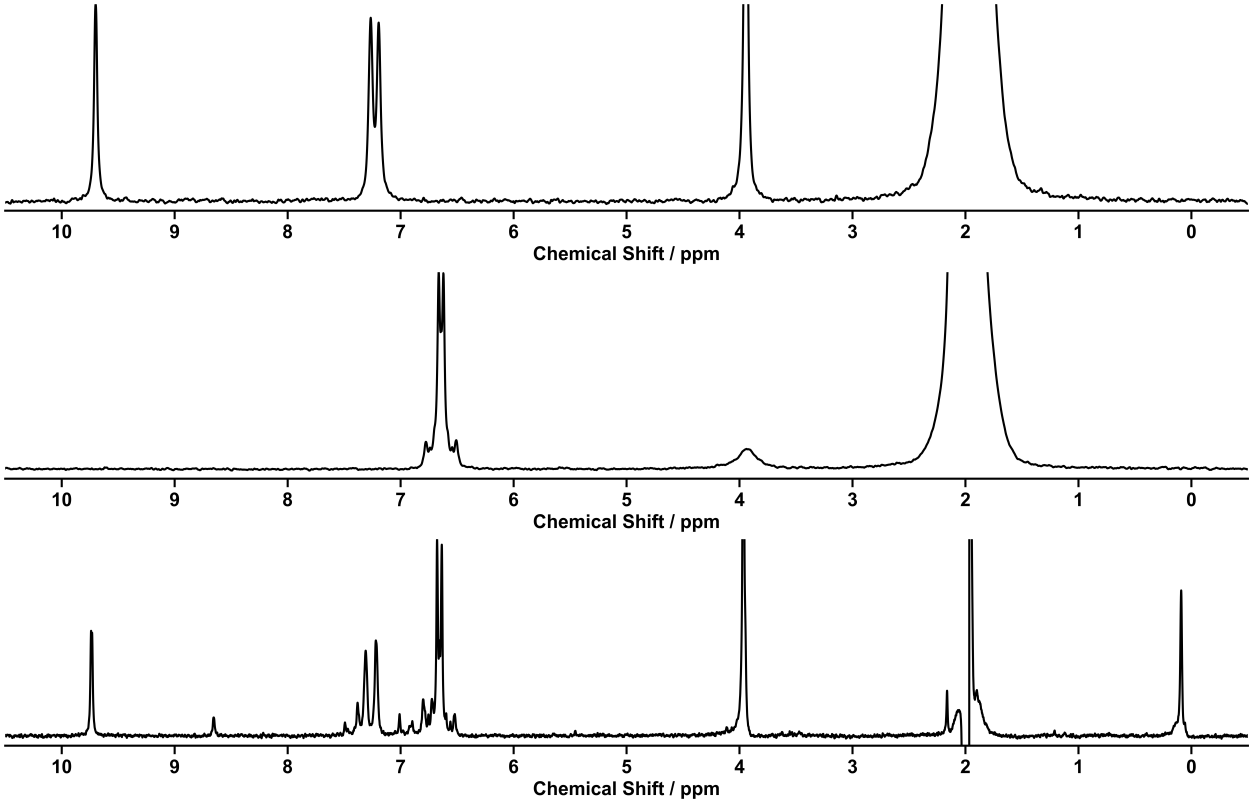
Reaction 126



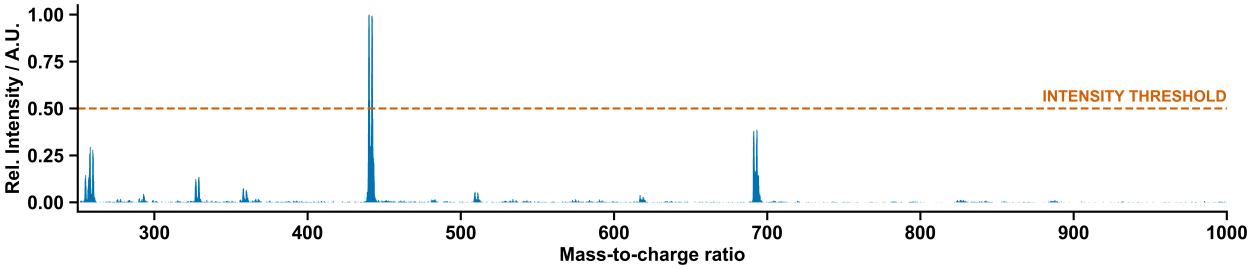
Scheme 105: Self-assembly of components 12, 15, with Silver(I) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 126.

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	
		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 105: Human labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 126. Decision motivations are also given.

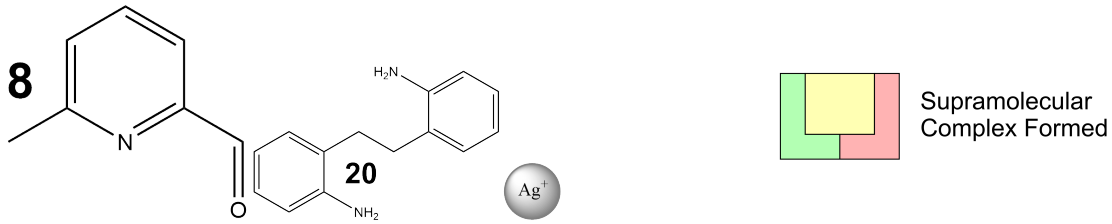


NMR Spectra 105: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 126.



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

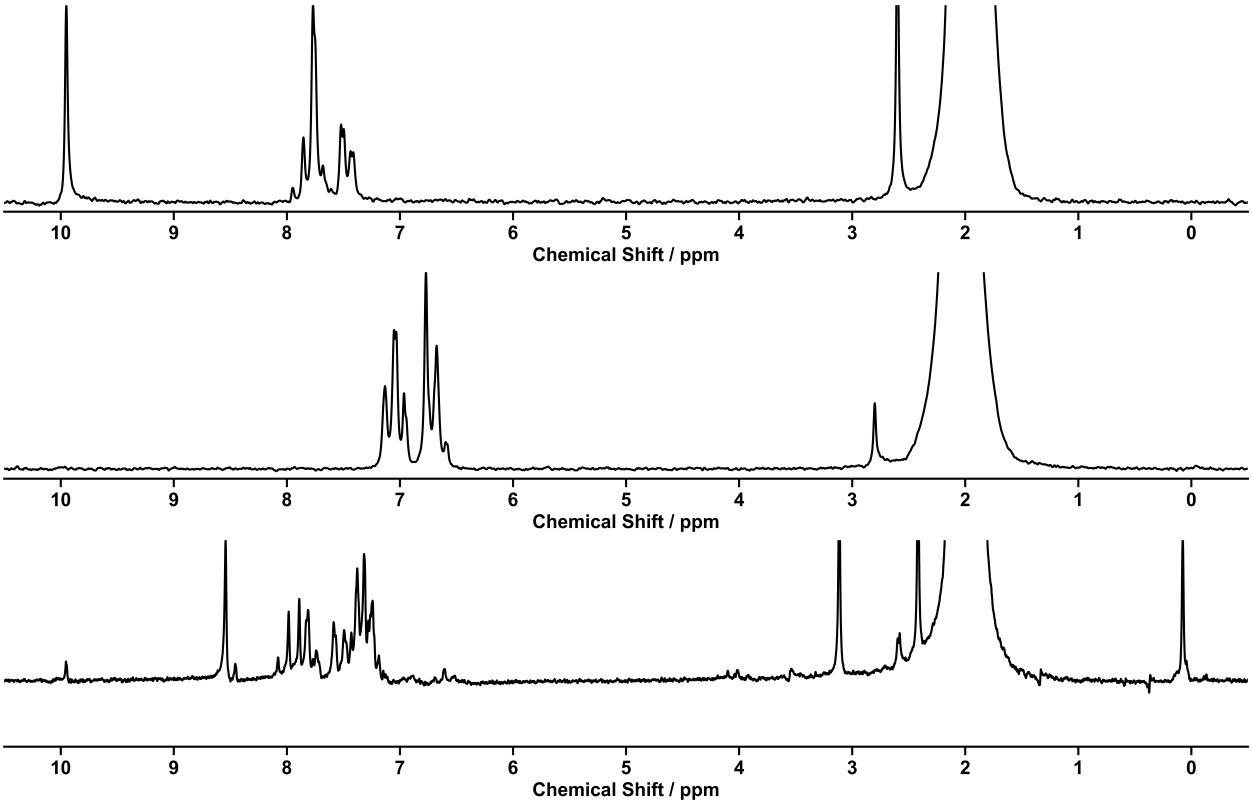
Reaction 127



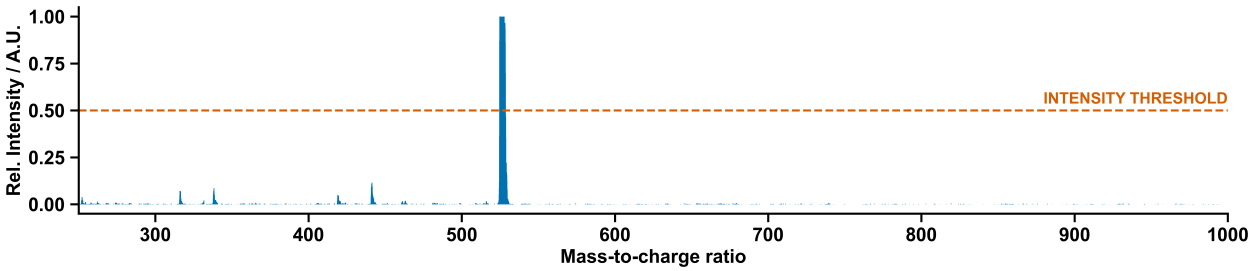
Scheme 106: Self-assembly of components 8, 20, with Silver(I) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 127.

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 labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 127. Decision motivations are also given.

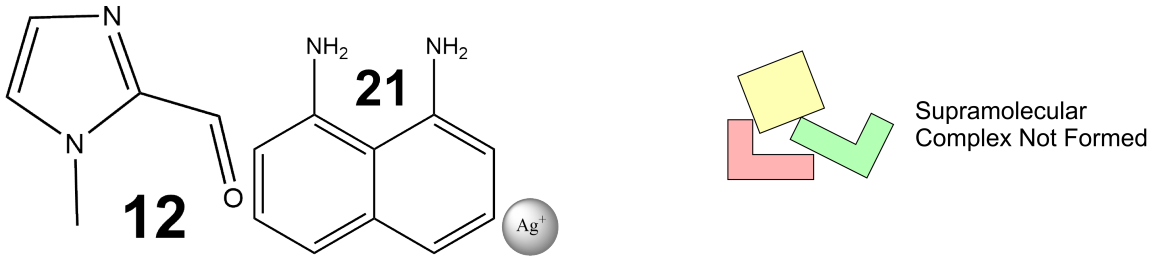


NMR Spectra 106: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 127.



