

Electronic Supplementary Information

Push-pull ruthenium diacetylide complexes: new dyes for p-type dye-sensitized solar cells.

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³¹P, ¹H, ¹³C NMR and HR-MS spectra of **SL1** and **SL2**

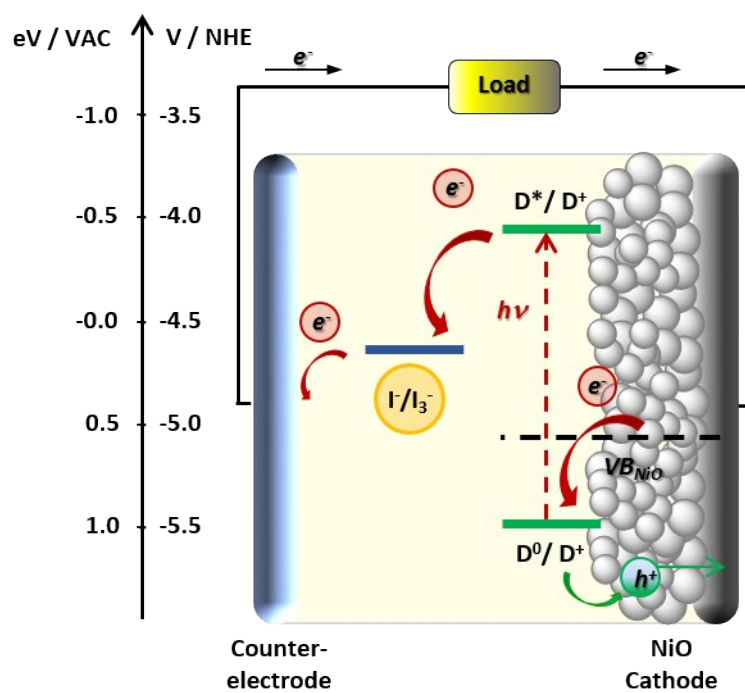


Figure S1. Schematic view of energy diagram and working principle of the p-type DSC.

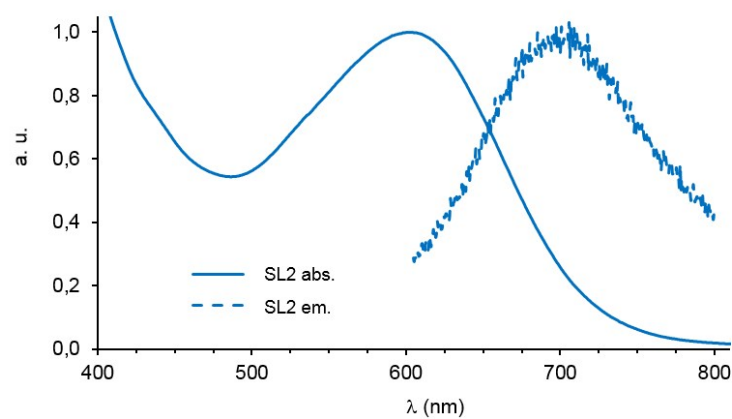
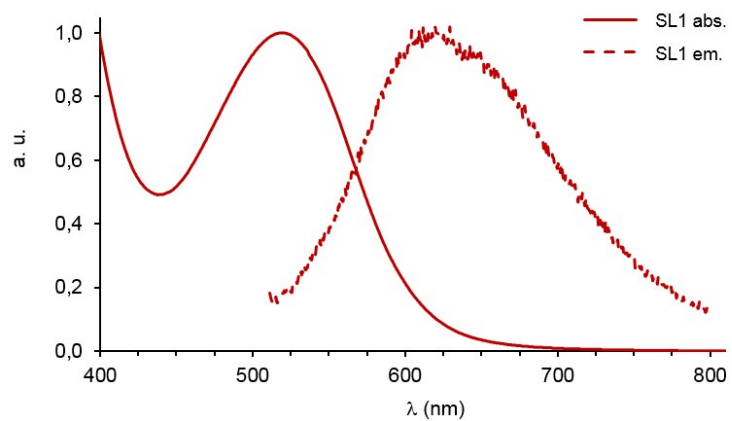


Figure S2. Normalized electronic absorption (plain) and fluorescence emission (dashed) spectra of **SL1** and **SL2** in CH_2Cl_2 .

