

[Dicyclohexyl(sulfanylidene)- λ^5 -phosphanyl]methanol

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SUPPLEMENTARY MATERIALS

Contents:

- Figure S1.** IR spectrum of $\text{Cy}_2\text{P}(\text{S})\text{CH}_2\text{OH}$ (**1**).
- Figure S2.** ^1H NMR spectrum (upper) and detail showing coupling (lower) of $\text{Cy}_2\text{P}(\text{S})\text{CH}_2\text{OH}$ (**1**).
- Figure S3.** $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of $\text{Cy}_2\text{P}(\text{S})\text{CH}_2\text{OH}$ (**1**).
- Figure S4.** $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of $\text{Cy}_2\text{P}(\text{S})\text{CH}_2\text{OH}$ (**1**).
- Figure S5.** COSY NMR spectrum (upper view) and enlarged view (lower) of $\text{Cy}_2\text{P}(\text{S})\text{CH}_2\text{OH}$ (**1**).
- Figure S6.** NOESY NMR spectrum (upper view) and enlarged view (lower) of $\text{Cy}_2\text{P}(\text{S})\text{CH}_2\text{OH}$ (**1**).
- Figure S7.** HSQC NMR spectrum (upper view) and enlarged view (lower) of $\text{Cy}_2\text{P}(\text{S})\text{CH}_2\text{OH}$ (**1**).
- Figure S8.** HMBC NMR spectrum (upper view) and enlarged view (lower) of $\text{Cy}_2\text{P}(\text{S})\text{CH}_2\text{OH}$ (**1**).
- Figure S9.** Negative-ion ESI mass spectrum of $\text{Cy}_2\text{P}(\text{S})\text{CH}_2\text{OH}$ (**1**) in methanol solution, with added sodium formate ionisation aid. Capillary exit voltage 90 V, Skimmer 1 voltage 30 V.
- Figure S10.** Positive-ion ESI mass spectrum of $\text{Cy}_2\text{P}(\text{S})\text{CH}_2\text{OH}$ (**1**) in methanol solution, with added sodium formate. Capillary exit voltage 90 V, Skimmer 1 voltage 30 V.

Figure S11. Positive-ion ESI mass spectrum of $\text{Cy}_2\text{P}(\text{S})\text{CH}_2\text{OH}$ (**1**) in methanol solution, with added sodium formate, showing the isotope pattern of the $[\text{2}(\textbf{1}) + \text{Na}]^+$ ion. Capillary exit voltage 90 V, Skimmer 1 voltage 30 V.

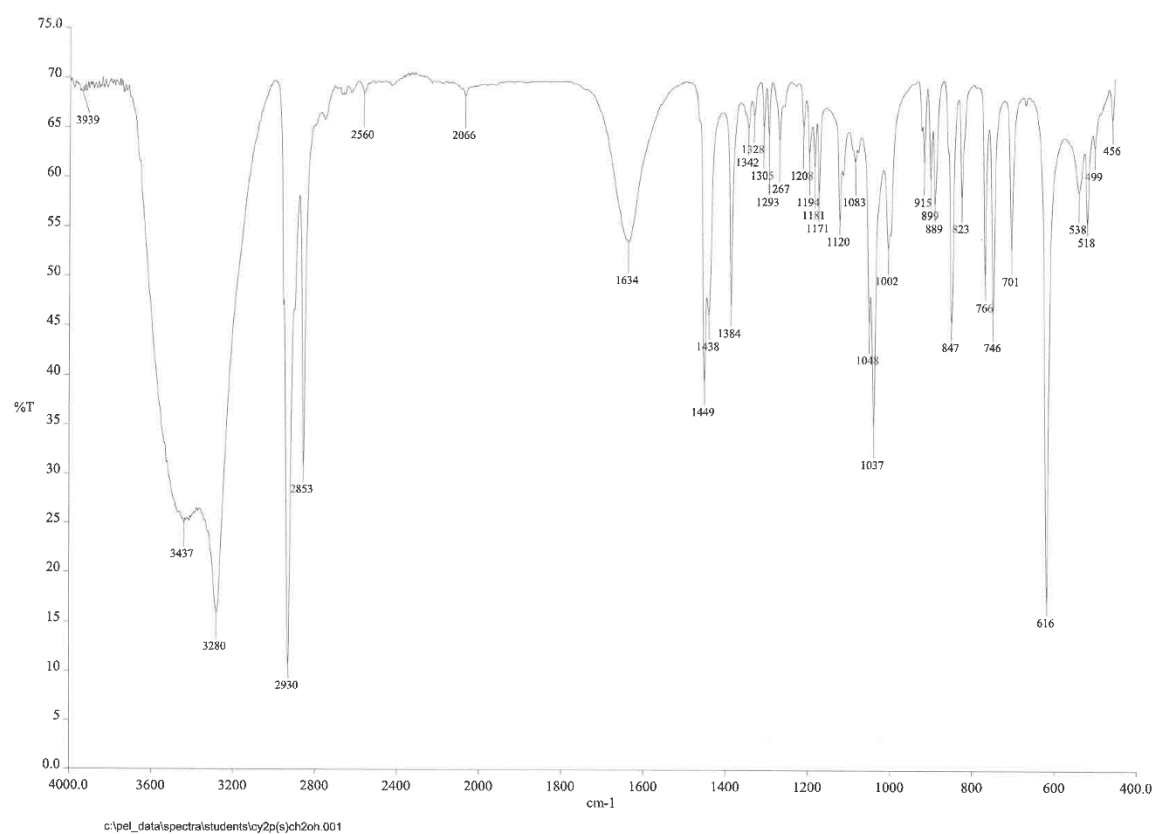
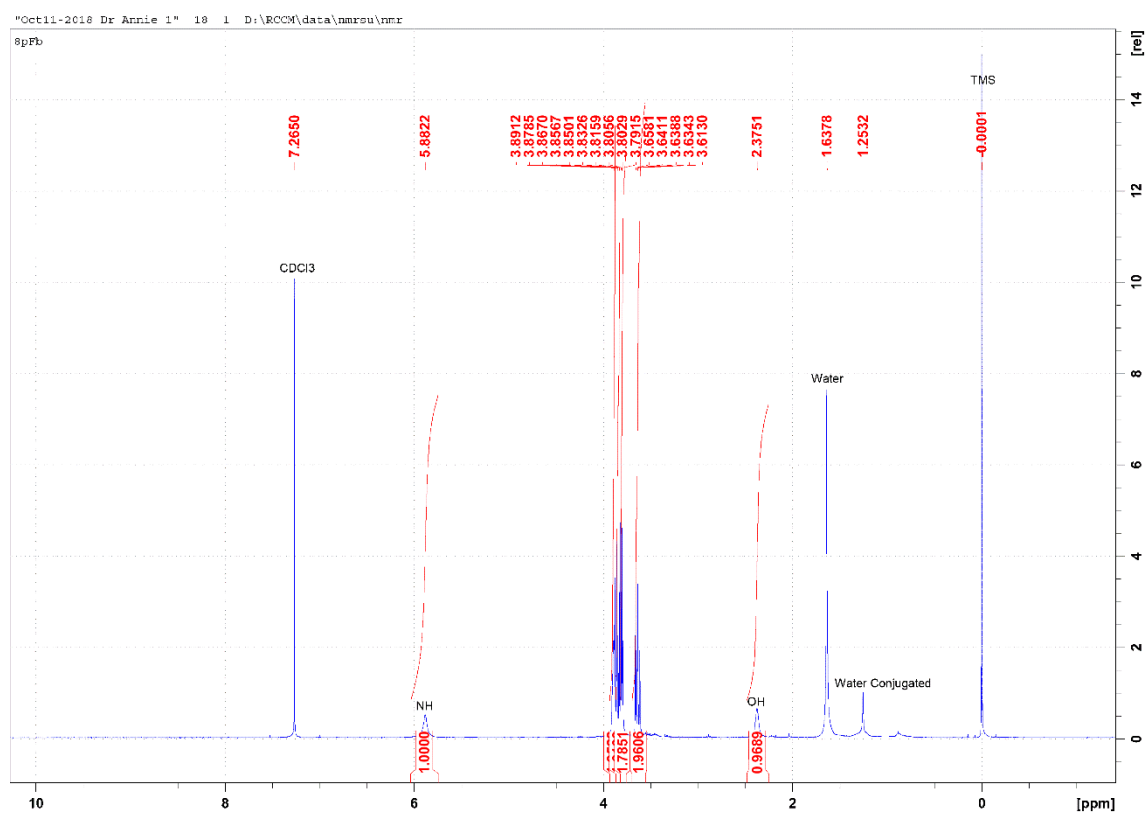


