Supporting Information

Fundamental Understanding of Fluorophenol-derived Dual Organocatalysts for Ring-opening Polymerization of Lactide

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Materials

L-lactide (LLA, 99.5%, supplied by Jinan Steel Biomaterials Co., LTD.) was recrystallized by anhydrous toluene three times to obtain white crystal and subsequently dried under vacuum for 72 h. 3-phenylpropanol (PPA, 99%, Acros) was dried over CaH_2 for 48h before distillation. Anhydrous dichloromethane CH_2Cl_2, >99.5%, was purchased from Sinopath Chemical Reagents Co., LTD. Toluene (> 99%, water content < 0.001%, Sinopsin Chemical Reagent Co., LTD.) was stored in a flask with 3 Å molecular sieve. 4-(N,N'-dimethylamino) pyridine (DMAP), 7-Methyl-1,5,7-triazabicyclo(4.4.0)dec-5-ene (MTBD) and fluorophenols were purchased from Sinophosphoric Chemical Reagent Co., LTD.

Instruments

^{1}H NMR and ^{13}C NMR spectra were measured at 298 K by a Bruker Ascend TM-400 spectrometer using $CDCl_3$ as solvent. **Size Exclusion Chromatography (SEC)** was applied to determine molecular weight and dispersity of polymer at a flow rate of 0.7 ml/min, 35˚ C in THF flow phase, polystyrene as standard. **Matrix-assisted laser desorption ionization time-of-flight (MALDI-TOF)** mass spectrometry was performed using a Voyager-DE STR (Applied Biosystems) spectrometer equipped with a nitrogen laser (337 nm), a delay extraction, and a reflector. The MALDI-TOF mass spectra re-present averages over 100 laser shots. This instrument operated at an accelerating potential of 20 kV. Polymer (2 μL) and matrix (20 μL, dithranol) solutions in CH_2Cl_2 (10 g·L^{-1}) were mixed with 2 μL of a sodium iodide solution (10 g·L^{-1} in methanol), which favors ionization. The final solution (1 μL) was deposited onto the sample target and dried in air at room temperature.

Experimental Procedures

1.1 Preparation of the dual catalysts
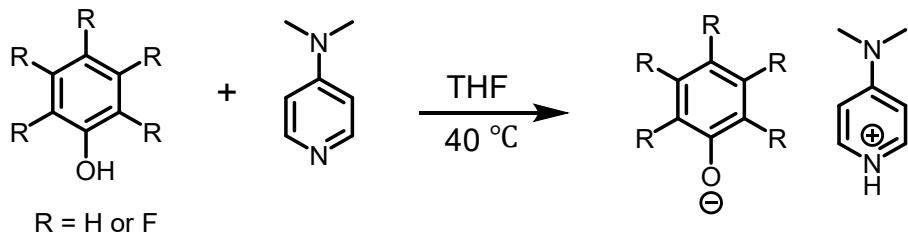
**Scheme S1**. Synthesis of fluorophenol/DMAP dual catalysts

Fluorophenol/DMAP catalysts were obtained by the reactions of fluorophenol and 4-(N,N-Dimethylamino) pyridine (DMAP). Taking *p*-fluorophenol and DMAP as an example, *p*-fluorophenol (689 mg, 6.15 mmol, 1.0 equiv.), DMAP (750 mg, 6.15 mmol, 1.0 equiv) and THF (5.0 mL) as the solvent were added into a 20 mL vial equipped with a stirrer. The mixture was stirred for 4 h at 40 °C. The solvent was removed by rotary steaming and the product was obtained by drying in vacuum for 24 hours.
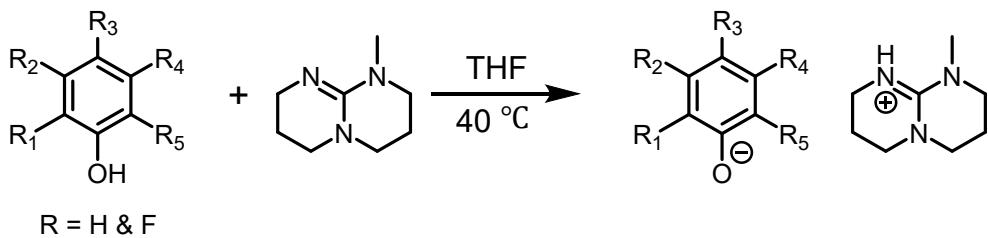
Scheme S2. Synthesis of fluorophenol/MTBD dual catalysts

Fluorophenol/MTBD catalysts were obtained by the reactions of fluorophenol and 7-methyl-1,5,7-triazabicyclo(4.4.0)dec-5-ene (MTBD). Taking *p*-fluorophenol and MTBD as an example, *p*-fluorophenol (689 mg, 6.15 mmol, 1.0 equiv.), MTBD (942 mg, 6.15 mmol, 1.0 equiv) and THF (5.0 mL) as the solvent were added into a 20 mL vial equipped with a stirrer. The mixture was stirred for 4 h at 40 °C. The solvent was removed by rotary steaming and the product was obtained by drying in vacuum for 24 hours.

1.2 General procedure for ring-opening polymerization of L-lactide
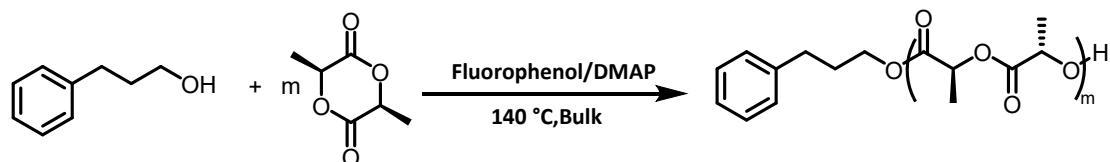
Scheme S3. Synthesis of polylactide catalyzed by fluorophenol/DMAP

A typical procedure for the polymerization is as follows: in an Ar-filled glove box, LLA (0.231 g, 1.6 mmol, 100 equiv) and catalyst **fluorophenol/DMAP** (0.016mmol, 1 equiv) were added into a dry Schlenk tube, and 3-phenylpropanol (2.18 μL, 0.016 mmol, 1 equiv) was dripped as initiator. The mixture was stirred for 1 h at 140 ˚C. A portion of the polymerization mixtures and then added a small amount of dichloromethane and benzoic acid to the mixtures for determining the monomer conversion that was directly determined from the ^{1}H NMR measurements of the polymerization mixtures. The polymer was isolated by reprecipitation in cold methanol. Yield, 85.2%; $M_{n,NMR}$, 12.6 kg·mol^{-1}; M_w/M_n, 1.09; ^{1}H NMR (CDCl$_3$) δ (ppm), 1.58 (m, 3H × *n*, (−

CH₃)*n*), 1.97 (q, 2H, ArCH₂*CH₂*–), 2.67 (t, 2H, Ar*CH₂*–), 4.15 (m, 2H, ArCH₂CH₂*CH₂*–), 4.36 (m, 1H, –*CH*(CH₃)OH), 5.10–5.23 (q, 1H × n − 1, (–*CH*(CH₃)O–)$_{n-1}$), 7.15–7.31 (m, 5H, aromatic).

1.3 Preparation of the fluorophenol/DMAP dual catalysts

o-FP/DMAP(a)
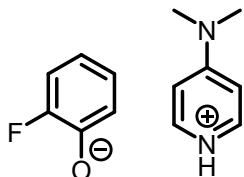
4-(N,N-Dimethylamino) pyridine *ortho*-fluorophenol (*o*-FP/DMAP) 1.35 g, yield = 94%. White crystal. ^{1}H NMR (400 MHz, CDCl₃) δ 8.20 (s, 2H), 7.07 – 7.01 (m, 1H), 6.98 (s, 2H), 6.78 (s, 1H), 6.50 (s, 2H), 3.02 (s, 6H). ^{13}C NMR (101 MHz, CDCl₃) δ 154.77, 153.24, 150.86, 148.75, 124.64, 119.60, 118.15, 115.95, 106.75, 39.72. ^{19}F NMR (376 MHz, CDCl₃) δ -138.41.
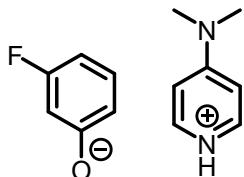
m-FP/DMAP(b)

4-(N,N-Dimethylamino) pyridine *meta*-fluorophenol (*m*-FP/DMAP) 1.36 g; yield = 95%. White crystal. ^{1}H NMR (400 MHz, CDCl₃) δ 8.18 (s, 2H), 7.11 (s, 1H), 6.64 (s, 1H), 6.58 (s, 1H), 6.52 (s, 3H), 3.03 (s, 6H). ^{13}C NMR (101 MHz, CDCl₃) δ 162.73, 159.69, 154.92, 148.35, 130.17, 111.83, 106.88, 105.90, 103.62, 39.72. ^{19}F NMR (376 MHz, CDCl₃) δ -112.78.
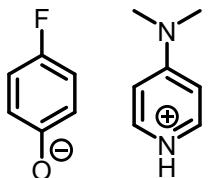
p-FP/DMAP (c)

4-(N,N-Dimethylamino) pyridine *p*-fluorophenol (*p*-FP/DMAP) 1.36 g; yield = 95%. White crystal. ^{1}H NMR (400 MHz, CDCl₃) δ 8.19 (s, 2H), 6.84 (d, *J* = 30.4 Hz, 3H), 6.51 (s, 2H), 3.02 (s, 6H). ^{13}C NMR (101 MHz, CDCl₃) δ 154.76, 153.83, 149.24, 116.50, 115.67, 106.10, 38.05. ^{19}F NMR (376 MHz, CDCl₃) δ -126.34.
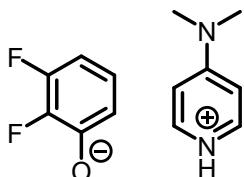
2,3-FP/DMAP(d)

4-(N,N-Dimethylamino) pyridine 2,3-difluorophenol (2,3-FP/DMAP) 1.46 g; yield = 94%. White crystal. ^{1}H NMR (400 MHz, CDCl$_3$) δ 8.18 (s, 2H), 6.83 (s, 1H), 6.74 (s, 1H), 6.58 (dddd, J = 10.1, 8.5, 6.8, 1.7 Hz, 1H), 6.51 (s, 2H), 3.03 (s, 6H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 154.94, 152.93, 150.53, 148.15, 142.42, 140.04, 123.29, 113.74, 106.76, 39.22. ^{19}F NMR (376 MHz, CDCl$_3$) δ -138.82, -162.04.

2,4-FP/DMAP (e)
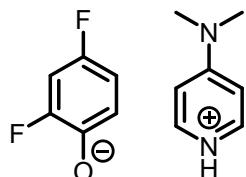
4-(N,N-Dimethylamino) pyridine 2,4-difluorophenol (2,4-FP/DMAP) 1.49 g; yield = 96%. Faint yellow crystal. ^{1}H NMR (400 MHz, CDCl$_3$) δ 8.18 (s, 2H), 6.91 (s, 1H), 6.81 (s, 1H), 6.70 (s, 1H), 6.50 (s, 2H), 3.02 (s, 6H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 156.51, 154.84, 154.10, 148.51, 142.01, 118.05, 110.89, 106.77, 104.23, 39.20. ^{19}F NMR (376 MHz, CDCl$_3$) δ -123.24, -133.32.

2,6-FP/DMAP (f)
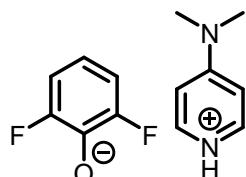
4-(N,N-Dimethylamino) pyridine 2,6-difluorophenol (2,6-FP/DMAP) 1.44 g; yield = 93%. White crystal. ^{1}H NMR (400 MHz, CDCl$_3$) δ 8.20 (s, 2H), 6.84 (s, 2H), 6.65 (s, 1H), 6.51 (s, 2H), 3.03 (s, 6H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 154.96, 152.36, 147.99, 135.84, 117.00, 111.42, 106.64, 39.23. ^{19}F NMR (376 MHz, CDCl$_3$) δ -133.72.

2,3,6-FP/DMAP(g)
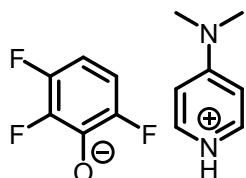
4-(N,N-Dimethylamino) pyridine 2,3,6-trifluorophenol (2,3,6-FP/DMAP) 1.54 g; yield = 93%. White crystal. ^{1}H NMR (400 MHz, CDCl$_3$) δ 8.17 (s, 2H), 6.71 (s, 1H), 6.53 (s, 2H), 6.41 (s, 1H), 3.06 (s, 6H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 155.12, 154.40, 152.89, 147.73, 134.82, 132.41, 106.97, 100.22, 39.25. ^{19}F NMR (376 MHz, CDCl$_3$) δ -138.50, -143.47, -156.88.

3,4,5-FP/DMAP (h)
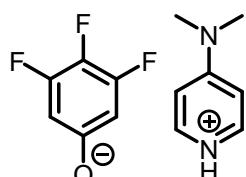
4-(N,N-Dimethylamino) pyridine 3,4,5-trifluorophenol (3,4,5-FP/DMAP) 1.58 g; yield = 95%. White crystal. ^{1}H NMR (400 MHz, CDCl$_3$) δ 8.13 (s, 2H), 6.54 (s, 2H), 6.43 (s, 2H), 3.05 (s, 6H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 155.33, 152.66, 150.22, 146.70, 134.54, 106.80, 100.08, 39.15. ^{19}F NMR (376 MHz, CDCl$_3$) δ -135.63, -174.88.

2,3,5,6-FP/DMAP (i)
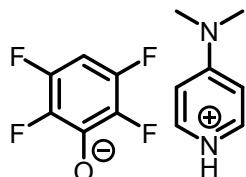
4-(N,N-Dimethylamino) pyridine 2, 3, 5, 6-tetrafluorphenol (2,3,5,6-FP/DMAP) 1.67 g; yield = 94%. White crystal. ^{1}H NMR (400 MHz, CDCl$_3$) δ 8.13 (s, 2H), 6.57 (s, 2H), 6.24 (s, 1H), 3.09 (s, 6H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 155.88, 147.90, 145.51, 143.91, 143.39, 106.65, 90.53, 39.50. ^{19}F NMR (376 MHz, CDCl$_3$) δ -144.06, -164.19.

2,3,4,5,6-FP/DMAP (j)
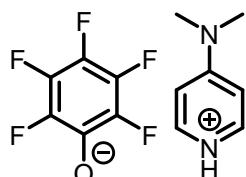
4-(N,N-Dimethylamino) pyridine pentafluorophenol (2,3,4,5,6-FP/DMAP) 1.71 g; yield = 91%. White crystal. ^{1}H NMR (400 MHz, CDCl$_3$) δ 8.13 (s, 1H), 6.57 (s, 1H), 3.09 (s, 3H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 155.75, 144.69, 141.29, 139.57, 139.01, 137.13, 106.59, 39.39. ^{19}F NMR (376 MHz, CDCl$_3$) δ -165.09, -167.82, -178.31.

1.4 Preparation of the fluorophenol/MTBD dual catalysts

o-FP/MTBD(a')
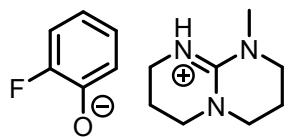
7-methyl-1,5,7-triazabicyclo(4.4.0)dec-5-ene (MTBD) *ortho*-fluorophenol (*o*-FP/MTBD) 1.47 g, yield = 90%. Yellow colorless liquid. ^{1}H NMR (400 MHz, CDCl$_3$) δ 6.91 – 6.86 (m, 1H), 6.85 (d, 1H), 6.80 (td, 1.6 Hz, 1H), 6.39 (tdd, 1H), 3.34 – 3.29 (m, 2H), 3.20 – 3.12 (m, 6H), 3.05 (s, 3H), 1.92 (q, 2H), 1.85 (qd, 2H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 155.45, 153.10, 151.81, 124.47, 120.17, 115.15, 114.00, 48.34, 48.12, 47.57, 40.08, 38.20, 21.78, 21.57. ^{19}F NMR (376 MHz, CDCl$_3$) δ -138.15.
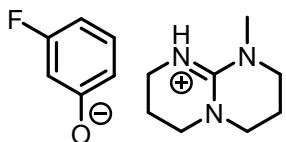
m-FP/MTBD(b')

7-methyl-1,5,7-triazabicyclo(4.4.0)dec-5-ene (MTBD) *meta*-fluorophenol (*m*-FP/MTBD) 1.52 g; yield = 93%. Yellow colorless liquid. ^{1}H NMR (400 MHz, CDCl$_3$) δ 6.92 (q, 1H), 6.44 (ddd, 1H), 6.35 (dt, 1H), 6.20 – 6.10 (m, 1H), 3.32 – 3.25 (m, 2H), 3.27 – 3.03 (m, 6H), 2.94 (s, 3H), 1.90 (p, 2H), 1.81 (p, 2H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 163.38, 160.29, 156.40, 148.79, 127.43, 111.06, 100.81, 45.55, 45.17, 44.86, 37.37, 34.95, 18.94, 18.89. ^{19}F NMR (376 MHz, CDCl$_3$) δ -114.42.

p-FP/MTBD(c')
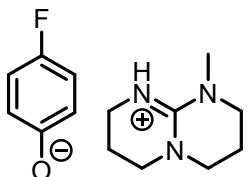
7-methyl-1,5,7-triazabicyclo(4.4.0)dec-5-ene (MTBD) *p*-fluorophenol (*p*-FP/MTBD) 1.50 g; yield = 92%. Yellow colorless liquid. ^{1}H NMR (400 MHz, CDCl$_3$) δ 6.79 – 6.69 (m, 4H), 3.31 – 3.16 (m, 2H), 3.16 – 3.04 (m, 6H), 2.95 (s, 3H), 2.89 – 2.80 (m, 2H), 1.91 – 1.74 (m, 2H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 156.52, 154.44, 114.28, 113.26, 45.56, 45.19, 44.88, 37.37, 34.96, 18.99, 18.93. ^{19}F NMR (376 MHz, CDCl$_3$) δ -130.10.

2,3-FP/MTBD(d')
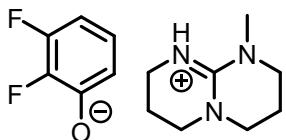
7-methyl-1,5,7-triazabicyclo(4.4.0)dec-5-ene (MTBD) 2,3-difluorophenol (2,3-FP/MTBD) 1.59 g; yield = 91%. Yellow colorless liquid. ^{1}H NMR (400 MHz, CDCl$_3$) δ 6.61 (tdd, 1H), 6.48 (tt, 1H), 6.10 (dddd, 1H), 3.34 – 3.20 (m, 2H), 3.15 (p, 6H), 3.09 – 3.03 (m, 3H), 3.00 (s, 2H), 1.87 (dq, 2H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 155.38, 150.90, 148.76, 141.16, 138.83, 120.37, 113.68, 45.50, 45.09, 44.64, 37.35, 35.01, 18.65, 18.55. ^{19}F NMR (376 MHz, Chloroform-*d*) δ -141.58, -165.82.

2,4-FP/MTBD(e')
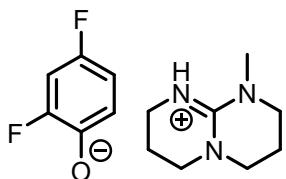
7-methyl-1,5,7-triazabicyclo(4.4.0)dec-5-ene (MTBD) 2,4-difluorophenol (2,4-FP/MTBD) 1.62 g; yield = 93%. Yellow colorless liquid. ^{1}H NMR (400 MHz, CDCl$_3$) 6.69 (s, 1H), 6.62 (s, 1H), 6.50 (s, 1H), 3.26 (s, 2H), 3.16 (s, 6H), 3.00 (s, 3H), 1.92 (s, 2H), 1.82 (s, 2H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 156.69, 151.21, 149.34, 148.73, 116.15, 107.59, 101.05, 45.45, 45.05, 44.60, 37.24, 34.92, 18.65, 18.56. ^{19}F NMR (376 MHz, Chloroform-*d*) δ -130.73, -134.35.

2,6-FP/MTBD(f')
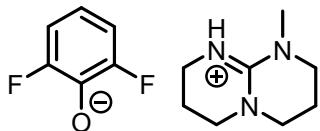
7-methyl-1,5,7-triazabicyclo(4.4.0)dec-5-ene (MTBD) 2,6-difluorophenol (2,6-FP/MTBD) 1.64 g; yield = 94%. Yellow colorless liquid. ^{1}H NMR (400 MHz, CDCl$_3$) δ 6.59 (s, 2H), 6.04 (s, 1H), 3.26 (s, 2H), 3.15 (s, 6H), 3.04 (s, 3H), 1.90 (s, 2H), 1.81 (s, 2H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 155.62, 152.07, 129.23, 110.49, 106.41, 48.45, 48.29, 48.21, 42.92, 37.50, 22.73, 22.70. ^{19}F NMR (376 MHz, CDCl$_3$) δ -137.18.
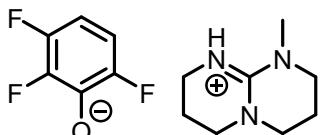
2,3.6-FP/MTBD(g')

7-methyl-1,5,7-triazabicyclo(4.4.0)dec-5-ene (MTBD) 2,3,6-trifluorophenol (2,3,6-FP/MTBD) 1.70 g; yield = 92%. Yellow colorless liquid. ^{1}H NMR (400 MHz, CDCl$_3$) δ 6.45 (s, 1H), 5.83 (s, 1H), 3.26 (s, 2H), 3.17 (s, 6H), 3.03 (s, 3H), 1.92 (s, 2H), 1.83 (s, 2H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 152.03, 149.75, 148.69, 147.76, 145.41, 142.99, 105.23, 45.43, 45.00, 44.45, 37.30, 34.97, 18.41, 18.27. ^{19}F NMR (376 MHz, CDCl$_3$) δ -141.65, -145.68, -162.25.

3,4,5-FP/MTBD(h')
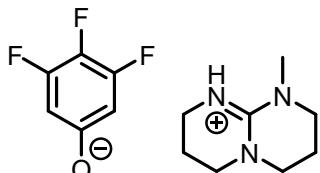
7-methyl-1,5,7-triazabicyclo(4.4.0)dec-5-ene (MTBD) 3,4,5-trifluorophenol (3,4,5-FP/MTBD) 1.72 g; yield = 93%. Yellow colorless liquid. ^{1}H NMR (400 MHz, CDCl$_3$) δ 6.09 (s, 2H), 3.28 (s, 2H), 3.20 (s, 6H), 2.99 (s, 3H), 1.97 (s, 2H), 1.87 (s, 2H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 160.45, 155.87, 150.16, 148.75, 147.76, 45.54, 45.11, 44.71, 37.39, 34.99, 18.71, 18.62. ^{19}F NMR (376 MHz, CDCl$_3$) δ -138.78, -182.55.

2,3,5,6-FP/MTBD(i')
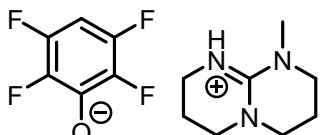
7-methyl-1,5,7-triazabicyclo(4.4.0)dec-5-ene (MTBD) 2, 3, 5, 6-tetrafluorphenol (2,3,5,6-FP/MTBD) 1.77 g; yield = 90%. Yellow colorless liquid. ^{1}H NMR (400 MHz, CDCl$_3$) δ 6.13 (s, 1H), 3.32 (s, 2H), 3.24 (s, 6H), 3.04 (s, 3H), 1.98 (s, 2H), 1.89 (s, 2H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 140.65, 137.42, 135.07, 130.74, 128.42, 37.48, 36.97, 36.48, 29.42, 26.93, 10.35, 10.20. ^{19}F NMR (376 MHz, CDCl$_3$) δ -144.72, -164.89.

2,3,4,5,6-FP/MTBD(j')
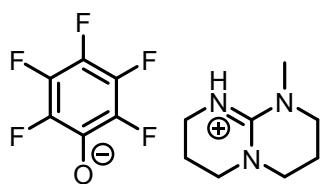
7-methyl-1,5,7-triazabicyclo(4.4.0)dec-5-ene (MTBD) pentafluorophenol (2,3,4,5,6-FP/MTBD) 1.84 g; yield = 89%. Yellow colorless liquid. ^{1}H NMR (400 MHz, CDCl$_3$) δ 3.29 (s, 2H), 3.23 (s, 6H), 3.05 (s, 3H), 1.98 (s, 2H), 1.88 (s, 2H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 148.67, 144.89, 139.88, 137.55, 135.25, 45.48, 44.99, 44.48, 37.35, 34.95, 18.38, 18.22. ^{19}F NMR (376 MHz, CDCl$_3$) δ -170.20, -170.99, -188.38.

Supporting Tables

Table S1. Pearson correlation coefficient between independent and dependent variables

dependent	independent variable	Fluorophenol/DMAP's pearson correlation (r)
k_{obs}	K_n	-0.14
k_{obs}	f^+	-0.35
k_{obs}	Q_{H1}	0.44
k_{obs}	Q_{O1}	-0.09
k_{obs}	Q_{H2}	-0.58
k_{obs}	Q_{O2}	-0.12
k_{obs}	$δ_F$	0.31
k_{obs}	Q_F	-0.12
k_{obs}	Int1	-0.07
k_{obs}	Int2	-0.38

Table S2. Summary of data from simulation and bench experiment for fluorophenol/DMAP dual catalyst

Entry	Catalyst	K_n	f^+	Q_{O1}	Q_F	Int1	Int2	Q_{H1}	$δ_F$	Q_{H2}	Q_{O2}	k_{obs}
1	a	-0.03	0.13	-0.765	-0.36	-5.91	-2.18	0.24	-138.41	0.29	-0.40	0.0287
2	b	-0.03	0.13	-0.769	-0.37	-8.34	-5.17	0.24	-112.77	0.31	-0.40	0.0350
3	c	-0.04	0.13	-0.782	-0.38	-5.87	-5.13	0.24	-126.34	0.30	-0.40	0.0257
4	d	-0.02	0.11	-0.758	-0.35	-3.04	-0.81	0.24	-150.43	0.29	-0.38	0.0344
5	e	-0.04	0.12	-0.769	-0.36	-8.95	-9.43	0.25	-128.27	0.27	-0.36	0.0387
6	f	-0.31	0.15	-0.761	-0.36	7.64	7.66	0.25	-133.72	0.27	-0.36	0.0324

7	g	-0.01	0.16	-0.753	-0.35	-4.93	3.92	0.24	-146.28	0.30	-0.39	0.0317
8	h	-0.02	0.11	-0.763	-0.35	-6.58	0.20	0.24	-155.25	0.31	-0.40	0.0286
9	i	-0.01	0.18	-0.747	-0.35	-4.08	6.75	0.24	-154.12	0.30	-0.35	0.0246
10	j	-0.01	0.18	-0.751	-0.34	-0.95	7.51	0.23	-170.40	0.30	-0.35	0.0316

Table S3. The combined independent variables for multi linear regression of fluorophenol/DMAP dual catalyst

Entry	Variable_1	Variable_2	Variable_3	Variable_4	Variable_5	Variable_6
1	f^+	Q_{O1}	Int1	Int2	Q_{H1}	δ_F
2	f^+	Q_F	Int1	Int2	Q_{H1}	δ_F
3	K_n	f^+	Q_{O1}	Q_F	Int1	δ_F
4	K_n	Q_F	Int1	Int2	Q_{H1}	δ_F
5	K_n	f^+	Q_{O1}	Q_F	Int1	Int2
6	K_n	f^+	Q_{O1}	Q_F	Int1	Q_{H1}
7	K_n	Q_{O1}	Q_F	Int1	Int2	Q_{H1}
8	K_n	Q_F	Int1	Int2	Q_{H1}	δ_F
9	f^+	Q_{O1}	Q_F	Int1	Int2	Q_{H1}
10	f^+	Q_{O1}	Q_F	Int1	Int2	Q_{H1}
11	K_n	f^+	Q_{O1}	Q_F	Int1	Int2
12	K_n	f^+	Q_{O1}	Q_F	Int1	δ_F
13	K_n	f^+	Q_F	Int1	Int2	Q_{H1}
14	K_n	Q_{O1}	Q_F	Int1	Int2	δ_F
15	K_n	f^+	Q_{O1}	Q_F	Int1	Int2
16	K_n	f^+	Q_{O1}	Q_F	Int1	Int2
17	K_n	f^+	Q_{O1}	Q_F	Int1	Int2
18	K_n	f^+	Q_{O1}	Q_F	Int1	Int2
19	K_n	f^+	Q_{O1}	Q_F	Int1	Q_{H1}
20	K_n	f^+	Q_{O1}	Q_F	Int2	Q_{H1}
21	K_n	f^+	Q_{O1}	Int1	Int2	Q_{H1}
22	K_n	f^+	Q_F	Int1	Int2	Q_{H1}
23	K_n	Q_{O1}	Q_F	Int1	Int2	Q_{H1}

Table S4. Pearson correlation coefficient between independent and dependent variables

dependent	independent variable	Fluorophenol/MTBD's pearson correlation (r)
k_{obs}	K_n	-0.27
k_{obs}	f^+	-0.41
k_{obs}	Q_{H1}	-0.50
k_{obs}	Q_{O1}	-0.30
k_{obs}	Q_{H2}	0.09
k_{obs}	Q_{O2}	-0.28
k_{obs}	δ_F	0.20
k_{obs}	Q_F	-0.32
k_{obs}	Int1	-0.39
k_{obs}	Int2	-0.34

Table S5. Summary of data from simulation and bench experiment for fluorophenol/MTBD dual catalyst

Entry	Catalyst	K_n	f^+	Q_{O1}	Q_F	Int1	Int2	Q_{H1}	δ_F	Q_{H2}	Q_{O2}	k_{obs}
1	a'	0.03	0.13	-0.765	-0.37	7.69	19.99	0.36	-138.15	0.28	-0.30	0.2103
2	b'	0.03	0.14	-0.769	-0.38	5.45	16.34	0.35	-114.42	0.28	-0.30	0.0793
3	c'	0.02	0.13	-0.782	-0.38	6.93	13.49	0.35	-130.10	0.28	-0.30	0.0736
4	d'	0.03	0.12	-0.758	-0.36	7.74	20.01	0.37	-153.72	0.28	-0.31	0.1048
5	e'	0.03	0.12	-0.769	-0.37	7.10	16.97	0.36	-132.54	0.28	-0.30	0.0200
6	f'	0.03	0.16	-0.761	-0.36	9.99	28.29	0.37	-137.18	0.28	-0.31	0.0358
7	g'	0.04	0.17	-0.753	-0.36	10.41	49.52	0.39	-149.87	0.28	-0.29	0.0255
8	h'	0.04	0.12	-0.763	-0.35	7.21	18.98	0.36	-160.67	0.28	-0.29	0.0538
9	i'	0.04	0.19	-0.747	-0.35	10.30	26.14	0.38	-154.80	0.27	-0.30	0.0080
10	j'	0.04	0.19	-0.751	-0.34	8.22	25.86	0.38	-176.51	0.27	-0.28	0.0475

Table S6. The combined independent variables for multi linear regression of fluorophenol/MTBD dual catalyst

Entry	Variable_1	Variable_2	Variable_3	Variable_4	Variable_5	Variable_6	Variab
1	f^+	Q_{H1}	Q_{O1}	Q_{H2}	Q_{O2}	Q_F	δ_F
2	Q_{H1}	Q_{O1}	Q_{H2}	Q_{O2}	Q_F	δ_F	Int1
3	K_n	f^+	Q_{H1}	Q_{O1}	Q_{H2}	Q_F	δ_F
4	K_n	f^+	Q_{H1}	Q_{O1}	Q_{H2}	Q_{O2}	Q_F
5	K_n	f^+	Q_{H1}	Q_{O1}	Q_{H2}	Q_F	δ_F
6	K_n	f^+	Q_{H1}	Q_{O1}	Q_{H2}	Q_F	δ_F
7	K_n	Q_{H1}	Q_{O1}	Q_{H2}	Q_{O2}	Q_F	δ_F
8	f^+	Q_{H1}	Q_{O1}	Q_{H2}	Q_{O2}	Q_F	δ_F
9	f^+	Q_{H1}	Q_{O1}	Q_{H2}	Q_{O2}	Q_F	δ_F
10	K_n	f^+	Q_{H1}	Q_{H2}	δ_F	Int1	Int2
11	K_n	f^+	Q_{H1}	Q_{O1}	Q_{H2}	δ_F	Int1
12	K_n	f^+	Q_{H1}	Q_{O1}	Q_{O2}	Q_F	δ_F
13	K_n	f^+	Q_{H1}	Q_{H2}	Q_{O2}	δ_F	Int1
14	K_n	f^+	Q_{H1}	Q_{H2}	Q_F	δ_F	Int1
15	K_n	f^+	Q_{O1}	Q_{H2}	Q_{O2}	Q_F	Int1
16	K_n	f^+	Q_{H1}	Q_{O1}	Q_{H2}	Q_{O2}	Q_F
17	K_n	f^+	Q_{H1}	Q_{O1}	Q_{H2}	Q_{O2}	Q_F
18	K_n	f^+	Q_{H1}	Q_{O1}	Q_{H2}	Q_{O2}	Q_F
19	K_n	f^+	Q_{H1}	Q_{O1}	Q_{H2}	Q_{O2}	δ_F
20	K_n	f^+	Q_{H1}	Q_{O1}	Q_{H2}	Q_F	δ_F
21	K_n	f^+	Q_{H1}	Q_{O1}	Q_{O2}	Q_F	δ_F
22	K_n	f^+	Q_{H1}	Q_{H2}	Q_{O2}	Q_F	δ_F
23	K_n	f^+	Q_{O1}	Q_{H2}	Q_{O2}	Q_F	δ_F
24	K_n	Q_{H1}	Q_{O1}	Q_{H2}	Q_{O2}	Q_F	δ_F

Supporting Figures
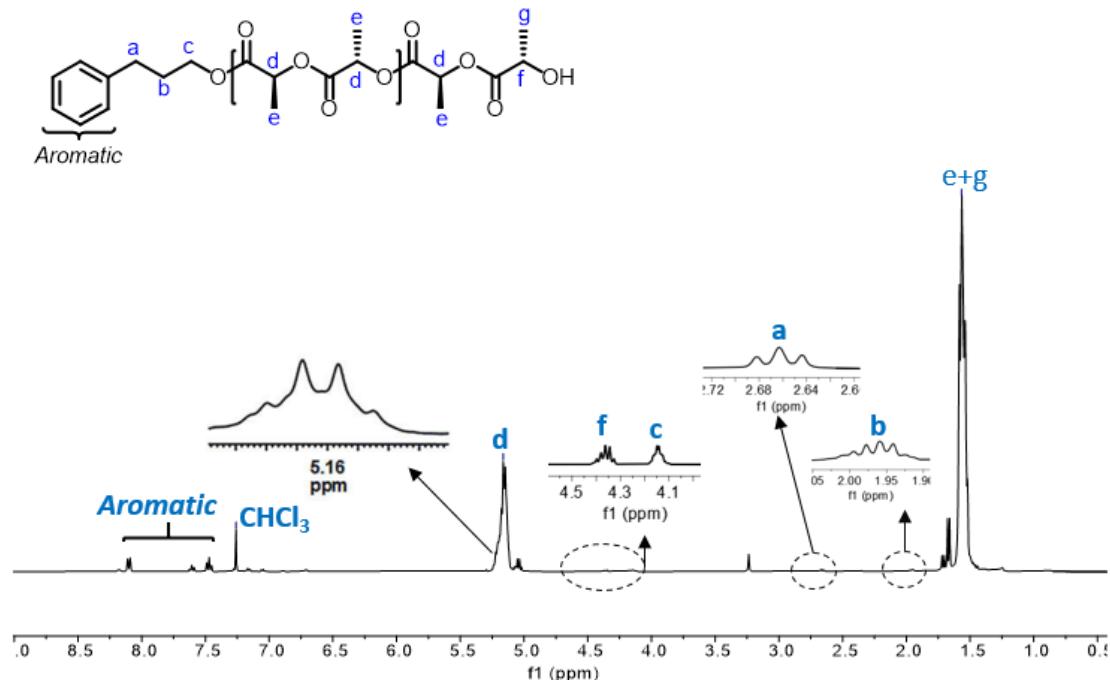
Figure S1. ^{1}H NMR spectrum of polylactide initiated by PPA in CDCl$_3$ (Table **1**, entry 1). Experimental conditions: 1.6 mmol LLA, [PPA]$_0$/[p-FP/DMAP]$_0$/[LLA]$_0$ = 1/1/100, at 140 °C, in bulk for 1 h.
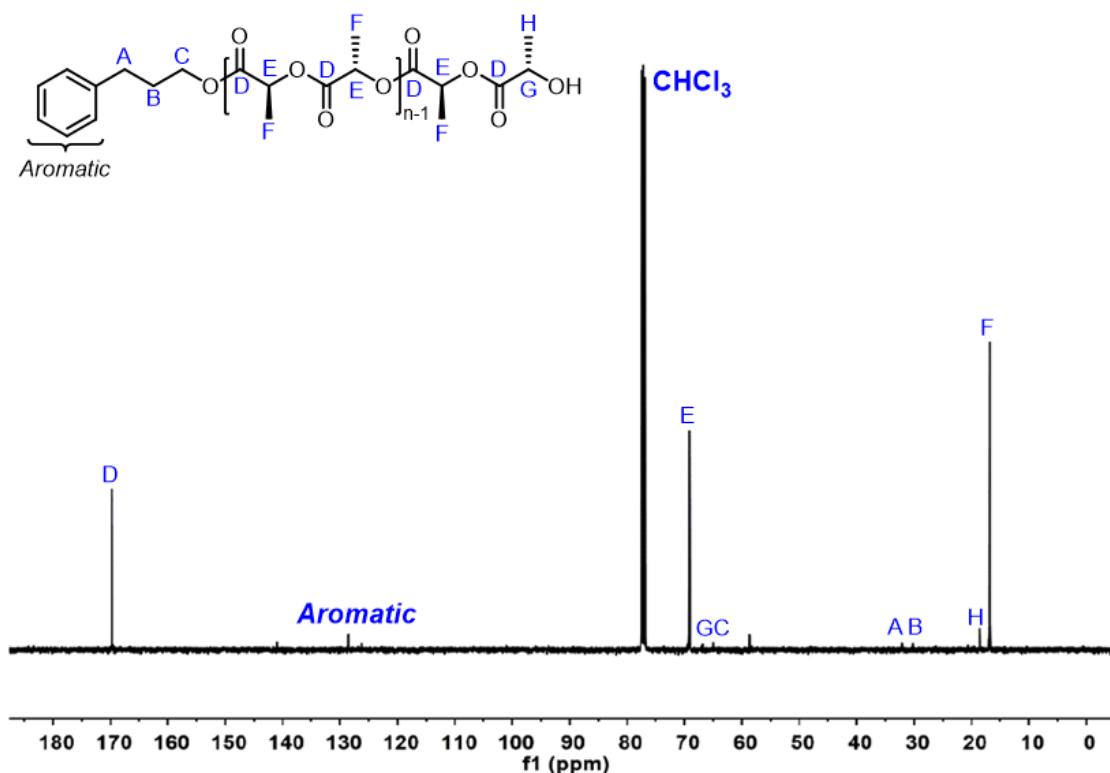
Figure S2. ^{13}C NMR spectrum of polylactide initiated by PPA in CDCl$_3$ (Table **1**, entry 1). Experimental

conditions: 1.6 mmol LLA, $[PPA]_0/[p\text{-}FP/DMAP]_0/[LLA]_0 = 1/1/100$, at 140 °C, in bulk for 1 h.
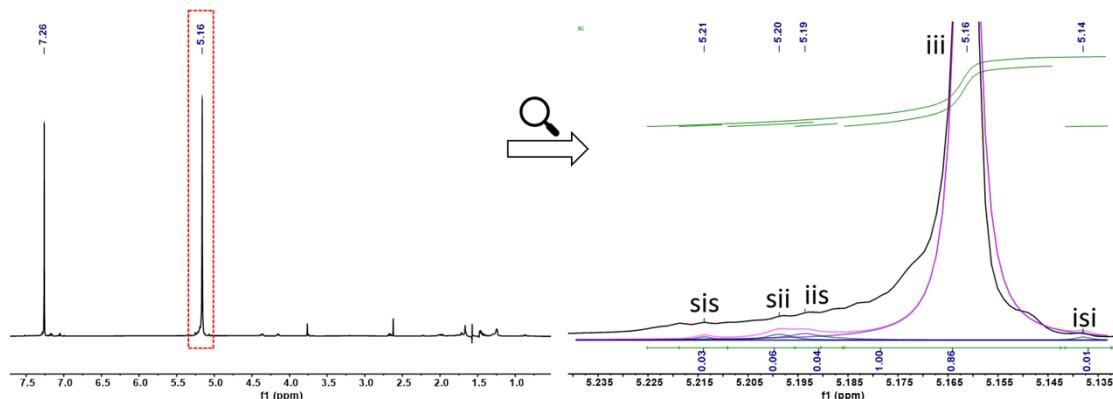
Figure S3. Stacked homonuclear decoupled ^{1}H NMR spectrum (400 MHz, CDCl$_3$) of PLA obtained (Table 1, entry 1)[2].

Cationic agent		[initiator] = PPA n				
		18	19	20	21	22
Na$^+$	Calc.	2751.90	2895.94	3039.98	3184.02	3328.06
	Exp.	2751.75	2895.85	3039.89	3184.21	3328.26
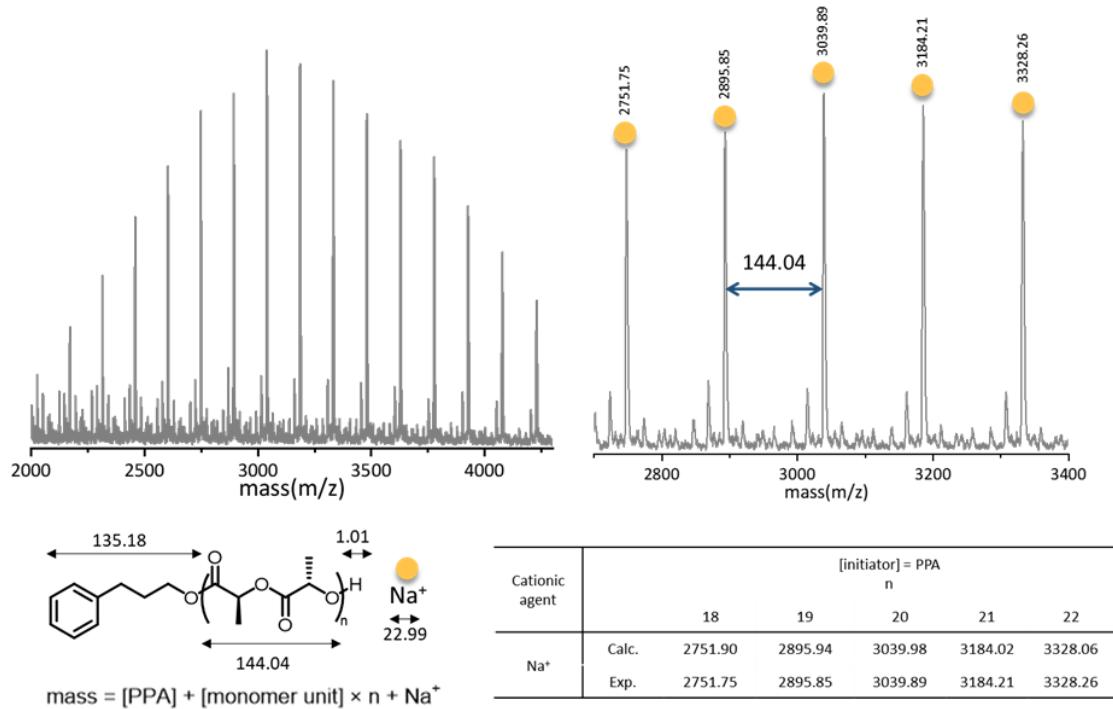
Figure S4. MALDI-TOF MS spectrum of PLLA obtained from LLA (Table **1**, entry 1), magnification between m/z = 2000 and m/z = 4250. Experimental conditions: $[M]_0/[I]_0$:100/1, 140 ˚C, 20min. Purification was performed by precipitation in methanol.
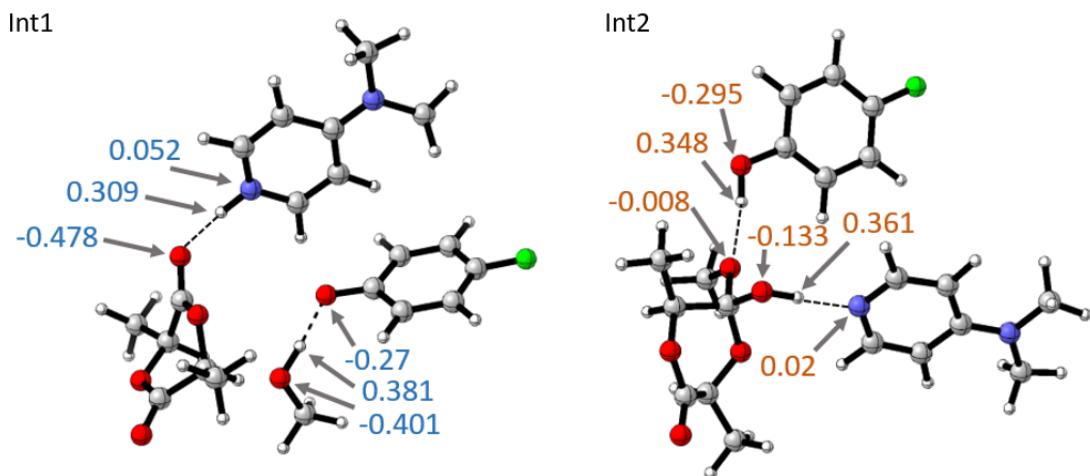
Figure S5. The mulliken charge distribution of involved atoms (Int1 and Int2) calculated with BY3LP/6-31G+(d,p).
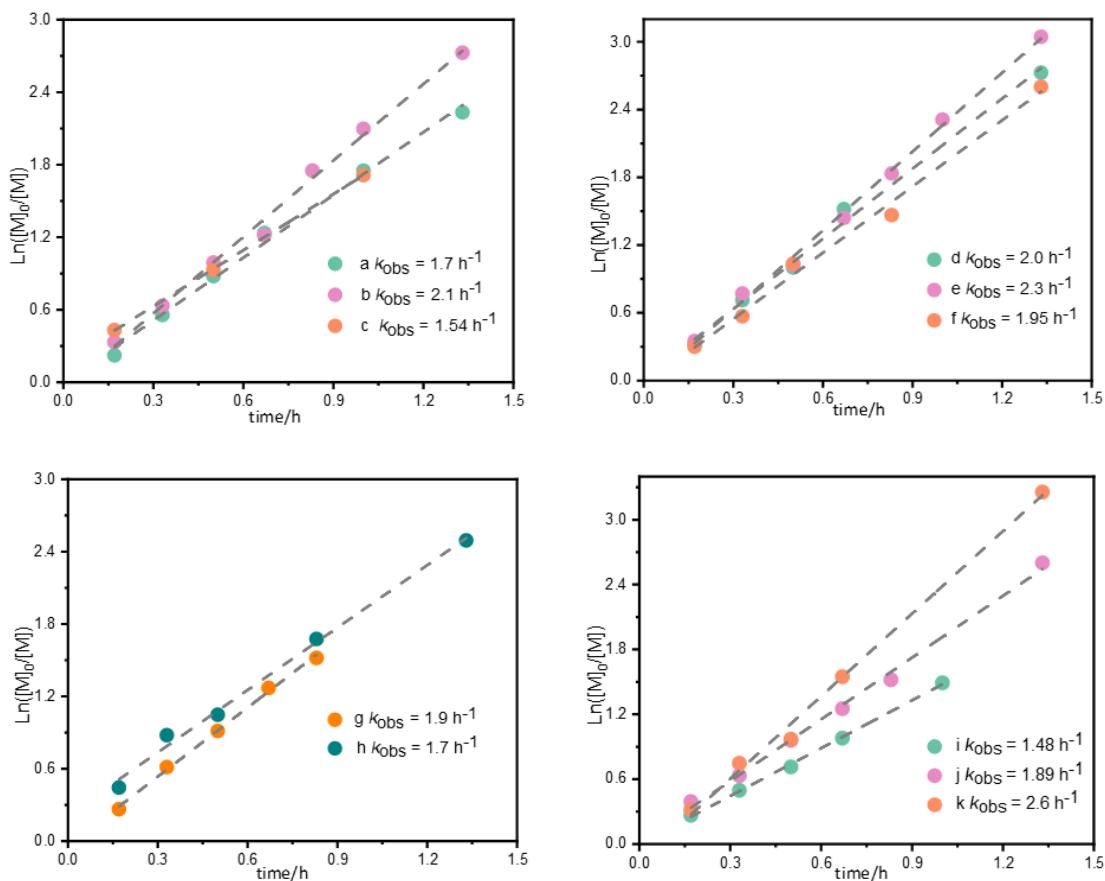
Figure S6. semilogarithmic kinetic plot of the ROP of LLAs using DMAP with fluorophenol. Experimental conditions: $[M]_0/[I]_0$:100/1, 140 ˚C.
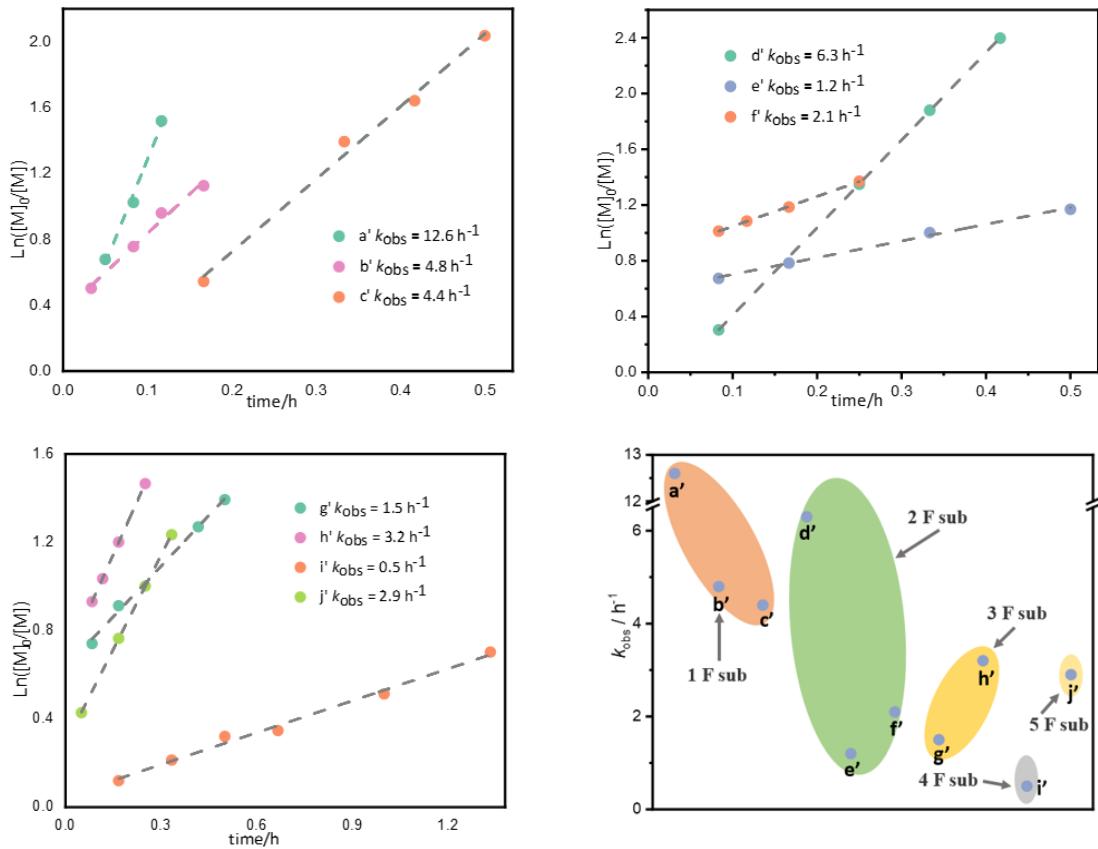
Figure S7. semilogarithmic kinetic plot of the ROP of LLAs using MTBD with fluorophenol. Experimental conditions: $[M]_0/[I]_0$:100/1, 140 °C.
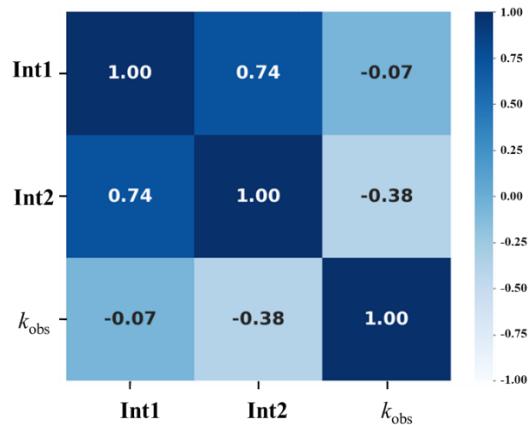
Figure S8. Heatmap representing the correlation between k_{obs} and single descriptor for fluorophenol/DMAP, deeper blue color represents stronger correlation.
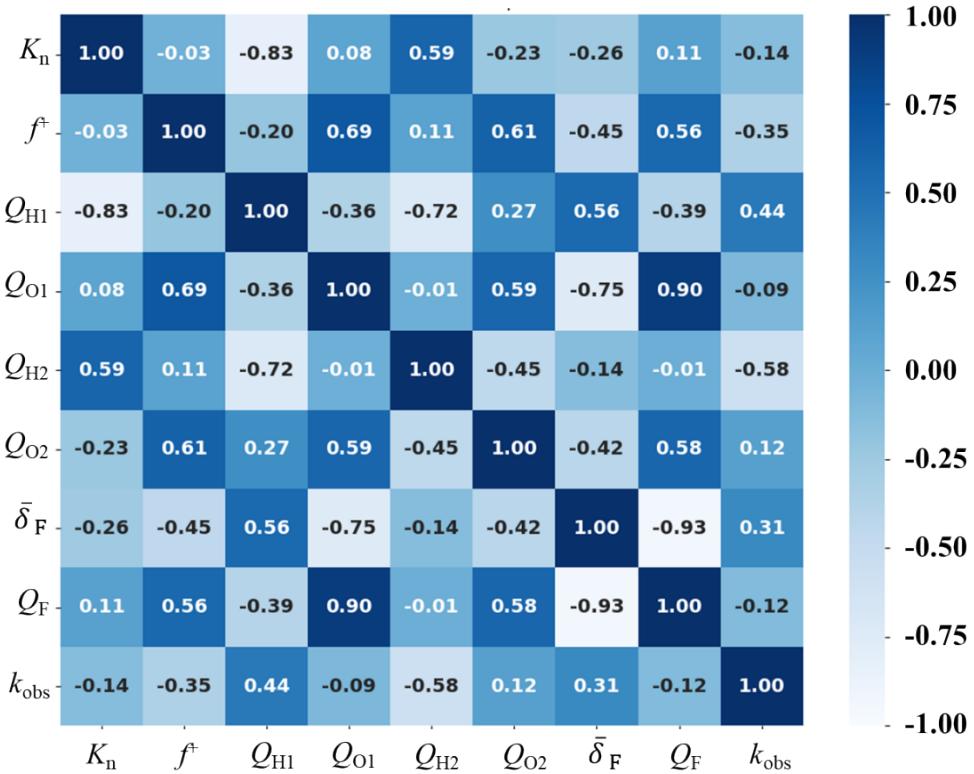
Figure S9. Heatmap representing the correlation between k_{obs} and single descriptor (electronic, thermodynamic, and bench results) for fluorophenol/DMAP, deeper blue color represents stronger correlation.
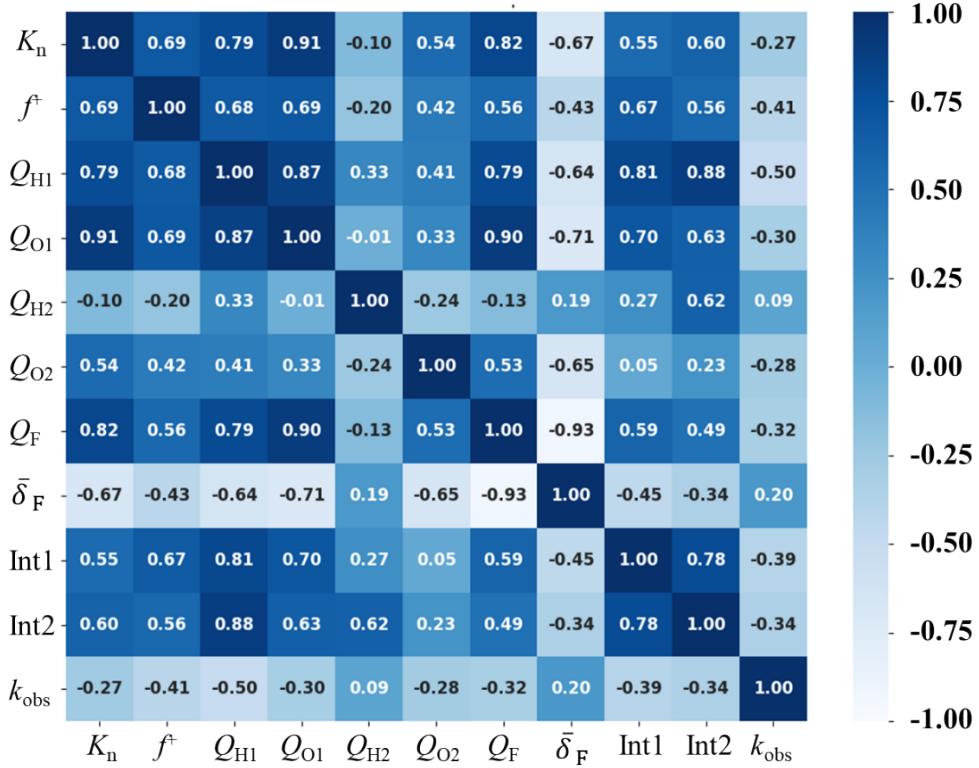
Figure S10. Heatmap representing the correlation between k_{obs} and single descriptor (electronic,