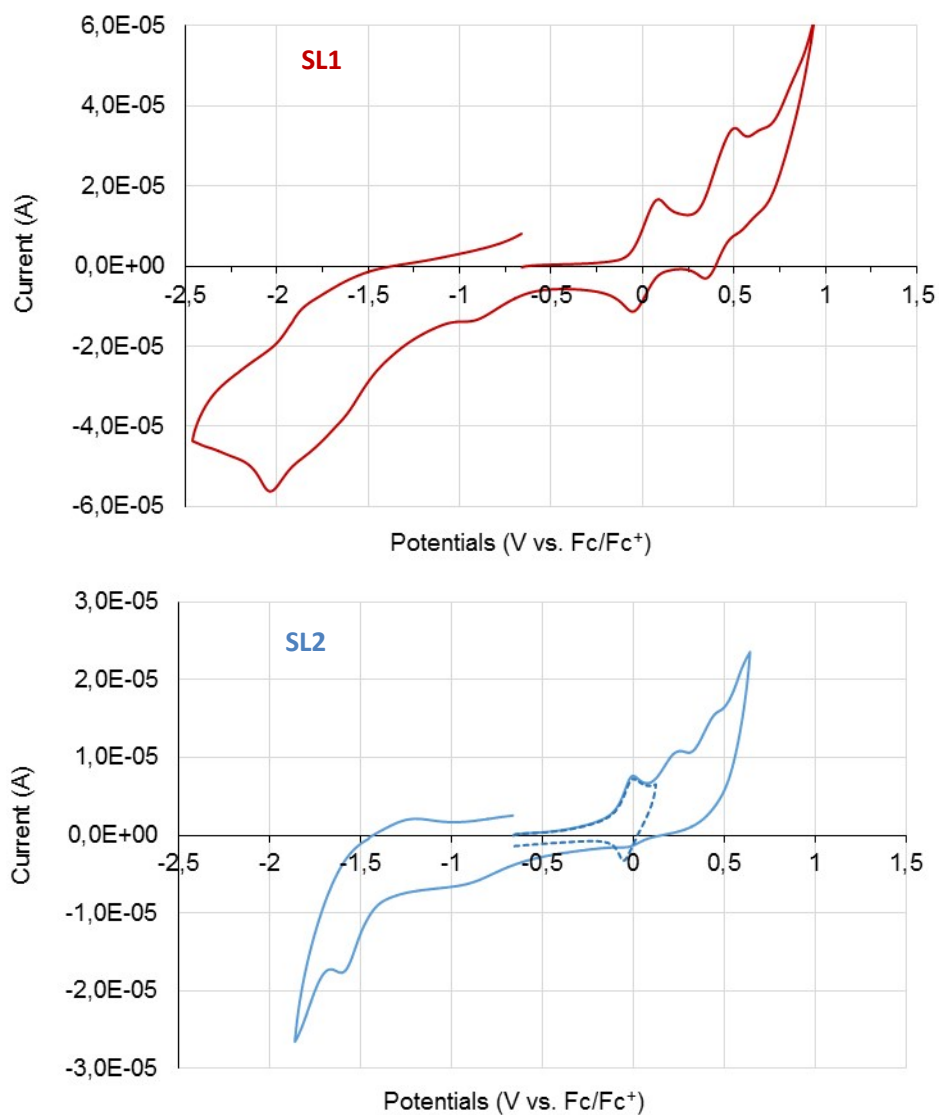


Figure S3. Cyclic voltammograms of **SL1** and **SL2** recorded in THF/ $n\text{Bu}_4\text{NPF}_6$ (0.1M) vs. Fc/Fc+ at 200 mV s⁻¹. The blue dotted line represents the reversibility of the first oxidation process isolated; the second oxidation process is only partly reversible.