Figure S1. IR spectrum of $\text{Cy}_2\text{P}(\text{S})\text{CH}_2\text{OH}$ (1).



¹H

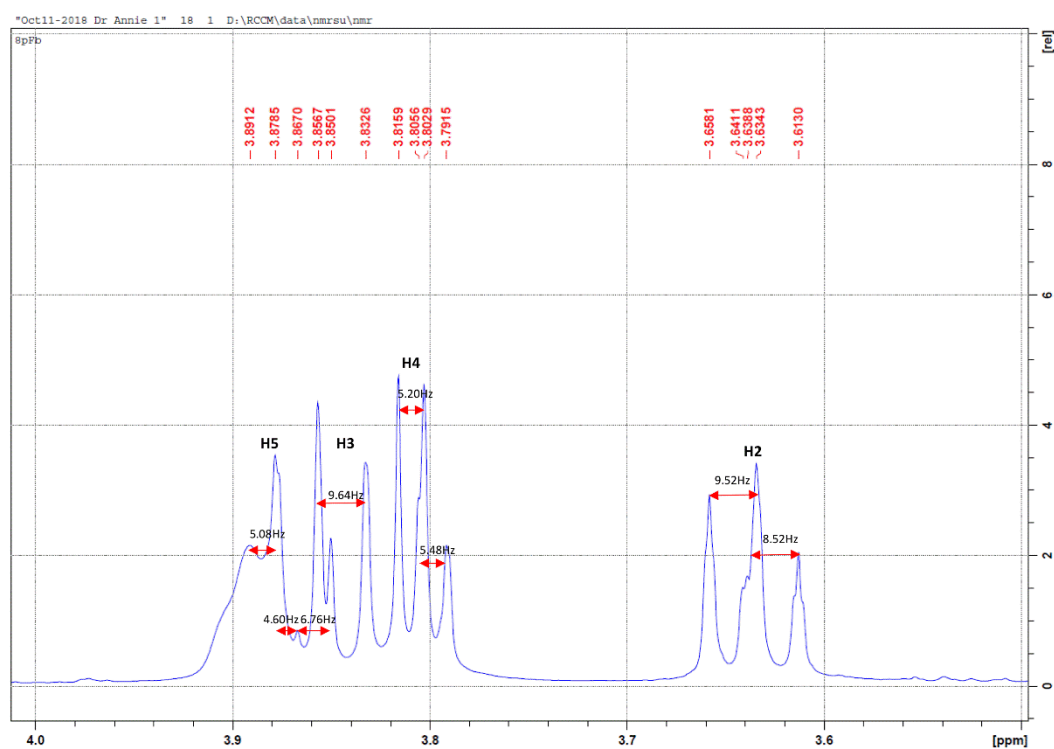


Figure S2. ¹H NMR spectrum (upper view) and detail showing coupling (lower) of Cy₂P(S)CH₂OH (**1**)