thermodynamic, and bench results) for fluorophenol/MTBD, deeper blue color represents stronger correlation.
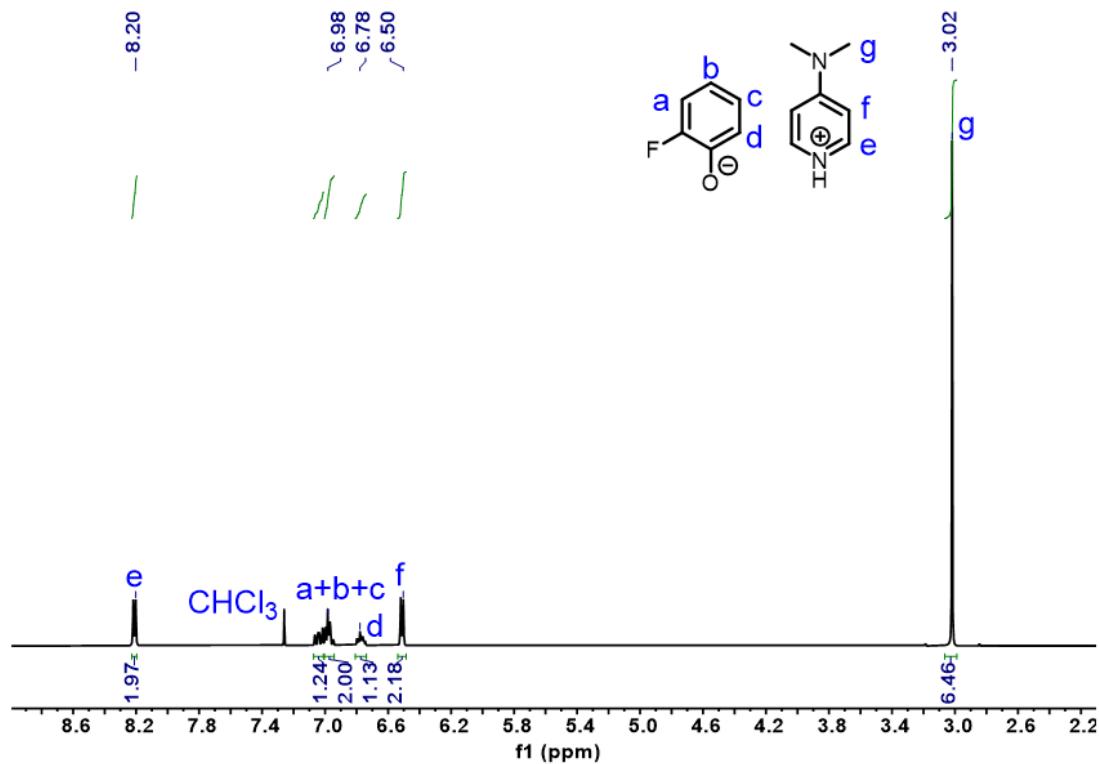
Figure S11. ^{1}H NMR spectrum (CDCl$_3$, 400 MHz) of *o*-FP/DMAP(a)
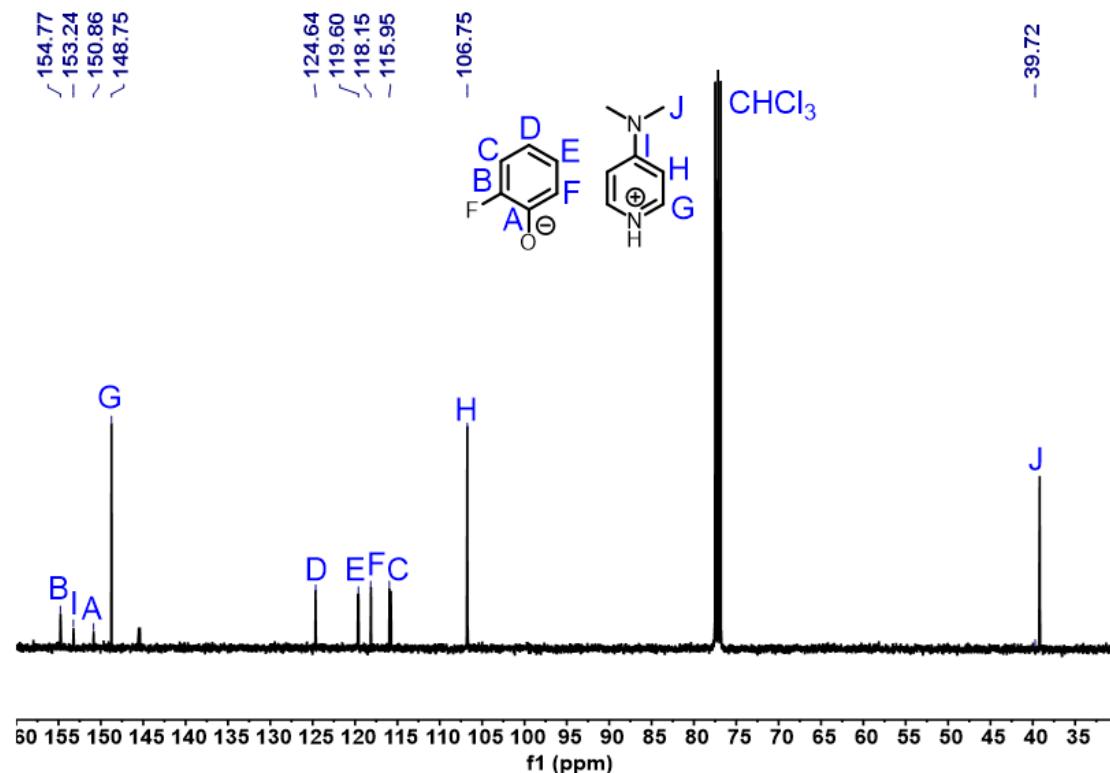
Figure S12. ^{13}C NMR spectrum (CDCl$_3$, 101 MHz) of *o*-FP/DMAP (a)
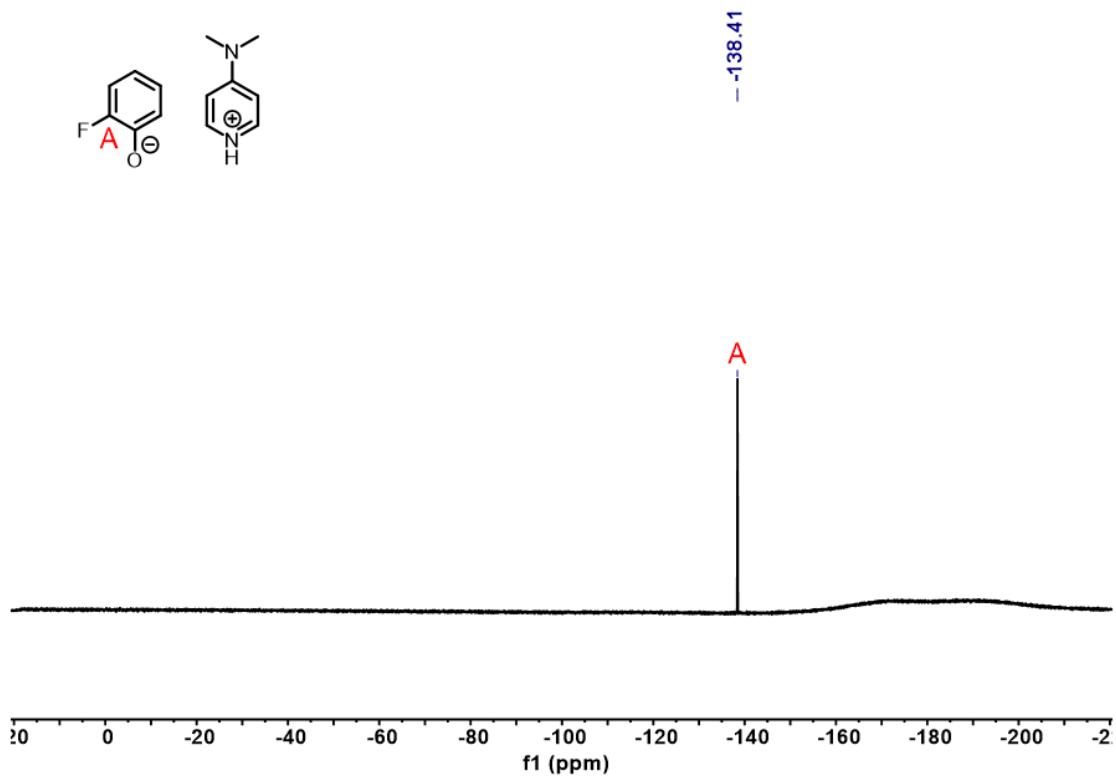
Figure S13. ^{19}F NMR spectrum (CDCl$_3$, 376 MHz) of *o*-FP/DMAP (a)
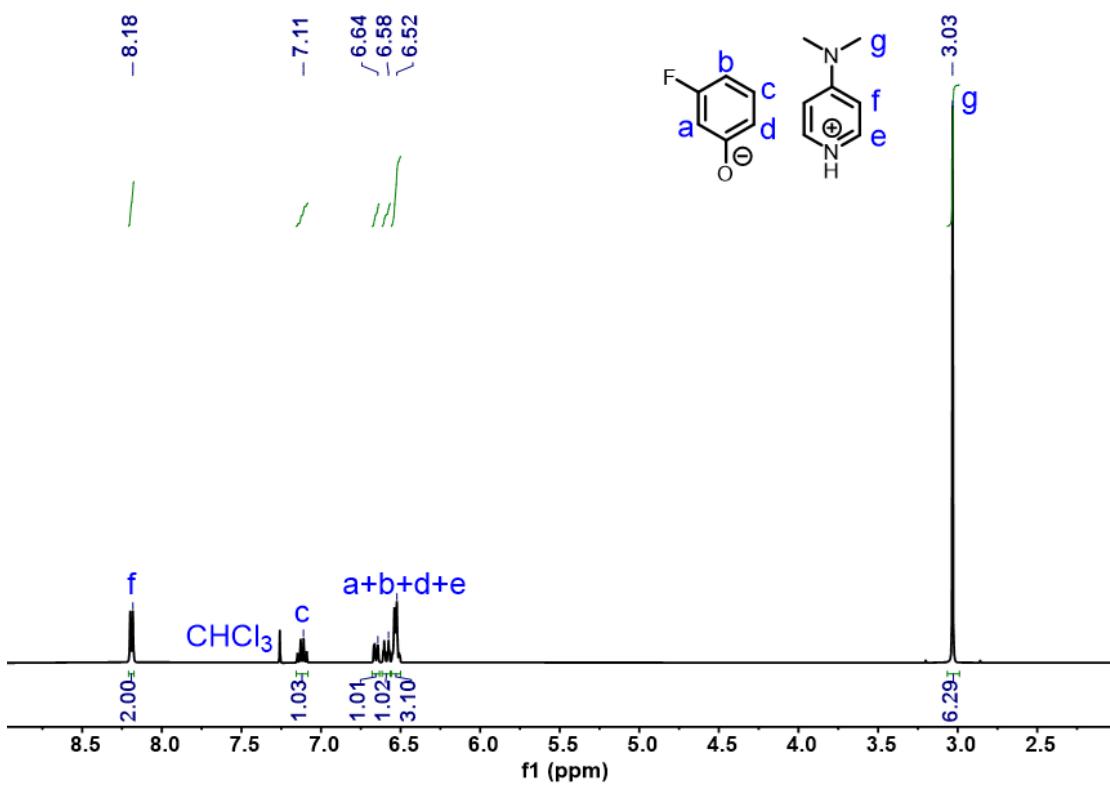
Figure S14. ^{1}H NMR spectrum (CDCl$_3$, 400 MHz) of *m*-FP/DMAP (b)
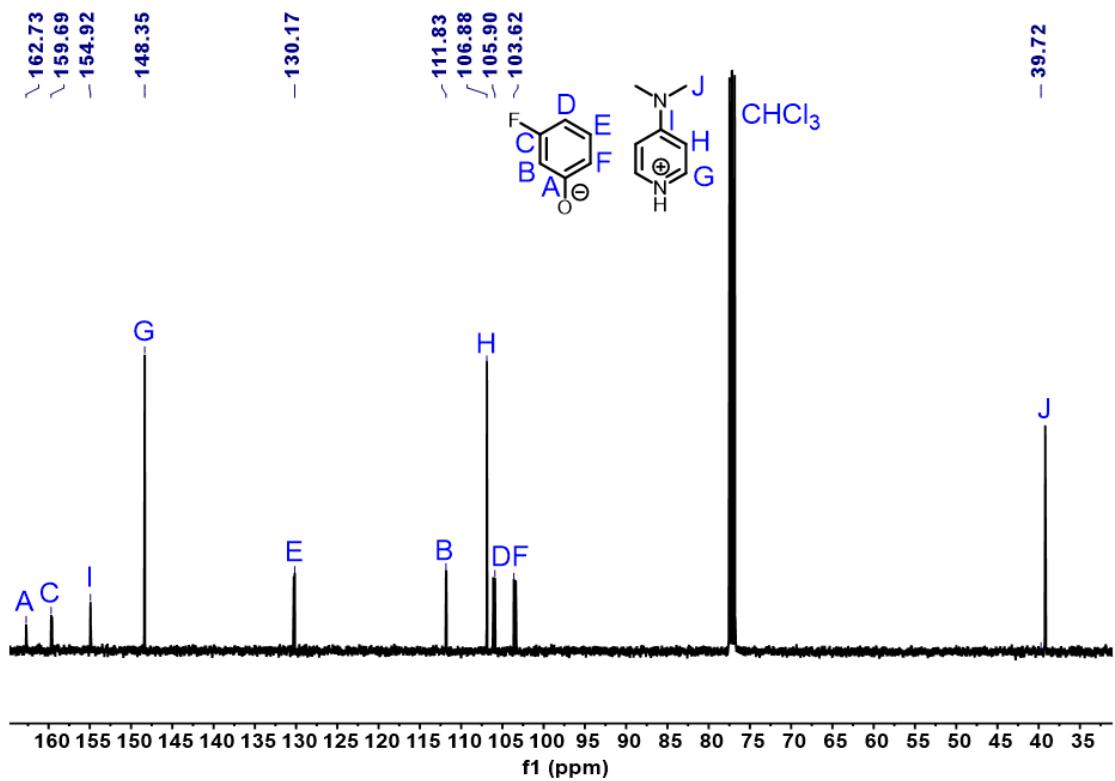
Figure S15. ¹³C NMR spectrum (CDCl₃, 101 MHz) of *m*-FP/DMAP (b)
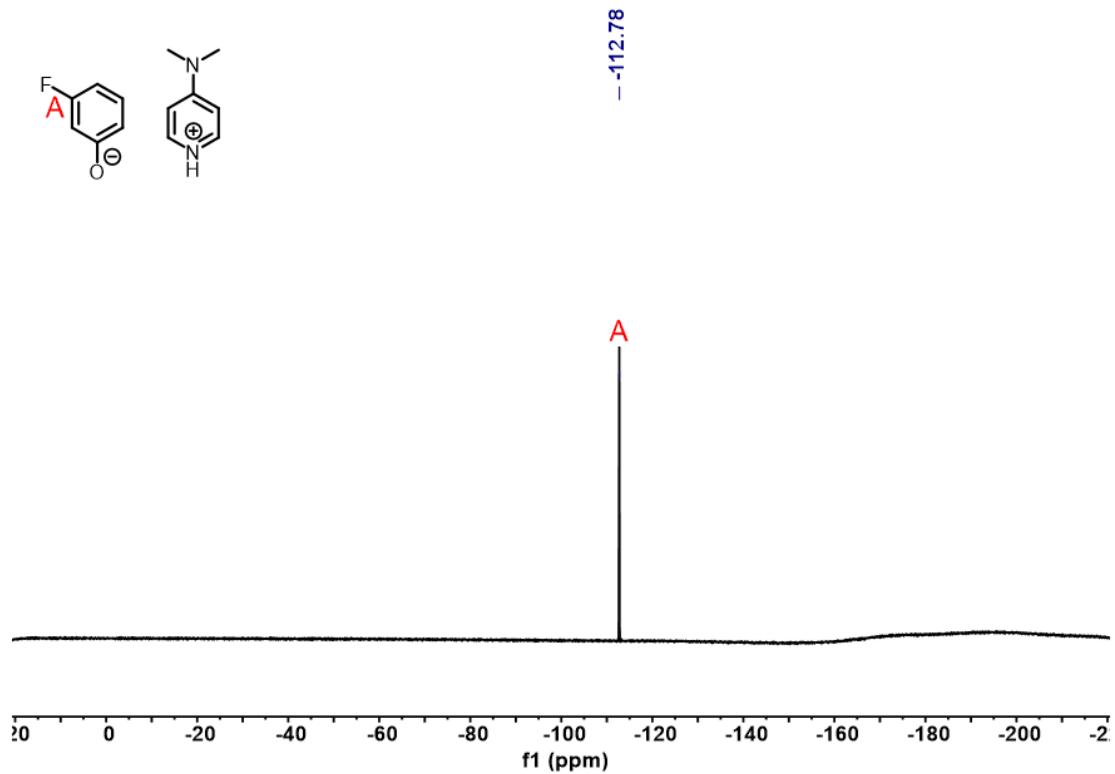
Figure S16. ¹⁹F NMR spectrum (CDCl₃, 376 MHz) of *m*-FP/DMAP (b)
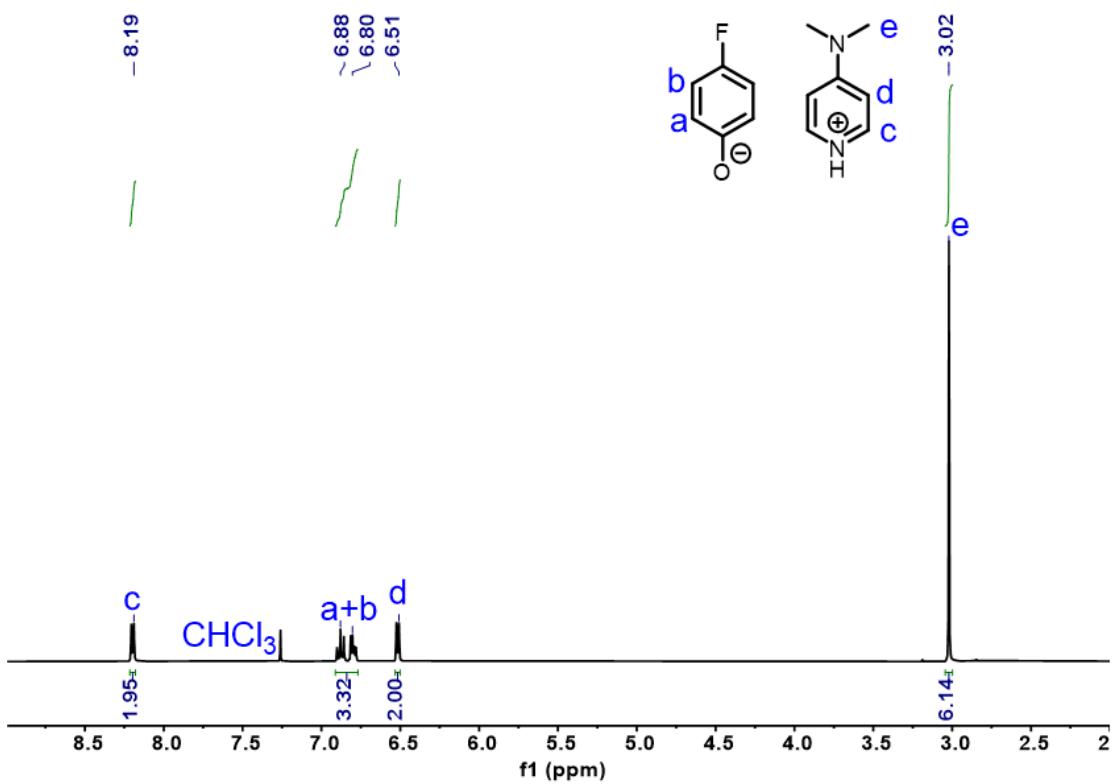
Figure S17. ^{1}H NMR spectrum (CDCl$_3$, 400 MHz) of *p*-FP/DMAP (c)
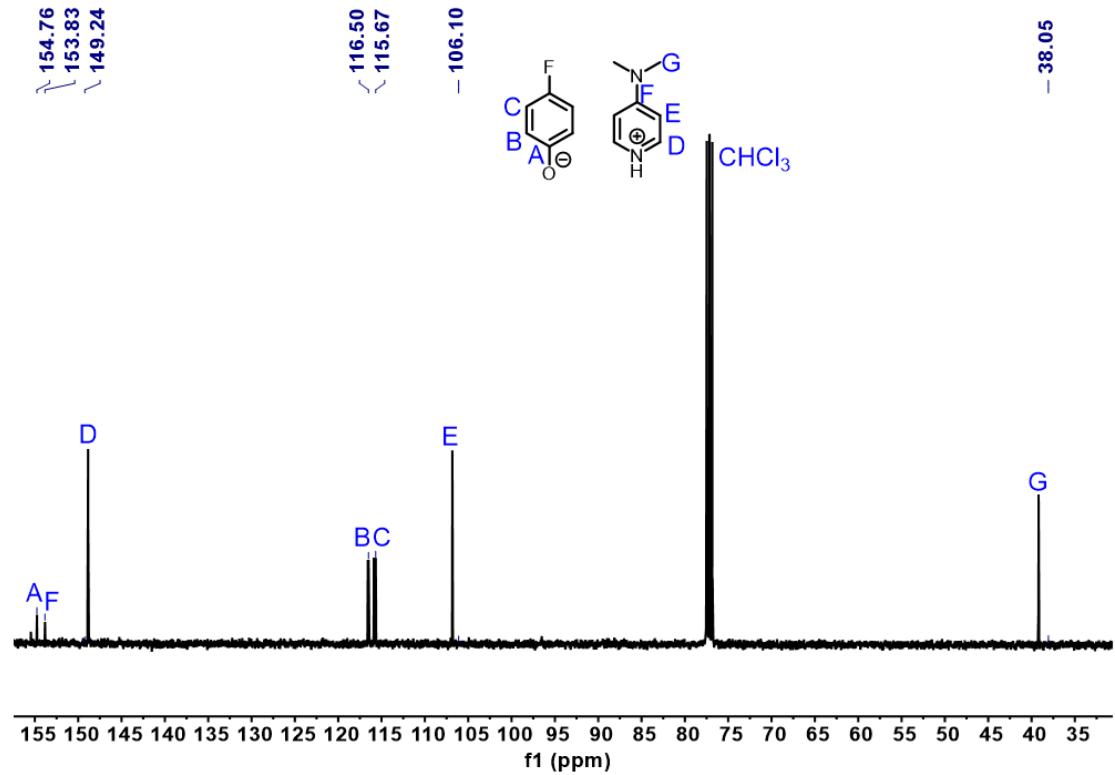
Figure S18. ^{13}C NMR spectrum (CDCl$_3$, 101 MHz) of *p*-FP/DMAP (c)
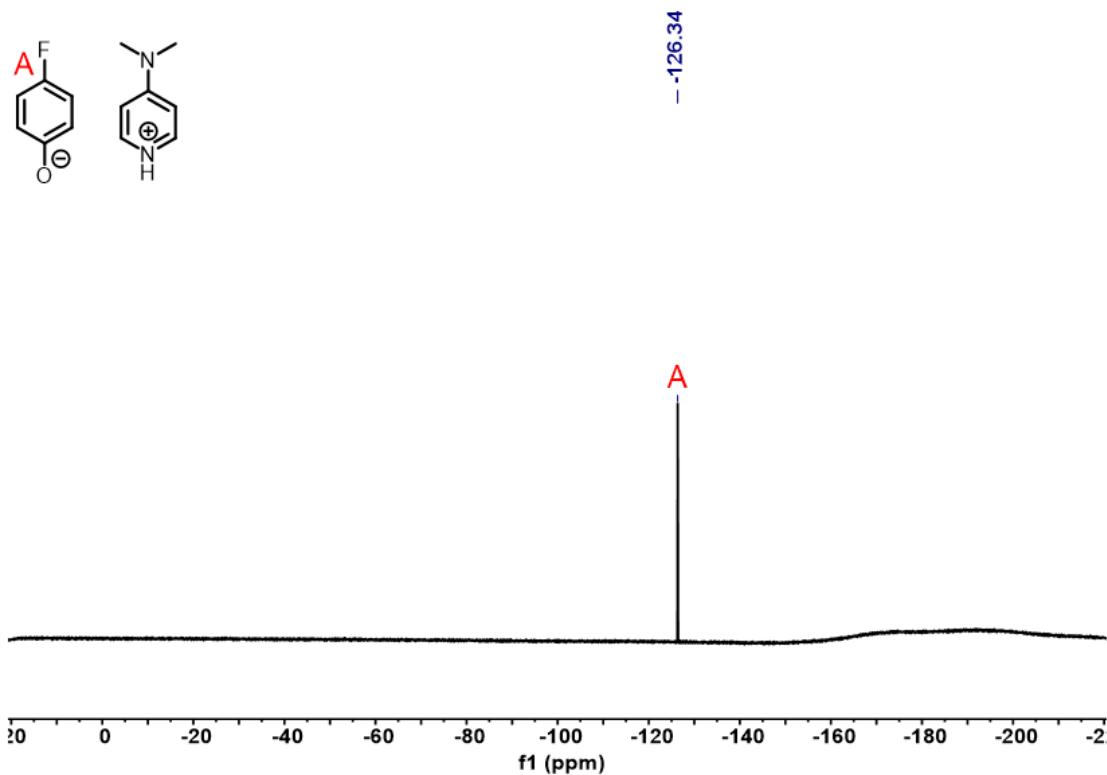
Figure S19. ^{19}F NMR spectrum (CDCl$_3$, 376 MHz) of *p*-FP/DMAP (c)
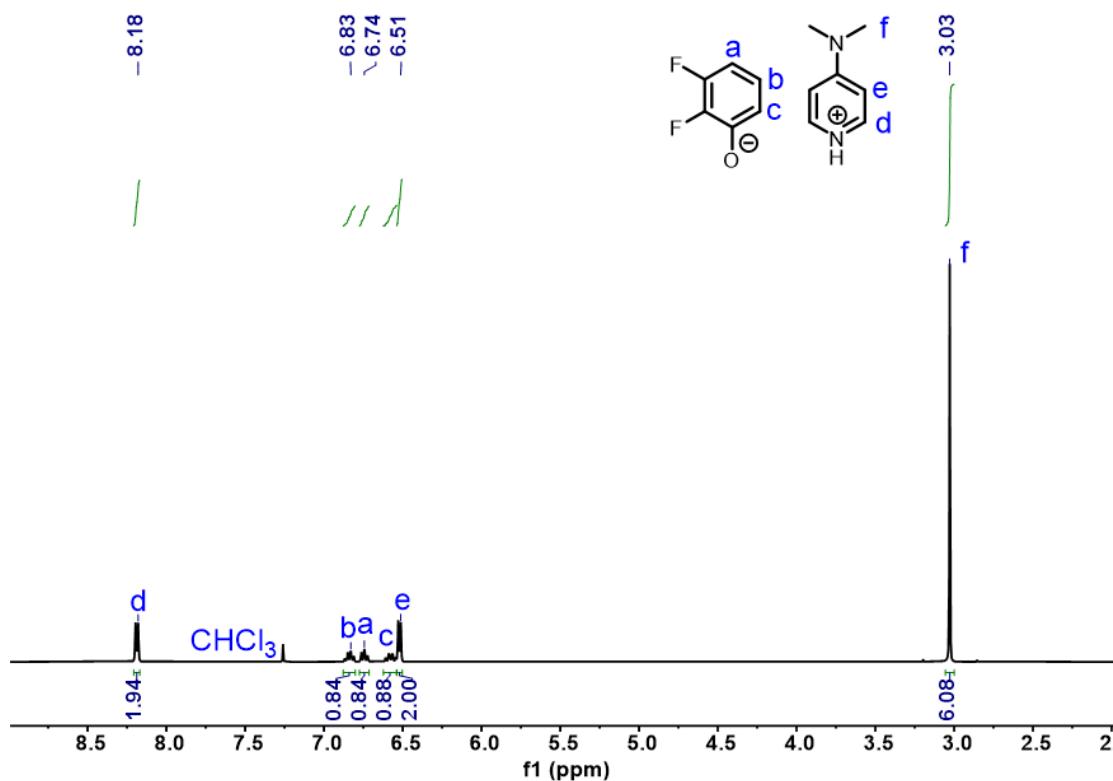
Figure S20. ^{1}H NMR spectrum (CDCl$_3$, 400 MHz) of 2,3-FP/DMAP (d)
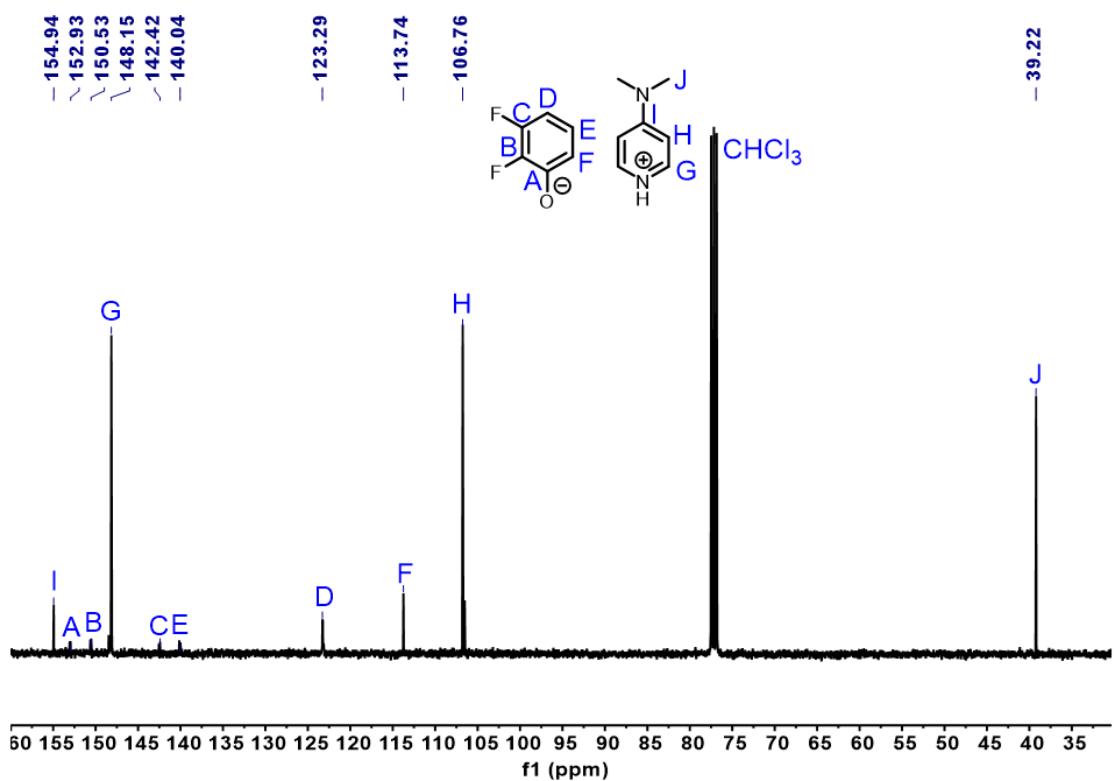
Figure S21. ¹³C NMR spectrum (CDCl₃, 101 MHz) of 2,3-FP/DMAP (d)
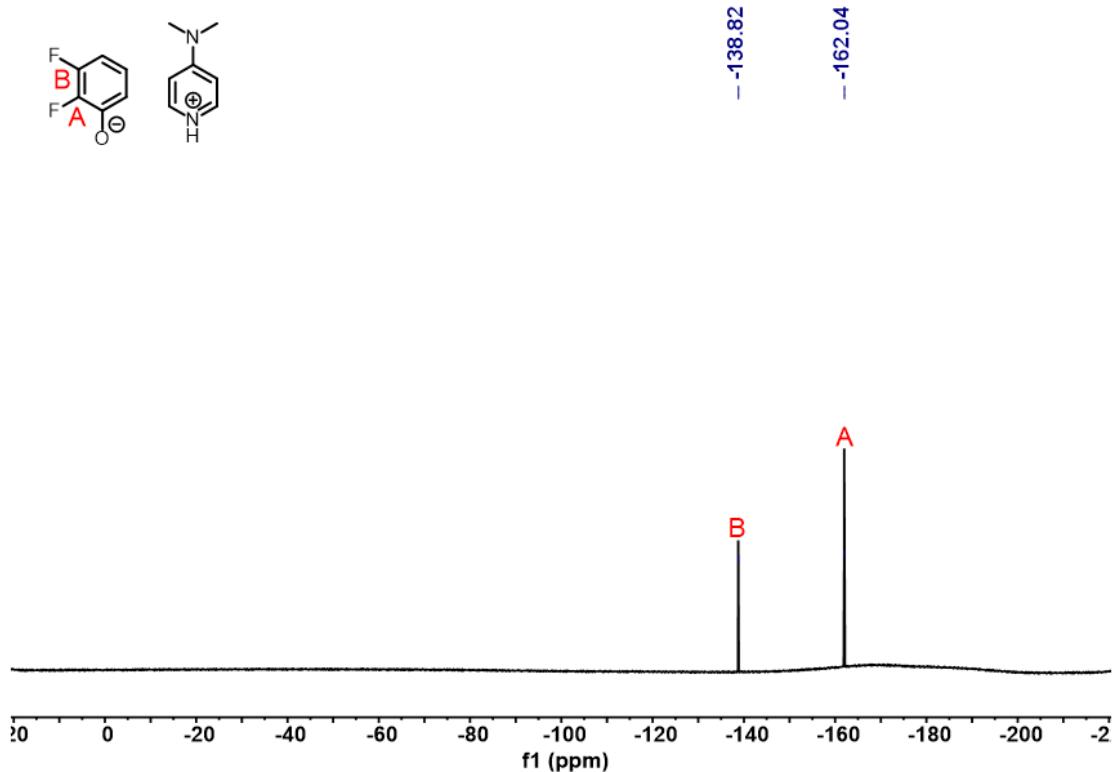
Figure S22. ¹⁹F NMR spectrum (CDCl₃, 376 MHz) of 2,3-FP/DMAP (d)
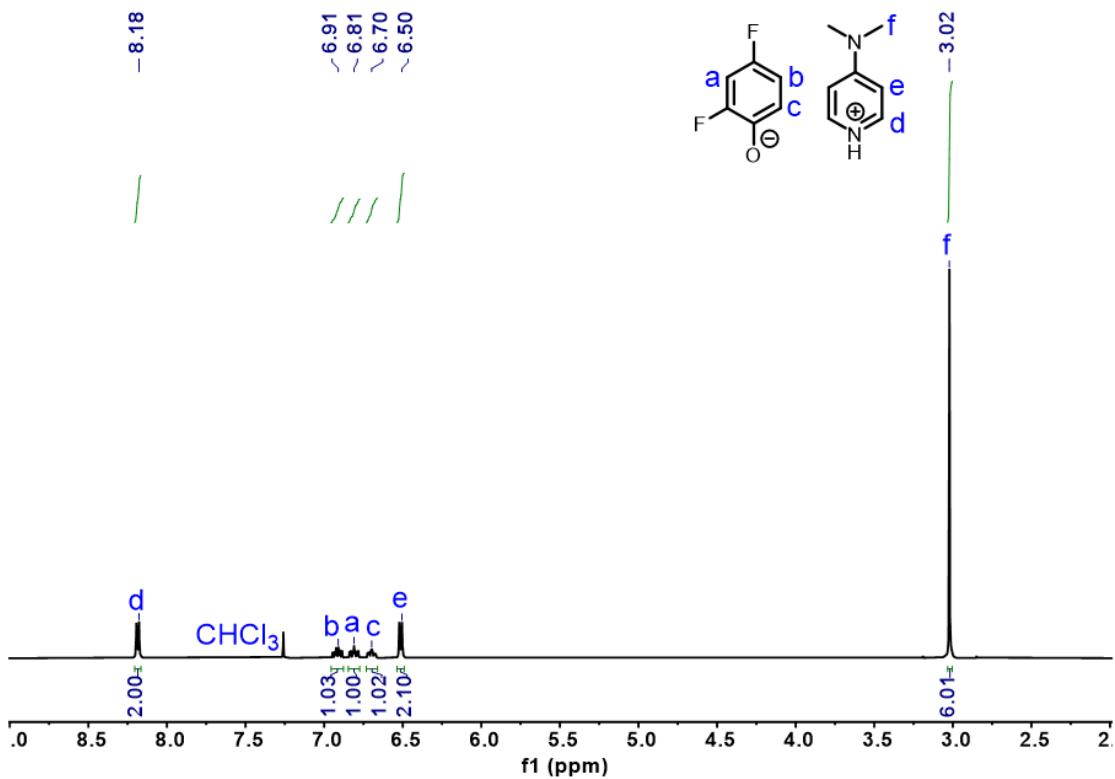
Figure S23. ^1H NMR spectrum (CDCl$_3$, 400 MHz) of 2,4-FP/DMAP (e)
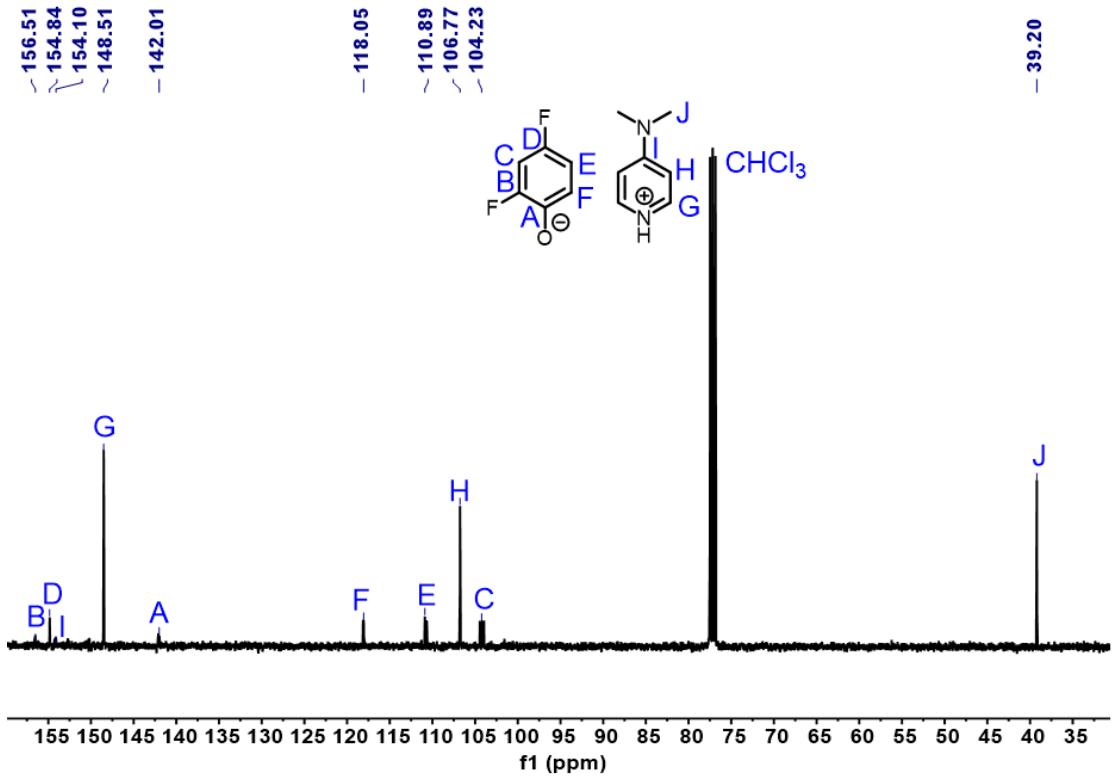
Figure S24. ^{13}C NMR spectrum (CDCl$_3$, 101 MHz) of 2,4-FP/DMAP (e)
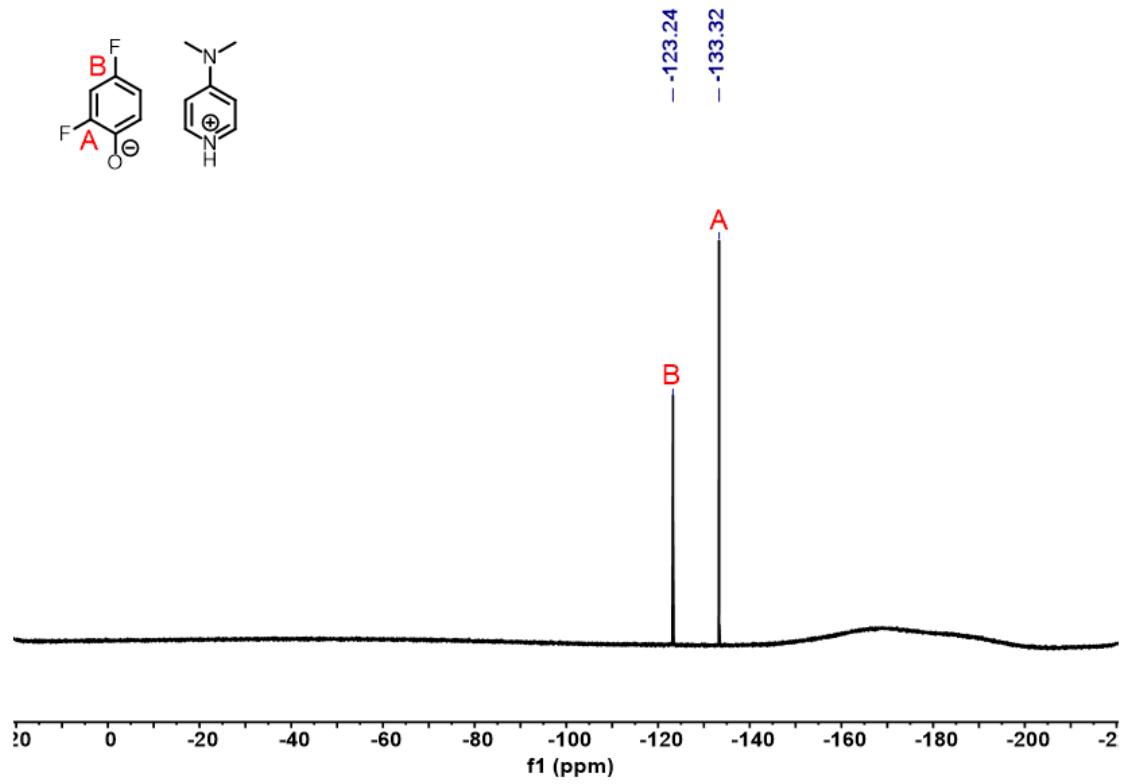
Figure S25. ^{19}F NMR spectrum (CDCl$_3$, 376 MHz) of 2,4-FP/DMAP (e)
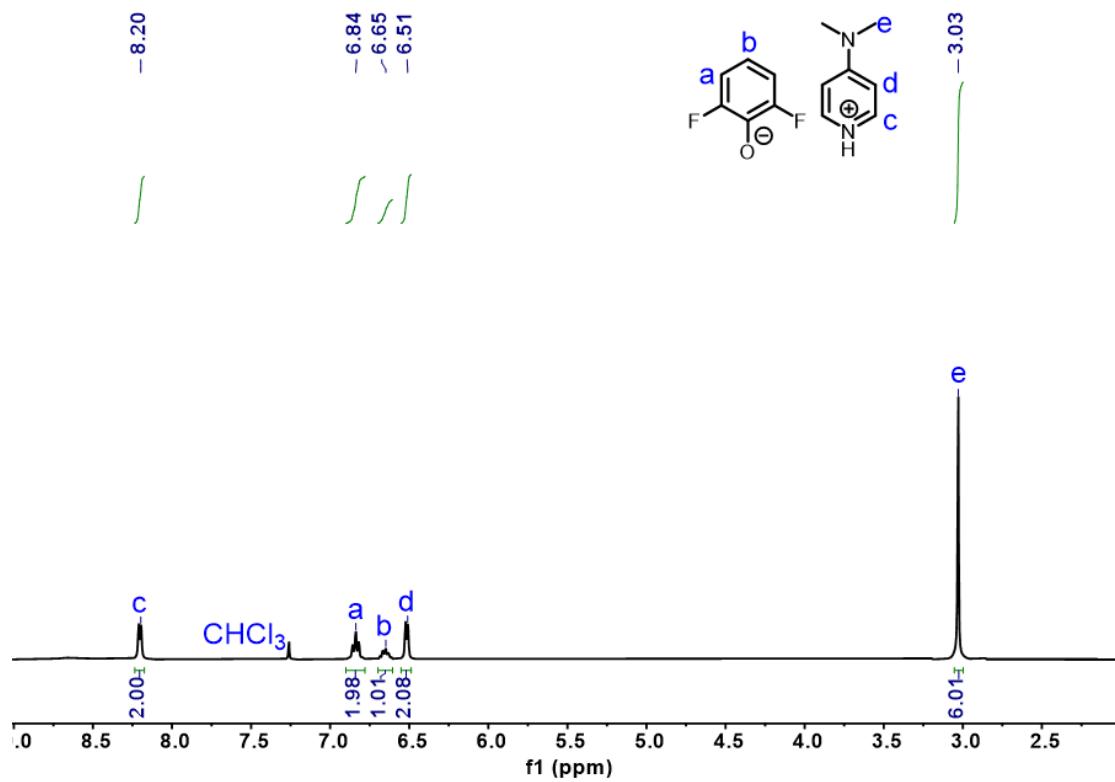
Figure S26. ^{1}H NMR spectrum (CDCl$_3$, 400 MHz) of 2,6-FP/DMAP (f)
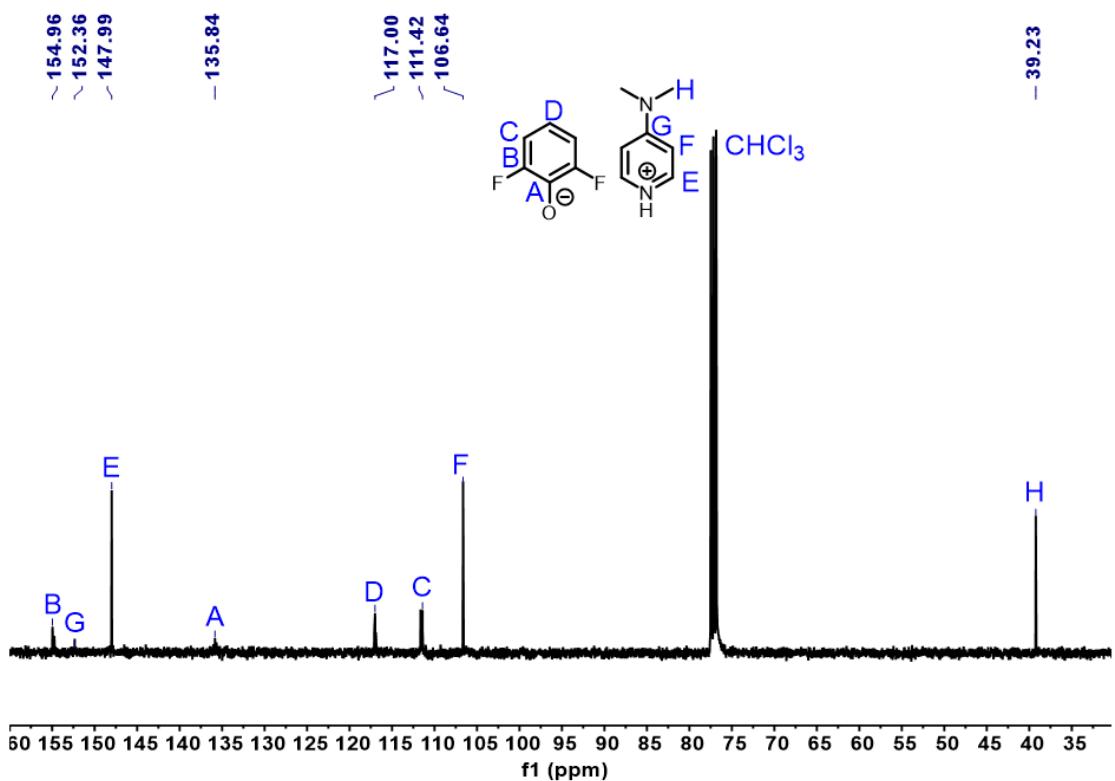
Figure S27. ^{13}C NMR spectrum (CDCl$_3$, 101 MHz) of 2,6-FP/DMAP (f)
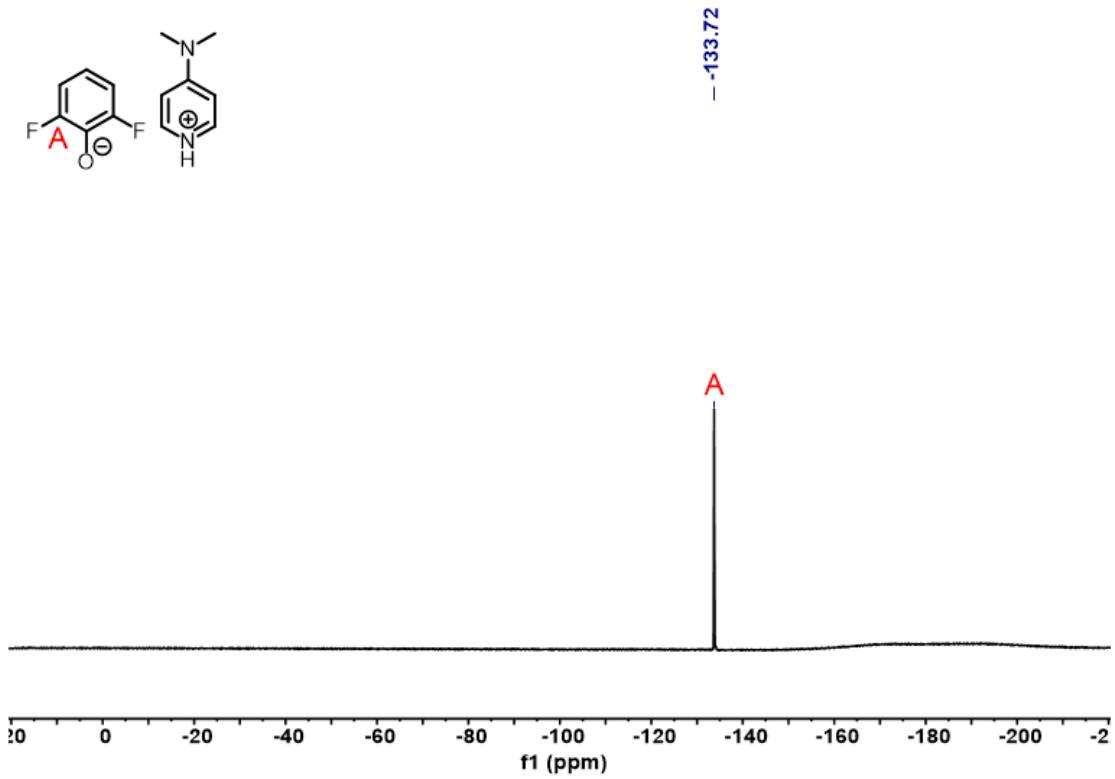
Figure S28. ^{19}F NMR spectrum (CDCl$_3$, 376 MHz) of 2,6-FP/DMAP (f)
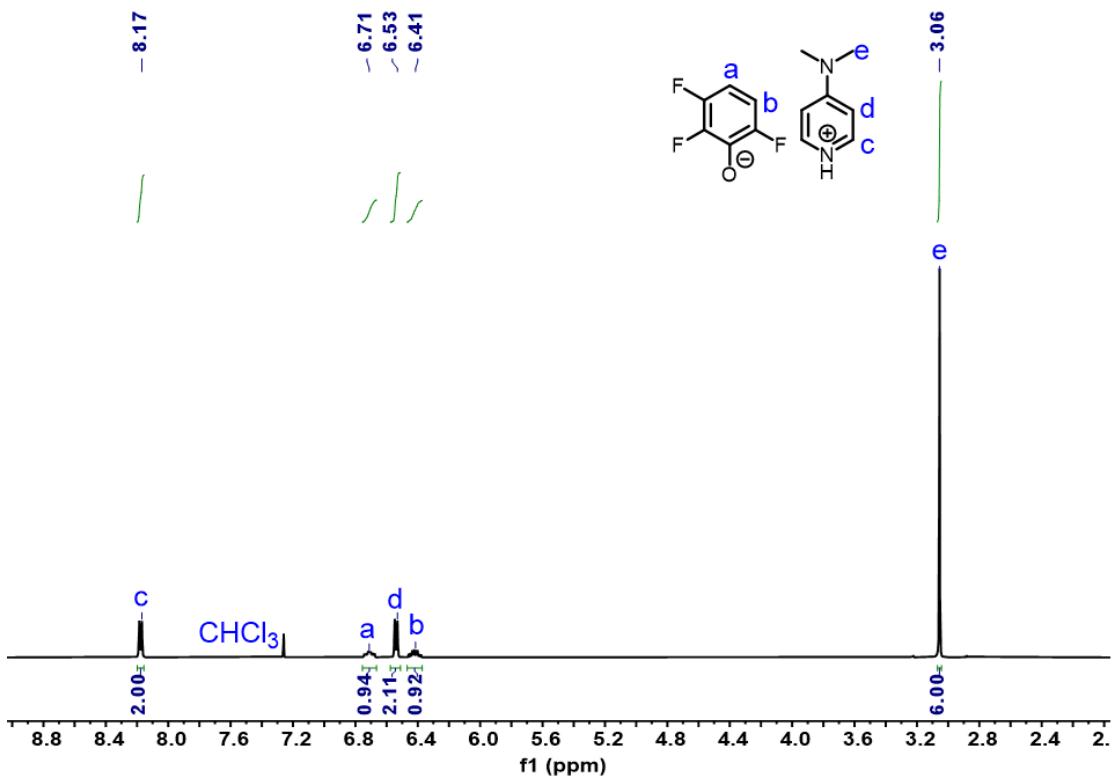
Figure S29. ^{1}H NMR spectrum (CDCl$_3$, 400 MHz) of 2,3,6-FP/DMAP (g)
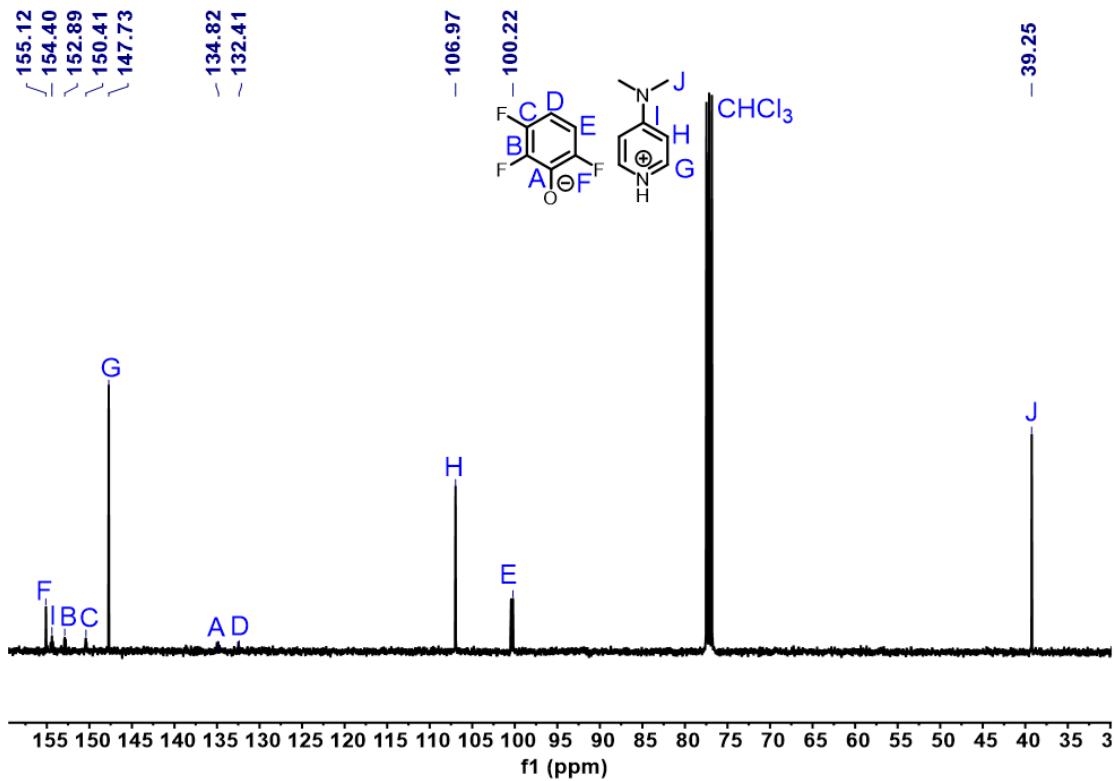
Figure S30. ^{13}C NMR spectrum (CDCl$_3$, 101 MHz) of 2,3,6-FP/DMAP (g)
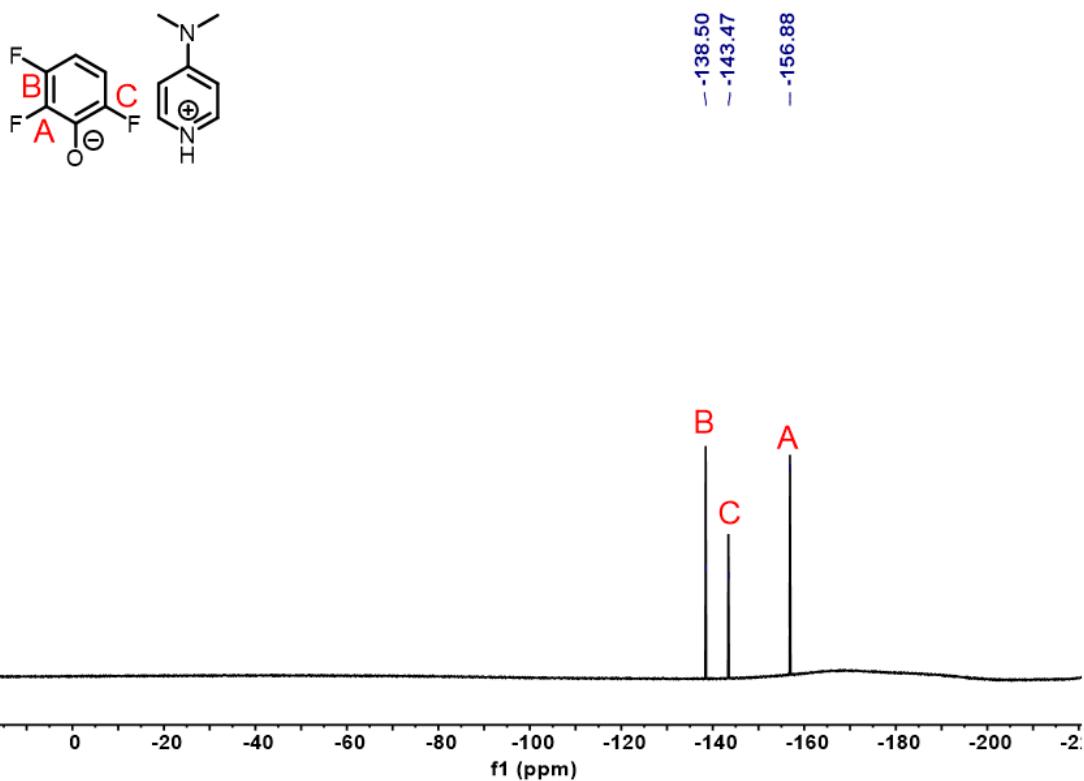
Figure S31. ^{19}F NMR spectrum (CDCl$_3$, 376 MHz) of 2,3,6-FP/DMAP (g)
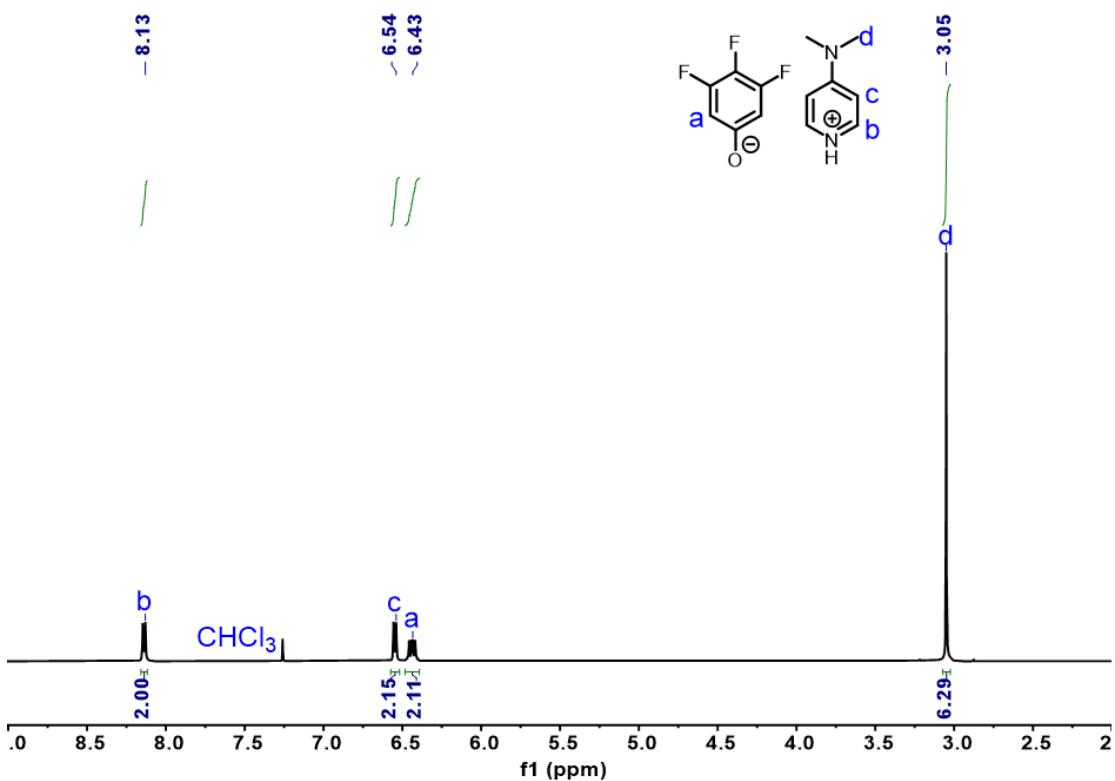
Figure S32. ^1H NMR spectrum (CDCl$_3$, 400 MHz) of 3,4,5-FP/DMAP (h)
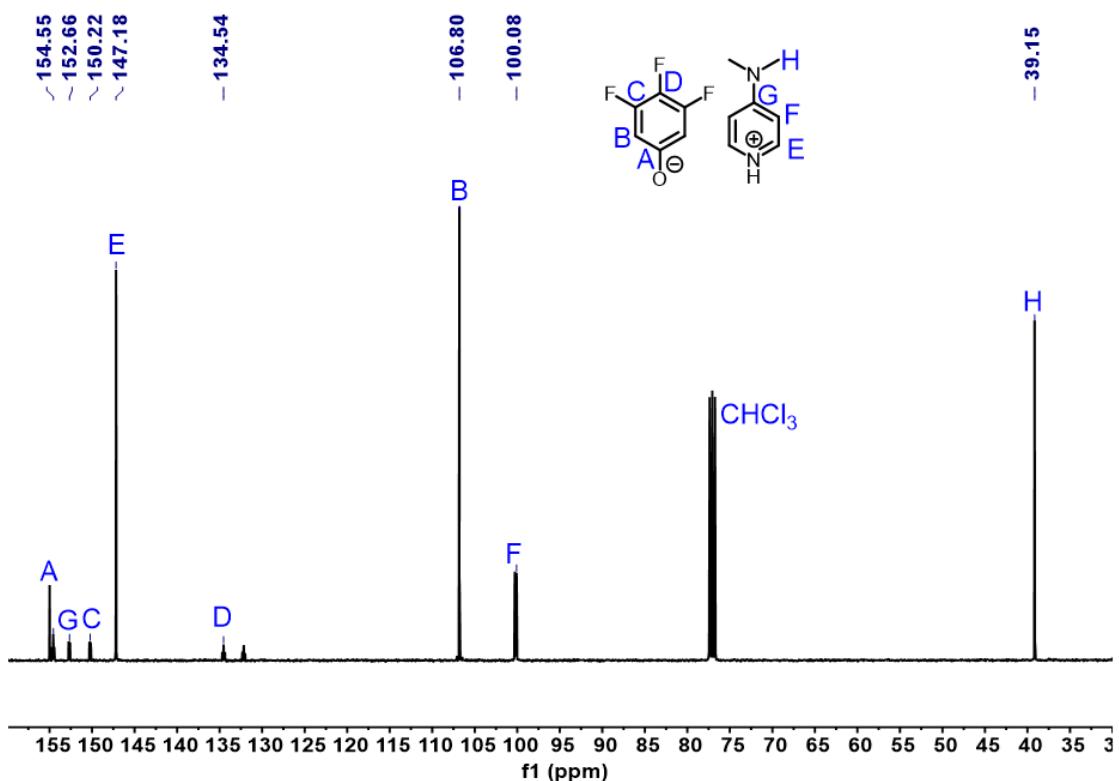
Figure S33. ^{13}C NMR spectrum (CDCl$_3$, 101 MHz) of 3,4,5-FP/DMAP (h)
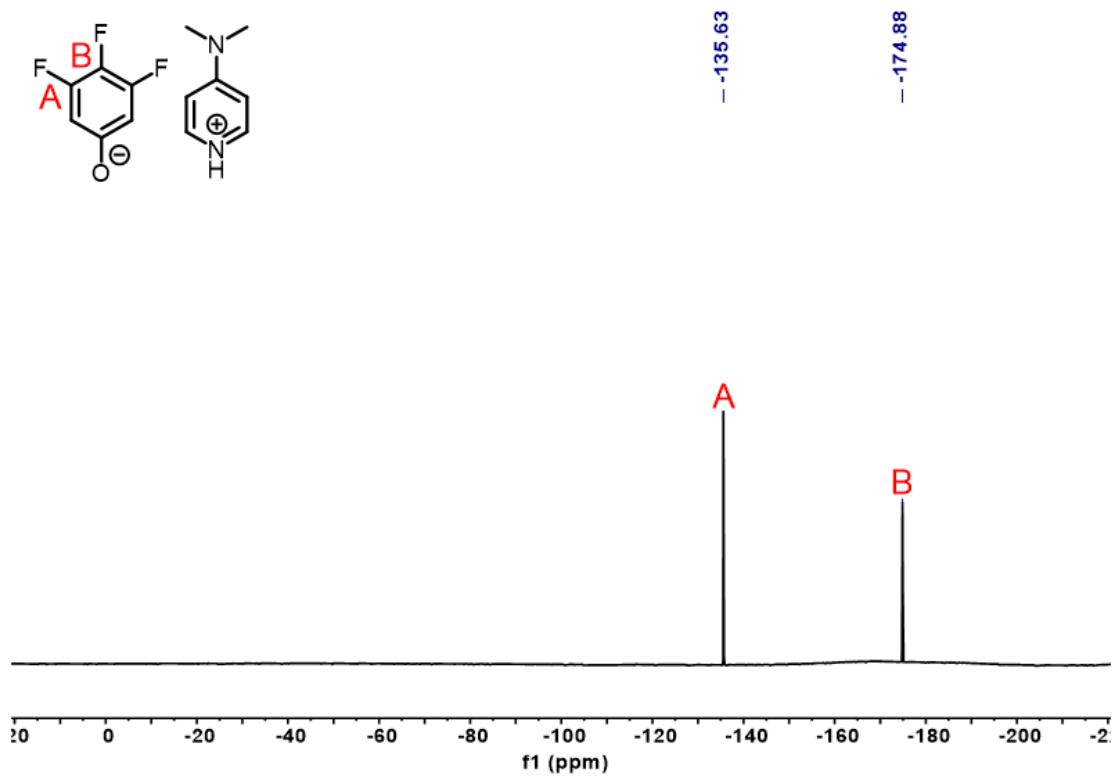
Figure S34. ^{19}F NMR spectrum (CDCl$_3$, 376 MHz) of 3,4,5-FP/DMAP (h)
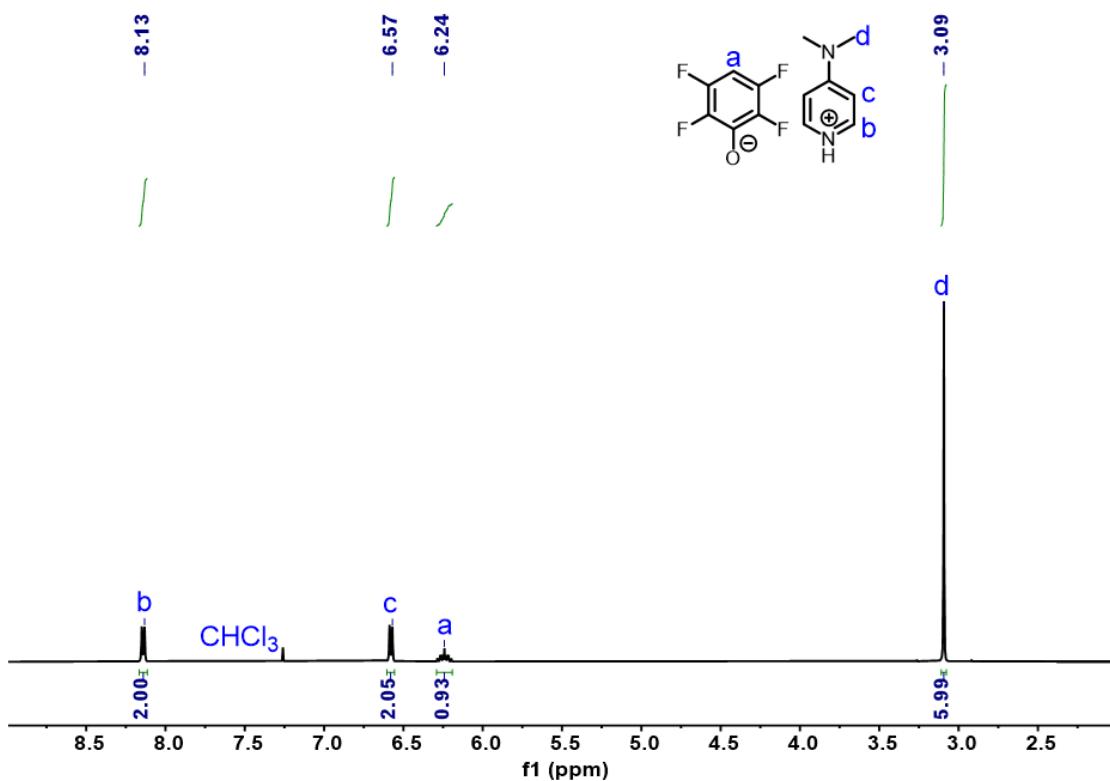
Figure S35. ^{1}H NMR spectrum (CDCl$_3$, 400 MHz) of 2,3,5,6-FP/DMAP (i)
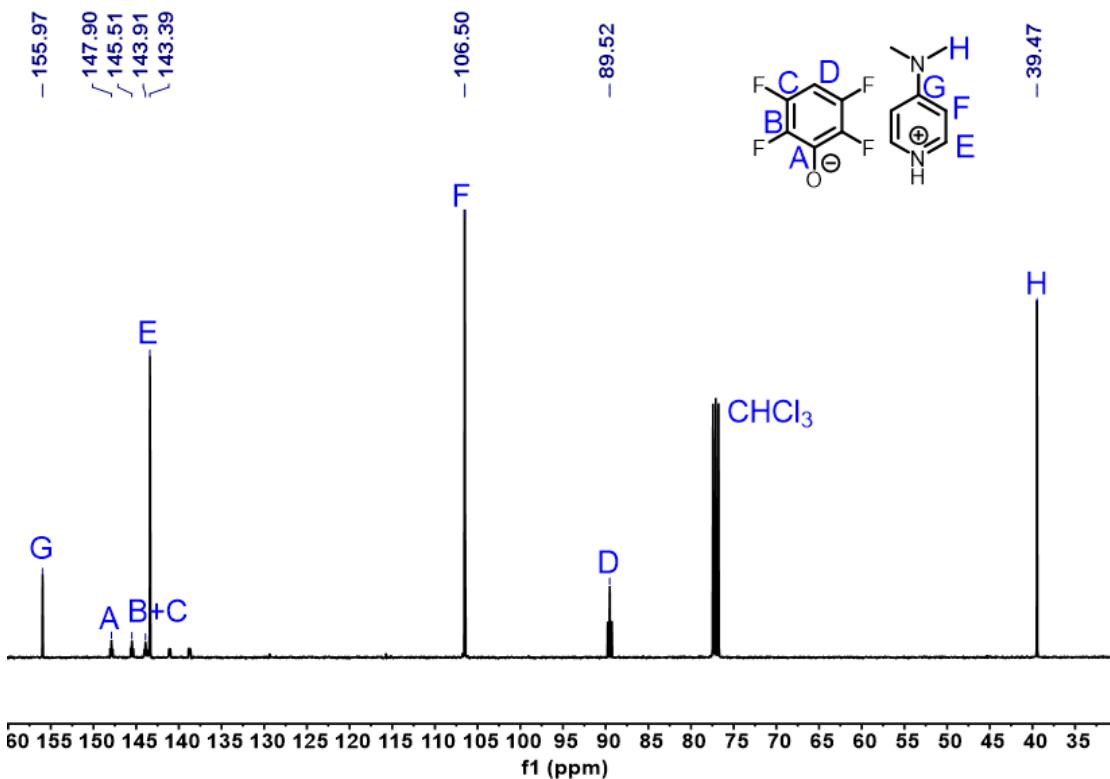
Figure S36. ^{13}C NMR spectrum (CDCl$_3$, 101 MHz) of 2,3,5,6-FP/DMAP (i)
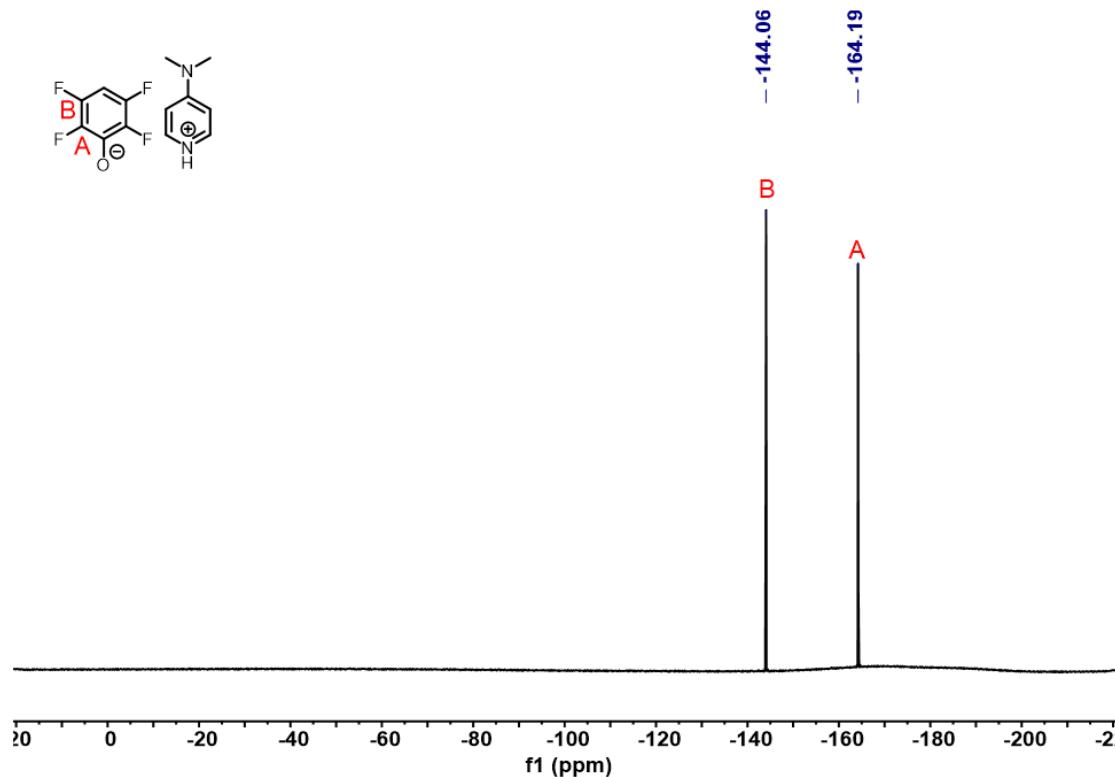
Figure S37. ^{19}F NMR spectrum (CDCl$_3$, 376 MHz) of 2,3,5,6-FP/DMAP (i)
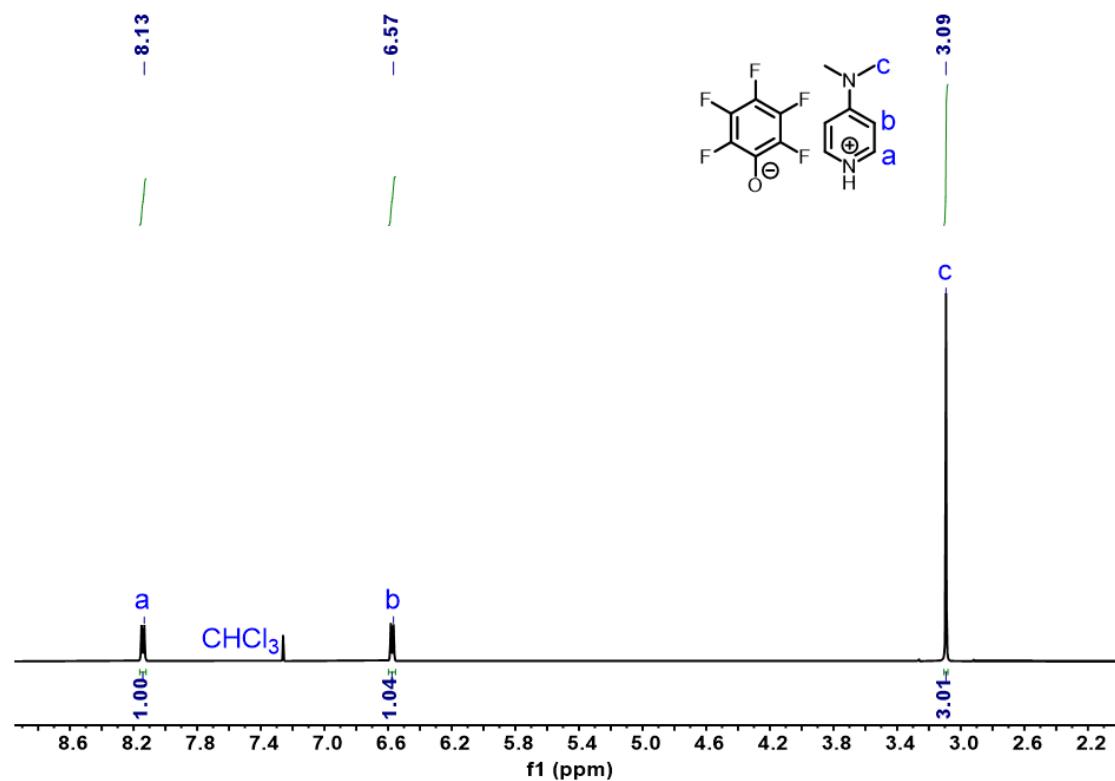
Figure S38. ^{1}H NMR spectrum (CDCl$_3$, 400 MHz) of 2,3,4,5,6-FP/DMAP (j)
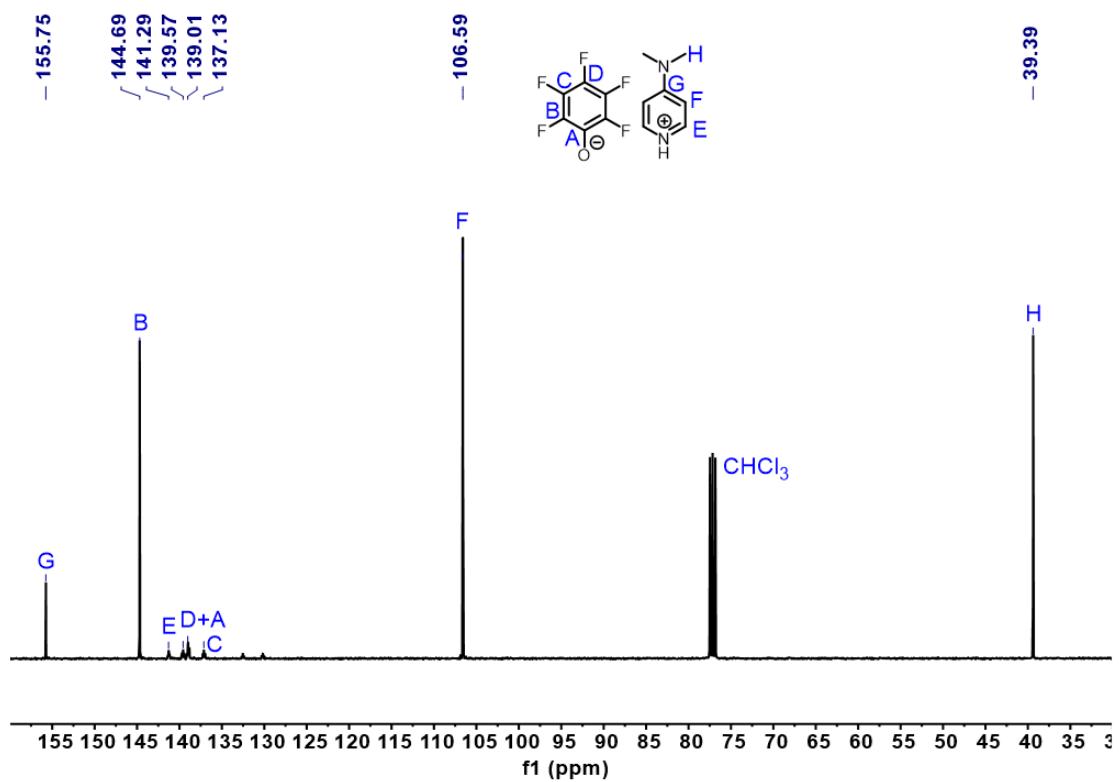
Figure S39. ^{13}C NMR spectrum (CDCl$_3$, 101 MHz) of 2,3,4,5,6-FP/DMAP (j)
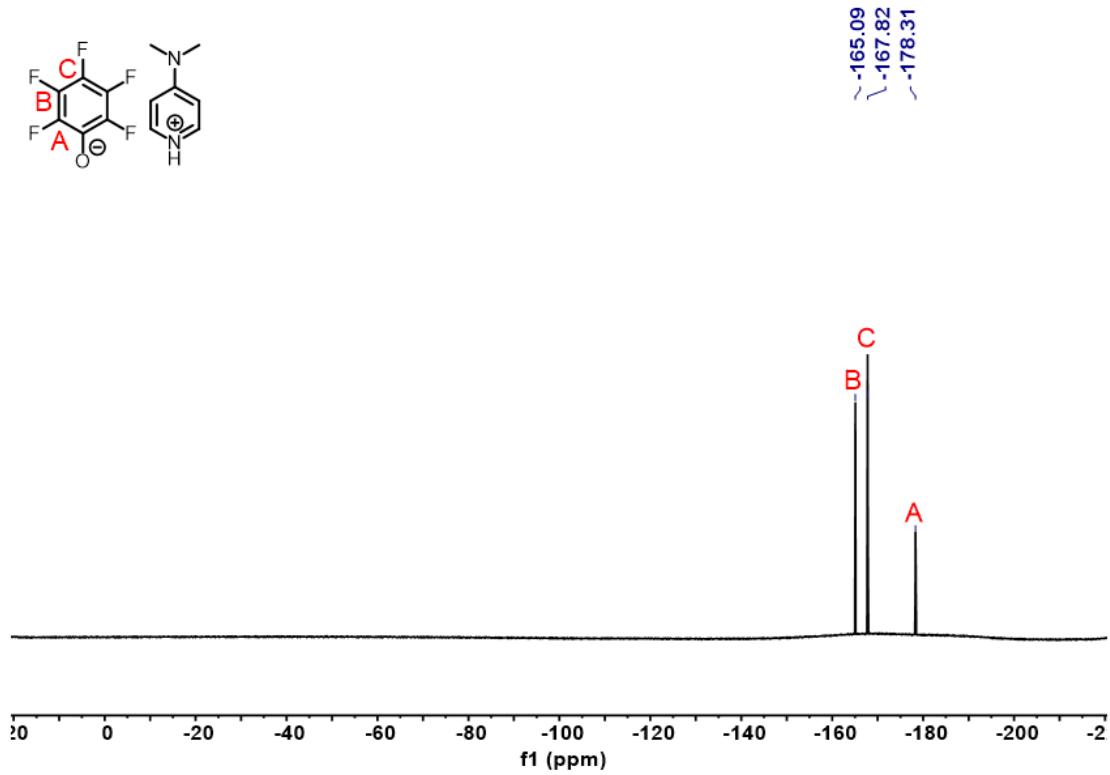
Figure S40. ^{19}F NMR spectrum (CDCl$_3$, 376 MHz) of 2,3,4,5,6-FP/DMAP (j)
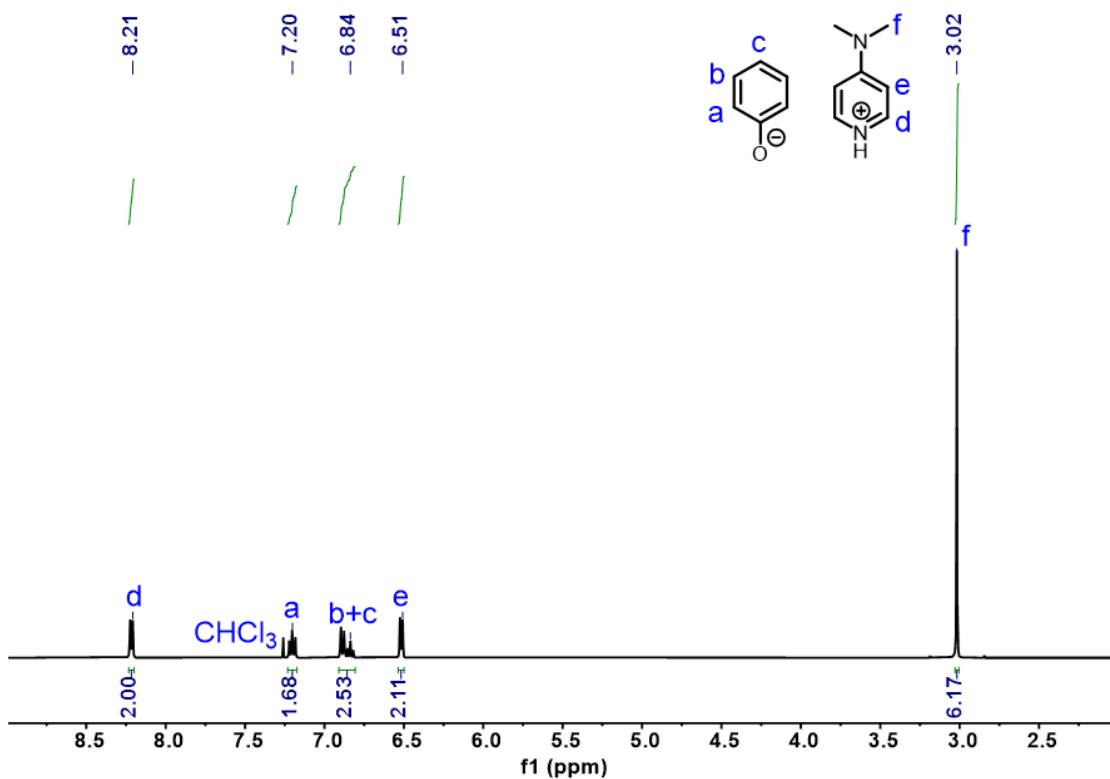
Figure S41. ^{1}H NMR spectrum (CDCl$_3$, 400 MHz) of Ph/DMAP (k)
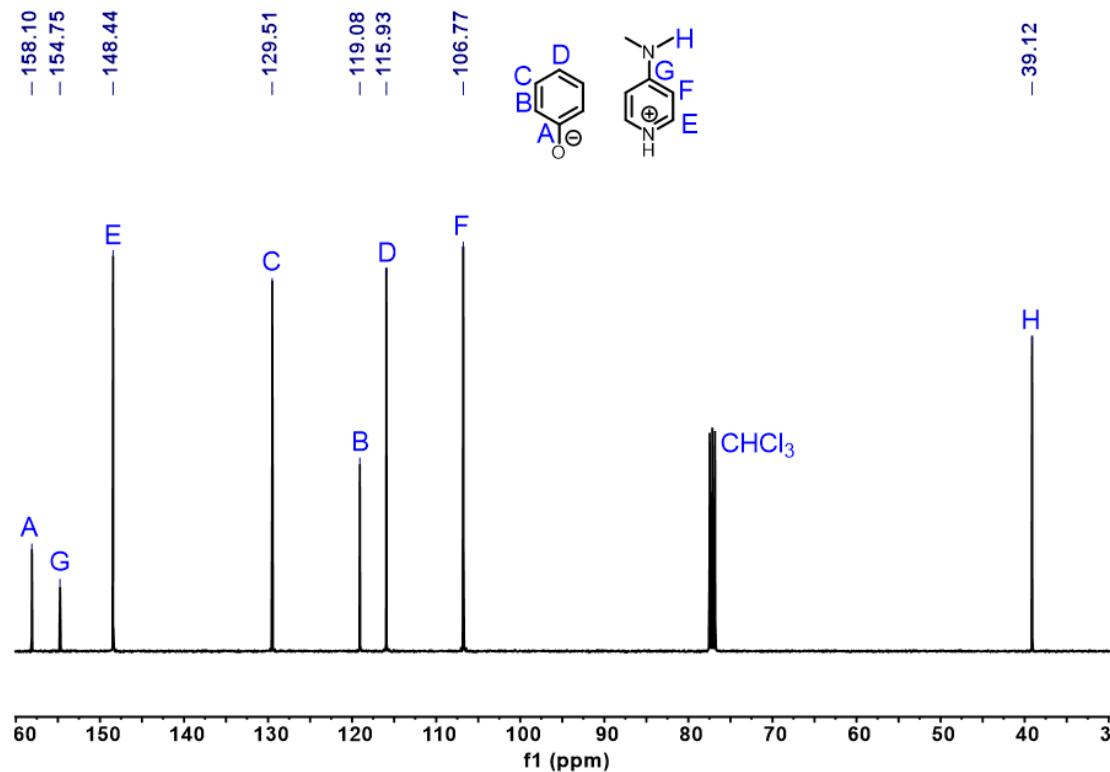
Figure S42. ^{13}C NMR spectrum (CDCl$_3$, 101 MHz) of Ph/DMAP (k)
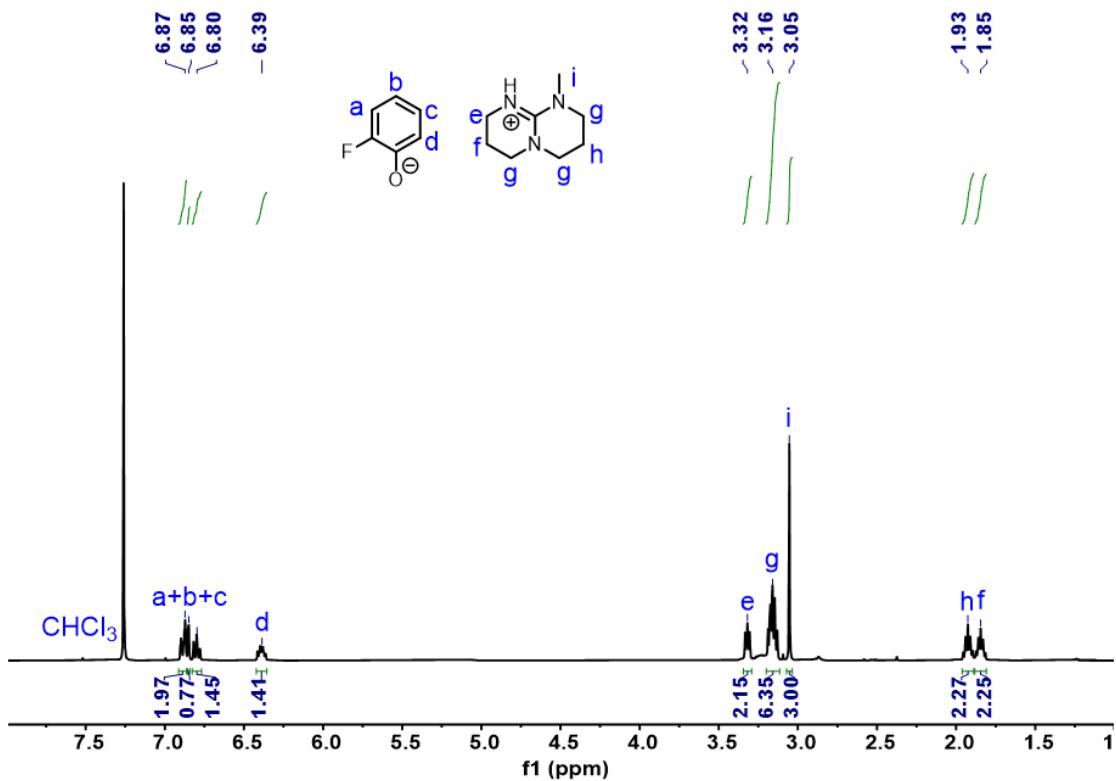
Figure S43. ^{1}H NMR spectrum (CDCl$_3$, 400 MHz) of *o*-FP/MTBD (a')
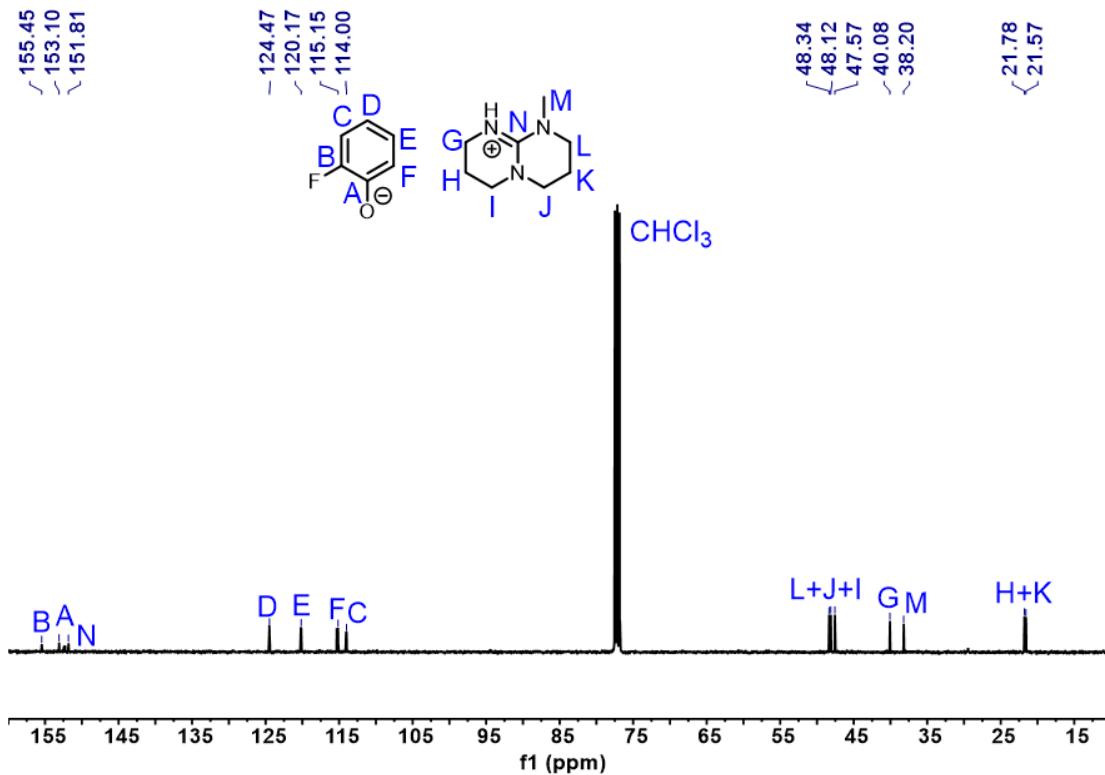
Figure S44. ^{13}C NMR spectrum (CDCl$_3$, 101 MHz) of *o*-FP/MTBD (a')
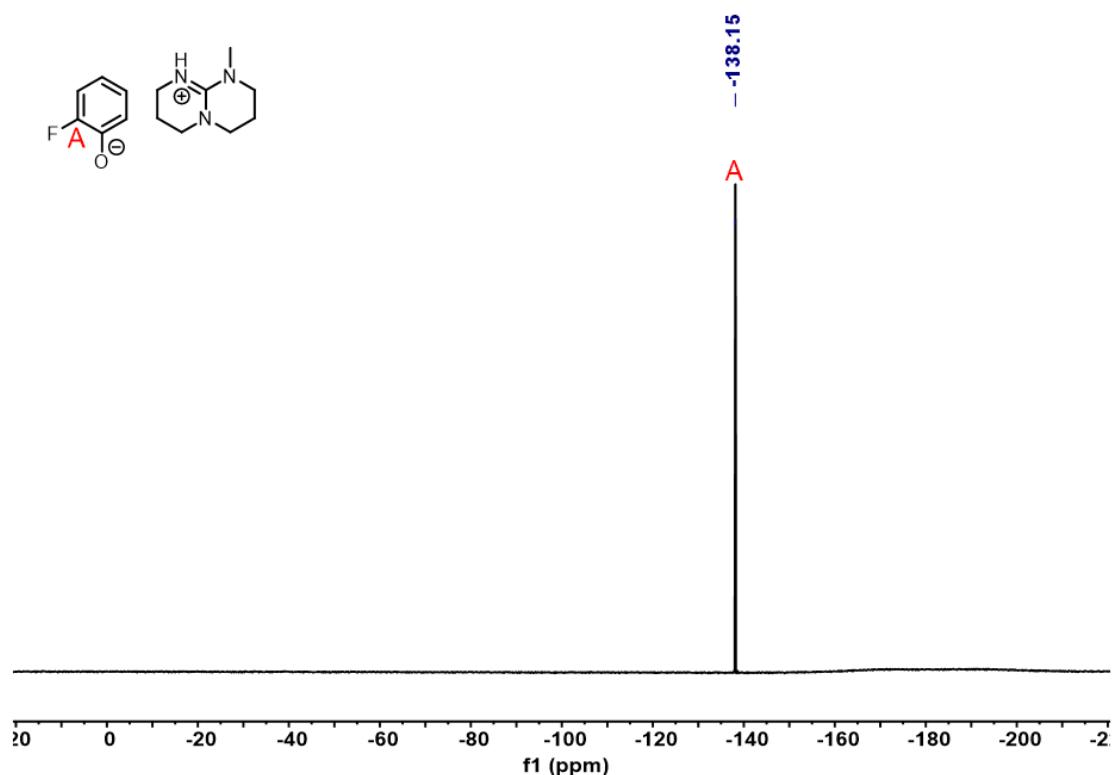
Figure S45. ^{19}F NMR spectrum (CDCl$_3$, 376 MHz) of *o*-FP/MTBD (a')
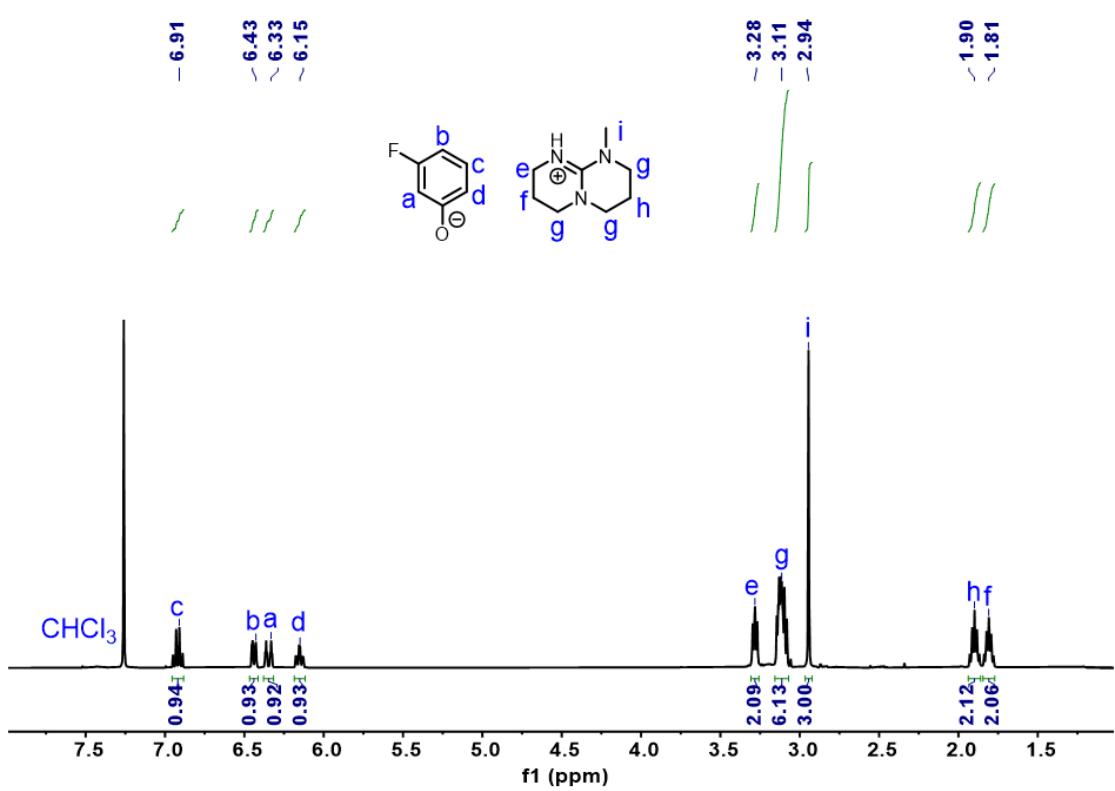
Figure S46. ^1H NMR spectrum (CDCl$_3$, 400 MHz) of *m*-FP/MTBD (b')
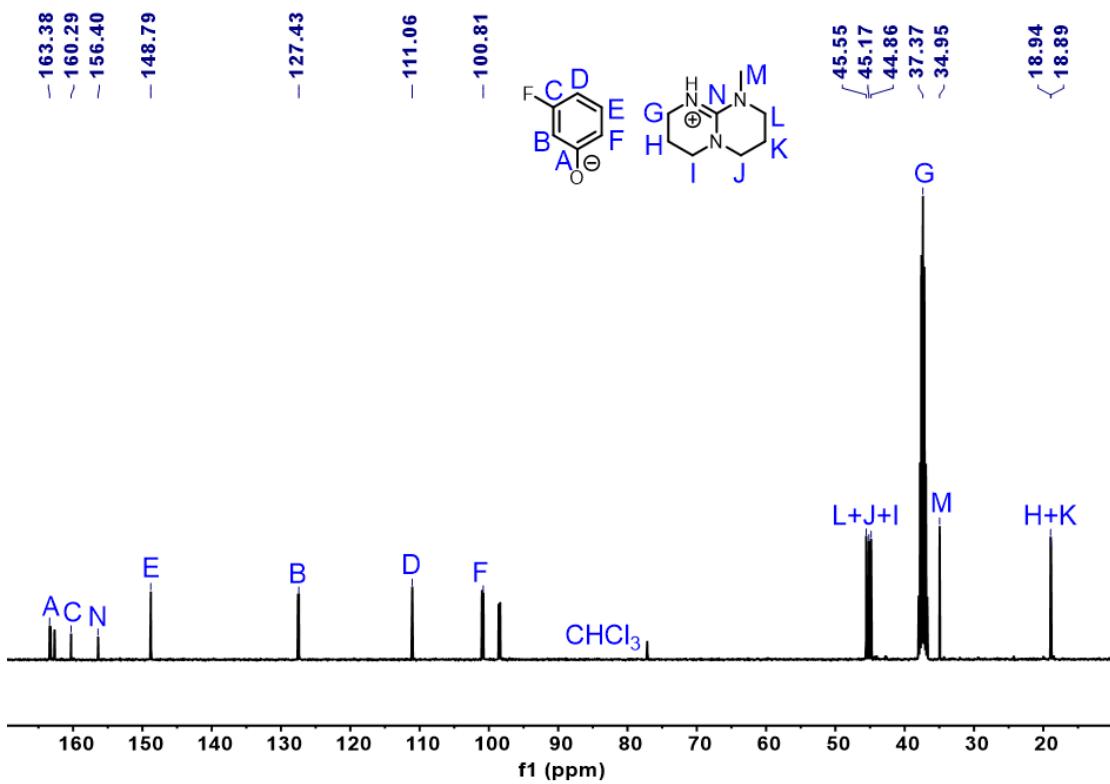
Figure S47. ^{13}C NMR spectrum (CDCl$_3$, 101 MHz) of *m*-FP/MTBD (b')
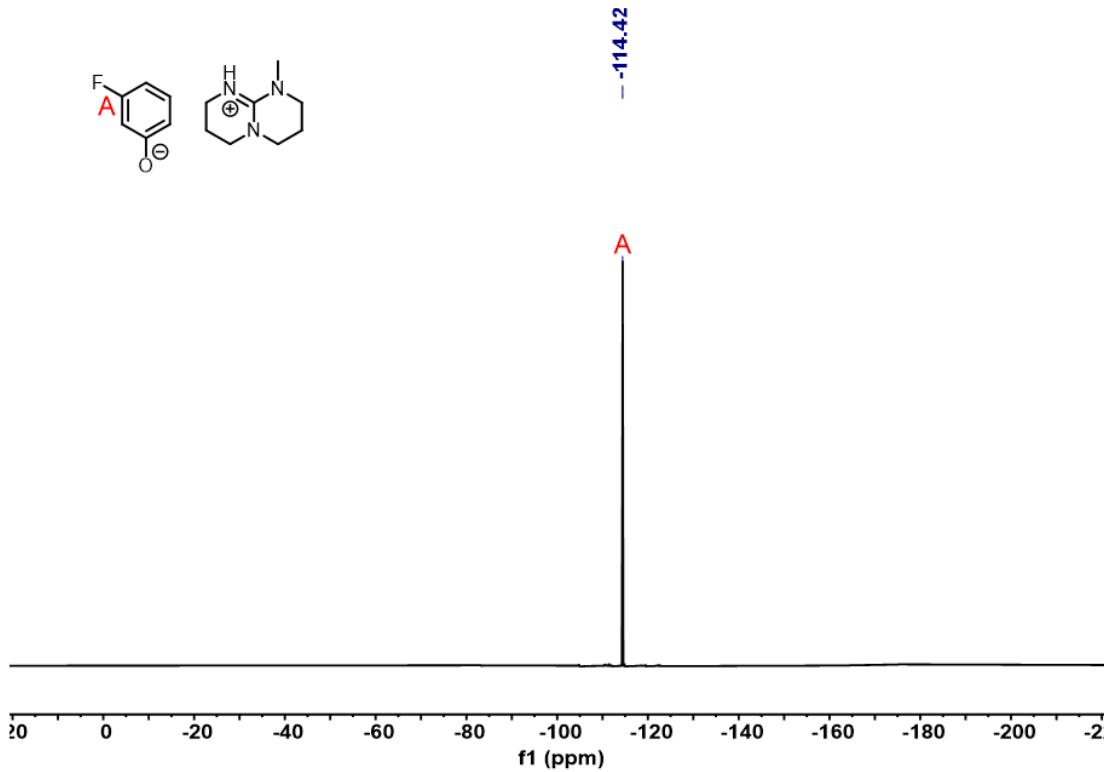
Figure S48. ^{19}F NMR spectrum (CDCl$_3$, 376 MHz) of *m*-FP/MTBD (b')
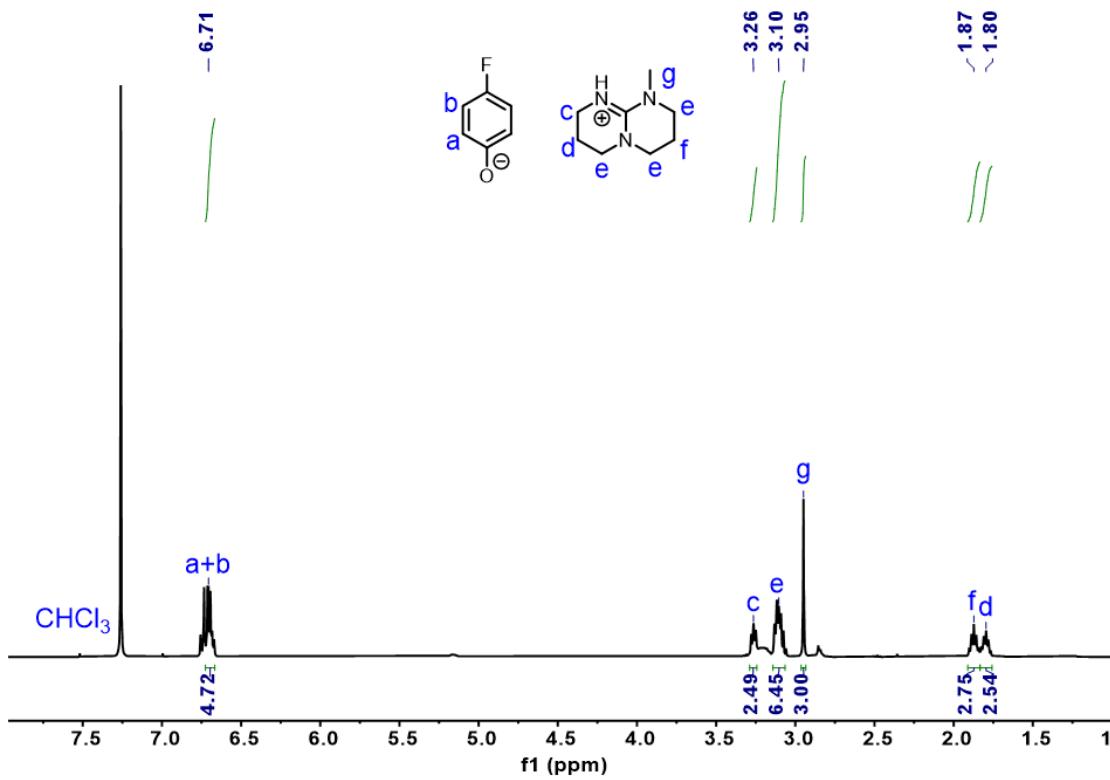
Figure S49. ^{1}H NMR spectrum (CDCl$_3$, 400 MHz) of *p*-FP/MTBD (c')
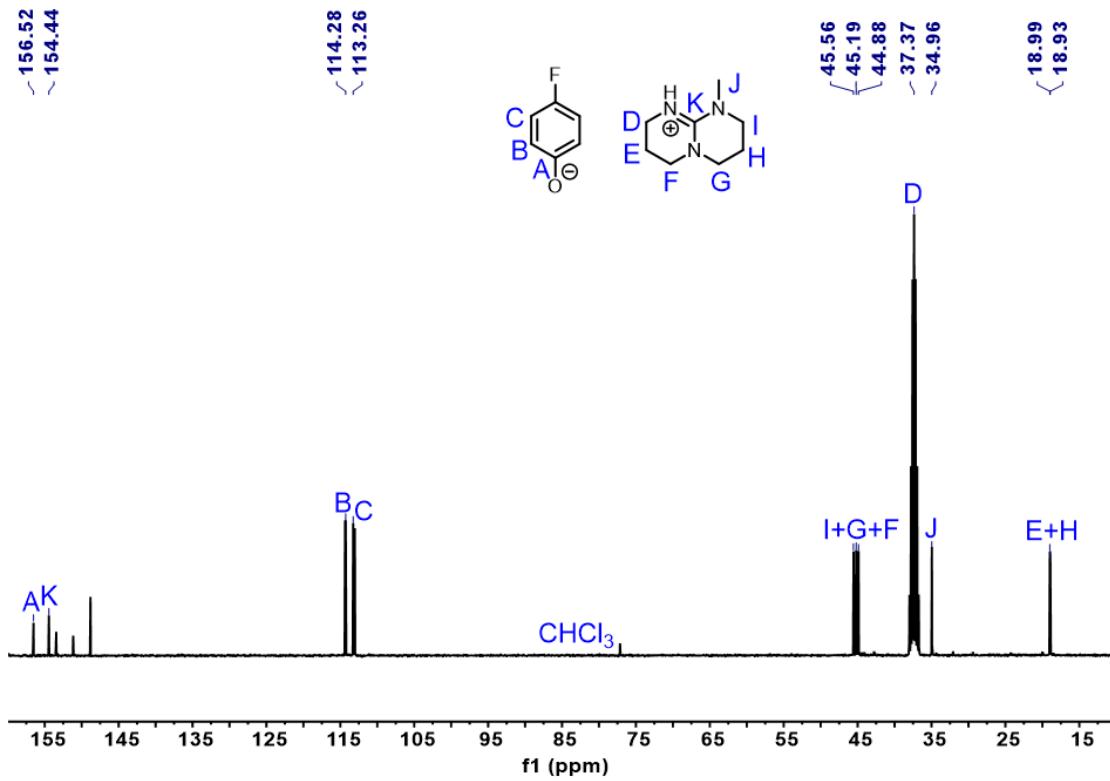
Figure S50. ^{13}C NMR spectrum (CDCl$_3$, 101 MHz) of *p*-FP/MTBD (c')