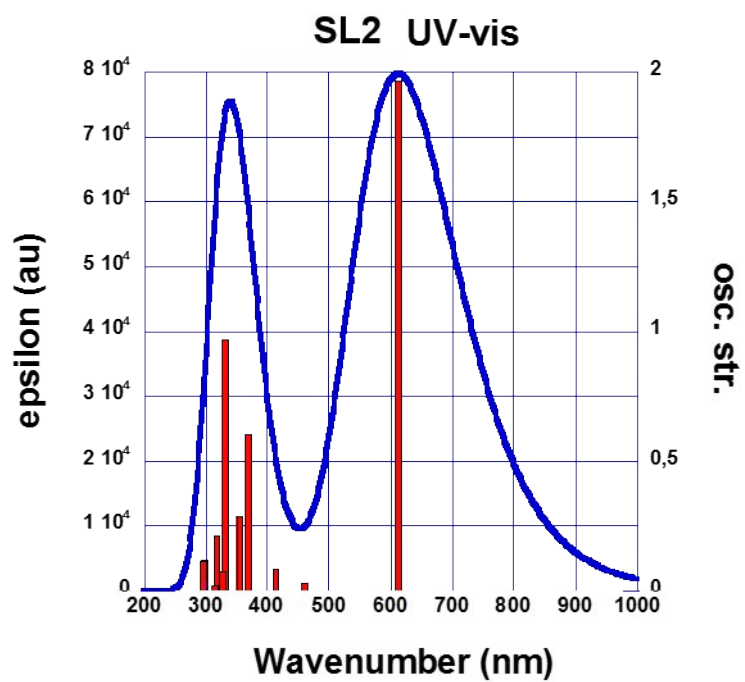
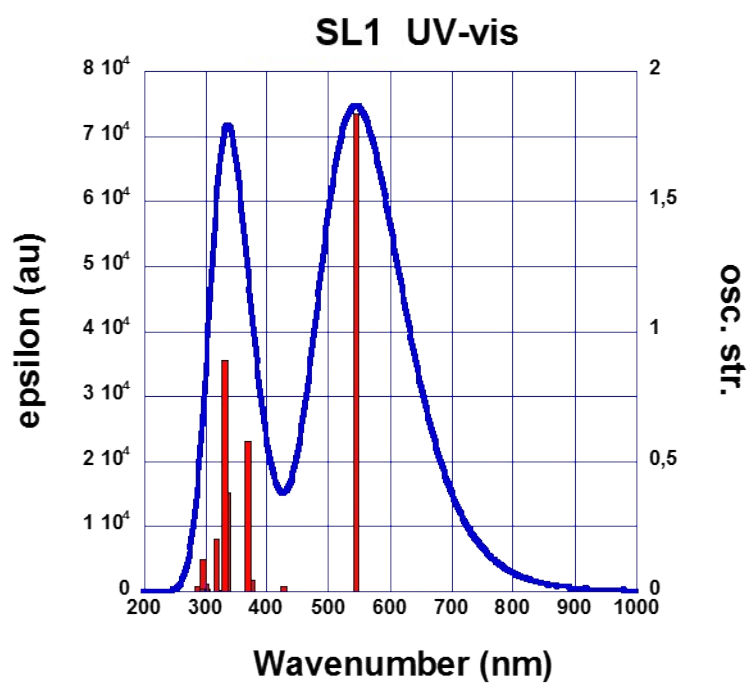
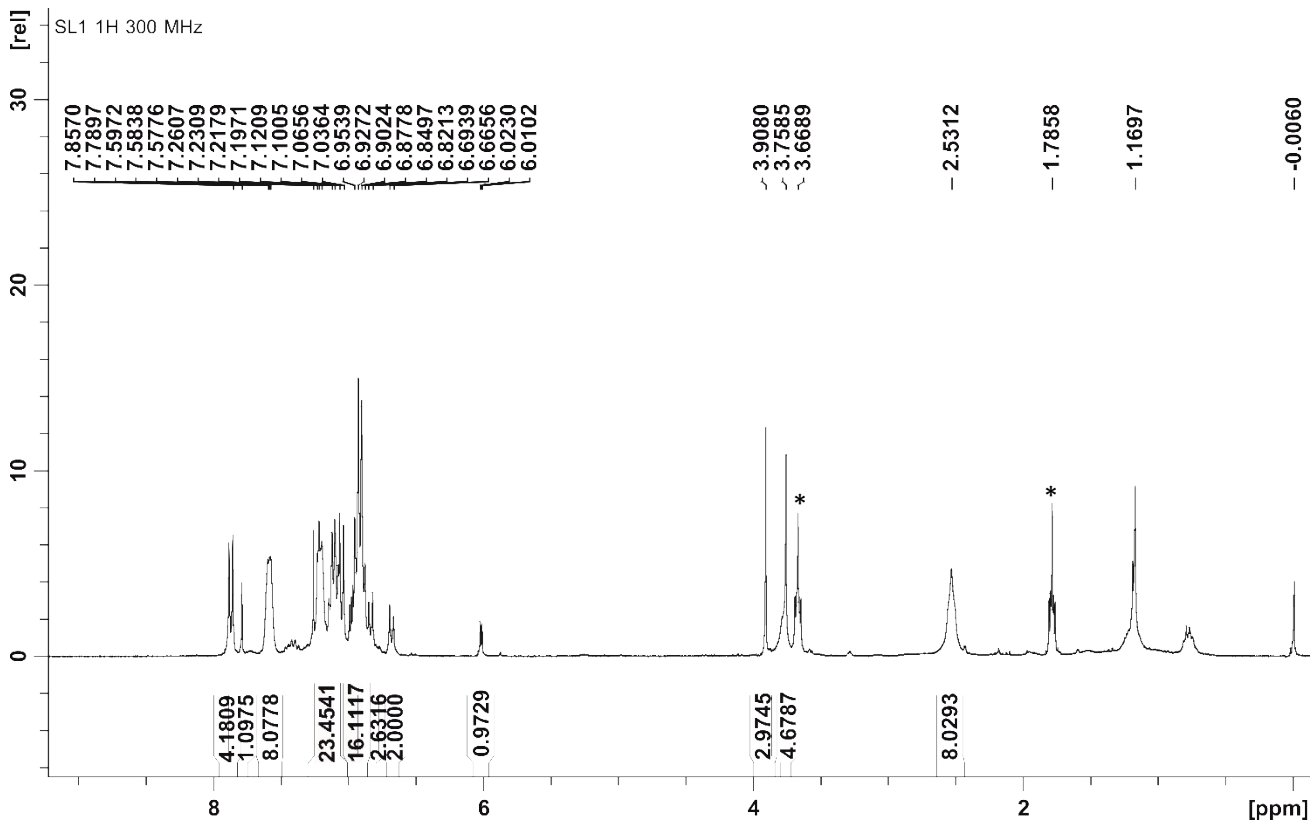