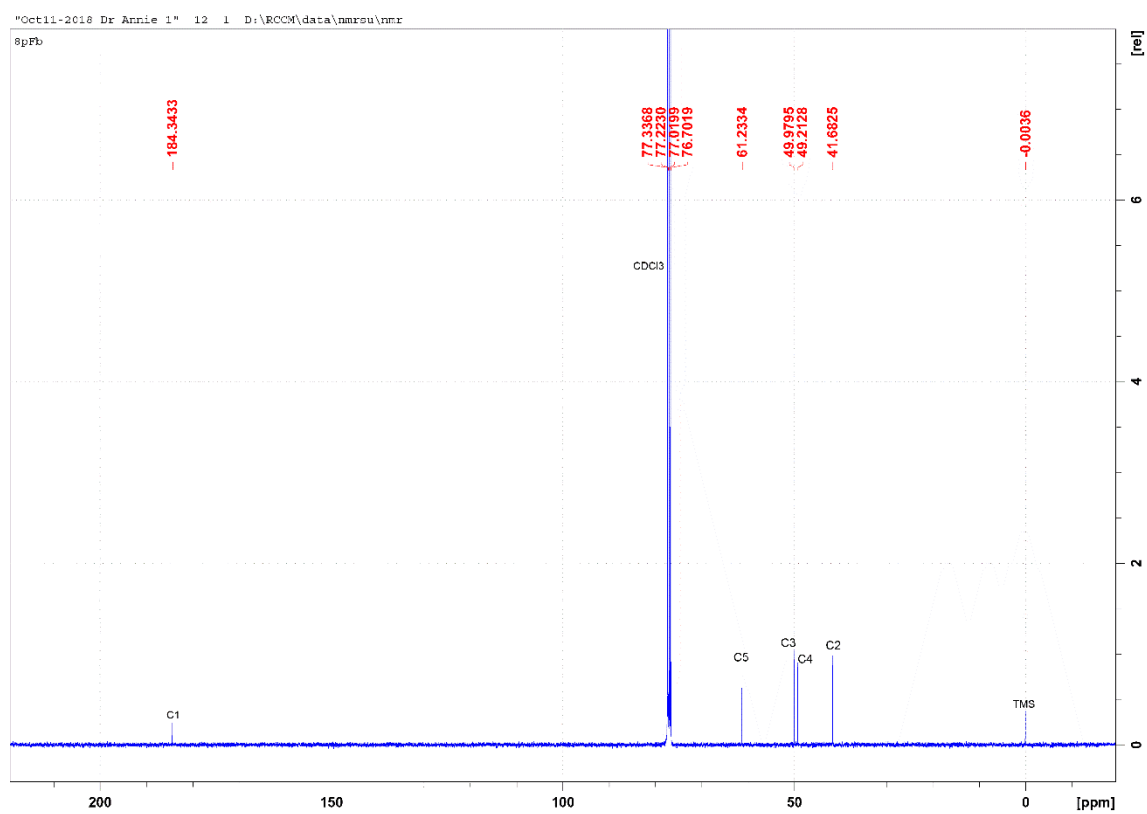


Figure S3. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of $\text{Cy}_2\text{P}(\text{S})\text{CH}_2\text{OH}$ (**1**).