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

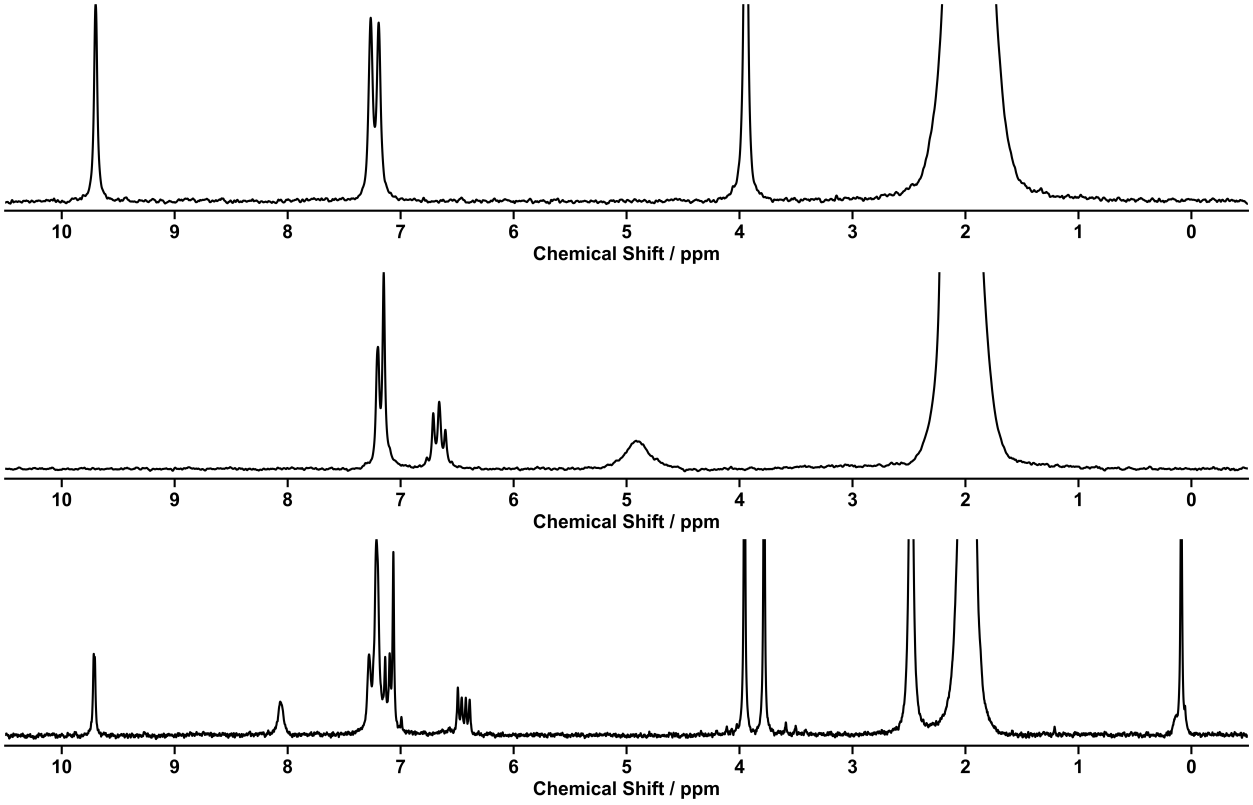
Reaction 128



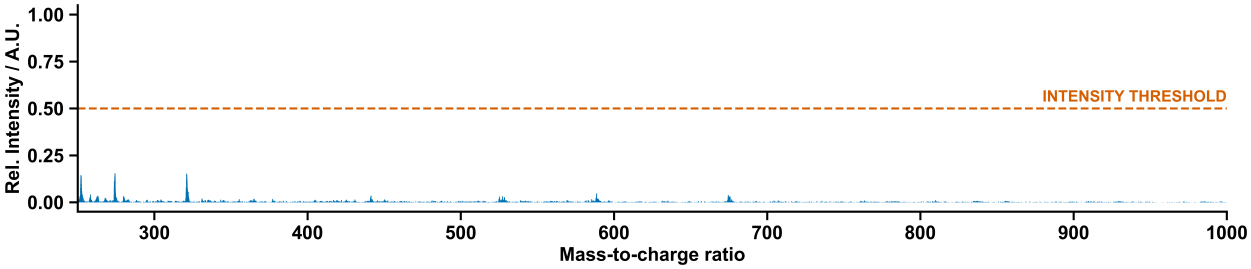
Scheme 107: Self-assembly of components 12, 21, with Silver(I) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 128.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: No reaction occured.	
	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 labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 128. Decision motivations are also given.

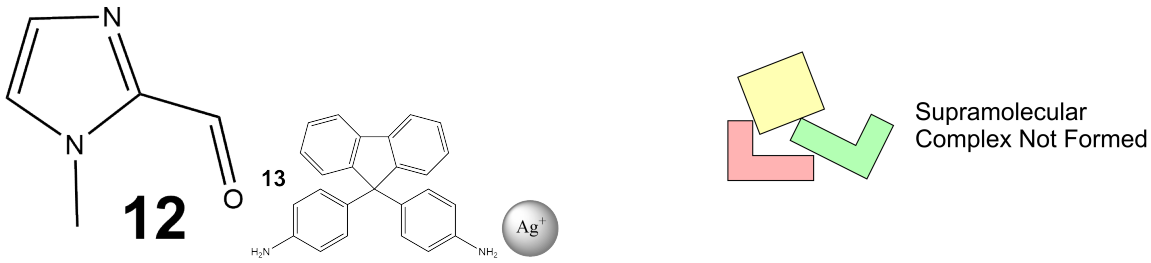


NMR Spectra 107: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 128.



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

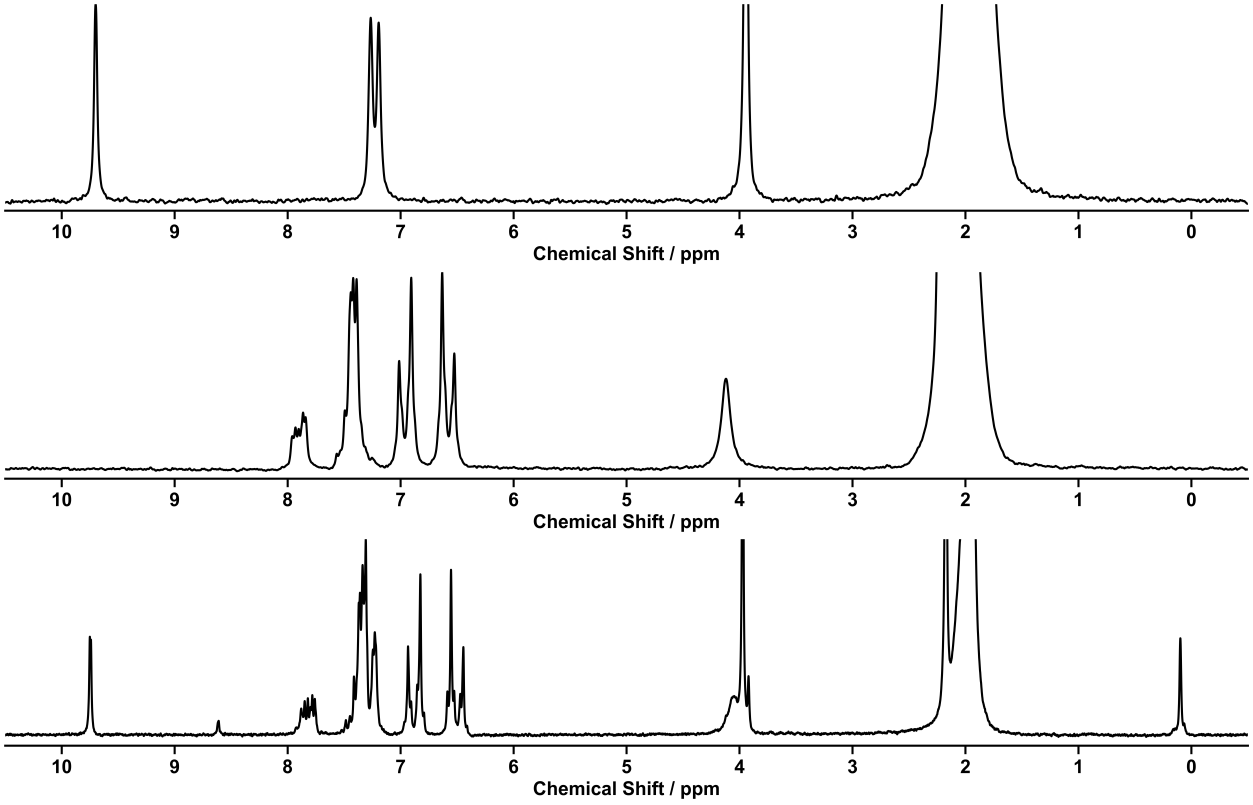
Reaction 129



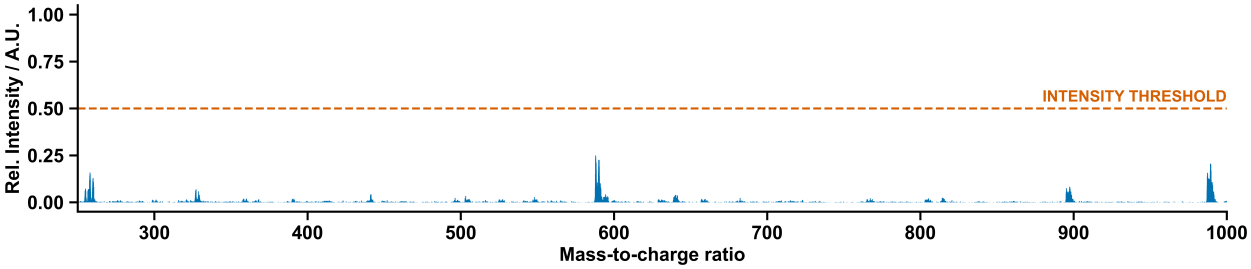
Scheme 108: Self-assembly of components 12, 13, with Silver(I) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 129.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: No reaction occured.	
	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 108: Human labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 129. Decision motivations are also given.

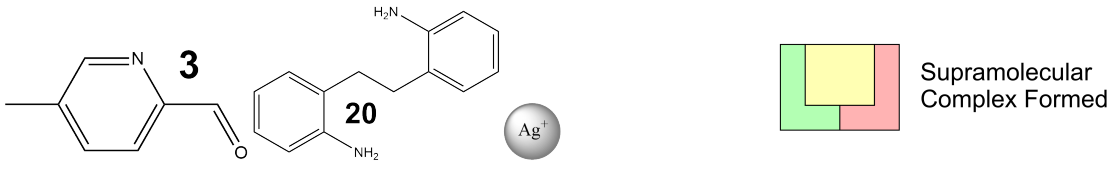


NMR Spectra 108: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 129.



