

Supplementary Material

Synthesis and properties of liquid phenyliodine dicarboxylates

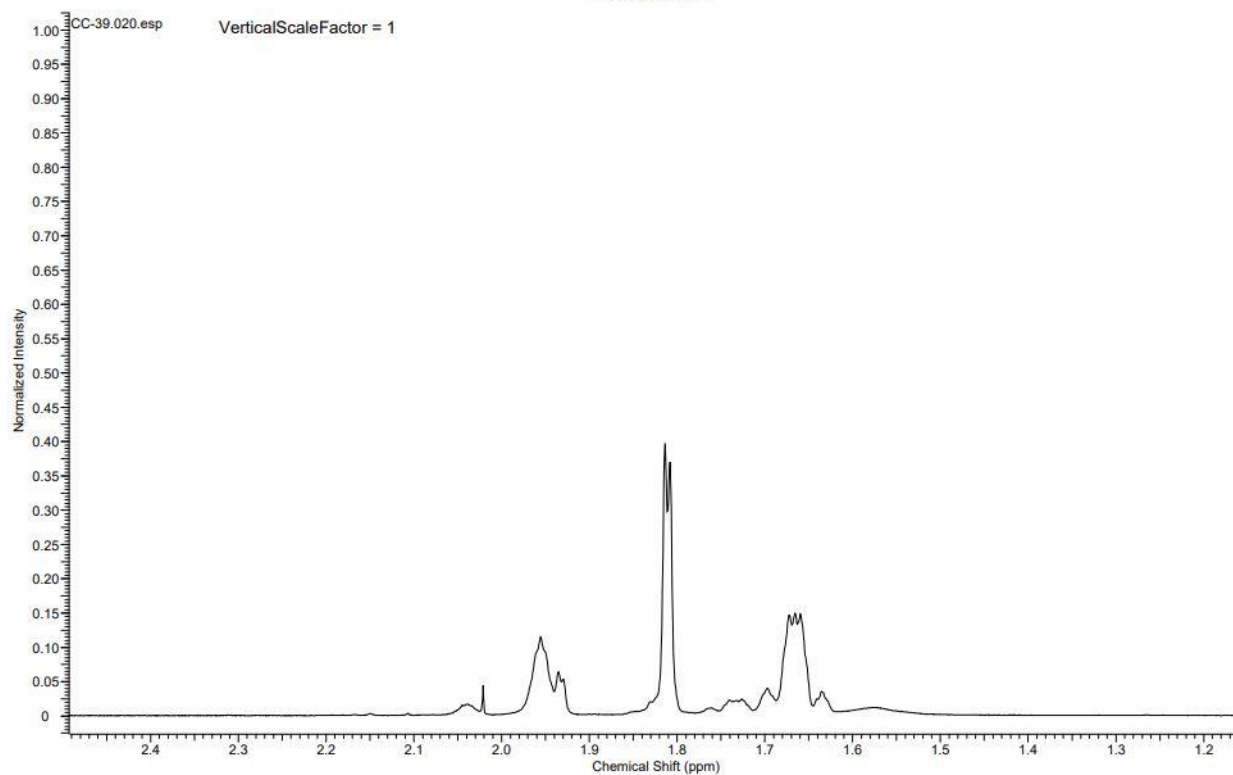
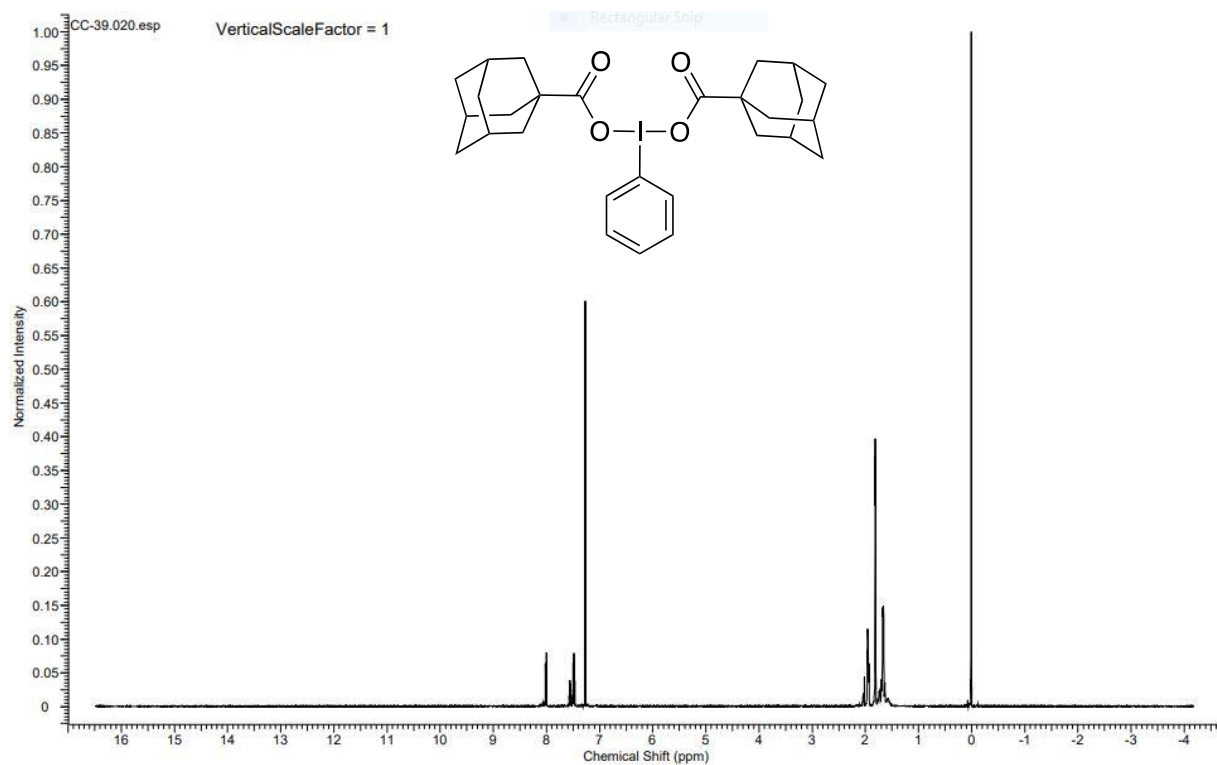
Christina Callovi, Su Wint War, Calvin N. Semczuk, Madison Fisher, Matthew Lucero Rodriguez, Joshua Plaut, Ivana Joshi, I. F. Dempsey Hyatt,* and Daniel L. Silverio*