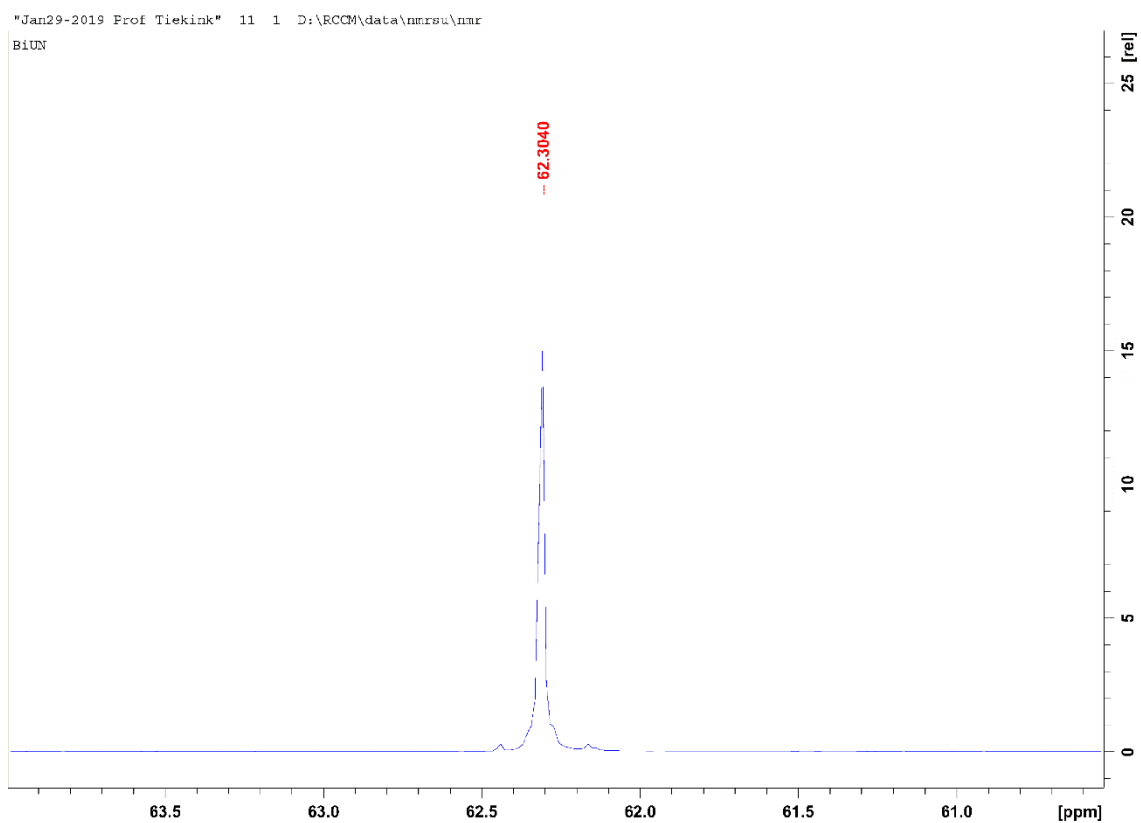


Figure S4. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of $\text{Cy}_2\text{P}(\text{S})\text{CH}_2\text{OH}$ (**1**).

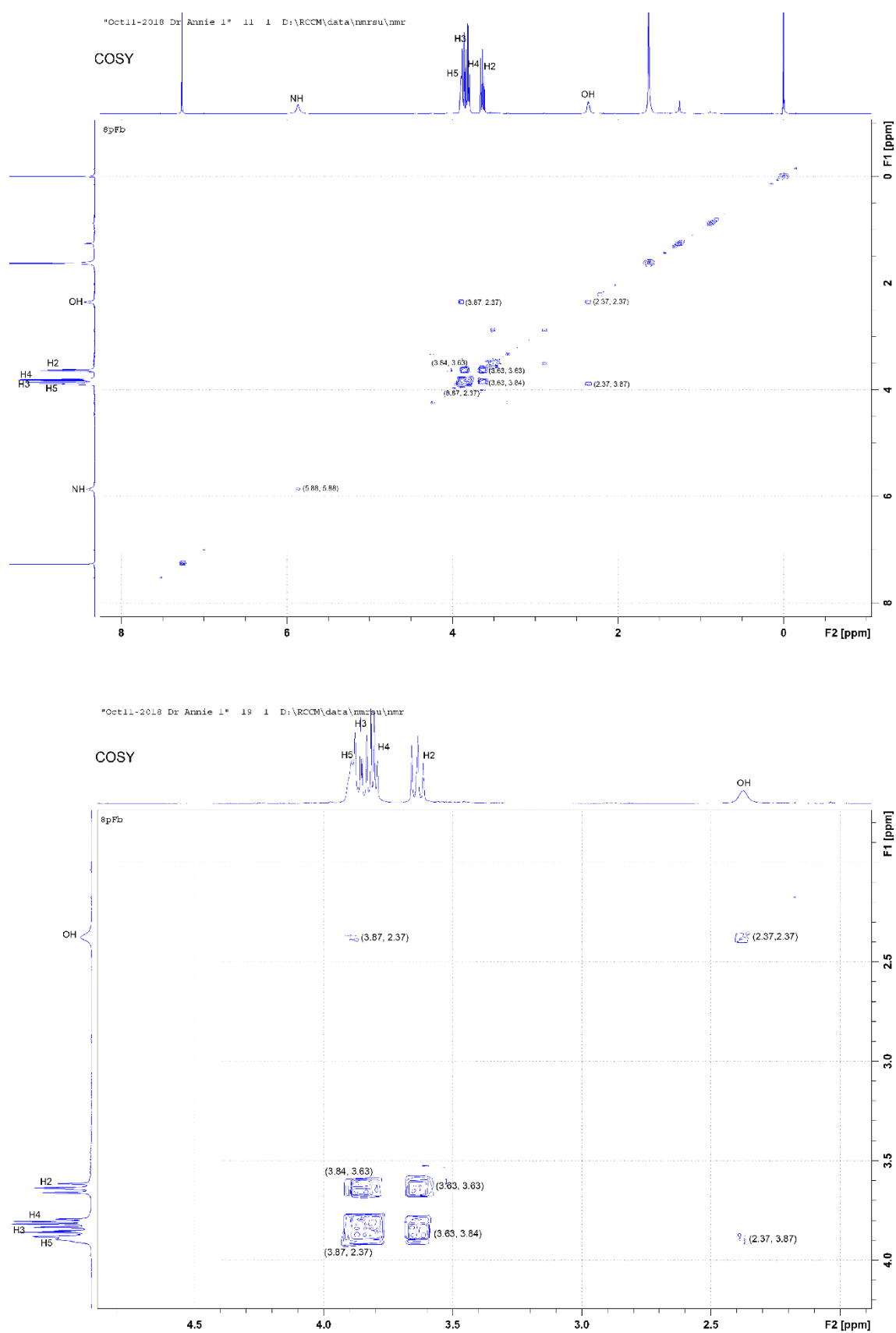


Figure S5. COSY NMR spectrum (upper view) and enlarged view (lower) of $\text{Cy}_2\text{P}(\text{S})\text{CH}_2\text{OH}$ (**1**).

