

C₃-triiodocyclotrimeratrylene as key intermediate to fluorescent probes: Application to selective choline recognition

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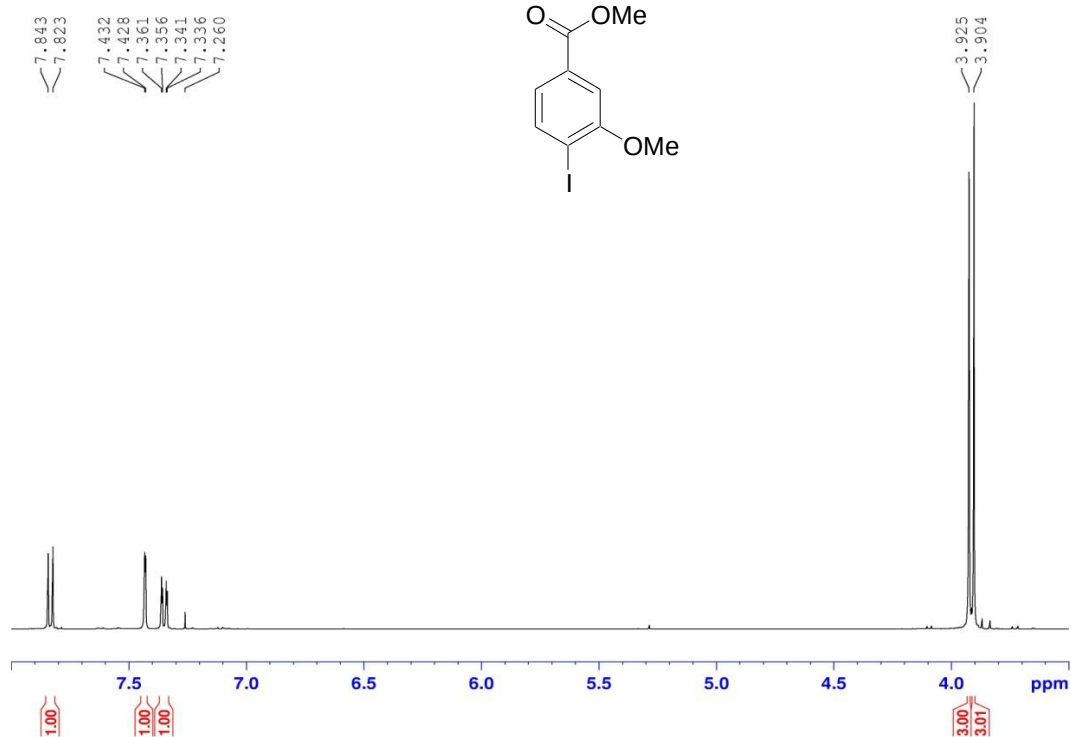
Supporting Information

1. ¹H, ¹³C NMR and ³¹P NMR spectra of all synthesized compounds
2. DOSY-NMR experiments
3. Fluorescence titration data

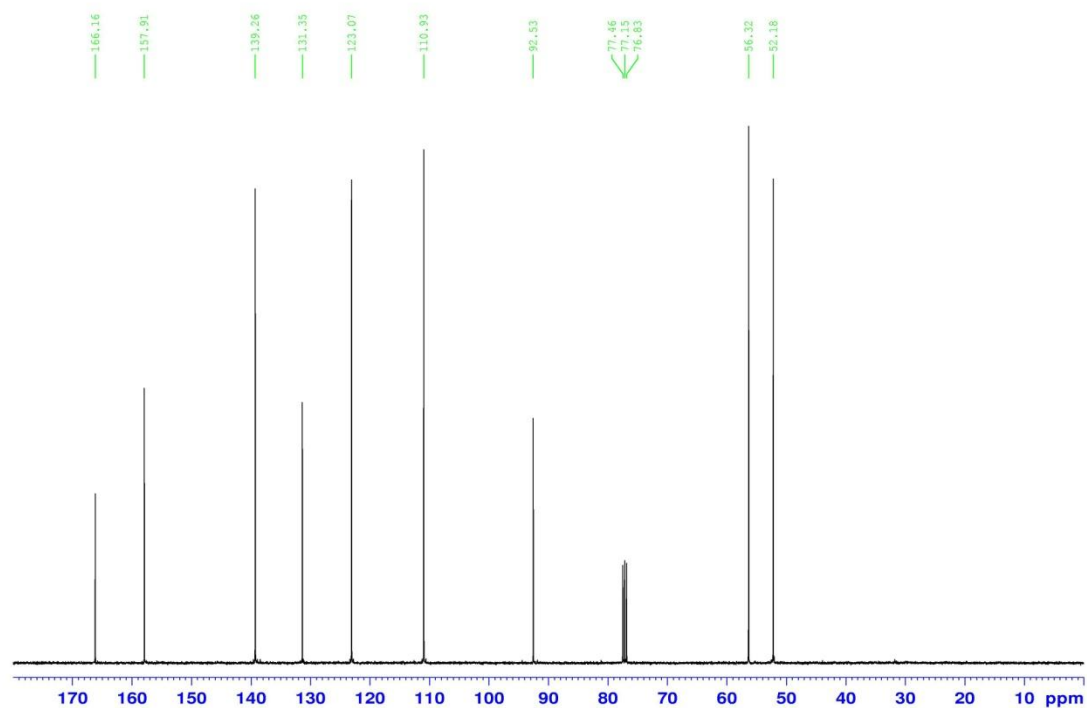
1. ^1H , ^{13}C MNR and ^{31}P NMR spectra of all synthesized compounds