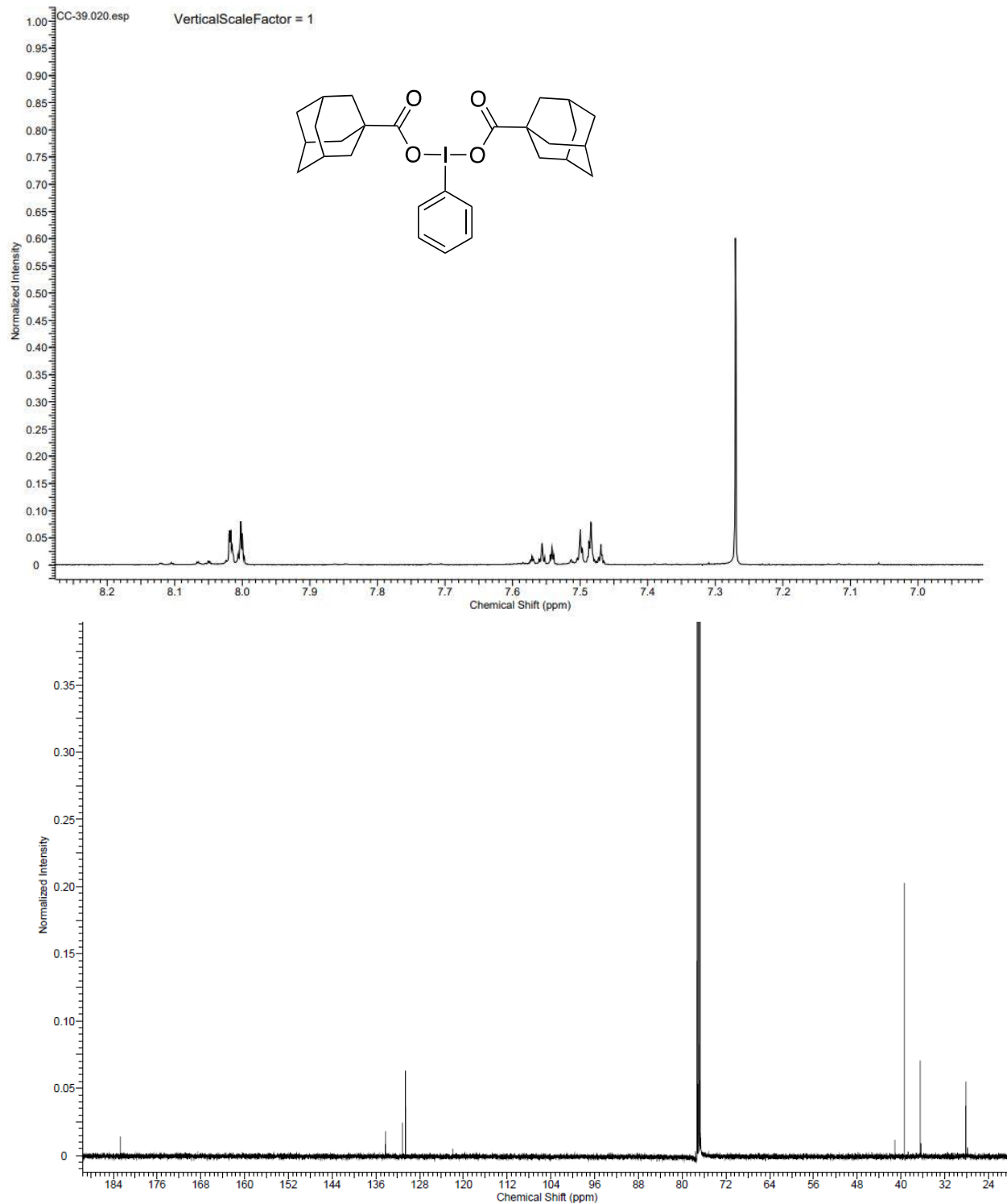
Department of Chemistry, Adelphi University, One South Avenue, Garden City, NY, 11530

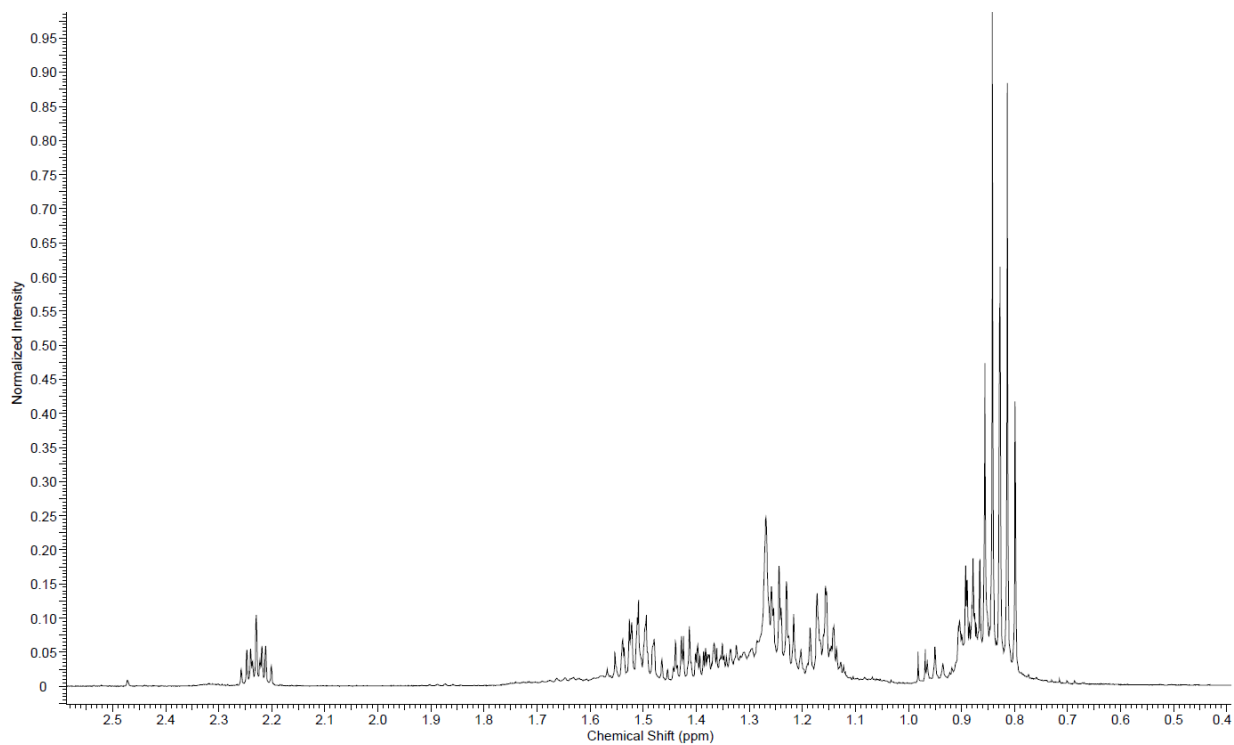
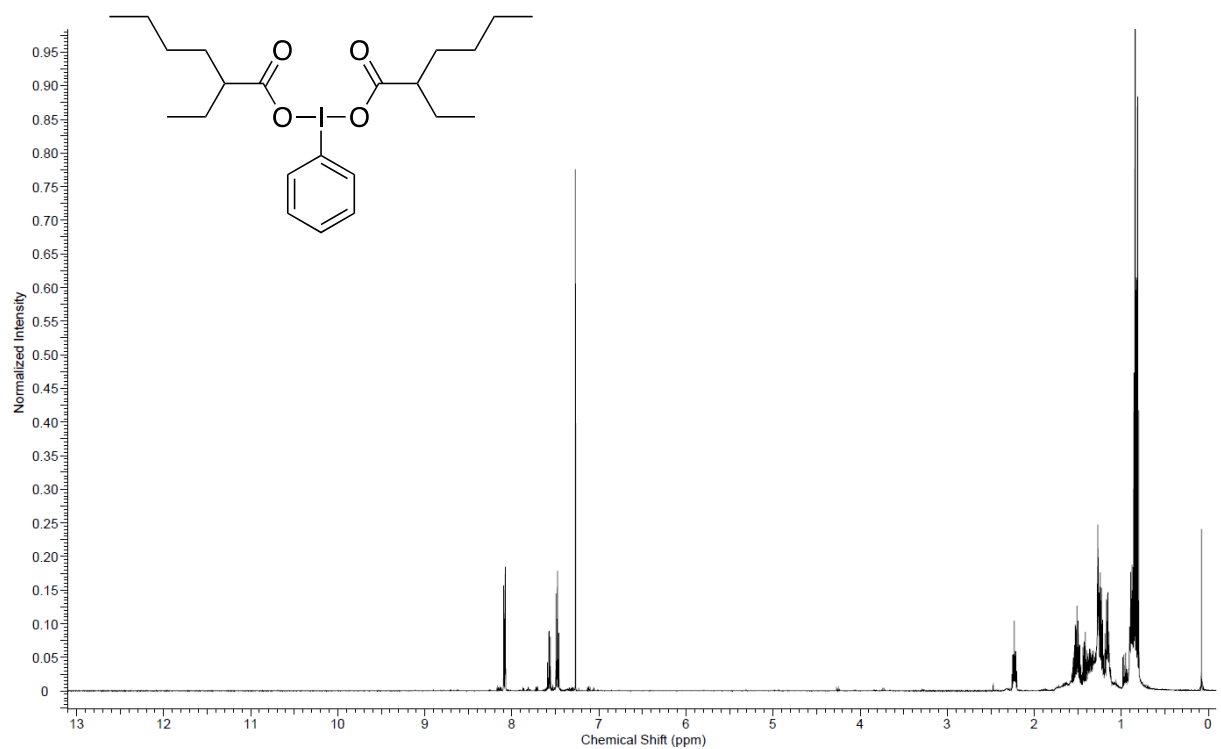
Email: dsilverio@adelphi.edu, ihyatt@adelphi.edu