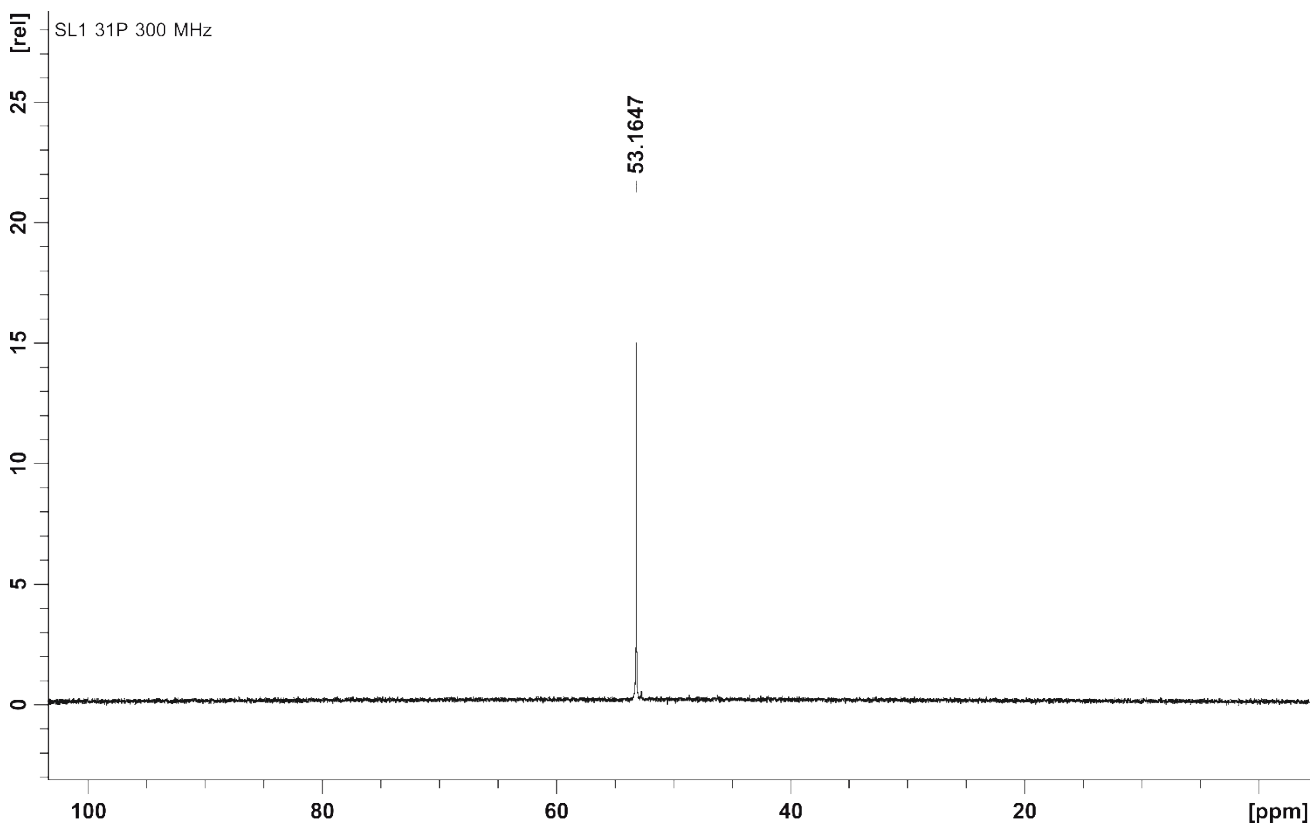
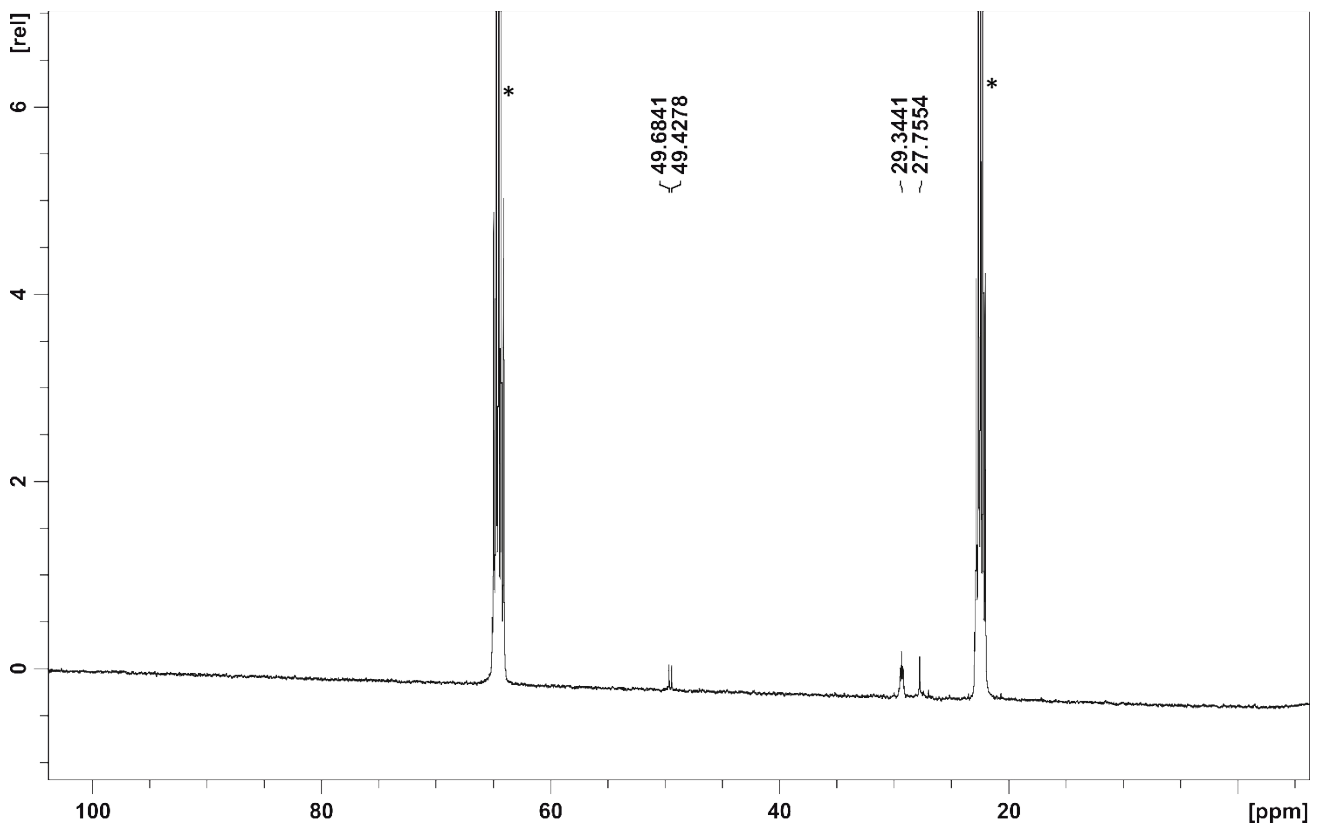
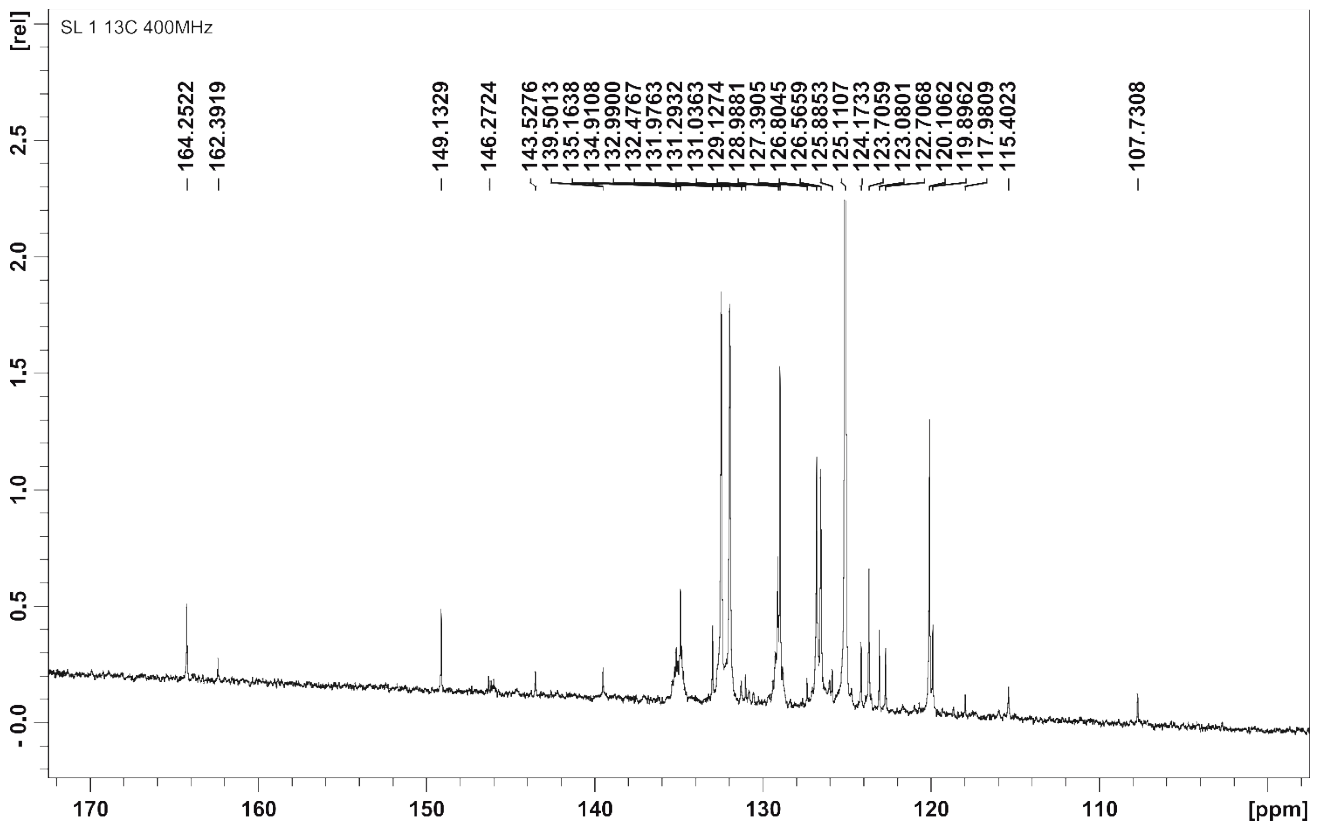