4-Iodo-3-methoxybenzoic acid methyl ester

^1H NMR, CDCl_3 , 400 MHz, 298K

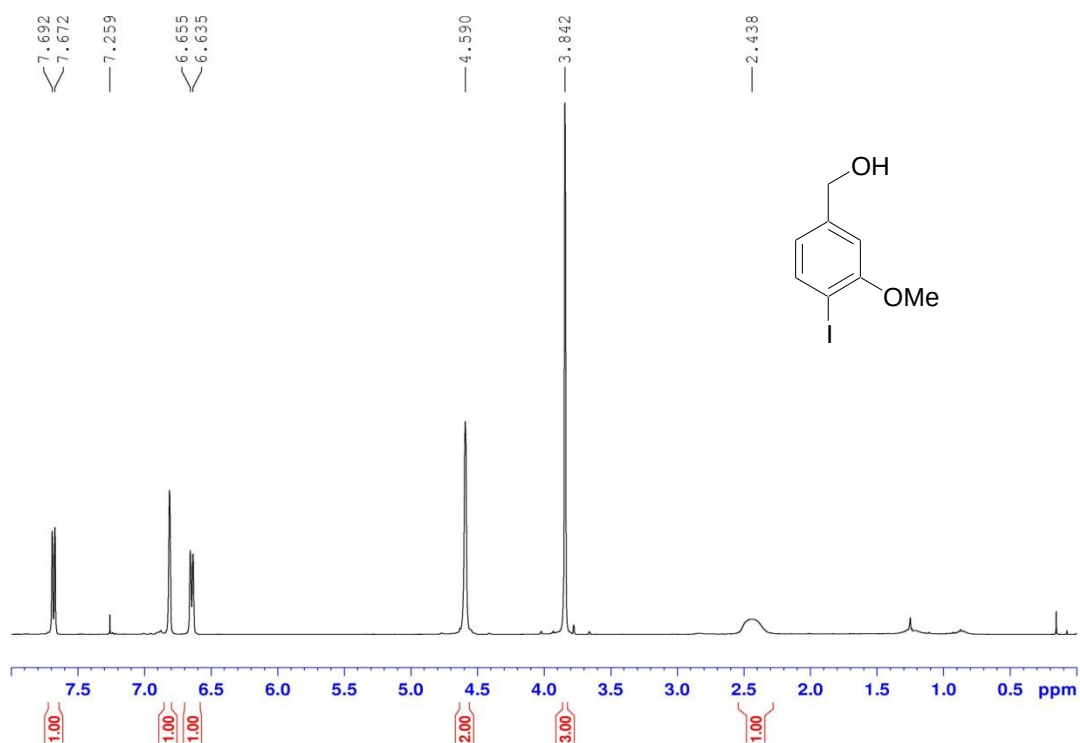


^{13}C NMR, CDCl_3 , 100 MHz, 298K

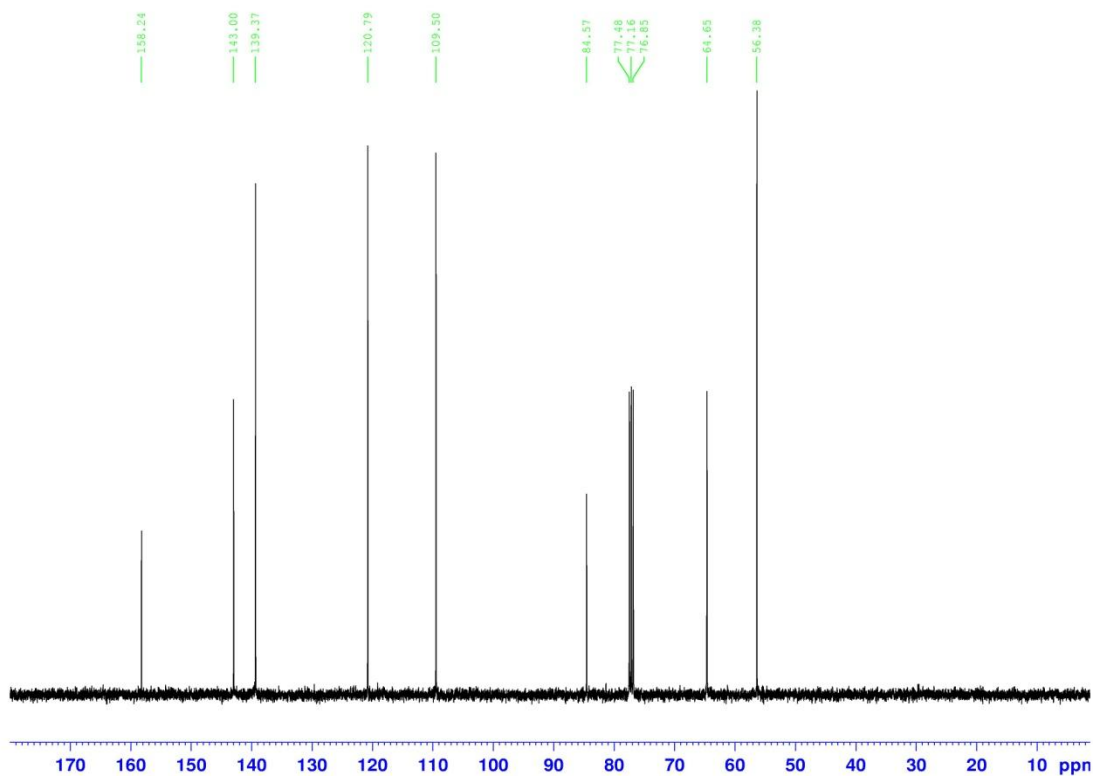


4-Iodo-3-methoxybenzyl alcohol (2)