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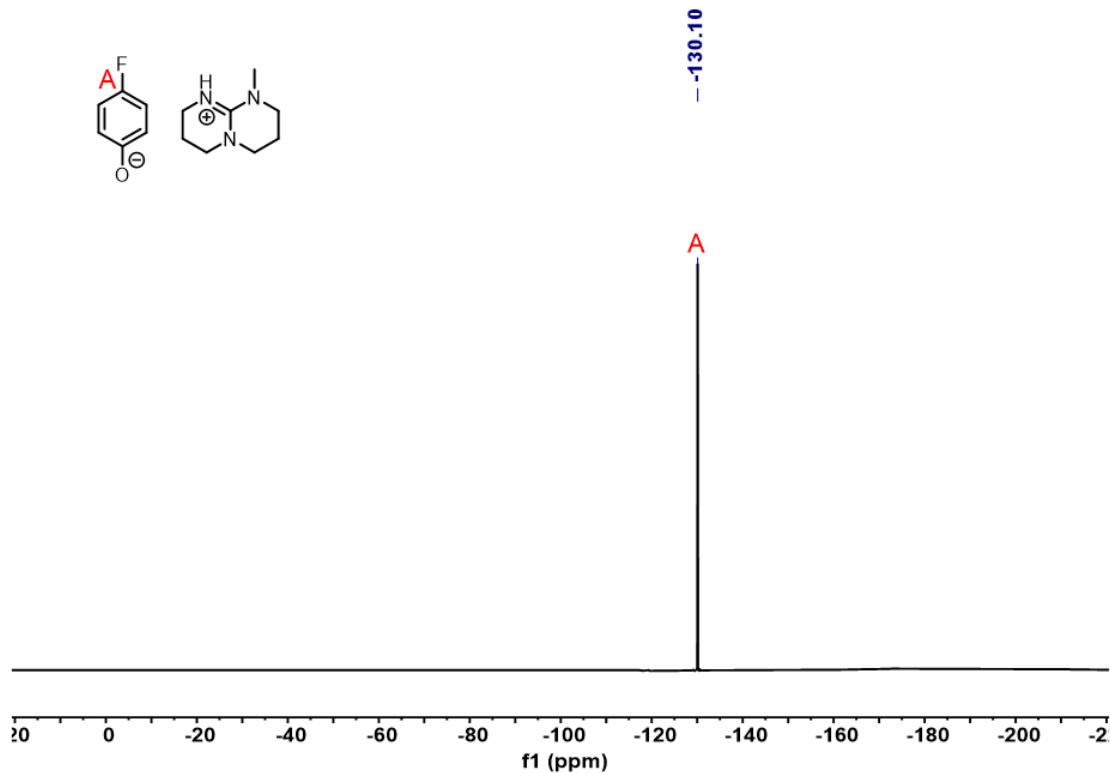
Figure S51. ^{19}F NMR spectrum (CDCl$_3$, 376 MHz) of *p*-FP/MTBD (c')
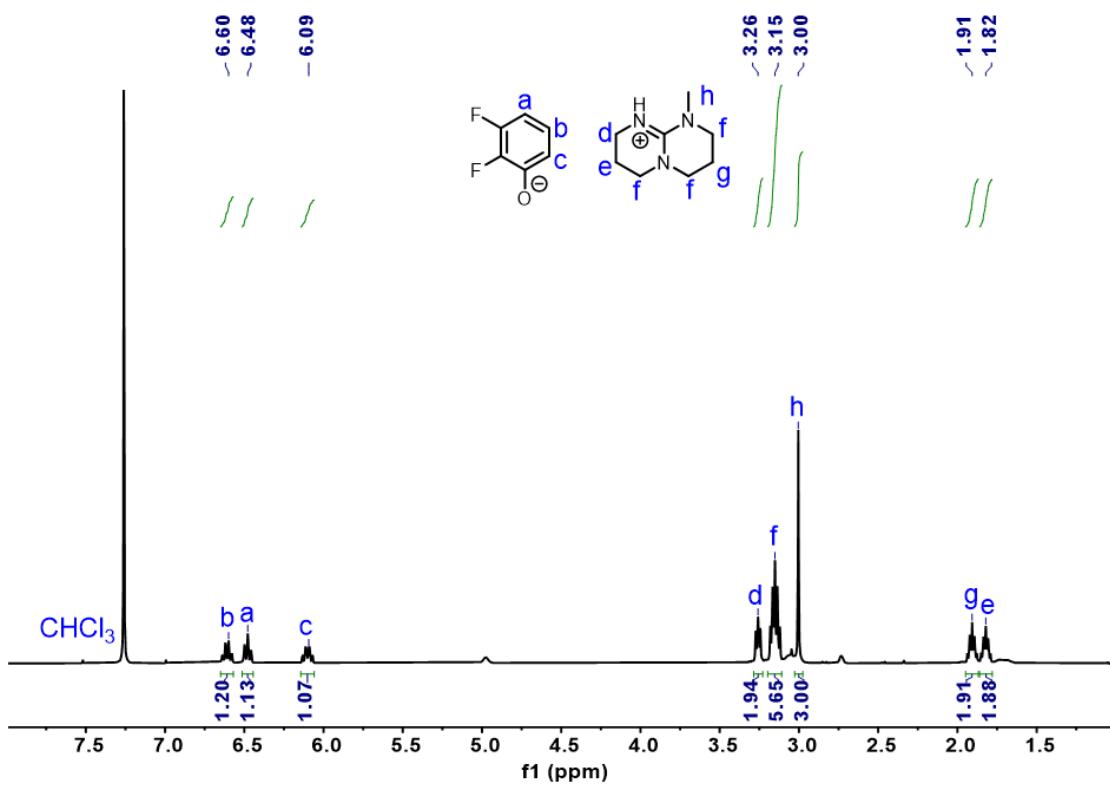
Figure S52. ^{1}H NMR spectrum (CDCl$_3$, 400 MHz) of 2,3-FP/MTBD (d')
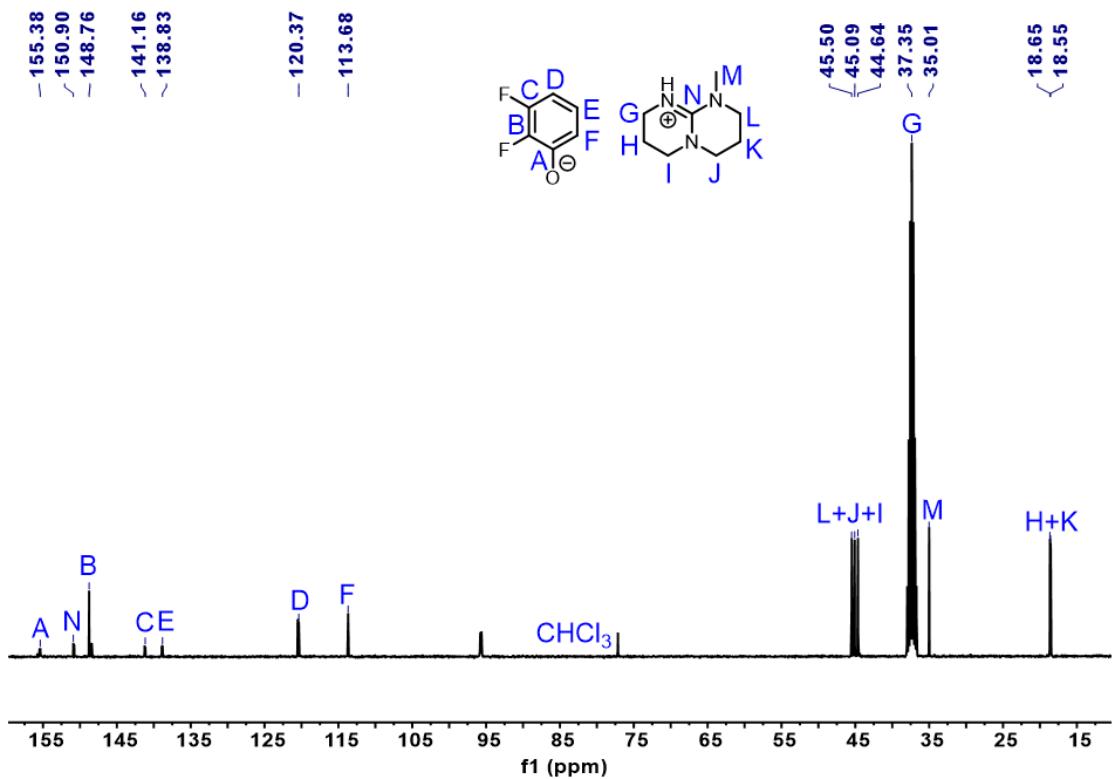
Figure S53. ^{13}C NMR spectrum (CDCl$_3$, 101 MHz) of 2,3-FP/MTBD (d')
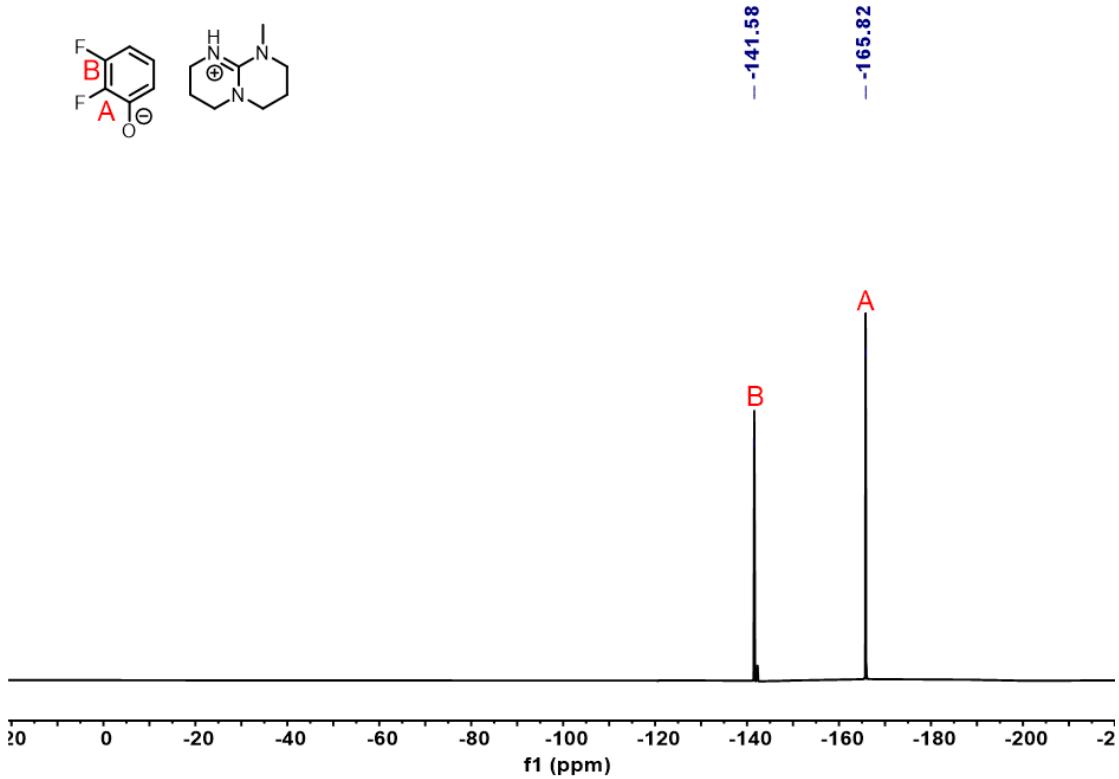
Figure S54. ^{19}F NMR spectrum (CDCl$_3$, 376 MHz) of 2,3-FP/MTBD (d')
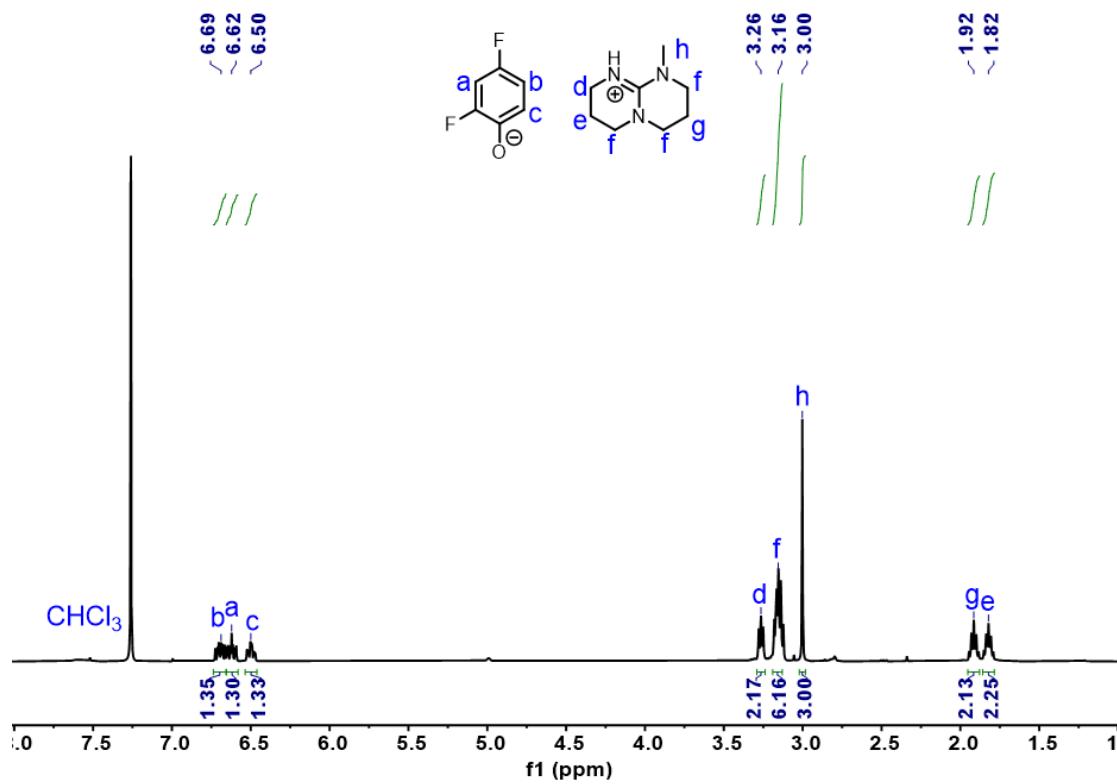
Figure S55. ^{1}H NMR spectrum (CDCl$_3$, 400 MHz) of 2,4-FP/MTBD (e')
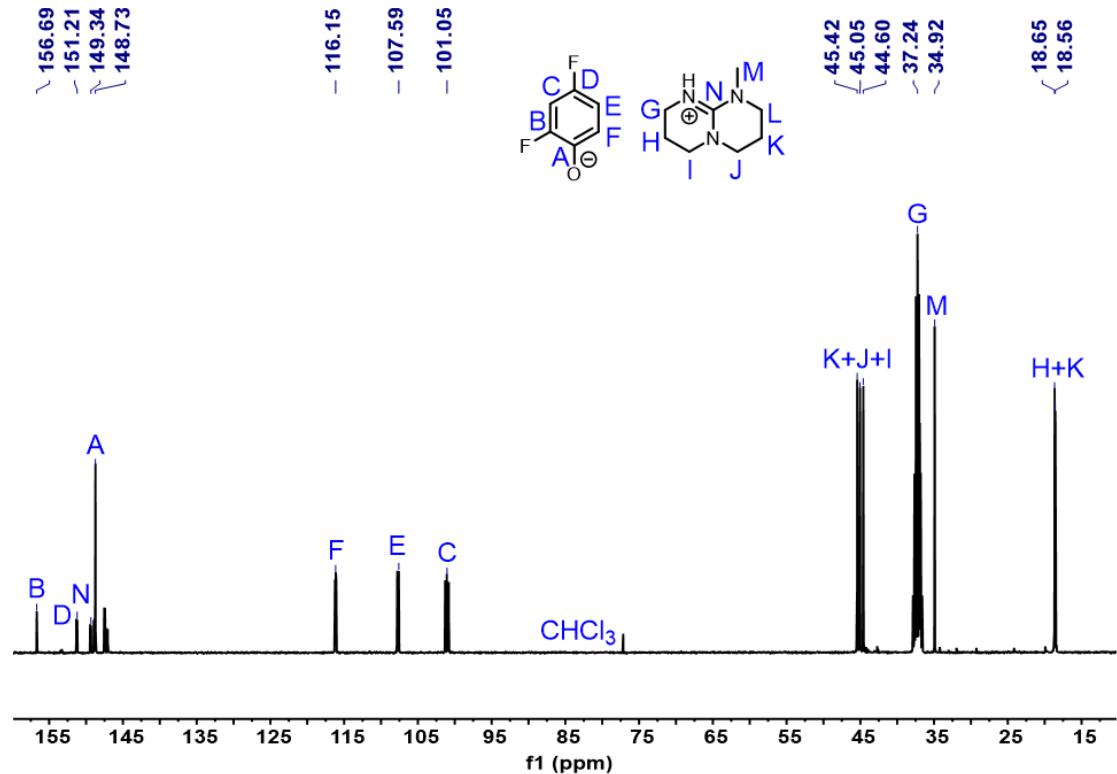
Figure S56. ^{13}C NMR spectrum (CDCl$_3$, 101 MHz) of 2,4-FP/MTBD (e')