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

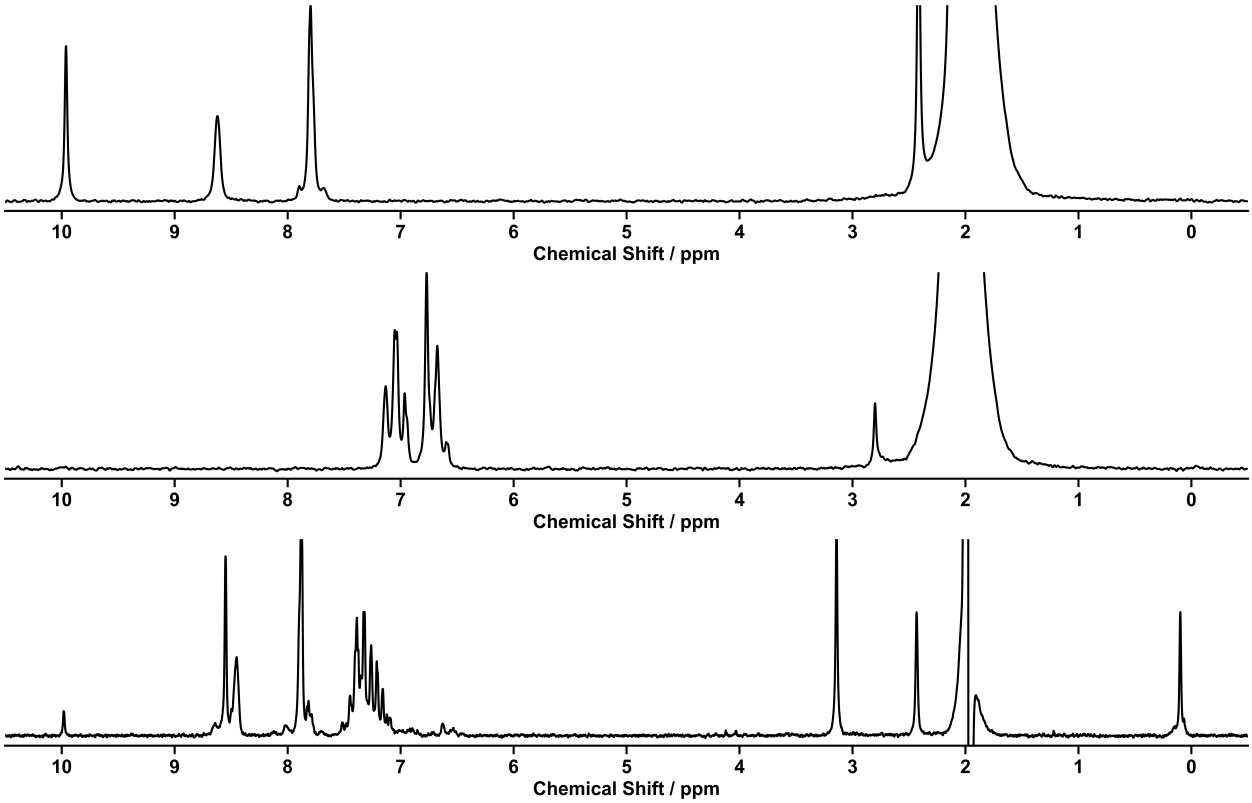
Reaction 131



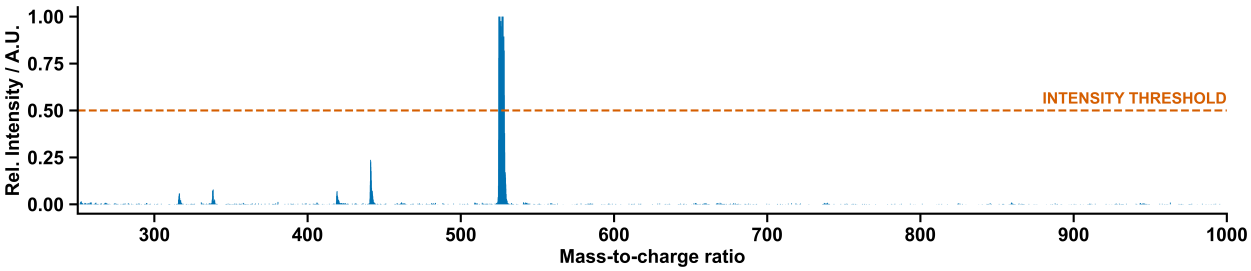
Scheme 109: Self-assembly of components 3, 20, with Silver(I) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 131.

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

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

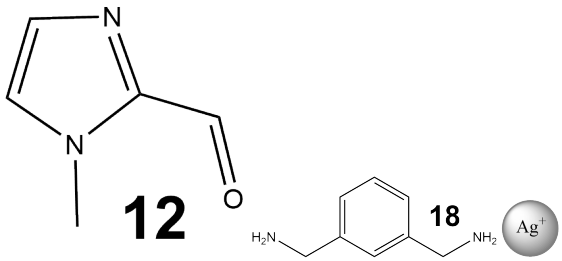


NMR Spectra 109: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 131.



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

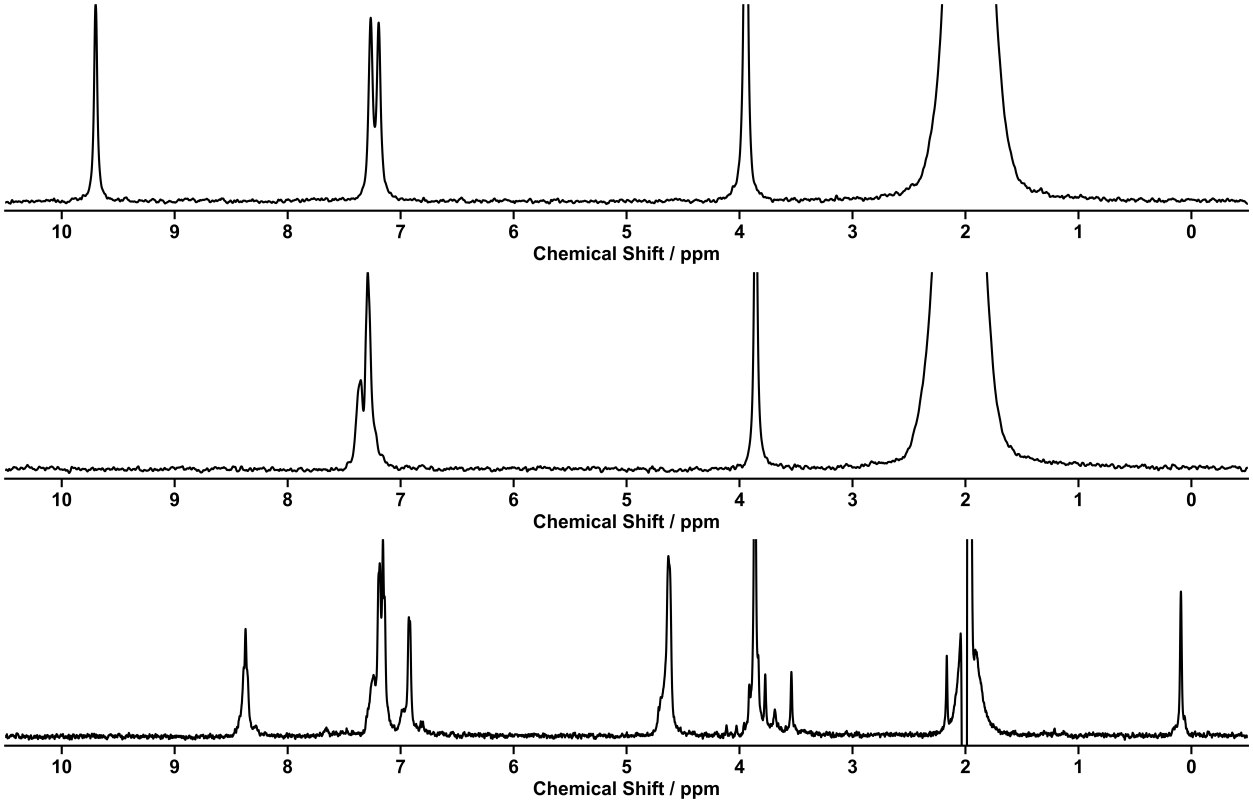
Reaction 132



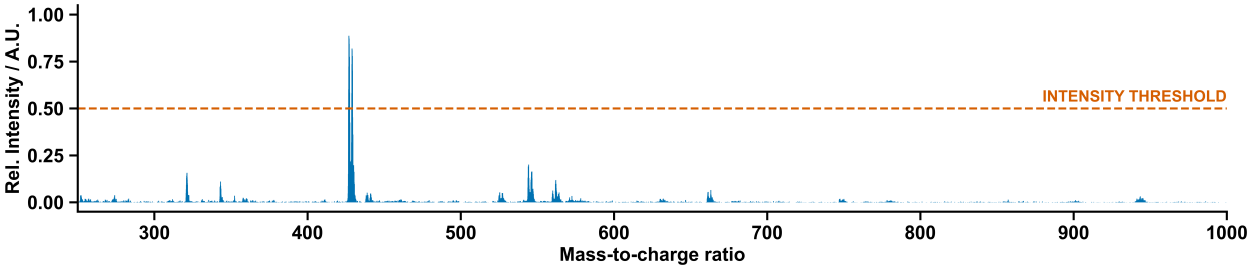
Scheme 110: Self-assembly of components 12, 18, with Silver(I) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 132.

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 labled and Decsision maker labled outcomes for the ^1H NMR spectroscopy and ULPC-MS spectrometry of reaction 132. Decision motivations are also given.

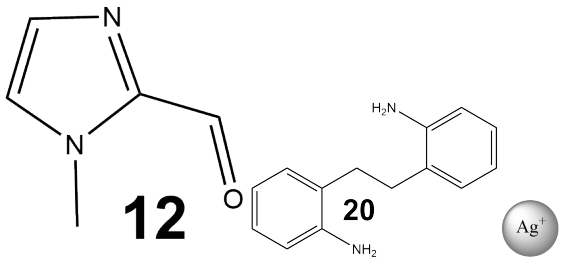


NMR Spectra 110: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 132.