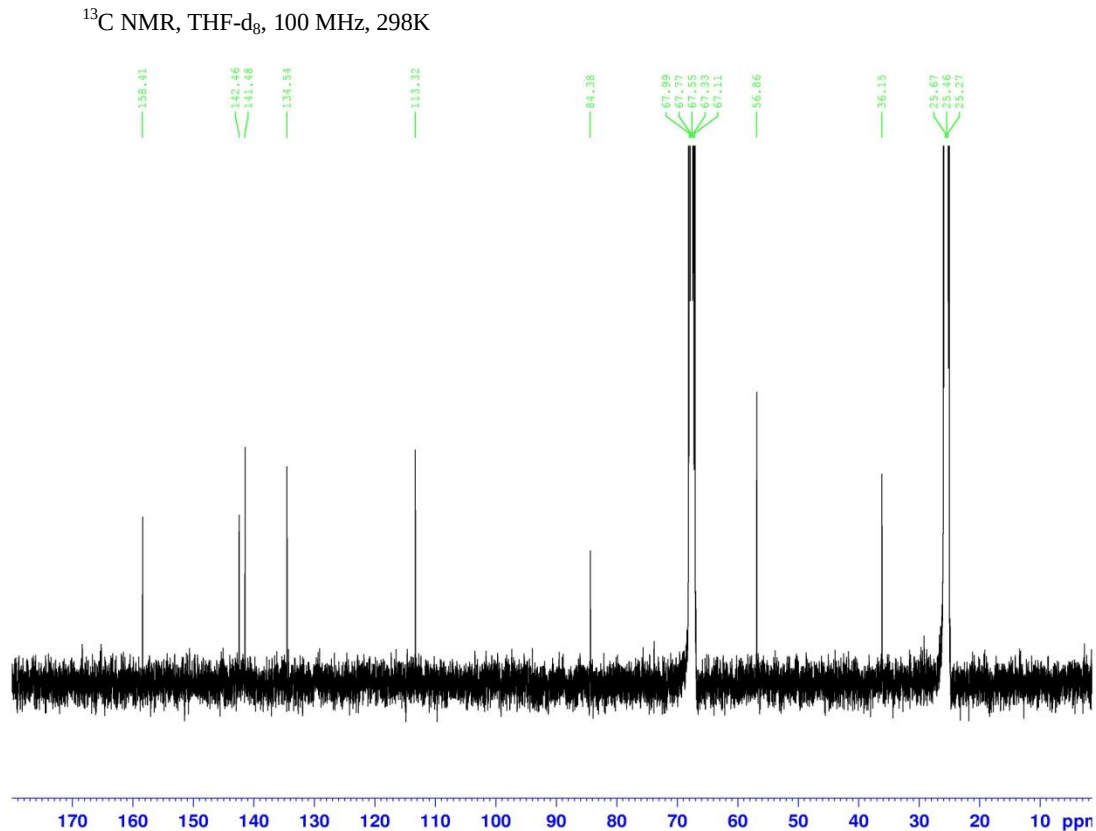
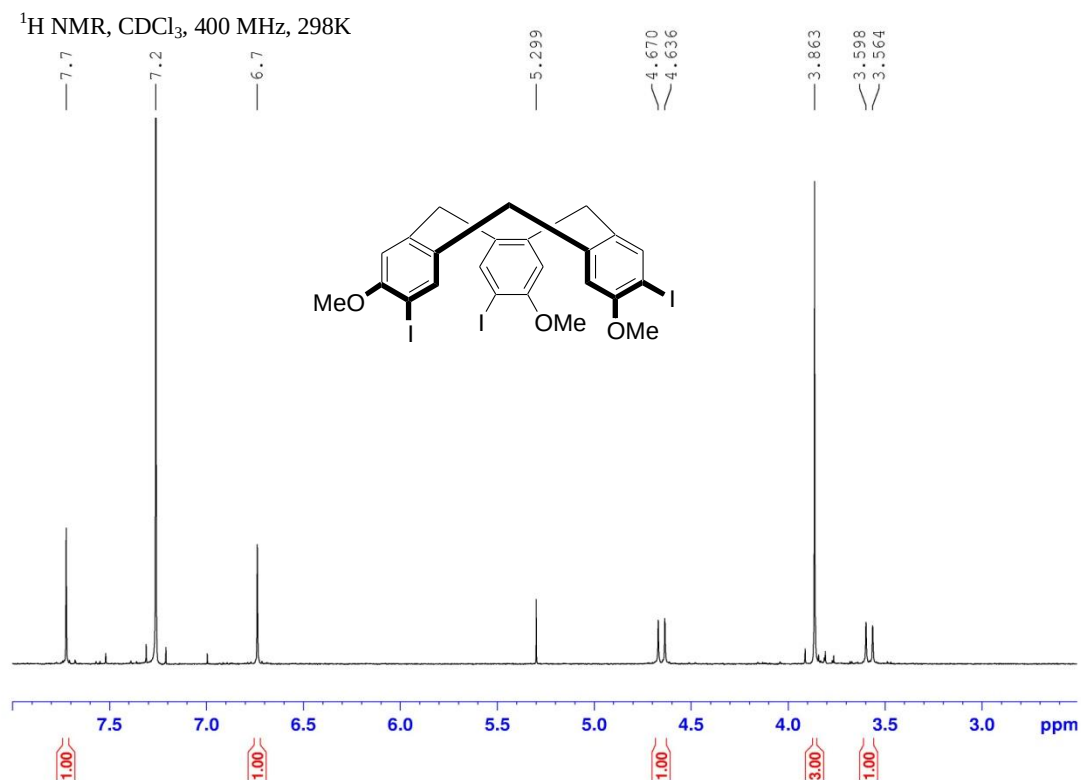
^1H NMR, CDCl_3 , 400 MHz, 298K