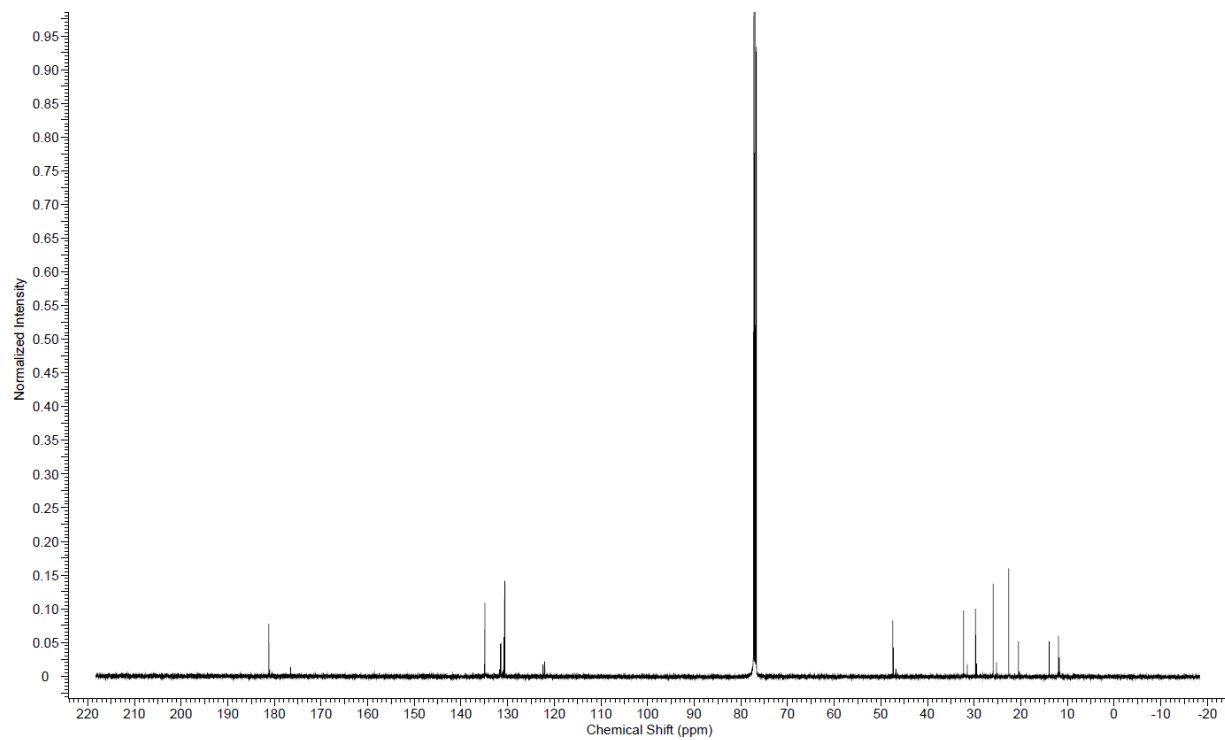
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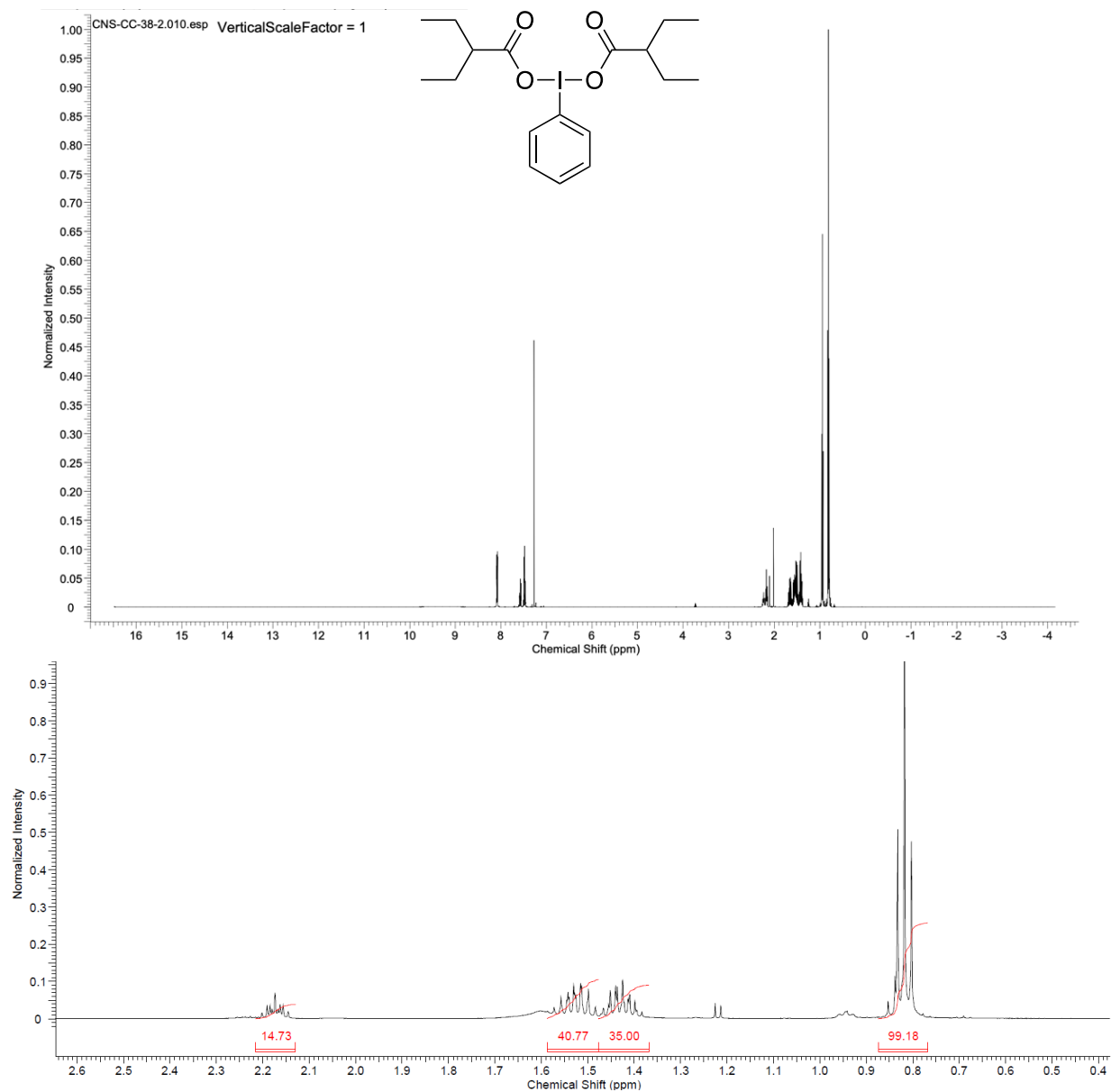
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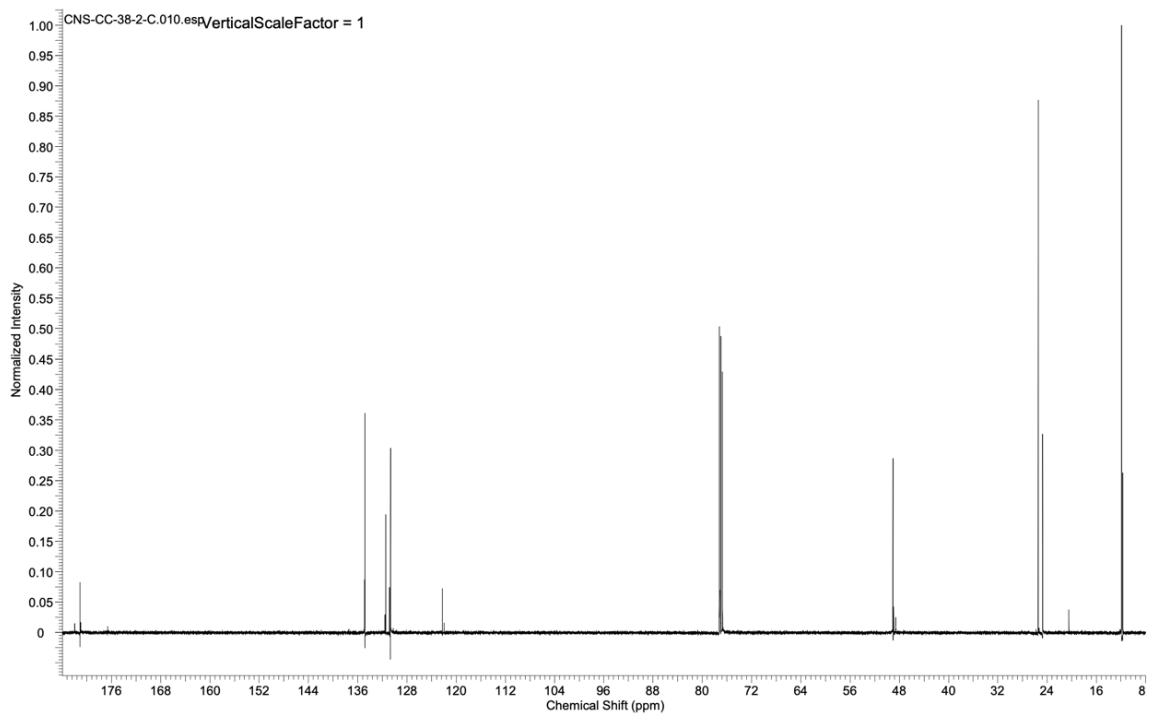