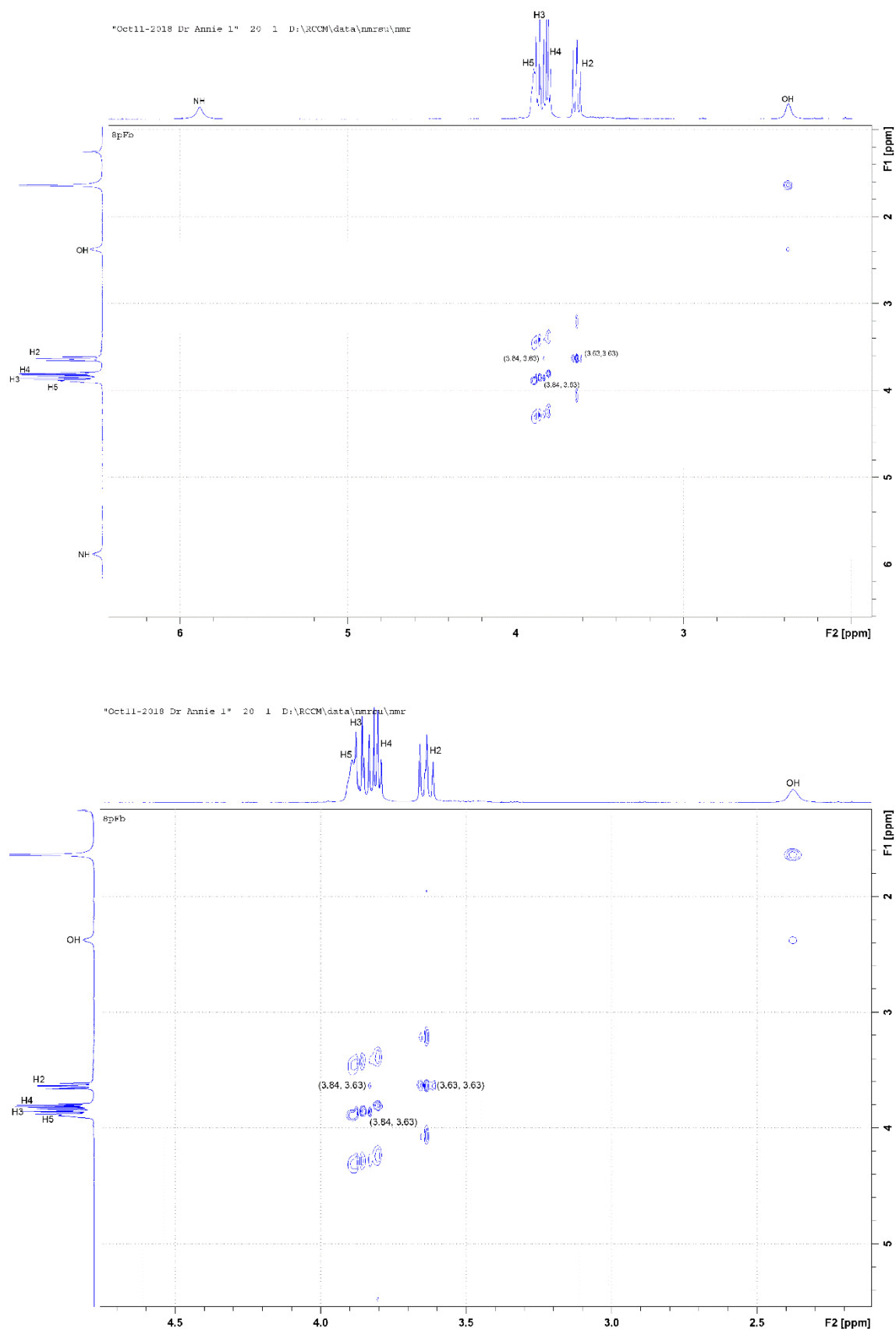


Figure S6. NOESY NMR spectrum (upper view) and enlarged view (lower) of $\text{Cy}_2\text{P}(\text{S})\text{CH}_2\text{OH}$ (1).