^{13}C NMR, CDCl_3 , 100 MHz, 298K

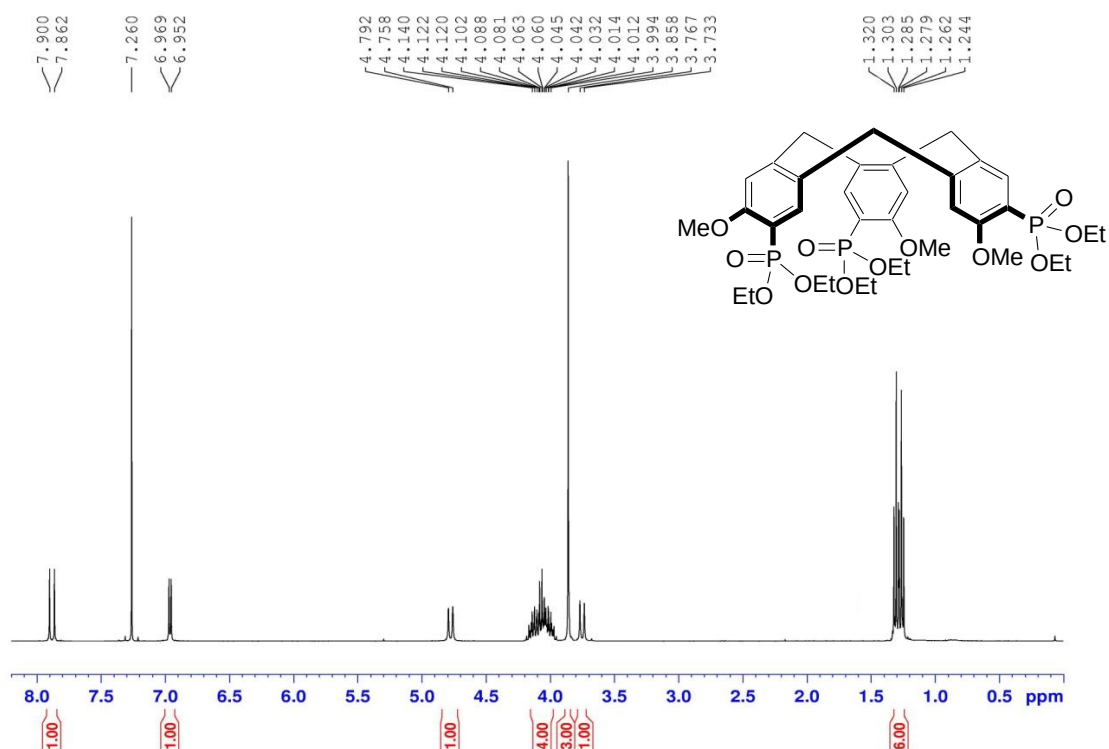


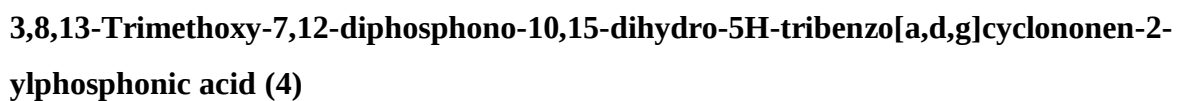
2,7,12-Triiodo-3,8,13-trimethoxy-10,15-dihydro-5H-tribenzo[*a,d,g*]cyclononene (1)

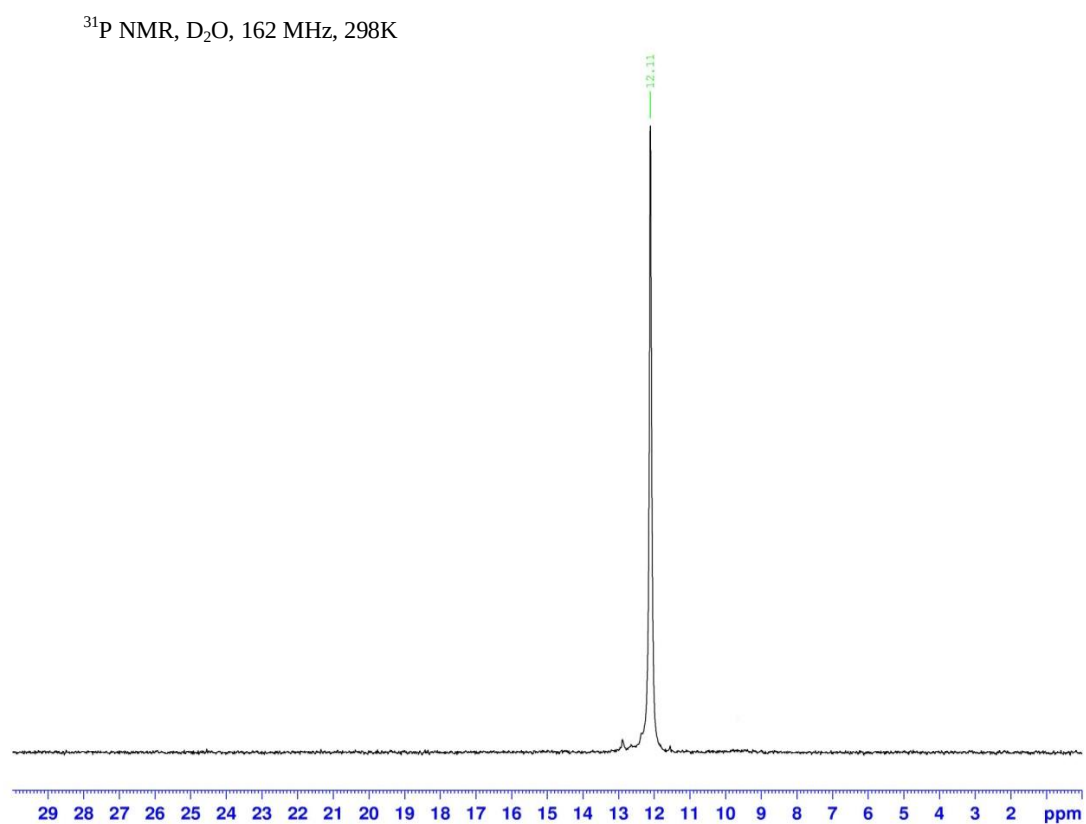
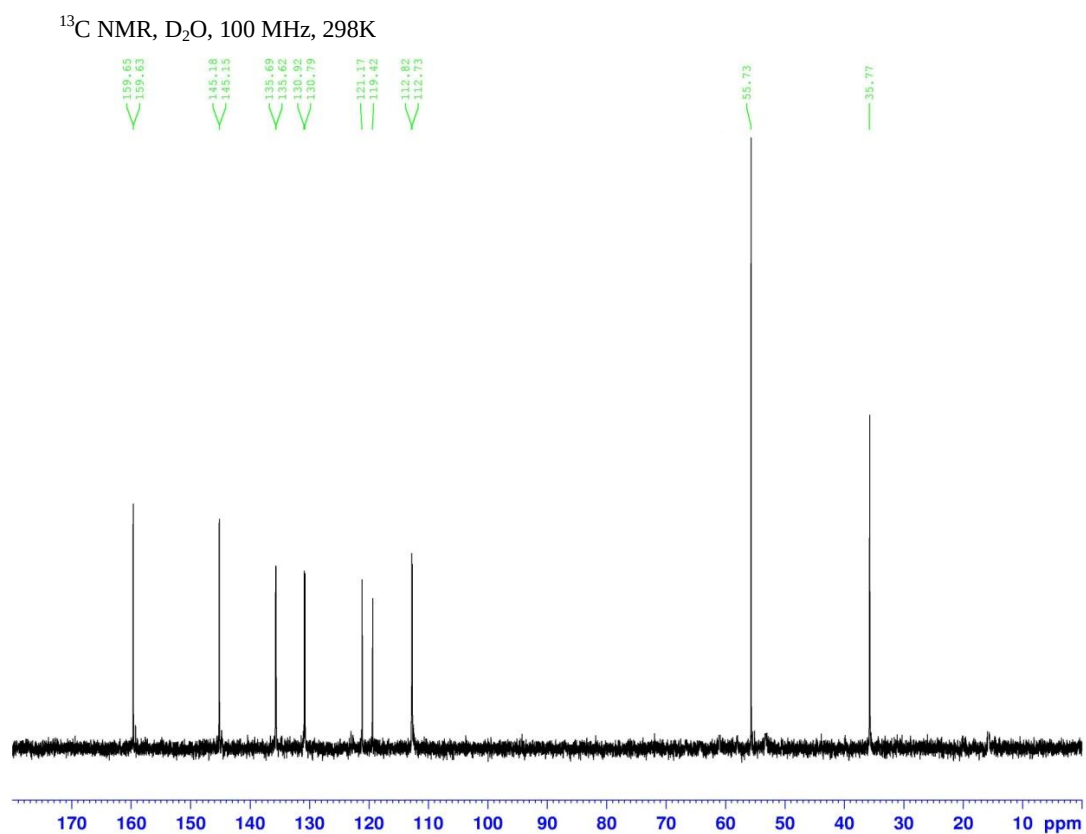