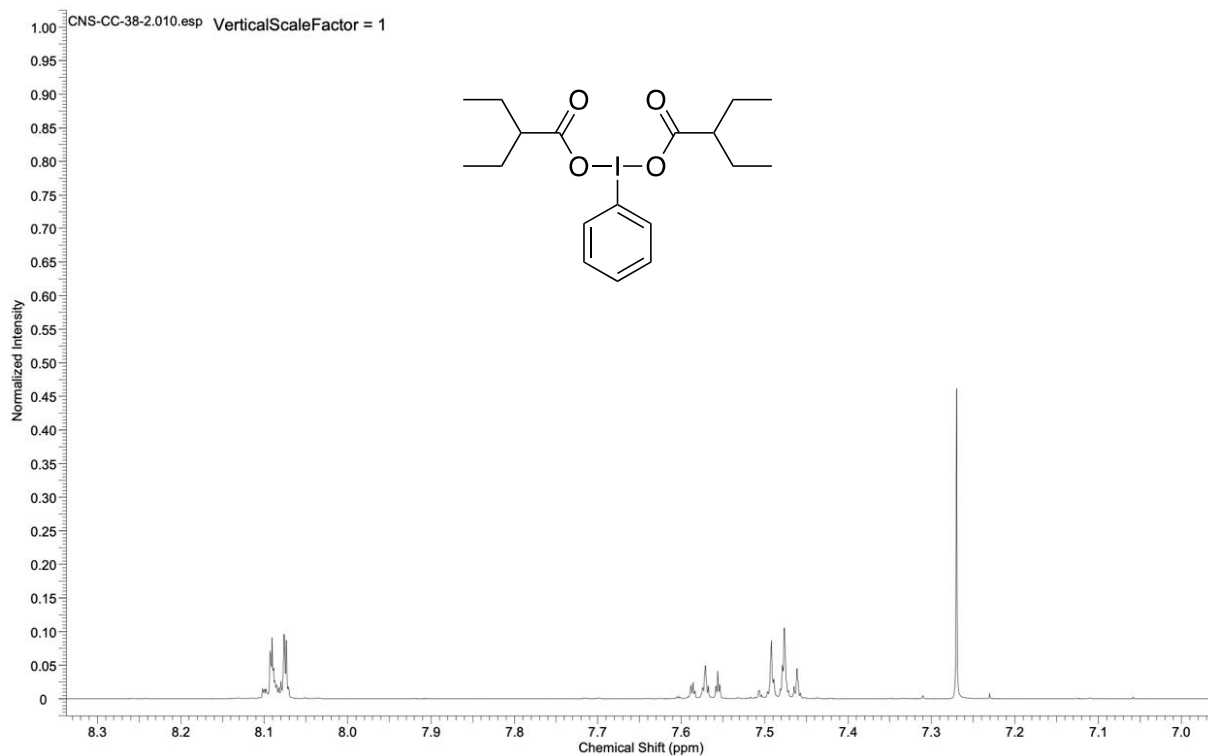
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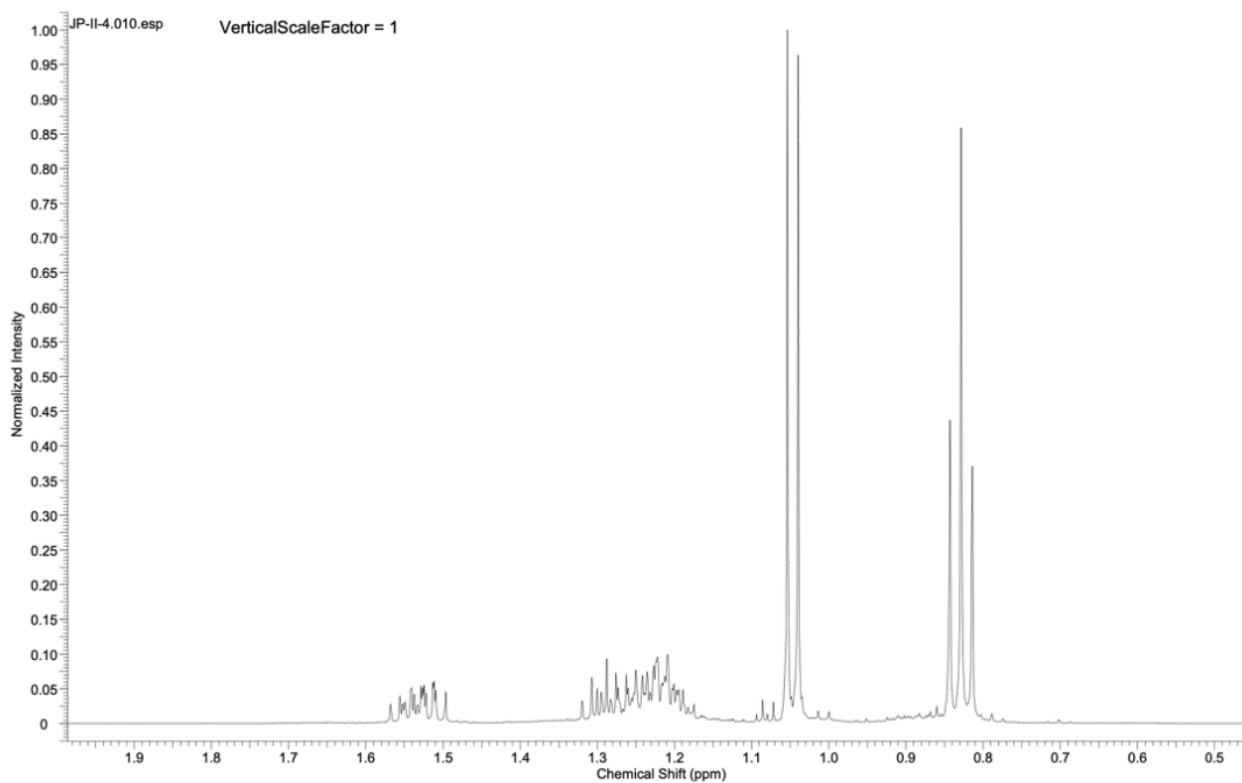
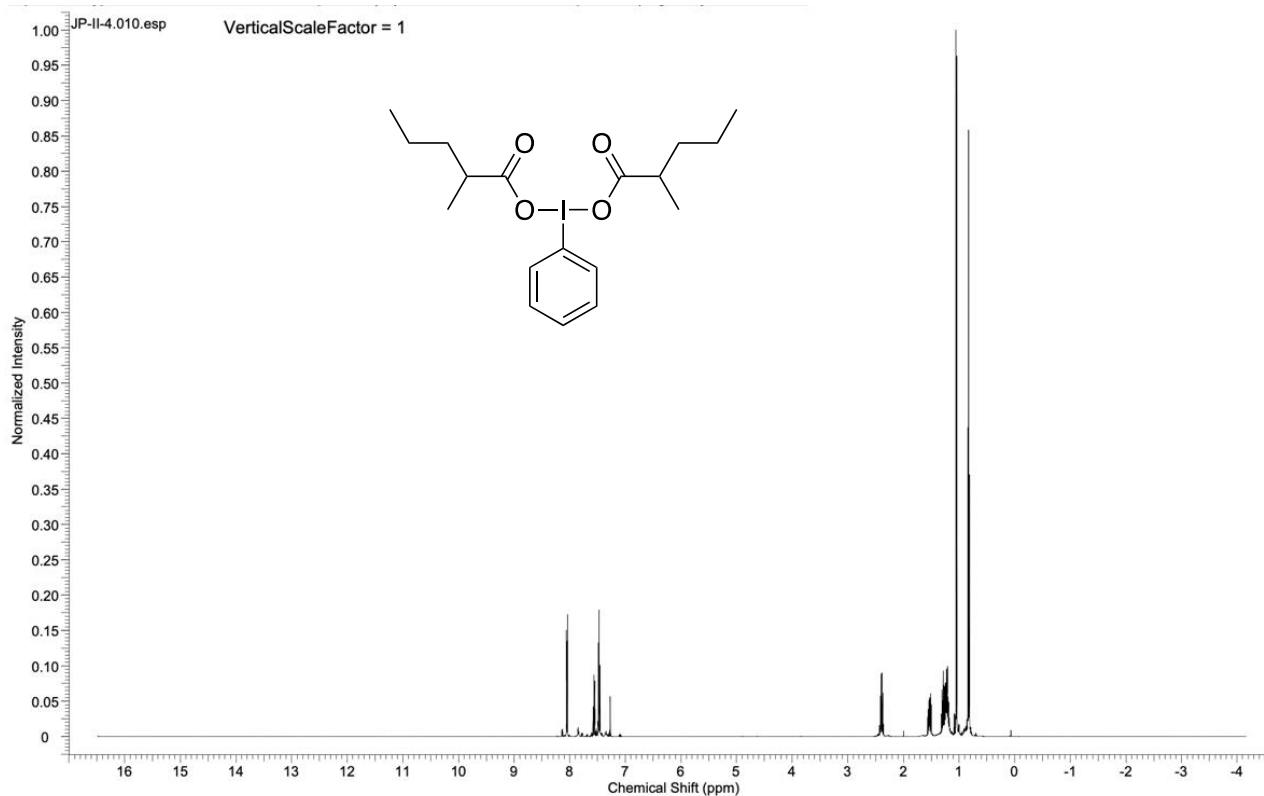