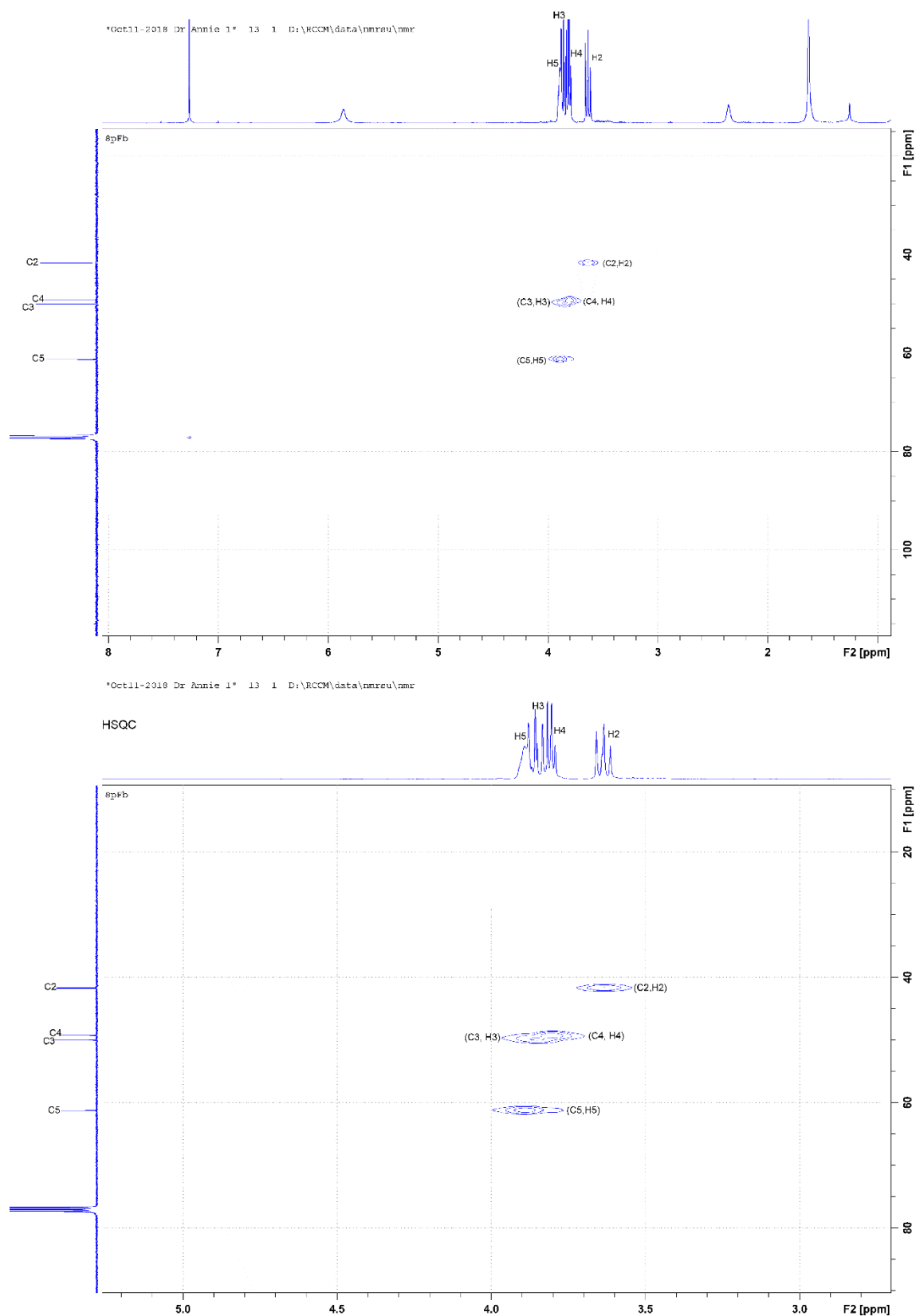


Figure S7. HSQC NMR spectrum (upper view) and enlarged view (lower) of Cy₂P(S)CH₂OH (1).

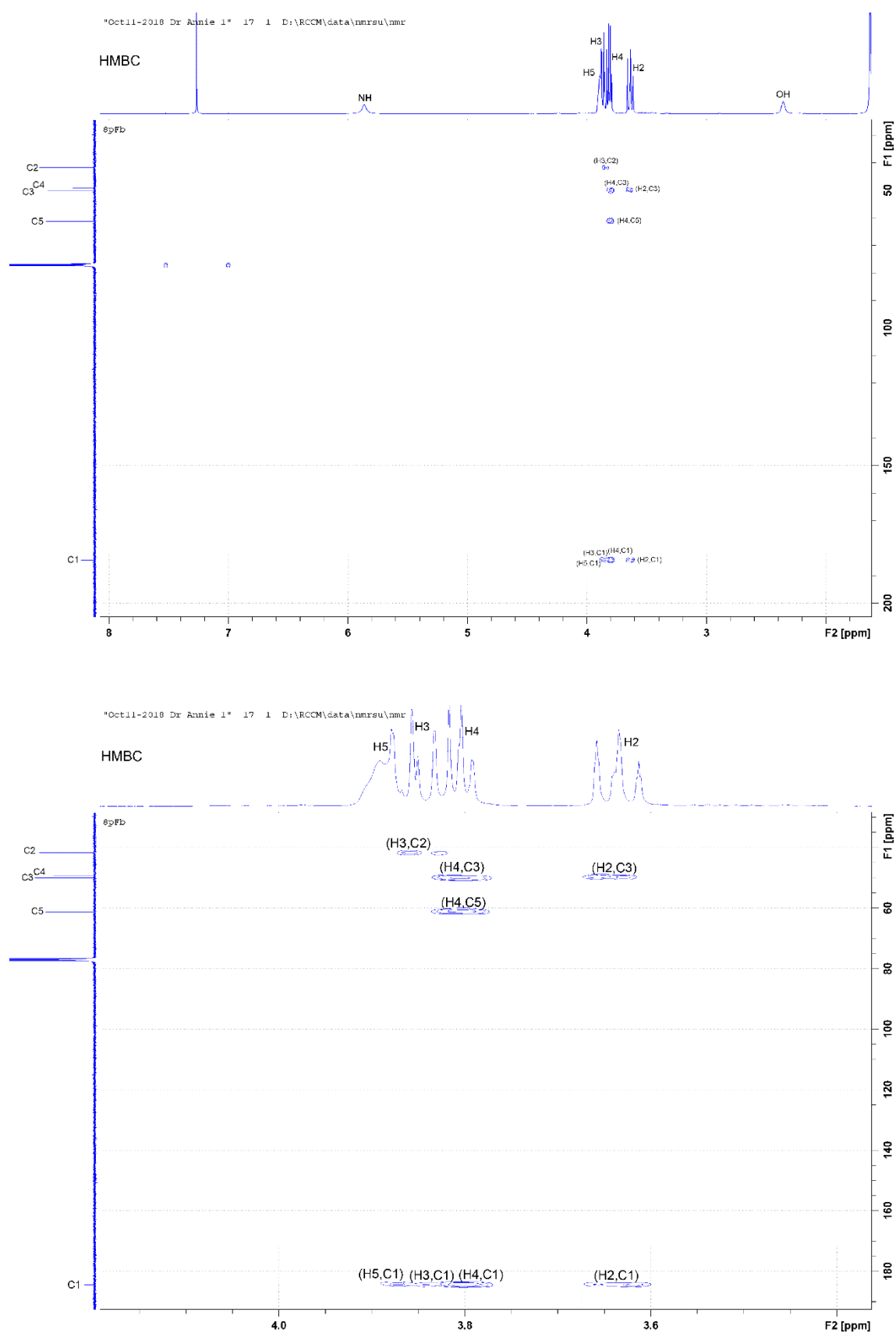


Figure S8. HMBC NMR spectrum (upper view) and enlarged view (lower) of $\text{Cy}_2\text{P}(\text{S})\text{CH}_2\text{OH}$ (**1**).