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

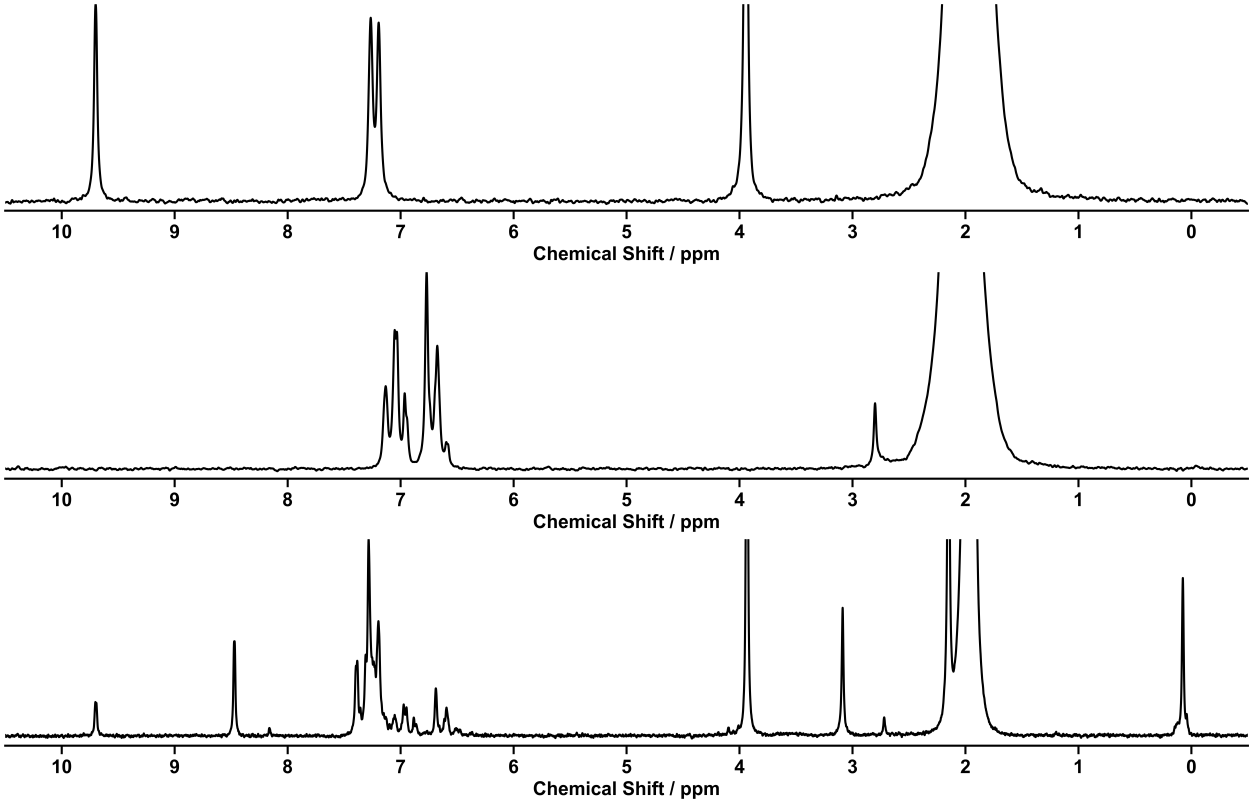
Reaction 133



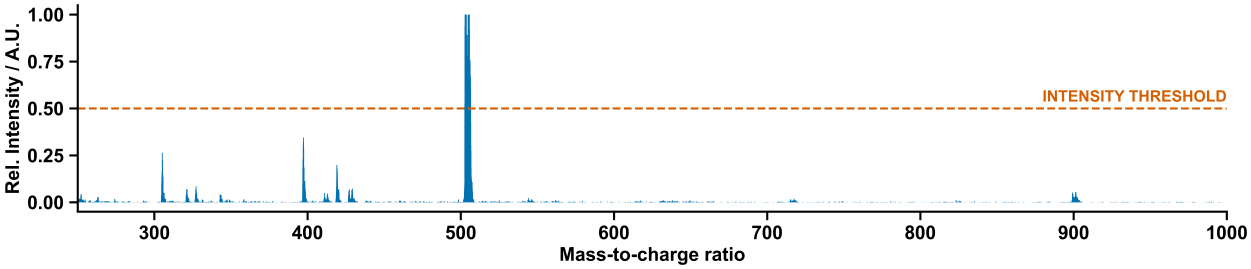
Scheme 111: Self-assembly of components 12, 20, with Silver(I) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 133.

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 labled and Decsision maker labled outcomes for the ^1H NMR spectroscopy and ULPC-MS spectrometry of reaction 133. Decision motivations are also given.

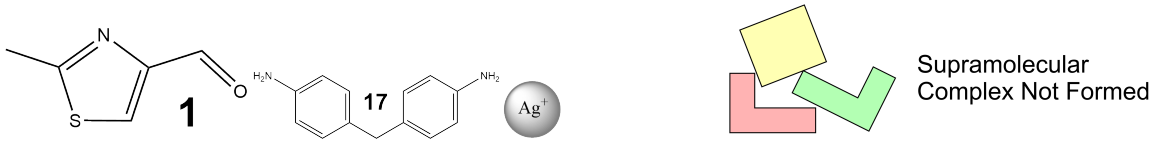


NMR Spectra 111: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 133.



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

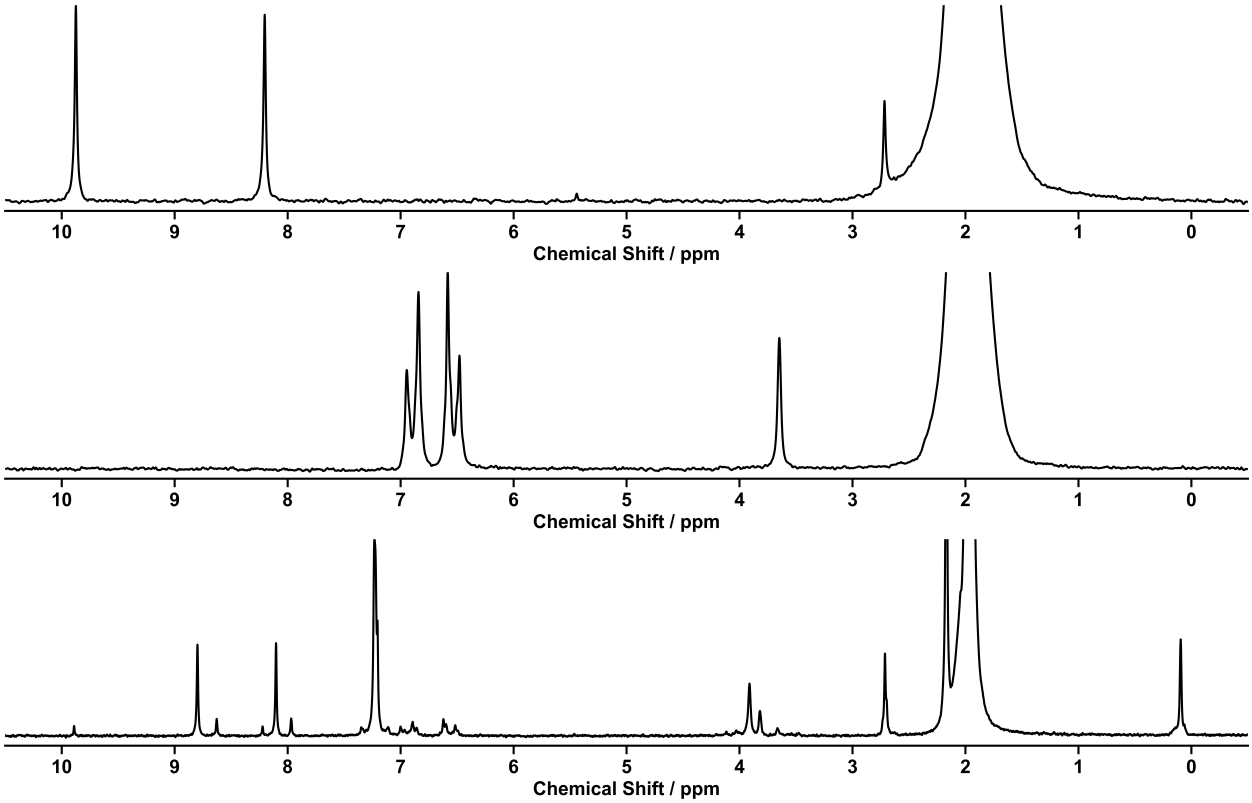
Reaction 134



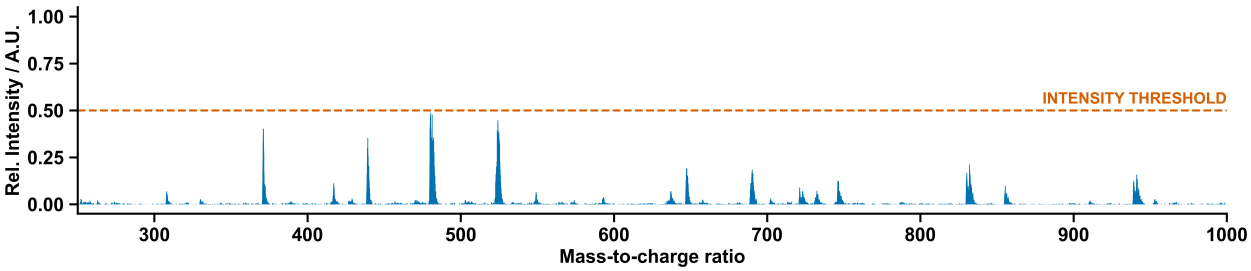
Scheme 112: Self-assembly of components 1, 17, with Silver(I) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 134.

<table>
<tr><td rowspan="2">Human Reaction Decision:
Failed</td><td>Human NMR Decision:
Pass</td><td colspan="2">NMR Spectra Category:
Single discrete species formed.</td></tr>
<tr><td>Human MS Decision:
Failed</td><td colspan="2">MS Spectra Category:
Reaction failed.</td></tr>
<tr><td rowspan="4">Decision Maker Reaction Decision:
N/A</td><td rowspan="2">Decision Maker NMR Decision:
N/A</td><td colspan="2">NMR Criteria 1:
N/A</td></tr>
<tr><td colspan="2">NMR Criteria 2:
N/A</td></tr>
<tr><td rowspan="2">Decision Maker MS Decision:
Pass</td><td>MS Criteria 1 and 2:
Pass</td><td>Number of predicted peaks found in MS spectra with appropriate intensity:
0</td></tr>
<tr><td>MS Criteria 3:
Pass</td><td>Number of counter-ions found:
0</td></tr>
</table>

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

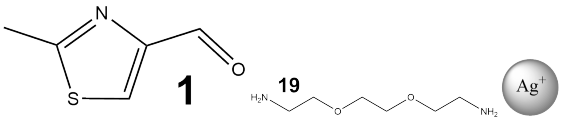


NMR Spectra 112: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 134.