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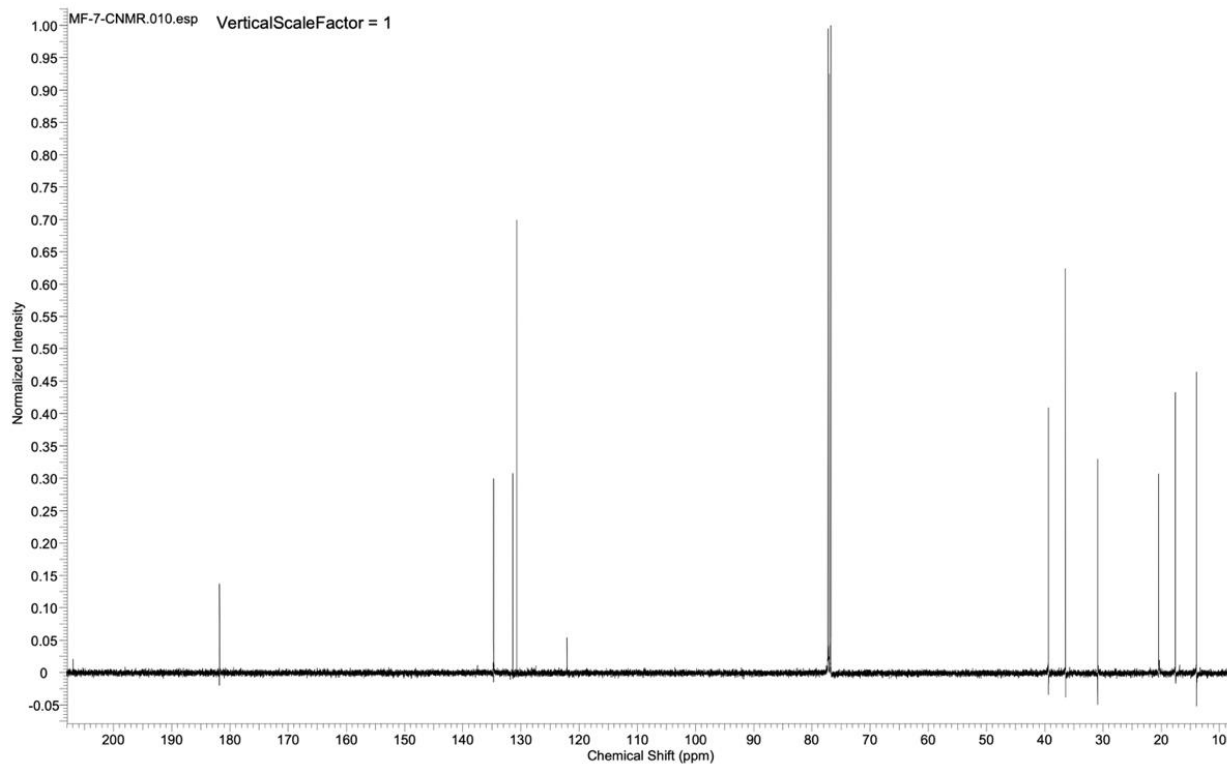
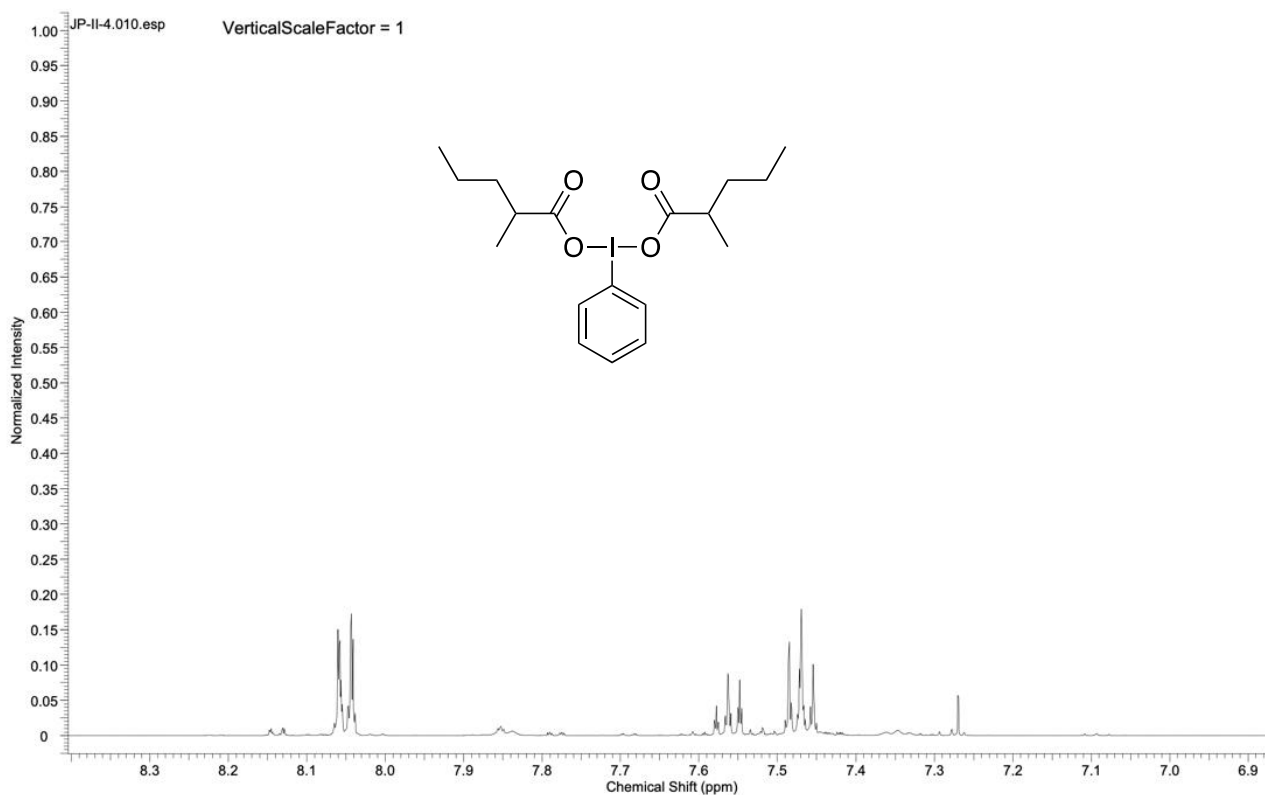
^1H NMR, & ^{13}C NMR, spectra of phenyl- λ^3 -iodanediyl bis(2-ethylhexanoate) (2b)