**Diethyl 12-[bis(hydroxymethoxy)(methylene)phosphoranyl]-7-(diethoxyphosphoryl)-
3,8,13-trimethoxy-10,15-dihydro-5*H*-tribenzo[*a,d,g*]cyclononen-2-ylphosphonate (3)**

¹H NMR, CDCl₃, 400 MHz, 298K

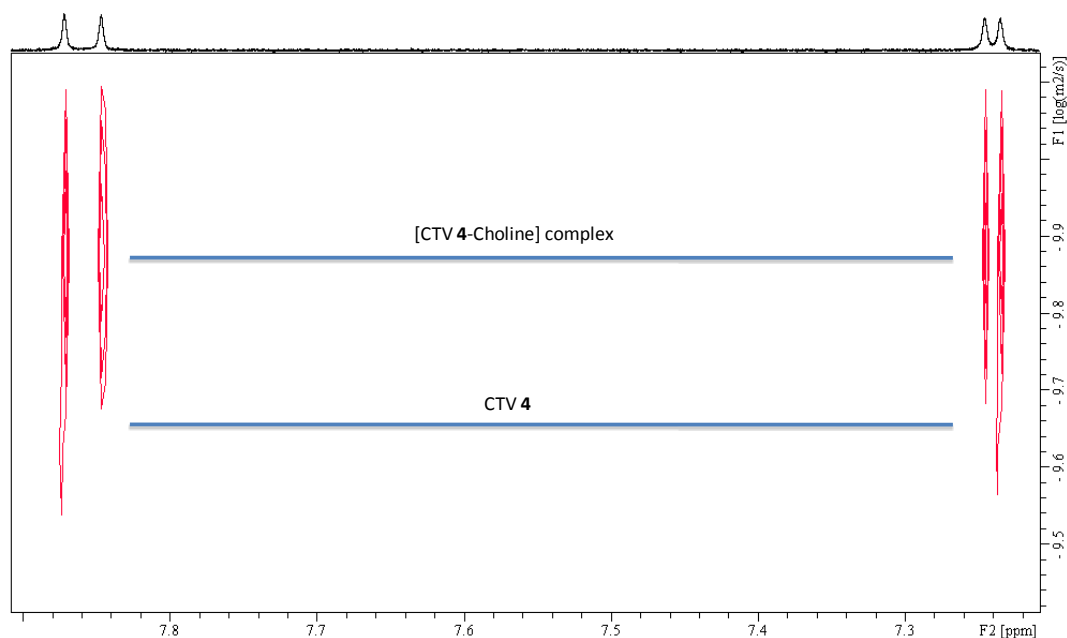




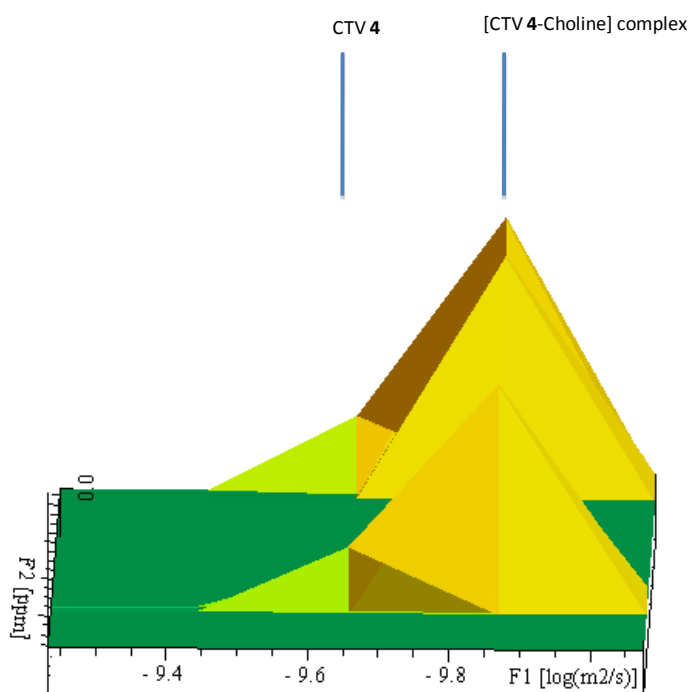


2. DOSY-NMR experiments

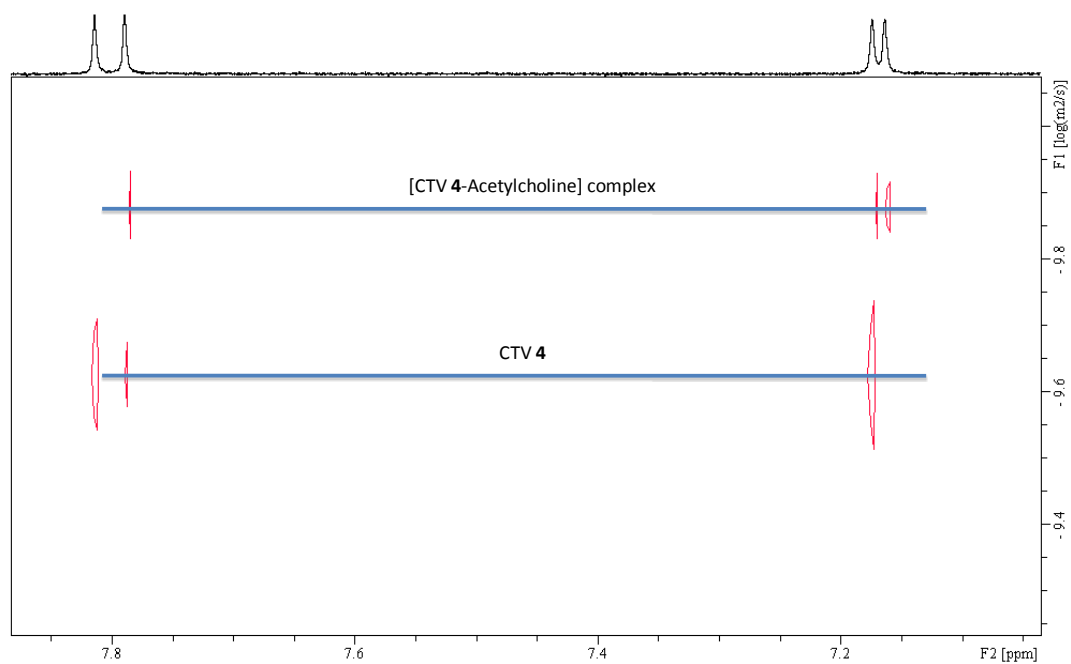
2D DOSY, 600.13 MHz, D₂O, at 25°C; aromatic region; 1 eq of CTV 4 and 40 eq of choline



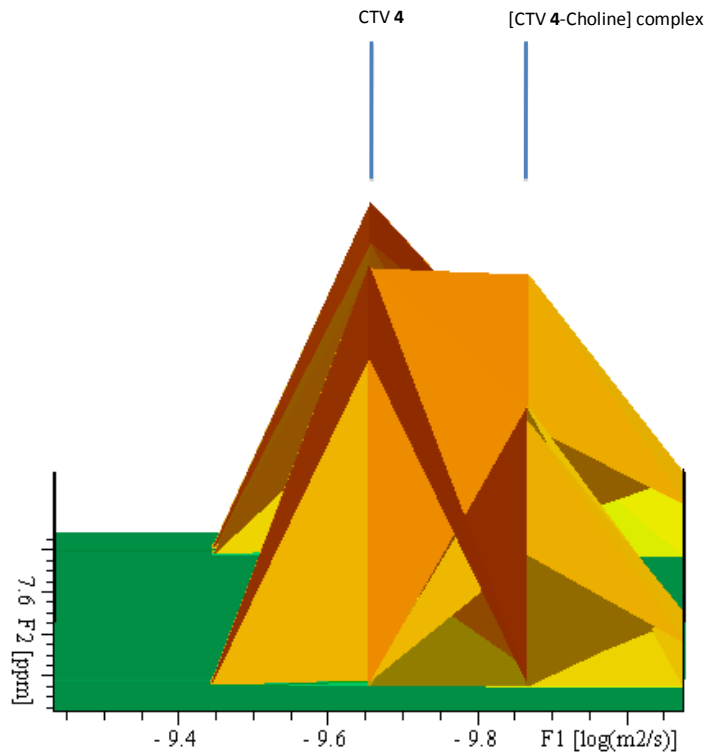
3D view of 2D DOSY; 1 eq of CTV 4 and 40 eq of choline