Figure S4. TD-DFT simulated absorption spectra of **SL1** and **SL2**. Absorption bands enlarged using Gaussian functions with full-width at half-height (FWHH) of 5 nm to reproduce the experimental spectra.

³¹P, ¹H, ¹³C NMR and HR-MS spectra of **SL1** and **SL2**

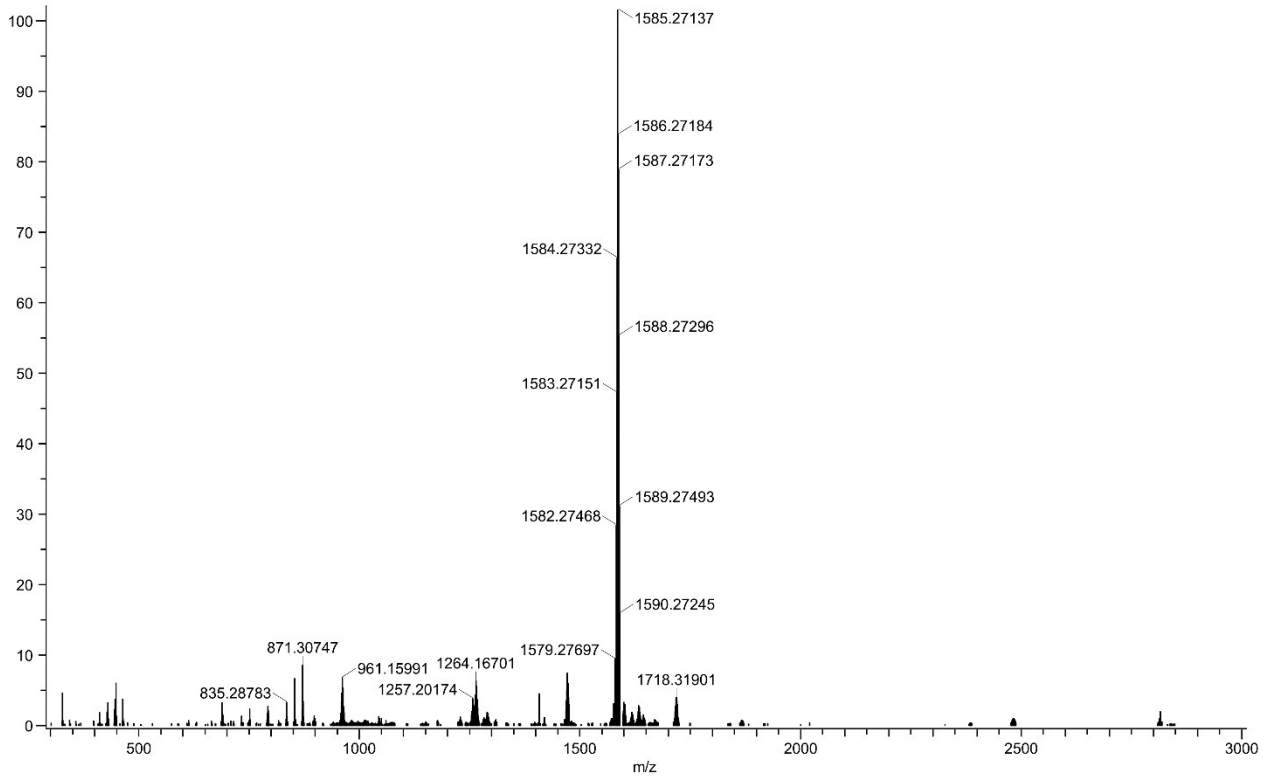
(* correspond to signals of solvent residuals)





Acq. Data Name: FD-04-05-15-SL1
 Creation Parameters: Average(MS[1] Time:0.69..0.76)
 x10³ Intensity (101643)

Experiment Date/Time: 5/4/2015 5:06:45 PM
 Ionization Mode: FD+(eiFi)

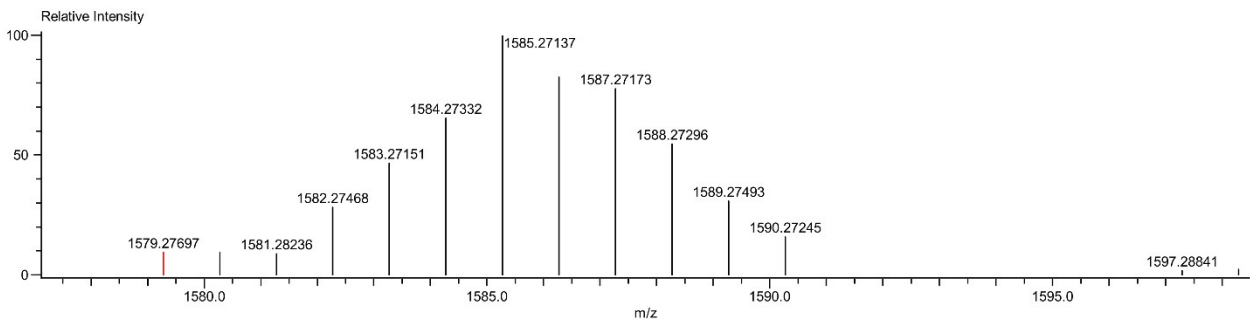


Data:FD-04-05-15-SL1
 Sample Name:
 Description:
 Ionization Mode:FD+(eiFi)
 History:Determine m/z[Peak Detect[Centroid,30,Area];Smooth[23]];Correct Base[];Average(MS[1] 0.69..0.76)