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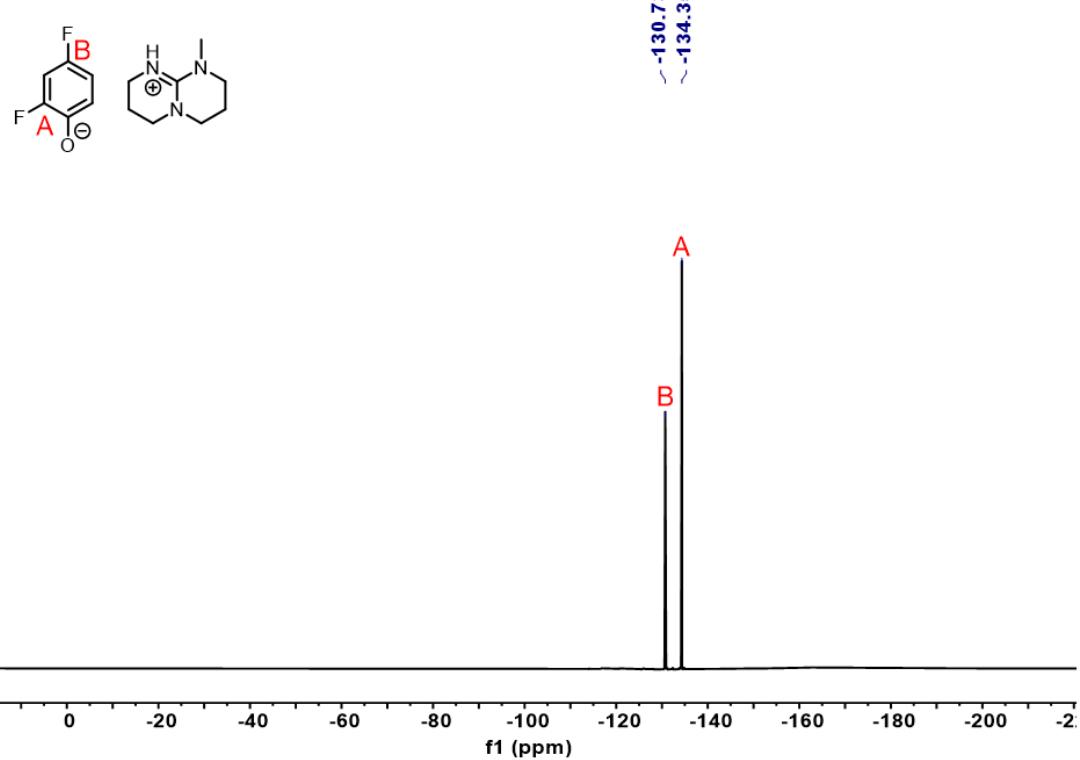
Figure S57. ^{19}F NMR spectrum (CDCl$_3$, 376 MHz) of 2,4-FP/MTBD (e')
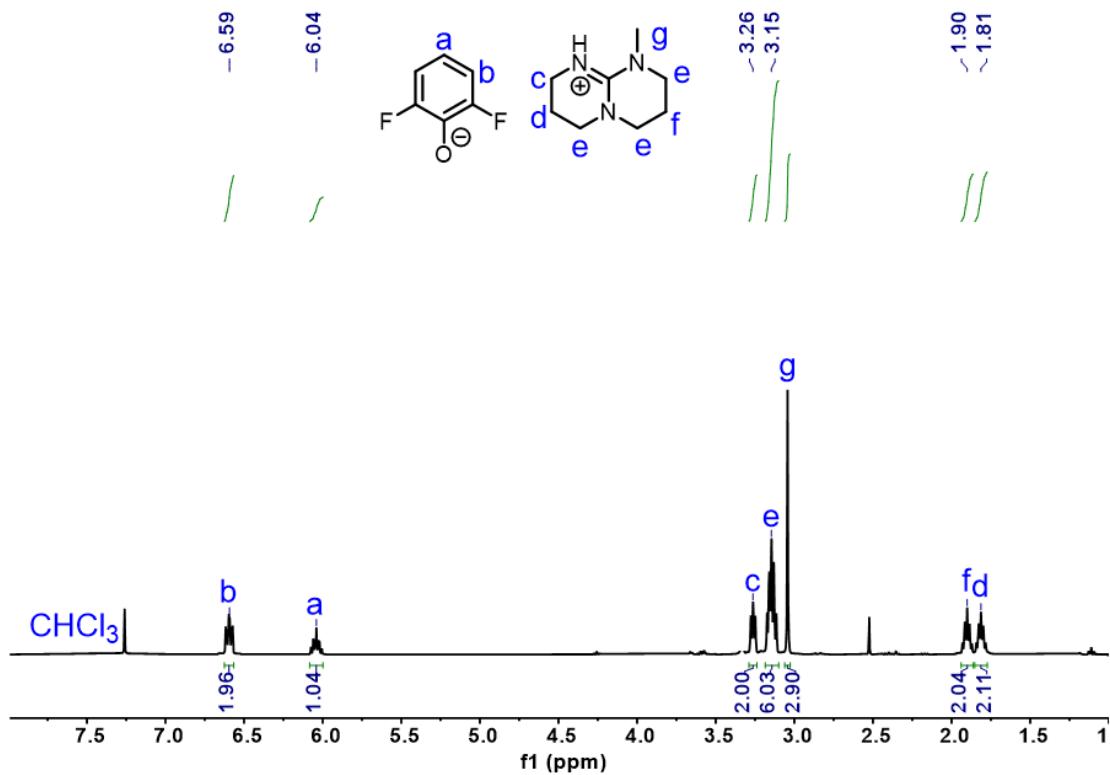
Figure S58. ^{1}H NMR spectrum (CDCl$_3$, 400 MHz) of 2,6-FP/MTBD (f')
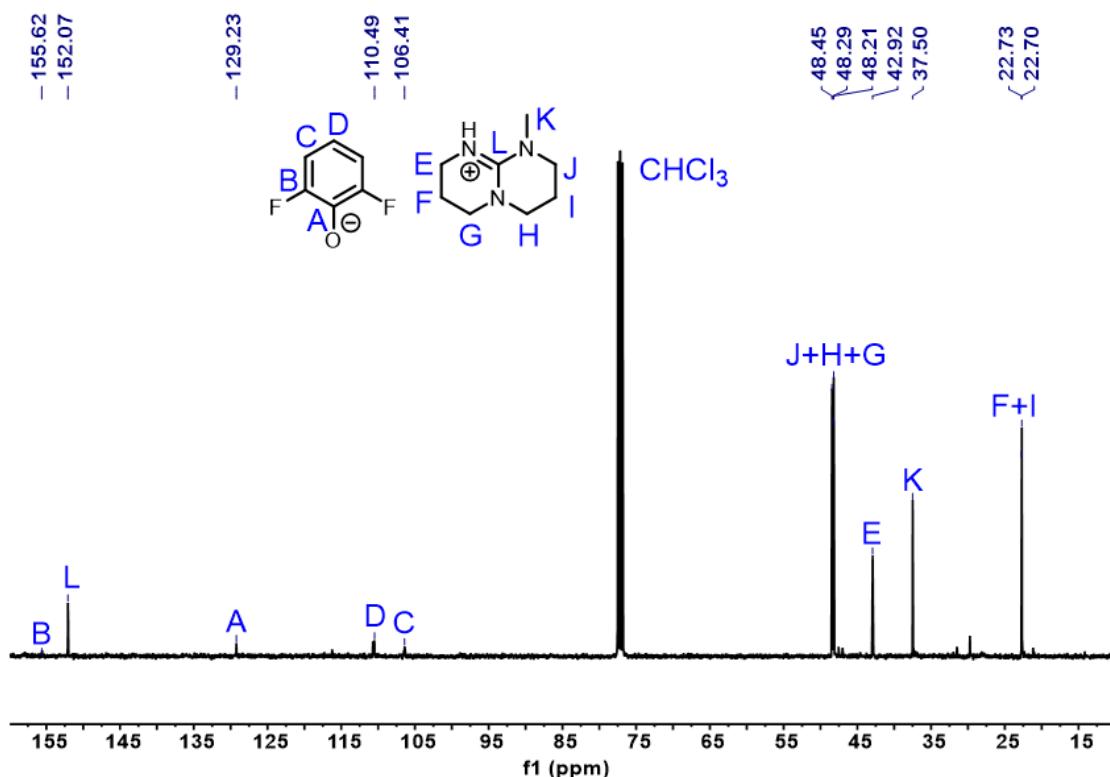
Figure S59. ^{13}C NMR spectrum (CDCl$_3$, 101 MHz) of 2,6-FP/MTBD (f')
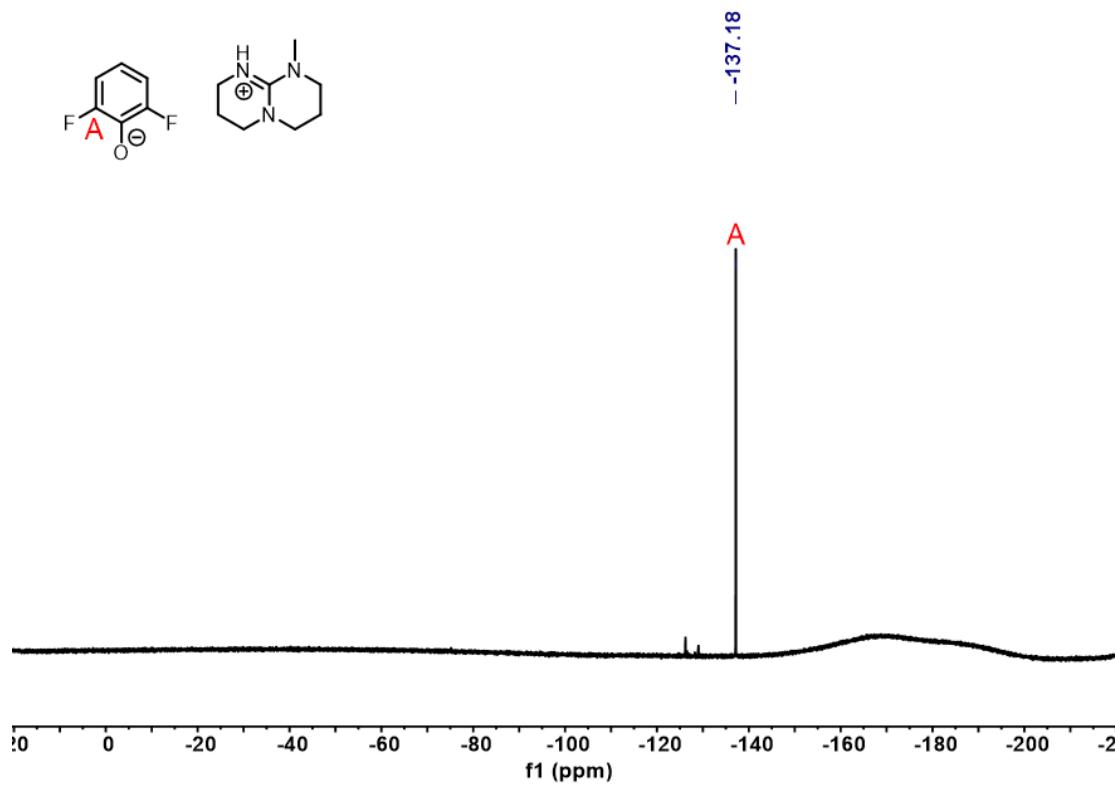
Figure S60. ^{19}F NMR spectrum (CDCl$_3$, 376 MHz) of 2,6-FP/MTBD (f')
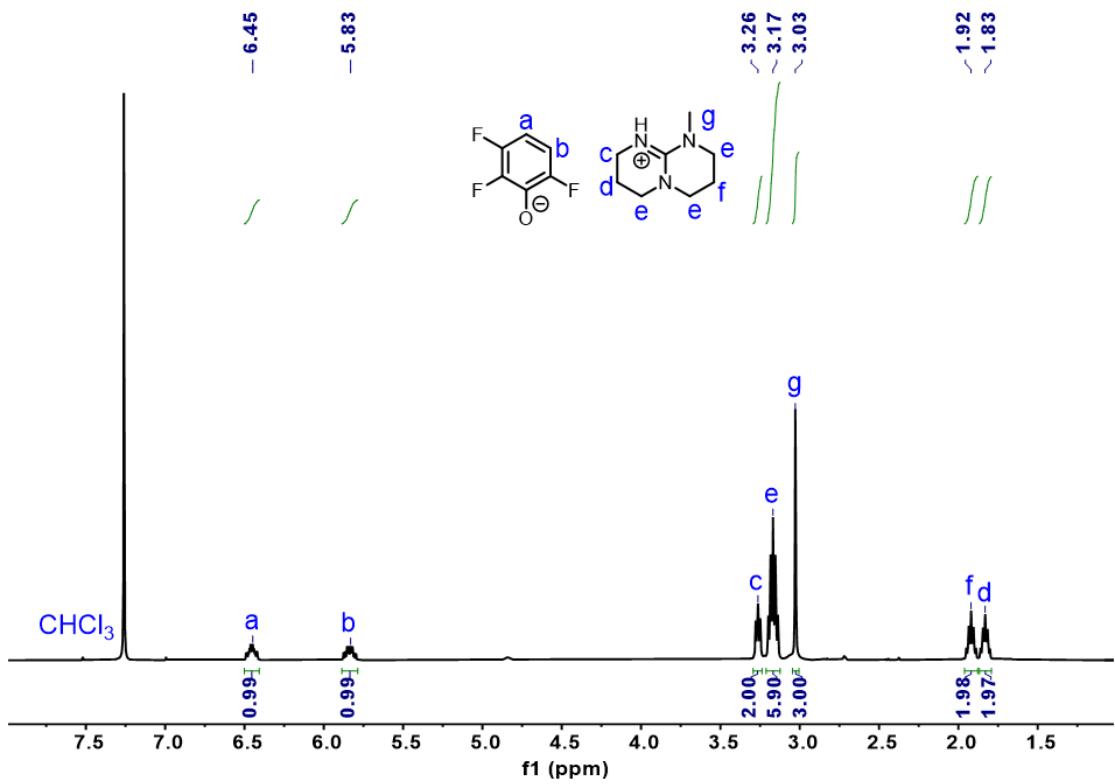
Figure S61. ^{1}H NMR spectrum (CDCl$_3$, 400 MHz) of 2,3,6-FP/MTBD (g')
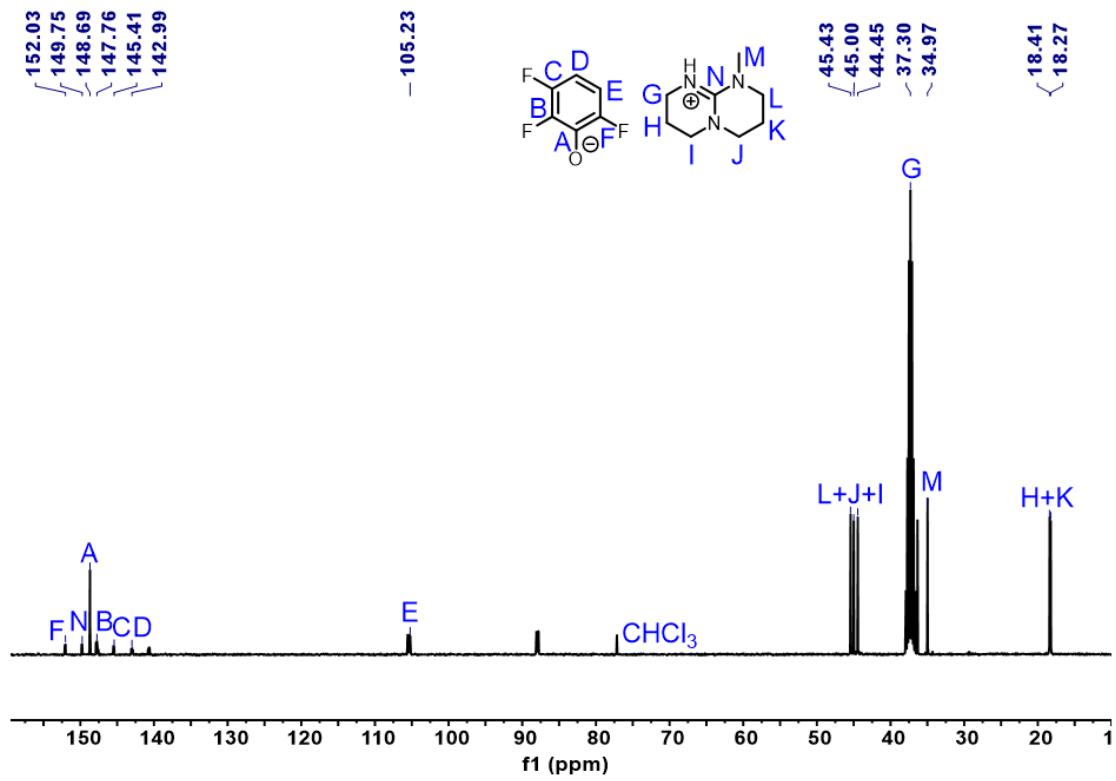
Figure S62. ^{13}C NMR spectrum (CDCl$_3$, 101 MHz) of 2,3,6-FP/MTBD (g')
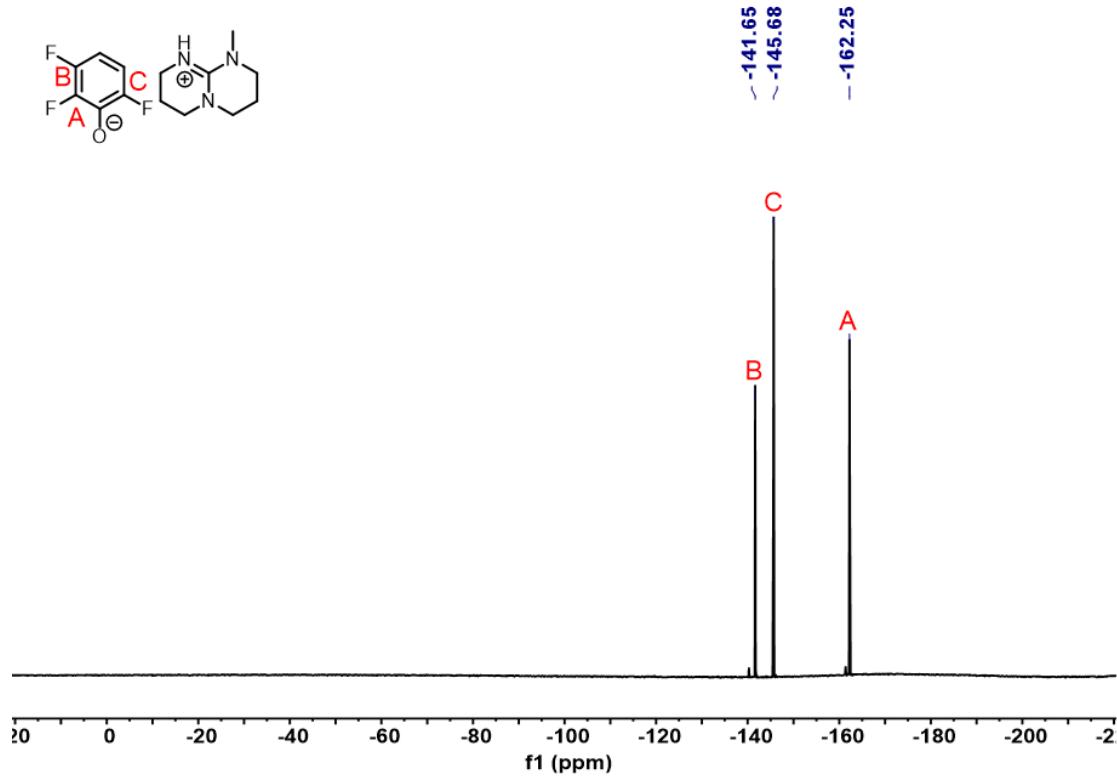
Figure S63. ^{19}F NMR spectrum (CDCl$_3$, 376 MHz) of 2,3,6-FP/MTBD (g')
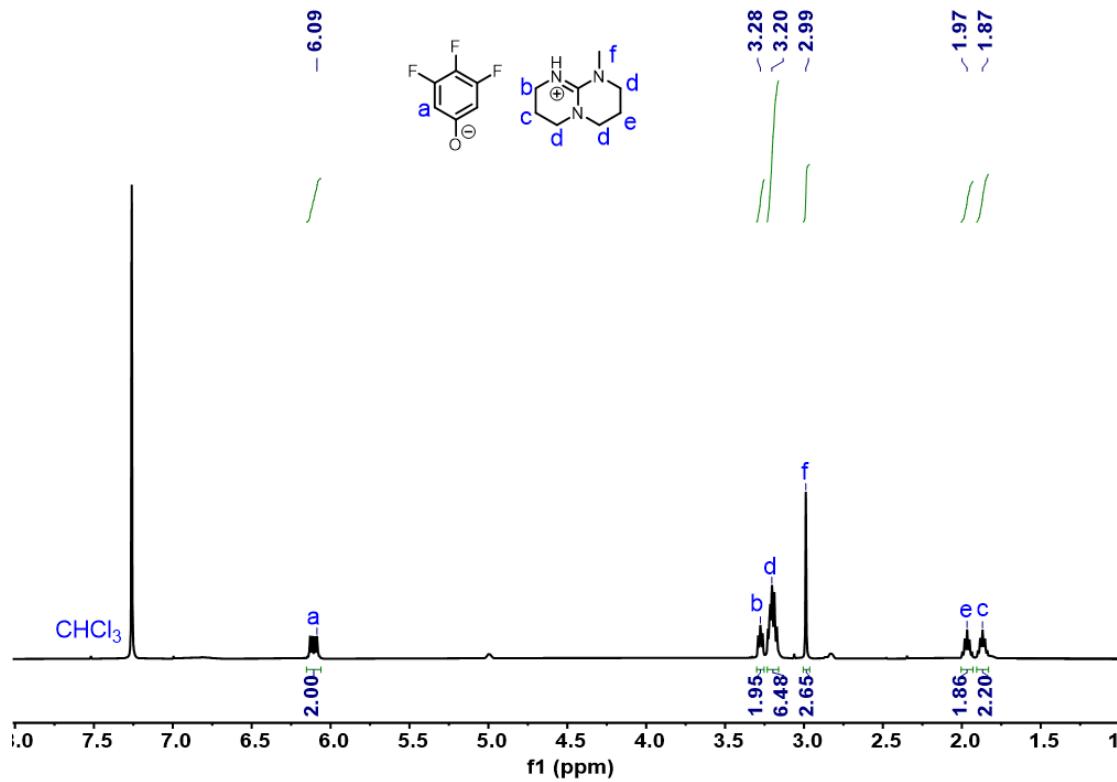
Figure S64. ^{1}H NMR spectrum (CDCl$_3$, 400 MHz) of 3,4,5-FP/MTBD (h')
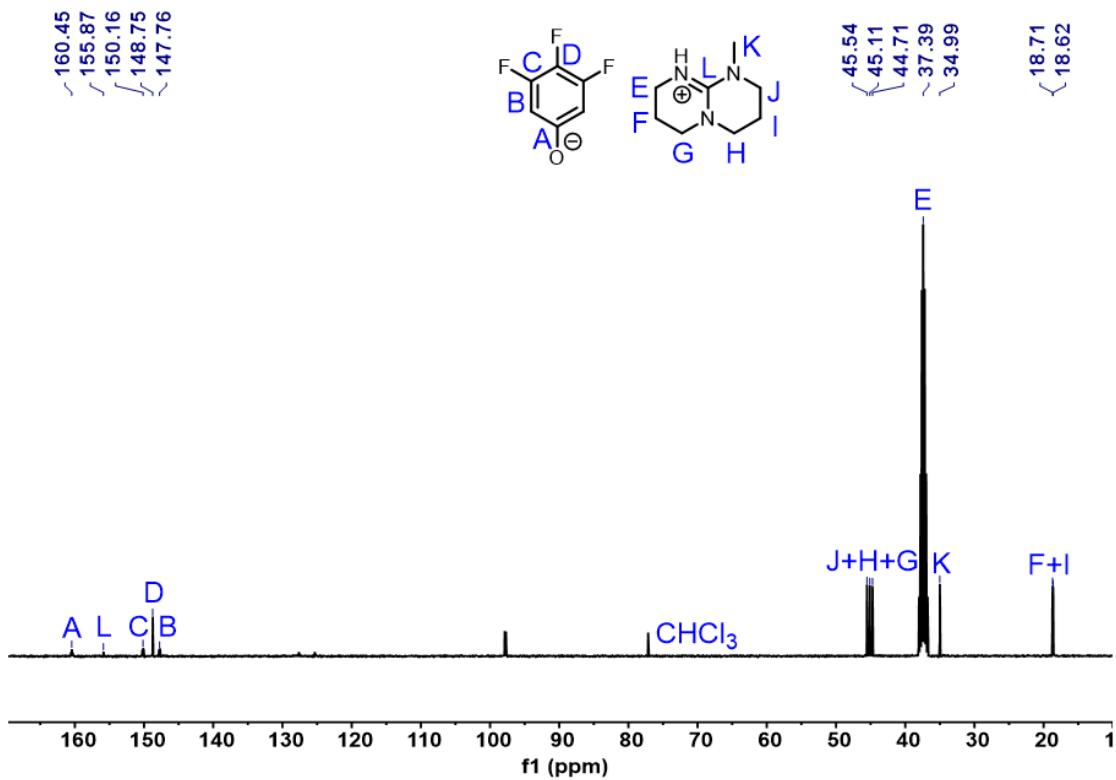
Figure S65. ^{13}C NMR spectrum (CDCl$_3$, 101 MHz) of 3,4,5-FP/MTBD (h')
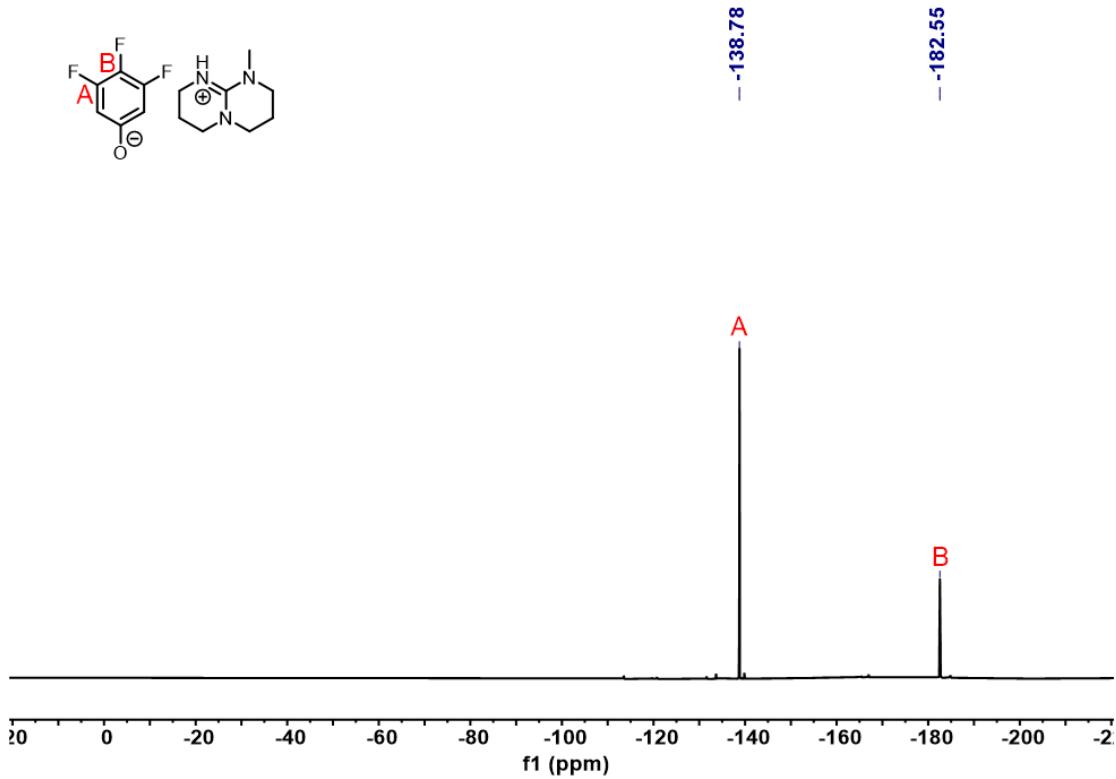
Figure S66. ^{19}F NMR spectrum (CDCl$_3$, 376 MHz) of 3,4,5-FP/MTBD (h')
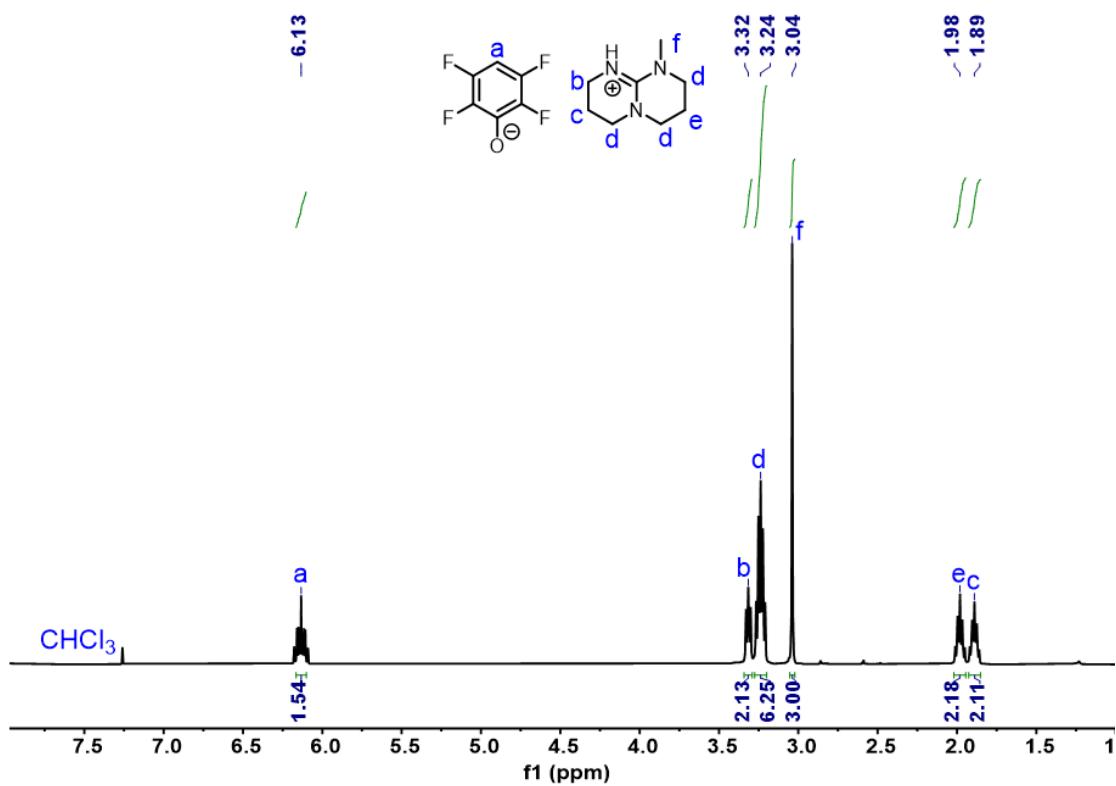
Figure S67. ¹H NMR spectrum (CDCl₃, 400 MHz) of 2,3,5,6-FP/MTBD (I')
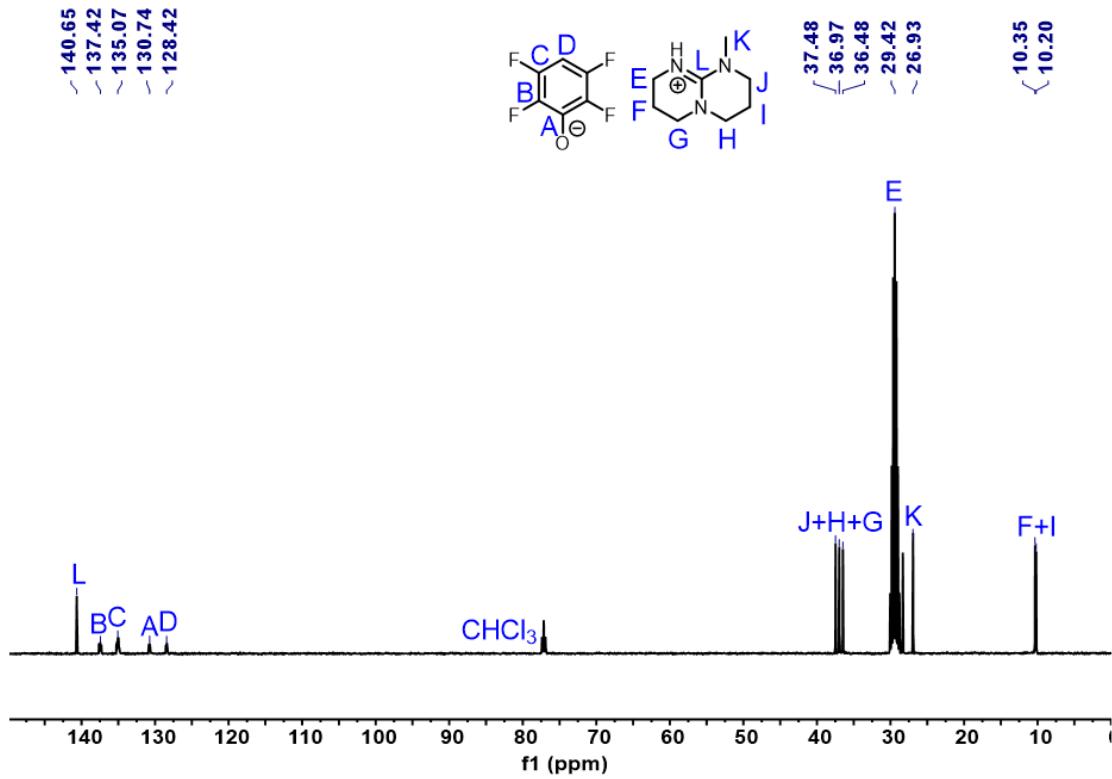
Figure S68. ¹³C NMR spectrum (CDCl₃, 101 MHz) of 2,3,5,6-FP/MTBD (I')