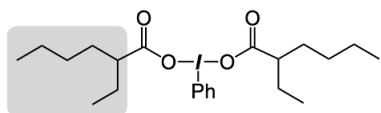
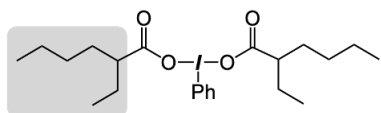
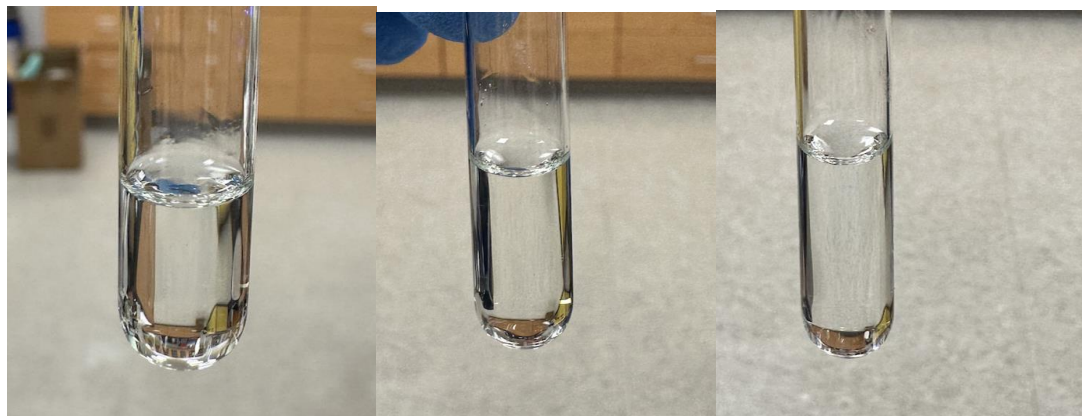
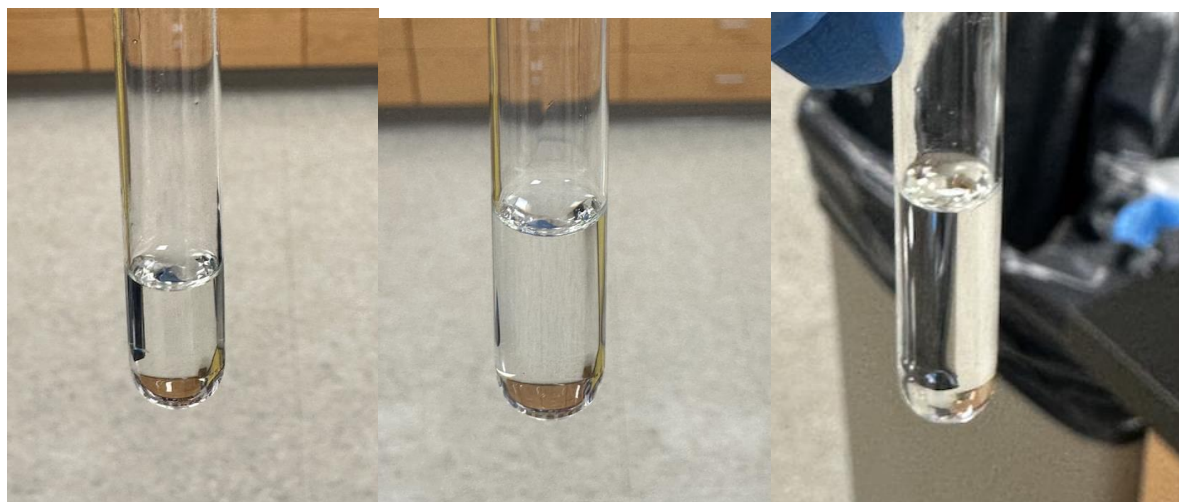
^1H NMR, & ^{13}C NMR, spectra of phenyl- λ^3 -iodanediyl bis(2-ethylhexanoate) (2b)