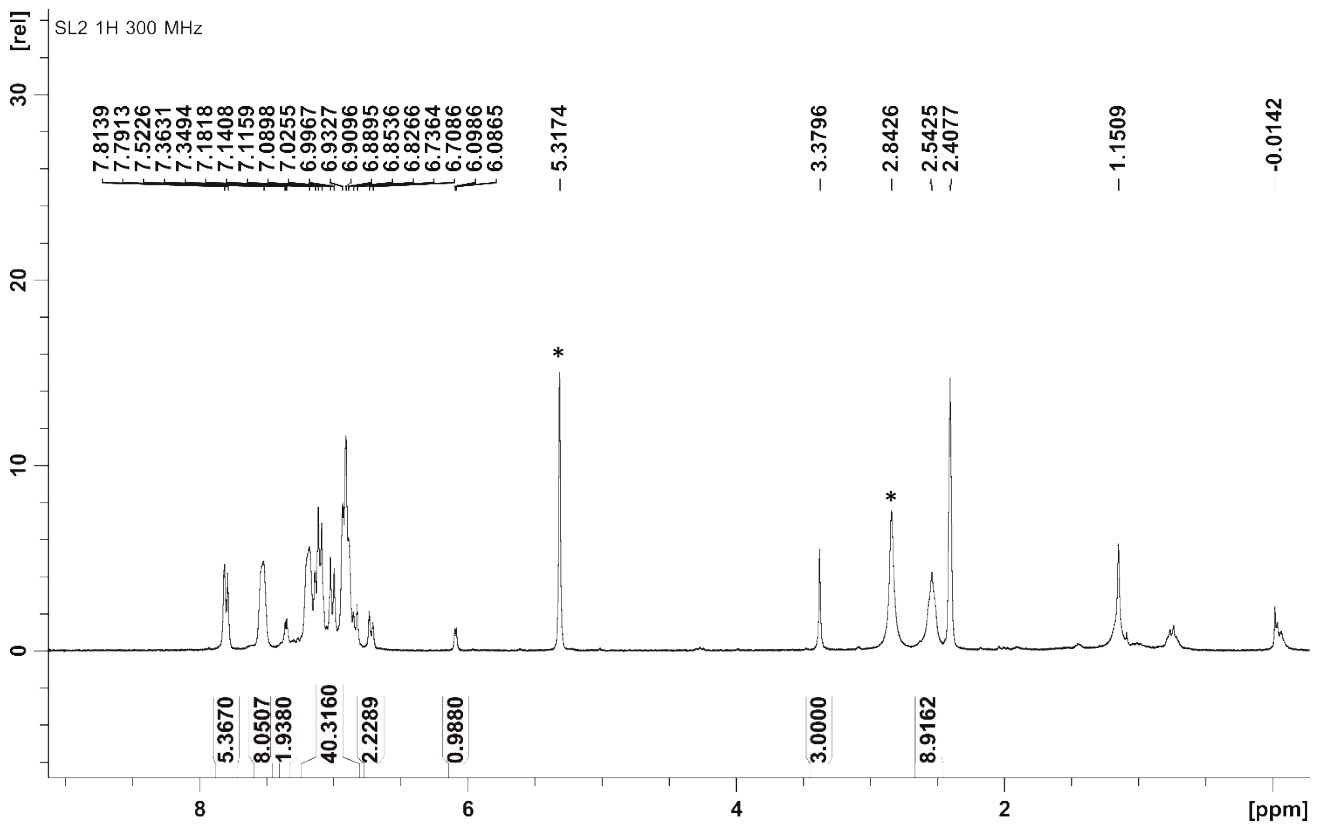
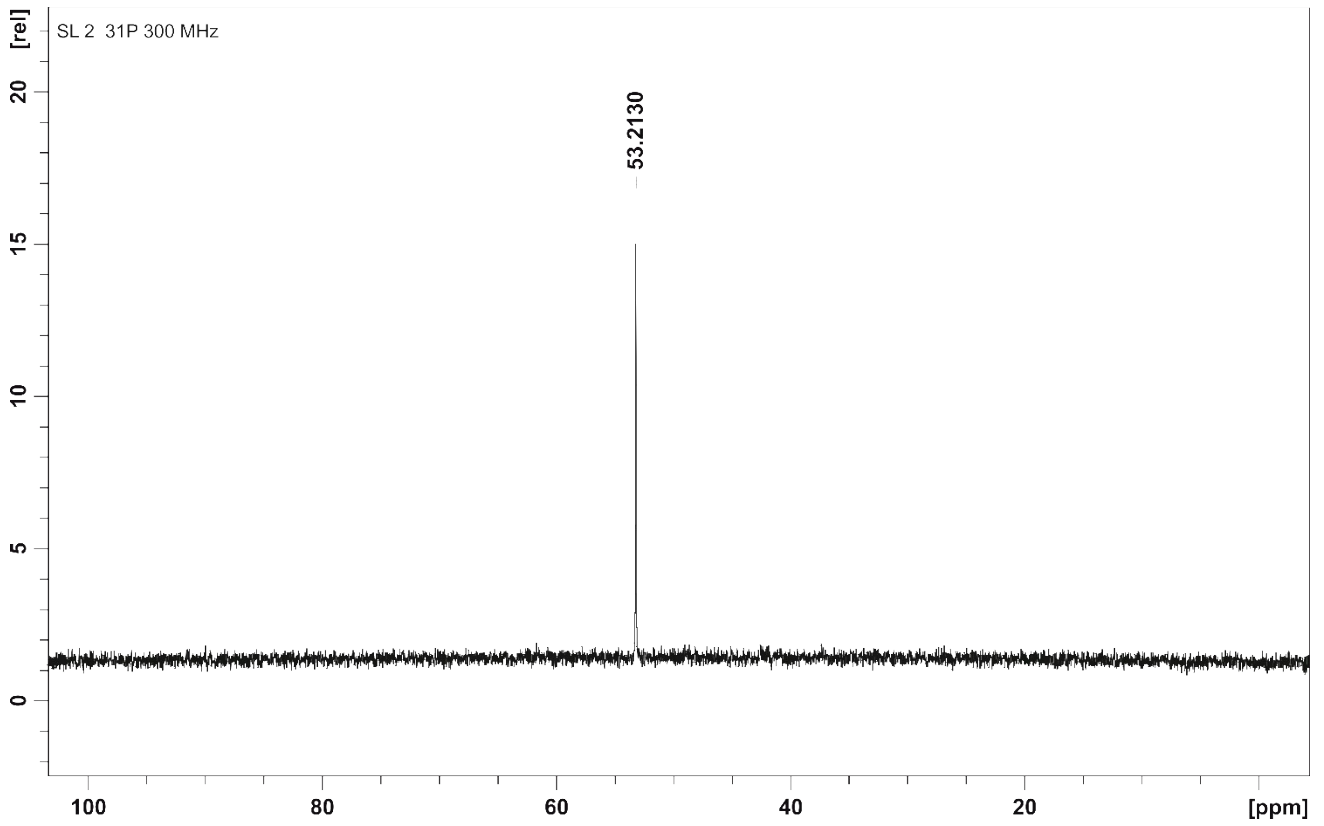
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 Operator:AccuTof
 Mass Calibration data:FD-141114-PEG1000
 Created:5/4/2015 5:23:18 PM
 Created by:AccuTof