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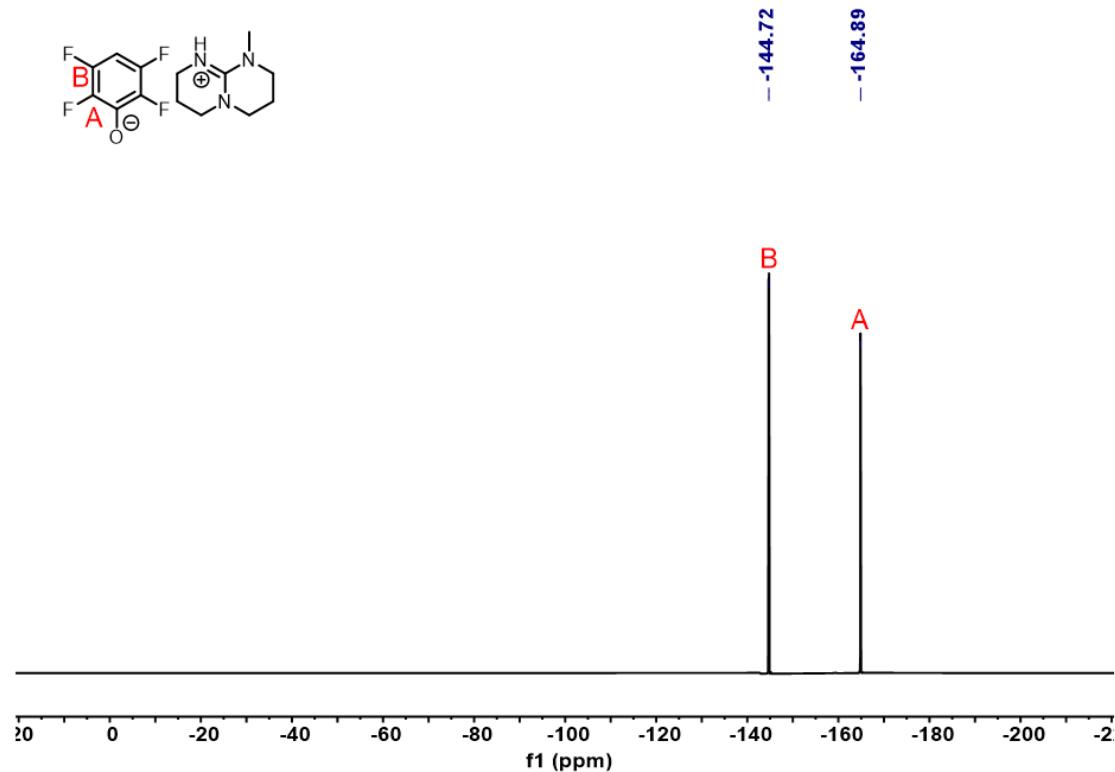
Figure S69. ^{19}F NMR spectrum (CDCl$_3$, 376 MHz) of 2,3,5,6-FP/MTBD (I')
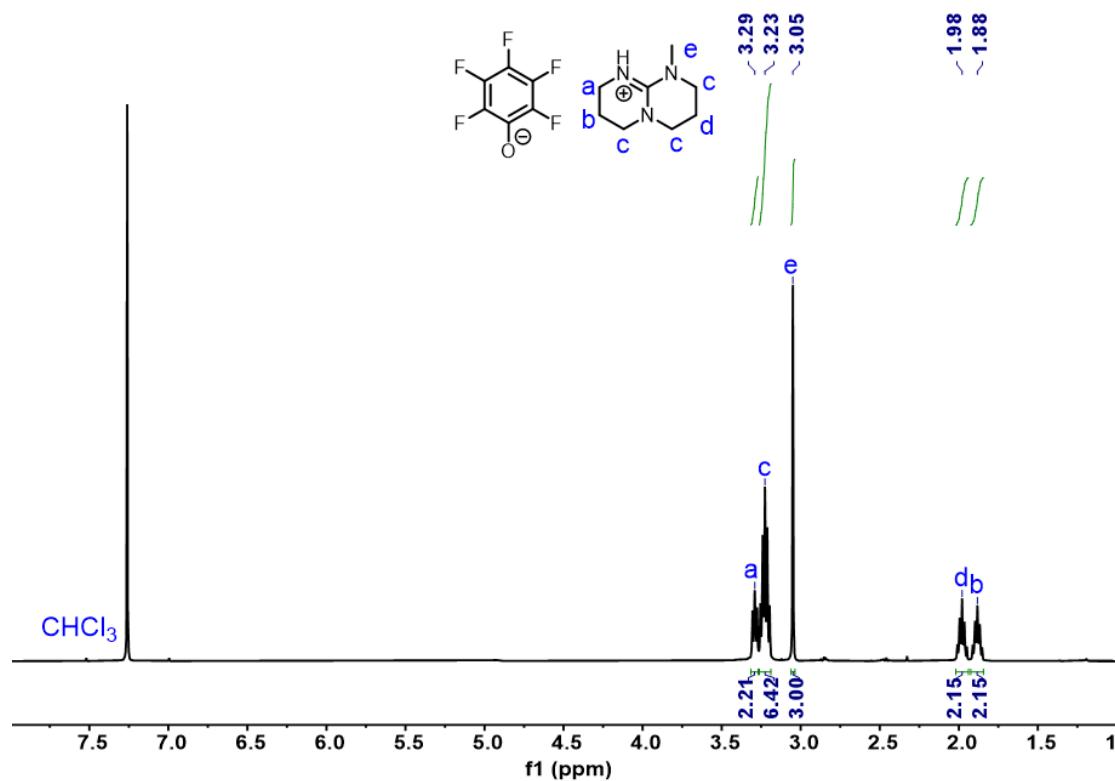
Figure S70. ^{1}H NMR spectrum (CDCl$_3$, 400 MHz) of 2,3,4,5,6-FP/MTBD (j')
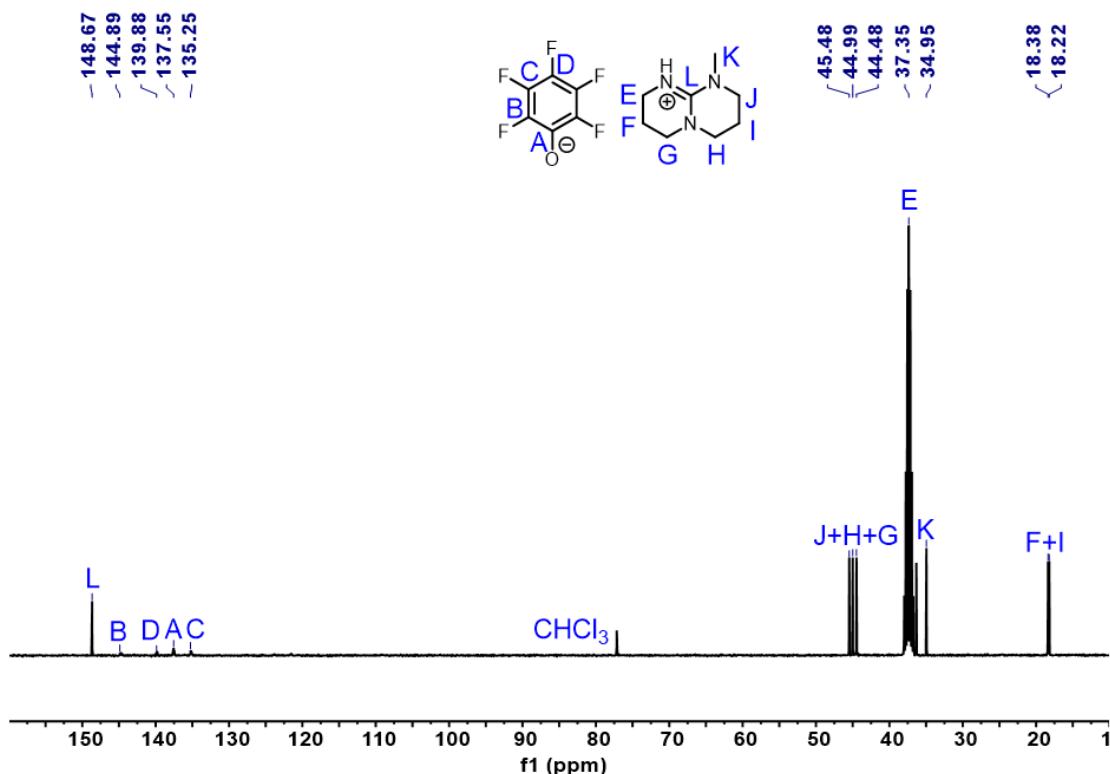
Figure S71. ^{13}C NMR spectrum (CDCl$_3$, 101 MHz) of 2,3,4,5,6-FP/MTBD (j')
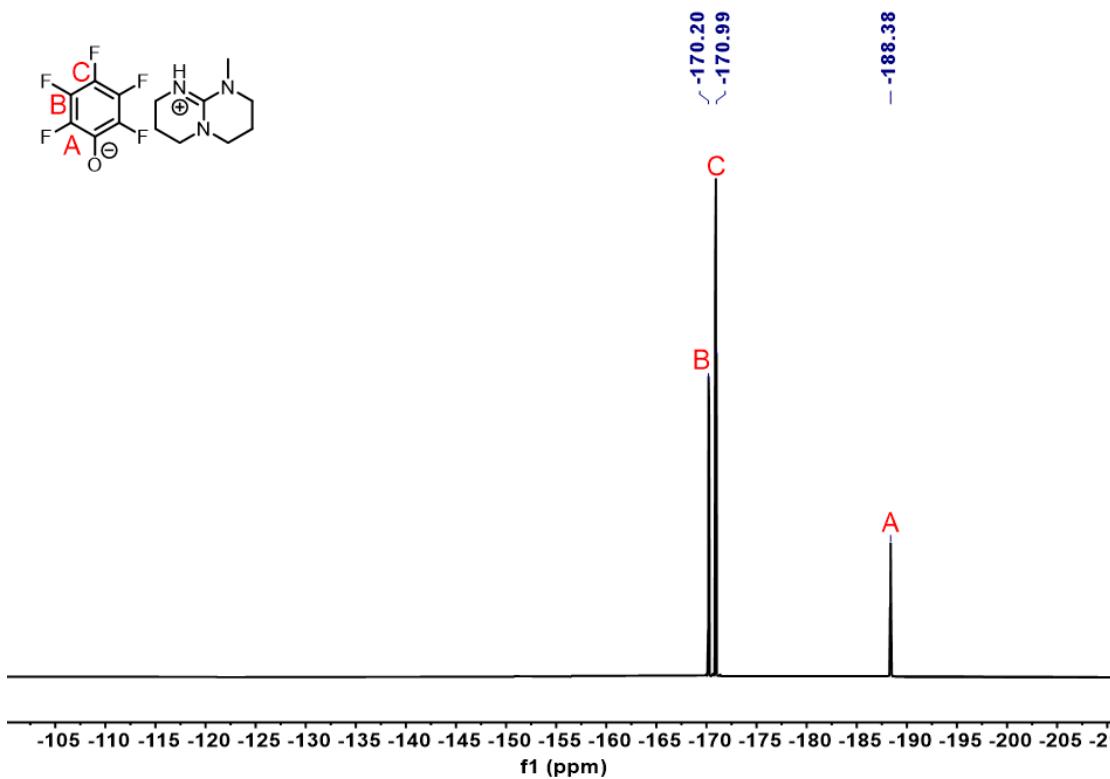
Figure S72. ^{19}F NMR spectrum (CDCl$_3$, 376 MHz) of 2,3,4,5,6-FP/MTBD (j')

Computational Study

Geometry optimizations of all structures were simulated at B3LYP, with 6-31+G(d,p) basis set for all elements. Single-point energy were obtained on optimized structures with B3LYP /aug-cc-pVTZ. Reported energies are free energies. All DFT calculations were performed using Gaussian 16 program[1].

Cartesian coordinates of the calculated species

o-FP/DMAP(a)
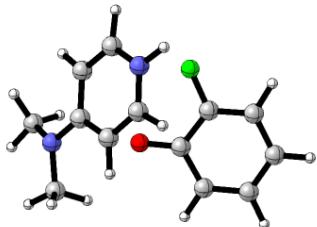
C	3.46099600	1.52420000	-0.50660400
C	2.13421300	1.79968700	-0.17867900
C	1.27138800	0.85183900	0.46865800
C	1.91807800	-0.40453900	0.71354500
C	3.23582700	-0.69549600	0.39875700
C	4.03340500	0.27522300	-0.22498600
H	4.06208000	2.29627300	-0.98574100
H	1.70825400	2.78010700	-0.38860700
H	3.63154600	-1.67749200	0.65273500
O	0.04743200	1.09616700	0.77521300
C	-2.11933100	-1.27303200	0.53092900
C	-1.41375200	-2.40681900	0.25259300
C	-0.48301700	-1.42067100	-1.68925300
C	-1.17369100	-0.26315300	-1.46995500
C	-1.99797200	-0.11643900	-0.30926100
H	-2.70969400	-1.25170200	1.43602300
H	-1.43486100	-3.27883100	0.89607300
H	0.20739900	-1.54135900	-2.51577200
H	-1.00064800	0.56508500	-2.14220400
C	-3.22213400	1.23026600	1.29452000
H	-3.74800400	2.18631100	1.31066000
H	-3.94620800	0.45159200	1.55523900
H	-2.40754800	1.25209400	2.03017800
C	-2.37654600	2.22730500	-0.82111900
H	-2.51224700	2.04634100	-1.89224600
H	-3.07700000	3.01162600	-0.52792500

H	-1.34656000	2.54404000	-0.61092400
H	5.06938000	0.06045600	-0.47309400
F	1.17813900	-1.40180200	1.32621200
N	-2.68149900	1.01674100	-0.05169300
N	-0.61353800	-2.48482700	-0.84403800
H	-0.01811500	-3.29127600	-0.96676100

m-FP/DMAP(b)
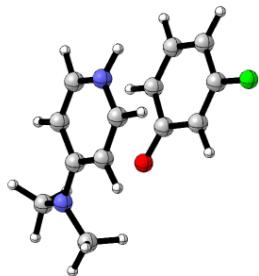
C	-2.56303800	1.68553900	0.51149600
C	-1.29406500	1.53074100	1.05837100
C	-0.71056100	0.22706000	1.27969700
C	-1.56706100	-0.89195900	0.96364300
C	-2.81719100	-0.68178500	0.41380800
C	-3.35188000	0.57881500	0.14160600
H	-2.96522100	2.68805500	0.36689700
H	-0.70359200	2.39892100	1.34443800
O	0.49494400	0.06833000	1.67356300
C	1.46225400	1.21350400	-1.00685800
C	0.28960100	1.34692200	-1.69626700
C	0.00445500	-0.99830000	-1.77411300
C	1.16873300	-1.19414500	-1.08520900
C	1.92457500	-0.07867900	-0.60372400
H	1.96750800	2.11513400	-0.69033800
H	-0.13000200	2.31285000	-1.94965400
H	-0.63258100	-1.81766500	-2.08559600
H	1.44107900	-2.20937400	-0.83275400
C	3.58636200	0.92327000	0.85281100
H	4.48897800	0.61636900	1.38436200
H	3.87240300	1.71006900	0.14726600
H	2.84890100	1.30772700	1.57067000
C	3.28971700	-1.54106800	0.77015800
H	3.37679900	-2.32687700	0.01299600
H	4.23996700	-1.49564200	1.30535200
H	2.48273800	-1.78342200	1.47529700
H	-4.35300200	0.68172800	-0.26496300
H	-1.21660500	-1.90152100	1.16018700

F	-3.57903300	-1.78387500	0.09654200
N	3.04201300	-0.23906000	0.14435200
N	-0.41811600	0.25494900	-2.10342500
H	-1.36431100	0.38116400	-2.44054700

p-FP/DMAP(c)
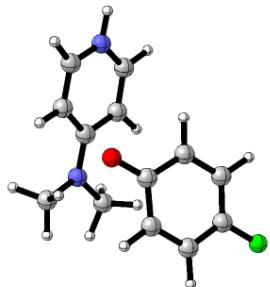
C	-3.14220400	0.60219000	0.35761000
C	-2.01956400	1.00779700	1.08156400
C	-0.90957900	0.13111600	1.34614800
C	-1.05949300	-1.20507300	0.83376700
C	-2.18381200	-1.61150500	0.10963300
C	-3.20538900	-0.69929800	-0.13288700
H	-3.97300700	1.28227300	0.17939800
H	-1.97627500	2.01625300	1.48999400
H	-0.26882100	-1.92109400	1.05194100
H	-2.27973900	-2.63191800	-0.25716500
O	0.15097000	0.52267100	1.96715400
C	1.68606600	-0.76479500	-1.30574900
C	2.47777900	-1.81584200	-0.92731700
C	3.30758000	-0.59108100	0.92753300
C	2.53019900	0.48594900	0.60828300
C	1.69359000	0.45751400	-0.55502000
H	1.03733800	-0.89563700	-2.16090300
H	2.48891900	-2.75906000	-1.46232700
H	3.93701400	-0.61698900	1.80902600
H	2.53216400	1.33716000	1.27180900
C	0.02540700	1.41787600	-2.05029100
H	-0.41878100	2.39907800	-2.21802000
H	0.55504200	1.12472900	-2.96476200
H	-0.78092200	0.70456900	-1.84002100
C	0.90046100	2.70178100	-0.05614000
H	1.88301100	3.19062000	-0.01905600
H	0.18162900	3.40526000	-0.47605300
H	0.58184200	2.39476100	0.95133400
F	-4.31172800	-1.09874100	-0.85167500
N	0.95307400	1.51242200	-0.91845700

| N | 3.28302500 | -1.72659700 | 0.16293900 |
| H | 3.83943900 | -2.52325500 | 0.43846200 |

2,3-FP/DMAP(d)
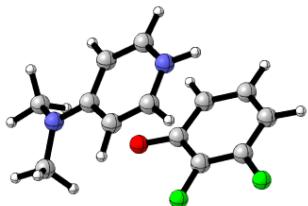
C	2.53332100	1.41629900	-1.28043300
C	1.26252700	1.01986600	-1.69056000
C	0.65485100	-0.21060100	-1.25520600
C	1.50108600	-1.00353600	-0.40030800
C	2.75834500	-0.58567200	0.00327900
C	3.30478200	0.63247300	-0.40630600
H	2.94759600	2.35258100	-1.65179300
H	0.68369400	1.63450300	-2.37701700
O	-0.53763300	-0.56164500	-1.54152500
C	-1.69194300	1.65151200	0.26293100
C	-0.59269600	2.25422900	0.80627600
C	-0.05359500	0.29975900	2.02294100
C	-1.13905200	-0.35544600	1.51422700
C	-1.98808200	0.28003300	0.55230300
H	-2.27122900	2.21110600	-0.45806400
H	-0.30063800	3.26711600	0.55521500
H	0.65116900	-0.17840800	2.69341700
H	-1.26956300	-1.39466900	1.78009000
C	-3.68052800	0.23076900	-1.18435700
H	-4.52021600	-0.40193700	-1.47723400
H	-4.08189100	1.22153900	-0.94806500
H	-2.96376000	0.29898500	-2.01397400
C	-3.09439300	-1.82611900	0.08336900
H	-3.14476300	-2.14681600	1.12876300
H	-4.00525500	-2.16908900	-0.41037900
H	-2.21746500	-2.26877700	-0.40814500
H	4.30463700	0.91211400	-0.08990800
F	3.47365200	-1.38820600	0.84565100
N	-3.03451200	-0.36277000	-0.01008300
N	0.20412500	1.59785300	1.69611000
H	1.08943500	2.00695100	1.96371200
F	1.03349000	-2.20279700	0.05151100

2,4-FP/DMAP(e)
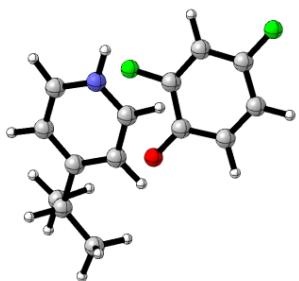
C	-3.13344300	1.44756300	0.58310600
C	-1.83429000	1.85363600	0.27942700
C	-0.92540300	1.08257300	-0.52906600
C	-1.48790900	-0.17468500	-0.94387900
C	-2.78238500	-0.60324800	-0.66687300
C	-3.59304700	0.22232500	0.10480400
H	-3.79391300	2.07235200	1.17943200
H	-1.47149100	2.81786900	0.62985100
O	0.26593000	1.44736100	-0.80631300
C	2.47597300	-1.66807800	-0.09310700
C	1.48796400	-2.60557500	0.10437700
C	0.22674400	-1.05503700	1.39057400
C	1.20698000	-0.08952500	1.21026600
C	2.34148200	-0.36061800	0.43468200
H	3.34058800	-1.93726300	-0.69110300
H	1.51959300	-3.60817300	-0.30727600
H	-0.68004700	-0.89310300	1.95941000
H	1.04561100	0.89041000	1.63707800
C	3.40639200	0.67430300	0.12947700
H	4.37123400	0.19658000	0.36803400
C	3.39980200	0.99823400	-1.38595100
H	4.19016600	1.72610300	-1.60474400
H	3.58864300	0.10616800	-1.99466800
H	2.42643700	1.41155500	-1.66840200
C	3.28285500	1.96025600	0.95610100
H	3.29334100	1.76097900	2.03531700
H	4.12873800	2.62039800	0.73422300
H	2.36117800	2.49437700	0.69849600
F	-0.70375300	-1.01519100	-1.69572800
H	-3.14966200	-1.54922800	-1.05594300
F	-4.86882700	-0.18628900	0.39562500
N	0.39688100	-2.28656200	0.83804900
H	-0.35308900	-2.96141500	0.92175700

2,6-FP/DMAP(f)
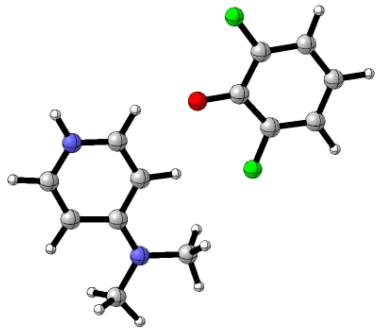
C	3.46767000	-1.85990500	0.00006000
C	2.32803300	-1.07311700	0.00002900
C	2.29441300	0.35447500	-0.00002400
C	3.61400300	0.90601800	-0.00003800
C	4.78457300	0.16376500	-0.00000900
C	4.72353300	-1.23772600	0.00004400
H	3.36692800	-2.94281400	0.00009700
H	5.73676700	0.68922400	-0.00002500
O	1.21217300	1.04281500	-0.00006300
C	-4.01658800	0.85229900	0.00004800
C	-3.72300300	2.19041900	0.00005600
C	-1.39078900	1.73807000	0.00003600
C	-1.62674200	0.38556100	0.00003800
C	-2.95783100	-0.11721300	0.00001100
H	-5.05845300	0.55788200	0.00009500
H	-4.49077800	2.95656500	0.00008200
H	-0.36042100	2.09820000	0.00002700
H	-0.73357200	-0.23180300	0.00005200
C	-2.09342200	-2.40219400	0.00000600
H	-2.50074000	-3.41378000	0.00005700
H	-1.46142300	-2.27534000	-0.88554800
H	-1.46142900	-2.27525300	0.88555100
C	-4.58337300	-1.94289600	-0.00011100
H	-5.13133700	-1.61215700	-0.89279200
H	-4.56461700	-3.03308700	-0.00046800
H	-5.13124800	-1.61272500	0.89284200
H	5.63357700	-1.83043800	0.00006600
F	3.71186600	2.27136800	-0.00008600
F	1.09489300	-1.71342000	0.00004800
N	-2.43175200	2.61728900	0.00002700
H	-2.23253500	3.60919500	0.00007000
N	-3.20993400	-1.44486900	-0.00004500

2,3,6-FP/DMAP(g)
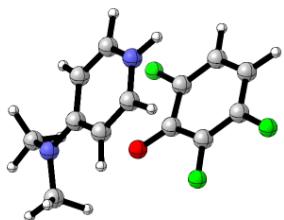
C	2.45991600	1.74420900	-0.12628800
C	1.20716300	1.58831200	-0.69177500
C	0.63180100	0.33163000	-1.09044100
C	1.52343700	-0.76929000	-0.84710100
C	2.77813400	-0.62231400	-0.27203100
C	3.27500900	0.62244900	0.10843500
H	2.80549100	2.74429700	0.12397400
O	-0.54518700	0.19302400	-1.55083900
C	-1.63772600	1.02347400	1.22859200
C	-0.55341500	1.08732200	2.05676300
C	-0.21825600	-1.24797400	1.89237000
C	-1.29245200	-1.37613200	1.05839000
C	-2.03703300	-0.22313300	0.64557200
H	-2.11874700	1.95169300	0.95456900
H	-0.18457500	2.02359700	2.45915600
H	0.40623900	-2.09001000	2.16832700
H	-1.49955900	-2.35514200	0.65006800
C	-3.59820900	0.91672100	-0.81825900
H	-4.44505900	0.65607100	-1.45521400
H	-3.96248900	1.60573000	-0.04952600
H	-2.81510800	1.39646400	-1.42068500
C	-3.24569200	-1.54091600	-0.99239700
H	-3.38221600	-2.40474300	-0.33409300
H	-4.14687000	-1.44410800	-1.60010700
H	-2.37522000	-1.69325100	-1.64466900
H	4.27143200	0.70804100	0.52845800
F	3.53492500	-1.73886100	-0.06397900
N	-3.07515100	-0.31180000	-0.20984500
N	0.13412000	-0.03631900	2.40709100
H	1.00552100	0.05302900	2.91195800
F	1.09840800	-2.01886600	-1.18159600
F	0.43709200	2.70604100	-0.88522500

3,4,5-FP/DMAP(h)
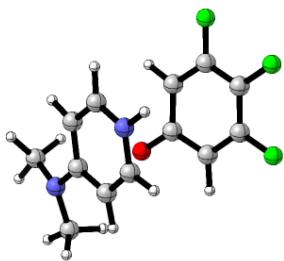
C	2.31680400	1.19174100	-0.48401500
C	1.02536000	1.21967500	-0.97833400
C	0.30014100	-0.00077200	-1.23211300
C	1.02547400	-1.22092000	-0.97732400
C	2.31692500	-1.19244200	-0.48303100
C	2.98973000	-0.00020500	-0.20526800
H	0.55532800	2.17481500	-1.19331700
O	-0.92180300	-0.00097100	-1.61047700
C	-1.82729700	1.21525100	1.04494600
C	-0.71987100	1.18486000	1.84402700
C	-0.71987400	-1.18201800	1.84584400
C	-1.82730100	-1.21362200	1.04681100
C	-2.41366800	0.00045200	0.56287600
H	-2.19140400	2.18069100	0.72269500
H	-0.21651700	2.08494100	2.17722000
H	-0.21651400	-2.08159200	2.18039600
H	-2.19143900	-2.17954700	0.72605400
C	-3.87487200	1.24186200	-0.92467100
H	-4.78497400	1.06241200	-1.49968400
H	-4.09445200	2.03237100	-0.19990800
H	-3.06951500	1.55955000	-1.60057100
C	-3.87506400	-1.24360700	-0.92215300
H	-4.09571200	-2.03233400	-0.19575300
H	-4.78454700	-1.06490900	-1.49836700
H	-3.06939800	-1.56334400	-1.59670700
H	0.55553500	-2.17630200	-1.19144300
F	2.97148300	-2.36085900	-0.23457000
N	-3.49921400	-0.00021400	-0.24263800
N	-0.18561000	0.00173700	2.26151400
H	0.69006600	0.00212600	2.76628200
F	4.25534400	0.00006400	0.28545600
F	2.97126300	2.36042800	-0.23652900

2,3,5,6-FP/DMAP(i)
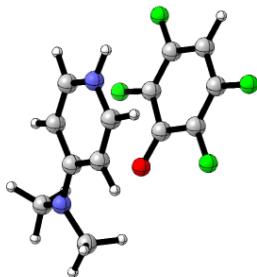
C	2.48901200	1.18553800	-0.23965300
C	1.22545500	1.19850900	-0.80618000
C	0.49535600	-0.00045500	-1.12195900
C	1.22465300	-1.19963700	-0.80518500
C	2.48821600	-1.18703600	-0.23866400
C	3.15726900	-0.00084400	0.06946000
O	-0.69006300	-0.00024200	-1.57583300
C	-1.65082200	1.21668300	1.15270300
C	-0.57682200	1.18505700	1.99611800
C	-0.57665100	-1.18064000	1.99862400
C	-1.65062400	-1.21418000	1.15524500
C	-2.22298700	0.00068900	0.65402700
H	-1.99206400	2.18204100	0.80664500
H	-0.08206000	2.08597000	2.34074100
H	-0.08182900	-2.08076400	2.34522400
H	-1.99184400	-2.18031300	0.81133100
C	-3.60433300	1.24376000	-0.90519100
H	-4.48287600	1.06100600	-1.52597900
H	-3.86300000	2.02999600	-0.18899300
H	-2.76539300	1.56429800	-1.53730100
C	-3.60323400	-1.24611800	-0.90299900
H	-3.86323300	-2.03075100	-0.18549500
H	-4.48060300	-1.06468100	-1.52581200
H	-2.76319200	-1.56804100	-1.53292500
H	4.15875800	-0.00100200	0.48299700
F	3.09438700	-2.37314300	0.04304100
N	-3.25658600	-0.00040000	-0.20930400
N	-0.05870600	0.00269500	2.43283800
H	0.79977000	0.00332800	2.96681500
F	0.62444200	-2.39555200	-1.05507900
F	0.62609500	2.39463900	-1.05716800
F	3.09598600	2.37148000	0.04105100