Generic Display Report

Analysis Info

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Method neglowaug2016.m
Sample Name
Comment Cy2P(S)CH₂OH in methanol

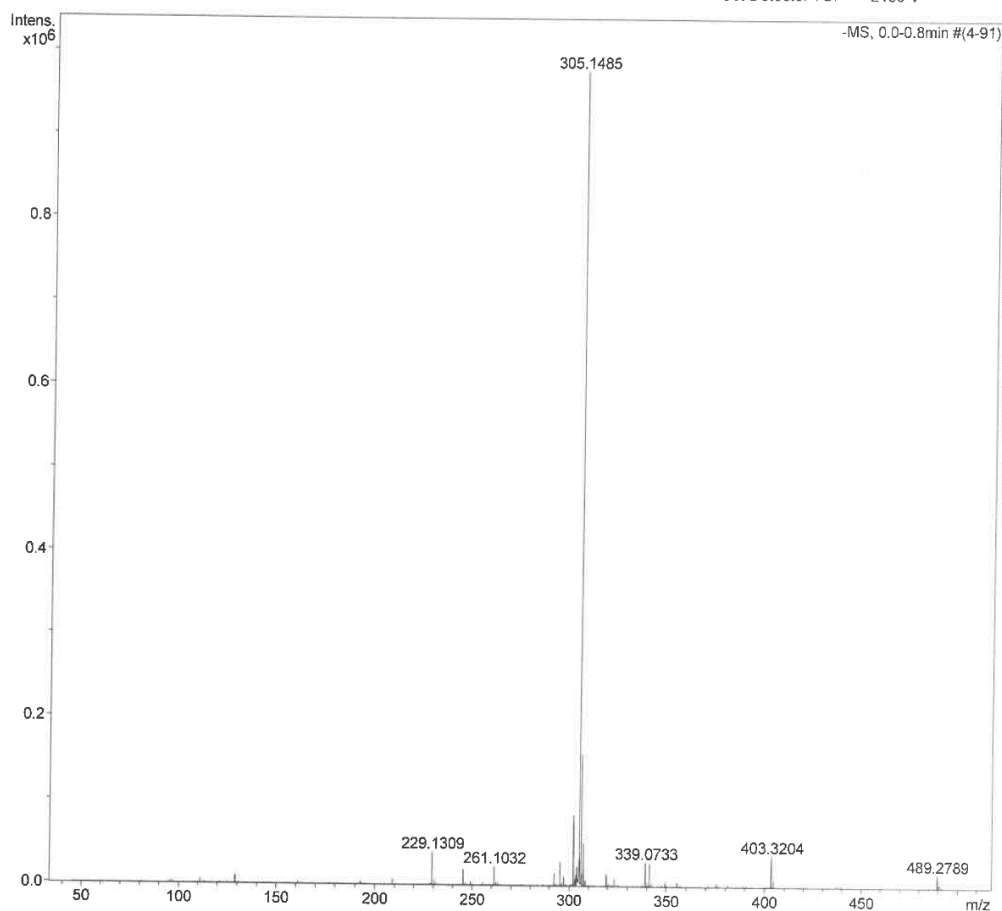
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Operator administrator
Instrument micrOTOF

negative ion + 3 drops sodium formate solution (0.002 M)

Acquisition Parameter

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		Set Hexapole 1	-25.0 V	Set Flight Tube	8600 V
				Set Detector TOF	2183 V



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Figure S9. Negative-ion ESI mass spectrum of Cy₂P(S)CH₂OH (**1**) in methanol solution, with added sodium formate ionisation aid. Capillary exit voltage 90 V, Skimmer 1 voltage 30 V.

Generic Display Report

Analysis Info

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Method poslowaug2016.m
Sample Name
Comment Cy2P(S)CH₂OH in methanol

Acquisition Date 5/13/2019 3:49:37 PM

Operator administrator
Instrument micrOTOF

positive ion + 3 drops sodium formate solution (0.002 M)

Acquisition Parameter

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Scan End	800 m/z	Set Skimmer 1	30.0 V	Set Reflector	1700 V
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				Set Detector TOF	2183 V