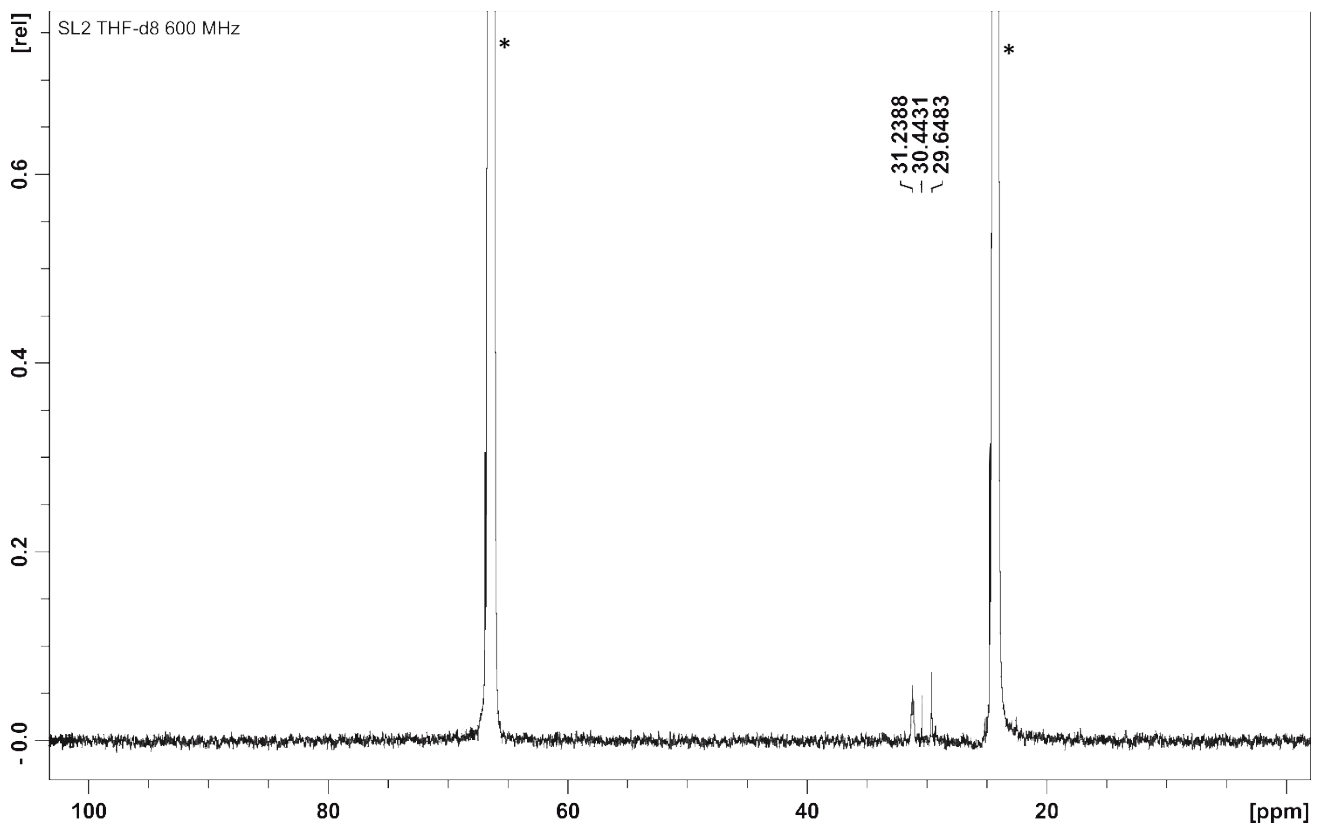
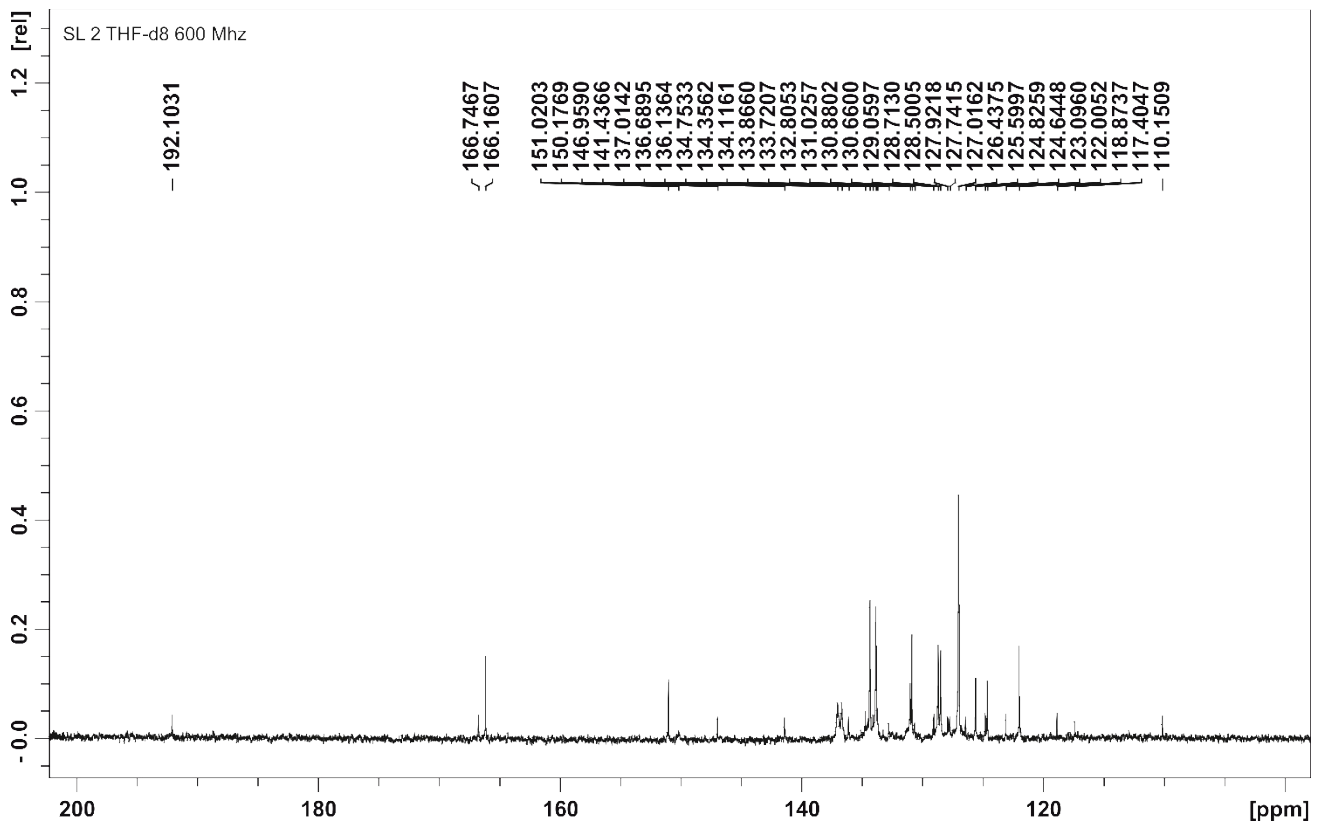
Charge number:1 Tolerance:5.00(ppm)
 Element:¹²C:0 .. 200, ¹H:0 .. 200, ¹⁴N:1 .. 1, ¹⁶O:8 .. 8, ³¹P:4 .. 4, ⁹⁶Ru:1 .. 1, ³²S:2 .. 2