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

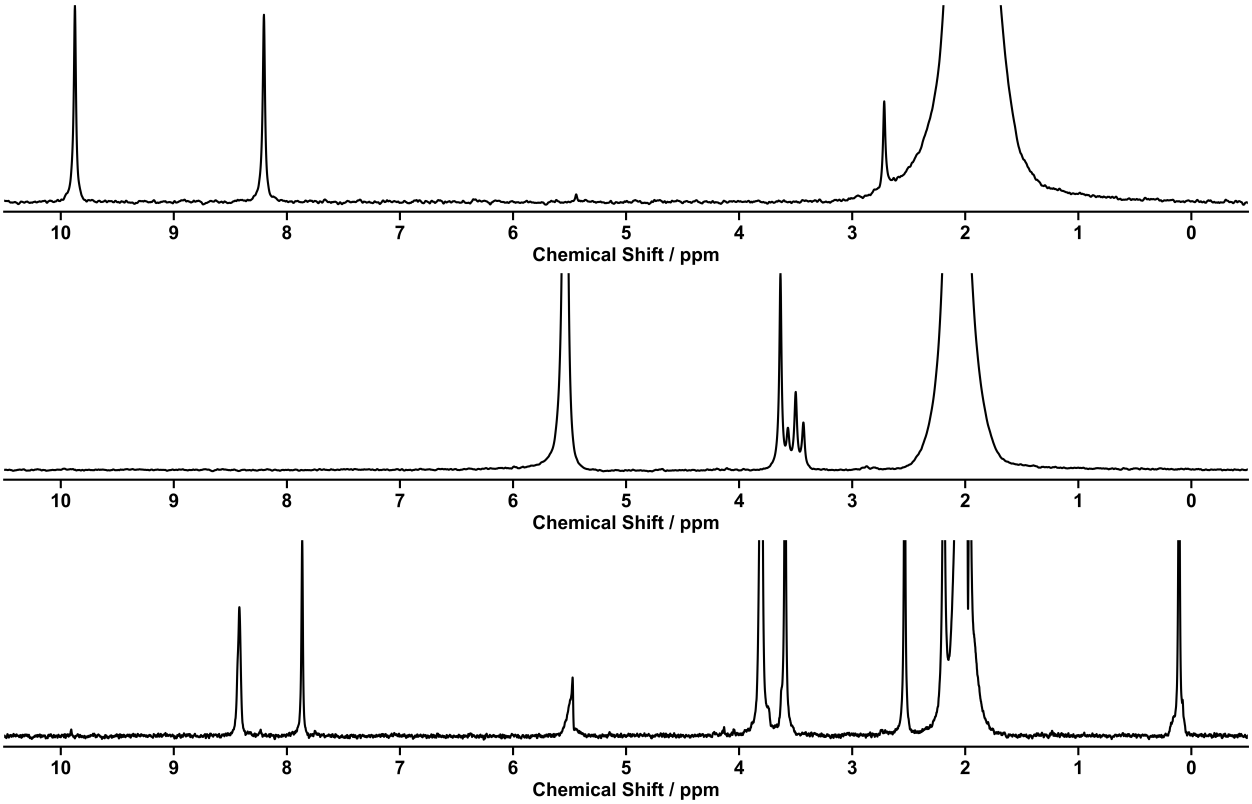
Reaction 135



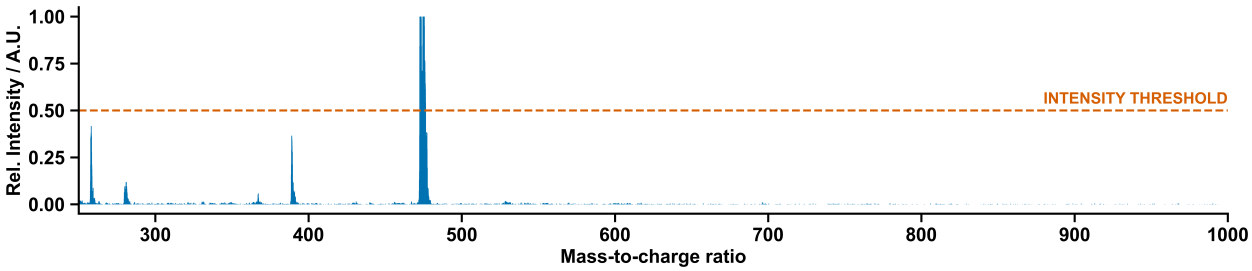
Scheme 113: Self-assembly of components 1, 19, with Silver(I) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 135.

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 labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 135. Decision motivations are also given.

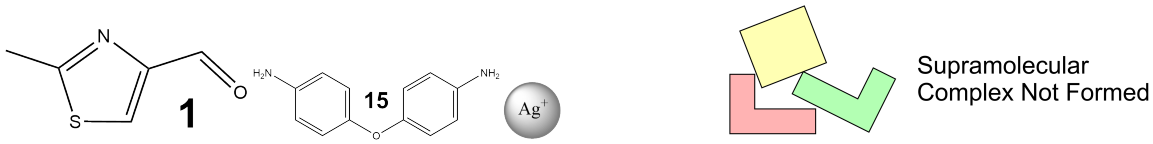


NMR Spectra 113: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 135.



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

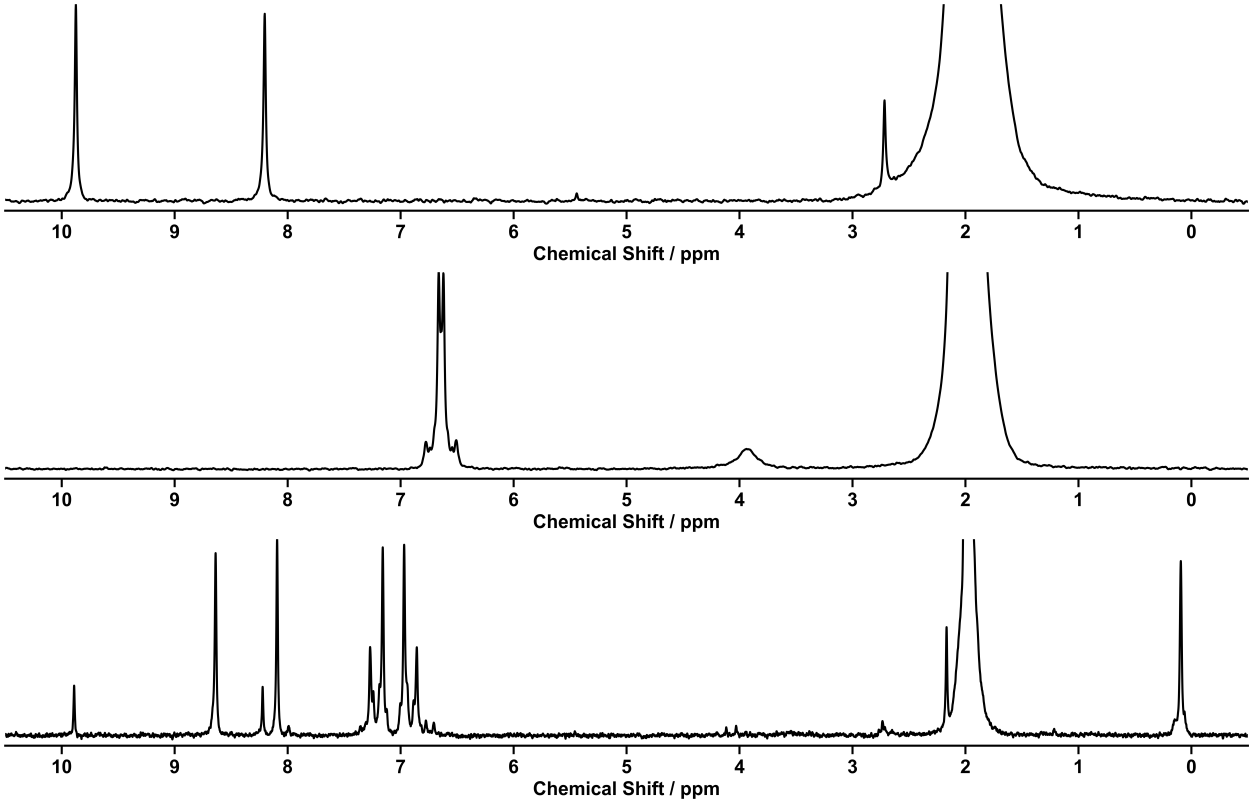
Reaction 136



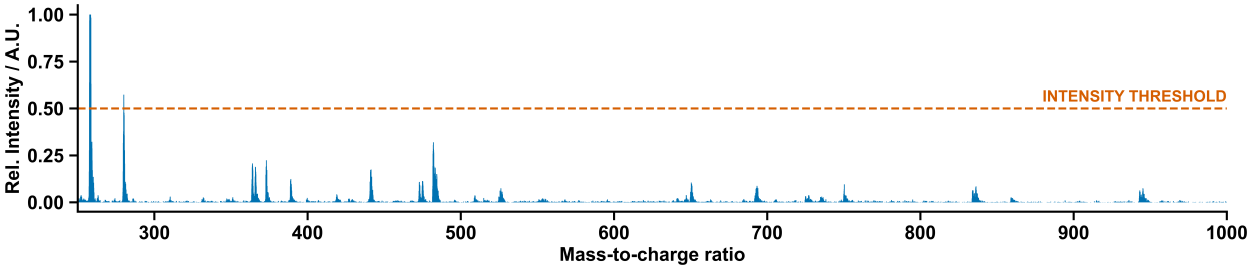
Scheme 114: Self-assembly of components 1, 15, with Silver(I) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 136.

<table>
<tr><td rowspan="2">Human Reaction Decision:
Failed</td><td>Human NMR Decision:
Pass</td><td colspan="2">NMR Spectra Category:
Single discrete species formed.</td></tr>
<tr><td>Human MS Decision:
Failed</td><td colspan="2">MS Spectra Category:
Reaction occurred, unknown product.</td></tr>
<tr><td rowspan="4">Decision Maker Reaction Decision:
N/A</td><td rowspan="2">Decision Maker NMR Decision:
N/A</td><td colspan="2">NMR Criteria 1:
N/A</td></tr>
<tr><td colspan="2">NMR Criteria 2:
N/A</td></tr>
<tr><td rowspan="2">Decision Maker MS Decision:
Pass</td><td>MS Criteria 1 and 2:
Pass</td><td>Number of predicted peaks found in MS spectra with appropriate intensity:
0</td></tr>
<tr><td>MS Criteria 3:
Pass</td><td>Number of counter-ions found:
0</td></tr>
</table>

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

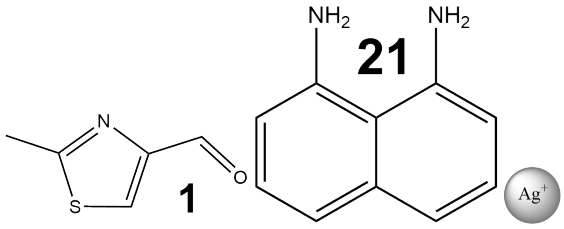


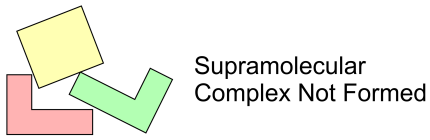
NMR Spectra 114: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 136.