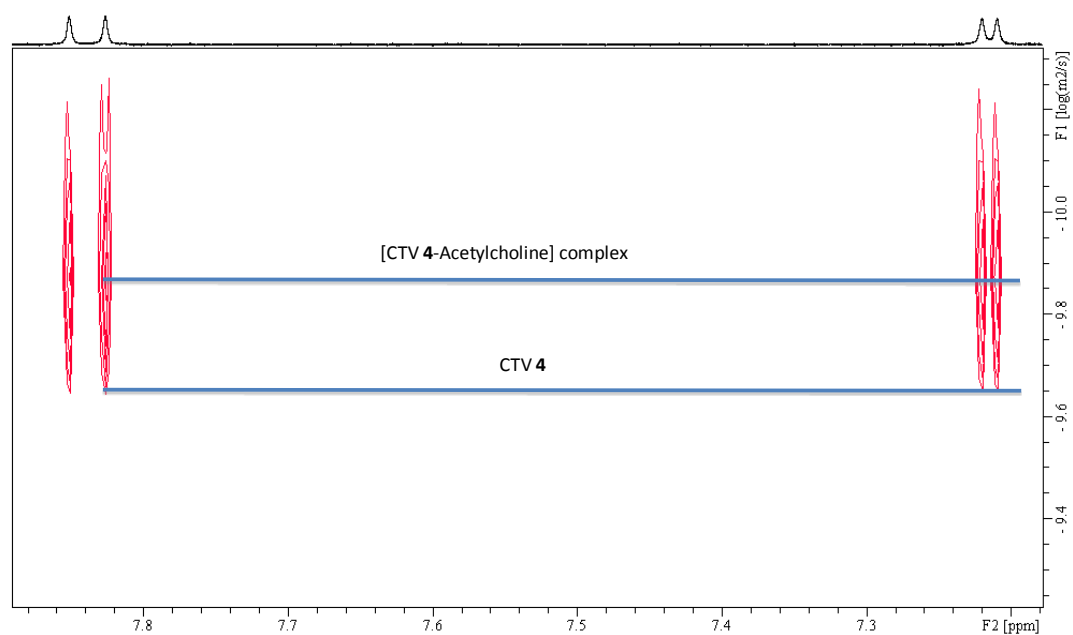
2D DOSY, 600.13 MHz, D₂O, at 25°C; aromatic region; 1 eq of CTV **4** and 40 eq of acetylcholine



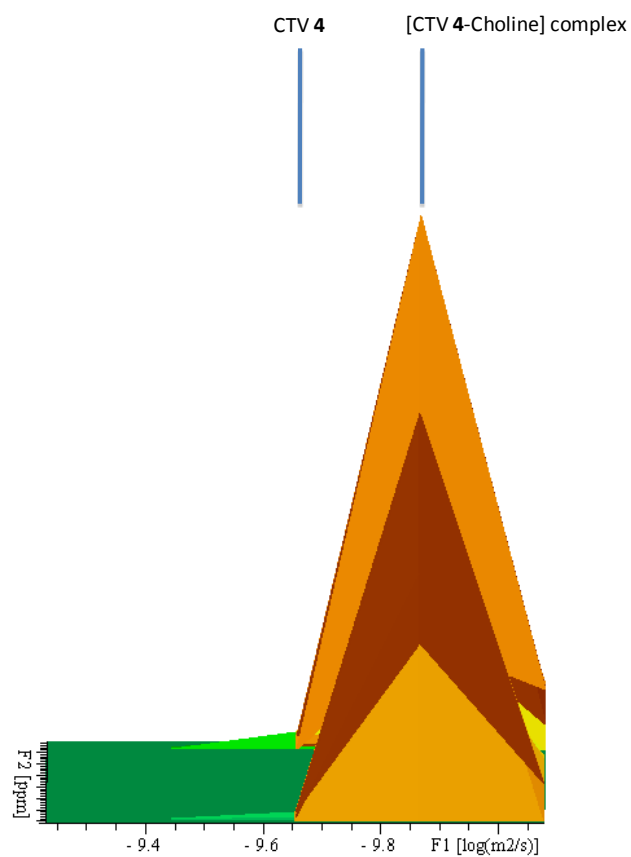
3D view of 2D DOSY; 1 eq of CTV **4** and 40 eq of acetylcholine



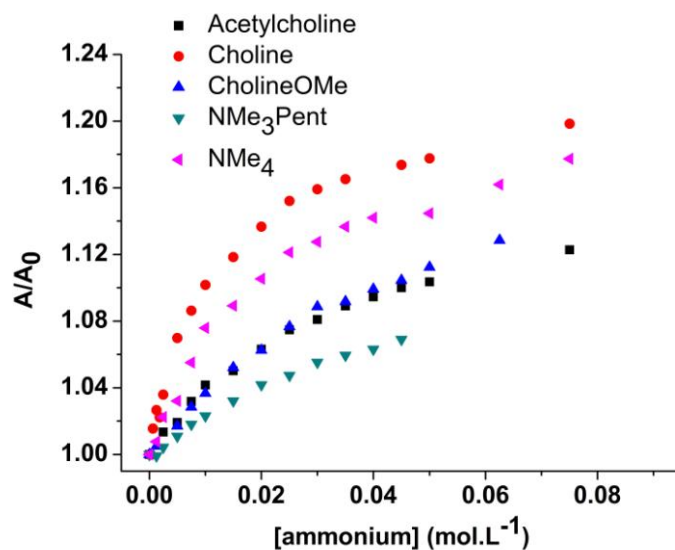
2D DOSY, 600,13 MHz, D₂O, at 25°C; aromatic region; 1 eq of CTV **4** and 200 eq of acetylcholine



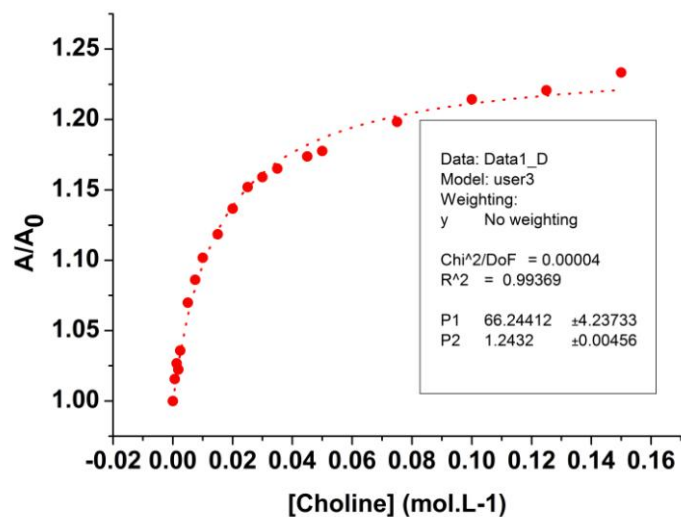
3D view of 2D DOSY; 1 eq of CTV **4** and 200 eq of acetylcholine