2,3,4,5,6-FP/DMAP(j)
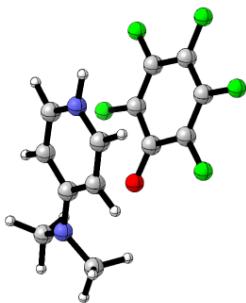
C	2.31012800	1.19325400	-0.33198000
C	1.01522300	1.19433100	-0.83416500
C	0.26880100	0.00144100	-1.11839300
C	1.00565000	-1.19645300	-0.83019100
C	2.30047400	-1.20420600	-0.32799500
C	2.96981000	-0.00768800	-0.06526700
O	-0.93462900	0.00559100	-1.53210100
C	-1.91396200	1.22343600	1.14719700
C	-0.87996100	1.19818400	2.03858500
C	-0.87923900	-1.16891900	2.05640400
C	-1.91311800	-1.20818500	1.16529100
C	-2.47334600	0.00361100	0.64072500
H	-2.23955600	2.18586500	0.77862300
H	-0.40255600	2.10155500	2.40104900
H	-0.40156500	-2.06653100	2.43262000
H	-2.23831400	-2.17630300	0.81152200
C	-3.83395700	1.23633200	-0.94431100
H	-4.70454800	1.04929600	-1.57490400
H	-4.10192800	2.02653600	-0.23593200
H	-2.98682900	1.55264900	-1.56725600
C	-3.83286300	-1.25343700	-0.92603200
H	-4.09900300	-2.03389200	-0.20626500
H	-4.70434200	-1.07674100	-1.55837900
H	-2.98638800	-1.57807800	-1.54566900
F	2.92175400	-2.37779200	-0.07106700
N	-3.49433000	-0.00335100	-0.23646300
N	-0.38181300	0.01809700	2.50640700
H	0.43095900	0.02285300	3.10708800
F	0.39825900	-2.39223900	-1.05158000
F	0.41769500	2.39426600	-1.05979400
F	2.94087900	2.36267000	-0.07900800
F	4.23055200	-0.01194400	0.42872800

Ph/DMAP(k)
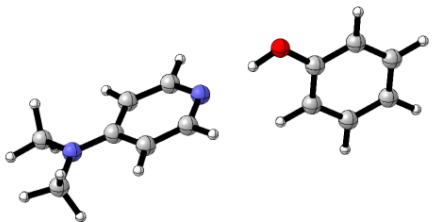
C	5.60275200	0.08392200	0.00450400
C	4.56199700	1.00847400	0.09214100
C	3.22570900	0.57494600	0.05412900
C	2.95357200	-0.79883600	-0.07313000
C	4.00625400	-1.71517400	-0.16000300
C	5.33597100	-1.28532200	-0.12224700
H	6.63196200	0.43614700	0.03548600
H	4.75975600	2.07279100	0.19070200
H	1.92173400	-1.14048400	-0.10326400
H	3.77976700	-2.77521800	-0.25813100
H	6.15003000	-2.00250000	-0.19020900
O	2.25441000	1.51581100	0.14335900
C	-2.42389900	0.28932500	-1.17905500
C	-1.06677800	0.56915400	-1.08982100
C	-1.06642000	0.34273100	1.18041000
C	-2.42352600	0.05069800	1.21303600
C	-3.16088200	0.01769100	0.00191100
H	-2.89393600	0.28504900	-2.15559000
H	-0.50083700	0.78091100	-1.99604400
H	-0.50022400	0.37138400	2.11045200
H	-2.89330400	-0.14622100	2.16965600
C	-5.21030000	-0.57301700	1.20907800
H	-6.26413000	-0.74564500	0.98322200
H	-4.81171200	-1.47826800	1.69037100
H	-5.15085400	0.25469100	1.92921300
C	-5.21058300	-0.32175800	-1.29779800
H	-5.15051300	0.63224900	-1.83955300
H	-4.81271800	-1.11395900	-1.94908000
H	-6.26455100	-0.53483400	-1.11039300
N	-0.37153500	0.60148800	0.05970800
H	1.34570800	1.11732100	0.10781200
N	-4.50341600	-0.25818800	-0.02548900

o-FP/MTBD(a')
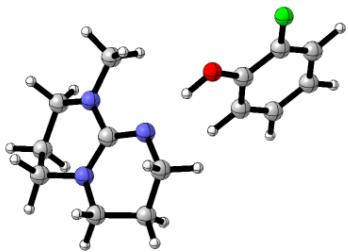
C	4.85737400	0.20750600	-0.53253500
C	3.93036600	0.14953500	0.49676400
C	2.55743600	-0.05982400	0.26943800
C	2.14747300	-0.21051800	-1.06771500
C	3.07255100	-0.15380700	-2.11583800
C	4.42916900	0.05474000	-1.85759700
H	2.72460000	-0.27508600	-3.13925100
O	1.72872200	-0.10334600	1.32724300
H	1.09167900	-0.37348600	-1.26920100
C	-1.89068000	0.02612600	0.34211500
N	-3.04556900	-0.54137000	-0.17900300
N	-1.88383000	1.40428200	0.44248100
C	-1.89530200	-2.70374700	-0.21086900
H	-2.03074800	-3.77990400	-0.04748700
H	-1.48619600	-2.56746400	-1.22077500
C	-0.93927800	-2.10807200	0.82199500
H	0.07004800	-2.51623300	0.68812000
H	-1.25574900	-2.40595800	1.83582400
C	-3.23754600	-1.98914600	-0.10448700
H	-3.73994500	-2.26544200	0.83945100
H	-3.90564900	-2.28189500	-0.92465400
C	-4.22926200	0.28740400	-0.36449900
H	-4.95842900	-0.29413900	-0.93944300
H	-4.70116300	0.54624200	0.60041700
C	-3.82200300	1.54585800	-1.12141800
H	-4.68483800	2.19813000	-1.29942100
H	-3.41984800	1.24854100	-2.09755100
C	-2.76732800	2.29829100	-0.31158900
H	-3.25589900	2.97247700	0.40878300
H	-2.16178000	2.93270700	-0.97786800
C	-0.76000800	2.07158900	1.08795700
H	-0.41338400	1.49198900	1.94432200
H	0.08850800	2.22134800	0.40452800
H	-1.10110800	3.05295000	1.43718100
N	-0.84773700	-0.64976800	0.74435000
H	0.76777700	-0.23478200	1.05209600
H	5.90286100	0.37126800	-0.28505700

H	5.14965000	0.09844100	-2.66976500
F	4.35689000	0.29993900	1.77740800

m-FP/MTBD(b')
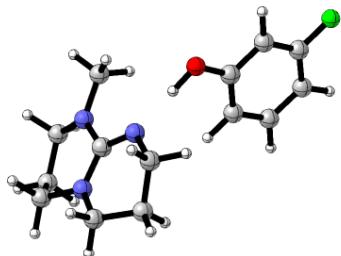
C	4.72306900	0.15459900	-0.16566900
C	3.79393900	0.02044300	0.85439300
C	2.43636100	-0.13014400	0.51750000
C	2.05999200	-0.13998000	-0.84069300
C	3.03181100	-0.00156500	-1.83477300
C	4.38519300	0.14906200	-1.51614900
H	2.72906800	-0.01211000	-2.87963500
O	1.55436700	-0.25842300	1.52815600
H	1.01216700	-0.25847100	-1.10199400
H	5.15329900	0.25725000	-2.27500000
C	-2.00790500	0.01115800	0.36027700
N	-3.13025500	-0.49867300	-0.27783000
N	-1.98606500	1.38045500	0.54665200
C	-2.01411000	-2.67745700	-0.36448800
H	-2.17814900	-3.75880500	-0.28116900
H	-1.52761300	-2.48623800	-1.33016300
C	-1.12963400	-2.16716300	0.77271800
H	-0.11985700	-2.58728600	0.68889300
H	-1.52741100	-2.52072600	1.73901200
C	-3.34946200	-1.94409000	-0.31263600
H	-3.92642100	-2.26986100	0.57096200
H	-3.95765100	-2.17040300	-1.19787300
C	-4.28320600	0.36462300	-0.49653500
H	-4.97770800	-0.16528400	-1.15779200
H	-4.82036600	0.57407800	0.44595900
C	-3.80064900	1.65799400	-1.14223700
H	-4.63709000	2.33801200	-1.34113700
H	-3.33299700	1.41223600	-2.10340500
C	-2.79572900	2.33735200	-0.21312300
H	-3.32449000	2.97734000	0.51008800
H	-2.13180000	2.99751000	-0.79319300
C	-0.90346700	1.98288500	1.31438300
H	-0.62768700	1.33942500	2.15074200

H	-0.00594300	2.16348800	0.70500600
H	-1.25623900	2.94426300	1.70542900
N	-1.00859400	-0.70913900	0.79454700
H	0.60543900	-0.34636300	1.20277200
H	4.10248300	0.02946800	1.89488000
F	6.03457800	0.29945000	0.17566300

p-FP/MTBD(c')
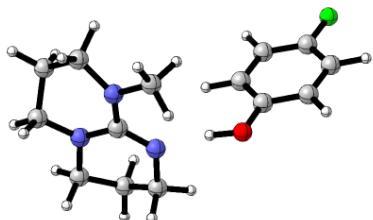
C	4.77362800	0.10898300	0.44348900
C	3.73189000	-0.14484700	1.33664900
C	2.40526700	-0.25109500	0.88205500
C	2.14227500	-0.09731500	-0.49160700
C	3.18433800	0.15783900	-1.39026000
C	4.48220200	0.25715300	-0.90849600
H	2.99213900	0.27689100	-2.45310900
O	1.44000000	-0.49873500	1.79681100
H	1.12055800	-0.18104400	-0.85234100
C	-1.99991000	-0.02316600	0.32819000
N	-3.05721100	-0.43590500	-0.47141900
N	-1.97584400	1.31960000	0.65583000
C	-1.97472700	-2.62491800	-0.66392600
H	-2.16466300	-3.70437400	-0.70772300
H	-1.38765800	-2.35242500	-1.55100300
C	-1.20448700	-2.25387200	0.60312200
H	-0.19825400	-2.69005200	0.57989800
H	-1.70572200	-2.69175300	1.48294800
C	-3.29580000	-1.86430700	-0.67410000
H	-3.96672900	-2.26014100	0.10886200
H	-3.81253200	-1.98556000	-1.63485000
C	-4.16664700	0.47544300	-0.71815900
H	-4.79541100	0.03390200	-1.49928300
H	-4.79749500	0.60271500	0.17998900
C	-3.59795400	1.81424500	-1.17291700
H	-4.39774900	2.53274800	-1.38670000
H	-3.03445600	1.65460900	-2.10024000
C	-2.68728800	2.36938500	-0.07890900
H	-3.28044200	2.94488100	0.64864600
H	-1.95667900	3.06886000	-0.51486200

C	-0.97119700	1.81237000	1.58962100
H	-0.79058600	1.07730000	2.37482700
H	-0.01347300	2.03610700	1.09735400
H	-1.35090500	2.73479100	2.04433400
N	-1.06315300	-0.80924300	0.78639900
H	0.52472300	-0.53050400	1.38563300
H	3.92921800	-0.26562100	2.39834400
F	5.50097400	0.50668100	-1.78508800
H	5.80124800	0.19185800	0.78639700

2,3-FP/MTBD(d')
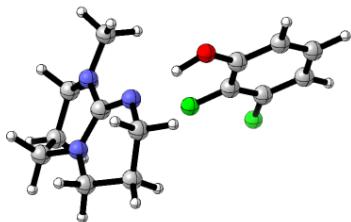
C	-3.25303900	0.95064000	0.89093200
C	-2.19049300	0.31534600	0.25332900
C	-2.40740100	-0.75663600	-0.63047900
C	-3.74424100	-1.14758900	-0.84468400
C	-4.79869700	-0.50164500	-0.20306900
C	-4.56845600	0.56050100	0.68018300
H	-5.81840900	-0.82887600	-0.38904300
O	-1.43256600	-1.40183400	-1.28199100
H	-3.92084300	-1.97288900	-1.52851100
C	1.92478700	-0.27638000	-0.43849300
N	2.91478400	-0.23767900	0.52397500
N	1.84209400	0.83249200	-1.25888900
C	1.92857000	-2.26481500	1.49946900
H	2.18102500	-3.20318300	2.00853700
H	1.17063000	-1.74801700	2.10239500
C	1.37575200	-2.52330400	0.09717900
H	0.43557200	-3.08465100	0.15097700
H	2.08129700	-3.15542500	-0.46914300
C	3.17498500	-1.39326900	1.38167600
H	4.01356700	-1.98582600	0.97678400
H	3.48736700	-1.02278100	2.36724200
C	3.87653500	0.85640900	0.52027100
H	4.44754500	0.80585600	1.45358100
H	4.59477900	0.75881500	-0.31238800
C	3.10921300	2.17155200	0.42194500
H	3.79064400	3.03040600	0.42693100
H	2.45537400	2.25730800	1.29796800

C	2.28266300	2.17464000	-0.86533300
H	2.87746700	2.58265100	-1.69652200
H	1.40426700	2.82894200	-0.74906900
C	0.94460000	0.81268800	-2.40535900
H	0.87853200	-0.19848800	-2.80871300
H	-0.06827900	1.15431500	-2.14752600
H	1.35130600	1.48334200	-3.17252100
N	1.11442500	-1.28395800	-0.63325600
H	-0.46745100	-1.19391400	-1.00435700
F	-0.92641900	0.75479100	0.49002600
F	-2.97244200	1.97678400	1.73073600
H	-5.37189900	1.07811600	1.19423600

2,4-FP/MTBD(e')
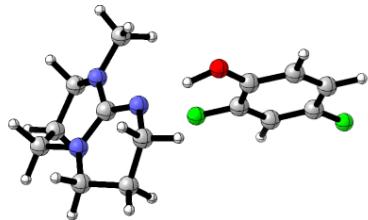
C	3.15854700	-0.86725700	1.02995400
C	2.10517200	-0.38100600	0.26373900
C	2.27629400	0.52895500	-0.79345300
C	3.59751000	0.92982200	-1.06259800
C	4.68072300	0.45800700	-0.31873800
C	4.44134700	-0.43292900	0.72046100
H	5.69540000	0.77695200	-0.53705600
O	1.28376100	1.00614600	-1.56309000
H	3.75163900	1.62927900	-1.87954900
C	-2.08382900	0.17039900	-0.39503000
N	-3.03950300	0.33271100	0.59184400
N	-2.07455800	-1.06023200	-1.02425200
C	-1.96108700	2.45891500	1.17502400
H	-2.16434500	3.48133500	1.51679500
H	-1.21536800	2.02027200	1.85085100
C	-1.42372000	2.44844700	-0.25664000
H	-0.45520700	2.95981500	-0.30798900
H	-2.10632900	3.01536600	-0.91289200
C	-3.24438100	1.63581400	1.22258100
H	-4.06149300	2.18056900	0.71814600
H	-3.56208100	1.46509200	2.25983500
C	-4.05479100	-0.69430700	0.78063100
H	-4.59420000	-0.46812500	1.70682800
H	-4.79260600	-0.69012400	-0.04093700

C	-3.35721300	-2.04768700	0.87456600
H	-4.08015800	-2.85724800	1.02936700
H	-2.68375000	-2.02977800	1.73975000
C	-2.56938100	-2.29714500	-0.41290600
H	-3.20771300	-2.79935800	-1.15561700
H	-1.72184500	-2.97201400	-0.21302500
C	-1.21344500	-1.26972500	-2.17994100
H	-1.12107100	-0.34332800	-2.74806600
H	-0.20673700	-1.60622800	-1.89360000
H	-1.67038200	-2.03966000	-2.81405100
N	-1.24159400	1.09382400	-0.77578600
H	0.33575000	0.88229400	-1.20797200
F	0.84630700	-0.82173800	0.55394100
H	2.97557400	-1.56790500	1.83821200
F	5.48635400	-0.89963100	1.46018600

2,6-FP/MTBD(f')
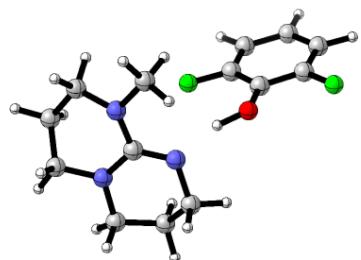
C	4.76621200	0.19990300	-0.41766600
C	3.81985700	-0.39865700	0.40172900
C	2.43380100	-0.16923800	0.28625000
C	2.07168200	0.73167800	-0.73064000
C	2.98488600	1.35004200	-1.57577800
C	4.34663900	1.08213800	-1.41916400
H	2.61688400	2.03158600	-2.33727700
O	1.59691800	-0.77895200	1.12882000
C	-1.93692900	-0.22633700	0.44028700
N	-3.00901800	-0.46684300	-0.39931100
N	-1.94572900	0.99191200	1.09203300
C	-1.83701700	-2.47349000	-1.19096700
H	-1.99427900	-3.50562300	-1.52761100
H	-1.23966800	-1.95779800	-1.95415200
C	-1.10130500	-2.43256600	0.14885000
H	-0.09381400	-2.85297300	0.04919500
H	-1.62883800	-3.06699700	0.88155300
C	-3.18293800	-1.77373300	-1.03203000
H	-3.86593100	-2.40020100	-0.43227300
H	-3.66103500	-1.61756400	-2.00826000

C	-4.13028800	0.46267800	-0.41232100
H	-4.77742500	0.19762300	-1.25543900
H	-4.73535200	0.37961000	0.50757300
C	-3.58027900	1.87652500	-0.57246300
H	-4.38872600	2.61655000	-0.60028000
H	-3.04208200	1.93185900	-1.52626300
C	-2.63833300	2.18348600	0.59312600
H	-3.20439400	2.61201600	1.43410100
H	-1.89590000	2.93916400	0.29084700
C	-0.94801200	1.26752700	2.11676400
H	-0.68718800	0.34719800	2.64059400
H	-0.03033400	1.70394800	1.69723100
H	-1.37704100	1.98112000	2.83113800
N	-0.96778800	-1.07261900	0.66961600
H	0.59721100	-0.73420500	0.89667500
F	4.23326600	-1.25264100	1.36863600
H	5.81552400	-0.03354400	-0.26273900
F	0.74360800	1.01443800	-0.88393000
H	5.07507800	1.55677700	-2.06976300

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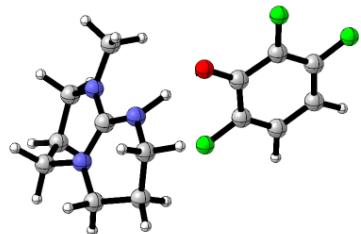
C	-4.36276800	0.01795900	0.40840800
C	-3.39354000	0.32387900	-0.53915200
C	-2.01219300	0.04365400	-0.34100500
C	-1.74214800	-0.56814500	0.91336900
C	-2.69613000	-0.88033700	1.86682300
C	-4.04295200	-0.58541700	1.62095000
H	-2.38492700	-1.35026300	2.79569200
O	-1.11995600	0.34141300	-1.23550000
C	2.22173500	0.20921800	-0.49565000
N	3.26992100	-0.49599100	0.01583100
N	2.13742800	1.54053200	-0.22634700
C	2.04614500	-2.57643900	-0.54289600
H	2.21118400	-3.61626300	-0.84764600
H	1.34657000	-2.57238400	0.30083100
C	1.45406200	-1.75199900	-1.68403400
H	0.45582200	-2.10484900	-1.95828500

H	2.08716900	-1.82407900	-2.58169300
C	3.37662100	-1.95586900	-0.12756900
H	4.15649200	-2.18689600	-0.87002700
H	3.70969500	-2.36488000	0.83498900
C	4.33436100	0.21334600	0.72347500
H	4.92925300	-0.52969900	1.26282600
H	5.00473400	0.72093000	0.01156900
C	3.70051500	1.21649900	1.68337100
H	4.46582800	1.76871400	2.24024100
H	3.08400800	0.67180900	2.40859400
C	2.84723800	2.19395800	0.88002400
H	3.47813400	2.98778300	0.45252700
H	2.10872100	2.68322800	1.53018600
C	1.19944600	2.40029600	-0.95346800
H	1.03203000	2.00830100	-1.95759700
H	0.22745500	2.46518900	-0.45262300
H	1.64575300	3.39879200	-1.02520100
N	1.31116000	-0.35420600	-1.28166600
H	0.24919700	-0.00562500	-1.21536900
F	-3.76922000	0.91178800	-1.69760300
F	-5.65806900	0.32175900	0.13178300
F	-0.42106100	-0.86743000	1.18651100
H	-4.82424700	-0.81213000	2.33816600

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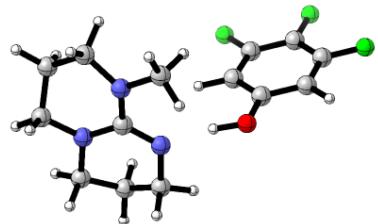
C	4.24024600	-0.10496600	0.53805900
C	3.22795900	-0.56231800	1.36722100
C	1.89641700	-0.53723000	0.91211200
C	1.61662100	-0.04690800	-0.37856200
C	2.66184900	0.40205500	-1.17615100
C	3.98443700	0.38502100	-0.74322900
O	0.94104600	-0.98706700	1.74232900
C	-2.41901900	-0.12318600	0.39944600
N	-3.44629500	-0.30948100	-0.51097100
N	-2.37600400	1.10500800	1.02866400
C	-2.38259300	-2.41566000	-1.18260100
H	-2.58925700	-3.44591800	-1.49685700

H	-1.73273100	-1.95893200	-1.94068500
C	-1.69163900	-2.38370500	0.17994200
H	-0.70013000	-2.84845700	0.11794800
H	-2.26729500	-2.98702900	0.90215600
C	-3.68689900	-1.63273800	-1.08700800
H	-4.41931900	-2.18985400	-0.47706000
H	-4.13337100	-1.49095700	-2.07960300
C	-4.51997700	0.67204500	-0.60026300
H	-5.10678200	0.44489000	-1.49698000
H	-5.20285300	0.60652500	0.26542800
C	-3.90020900	2.06107700	-0.69533700
H	-4.67239300	2.83462000	-0.77755200
H	-3.28253000	2.10652100	-1.60052900
C	-3.05161400	2.31396100	0.54837500
H	-3.68460000	2.69440600	1.36529900
H	-2.29980900	3.09116200	0.34169300
C	-1.42213200	1.33283500	2.10676700
H	-1.28785400	0.42256400	2.69248400
H	-0.43887800	1.65684600	1.73600600
H	-1.82221900	2.11940500	2.75718600
N	-1.51841700	-1.02517800	0.69638800
H	0.01178500	-0.91628700	1.34073600
F	5.51963700	-0.12649000	0.96889800
F	2.39672600	0.87354600	-2.41558500
F	4.98368700	0.82616900	-1.53304100
H	0.60137800	-0.01885900	-0.75984900
H	3.46236900	-0.93726700	2.35790100

2,3,5,6-FP/MTBD(I')
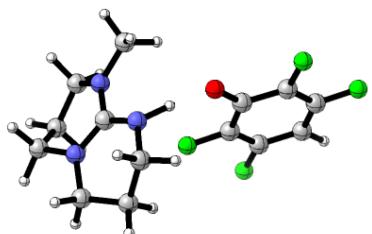
C	4.20530900	0.12469200	0.01504900
C	3.25717800	-0.83400100	0.33809400
C	1.85741000	-0.60445000	0.18688000
C	1.53999900	0.68873100	-0.31720900
C	2.50107100	1.63666700	-0.63623200
C	3.85878600	1.38244200	-0.47971600
O	0.97749900	-1.49911400	0.49635500
C	-2.32993600	-0.55728800	0.28864900

N	-3.32294500	-0.07184700	-0.50314700
N	-2.21845900	-0.08905700	1.55886400
C	-2.12989200	-1.03773200	-2.45160500
H	-2.31414800	-1.46873800	-3.44221600
H	-1.33819400	-0.28549100	-2.54847200
C	-1.68515500	-2.10628600	-1.45430700
H	-0.72541400	-2.54766600	-1.73666600
H	-2.42351600	-2.92076800	-1.40569600
C	-3.41187500	-0.38828400	-1.93814800
H	-4.27220300	-1.05524500	-2.10098800
H	-3.61339900	0.54572100	-2.47814500
C	-4.29398500	0.86143200	0.06856600
H	-4.84446400	1.31922300	-0.75822400
H	-5.02219400	0.32350000	0.69527700
C	-3.54160800	1.90988100	0.88480200
H	-4.23149400	2.63841400	1.32513700
H	-2.85762100	2.45212400	0.22118900
C	-2.76506400	1.20403900	1.99377200
H	-3.41816300	1.01528700	2.85833900
H	-1.93573400	1.83461400	2.34256200
C	-1.34606700	-0.75088700	2.53216700
H	-1.29545600	-1.82050300	2.32278700
H	-0.32628500	-0.35134800	2.50823300
H	-1.77783300	-0.59878100	3.52772800
N	-1.50310900	-1.51395400	-0.13013000
H	-0.45691000	-1.46605200	0.20003700
F	3.66331100	-2.03271100	0.81345800
F	5.51741600	-0.17157600	0.18606700
F	0.21635200	1.00568500	-0.49194500
H	4.61066300	2.12152000	-0.72916100
F	2.09591300	2.84386500	-1.11160600

2,3,4,5,6-FP/MTBD(j')
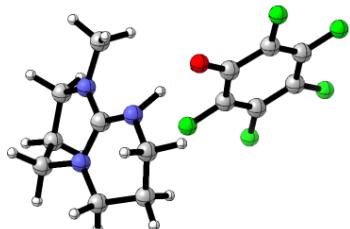
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C	-2.96077500	1.20391100	0.21888500
C	-1.58695000	0.84068900	0.11073600
C	-1.38360600	-0.54607400	-0.12593100

C	-2.41385100	-1.47201400	-0.24765500
C	-3.73898500	-1.06274800	-0.13507400
O	-0.63323900	1.70678100	0.23207600
C	2.60890400	0.53409600	0.14047600
N	3.54223500	-0.17767900	-0.54598700
N	2.52423600	0.37766100	1.48692100
C	2.33235500	0.39579200	-2.63381200
H	2.50213300	0.58373400	-3.70002000
H	1.50453900	-0.31709000	-2.54082400
C	1.97175800	1.68254100	-1.89373200
H	1.02248100	2.09745400	-2.24359800
H	2.74596700	2.44849600	-2.05104100
C	3.60015000	-0.18788700	-2.01685000
H	4.48320400	0.38361400	-2.34130100
H	3.74376300	-1.22638200	-2.34126400
C	4.49423000	-1.00490100	0.19583100
H	4.98040200	-1.67599400	-0.51798300
H	5.27800600	-0.37856200	0.64974200
C	3.73394200	-1.78682600	1.26422900
H	4.41003800	-2.42780300	1.84088300
H	2.99534400	-2.43192600	0.77366400
C	3.04440200	-0.79735700	2.19983500
H	3.74909600	-0.43885900	2.96450300
H	2.21171700	-1.28339700	2.72642700
C	1.72917300	1.29786800	2.30458500
H	1.72769800	2.29215300	1.85510000
H	0.68903500	0.96813400	2.40112300
H	2.19276000	1.35174200	3.29587400
N	1.81374000	1.41497200	-0.46508900
H	0.78442700	1.51312500	-0.10029200
F	-3.26902900	2.49817000	0.44675500
F	-5.27743100	0.70162000	0.21220200
F	-0.09745500	-1.00178800	-0.24002100
F	-2.12909100	-2.77288900	-0.47321200
F	-4.74967900	-1.95093100	-0.25134200

o-FP/DMAP(a)_Int1
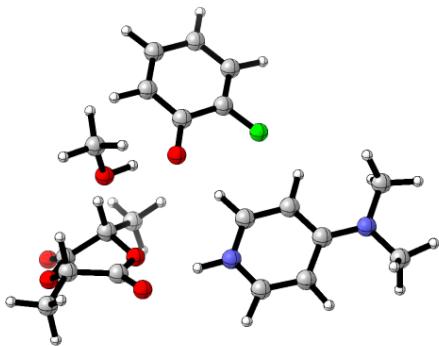
O	-1.85718900	1.20273800	0.90097300
C	-2.14704100	2.10011400	-0.03606600
O	-1.28133000	2.86223900	-0.43643900
H	-3.04575600	-1.44946400	2.58178200
C	-2.33694000	-0.64748000	2.35885700
H	-2.24183700	-0.01330300	3.24617600
H	-1.36870600	-1.08600500	2.10357800
C	-2.84191900	0.14874000	1.17487100
H	-2.88688000	-0.47954200	0.27520300
C	-3.58277700	2.10185100	-0.53574700
H	-3.63745600	1.27348900	-1.25632900
O	-4.49006400	1.83194100	0.56739200
C	-4.21043000	0.79131700	1.39212400
O	-5.00796000	0.43538600	2.21925900
C	-4.00783500	3.41231200	-1.17071100
H	-3.94201300	4.23537700	-0.45204200
H	-3.35844600	3.63599500	-2.02141800
H	-5.04106000	3.32836100	-1.52006300
C	3.60398800	2.83280300	0.03914500
C	2.25282600	3.05316900	-0.07723100
C	1.79487600	0.73568200	-0.12584700
C	3.13856000	0.45132000	-0.00914100
C	4.10132000	1.49364100	0.08161400
H	4.26369900	3.68886100	0.09967600
H	1.82542600	4.05012400	-0.11023000
H	1.03283900	-0.06010900	-0.20869700
H	3.41415800	-0.59438800	0.01985300
C	5.90003500	-0.15477800	0.24688500
H	6.98439900	-0.15493900	0.36429500
H	5.46120300	-0.69913600	1.09219500
H	5.65260100	-0.69048800	-0.67842600
C	6.39543700	2.32206000	0.28715700
H	6.21281800	2.95570900	1.16552600
H	7.39777800	1.90169000	0.37696700
H	6.37056000	2.95205500	-0.61224900

N	1.37775200	2.02611100	-0.15705400
H	0.36813600	2.24682700	-0.23354300
C	1.23194300	-4.61400200	0.45430700
C	1.05994900	-3.25970100	0.22691500
C	-0.09908900	-2.67631600	-0.35290000
C	-1.10788300	-3.62115100	-0.69576400
C	-0.95646200	-4.99188900	-0.47696700
C	0.21057800	-5.50657400	0.09932900
H	2.15921000	-4.95915700	0.90644600
H	-1.76279700	-5.66660200	-0.75968000
O	-0.21511200	-1.38767300	-0.54063500
C	-2.01773200	-0.64630600	-3.31921300
H	-2.82670000	-0.13664400	-3.85800200
H	-2.14178300	-1.73099100	-3.46536900
H	-1.06086200	-0.34772300	-3.77739600
O	-2.08845000	-0.28177200	-1.95325800
H	-1.35968800	-0.76549200	-1.44667500
H	-2.02270600	-3.23654200	-1.14344800
N	5.42756900	1.23087700	0.20366000
H	0.32940900	-6.57276700	0.27160200
F	2.09106900	-2.40842900	0.58733100

m-FP/DMAP(b)_Int1

O	-2.61317500	1.18366300	0.72651900
C	-2.79975000	1.36675200	-0.57885300
O	-2.03670100	2.07944800	-1.21210100
H	-3.76600500	-0.44606800	3.42925600
C	-3.17804300	0.30443100	2.89398300
H	-3.46796900	1.29415200	3.26113800
H	-2.11634600	0.13610000	3.09766100
C	-3.43955300	0.17288500	1.40832500
H	-3.11885500	-0.80858800	1.02338700
C	-3.97989500	0.63191500	-1.19044800
H	-3.65550800	-0.41816400	-1.28739900
O	-5.11182400	0.68798100	-0.27645500
C	-4.90252500	0.37515000	1.02407800

O	-5.82631800	0.26902800	1.78844200
C	-4.43370300	1.19727800	-2.52210900
H	-4.74710400	2.24123200	-2.42135200
H	-3.61278500	1.14443600	-3.24242200
H	-5.27526200	0.60763500	-2.89705500
C	2.61962600	3.50884300	0.02834500
C	1.28060900	3.47714600	-0.27830100
C	1.30555400	1.12603500	-0.49168600
C	2.64801100	1.09041900	-0.18607200
C	3.36430500	2.28929600	0.08835300
H	3.08175800	4.46840300	0.22197800
H	0.67577400	4.37662300	-0.33068200
H	0.72737700	0.20982500	-0.69855000
H	3.12209800	0.11736600	-0.16413500
C	5.41091700	0.99956100	0.44716300
H	6.45122100	1.19813000	0.70702900
H	4.98626900	0.33122300	1.20612700
H	5.38905000	0.48474400	-0.52102000
C	5.39712700	3.51800500	0.67120200
H	4.97450100	4.03627700	1.54246300
H	6.44089400	3.28848000	0.88800600
H	5.37056400	4.19820100	-0.19063200
N	0.64608800	2.31059200	-0.53165900
H	-0.36797800	2.30408900	-0.74644900
C	3.32802800	-3.10461900	-0.42357000
C	2.29040000	-2.36842800	-0.97448700
C	1.03319900	-2.28712000	-0.29956500
C	0.92355200	-3.01697800	0.92406500
C	1.99202400	-3.75200400	1.43148200
C	3.23112500	-3.80894600	0.77202800
H	1.86811700	-4.29507400	2.36715300
O	0.06289400	-1.55394100	-0.77678800
C	-2.71391000	-3.44150200	-0.91451300
H	-3.79234800	-3.62575800	-0.83340300
H	-2.19243200	-4.15334800	-0.25636800
H	-2.40487500	-3.64420700	-1.95164300
O	-2.45972100	-2.09588400	-0.54375700
H	-1.46491400	-1.92251400	-0.61471800
H	-0.02291800	-2.98027300	1.45950400
N	4.68477100	2.27298200	0.39172900
H	4.07288200	-4.37770500	1.15347200
F	4.52518100	-3.13431700	-1.10131000
H	2.41834500	-1.87245700	-1.93345100

p-FP/DMAP(c)_Int1
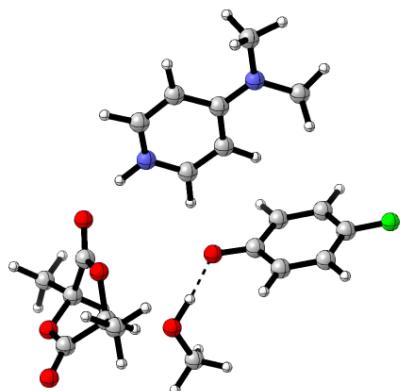
O	-2.73742900	1.16513800	0.73443100
C	-2.89859400	1.24731800	-0.58523600
O	-2.18294800	1.98548800	-1.24373900
H	-3.84031800	-0.37262100	3.51093100
C	-3.29987500	0.38815000	2.94121000
H	-3.68459200	1.37156900	3.22983800
H	-2.23539800	0.32697800	3.18694000
C	-3.49815500	0.13448400	1.46150000
H	-3.08377300	-0.83977500	1.15478100
C	-3.98861100	0.37008800	-1.17600200
H	-3.57565200	-0.65336200	-1.18795000
O	-5.15150000	0.38961300	-0.29948500
C	-4.95947200	0.18279200	1.02426100
O	-5.89541300	0.04747500	1.76923600
C	-4.44345400	0.80011400	-2.55680400
H	-4.84705700	1.81748900	-2.54063300
H	-3.59694100	0.76814300	-3.24813600
H	-5.21878100	0.11481200	-2.91135200
C	2.51175500	1.18818000	-0.28802600
C	1.16743400	1.20712100	-0.58728200
C	1.09069200	3.54683600	-0.27964500
C	2.42939700	3.59495800	0.02605300
C	3.20064900	2.39037100	0.03744200
H	3.00852800	0.22648800	-0.30826600
H	0.60713300	0.28561800	-0.81995600
H	0.46645300	4.43436300	-0.29452000
H	2.87085600	4.55563000	0.25845000
C	5.20476900	3.64023800	0.67362800
H	6.25374100	3.42596700	0.88078100
H	5.16190100	4.35370800	-0.16017600
H	4.77158900	4.11359500	1.56509400
C	5.27388400	1.13305800	0.35627000
H	5.27478200	0.65984200	-0.63326000

H	6.30622700	1.34257700	0.63837300
H	4.85464300	0.42376100	1.07993900
N	0.48176000	2.37725700	-0.57764700
H	-0.53259300	2.34927200	-0.78685500
C	3.45570600	-2.88080100	-1.07807500
C	2.24490200	-2.29625300	-1.46248200
C	1.16401900	-2.12186500	-0.54795700
C	1.37974400	-2.60254200	0.77754800
C	2.58693700	-3.19075300	1.16550300
C	3.61281400	-3.31286700	0.23453300
H	4.26811900	-3.01385300	-1.78945500
H	2.73615200	-3.55203800	2.18058900
O	0.05911000	-1.51120900	-0.90753700
C	-2.52700600	-3.60473400	-0.48006400
H	-3.57419300	-3.85182300	-0.26552200
H	-1.88847000	-4.20457600	0.18687500
H	-2.30794300	-3.89784100	-1.51853100
O	-2.34301400	-2.21330900	-0.27684200
H	-1.38095000	-1.97711800	-0.49345700
H	0.57313300	-2.49584300	1.50047600
H	2.09967900	-1.96606600	-2.48931900
F	4.80683500	-3.87955600	0.61779700
N	4.52060400	2.39162500	0.34441700

2,3-FP/DMAP(d)_Int1
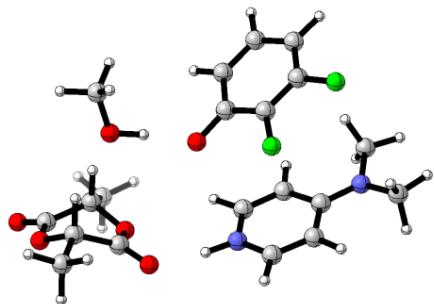
O	-2.94335700	0.93073100	0.81548100
C	-3.06478800	1.22624200	-0.48094800
O	-2.31537500	2.03631200	-0.99647500
H	-4.17867000	-0.97949800	3.28794700
C	-3.59431100	-0.16142800	2.85830300
H	-3.95652800	0.78024500	3.28294700
H	-2.54199700	-0.30025400	3.12409300
C	-3.74872300	-0.17764500	1.35147900
H	-3.34034000	-1.10193800	0.91315900
C	-4.16027200	0.48441500	-1.22883500
H	-3.76255000	-0.52873400	-1.39978100

O	-5.34605000	0.38811300	-0.39056600
C	-5.19552200	-0.02856500	0.88838700
O	-6.15480300	-0.26128500	1.57718900
C	-4.56880600	1.14456100	-2.53120100
H	-4.95146200	2.15504000	-2.35661400
H	-3.70472300	1.20638000	-3.19828000
H	-5.34878200	0.54645300	-3.01127200
C	2.01016200	1.26782400	1.27520300
C	0.69384200	1.40441500	0.90096100
C	1.28021200	2.86663300	-0.84510000
C	2.61463300	2.75682300	-0.54457100
C	3.03606300	1.91745200	0.53239000
H	2.24027300	0.59877400	2.09291900
H	-0.11342800	0.87715900	1.39059400
H	0.91802000	3.46806600	-1.67188300
H	3.32709900	3.28511000	-1.16395600
C	5.37873200	2.30244300	-0.04836500
H	6.35890600	2.05716500	0.36204400
H	5.31716900	1.88970900	-1.06415400
H	5.29852200	3.39543100	-0.09790300
C	4.74525700	0.79166400	1.86796500
H	4.43613000	-0.23306500	1.62353300
H	5.83141500	0.81260400	1.96513400
H	4.31398000	1.07694500	2.83520200
N	0.34300300	2.20766300	-0.12920900
H	-0.64648900	2.22826200	-0.42306700
C	3.61679000	-1.93787900	-0.66134700
C	2.40286300	-1.29573300	-0.86083200
C	1.21722700	-1.65698800	-0.14889500
C	1.39120900	-2.73619500	0.77360000
C	2.61579100	-3.37711000	0.95355800
C	3.76078500	-2.98789400	0.24220600
H	2.68874200	-4.19957600	1.66248200
O	0.10577100	-1.01887900	-0.32239300
C	-2.18111500	-3.35151400	-1.26294700
H	-3.20004400	-3.72631200	-1.41834400
H	-1.64462700	-4.06914000	-0.62335900
H	-1.67303700	-3.31370000	-2.23879400
O	-2.26557000	-2.06824500	-0.66348900
H	-1.33505300	-1.71559600	-0.52542300
H	0.51657200	-3.05090600	1.33941500
N	4.34701500	1.73676200	0.82120400
H	4.72243800	-3.47686900	0.36030300
F	4.70261000	-1.50646700	-1.37113400

| F | 2.34774900 | -0.27751300 | -1.76608100 |

2,4-FP/DMAP(e)_Int1
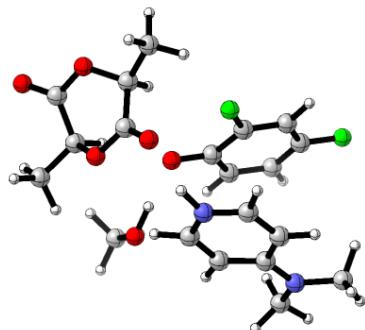
O	-2.97125600	0.78244300	-1.00367100
C	-2.70701900	-0.46555200	-1.38892200
O	-2.10495000	-0.66954400	-2.42939800
H	-4.25746300	2.62615600	1.48929400
C	-3.85714800	2.44560200	0.48785800
H	-4.62430200	2.72172800	-0.24265200
H	-2.96404800	3.05962000	0.34137000
C	-3.48634800	0.98294200	0.35707300
H	-2.66319100	0.71436300	1.03584800
C	-3.18981400	-1.56393100	-0.45478600
H	-2.45355200	-1.59646900	0.36145000
O	-4.49004600	-1.21283800	0.09380800
C	-4.65358000	0.03074000	0.60389000
O	-5.65541500	0.32268000	1.20375400
C	-3.32084800	-2.92089300	-1.11844700
H	-4.03271800	-2.88321700	-1.94900200
H	-2.34594300	-3.23635400	-1.49756900
H	-3.67059600	-3.65028700	-0.38204500
C	1.88052200	1.74719300	-1.01528300
C	0.62403700	1.44308600	-1.47893100
C	1.47547000	-0.28680000	-2.83023300
C	2.75818800	-0.03686200	-2.41051600
C	3.00692200	0.99363400	-1.45101900
H	1.94884800	2.52297900	-0.26460200
H	-0.25633000	1.96439200	-1.12417900
H	1.23374400	-1.08728700	-3.52091200
H	3.55409200	-0.66452800	-2.78917100
C	5.37125300	0.37386500	-1.35618800
H	6.28546700	0.76409300	-0.90730200
H	5.23024900	-0.65938300	-1.01041700
H	5.50683100	0.37151400	-2.44446100
C	4.44274800	2.20163000	0.11117300

H	3.89376300	1.90502900	1.01423900
H	5.50545400	2.25631600	0.35056200
H	4.11106500	3.20045700	-0.19613600
N	0.43466000	0.44854300	-2.37819900
H	-0.52997700	0.15994200	-2.60146400
C	1.92195300	-2.59497100	1.01306000
C	0.80892700	-1.81802000	0.72696400
C	0.49711400	-0.57511600	1.34942200
C	1.44894900	-0.17843200	2.33392500
C	2.58390100	-0.93443100	2.65077200
C	2.80857100	-2.12913500	1.98078700
H	3.28044300	-0.60664500	3.41848100
O	-0.55053900	0.12683200	1.02019800
C	-0.55272100	3.34881800	2.39844200
H	-0.46578400	4.43659100	2.29060700
H	0.17221900	3.02404400	3.16345400
H	-1.56379900	3.12404800	2.77507100
O	-0.30374900	2.75893900	1.13731700
H	-0.39949200	1.76413400	1.20411400
H	1.26076600	0.75177800	2.86527700
N	4.25056000	1.23029700	-0.96871400
F	-0.05377900	-2.28323600	-0.23773600
F	3.92049100	-2.87745800	2.27323400
H	2.08847100	-3.53695700	0.49873800

2,6-FP/DMAP(f)_Int1
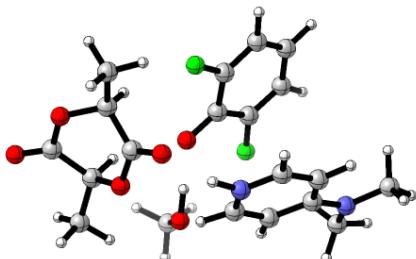
O	2.67751000	0.68946900	1.22097200
C	2.64602500	-0.63915100	1.31417500
O	2.02096200	-1.17481300	2.21415300
H	3.74016700	3.23965000	-0.68641400
C	3.31264100	2.77608800	0.20698700
H	3.96264800	3.00712000	1.05722800
H	2.30886500	3.17635200	0.37224900
C	3.22218000	1.27948000	-0.01001200
H	2.50235000	1.03576100	-0.80591800
C	3.41516400	-1.40026500	0.24634000
H	2.76216500	-1.41634900	-0.63735300

O	4.64156800	-0.69568100	-0.08452100
C	4.56762100	0.63302200	-0.33491200
O	5.51525900	1.22681600	-0.77944200
C	3.78934400	-2.81273200	0.65337100
H	4.42339900	-2.80740200	1.54557900
H	2.88182600	-3.38356300	0.86377700
H	4.33117900	-3.29268000	-0.16667100
C	-2.10578100	1.23322000	1.28181300
C	-0.84021500	0.87605700	1.67663100
C	-1.62582400	-1.15438600	2.57233300
C	-2.91556200	-0.86324900	2.20342100
C	-3.20107700	0.35426800	1.50916100
H	-2.20135000	2.16014100	0.73253500
H	0.02046600	1.49901900	1.46940400
H	-1.35636800	-2.08299700	3.06391500
H	-3.68713600	-1.59242100	2.41316600
C	-5.54534500	-0.29690300	1.26483100
H	-6.46932700	0.15288800	0.89933200
H	-5.37295900	-1.23062000	0.71183600
H	-5.68473600	-0.53344400	2.32706000
C	-4.67457300	1.85153700	0.26321400
H	-4.06296800	1.83448800	-0.64710400
H	-5.72654700	1.88986300	-0.02244600
H	-4.44135300	2.76042800	0.83185200
N	-0.61336700	-0.29372000	2.31976700
H	0.36395900	-0.57654100	2.49454000
C	-1.30039100	-2.96083600	-1.93353800
C	-0.39236600	-2.04121800	-1.43346400
C	-0.53537600	-0.62264200	-1.47959300
C	-1.76220200	-0.24698200	-2.10421400
C	-2.70172400	-1.12537600	-2.62389700
C	-2.47787400	-2.50524600	-2.54027600
H	-3.59195600	-0.72043000	-3.09951500
O	0.33319600	0.20595700	-0.99742200
C	-0.02794100	3.68529300	-1.67959700
H	-0.12448000	4.71684200	-1.31989300
H	-0.87351300	3.46611800	-2.34836800
H	0.90123800	3.61621300	-2.26868200
O	-0.01042700	2.82790300	-0.55171600
H	0.05004100	1.88302000	-0.85665800
N	-4.44929900	0.65130300	1.07542000
F	0.75148800	-2.52620000	-0.84239300
H	-1.07472200	-4.02095400	-1.84943200
F	-2.02385000	1.10039800	-2.20001400

H	-3.19587400	-3.20843800	-2.95150100

2,3,6-FP/DMAP(g)_Int1
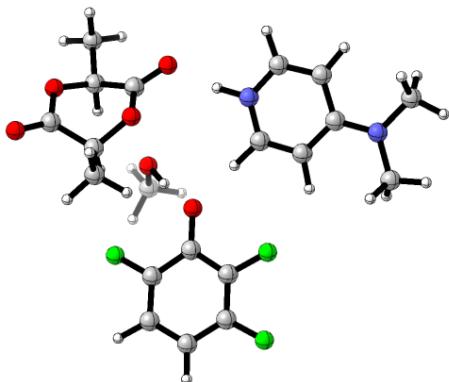
O	-2.02658600	1.31280300	0.92898000
C	-2.30576100	2.23839300	0.01798900
O	-1.45392400	3.05157000	-0.30593000
H	-3.19342900	-1.43485300	2.46418400
C	-2.51655700	-0.58976200	2.31479900
H	-2.51358900	0.01971100	3.22419700
H	-1.51121900	-0.97036400	2.11661400
C	-2.98484700	0.21509900	1.12141000
H	-2.95360100	-0.39361800	0.20756000
C	-3.71169000	2.20607100	-0.55888500
H	-3.69300600	1.40706400	-1.31333500
O	-4.66494400	1.85632900	0.48031000
C	-4.38755400	0.79691100	1.28167500
O	-5.21364100	0.38025700	2.05027700
C	-4.15495100	3.52383400	-1.16562500
H	-4.15994200	4.31942500	-0.41377300
H	-3.47159800	3.80542000	-1.97129200
H	-5.16437900	3.41452100	-1.57275700
C	3.40887400	3.35762200	0.21148300
C	2.04406300	3.48713800	0.11803900
C	1.75959800	1.15881400	-0.14764500
C	3.12041800	0.96313500	-0.05974800
C	4.00512400	2.06161600	0.12565200
H	4.00394100	4.25100300	0.35101500
H	1.54451200	4.44859300	0.17873100
H	1.05923200	0.32120100	-0.29235900
H	3.47480500	-0.05601400	-0.13456900
C	5.92131600	0.54209000	0.12603400
H	7.00481500	0.61284200	0.22810900
H	5.54131100	-0.10842800	0.92342800
H	5.69527000	0.07592300	-0.84114500