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

Reaction 137

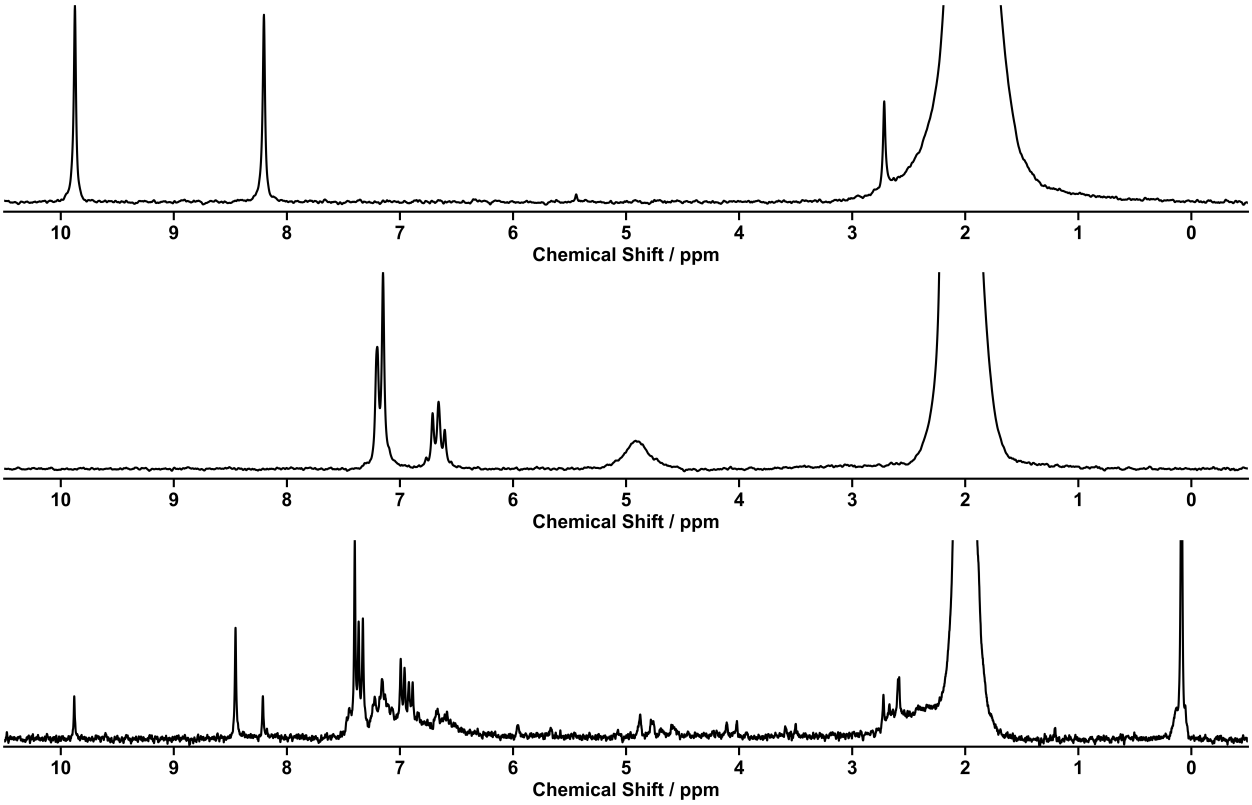




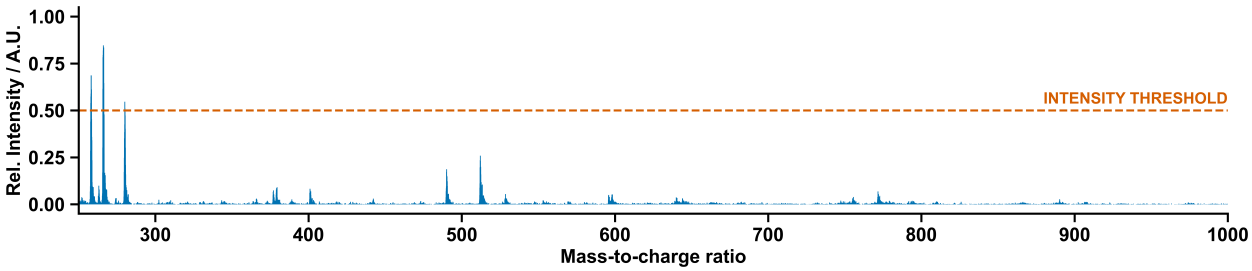
Scheme 115: Self-assembly of components 1, 21, with Silver(I) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 137.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: No reaction occured.	
	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 labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 137. Decision motivations are also given.

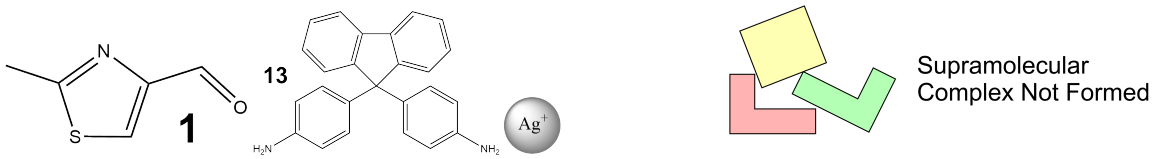


NMR Spectra 115: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 137.



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

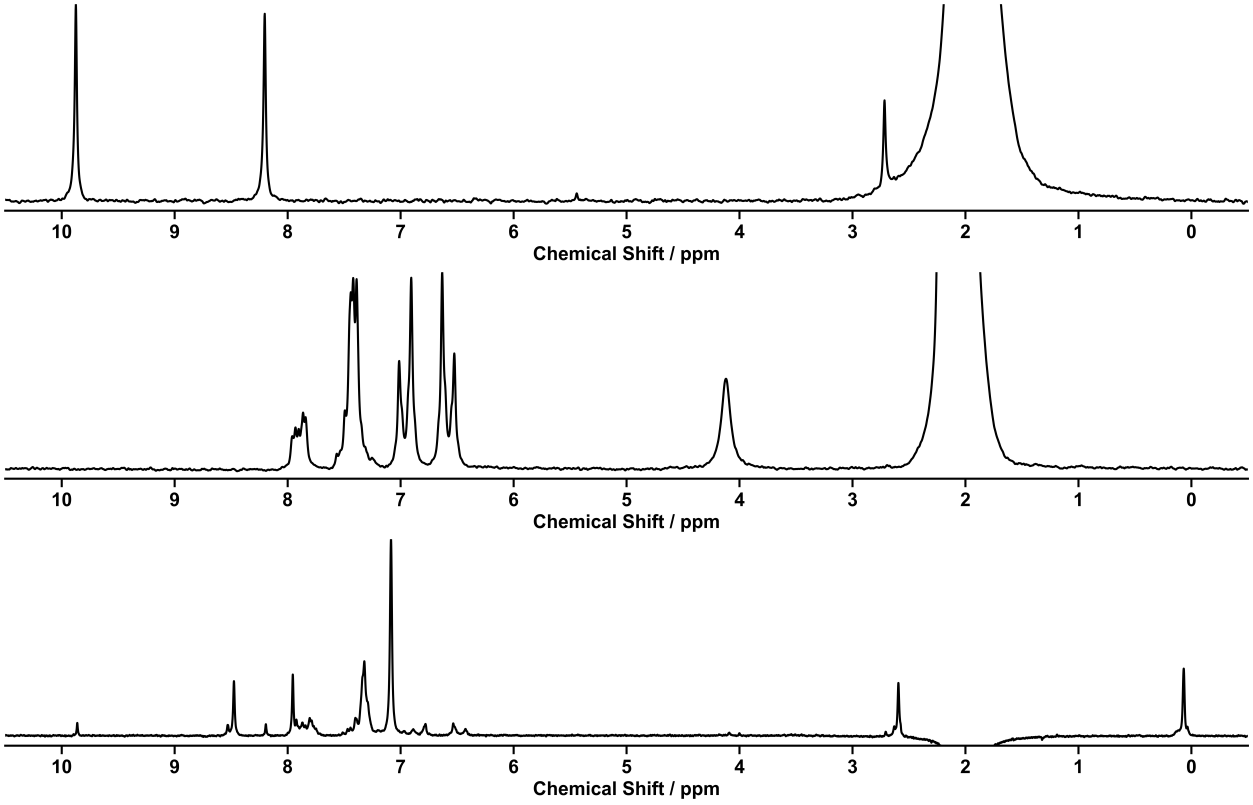
Reaction 138



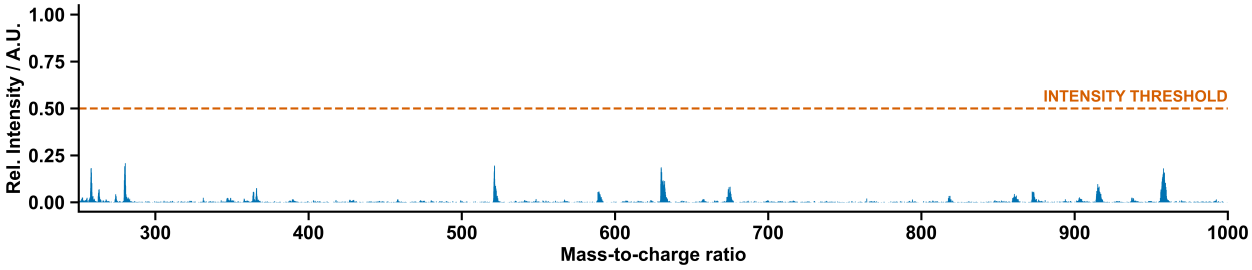
Scheme 116: Self-assembly of components 1, 13, with Silver(I) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 138.

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 labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 138. Decision motivations are also given.

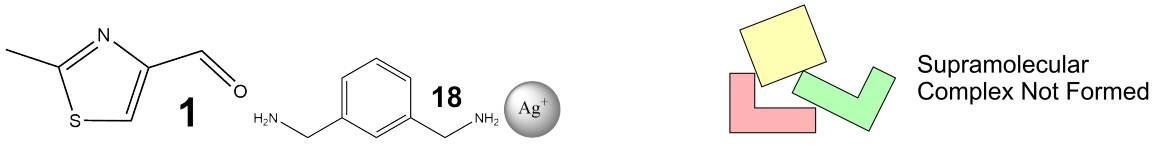


NMR Spectra 116: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 138.