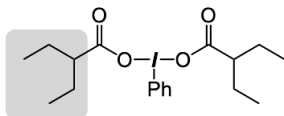
^1H NMR, & ^{13}C NMR spectra of phenyl- λ^3 -iodanediyl bis(2-ethylbutanoate) (**2c**)

^1H NMR, & ^{13}C NMR spectra of phenyl- λ^3 -iodanediyl bis(2-ethylbutanoate) (**2c**)

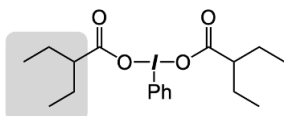
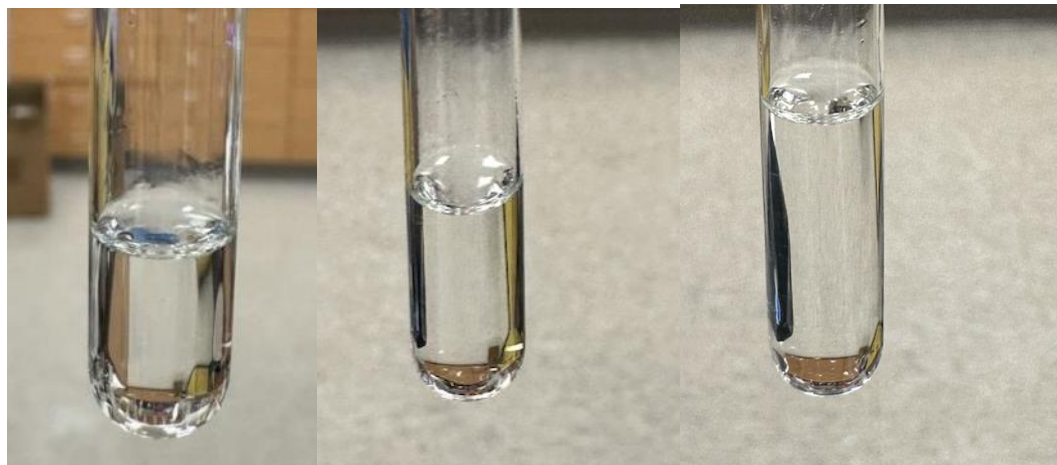
^1H NMR & ^{13}C NMR of phenyl- λ^3 -iodanediyl bis(2-methylpentanoate) (2d)

^1H NMR & ^{13}C NMR of phenyl- λ^3 -iodanediyl bis(2-methylpentanoate) (2d)

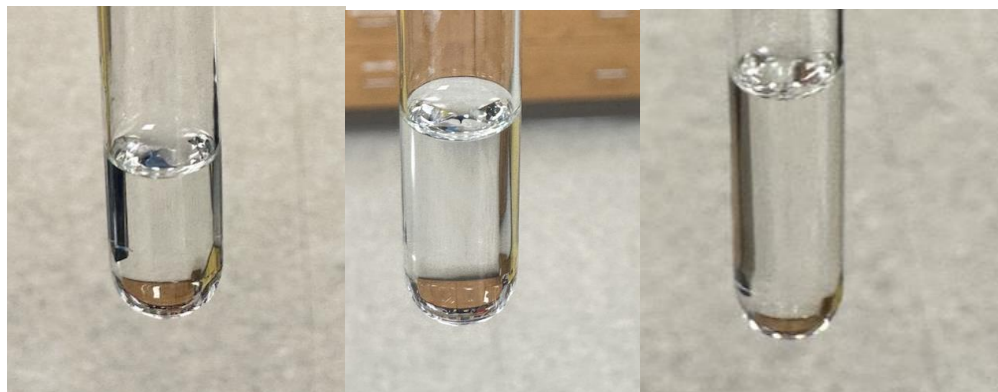
Pictures for Miscibility of **2b** to **2d**compound **2b** with hexanes (2:1,1:1,1:2)compound **2b** with acetonitrile (2:1,1:1,1:2)

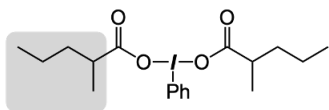


compound **2c** with hexanes (2:1,1:1,1:2)

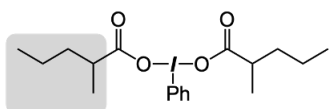
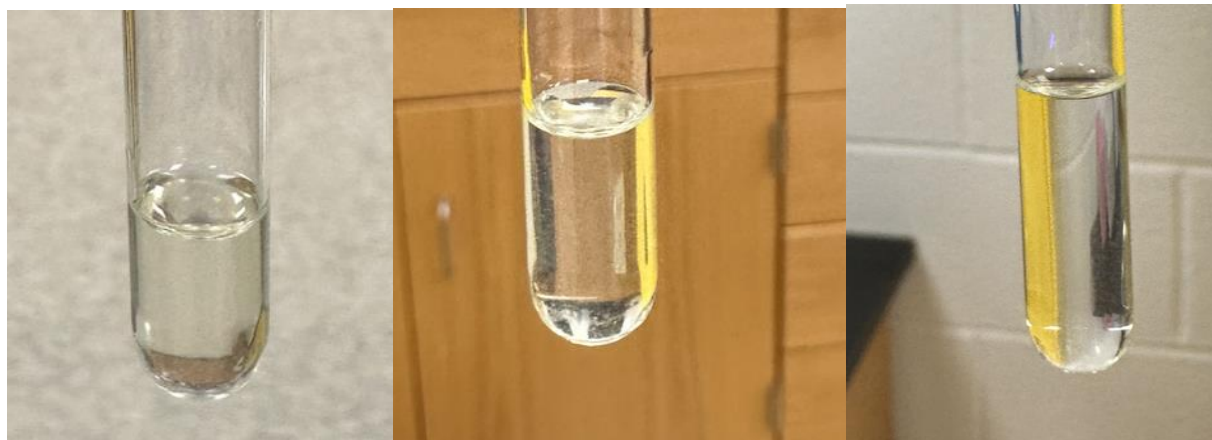


with acetonitrile (2:1,1:1,1:2)

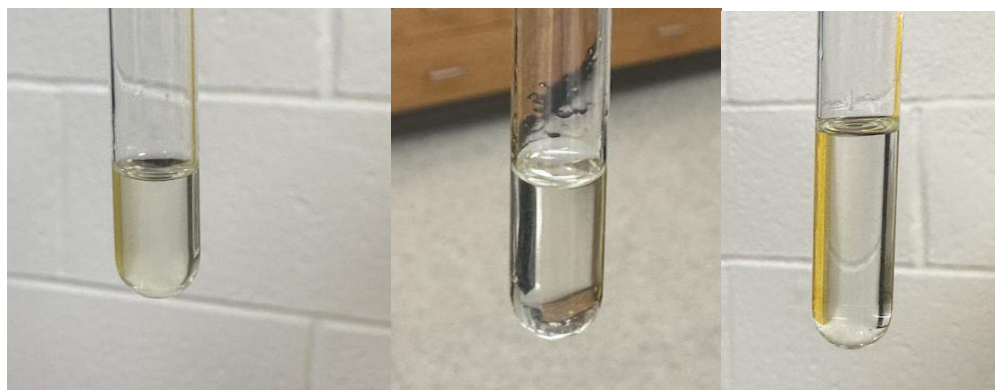




compound **2d** with hexanes (2:1,1:1,1:2)

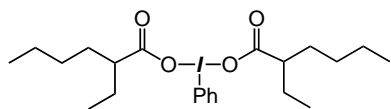


compound **2d** with acetonitrile (2:1,1:1,1:2)