C	6.23314000	3.03427900	0.40390100
H	6.01268000	3.56399800	1.34040800
H	7.26440700	2.68259200	0.44969700
H	6.15288800	3.74468800	-0.42983200
N	1.24576000	2.41048000	-0.05619700
H	0.22082000	2.56044700	-0.11641300
C	1.60813700	-4.29144400	0.17997700
C	1.39333600	-2.94980300	-0.10865300
C	0.10153000	-2.38979800	-0.31114800
C	-0.94031100	-3.35355000	-0.17988900
C	-0.74523500	-4.69342600	0.10432400
C	0.55363900	-5.18921500	0.29174500
H	-1.60916100	-5.34768900	0.18127200
O	-0.09330600	-1.13731800	-0.57564200
C	-2.21650600	-0.69950400	-3.23476400
H	-2.99513300	-0.16817800	-3.79605700
H	-2.54209600	-1.74135100	-3.09373900
H	-1.29828400	-0.70093000	-3.84301900
O	-2.02853100	-0.03312200	-1.99739200
H	-1.32033500	-0.51493400	-1.48588900
N	5.34728800	1.88729300	0.21663000
F	2.47741800	-2.12051900	-0.20692100
F	-2.22297000	-2.89860000	-0.35063500
H	0.74664200	-6.23234400	0.51694100
F	2.88844000	-4.72069200	0.35423700

3,4,5-FP/DMAP(h)_Int1
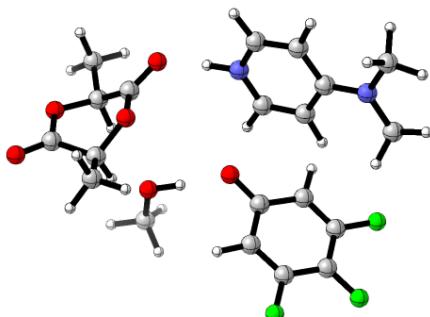
O	-3.03760300	0.93860200	0.80318400
C	-3.27797800	1.19950500	-0.47976600
O	-2.64566800	2.07082000	-1.05617300
H	-3.87258300	-1.06735500	3.36675200
C	-3.41850700	-0.19284700	2.89299600
H	-3.85110300	0.70581200	3.34416500
H	-2.33992500	-0.20963700	3.07575800
C	-3.68546100	-0.24052600	1.40317700

H	-3.22318100	-1.12402500	0.93454600
C	-4.34590600	0.34704400	-1.14334500
H	-3.86682700	-0.62744000	-1.33650600
O	-5.45226700	0.14871700	-0.21895100
C	-5.16980700	-0.23721900	1.04794600
O	-6.04952800	-0.55101400	1.80672200
C	-4.90983300	0.94825300	-2.41603500
H	-5.37654300	1.91881300	-2.22033300
H	-4.10674600	1.08468300	-3.14538100
H	-5.65981800	0.27067700	-2.83416400
C	1.74524100	4.12683200	0.26100100
C	0.41961600	3.90353000	-0.02261200
C	0.82900100	1.63335000	-0.52116400
C	2.16943400	1.79096700	-0.24814300
C	2.68574200	3.05414200	0.15854000
H	2.04740600	5.12157400	0.56246000
H	-0.32850700	4.68653500	0.04654200
H	0.40338800	0.66369400	-0.82281300
H	2.80092400	0.91811500	-0.35335600
C	4.93132800	2.10030600	0.32845400
H	5.93312400	2.44391800	0.58781500
H	4.65630200	1.28965300	1.01432200
H	4.95799900	1.70088700	-0.69262100
C	4.50217900	4.53483900	0.85815500
H	4.03183800	4.86208700	1.79506500
H	5.57723400	4.46398600	1.02609400
H	4.32775700	5.29931300	0.08946700
N	-0.02078200	2.68360600	-0.40440400
H	-1.02747700	2.52837100	-0.59870000
C	3.53312300	-2.21785600	-0.97769100
C	2.35432100	-1.64035500	-1.42411600
C	1.14419000	-1.77976500	-0.67534300
C	1.22078600	-2.55484300	0.52252200
C	2.42072500	-3.11807200	0.92461000
C	3.60244800	-2.96234800	0.19837000
O	0.04545500	-1.19555000	-1.06033200
C	-2.42824700	-3.47795200	-1.21100600
H	-3.46124700	-3.83038300	-1.10341000
H	-1.77453800	-4.14662700	-0.63046500
H	-2.14421500	-3.55459900	-2.27169600
O	-2.36237300	-2.13851600	-0.74483100
H	-1.41610300	-1.80768500	-0.84848200
N	4.00000500	3.22856900	0.43530300
F	4.67570000	-2.05713300	-1.69985000

H	0.33460700	-2.69950100	1.13356900
H	2.34476200	-1.09876400	-2.36588400
F	2.47363800	-3.83989400	2.07289200
F	4.76848700	-3.51005100	0.61970400

2,3,5,6-FP/DMAP(i)_Int1
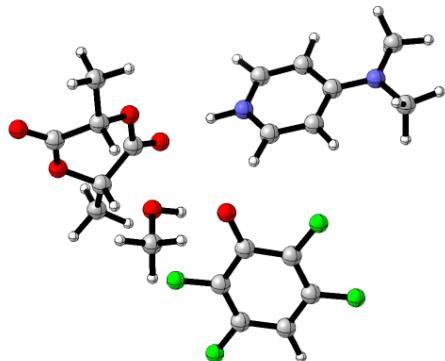
O	-2.50423800	2.28952200	0.01344400
C	-2.35522200	1.40859300	-0.97580300
O	-1.39320700	1.49006300	-1.72203600
H	-4.47277900	3.17410000	2.58742000
C	-3.68268000	3.31100300	1.84420400
H	-3.92517700	4.19349000	1.24348500
H	-2.73185700	3.47280100	2.36110500
C	-3.59048100	2.06920200	0.98160300
H	-3.30676900	1.18465300	1.57326800
C	-3.43261100	0.34231300	-1.08595100
H	-3.23433700	-0.38264900	-0.28092100
O	-4.73470300	0.95257600	-0.84819500
C	-4.88231800	1.75030600	0.23355800
O	-5.96820900	2.15880600	0.55631300
C	-3.48049600	-0.34702600	-2.43475600
H	-3.65742400	0.37295200	-3.23996400
H	-2.53303600	-0.86132800	-2.61367100
H	-4.28595500	-1.08679700	-2.43091100
C	3.20347900	3.35329800	-1.09337000
C	1.88774100	3.16513300	-1.44280500
C	1.70251700	1.28590700	-0.02833700
C	3.01688700	1.41717700	0.35930900
C	3.82780600	2.46247700	-0.16566700
H	3.74319000	4.17714000	-1.54237400
H	1.37644400	3.81037400	-2.14979900
H	1.04850400	0.48176600	0.34464200
H	3.40081800	0.68364700	1.05606800
C	5.73856700	1.65924000	1.13151600

H	6.78405200	1.93277200	1.27786200
H	5.23585000	1.68574600	2.10653300
H	5.70100700	0.63289800	0.74604400
C	5.93790700	3.68535100	-0.36534300
H	5.51927800	4.66941800	-0.11625300
H	6.94230000	3.62979400	0.05571300
H	6.02133100	3.60339700	-1.45740100
N	1.16168500	2.15320600	-0.91873100
H	0.17679100	2.00992400	-1.21426700
C	0.28426200	-4.27147400	-0.80136300
C	-0.27063900	-3.07577200	-0.37085400
C	0.46509800	-2.10843900	0.37369100
C	1.81708900	-2.48416100	0.62212600
C	2.36000800	-3.68109400	0.18008500
C	1.61123700	-4.60765100	-0.53982200
O	-0.03594600	-0.98551200	0.77457900
C	-2.70794800	-1.72936400	2.80200100
H	-3.69474400	-1.53974500	3.24026300
H	-1.96686500	-1.75190800	3.61562400
H	-2.72867400	-2.71839200	2.31986000
O	-2.43386000	-0.69516600	1.86905200
H	-1.53239600	-0.84997700	1.47419500
N	5.12781300	2.60403500	0.19251100
F	-0.48812200	-5.13582200	-1.50506100
F	3.66108800	-3.95268300	0.46140600
F	-1.56857000	-2.80099900	-0.66968300
F	2.60854200	-1.62085700	1.32635900
H	2.03761100	-5.54393500	-0.87956300

2,3,4,5,6-FP/DMAP(j)_Int1
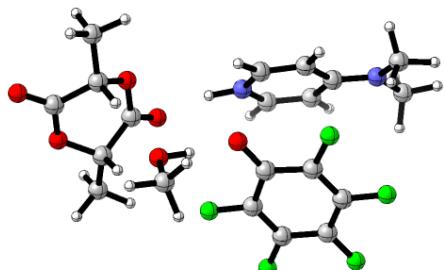
O	-3.37910300	1.51205700	-0.23289900
C	-3.02407800	0.59136100	-1.12975100
O	-2.11035900	0.81696300	-1.90503700
H	-5.52044700	2.18184400	2.26713900
C	-4.78027700	2.41984400	1.49850200
H	-5.22193800	3.14592400	0.80858500
H	-3.90078400	2.86178700	1.97663000

C	-4.38615000	1.14785000	0.77620100
H	-3.90145400	0.42888600	1.45568000
C	-3.81015900	-0.70856600	-1.09438400
H	-3.43792900	-1.26444900	-0.21868200
O	-5.22170400	-0.41245500	-0.88997700
C	-5.56045100	0.44491000	0.09986500
O	-6.71337300	0.61188600	0.40396200
C	-3.68544200	-1.53654100	-2.35779400
H	-4.03615900	-0.97806900	-3.23136100
H	-2.63899200	-1.81456000	-2.50779000
H	-4.28344600	-2.44636200	-2.25227300
C	1.92902900	2.43828400	0.45655900
C	0.63498300	2.18546400	0.07024400
C	1.32138400	1.74463800	-2.13720900
C	2.63746900	1.97146600	-1.81913300
C	2.99712600	2.30998700	-0.47719600
H	2.11193500	2.66412100	1.49791300
H	-0.19362200	2.19693900	0.76578400
H	1.00440800	1.45331300	-3.13298000
H	3.38291000	1.85119200	-2.59420900
C	5.36748000	2.28798300	-1.07664300
H	6.31847000	2.52133700	-0.59691600
H	5.40758900	1.24953100	-1.43206300
H	5.25162900	2.95622900	-1.93888400
C	4.62664900	2.72303700	1.29811900
H	4.27932800	1.90070400	1.93511100
H	5.71057700	2.79742400	1.39048000
H	4.18858400	3.66421400	1.65381400
N	0.34392900	1.85596200	-1.20963200
H	-0.62592900	1.59194100	-1.45969200
C	1.83412500	-2.63384300	-0.73356300
C	0.76089800	-1.91166800	-0.22632600
C	0.86945200	-0.98042300	0.85133100
C	2.19568100	-0.87345800	1.36904700
C	3.27715700	-1.58519000	0.86361300
C	3.11158600	-2.47521700	-0.19597600
O	-0.11669300	-0.28103000	1.29098800
C	-2.50036900	-2.04818400	2.97585500
H	-3.52923600	-2.32260500	3.23614300
H	-2.02650900	-1.59610700	3.86026100
H	-1.95289400	-2.96824100	2.72003900
O	-2.54844100	-1.14295400	1.88326600
H	-1.61883800	-0.86411800	1.65750000
N	4.28779100	2.48396700	-0.10880100

F	1.65097400	-3.48649000	-1.76291300
F	4.50970900	-1.40466900	1.39307800
F	-0.45820200	-2.09195300	-0.79658500
F	2.42573000	-0.02102900	2.40453300
F	4.16418000	-3.16213700	-0.69386800

Ph/DMAP(k)_Int1
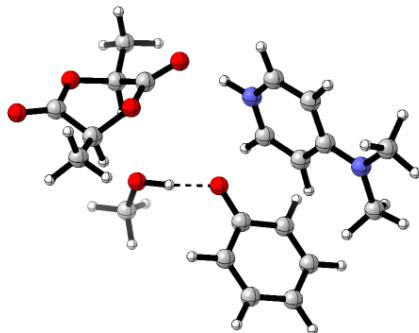
O	2.41415800	-1.29518900	0.69698900
C	2.57732100	-1.37694300	-0.62248900
O	1.79295200	-2.02619300	-1.29628700
H	3.64503300	0.08721500	3.50123800
C	3.03305600	-0.60596800	2.91776700
H	3.30877500	-1.62764300	3.19819300
H	1.97858400	-0.43494800	3.15451500
C	3.27193400	-0.35856200	1.44306500
H	2.96557000	0.65733800	1.14414500
C	3.75944500	-0.61292500	-1.19281800
H	3.45684000	0.44859200	-1.19439800
O	4.90557400	-0.76629700	-0.30719700
C	4.72394500	-0.55640400	1.01751300
O	5.66199700	-0.53046600	1.77178800
C	4.17919100	-1.07174000	-2.57544700
H	4.47294600	-2.12621900	-2.56952000
H	3.34716400	-0.94204100	-3.27292200
H	5.02574000	-0.46788600	-2.91488100
C	-2.95454700	-3.14579600	0.00544500
C	-1.62252800	-3.23709900	-0.31925600
C	-1.45578600	-0.90001000	-0.61076200
C	-2.78650600	-0.74123600	-0.29272400
C	-3.59293600	-1.86624700	0.03710300
H	-3.49208000	-4.05628200	0.23762000
H	-1.09591000	-4.18546000	-0.34894100
H	-0.80597500	-0.03942600	-0.84277000
H	-3.17730700	0.26871200	-0.30021200
C	-5.51591600	-0.39830500	0.39250900

H	-6.55330500	-0.49609800	0.71461500
H	-4.99708900	0.26744600	1.09225200
H	-5.50279500	0.06665700	-0.60113400
C	-5.71108900	-2.90150200	0.68928100
H	-5.31656500	-3.43505400	1.56450300
H	-6.72651100	-2.57794500	0.92062700
H	-5.76140600	-3.60094600	-0.15615100
N	-0.89744800	-2.13605900	-0.61813100
H	0.11185600	-2.21406800	-0.83822900
C	-3.31655500	3.41281600	-0.86288600
C	-2.20077600	2.70864500	-1.31992500
C	-1.10138500	2.40675800	-0.46101300
C	-1.20330300	2.88093900	0.88081200
C	-2.32292600	3.58580200	1.32502500
C	-3.39821300	3.85580500	0.46562500
O	-0.08308700	1.69619900	-0.88377000
C	2.71588600	3.48141100	-0.45170300
H	3.78484500	3.61273100	-0.24185100
H	2.14803300	4.12899100	0.23413700
H	2.52117200	3.81956700	-1.48131900
O	2.38832800	2.11264700	-0.27769500
H	1.40227700	1.98563300	-0.48391100
N	-4.90048900	-1.72944900	0.36720900
H	-0.37794200	2.67421100	1.56068200
H	-2.35811900	3.93203900	2.35783700
H	-4.26292300	4.41558600	0.81448500
H	-4.12889600	3.63226300	-1.55619300
H	-2.13570200	2.38334400	-2.35732000

o-FP/DMAP(a)_Int2
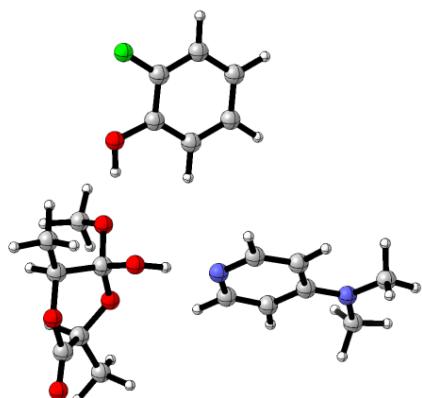
O	1.90018000	-1.78407800	0.74958200
C	2.20003400	-0.60646300	0.00492900
O	1.37213800	-0.47510500	-1.05872800
H	2.96508300	-4.88162000	1.42570500

C	2.22580500	-4.08356900	1.31616400
H	1.46505100	-4.41456700	0.60259500
H	1.75307700	-3.89608000	2.28588200
C	2.89958500	-2.81498000	0.82241800
H	3.68019700	-2.51252600	1.54401200
C	3.66757000	-0.61169700	-0.47828000
H	4.32609900	-0.55312400	0.39902500
O	3.94579000	-1.86513600	-1.15481800
C	3.60528700	-3.00833800	-0.52436100
O	3.87808300	-4.08188900	-0.99950800
C	3.99810600	0.50444200	-1.45174700
H	3.36577500	0.42831600	-2.33954900
H	3.83167000	1.47956100	-0.98376900
H	5.04923600	0.43015900	-1.74816800
C	-2.93206200	-2.30200300	0.59250700
C	-1.61901000	-1.90219900	0.38530100
C	-2.21513000	-0.47641400	-1.29820500
C	-3.55911700	-0.80251000	-1.17990700
C	-3.96736100	-1.74572800	-0.20208400
H	-3.13920700	-3.03815400	1.36043900
H	-0.81671700	-2.32474300	0.98779900
H	-1.90011900	0.24943800	-2.04612300
H	-4.27184600	-0.32636000	-1.84295400
C	-6.30063500	-1.55897800	-0.92772400
H	-7.27862200	-1.93300000	-0.61942300
H	-6.33141200	-0.46215500	-0.88387300
H	-6.13291000	-1.85847200	-1.97309800
C	-5.64558600	-3.12625600	0.93034700
H	-5.32976900	-2.85106200	1.94548800
H	-6.73107000	-3.24060500	0.93812700
H	-5.19997200	-4.10128700	0.68207600
N	-1.23948800	-1.00274700	-0.53826700
H	0.41676500	-0.67117300	-0.80167300
C	-1.07200600	5.61933900	0.07560300
C	0.17339600	5.01748100	-0.02696100
C	0.35581900	3.63724200	0.15487100
C	-0.77757600	2.86411900	0.44776000
C	-2.03885300	3.45935300	0.55632000
C	-2.19381000	4.83533700	0.37176100
H	-1.14756500	6.69269300	-0.07577600
H	-2.90087000	2.83773500	0.78625400
O	1.60716100	3.13464200	0.04071200
C	2.48622700	0.48309700	2.20503200
H	2.12073800	-0.39585800	2.74568100

H	2.12292900	1.39123200	2.69254100
H	3.58461000	0.49847400	2.21363500
O	1.95969300	0.51671800	0.87409300
H	1.61160300	2.17216400	0.21972800
H	-0.65804400	1.79174900	0.58384400
N	-5.28177800	-2.09692100	-0.03495500
F	1.25757800	5.78202300	-0.31052300
H	-3.17250900	5.29986400	0.45571400

m-FP/DMAP(b)_Int2
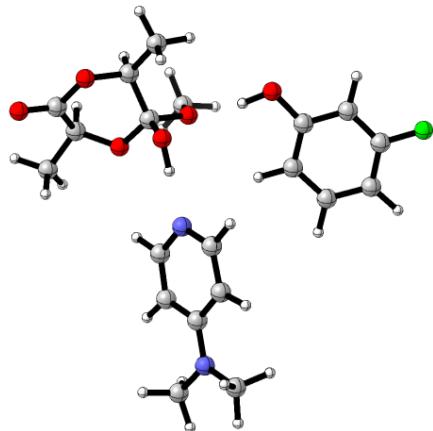
O	-2.64510300	0.55076700	0.76839600
C	-2.33955800	-0.59178600	-0.02736700
O	-1.58113900	-0.25575400	-1.09745900
H	-5.08522400	2.69325000	1.56973000
C	-4.05096700	2.36914300	1.42589900
H	-3.56908700	3.05746800	0.72480600
H	-3.52579600	2.40615400	2.38597900
C	-4.02117000	0.95133300	0.88183400
H	-4.53697900	0.27829600	1.59079300
C	-3.62850700	-1.29592200	-0.50672300
H	-4.15290900	-1.70253100	0.36874900
O	-4.50403500	-0.32211400	-1.13137400
C	-4.75788700	0.81801100	-0.45568900
O	-5.53424200	1.63273500	-0.88699300
C	-3.38469200	-2.39529100	-1.52383500
H	-2.89069700	-1.98602100	-2.40831700
H	-2.74804100	-3.17480700	-1.09408400
H	-4.34079300	-2.84111100	-1.81606100
C	1.29522000	3.42704000	0.55742000
C	0.33582500	2.44588800	0.34805200
C	1.56251800	1.46132800	-1.30975700
C	2.58541200	2.39153100	-1.18796200
C	2.48057100	3.42524300	-0.22217800

H	1.11543000	4.18048000	1.31541100
H	-0.57761600	2.43873900	0.94035500
H	1.64282100	0.66496000	-2.04776800
H	3.44776900	2.30663800	-1.83865800
C	4.62686800	4.37128500	-0.93232500
H	5.30534300	5.16757600	-0.62083900
H	5.17566800	3.42189400	-0.87681500
H	4.34841700	4.54870600	-1.98198200
C	3.27720700	5.45550400	0.89490700
H	3.11472900	5.07723700	1.91294000
H	4.17605700	6.07462400	0.90876700
H	2.42406800	6.09551300	0.62368700
N	0.44411100	1.46538100	-0.56444400
H	-0.83910100	0.37577500	-0.83380900
C	3.66556400	-4.20407000	0.06918300
C	2.31057300	-4.36825600	-0.17791700
C	1.45102100	-3.28599400	0.06668300
C	1.97149400	-2.07180000	0.54661900
C	3.34330900	-1.95340600	0.78335600
C	4.21724600	-3.01968300	0.54890600
H	3.73817300	-1.01126200	1.15642100
O	0.13021400	-3.47457200	-0.17722200
C	-2.00040100	-1.76801700	2.11952500
H	-2.12378200	-0.84609500	2.69691800
H	-1.21627400	-2.38078300	2.57139800
H	-2.93757200	-2.34131200	2.12412500
O	-1.55460500	-1.48021000	0.79013600
H	-0.38634400	-2.67643600	0.05442300
H	1.30381000	-1.23265400	0.72290800
N	3.46518300	4.36375600	-0.05189700
H	5.28510500	-2.94595500	0.72752100
F	4.49340500	-5.25796600	-0.16970700
H	1.92052800	-5.30988900	-0.55052200

p-FP/DMAP(c)_Int2
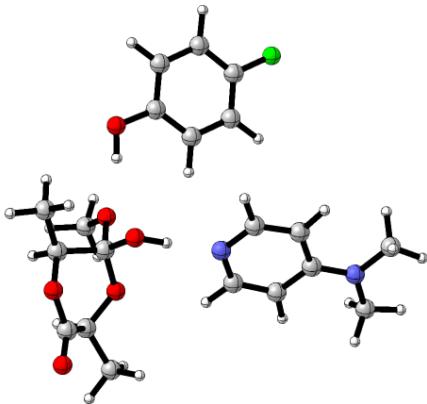
O	-2.62343500	0.73702700	0.77810600
C	-2.45501900	-0.43070300	-0.02193100
O	-1.68903600	-0.17407700	-1.10885300
H	-4.80461200	3.13170700	1.61118800
C	-3.81393400	2.69755400	1.45153800
H	-3.27260700	3.32731600	0.73890900
H	-3.27125700	2.68112600	2.40242000
C	-3.94632300	1.28284100	0.91456400
H	-4.51745900	0.67106500	1.63658000
C	-3.81989300	-0.99681200	-0.47269600
H	-4.36569300	-1.34518700	0.41473000
O	-4.60151000	0.06222600	-1.08302800
C	-4.71954700	1.22458300	-0.40762300
O	-5.41464700	2.11536800	-0.82693400
C	-3.71315900	-2.11689100	-1.49087000
H	-3.19808800	-1.76208000	-2.38679300
H	-3.15208800	-2.95783000	-1.07171800
H	-4.71634900	-2.46116700	-1.76177900
C	1.63335900	3.10525500	0.58069000
C	0.55780500	2.25636300	0.35870600
C	1.59597300	1.24234000	-1.40691100
C	2.72532900	2.03855900	-1.27818000
C	2.77772700	3.01877500	-0.25380900
H	1.57567500	3.82149100	1.39204700
H	-0.32579700	2.31564500	0.99196100
H	1.55507800	0.48732300	-2.19027800
H	3.54934800	1.89115400	-1.96634400
C	5.02595100	3.69715600	-0.95503900
H	5.77938100	4.43112700	-0.66380900
H	5.47808900	2.69784100	-0.88079300
H	4.76328100	3.88009100	-2.00642900
C	3.88235500	4.81580900	0.99292300
H	3.79707100	4.34132300	1.98117500
H	4.82592500	5.36342800	0.96199500

H	3.06499600	5.54312800	0.88759400
N	0.51471100	1.32886300	-0.61298900
H	-0.88336800	0.38164800	-0.86275700
C	3.21735900	-4.59919300	-0.06655400
C	1.83023700	-4.63548300	-0.21917500
C	1.06106900	-3.48285600	0.00178100
C	1.69590300	-2.28867700	0.37670800
C	3.08565200	-2.24939600	0.53249100
C	3.82247100	-3.40451000	0.30854300
H	3.82525600	-5.48365900	-0.23456000
H	3.59035100	-1.33221300	0.82246200
O	-0.28699500	-3.58133500	-0.15957200
C	-2.19431200	-1.63307700	2.12044100
H	-2.20493600	-0.70308200	2.69796700
H	-1.47104800	-2.32701600	2.55613800
H	-3.18748600	-2.10200700	2.14753300
O	-1.74975500	-1.39567200	0.78066700
H	-0.72514700	-2.73227700	0.04689100
H	1.10491500	-1.39079800	0.53847500
H	1.32779400	-5.55354000	-0.51084300
F	5.17974800	-3.36618600	0.45917400
N	3.86672300	3.83156600	-0.08146900

2,3-FP/DMAP(d)_Int2
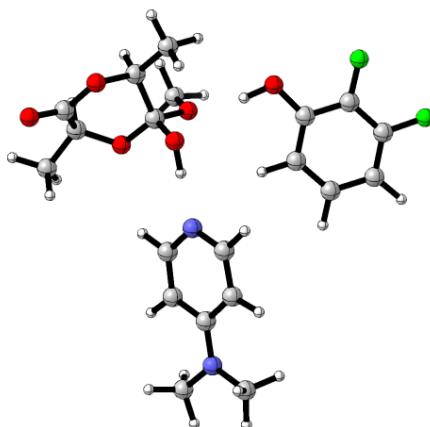
O	-2.59561300	-1.03592700	0.75409700
C	-1.61764800	-1.76553300	0.01981800
O	-1.15187300	-1.04552800	-1.02838100
H	-5.87665300	-0.79888900	1.35967300
C	-4.84970400	-0.43314000	1.27606500
H	-4.83844900	0.40292000	0.57013400
H	-4.51263200	-0.08163400	2.25677000
C	-3.93904500	-1.54813100	0.79199900
H	-3.98443700	-2.39133200	1.50493100

C	-2.18808300	-3.10923500	-0.48626700
H	-2.41156500	-3.74504100	0.38123300
O	-3.43509300	-2.86596900	-1.18706700
C	-4.36515800	-2.10787300	-0.56976700
O	-5.44860800	-1.93098500	-1.06687800
C	-1.27160500	-3.84370600	-1.44716700
H	-1.07265500	-3.22399100	-2.32478900
H	-0.32053600	-4.08072800	-0.96047900
H	-1.74795900	-4.77710200	-1.76342100
C	-1.25515400	3.63341300	0.62018700
C	-1.36727300	2.26400200	0.42318200
C	0.15717100	2.28483700	-1.27930300
C	0.34845500	3.65534300	-1.17188900
C	-0.36767600	4.38762000	-0.19012100
H	-1.85509100	4.10109000	1.39208500
H	-2.04786300	1.67683100	1.03734100
H	0.70678500	1.72096000	-2.03129300
H	1.04382400	4.13964000	-1.84735700
C	0.65387700	6.48465900	-0.94098200
H	0.66829400	7.53355800	-0.63944400
H	1.68581100	6.11086900	-0.90563100
H	0.30251300	6.43197600	-1.98227200
C	-1.02407200	6.46241900	0.93604500
H	-0.87033900	6.07602000	1.95243700
H	-0.73416800	7.51468800	0.93162000
H	-2.09739600	6.40163300	0.70152400
N	-0.68074700	1.57485700	-0.50428300
H	-0.98576500	-0.08556400	-0.76632600
C	5.32236200	-1.06399900	0.07361600
C	4.31747100	-2.02257400	-0.00943400
C	2.97450600	-1.66237300	0.18559800
C	2.67841300	-0.31797600	0.46226200
C	3.70145300	0.62988400	0.54392900
C	5.03752800	0.26917000	0.35047900
H	3.45146900	1.66510800	0.76066600
O	2.04724100	-2.63983100	0.09665400
C	-0.76539900	-2.48357700	2.22782800
H	-1.44775200	-1.81544600	2.76289900
H	0.20213300	-2.50331200	2.73563400
H	-1.17292600	-3.50349000	2.21401600
O	-0.50488300	-1.99252600	0.90802300
H	1.15005200	-2.28760200	0.27594300
H	1.64084300	-0.02821200	0.60529600
N	-0.21103300	5.74004900	-0.03413600

H	5.84920300	0.98733900	0.40901700
F	6.60163500	-1.45585000	-0.12054200
F	4.63679100	-3.30391400	-0.27604800

2,4-FP/DMAP(e)_Int2
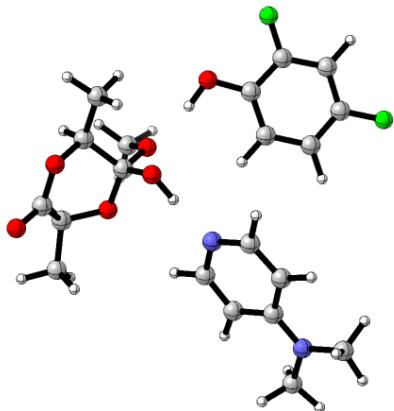
O	-2.73002100	0.72894100	0.76913600
C	-2.43549700	-0.45199700	0.03030600
O	-1.63323600	-0.18335100	-1.02819400
H	-5.10453200	3.01542100	1.33654700
C	-4.08060100	2.63970800	1.26057900
H	-3.53519200	3.26619200	0.54823800
H	-3.59930100	2.70742400	2.24175400
C	-4.09079900	1.19385200	0.79534200
H	-4.66599800	0.58319900	1.51491000
C	-3.72895800	-1.13781000	-0.46241500
H	-4.29975000	-1.48126800	0.41112500
O	-4.54428300	-0.16722400	-1.16806000
C	-4.77631300	1.01706300	-0.56428700
O	-5.50109000	1.83681800	-1.06921700
C	-3.48722300	-2.29464200	-1.41428400
H	-2.94488900	-1.94771600	-2.29714200
H	-2.89805000	-3.07511200	-0.92297100
H	-4.44753300	-2.71956800	-1.72319100
C	1.32739900	3.42441500	0.68851900
C	0.35558100	2.45654900	0.47577000
C	1.43799800	1.63323400	-1.36109000
C	2.46597300	2.55832000	-1.24512300
C	2.44145800	3.50326800	-0.18685500
H	1.21292200	4.10543000	1.52375600
H	-0.50477300	2.39038700	1.13959500
H	1.45595300	0.90617000	-2.17144800
H	3.27023500	2.53887600	-1.97117200
C	4.53979500	4.50022700	-0.96693300

H	5.22645800	5.29015800	-0.65769700
H	5.10171000	3.55661800	-0.99592500
H	4.19397000	4.72826800	-1.98562600
C	3.34785100	5.40806300	1.05953100
H	3.31324500	4.91749300	2.04209500
H	4.23247100	6.04678800	1.03459900
H	2.46046300	6.05049700	0.96244300
N	0.38779300	1.55965900	-0.52494200
H	-0.90262100	0.46437800	-0.77572600
C	3.47348400	-4.19984900	-0.01239700
C	2.09033200	-4.32413100	-0.01360800
C	1.23307800	-3.22371000	0.14787500
C	1.82192900	-1.96274000	0.31449400
C	3.21304100	-1.80679800	0.32194900
C	4.01273800	-2.92847500	0.15815500
H	3.66593000	-0.82873600	0.45150100
O	-0.10307100	-3.44388200	0.13531800
C	-2.20505700	-1.55302200	2.23144400
H	-2.32972400	-0.60691800	2.76777200
H	-1.45301000	-2.16495500	2.73570000
H	-3.15412900	-2.10585000	2.22007000
O	-1.70187100	-1.32557200	0.90989600
H	-0.59298400	-2.60944300	0.28619000
H	1.17896300	-1.09454300	0.43295700
N	3.43255300	4.43375500	-0.02097600
F	5.36822700	-2.79064800	0.16222700
H	4.10572600	-5.07235400	-0.14021900
F	1.54769800	-5.55265500	-0.17551200

2,6-FP/DMAP(f)_Int2
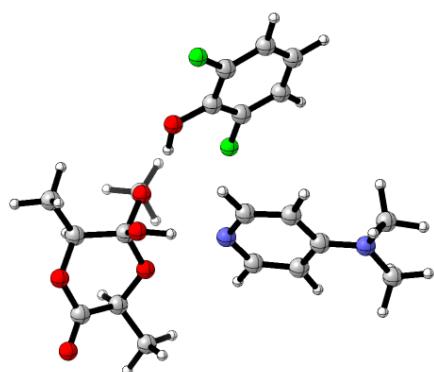
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C	2.58819600	0.42208400	-0.07394600
O	1.87444300	0.09644000	-1.17628500
H	4.98680900	-3.07984500	1.61162000

C	3.99177300	-2.65849800	1.44458400
H	3.46254000	-3.29571600	0.72944200
H	3.44167600	-2.64718800	2.39123800
C	4.10775500	-1.24232400	0.90660600
H	4.67248200	-0.62410800	1.62901900
C	3.94392400	1.02495100	-0.50212500
H	4.46336400	1.39503700	0.39230000
O	4.76638200	-0.01593800	-1.08915900
C	4.89062900	-1.17530300	-0.41001100
O	5.60600300	-2.05569000	-0.81800500
C	3.81939900	2.13315100	-1.53085200
H	3.33395500	1.75390100	-2.43328600
H	3.21649800	2.95224800	-1.12667400
H	4.81400400	2.51354700	-1.78490600
C	-1.70527400	-2.93533300	0.46894500
C	-0.54641800	-2.20068700	0.25766400
C	-1.47851900	-1.04496400	-1.47994600
C	-2.68611100	-1.71852900	-1.35885800
C	-2.83907500	-2.70490100	-0.35151200
H	-1.71896100	-3.67339100	1.26245800
H	0.32741000	-2.36633700	0.88568700
H	-1.35788000	-0.28279900	-2.24808700
H	-3.49165400	-1.47190200	-2.04041800
C	-5.12575200	-3.17742600	-1.09622500
H	-5.97307200	-3.78798000	-0.77852600
H	-5.44801500	-2.12771300	-1.09297000
H	-4.86997400	-3.45687600	-2.12946200
C	-4.09877800	-4.45399600	0.81435200
H	-3.88519100	-4.07498800	1.82279700
H	-5.11237900	-4.85923800	0.81792600
H	-3.40108000	-5.27786100	0.60055200
N	-0.40982100	-1.26449800	-0.69555400
H	1.04233600	-0.42217100	-0.93337500
C	-3.94732600	3.36282300	-0.20051600
C	-2.66269800	3.22497000	-0.70846300
C	-1.61244200	2.63722100	0.01727700
C	-1.94597900	2.19198500	1.30414200
C	-3.21718000	2.30797100	1.85059300
C	-4.22804500	2.90007400	1.08939200
H	-3.39403800	1.93859800	2.85633400
O	-0.39443900	2.55022300	-0.54386500
C	2.24971100	1.70875100	2.00039800
H	2.38020700	0.80505100	2.60452300
H	1.45287700	2.31806700	2.43101700

H	3.17997200	2.29325000	1.99193400
O	1.82112100	1.37896500	0.67503800
H	0.25564700	2.05468600	0.00031200
N	-4.01346000	-3.39255700	-0.17976400
H	-4.70726500	3.83059200	-0.81937200
F	-2.39237100	3.66989900	-1.95729000
F	-0.95167500	1.62209500	2.04206700
H	-5.22814400	3.00421400	1.49949900

2,3,6-FP/DMAP(g)_Int2
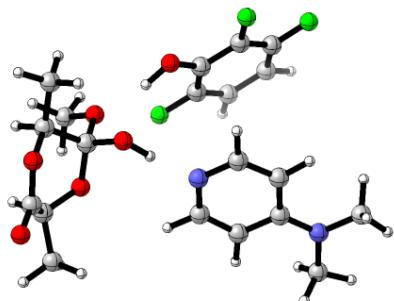
O	-2.99556100	0.53195000	0.77639200
C	-2.77470600	-0.55667400	-0.11814400
O	-2.04356400	-0.17534400	-1.19078600
H	-5.22954900	2.86840500	1.63497400
C	-4.22935700	2.45494900	1.47953000
H	-3.68307000	3.11784100	0.80154300
H	-3.70444400	2.41104300	2.43942000
C	-4.32766200	1.05844900	0.88927000
H	-4.91018300	0.41434500	1.57377600
C	-4.11453900	-1.15448400	-0.60017900
H	-4.65216000	-1.56213600	0.26668000
O	-4.93032300	-0.09743700	-1.16641700
C	-5.07554400	1.03649400	-0.44913200
O	-5.78413000	1.92862100	-0.84269200
C	-3.95694700	-2.22131100	-1.66741100
H	-3.45000000	-1.80517100	-2.54135700
H	-3.36128900	-3.05330600	-1.27906700
H	-4.94250400	-2.59546300	-1.96252600
C	1.44723000	2.92475100	0.55166500
C	0.31494400	2.14808400	0.34690100
C	1.21294100	1.15286200	-1.50453900
C	2.39177600	1.87715000	-1.39652100
C	2.54861300	2.80391000	-0.33432000
H	1.46569800	3.61125400	1.39008000
H	-0.53358800	2.23108700	1.02407800
H	1.09008200	0.43632000	-2.31508200

H	3.17248200	1.71568200	-2.13047100
C	4.77254300	3.43234800	-1.15045900
H	5.60500000	4.06299600	-0.83289700
H	5.14233300	2.40141000	-1.22791500
H	4.45517400	3.76176200	-2.15123400
C	3.78227800	4.53463200	0.88482900
H	3.64203200	4.08037000	1.87497400
H	4.77326300	4.99183200	0.86451500
H	3.03440800	5.33255700	0.76225700
N	0.17543000	1.26748500	-0.65770400
H	-1.24087200	0.37319100	-0.91564400
C	3.98598700	-2.52850100	0.00034900
C	2.72469200	-2.63516900	-0.58015800
C	1.56407000	-2.29544200	0.13525800
C	1.75892200	-1.85187800	1.45275400
C	3.00930100	-1.74108400	2.04116400
C	4.14823900	-2.08512800	1.30695800
H	3.08174100	-1.39218200	3.06657400
O	0.37592500	-2.42932000	-0.47124900
C	-2.47115400	-1.94183100	1.89881500
H	-2.62145100	-1.07254500	2.54706000
H	-1.68301900	-2.57111400	2.31653000
H	-3.39723500	-2.52884500	1.83420800
O	-2.01106800	-1.53944100	0.60371000
H	-0.37236600	-2.03173100	0.02916900
N	3.69589800	3.53716100	-0.17349100
F	2.60907000	-3.06243700	-1.84935800
F	0.64960400	-1.52290100	2.17138800
H	5.14428400	-2.01707900	1.73154200
F	5.06532000	-2.86333400	-0.74139200

3,4,5-FP/DMAP(h)_Int2
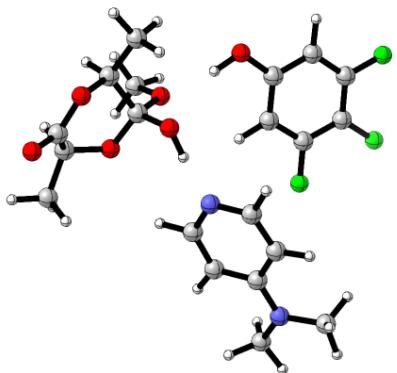
O	-3.04139500	0.41319200	0.81257700
C	-2.70877500	-0.71143200	0.00598200

O	-2.05915900	-0.34144500	-1.12241900
H	-5.52951200	2.52908100	1.53815600
C	-4.48939800	2.22861500	1.38579300
H	-4.04672600	2.88556000	0.63093400
H	-3.94116000	2.34164900	2.32681900
C	-4.42745700	0.78085600	0.93005300
H	-4.90283900	0.13719400	1.69278100
C	-3.97191400	-1.51847000	-0.36487300
H	-4.42489900	-1.90809500	0.55720300
O	-4.93332700	-0.63037200	-0.98823400
C	-5.20333100	0.53905100	-0.37008700
O	-6.03185700	1.29353300	-0.81268900
C	-3.71280700	-2.65180200	-1.34010100
H	-3.28240800	-2.26011800	-2.26499400
H	-3.01570200	-3.37467400	-0.90483700
H	-4.65438300	-3.16199700	-1.56663200
C	0.92051200	3.25222500	0.55924700
C	-0.09371400	2.33449800	0.32671400
C	0.84559000	1.64879900	-1.64109800
C	1.90713500	2.53191600	-1.51183000
C	1.97870400	3.38051900	-0.37710700
H	0.88749000	3.84844800	1.46347600
H	-0.90779300	2.22630300	1.04153500
H	0.79339300	0.99084200	-2.50716400
H	2.67125700	2.54477500	-2.27987200
C	4.13750300	4.26967000	-1.11786300
H	4.82747300	5.06606300	-0.83274300
H	4.68527800	3.31546800	-1.10084100
H	3.81036300	4.46448900	-2.14705700
C	3.10289000	5.02888300	1.04274100
H	3.24498200	4.37706900	1.91823000
H	3.95577100	5.70719900	0.97906000
H	2.20421300	5.63741100	1.20536400
N	-0.15255000	1.52926300	-0.74812000
H	-1.36961700	0.37501100	-0.92914800
C	3.70750600	-3.42366000	-0.13562600
C	2.38348600	-3.78669500	-0.33096100
C	1.37097600	-2.85374500	-0.05592000
C	1.70352400	-1.57101900	0.41012900
C	3.04288000	-1.25032400	0.59417400
C	4.06478500	-2.15757400	0.32844300
O	0.09261100	-3.24668300	-0.25795400
C	-2.14952100	-1.85737500	2.12529500
H	-2.39200000	-0.95919300	2.70201800

H	-1.26791400	-2.34037000	2.55453800
H	-2.98834400	-2.56544200	2.16088300
O	-1.79592300	-1.51658700	0.77949200
H	-0.54120100	-2.54196900	-0.00654600
N	3.00575800	4.26962700	-0.19793200
F	4.69033900	-4.30976500	-0.39612800
H	0.94029800	-0.82603400	0.61114600
H	2.13677200	-4.77936300	-0.69225300
F	5.35693900	-1.82298200	0.51230700
F	3.37891300	-0.01972800	1.04021000

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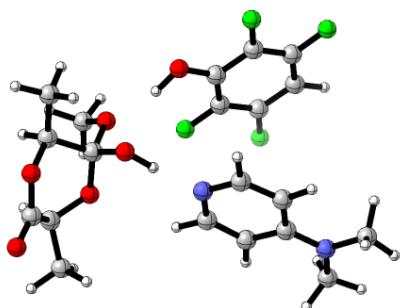
O	-3.01734900	0.55962100	0.75395200
C	-2.86341200	-0.56581900	-0.10433900
O	-2.16487800	-0.24811800	-1.21875100
H	-5.15969500	2.97340600	1.63270100
C	-4.17663300	2.53181200	1.44827100
H	-3.64652400	3.15766100	0.72394100
H	-3.61063900	2.50916600	2.38524100
C	-4.33242400	1.11866100	0.91300000
H	-4.89307000	0.51054000	1.64659200
C	-4.23536500	-1.14887900	-0.50620100
H	-4.74146500	-1.51545900	0.39729700
O	-5.05276800	-0.09302500	-1.07169000
C	-5.14302600	1.06714800	-0.38750400
O	-5.85186100	1.95990300	-0.77846800
C	-4.14878900	-2.25407800	-1.54209300
H	-3.67467700	-1.87868000	-2.45216800
H	-3.55350200	-3.08573000	-1.15257700
H	-5.15445900	-2.61572800	-1.77904600
C	1.40787800	2.77643900	0.45934700
C	0.27256600	2.00103600	0.27037400
C	0.98436400	1.28502900	-1.78068800
C	2.15640500	2.02361900	-1.69923100
C	2.40767700	2.81181200	-0.54656100
H	1.50967000	3.33759500	1.38078600

H	-0.49833100	1.96546000	1.03800000
H	0.78936800	0.67646000	-2.66243900
H	2.86056400	1.97848600	-2.52171800
C	4.56711800	3.53220700	-1.45359300
H	5.38012900	4.20507700	-1.17506300
H	4.98781100	2.52476900	-1.58755900
H	4.16615000	3.86965700	-2.41910500
C	3.78756800	4.31377200	0.81144800
H	3.85148700	3.65579200	1.69039700
H	4.73325100	4.85105400	0.72005400
H	2.99544600	5.05368900	0.99088500
N	0.04063000	1.25627200	-0.82398900
H	-1.36277600	0.32863000	-1.00215700
C	3.82402000	-2.51045900	-0.23920600
C	2.53130500	-2.77506400	-0.67736200
C	1.41530300	-2.30183300	0.03641500
C	1.67249600	-1.56385500	1.20286000
C	2.97264000	-1.30533900	1.62368000
C	4.07159900	-1.77290600	0.91457000
O	0.19379200	-2.59537100	-0.42292500
C	-2.48460200	-1.85854100	1.96703100
H	-2.52060500	-0.95552800	2.58430100
H	-1.71609900	-2.53147800	2.35365500
H	-3.45296400	-2.37554400	1.99800300
O	-2.09678100	-1.54553600	0.62437900
H	-0.53414100	-2.10206100	0.02479300
N	3.54664500	3.56153500	-0.41345300
F	4.86130800	-2.98079100	-0.96131300
F	3.15791500	-0.58558400	2.75081800
F	0.62709100	-1.10360900	1.92656600
F	2.33691100	-3.48729600	-1.79990700
H	5.08374100	-1.57475500	1.24850800

2,3,4,5,6-FP/DMAP(j)_Int2
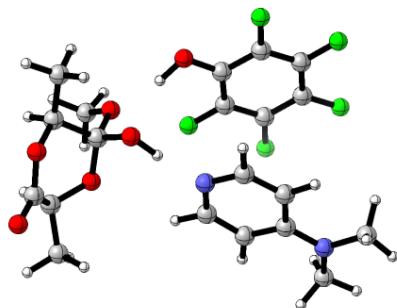
O	-3.17080200	0.62665400	0.73439800
C	-3.02328100	-0.54989300	-0.05109800

O	-2.29897400	-0.31211100	-1.16910800
H	-5.29363000	3.10853200	1.45715200
C	-4.31400200	2.64627600	1.30869300
H	-3.76832200	3.22558200	0.55772700
H	-3.75899200	2.66834400	2.25220800
C	-4.48135600	1.20808500	0.84926500
H	-5.05628000	0.64682700	1.60850200
C	-4.39761700	-1.13536600	-0.44104300
H	-4.92163000	-1.44477100	0.47360400
O	-5.19134300	-0.10142000	-1.07596100
C	-5.27719000	1.09506200	-0.45640100
O	-5.97022200	1.97310000	-0.90433400
C	-4.31254600	-2.29730800	-1.41307100
H	-3.82021900	-1.97964000	-2.33536800
H	-3.73573200	-3.11482600	-0.96959000
H	-5.32007000	-2.65710800	-1.64472700
C	1.29848900	2.74945000	0.39582500
C	0.14343100	1.99972100	0.22476000
C	0.84772800	1.19632000	-1.79605100
C	2.03940500	1.90445900	-1.73080600
C	2.30567900	2.72469900	-0.60356400
H	1.41085600	3.33605200	1.29993600
H	-0.63214800	2.01040700	0.98846900
H	0.64183200	0.56450600	-2.65887600
H	2.74747200	1.81124000	-2.54585800
C	4.50822800	3.32047300	-1.49642300
H	5.32558400	4.00060600	-1.25012300
H	4.91445400	2.29907700	-1.54486800
H	4.13448200	3.59253600	-2.49208900
C	3.73774800	4.19424100	0.73453000
H	3.80910800	3.53565300	1.61283400
H	4.68775600	4.72024000	0.62445600
H	2.95923700	4.94446200	0.92573300
N	-0.10218100	1.22381300	-0.84509800
H	-1.50616600	0.28627800	-0.97894300
C	3.55177800	-2.29978100	-0.42902000
C	2.24779500	-2.71022300	-0.69293200
C	1.16778800	-2.29306200	0.10362100
C	1.46970300	-1.45589700	1.18797600
C	2.76908900	-1.03377000	1.45680500
C	3.81966500	-1.45438900	0.64654300
O	-0.06106500	-2.73581600	-0.19487000
C	-2.69638400	-1.72048400	2.10359900
H	-2.72837700	-0.77921700	2.66097600

H	-1.94220500	-2.37725200	2.54293200
H	-3.67208400	-2.22190200	2.15349900
O	-2.28616500	-1.49844700	0.74933500
H	-0.78452600	-2.18543200	0.19194900
N	3.46309300	3.44780000	-0.48766600
F	4.55558600	-2.70719400	-1.21969100
F	3.00989100	-0.22332200	2.49975400
F	0.47125700	-1.04661900	1.99784600
F	2.01984200	-3.51534100	-1.74108600
F	5.07530200	-1.04517500	0.89394400

p-FP/DMAP(c)_TS1
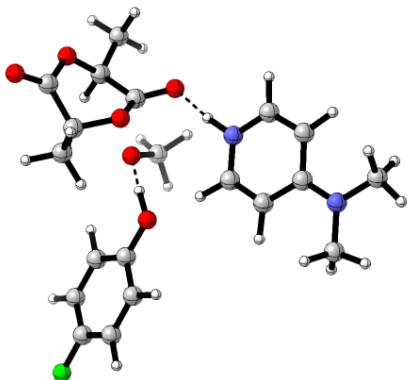
O	0.94806200	1.81056700	-0.79611600
C	0.99287600	2.37383400	0.43665500
O	-0.08438600	2.65177300	0.98330600
H	2.94050300	0.65548300	-3.23314900
C	1.98566800	0.85117200	-2.73748400
H	1.37753400	1.47663200	-3.39899200
H	1.47223000	-0.09722000	-2.55472600
C	2.23171800	1.54965300	-1.41494000
H	2.80623100	0.90300600	-0.73679700
C	2.29642200	3.13704500	0.74466200
H	3.03248500	2.42290500	1.12107700
O	2.82331700	3.71217600	-0.49103400
C	2.95843900	2.88947700	-1.55759700
O	3.58249600	3.23499500	-2.52890200
C	2.09995600	4.28086900	1.72006200
H	1.36459200	4.99595500	1.33920600
H	1.73974000	3.89047800	2.67611000
H	3.05334700	4.79447900	1.87834700
C	-4.59396200	1.28379000	0.19162800
C	-3.38788700	1.90034200	0.43479500
C	-2.20377400	-0.10166600	0.11690400
C	-3.37468900	-0.78469600	-0.13630800