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

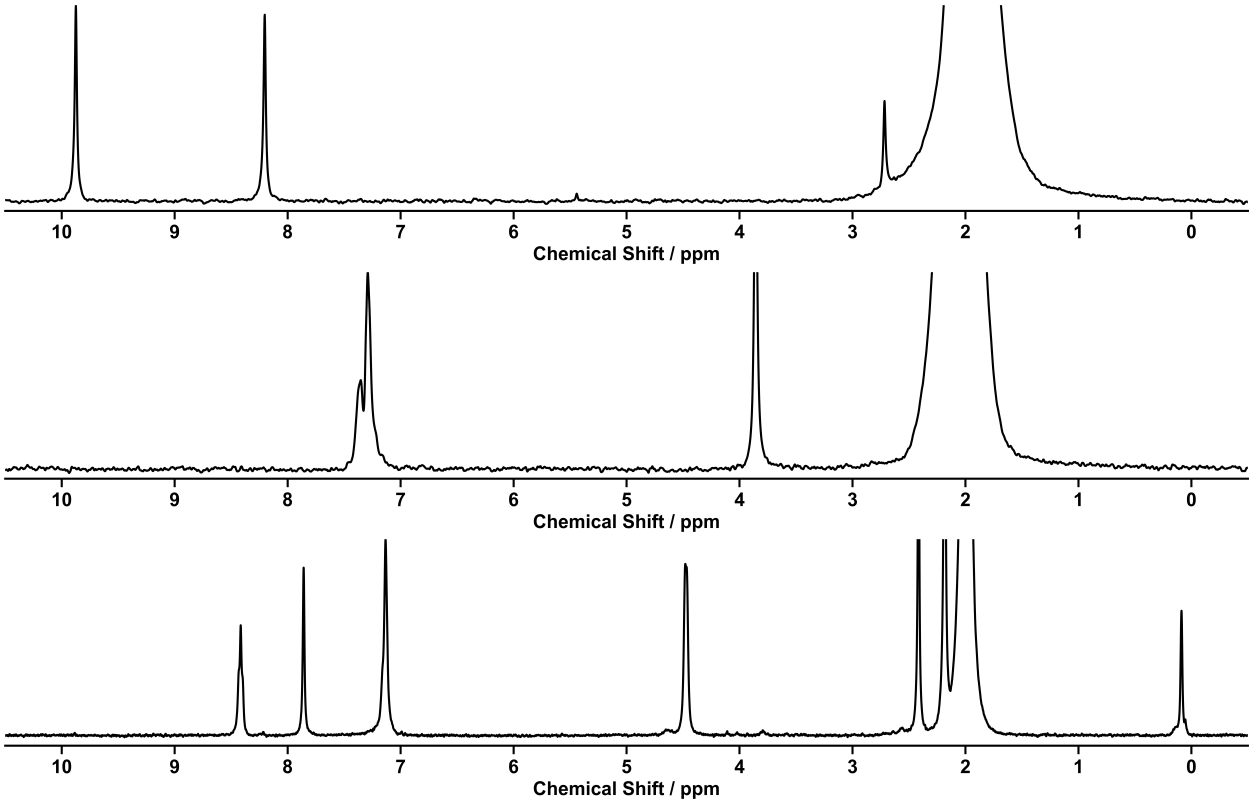
Reaction 139



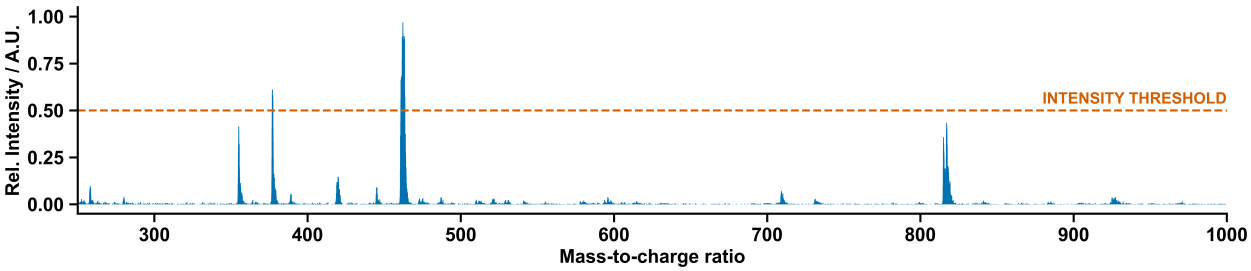
Scheme 117: Self-assembly of components 1, 18, with Silver(I) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 139.

<table>
<tr><td rowspan="2">Human Reaction Decision:
Failed</td><td>Human NMR Decision:
Pass</td><td colspan="2">NMR Spectra Category:
Single discrete species formed.</td></tr>
<tr><td>Human MS Decision:
Failed</td><td colspan="2">MS Spectra Category:
Reaction occurred, unknown product.</td></tr>
<tr><td rowspan="4">Decision Maker Reaction Decision:
N/A</td><td rowspan="2">Decision Maker NMR Decision:
N/A</td><td colspan="2">NMR Criteria 1:
N/A</td></tr>
<tr><td colspan="2">NMR Criteria 2:
N/A</td></tr>
<tr><td rowspan="2">Decision Maker MS Decision:
Pass</td><td>MS Criteria 1 and 2:
Pass</td><td>Number of predicted peaks found in MS spectra with appropriate intensity:
3</td></tr>
<tr><td>MS Criteria 3:
Pass</td><td>Number of counter-ions found:
2</td></tr>
</table>

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

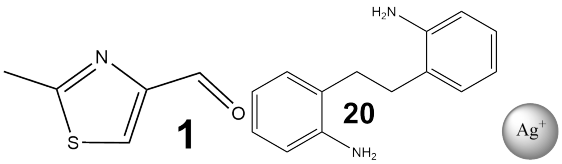


NMR Spectra 117: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 139.



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

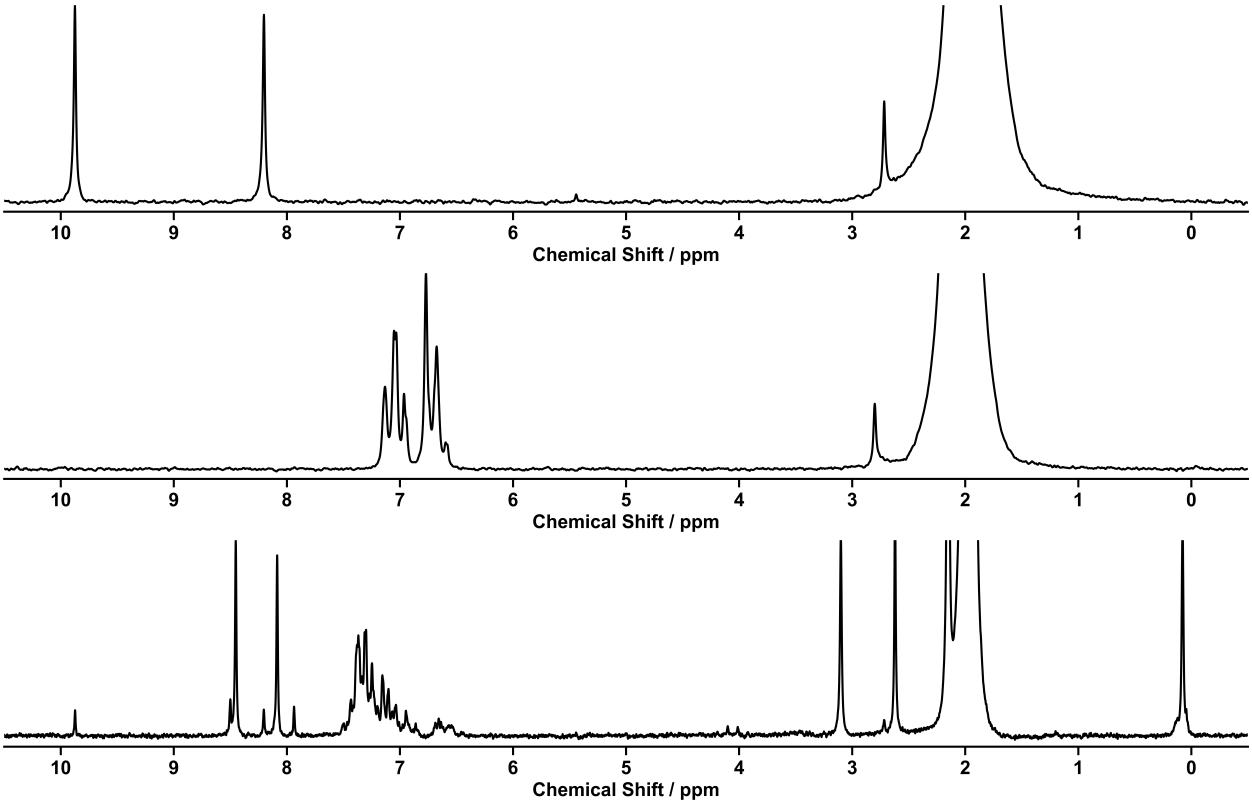
Reaction 140



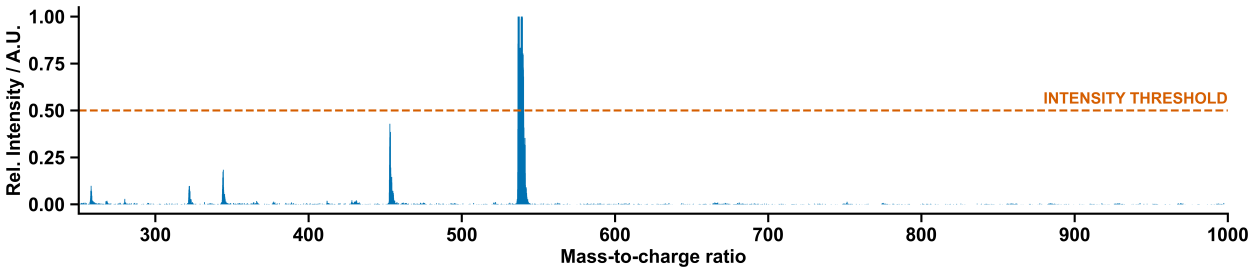
Scheme 118: Self-assembly of components 1, 20, with Silver(I) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 140.

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 labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 140. Decision motivations are also given.

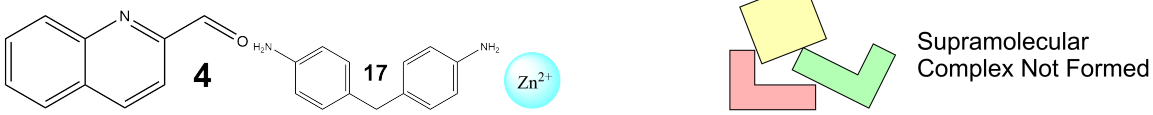


NMR Spectra 118: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 140.