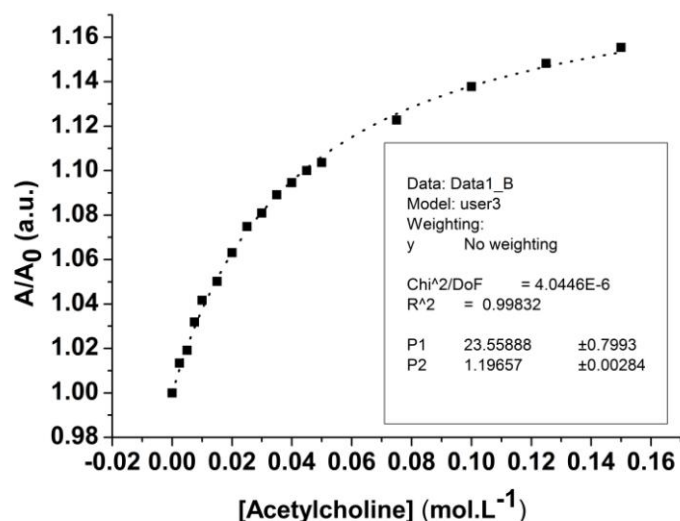
3. Fluorescence titration data



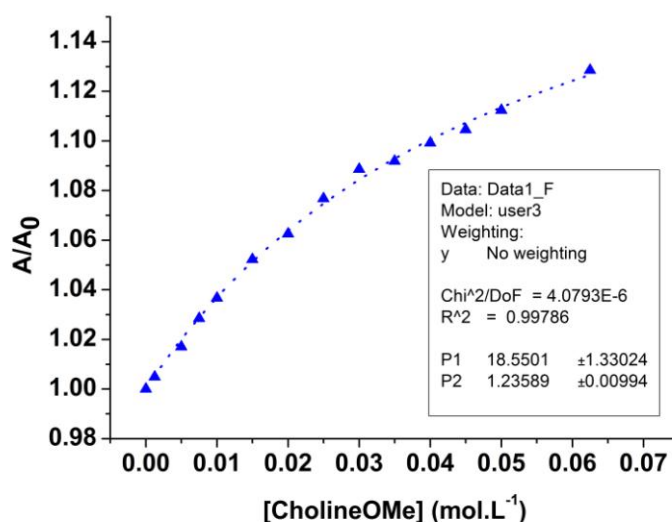
Relative fluorescence area of **4** (10^{-5} M) with increasing ammonium concentrations (0 to 0.08 M)
(●) choline, (◀) tetramethylammonium, (▲) methoxycholine, (■) acetylcholine and
(▼) trimethylpentylammonium



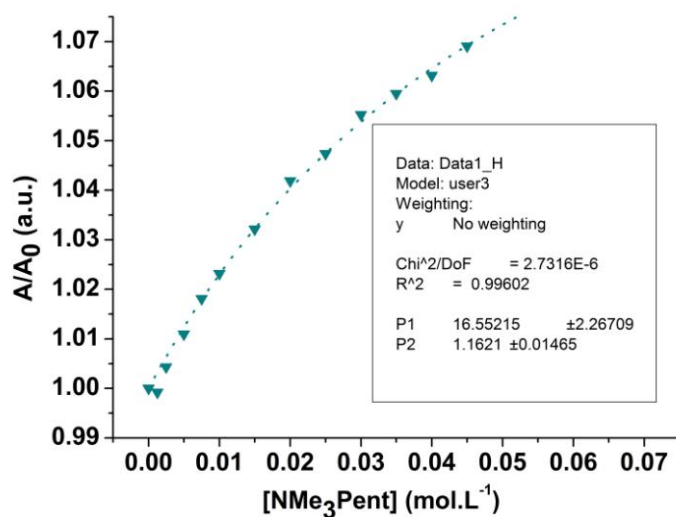
Relative fluorescence area of **4** (10^{-5} M) with increasing choline concentrations (0 to 0.16 M)
fitted with a 1:1 binding model.



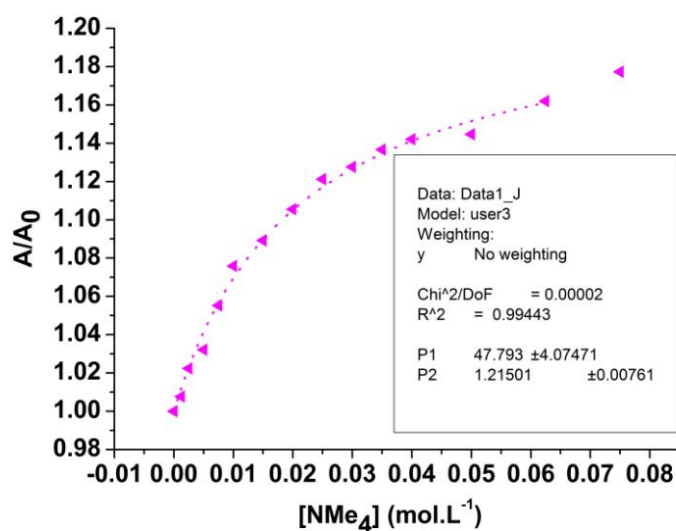
Relative fluorescence area of **4** (10^{-5} M) with increasing acetylcholine concentrations (0 to 0.16 M) fitted with a 1:1 binding model.



Relative fluorescence area of **4** (10^{-5} M) with increasing methoxycholine concentrations (0 to 0.07 M) fitted with a 1:1 binding model.



Relative fluorescence area of **4** (10^{-5} M) with increasing trimethylpentylammonium concentrations (0 to 0.07 M) fitted with a 1:1 binding model.



Relative fluorescence area of **4** (10^{-5} M) with increasing tetramethylammonium concentrations (0 to 0.08 M) fitted with a 1:1 binding model.