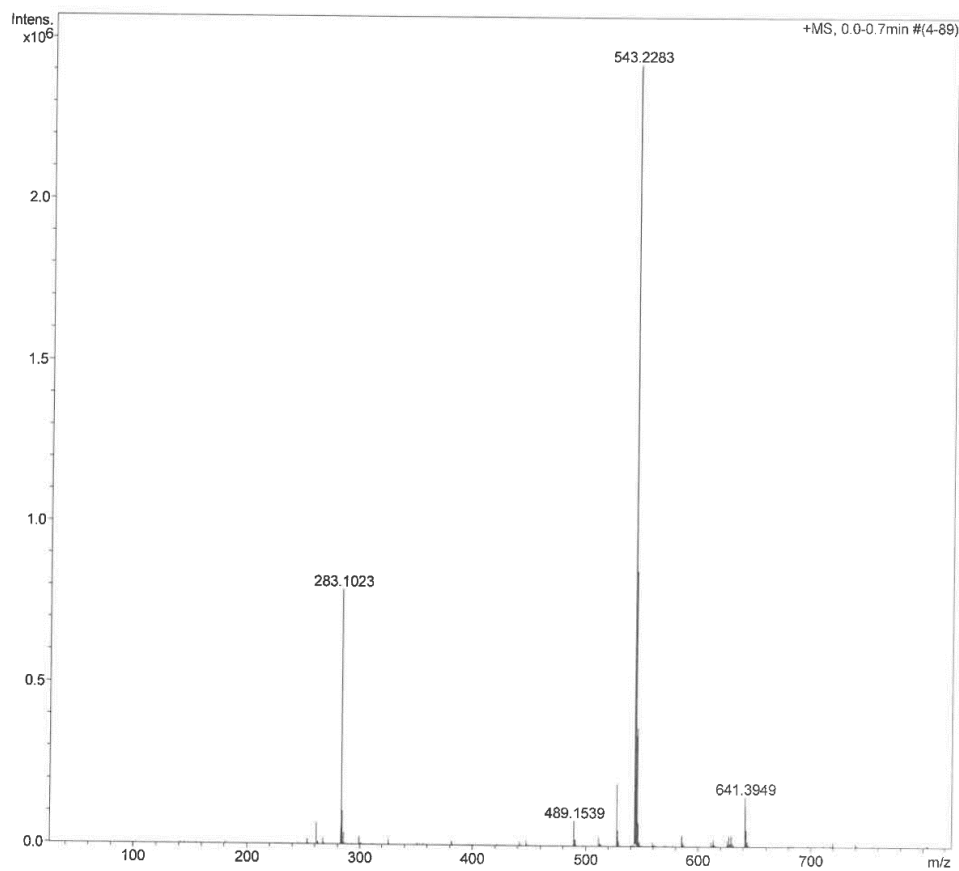


Figure S10. Positive-ion ESI mass spectrum of Cy₂P(S)CH₂OH (**1**) in methanol solution, with added sodium formate. Capillary exit voltage 90 V, Skimmer 1 voltage 30 V.

Generic Display Report

Analysis Info

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Method poslowaug2016.m
Sample Name
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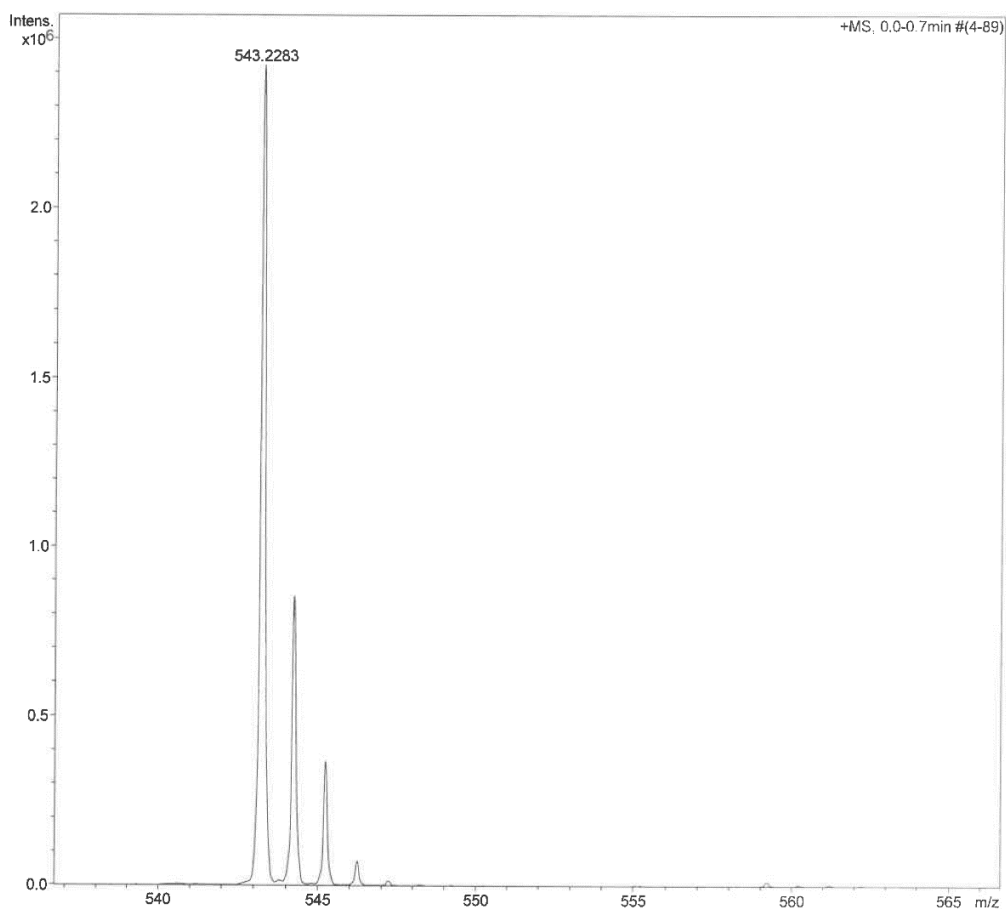
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Operator administrator
Instrument micrOTOF

positive ion + 3 drops sodium formate solution (0.002 M)

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Corrector Fill	53 V
n/a	n/a	Set Capillary Exit	90.0 V	Set Pulsar Pull	790 V
Scan Begin	50 m/z	Set Hexapole RF	80.0 V	Set Pulsar Push	790 V
Scan End	800 m/z	Set Skimmer 1	30.0 V	Set Reflector	1700 V
		Set Hexapole 1	23.0 V	Set Flight Tube	8600 V
				Set Detector TOF	2183 V



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Figure S11. Positive-ion ESI mass spectrum of Cy₂P(S)CH₂OH (**1**) in methanol solution, with added sodium formate, showing the isotope pattern of the [2(**1**) + Na]⁺ ion. Capillary exit voltage 90 V, Skimmer 1 voltage 30 V.