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

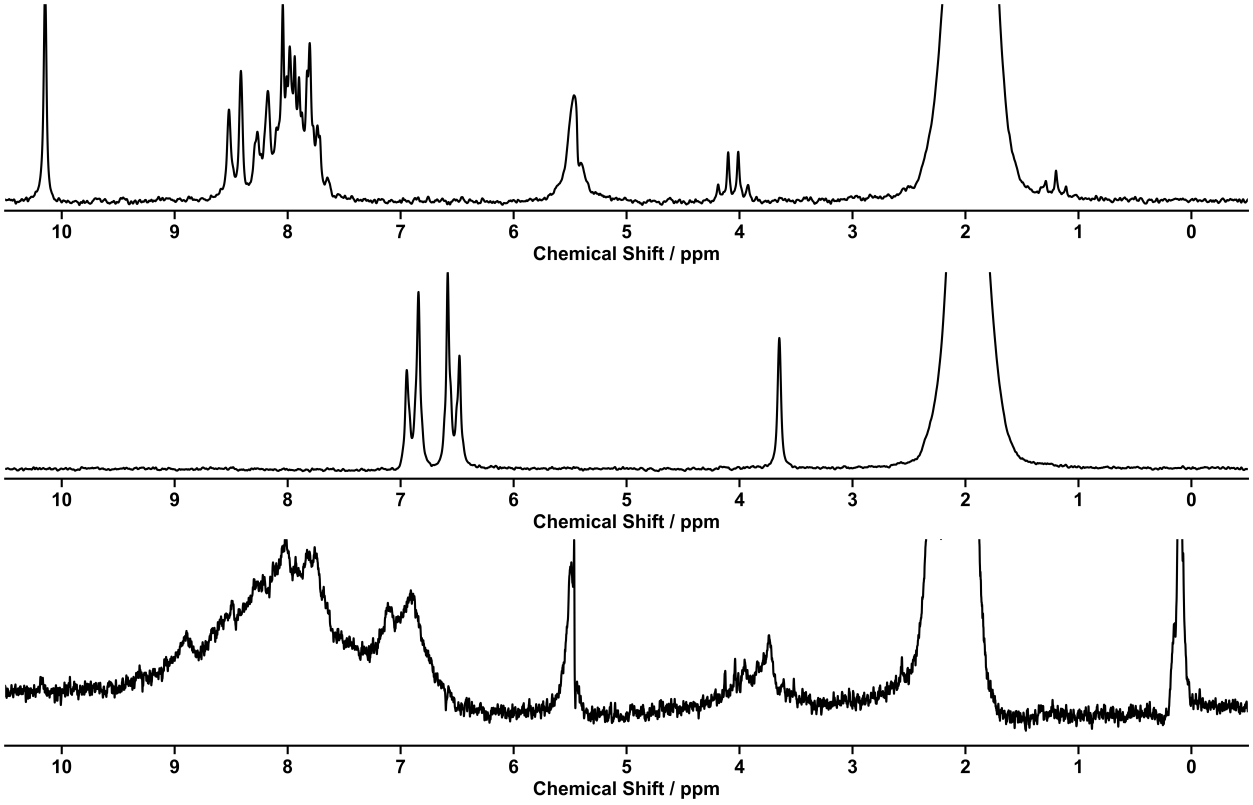
Reaction 141



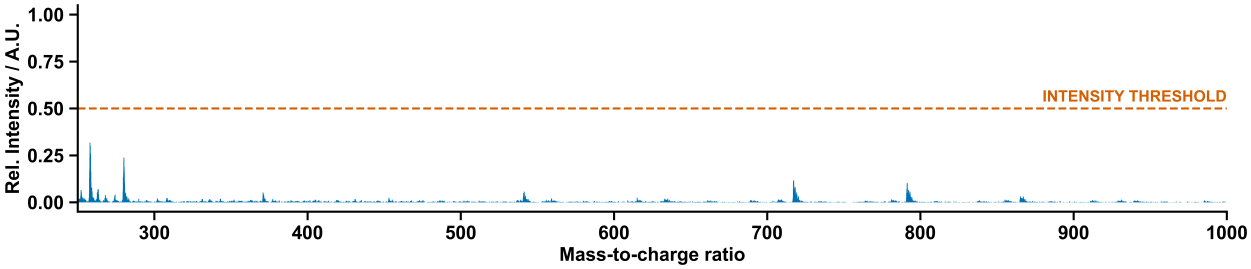
Scheme 119: Self-assembly of components 4, 17, with Zinc(II) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 141.

Human Reaction Decision: Failed	Human NMR Decision: Failed	NMR Spectra Category: Oligomers formed.	
	Human MS Decision: Failed	MS Spectra Category: Reaction failed.	
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 119: Human labled and Decsision maker labled outcomes for the ^{1}H NMR spectroscopy and ULPC-MS spectrometry of reaction 141. Decision motivations are also given.

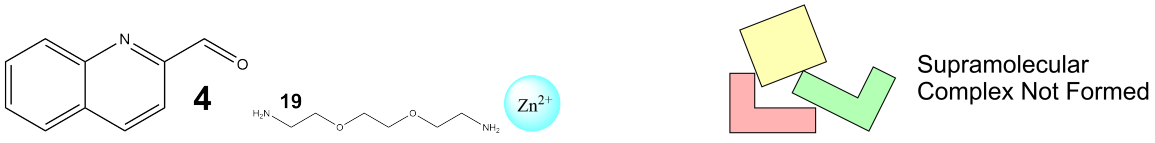


NMR Spectra 119: The stacked ^{1}H NMR spectra of the aldehyde (top), amine (middle), and reaction sample (bottom) for reaction 141.



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

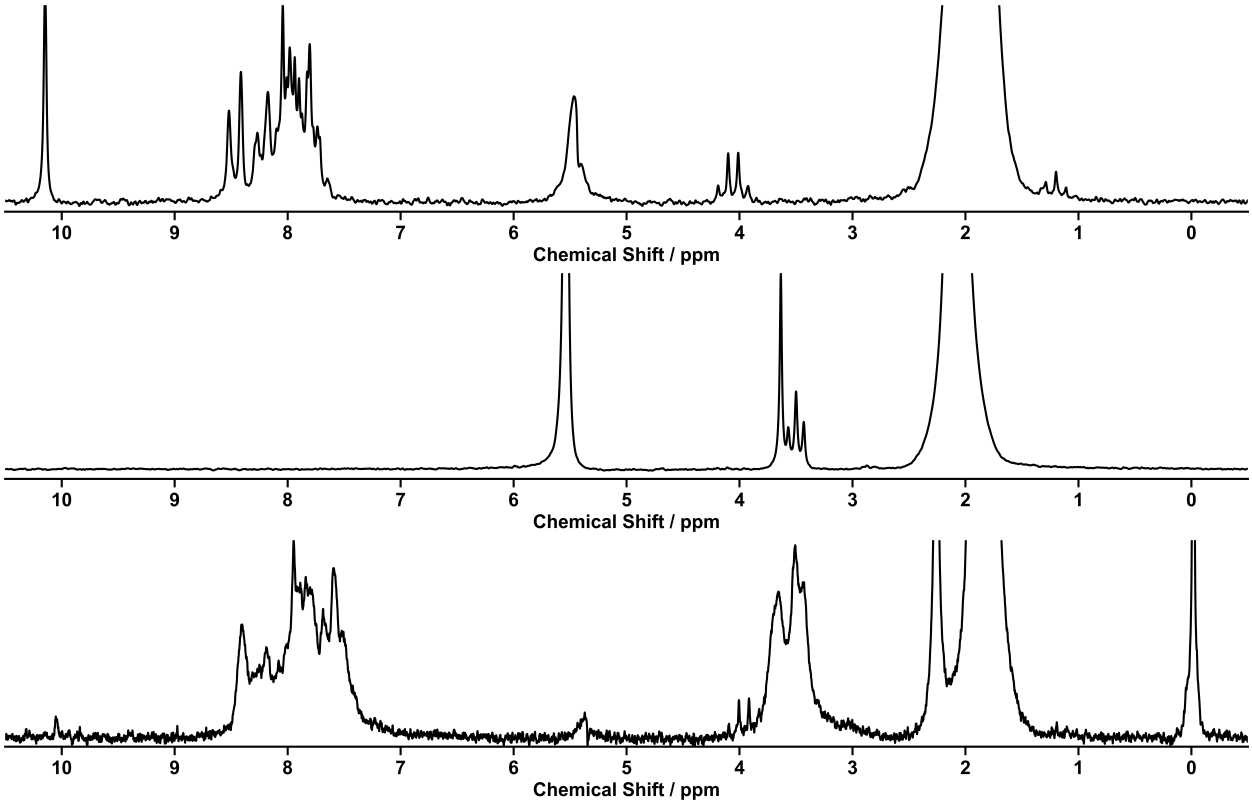
Reaction 142



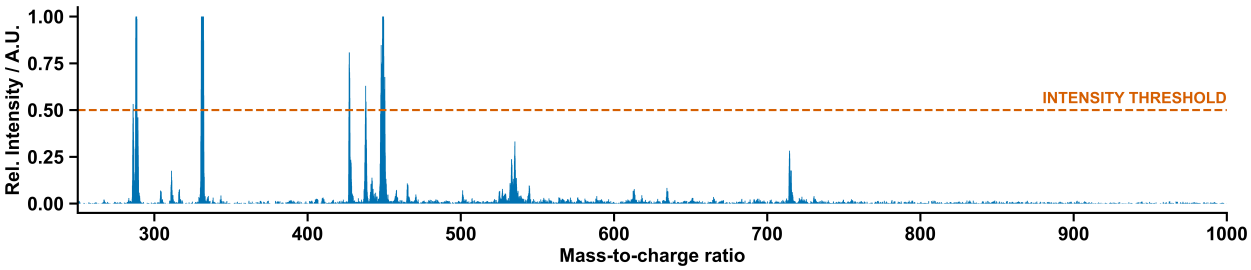
Scheme 120: Self-assembly of components 4, 19, with Zinc(II) in a 3.0:1.5:1.0 molar ratio in CH_3CN at 60°C for 40h. These are the reagents (starting materials) for reaction 142.

<table>
<tr><td rowspan="2">Human Reaction Decision:
Failed</td><td>Human NMR Decision:
Failed</td><td colspan="2">NMR Spectra Category:
Oligomers formed.</td></tr>
<tr><td>Human MS Decision:
Failed</td><td colspan="2">MS Spectra Category:
Reaction occurred, unknown product.</td></tr>
<tr><td rowspan="4">Decision Maker Reaction Decision:
N/A</td><td rowspan="2">Decision Maker NMR Decision:
N/A</td><td colspan="2">NMR Criteria 1:
N/A</td></tr>
<tr><td colspan="2">NMR Criteria 2:
N/A</td></tr>
<tr><td rowspan="2">Decision Maker MS Decision:
Pass</td><td>MS Criteria 1 and 2:
Pass</td><td>Number of predicted peaks found in MS spectra with appropriate intensity:
1</td></tr>
<tr><td>MS Criteria 3:
Pass</td><td>Number of counter-ions found:
1</td></tr>
</table>

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



NMR Spectra 120: The stacked ^{1}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.