Unsaturation Number:-20.0 .. 100.0 (Fraction:Both)



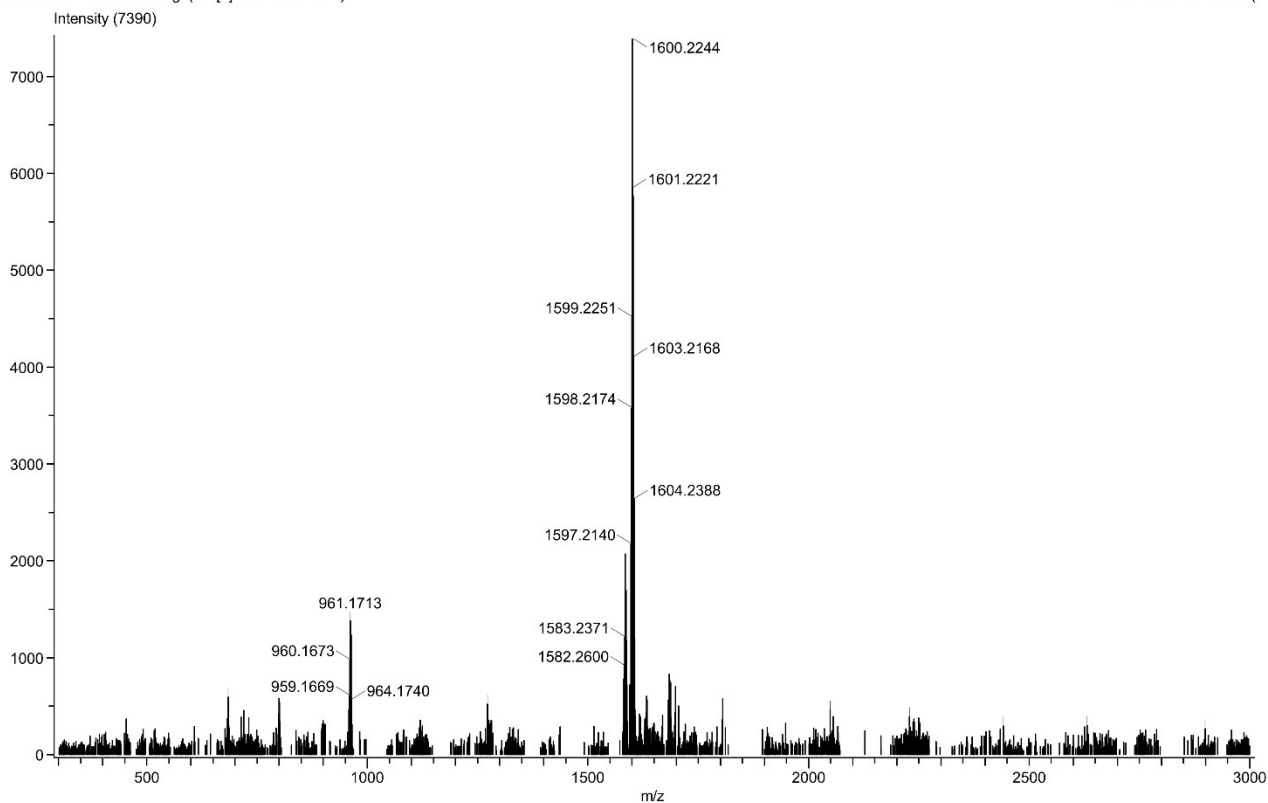
Mass	Intensity	Relative Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
1579.27697	9354.72	9.20	1579.28041	-3.44	-2.18	¹² C ₉₀ ¹ H ₇₃ ¹⁴ N ₁ ¹⁶ O ₈ ³¹ P ₄ ⁹⁶ Ru ₁ ³² S ₂	63.5





Acq. Data Name: FD-05-05-15-SL2
 Creation Parameters: Average(MS[1] Time:0.68..0.69)

Experiment Date/Time: 5/5/2015 11:04:14 AM
 Ionization Mode: FD+(eIFi)

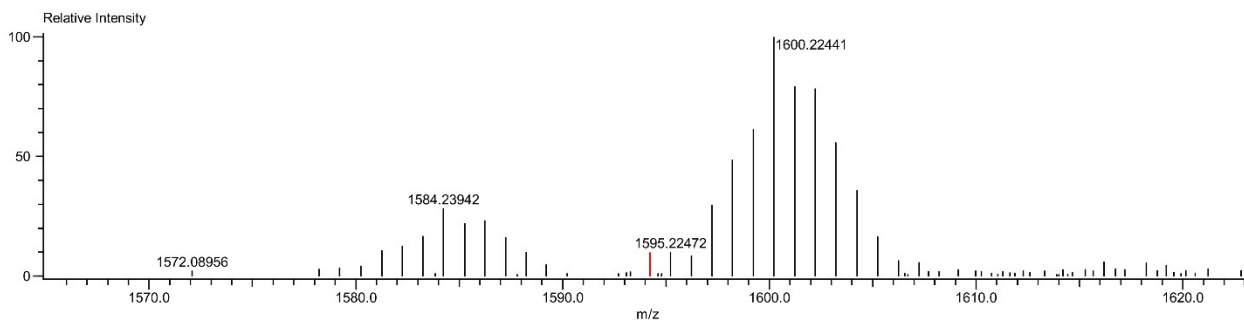


Data:FD-05-05-15-SL2
 Sample Name:
 Description:
 Ionization Mode:FD+(eIFi)
 History:Determine m/z[Peak Detect[Centroid,30,Area];Smooth[9]];Correct Base[];Average(MS[1] 0.68..0.69)

Acquired:5/5/2015 11:04:14 AM
 Operator:AccuTof
 Mass Calibration data:FD-141114-PEG1000
 Created:5/5/2015 11:19:46 AM
 Created by:AccuTof

Charge number:1
 Tolerance:5.00(ppm)
 Element:¹²C:0 .. 200, ¹H:0 .. 200, ¹⁴N:2 .. 2, ¹⁶O:5 .. 5, ³¹P:4 .. 4, ⁹⁶Ru:1 .. 1, ³²S:4 .. 4

Unsaturation Number:-20.0 .. 100.0 (Fraction:Both)



Mass	Intensity	Relative Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
1594.22185	704.37	9.53	1594.21940	2.45	1.53	¹² C ₈₉ ¹ H ₇₀ ¹⁴ N ₂ ¹⁶ O ₅ ³¹ P ₄ ⁹⁶ Ru ₁ ³² S ₄	66.5