Solubility data for **phenyl- λ 3-iodanediyl bis(1-adamantoate) (2a)**

Solvent	Solubility (g/ml)
Hexanes	0.005
	0.0051
	0.0044
	0.0053
	0.0042
	0.0046
	0.004
	0.0042
Average	0.0046
Standard Deviation (SD)	0.000481
%RSD	10.5%

Partition Coefficient of Compound **2b** in Acetonitrile and Hexanes**Compound 2b**

Molar mass = 490.42 g/mol

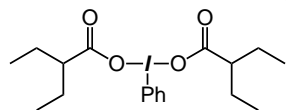
Density = 1.3 g/ml

Acetonitrile layer (0.10 ml of 2b)

	Mass dissolved (g)	Concentration (mol/L)
Trial 1 Vial 1	0.0202	0.0412
Trial 1 Vial 2	0.0184	0.0375
Trial 2 Vial 1	0.0182	0.0371
Trial 3 Vial 1	0.0193	0.0394
Trial 3 Vial 2	0.0198	0.0404
Average	0.0192	0.0391
Standard deviation (SD)	0.00087	0.00177
%RSD	4.52	4.52

Hexanes layer (0.10 ml 2b)

	Mass dissolved (g)	Concentration (mol/L)
Trial 1 Vial 1	0.0095	0.0194
Trial 1 Vial 2	0.0103	0.0210
Trial 2 Vial 1	0.0081	0.0165
Trial 2 Vial 2	0.0109	0.0222
Trial 3 Vial 1	0.0082	0.0167
Trial 3 Vial 2	0.0086	0.0175
Average	0.00927	0.0189
Standard deviation (SD)	0.00116	0.00237
%RSD	12.5	12.5

Partition Coefficient of Compound **2c** in Acetonitrile and Hexanes**Compound 2c**

Molar mass = 434.10 g/mol

Density = 1.3 g/ml

Acetonitrile layer (0.10 ml of 2c)

	Mass dissolved (g)	Concentration (mol/L)
Trial 1 Vial 1	0.0217	0.0500
Trial 1 Vial 2	0.0217	0.0500
Trial 2 Vial 1	0.0202	0.0465
Trial 2 Vial 2	0.0206	0.0475
Average	0.0211	0.0485
Standard deviation (SD)	0.000768	0.00178
%RSD	3.65%	3.67%

Hexanes layer (0.10 ml)

	Mass dissolved (g)	Concentration (mol/L)
Trial 1 Vial 1 (SW-1-67)	0.004	0.00921
Trial 1 Vial 2	0.0037	0.00852
Trial 2 Vial 1 (SW-1-68)	0.0038	0.00875
Trial 2 Vial 2	0.0037	0.00852
Average	0.0038	0.00875
Standard deviation (SD)	0.000141	0.000325
%RSD	3.72%	3.72%

Partition Coefficient = 0.12

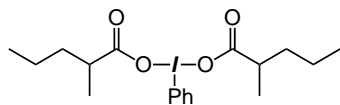
Acetonitrile layer (0.20 ml 2c)

	Mass dissolved (g)	Concentration (mol/L)
Trial 1 Vial 1	0.0451	0.104
Trial 1 Vial 2	0.0415	0.0956
Trial 2 Vial 1	0.0423	0.0974
Trial 2 Vial 2	0.0435	0.100
Trial 3 Vial 1	0.0413	0.0951
Trial 3 Vial 2	0.0419	0.0965
Average	0.0426	0.0981
Standard deviation (SD)	0.00145	0.00337
%RSD	3.41%	3.43%

Hexanes layer (0.20 ml of 2c)

	Mass dissolved (g)	Concentration (mol/L)
Trial 1 Vial 1	0.0076	0.0175
Trial 1 Vial 2	0.0076	0.0175
Trial 2 Vial 1	0.0063	0.0145
Trial 2 Vial 2	0.0068	0.0157
Trial 3 Vial 1	0.0073	0.0168
Trial 3 Vial 2	0.0072	0.0166
Average	0.00713	0.0164
Standard deviation (SD)	0.000505	0.00116
%RSD	7.07%	7.05%

Partition Coefficient = 0.11

Partition Coefficient of Compound **2d** in Acetonitrile and Hexanes**Compound 2d (I)**

Molar mass = 434.10 g/mol

Density = 1.3 g/ml

Acetonitrile layer (0.1 ml 2d)

	Mass dissolved (g)	Concentration (mol/L)
Trial 1 Vial 1	0.0296	0.0682
Trial 1 Vial 2	0.0303	0.0698
Trial 2 Vial 1	0.0298	0.0686
Trial 2 Vial 2	0.0285	0.0657
Average	0.0296	0.0681
Standard deviation (SD)	0.000759	0.00172
%RSD	2.57%	2.53%

Hexanes layer (0.1 ml 2d)

	Mass dissolved (g)	Concentration (mol/L)
Trial 1 Vial 1	0.0044	0.0101
Trial 1 Vial 2	0.0054	0.0124
Trial 2 Vial 1	0.0047	0.0108
Trial 2 Vial 2	0.0048	0.0111
Average	0.00483	0.0111
Standard deviation (SD)	0.000419	0.000963
%RSD	8.69%	8.67%

Partition Coefficient = 0.11

Acetonitrile layer (0.2 ml 2d)

	Mass dissolved (g)	Concentration (mol/L)
Trial 1 Vial 1	0.0606	0.14
Trial 1 Vial 2	0.0601	0.138
Trial 2 Vial 1	0.06	0.138
Trial 2 Vial 2	0.0609	0.14
Average	0.0604	0.139
Standard deviation (SD)	0.000424	0.00115
%RSD	0.702%	0.831%

Hexanes layer (0.2 ml 2d)

	Mass dissolved (g)	Concentration (mol/L)
Trial 1 Vial 1	0.011	0.0253
Trial 1 Vial 2	0.0109	0.0251
Trial 2 Vial 1	0.0111	0.0256
Trial 2 Vial 2	0.0111	0.0256
Average	0.011025	0.0254
Standard deviation (SD)	0.0000957	0.000245
%RSD	0.868%	0.964%

Partition Coefficient = 0.12

Absorbance Data for Filtered vs. Unfiltered $\text{PhI}(\text{OAc})_2$ **1a**

Made 20%, 40%, 60%, 80% solution in CH_2Cl_2 of unfiltered PIDA and filtered PIDA. Allowed the solutions to stir for an hour before measurement and the filtration. Absorbances were measured with a Genesys 10S Vis Spectrophotometer equipped with Thermo electron quartz cuvettes with a 10 mm path length immediately following filtration as described in the experimental section of the manuscript.

20% saturation of unfiltered PIDA = 0.884 A

40% saturation of unfiltered PIDA = 1.464 A

60% saturation of unfiltered PIDA = 1.897 A

80% saturation of unfiltered PIDA = 2.216 A

20% saturation of filtered PIDA = 0.000 A

40% saturation of filtered PIDA = 0.000 A

60% saturation of filtered PIDA = 0.000 A

80% saturation of filtered PIDA = 0.001 A

Absorbance vs. Time Stored for Filtered $\text{PhI}(\text{OAc})_2$ **1a**

Filtered **1a** was stored as a solid at 2 °C in a vial. 60% saturated solutions in CH_2Cl_2 were made to measure the absorbance. Following measurement, the solvent was removed in vacuo and the obtained solid **1a** was added back into the vial it came from.

Date	Absorbance (stored under nitrogen atmosphere)	Absorbance (stored under air atmosphere)
07/25/22	0.000 A	0.000 A
07/26/22	0.000 A	0.000 A
07/27/22	0.000 A	0.000 A
07/28/22	0.000 A	0.000 A
08/01/22	0.000 A	0.000 A
08/02/22	0.001 A	0.001 A
08/03/22	0.000 A	0.001 A