C	-4.62812800	-0.11079900	-0.10809800
H	-5.49715800	1.87880600	0.23424200
H	-3.31336600	2.95817100	0.66680700
H	-1.22586800	-0.59053400	0.10682700
H	-3.30546800	-1.84301800	-0.35311200
C	-7.06589100	-0.03515300	-0.31580500
H	-7.09186600	0.76857100	-1.06365300
H	-7.87716800	-0.72938700	-0.53774800
H	-7.25181600	0.39970300	0.67530900
C	-5.79526800	-2.19059600	-0.65432400
H	-5.37483400	-2.77416600	0.17497500
H	-6.82241300	-2.52005000	-0.81515300
H	-5.22015700	-2.40763000	-1.56390300
N	-2.22400200	1.22028700	0.39839200
H	-1.31583100	1.75003000	0.59479400
C	3.33764400	-3.74395700	0.76100000
C	2.61337000	-2.55028500	0.82935600
C	1.34186300	-2.44031000	0.22628300
C	0.82584200	-3.56475300	-0.45013600
C	1.54571500	-4.75993400	-0.51999400
C	2.79263300	-4.83093400	0.08930800
H	4.31663200	-3.83227100	1.22463100
H	1.14983800	-5.62719400	-1.04183000
O	0.61739800	-1.31029900	0.27243000
C	1.34110600	0.60194700	2.77650700
H	0.42824800	1.18096800	3.01442200
H	2.17173600	1.03832300	3.36073500
H	1.18479600	-0.42398700	3.15335700
O	1.61695700	0.60232400	1.40168700
H	1.10429100	-0.45860400	0.79900200
H	-0.14869800	-3.48562000	-0.92650200
H	3.02590800	-1.68901900	1.34830700
F	3.50084600	-6.00062700	0.02346000
N	-5.79653500	-0.75910400	-0.35261200

p-FP/DMAP(c)_TS2
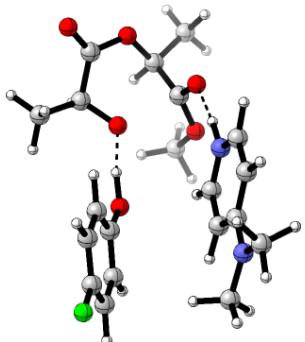
O	-2.14718200	0.78907600	-0.05646000
C	-2.83886400	-1.16633700	0.60785300
O	-2.29328000	-1.96047900	-0.16240000
H	-3.28053100	3.29249600	-2.03303500
C	-2.49682600	2.69629100	-1.55299200
H	-1.84954400	2.29273700	-2.33896700
H	-1.90444500	3.34900200	-0.90233500
C	-3.10035800	1.56106200	-0.71994800
H	-3.81546200	2.03421500	-0.00319600
C	-4.28562700	-0.72653700	0.37628100
H	-4.50572300	0.17040700	0.96245700
O	-4.50528300	-0.45994800	-1.01171700
C	-3.96334600	0.64838600	-1.60870600
O	-4.20316600	0.83016000	-2.77698900
C	-5.25039800	-1.85102400	0.75664000
H	-5.04760700	-2.73680700	0.14699300
H	-5.14132200	-2.11711800	1.81444300
H	-6.28053200	-1.52616700	0.57869700
C	2.36730000	-1.24921000	0.76611800
C	0.99287600	-1.31448600	0.78111400
C	0.98245100	-2.89505300	-0.94742400
C	2.35674600	-2.88588200	-1.02309000
C	3.11062200	-2.03467400	-0.15993200
H	2.85102300	-0.55471200	1.44019400
H	0.38364000	-0.70374200	1.44031900
H	0.36968100	-3.50941700	-1.59949300
H	2.83735200	-3.51594000	-1.76046100
C	5.19707300	-2.76569800	-1.20608500
H	6.26637500	-2.59963700	-1.07046700
H	5.00161400	-3.83736600	-1.07179900
H	4.93465500	-2.48539900	-2.23563000
C	5.19603800	-1.02039100	0.61914500
H	5.05740600	-1.25008000	1.68358600
H	6.26014000	-1.09383700	0.39177900
H	4.87435500	0.01222400	0.43424000

N	0.31867200	-2.12630600	-0.06068200
H	-0.75220400	-2.10041600	-0.05876800
C	2.31244900	2.27739700	-1.07502700
C	1.05982400	1.95013300	-0.54679000
C	0.80625100	2.07290400	0.83599700
C	1.84194800	2.54504900	1.66922200
C	3.09657100	2.86813800	1.14595200
C	3.31351900	2.72177000	-0.22023800
H	2.51017900	2.18960000	-2.14024700
H	3.89409100	3.24028400	1.78400900
O	-0.36353600	1.73556300	1.40038700
C	-2.79251200	-0.09879200	2.79413500
H	-2.73990200	0.89745300	2.34853700
H	-2.11165200	-0.15493000	3.64569700
H	-3.80970200	-0.33096100	3.13183200
O	-2.31894500	-1.08489400	1.86076300
H	-1.10195900	1.40391600	0.72128400
H	1.64151500	2.65777000	2.73175100
H	0.26840700	1.59081400	-1.19790200
F	4.54744300	3.02698900	-0.73524500
N	4.46416900	-1.96674900	-0.22622400

p-FP/DMAP(c)_Int3
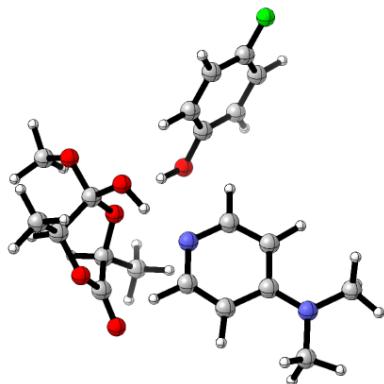
O	1.28675100	-1.78365800	0.69875200
C	1.37922100	-2.11428600	-0.70655900
O	0.85689900	-1.09002800	-1.43811900
H	-0.00064900	-2.72241200	3.64532500
C	0.46521500	-2.02927900	2.93943600
H	-0.17705800	-1.14939000	2.84129800
H	1.43779700	-1.71445900	3.32936800
C	0.64475200	-2.71182900	1.59415500
H	1.28417200	-3.60335400	1.71815600
C	0.68051600	-3.47644100	-0.95803200
H	1.26840900	-4.27571400	-0.48805600

O	-0.63146900	-3.47375200	-0.33034000
C	-0.68193300	-3.18709700	0.99243300
O	-1.71205500	-3.30956000	1.60540300
C	0.48098000	-3.78416700	-2.42965200
H	-0.14571600	-3.02127100	-2.89885500
H	1.45050900	-3.79366100	-2.93709400
H	0.00710500	-4.76437100	-2.54376400
C	-2.67565100	1.98626700	-0.32860900
C	-1.54423800	1.21962000	-0.56733000
C	-2.75904900	-0.71468300	-0.68693700
C	-3.95285900	-0.04690400	-0.45389900
C	-3.94648300	1.35907400	-0.26899900
H	-2.56051300	3.05443600	-0.18726300
H	-0.56756700	1.69911200	-0.61265400
H	-2.76117900	-1.79483200	-0.81796800
H	-4.86971800	-0.62260400	-0.40848700
C	-6.36856600	1.37013800	0.10128600
H	-7.16511300	2.10368300	0.23937400
H	-6.60573000	0.78226000	-0.79518600
H	-6.37040300	0.69297700	0.96875900
C	-5.03221700	3.49829200	0.23082400
H	-4.55442500	4.04197900	-0.59466400
H	-6.04611800	3.88691900	0.34317200
H	-4.47624000	3.71598100	1.15533300
N	-1.55758100	-0.11332300	-0.75003200
H	-0.07405400	-0.83656100	-1.13480400
C	3.40134300	4.07182200	0.91330800
C	2.98983400	2.95464700	1.64257400
C	2.58675100	1.78558100	0.98065900
C	2.59760300	1.73869000	-0.42182600
C	3.01031300	2.85788500	-1.15395900
C	3.40358900	4.00383900	-0.47570500
H	3.71766100	4.98419100	1.41092100
H	3.02792600	2.83739900	-2.24000400
O	2.19747100	0.73187900	1.75630800
C	3.63202100	-2.91477200	-0.28284700
H	3.61223200	-2.57540900	0.75940100
H	4.62372200	-2.72658100	-0.70104400
H	3.43729600	-3.99672700	-0.32397100
O	2.72874800	-2.16656600	-1.09204000
H	1.91255500	-0.02656500	1.21614900
H	2.28768800	0.83422800	-0.94112400
H	2.97726900	2.97458000	2.72886400
F	3.80475500	5.09576400	-1.19116500

| N | -5.09817000 | 2.06895000 | -0.04601300 |

p-FP/DMAP(c)_Int4
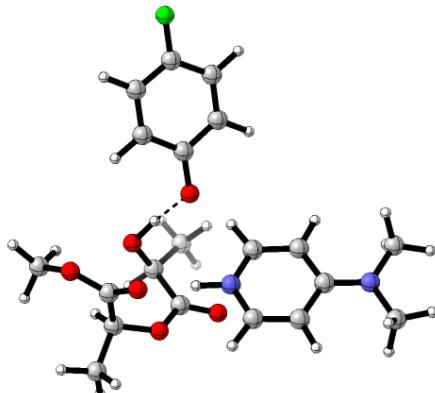
O	2.05132400	-1.28768800	1.04949800
C	1.36246100	-2.59138400	-1.25513800
O	0.49557700	-1.95463600	-1.82650900
H	0.68293600	-1.31952100	4.15829400
C	1.23297600	-0.85917800	3.33066200
H	0.72921600	0.06542600	3.03528900
H	2.24607000	-0.61204000	3.66513100
C	1.33016500	-1.81360700	2.14118700
H	1.85750500	-2.72555200	2.47540600
C	1.02684300	-3.57214000	-0.12129400
H	1.87051100	-3.67371900	0.56084700
O	-0.13336200	-3.10751200	0.58003500
C	-0.06588100	-2.27338800	1.67469200
O	-1.11226100	-1.95733500	2.18356300
C	0.66297800	-4.93672700	-0.71622200
H	-0.20448600	-4.84242500	-1.37708200
H	1.49932200	-5.34678700	-1.29377700
H	0.41720400	-5.63432900	0.09067300
C	-2.78587500	1.32189800	0.04400000
C	-1.64430300	0.61560900	-0.26846500
C	-2.91802600	-0.98435900	-1.44518400
C	-4.09112900	-0.32572900	-1.16590200
C	-4.06285300	0.87598300	-0.39514000
H	-2.67361200	2.21576000	0.64392400
H	-0.62895300	0.89786900	0.06856900
H	-2.88832000	-1.90411800	-2.01955900
H	-5.01868500	-0.74402700	-1.53459500
C	-6.50031000	1.05386700	-0.53984500
H	-7.27876700	1.74045600	-0.20489300
H	-6.55225700	0.99089900	-1.63486400

H	-6.71612100	0.06231500	-0.11926500
C	-5.14028000	2.77083200	0.71466900
H	-4.52010400	3.53824100	0.23429000
H	-6.14824800	3.17158100	0.82901500
H	-4.73543100	2.56711800	1.71473400
N	-1.73051800	-0.51364600	-1.00977600
H	-0.87226600	-1.04691600	-1.23295000
C	3.73829100	3.06099600	-0.91246500
C	2.98514000	1.93928700	-0.55699700
C	1.82976100	2.04420700	0.26318000
C	1.47638800	3.34801100	0.70213500
C	2.22206100	4.47499400	0.34448500
C	3.34430100	4.31428100	-0.45852800
H	4.62092200	2.96971200	-1.54114700
H	1.94418600	5.46826100	0.68933800
O	1.10381200	0.99066000	0.59871500
C	3.73292400	-3.05206700	-0.99237000
H	3.77888100	-2.54459000	-0.02469000
H	4.60422600	-2.79545100	-1.59702000
H	3.68574000	-4.14099000	-0.87593600
O	2.60432500	-2.55536700	-1.74361000
H	1.71570400	-0.31780600	0.84210100
H	0.60630500	3.45425200	1.34762700
H	3.27677400	0.95491300	-0.91670600
F	4.08175100	5.41936000	-0.81154900
N	-5.20135600	1.55421000	-0.09552600

o-FP/MTBD(a')_Int1

O	-2.67955500	-0.54520600	-1.47321600
C	-2.15734200	-1.48527300	-0.67878000
O	-1.28130100	-2.21885400	-1.09352500
H	-4.78581000	2.06665800	-1.53718700
C	-4.13167100	1.30441300	-1.96874800
H	-4.72011700	0.69642800	-2.66320100

H	-3.31867600	1.79778000	-2.50799800
C	-3.55660500	0.45162900	-0.85670600
H	-2.92413200	1.05579500	-0.19194200
C	-2.73951900	-1.55594900	0.72636100
H	-2.26032000	-0.73872100	1.28527700
O	-4.17581900	-1.31928900	0.68216100
C	-4.62237900	-0.25391600	-0.02078300
O	-5.77803000	0.08041300	0.03299900
C	-2.51277200	-2.88821000	1.41335800
H	-2.92705200	-3.71165300	0.82295700
H	-1.43914000	-3.04063700	1.55113900
H	-2.99901000	-2.87424700	2.39352000
C	0.17120500	4.20393400	0.27223600
C	-0.34534500	2.92283200	0.17537200
C	0.06357200	1.81548500	0.97581200
C	1.08926700	2.14363400	1.91410800
C	1.62265400	3.42970000	2.02984500
C	1.17807100	4.47463800	1.21100800
H	-0.22203600	4.97898900	-0.38202700
H	2.39294600	3.61913700	2.77620500
O	-0.44922200	0.62637500	0.83824100
C	0.23413300	-1.26460300	3.59753500
H	0.68972900	-2.09878300	4.14541700
H	-0.85749400	-1.32095400	3.74197300
H	0.58506300	-0.32499900	4.05382700
O	0.60334400	-1.37461500	2.23575800
H	0.22280200	-0.59619000	1.73086000
H	1.44562600	1.34634100	2.56335900
H	1.58564900	5.47726600	1.30600700
F	-1.33386300	2.69886300	-0.76088200
C	2.42355700	-0.94975200	-1.13414300
N	3.65878200	-1.10603400	-0.60032600
N	2.06576100	0.22467500	-1.68961600
C	2.85054000	-3.14111900	0.55846900
H	3.18470700	-4.11873500	0.92408800
H	2.31899000	-2.61985500	1.36399500
C	1.90229500	-3.30509400	-0.62327900
H	0.95932000	-3.76659200	-0.32162500
H	2.34978500	-3.92953700	-1.41073000
C	4.06187800	-2.33160800	0.10939700
H	4.71331000	-2.92911400	-0.54770800
H	4.65968100	-2.02548200	0.97622600
C	4.64609600	-0.03446800	-0.75442600
H	5.44328200	-0.21596100	-0.02778900

H	5.09695700	-0.07240900	-1.75870900
C	3.96765200	1.30774300	-0.50476300
H	4.67751900	2.13258700	-0.62941500
H	3.59062300	1.34069500	0.52350900
C	2.81368800	1.48036700	-1.48357900
H	3.17985900	1.81343500	-2.46565200
H	2.11158700	2.23319900	-1.10805600
C	0.76819800	0.36926400	-2.36094200
H	0.56454000	-0.49953600	-2.99327800
H	-0.03917800	0.50378700	-1.63196200
H	0.82175500	1.25330600	-3.00143300
N	1.56866800	-1.98681500	-1.17049200
H	0.57314500	-1.79702800	-1.27212100

m-FP/MTBD(b')_Int1

O	-2.67955500	-0.54520600	-1.47321600
C	-2.15734200	-1.48527300	-0.67878000
O	-1.28130100	-2.21885400	-1.09352500
H	-4.78581000	2.06665800	-1.53718700
C	-4.13167100	1.30441300	-1.96874800
H	-4.72011700	0.69642800	-2.66320100
H	-3.31867600	1.79778000	-2.50799800
C	-3.55660500	0.45162900	-0.85670600
H	-2.92413200	1.05579500	-0.19194200
C	-2.73951900	-1.55594900	0.72636100
H	-2.26032000	-0.73872100	1.28527700
O	-4.17581900	-1.31928900	0.68216100
C	-4.62237900	-0.25391600	-0.02078300
O	-5.77803000	0.08041300	0.03299900
C	-2.51277200	-2.88821000	1.41335800
H	-2.92705200	-3.71165300	0.82295700
H	-1.43914000	-3.04063700	1.55113900
H	-2.99901000	-2.87424700	2.39352000
C	0.17120500	4.20393400	0.27223600

C	-0.34534500	2.92283200	0.17537200
C	0.06357200	1.81548500	0.97581200
C	1.08926700	2.14363400	1.91410800
C	1.62265400	3.42970000	2.02984500
C	1.17807100	4.47463800	1.21100800
H	2.39294600	3.61913700	2.77620500
O	-0.44922200	0.62637500	0.83824100
C	0.23413300	-1.26460300	3.59753500
H	0.68972900	-2.09878300	4.14541700
H	-0.85749400	-1.32095400	3.74197300
H	0.58506300	-0.32499900	4.05382700
O	0.60334400	-1.37461500	2.23575800
H	0.22280200	-0.59619000	1.73086000
H	1.44562600	1.34634100	2.56335900
H	1.58564900	5.47726600	1.30600700
C	2.42355700	-0.94975200	-1.13414300
N	3.65878200	-1.10603400	-0.60032600
N	2.06576100	0.22467500	-1.68961600
C	2.85054000	-3.14111900	0.55846900
H	3.18470700	-4.11873500	0.92408800
H	2.31899000	-2.61985500	1.36399500
C	1.90229500	-3.30509400	-0.62327900
H	0.95932000	-3.76659200	-0.32162500
H	2.34978500	-3.92953700	-1.41073000
C	4.06187800	-2.33160800	0.10939700
H	4.71331000	-2.92911400	-0.54770800
H	4.65968100	-2.02548200	0.97622600
C	4.64609600	-0.03446800	-0.75442600
H	5.44328200	-0.21596100	-0.02778900
H	5.09695700	-0.07240900	-1.75870900
C	3.96765200	1.30774300	-0.50476300
H	4.67751900	2.13258700	-0.62941500
H	3.59062300	1.34069500	0.52350900
C	2.81368800	1.48036700	-1.48357900
H	3.17985900	1.81343500	-2.46565200
H	2.11158700	2.23319900	-1.10805600
C	0.76819800	0.36926400	-2.36094200
H	0.56454000	-0.49953600	-2.99327800
H	-0.03917800	0.50378700	-1.63196200
H	0.82175500	1.25330600	-3.00143300
N	1.56866800	-1.98681500	-1.17049200
H	0.57314500	-1.79702800	-1.27212100
H	-1.11190494	2.74915214	-0.55065910
F	-0.31680100	5.16576527	-0.53969426

p-FP/MTBD(c')_Int1

O	-2.67955500	-0.54520600	-1.47321600
C	-2.15734200	-1.48527300	-0.67878000
O	-1.28130100	-2.21885400	-1.09352500
H	-4.78581000	2.06665800	-1.53718700
C	-4.13167100	1.30441300	-1.96874800
H	-4.72011700	0.69642800	-2.66320100
H	-3.31867600	1.79778000	-2.50799800
C	-3.55660500	0.45162900	-0.85670600
H	-2.92413200	1.05579500	-0.19194200
C	-2.73951900	-1.55594900	0.72636100
H	-2.26032000	-0.73872100	1.28527700
O	-4.17581900	-1.31928900	0.68216100
C	-4.62237900	-0.25391600	-0.02078300
O	-5.77803000	0.08041300	0.03299900
C	-2.51277200	-2.88821000	1.41335800
H	-2.92705200	-3.71165300	0.82295700
H	-1.43914000	-3.04063700	1.55113900
H	-2.99901000	-2.87424700	2.39352000
C	0.17120500	4.20393400	0.27223600
C	-0.34534500	2.92283200	0.17537200
C	0.06357200	1.81548500	0.97581200
C	1.08926700	2.14363400	1.91410800
C	1.62265400	3.42970000	2.02984500
C	1.17807100	4.47463800	1.21100800
H	2.39294600	3.61913700	2.77620500
O	-0.44922200	0.62637500	0.83824100
C	0.23413300	-1.26460300	3.59753500
H	0.68972900	-2.09878300	4.14541700
H	-0.85749400	-1.32095400	3.74197300
H	0.58506300	-0.32499900	4.05382700
O	0.60334400	-1.37461500	2.23575800
H	0.22280200	-0.59619000	1.73086000

H	1.44562600	1.34634100	2.56335900
C	2.42355700	-0.94975200	-1.13414300
N	3.65878200	-1.10603400	-0.60032600
N	2.06576100	0.22467500	-1.68961600
C	2.85054000	-3.14111900	0.55846900
H	3.18470700	-4.11873500	0.92408800
H	2.31899000	-2.61985500	1.36399500
C	1.90229500	-3.30509400	-0.62327900
H	0.95932000	-3.76659200	-0.32162500
H	2.34978500	-3.92953700	-1.41073000
C	4.06187800	-2.33160800	0.10939700
H	4.71331000	-2.92911400	-0.54770800
H	4.65968100	-2.02548200	0.97622600
C	4.64609600	-0.03446800	-0.75442600
H	5.44328200	-0.21596100	-0.02778900
H	5.09695700	-0.07240900	-1.75870900
C	3.96765200	1.30774300	-0.50476300
H	4.67751900	2.13258700	-0.62941500
H	3.59062300	1.34069500	0.52350900
C	2.81368800	1.48036700	-1.48357900
H	3.17985900	1.81343500	-2.46565200
H	2.11158700	2.23319900	-1.10805600
C	0.76819800	0.36926400	-2.36094200
H	0.56454000	-0.49953600	-2.99327800
H	-0.03917800	0.50378700	-1.63196200
H	0.82175500	1.25330600	-3.00143300
N	1.56866800	-1.98681500	-1.17049200
H	0.57314500	-1.79702800	-1.27212100
H	-1.11190494	2.74915214	-0.55065910
H	-0.21558494	4.96627434	-0.37129391
F	1.68451160	5.72046463	1.32905007

2,3-FP/MTBD(d')_Int1

| O | -2.67955500 | -0.54520600 | -1.47321600 |

C	-2.15734200	-1.48527300	-0.67878000
O	-1.28130100	-2.21885400	-1.09352500
H	-4.78581000	2.06665800	-1.53718700
C	-4.13167100	1.30441300	-1.96874800
H	-4.72011700	0.69642800	-2.66320100
H	-3.31867600	1.79778000	-2.50799800
C	-3.55660500	0.45162900	-0.85670600
H	-2.92413200	1.05579500	-0.19194200
C	-2.73951900	-1.55594900	0.72636100
H	-2.26032000	-0.73872100	1.28527700
O	-4.17581900	-1.31928900	0.68216100
C	-4.62237900	-0.25391600	-0.02078300
O	-5.77803000	0.08041300	0.03299900
C	-2.51277200	-2.88821000	1.41335800
H	-2.92705200	-3.71165300	0.82295700
H	-1.43914000	-3.04063700	1.55113900
H	-2.99901000	-2.87424700	2.39352000
C	0.17120500	4.20393400	0.27223600
C	-0.34534500	2.92283200	0.17537200
C	0.06357200	1.81548500	0.97581200
C	1.08926700	2.14363400	1.91410800
C	1.62265400	3.42970000	2.02984500
C	1.17807100	4.47463800	1.21100800
H	2.39294600	3.61913700	2.77620500
O	-0.44922200	0.62637500	0.83824100
C	0.23413300	-1.26460300	3.59753500
H	0.68972900	-2.09878300	4.14541700
H	-0.85749400	-1.32095400	3.74197300
H	0.58506300	-0.32499900	4.05382700
O	0.60334400	-1.37461500	2.23575800
H	0.22280200	-0.59619000	1.73086000
H	1.44562600	1.34634100	2.56335900
C	2.42355700	-0.94975200	-1.13414300
N	3.65878200	-1.10603400	-0.60032600
N	2.06576100	0.22467500	-1.68961600
C	2.85054000	-3.14111900	0.55846900
H	3.18470700	-4.11873500	0.92408800
H	2.31899000	-2.61985500	1.36399500
C	1.90229500	-3.30509400	-0.62327900
H	0.95932000	-3.76659200	-0.32162500
H	2.34978500	-3.92953700	-1.41073000
C	4.06187800	-2.33160800	0.10939700
H	4.71331000	-2.92911400	-0.54770800
H	4.65968100	-2.02548200	0.97622600

C	4.64609600	-0.03446800	-0.75442600
H	5.44328200	-0.21596100	-0.02778900
H	5.09695700	-0.07240900	-1.75870900
C	3.96765200	1.30774300	-0.50476300
H	4.67751900	2.13258700	-0.62941500
H	3.59062300	1.34069500	0.52350900
C	2.81368800	1.48036700	-1.48357900
H	3.17985900	1.81343500	-2.46565200
H	2.11158700	2.23319900	-1.10805600
C	0.76819800	0.36926400	-2.36094200
H	0.56454000	-0.49953600	-2.99327800
H	-0.03917800	0.50378700	-1.63196200
H	0.82175500	1.25330600	-3.00143300
N	1.56866800	-1.98681500	-1.17049200
H	0.57314500	-1.79702800	-1.27212100
F	-1.31250007	2.70370320	-0.74064855
F	-0.31680100	5.16576527	-0.53969426
H	1.57947207	5.46207096	1.30456727

2,4-FP/MTBD(e')_Int1

O	-2.67955500	-0.54520600	-1.47321600
C	-2.15734200	-1.48527300	-0.67878000
O	-1.28130100	-2.21885400	-1.09352500
H	-4.78581000	2.06665800	-1.53718700
C	-4.13167100	1.30441300	-1.96874800
H	-4.72011700	0.69642800	-2.66320100
H	-3.31867600	1.79778000	-2.50799800
C	-3.55660500	0.45162900	-0.85670600
H	-2.92413200	1.05579500	-0.19194200
C	-2.73951900	-1.55594900	0.72636100
H	-2.26032000	-0.73872100	1.28527700
O	-4.17581900	-1.31928900	0.68216100
C	-4.62237900	-0.25391600	-0.02078300
O	-5.77803000	0.08041300	0.03299900

C	-2.51277200	-2.88821000	1.41335800
H	-2.92705200	-3.71165300	0.82295700
H	-1.43914000	-3.04063700	1.55113900
H	-2.99901000	-2.87424700	2.39352000
C	0.17120500	4.20393400	0.27223600
C	-0.34534500	2.92283200	0.17537200
C	0.06357200	1.81548500	0.97581200
C	1.08926700	2.14363400	1.91410800
C	1.62265400	3.42970000	2.02984500
C	1.17807100	4.47463800	1.21100800
H	2.39294600	3.61913700	2.77620500
O	-0.44922200	0.62637500	0.83824100
C	0.23413300	-1.26460300	3.59753500
H	0.68972900	-2.09878300	4.14541700
H	-0.85749400	-1.32095400	3.74197300
H	0.58506300	-0.32499900	4.05382700
O	0.60334400	-1.37461500	2.23575800
H	0.22280200	-0.59619000	1.73086000
H	1.44562600	1.34634100	2.56335900
C	2.42355700	-0.94975200	-1.13414300
N	3.65878200	-1.10603400	-0.60032600
N	2.06576100	0.22467500	-1.68961600
C	2.85054000	-3.14111900	0.55846900
H	3.18470700	-4.11873500	0.92408800
H	2.31899000	-2.61985500	1.36399500
C	1.90229500	-3.30509400	-0.62327900
H	0.95932000	-3.76659200	-0.32162500
H	2.34978500	-3.92953700	-1.41073000
C	4.06187800	-2.33160800	0.10939700
H	4.71331000	-2.92911400	-0.54770800
H	4.65968100	-2.02548200	0.97622600
C	4.64609600	-0.03446800	-0.75442600
H	5.44328200	-0.21596100	-0.02778900
H	5.09695700	-0.07240900	-1.75870900
C	3.96765200	1.30774300	-0.50476300
H	4.67751900	2.13258700	-0.62941500
H	3.59062300	1.34069500	0.52350900
C	2.81368800	1.48036700	-1.48357900
H	3.17985900	1.81343500	-2.46565200
H	2.11158700	2.23319900	-1.10805600
C	0.76819800	0.36926400	-2.36094200
H	0.56454000	-0.49953600	-2.99327800
H	-0.03917800	0.50378700	-1.63196200
H	0.82175500	1.25330600	-3.00143300

N	1.56866800	-1.98681500	-1.17049200
H	0.57314500	-1.79702800	-1.27212100
F	-1.31250007	2.70370320	-0.74064855
F	1.68451160	5.72046463	1.32905007
H	-0.21558494	4.96627434	-0.37129391

2,6-FP/MTBD(f')_Int1

O	-2.67955500	-0.54520600	-1.47321600
C	-2.15734200	-1.48527300	-0.67878000
O	-1.28130100	-2.21885400	-1.09352500
H	-4.78581000	2.06665800	-1.53718700
C	-4.13167100	1.30441300	-1.96874800
H	-4.72011700	0.69642800	-2.66320100
H	-3.31867600	1.79778000	-2.50799800
C	-3.55660500	0.45162900	-0.85670600
H	-2.92413200	1.05579500	-0.19194200
C	-2.73951900	-1.55594900	0.72636100
H	-2.26032000	-0.73872100	1.28527700
O	-4.17581900	-1.31928900	0.68216100
C	-4.62237900	-0.25391600	-0.02078300
O	-5.77803000	0.08041300	0.03299900
C	-2.51277200	-2.88821000	1.41335800
H	-2.92705200	-3.71165300	0.82295700
H	-1.43914000	-3.04063700	1.55113900
H	-2.99901000	-2.87424700	2.39352000
C	0.17120500	4.20393400	0.27223600
C	-0.34534500	2.92283200	0.17537200
C	0.06357200	1.81548500	0.97581200
C	1.08926700	2.14363400	1.91410800
C	1.62265400	3.42970000	2.02984500
C	1.17807100	4.47463800	1.21100800
H	2.39294600	3.61913700	2.77620500
O	-0.44922200	0.62637500	0.83824100
C	0.23413300	-1.26460300	3.59753500

H	0.68972900	-2.09878300	4.14541700
H	-0.85749400	-1.32095400	3.74197300
H	0.58506300	-0.32499900	4.05382700
O	0.60334400	-1.37461500	2.23575800
H	0.22280200	-0.59619000	1.73086000
C	2.42355700	-0.94975200	-1.13414300
N	3.65878200	-1.10603400	-0.60032600
N	2.06576100	0.22467500	-1.68961600
C	2.85054000	-3.14111900	0.55846900
H	3.18470700	-4.11873500	0.92408800
H	2.31899000	-2.61985500	1.36399500
C	1.90229500	-3.30509400	-0.62327900
H	0.95932000	-3.76659200	-0.32162500
H	2.34978500	-3.92953700	-1.41073000
C	4.06187800	-2.33160800	0.10939700
H	4.71331000	-2.92911400	-0.54770800
H	4.65968100	-2.02548200	0.97622600
C	4.64609600	-0.03446800	-0.75442600
H	5.44328200	-0.21596100	-0.02778900
H	5.09695700	-0.07240900	-1.75870900
C	3.96765200	1.30774300	-0.50476300
H	4.67751900	2.13258700	-0.62941500
H	3.59062300	1.34069500	0.52350900
C	2.81368800	1.48036700	-1.48357900
H	3.17985900	1.81343500	-2.46565200
H	2.11158700	2.23319900	-1.10805600
C	0.76819800	0.36926400	-2.36094200
H	0.56454000	-0.49953600	-2.99327800
H	-0.03917800	0.50378700	-1.63196200
H	0.82175500	1.25330600	-3.00143300
N	1.56866800	-1.98681500	-1.17049200
H	0.57314500	-1.79702800	-1.27212100
F	-1.31250007	2.70370320	-0.74064855
H	-0.21558494	4.96627434	-0.37129391
F	1.53135623	1.15453410	2.71955104
H	1.57947207	5.46207096	1.30456727

2,3,6-FP/MTBD(g')_Int1

O	-2.67955500	-0.54520600	-1.47321600
C	-2.15734200	-1.48527300	-0.67878000
O	-1.28130100	-2.21885400	-1.09352500
H	-4.78581000	2.06665800	-1.53718700
C	-4.13167100	1.30441300	-1.96874800
H	-4.72011700	0.69642800	-2.66320100
H	-3.31867600	1.79778000	-2.50799800
C	-3.55660500	0.45162900	-0.85670600
H	-2.92413200	1.05579500	-0.19194200
C	-2.73951900	-1.55594900	0.72636100
H	-2.26032000	-0.73872100	1.28527700
O	-4.17581900	-1.31928900	0.68216100
C	-4.62237900	-0.25391600	-0.02078300
O	-5.77803000	0.08041300	0.03299900
C	-2.51277200	-2.88821000	1.41335800
H	-2.92705200	-3.71165300	0.82295700
H	-1.43914000	-3.04063700	1.55113900
H	-2.99901000	-2.87424700	2.39352000
C	0.17120500	4.20393400	0.27223600
C	-0.34534500	2.92283200	0.17537200
C	0.06357200	1.81548500	0.97581200
C	1.08926700	2.14363400	1.91410800
C	1.62265400	3.42970000	2.02984500
C	1.17807100	4.47463800	1.21100800
H	2.39294600	3.61913700	2.77620500
O	-0.44922200	0.62637500	0.83824100
C	0.23413300	-1.26460300	3.59753500
H	0.68972900	-2.09878300	4.14541700
H	-0.85749400	-1.32095400	3.74197300
H	0.58506300	-0.32499900	4.05382700
O	0.60334400	-1.37461500	2.23575800
H	0.22280200	-0.59619000	1.73086000
H	1.58564900	5.47726600	1.30600700
F	-1.33386300	2.69886300	-0.76088200
C	2.42355700	-0.94975200	-1.13414300

N	3.65878200	-1.10603400	-0.60032600
N	2.06576100	0.22467500	-1.68961600
C	2.85054000	-3.14111900	0.55846900
H	3.18470700	-4.11873500	0.92408800
H	2.31899000	-2.61985500	1.36399500
C	1.90229500	-3.30509400	-0.62327900
H	0.95932000	-3.76659200	-0.32162500
H	2.34978500	-3.92953700	-1.41073000
C	4.06187800	-2.33160800	0.10939700
H	4.71331000	-2.92911400	-0.54770800
H	4.65968100	-2.02548200	0.97622600
C	4.64609600	-0.03446800	-0.75442600
H	5.44328200	-0.21596100	-0.02778900
H	5.09695700	-0.07240900	-1.75870900
C	3.96765200	1.30774300	-0.50476300
H	4.67751900	2.13258700	-0.62941500
H	3.59062300	1.34069500	0.52350900
C	2.81368800	1.48036700	-1.48357900
H	3.17985900	1.81343500	-2.46565200
H	2.11158700	2.23319900	-1.10805600
C	0.76819800	0.36926400	-2.36094200
H	0.56454000	-0.49953600	-2.99327800
H	-0.03917800	0.50378700	-1.63196200
H	0.82175500	1.25330600	-3.00143300
N	1.56866800	-1.98681500	-1.17049200
H	0.57314500	-1.79702800	-1.27212100
F	-0.31680100	5.16576527	-0.53969426
F	1.53135623	1.15453410	2.71955104

3,4,5-FP/MTBD(h')_Int1

O	-2.67955500	-0.54520600	-1.47321600
C	-2.15734200	-1.48527300	-0.67878000
O	-1.28130100	-2.21885400	-1.09352500
H	-4.78581000	2.06665800	-1.53718700
C	-4.13167100	1.30441300	-1.96874800

H	-4.72011700	0.69642800	-2.66320100
H	-3.31867600	1.79778000	-2.50799800
C	-3.55660500	0.45162900	-0.85670600
H	-2.92413200	1.05579500	-0.19194200
C	-2.73951900	-1.55594900	0.72636100
H	-2.26032000	-0.73872100	1.28527700
O	-4.17581900	-1.31928900	0.68216100
C	-4.62237900	-0.25391600	-0.02078300
O	-5.77803000	0.08041300	0.03299900
C	-2.51277200	-2.88821000	1.41335800
H	-2.92705200	-3.71165300	0.82295700
H	-1.43914000	-3.04063700	1.55113900
H	-2.99901000	-2.87424700	2.39352000
C	0.17120500	4.20393400	0.27223600
C	-0.34534500	2.92283200	0.17537200
C	0.06357200	1.81548500	0.97581200
C	1.08926700	2.14363400	1.91410800
C	1.62265400	3.42970000	2.02984500
C	1.17807100	4.47463800	1.21100800
O	-0.44922200	0.62637500	0.83824100
C	0.23413300	-1.26460300	3.59753500
H	0.68972900	-2.09878300	4.14541700
H	-0.85749400	-1.32095400	3.74197300
H	0.58506300	-0.32499900	4.05382700
O	0.60334400	-1.37461500	2.23575800
H	0.22280200	-0.59619000	1.73086000
C	2.42355700	-0.94975200	-1.13414300
N	3.65878200	-1.10603400	-0.60032600
N	2.06576100	0.22467500	-1.68961600
C	2.85054000	-3.14111900	0.55846900
H	3.18470700	-4.11873500	0.92408800
H	2.31899000	-2.61985500	1.36399500
C	1.90229500	-3.30509400	-0.62327900
H	0.95932000	-3.76659200	-0.32162500
H	2.34978500	-3.92953700	-1.41073000
C	4.06187800	-2.33160800	0.10939700
H	4.71331000	-2.92911400	-0.54770800
H	4.65968100	-2.02548200	0.97622600
C	4.64609600	-0.03446800	-0.75442600
H	5.44328200	-0.21596100	-0.02778900
H	5.09695700	-0.07240900	-1.75870900
C	3.96765200	1.30774300	-0.50476300
H	4.67751900	2.13258700	-0.62941500
H	3.59062300	1.34069500	0.52350900

C	2.81368800	1.48036700	-1.48357900
H	3.17985900	1.81343500	-2.46565200
H	2.11158700	2.23319900	-1.10805600
C	0.76819800	0.36926400	-2.36094200
H	0.56454000	-0.49953600	-2.99327800
H	-0.03917800	0.50378700	-1.63196200
H	0.82175500	1.25330600	-3.00143300
N	1.56866800	-1.98681500	-1.17049200
H	0.57314500	-1.79702800	-1.27212100
F	-0.31680100	5.16576527	-0.53969426
F	1.68451160	5.72046463	1.32905007
F	2.57741316	3.66450279	2.95494100
H	-1.11190494	2.74915214	-0.55065910
H	1.43966365	1.35968074	2.55249619

2,3,5,6-FP/MTBD(I')_Int1

O	-2.67955500	-0.54520600	-1.47321600
C	-2.15734200	-1.48527300	-0.67878000
O	-1.28130100	-2.21885400	-1.09352500
H	-4.78581000	2.06665800	-1.53718700
C	-4.13167100	1.30441300	-1.96874800
H	-4.72011700	0.69642800	-2.66320100
H	-3.31867600	1.79778000	-2.50799800
C	-3.55660500	0.45162900	-0.85670600
H	-2.92413200	1.05579500	-0.19194200
C	-2.73951900	-1.55594900	0.72636100
H	-2.26032000	-0.73872100	1.28527700
O	-4.17581900	-1.31928900	0.68216100
C	-4.62237900	-0.25391600	-0.02078300
O	-5.77803000	0.08041300	0.03299900
C	-2.51277200	-2.88821000	1.41335800
H	-2.92705200	-3.71165300	0.82295700
H	-1.43914000	-3.04063700	1.55113900
H	-2.99901000	-2.87424700	2.39352000
C	0.17120500	4.20393400	0.27223600

C	-0.34534500	2.92283200	0.17537200
C	0.06357200	1.81548500	0.97581200
C	1.08926700	2.14363400	1.91410800
C	1.62265400	3.42970000	2.02984500
C	1.17807100	4.47463800	1.21100800
O	-0.44922200	0.62637500	0.83824100
C	0.23413300	-1.26460300	3.59753500
H	0.68972900	-2.09878300	4.14541700
H	-0.85749400	-1.32095400	3.74197300
H	0.58506300	-0.32499900	4.05382700
O	0.60334400	-1.37461500	2.23575800
H	0.22280200	-0.59619000	1.73086000
H	1.58564900	5.47726600	1.30600700
F	-1.33386300	2.69886300	-0.76088200
C	2.42355700	-0.94975200	-1.13414300
N	3.65878200	-1.10603400	-0.60032600
N	2.06576100	0.22467500	-1.68961600
C	2.85054000	-3.14111900	0.55846900
H	3.18470700	-4.11873500	0.92408800
H	2.31899000	-2.61985500	1.36399500
C	1.90229500	-3.30509400	-0.62327900
H	0.95932000	-3.76659200	-0.32162500
H	2.34978500	-3.92953700	-1.41073000
C	4.06187800	-2.33160800	0.10939700
H	4.71331000	-2.92911400	-0.54770800
H	4.65968100	-2.02548200	0.97622600
C	4.64609600	-0.03446800	-0.75442600
H	5.44328200	-0.21596100	-0.02778900
H	5.09695700	-0.07240900	-1.75870900
C	3.96765200	1.30774300	-0.50476300
H	4.67751900	2.13258700	-0.62941500
H	3.59062300	1.34069500	0.52350900
C	2.81368800	1.48036700	-1.48357900
H	3.17985900	1.81343500	-2.46565200
H	2.11158700	2.23319900	-1.10805600
C	0.76819800	0.36926400	-2.36094200
H	0.56454000	-0.49953600	-2.99327800
H	-0.03917800	0.50378700	-1.63196200
H	0.82175500	1.25330600	-3.00143300
N	1.56866800	-1.98681500	-1.17049200
H	0.57314500	-1.79702800	-1.27212100
F	-0.31680100	5.16576527	-0.53969426
F	1.53135623	1.15453410	2.71955104
F	2.57741316	3.66450279	2.95494100

2,3,4,5,6-FP/MTBD(j')_Int1

O	-2.67955500	-0.54520600	-1.47321600
C	-2.15734200	-1.48527300	-0.67878000
O	-1.28130100	-2.21885400	-1.09352500
H	-4.78581000	2.06665800	-1.53718700
C	-4.13167100	1.30441300	-1.96874800
H	-4.72011700	0.69642800	-2.66320100
H	-3.31867600	1.79778000	-2.50799800
C	-3.55660500	0.45162900	-0.85670600
H	-2.92413200	1.05579500	-0.19194200
C	-2.73951900	-1.55594900	0.72636100
H	-2.26032000	-0.73872100	1.28527700
O	-4.17581900	-1.31928900	0.68216100
C	-4.62237900	-0.25391600	-0.02078300
O	-5.77803000	0.08041300	0.03299900
C	-2.51277200	-2.88821000	1.41335800
H	-2.92705200	-3.71165300	0.82295700
H	-1.43914000	-3.04063700	1.55113900
H	-2.99901000	-2.87424700	2.39352000
C	0.17120500	4.20393400	0.27223600
C	-0.34534500	2.92283200	0.17537200
C	0.06357200	1.81548500	0.97581200
C	1.08926700	2.14363400	1.91410800
C	1.62265400	3.42970000	2.02984500
C	1.17807100	4.47463800	1.21100800
O	-0.44922200	0.62637500	0.83824100
C	0.23413300	-1.26460300	3.59753500
H	0.68972900	-2.09878300	4.14541700
H	-0.85749400	-1.32095400	3.74197300
H	0.58506300	-0.32499900	4.05382700
O	0.60334400	-1.37461500	2.23575800
H	0.22280200	-0.59619000	1.73086000
F	-1.33386300	2.69886300	-0.76088200

C	2.42355700	-0.94975200	-1.13414300
N	3.65878200	-1.10603400	-0.60032600
N	2.06576100	0.22467500	-1.68961600
C	2.85054000	-3.14111900	0.55846900
H	3.18470700	-4.11873500	0.92408800
H	2.31899000	-2.61985500	1.36399500
C	1.90229500	-3.30509400	-0.62327900
H	0.95932000	-3.76659200	-0.32162500
H	2.34978500	-3.92953700	-1.41073000
C	4.06187800	-2.33160800	0.10939700
H	4.71331000	-2.92911400	-0.54770800
H	4.65968100	-2.02548200	0.97622600
C	4.64609600	-0.03446800	-0.75442600
H	5.44328200	-0.21596100	-0.02778900
H	5.09695700	-0.07240900	-1.75870900
C	3.96765200	1.30774300	-0.50476300
H	4.67751900	2.13258700	-0.62941500
H	3.59062300	1.34069500	0.52350900
C	2.81368800	1.48036700	-1.48357900
H	3.17985900	1.81343500	-2.46565200
H	2.11158700	2.23319900	-1.10805600
C	0.76819800	0.36926400	-2.36094200
H	0.56454000	-0.49953600	-2.99327800
H	-0.03917800	0.50378700	-1.63196200
H	0.82175500	1.25330600	-3.00143300
N	1.56866800	-1.98681500	-1.17049200
H	0.57314500	-1.79702800	-1.27212100
F	-0.31680100	5.16576527	-0.53969426
F	1.53135623	1.15453410	2.71955104
F	2.57741316	3.66450279	2.95494100
F	1.68451160	5.72046463	1.32905007

o-FP/MTBD(a')_Int2

O	1.66037827	-1.90776036	0.89874642
C	1.96023227	-0.73014536	0.15409342
O	1.13233627	-0.59878736	-0.90956358

H	2.72528127	-5.00530236	1.57486942
C	1.98600327	-4.20725136	1.46532842
H	1.22524927	-4.53824936	0.75175942
H	1.51327527	-4.01976236	2.43504642
C	2.65978327	-2.93866236	0.97158242
H	3.44039527	-2.63620836	1.69317642
C	3.42776827	-0.73537936	-0.32911558
H	4.08629727	-0.67680636	0.54818942
O	3.70598827	-1.98881836	-1.00565358
C	3.36548527	-3.13202036	-0.37519658
O	3.63828127	-4.20557136	-0.85034358
C	3.75830427	0.38075964	-1.30258258
H	3.12597327	0.30463364	-2.19038458
H	3.59186827	1.35587864	-0.83460458
H	4.80943427	0.30647664	-1.59900358
H	0.17696327	-0.79485536	-0.65250858
C	-1.07200600	5.61933900	0.07560300
C	0.17339600	5.01748100	-0.02696100
C	0.35581900	3.63724200	0.15487100
C	-0.77757600	2.86411900	0.44776000
C	-2.03885300	3.45935300	0.55632000
C	-2.19381000	4.83533700	0.37176100
O	1.60716100	3.13464200	0.04071200
C	2.24642527	0.35941464	2.35419642
H	1.88093627	-0.51954036	2.89484542
H	1.88312727	1.26754964	2.84170542
H	3.34480827	0.37479164	2.36279942
O	1.71989127	0.39303564	1.02325742
H	1.61160300	2.17216400	0.21972800
C	-2.40260550	-1.21906873	0.00797865
N	-3.42191629	-2.17361938	-0.15744936
N	-1.14906340	-1.47877918	0.17232281
N	-2.79075657	0.12145698	-0.12062267
C	-1.66195927	-3.84903349	-0.45102625
H	-1.37271833	-4.88573624	-0.23566271
H	-1.66429584	-3.72281678	-1.54200729
C	-0.68658716	-2.85859241	0.19057818
H	0.28611207	-2.90028793	-0.31908900
H	-0.49021719	-3.15532105	1.23472548
C	-3.06007303	-3.56914799	0.08655186
H	-3.10557843	-3.80472700	1.16705152
H	-3.80995846	-4.19789322	-0.41135987
C	-4.80801593	-1.85494433	0.17343335
H	-5.44915464	-2.59902535	-0.31736417

H	-4.98370346	-1.95090712	1.26313260
C	-5.16691406	-0.44864680	-0.28351254
H	-6.17096331	-0.18419317	0.06996712
H	-5.16566777	-0.40156355	-1.37971375
C	-4.13762957	0.52747289	0.26950713
H	-4.23505127	0.59679678	1.37139911
H	-4.31188096	1.53436370	-0.12804380
C	-1.75940139	1.12556867	0.11113831
H	-0.85056298	0.85172395	-0.42534482
H	-2.12986795	2.08860982	-0.25770515
H	-1.50147135	1.22723200	1.17854903
F	1.25229779	5.77829951	-0.30914199
H	-0.65997386	1.80906259	0.58164690
H	-2.88710762	2.84765933	0.78258303
H	-3.15756328	5.29277020	0.45443195
H	-1.14641024	6.67628909	-0.07346250

m-FP/MTBD(b')_Int2

O	1.66037827	-1.90776036	0.89874642
C	1.96023227	-0.73014536	0.15409342
O	1.13233627	-0.59878736	-0.90956358
H	2.72528127	-5.00530236	1.57486942
C	1.98600327	-4.20725136	1.46532842
H	1.22524927	-4.53824936	0.75175942
H	1.51327527	-4.01976236	2.43504642
C	2.65978327	-2.93866236	0.97158242
H	3.44039527	-2.63620836	1.69317642
C	3.42776827	-0.73537936	-0.32911558
H	4.08629727	-0.67680636	0.54818942
O	3.70598827	-1.98881836	-1.00565358
C	3.36548527	-3.13202036	-0.37519658
O	3.63828127	-4.20557136	-0.85034358
C	3.75830427	0.38075964	-1.30258258
H	3.12597327	0.30463364	-2.19038458
H	3.59186827	1.35587864	-0.83460458
H	4.80943427	0.30647664	-1.59900358

H	0.17696327	-0.79485536	-0.65250858
C	-1.07200600	5.61933900	0.07560300
C	0.17339600	5.01748100	-0.02696100
C	0.35581900	3.63724200	0.15487100
C	-0.77757600	2.86411900	0.44776000
C	-2.03885300	3.45935300	0.55632000
C	-2.19381000	4.83533700	0.37176100
O	1.60716100	3.13464200	0.04071200
C	2.24642527	0.35941464	2.35419642
H	1.88093627	-0.51954036	2.89484542
H	1.88312727	1.26754964	2.84170542
H	3.34480827	0.37479164	2.36279942
O	1.71989127	0.39303564	1.02325742
H	1.61160300	2.17216400	0.21972800
C	-2.40260550	-1.21906873	0.00797865
N	-3.42191629	-2.17361938	-0.15744936
N	-1.14906340	-1.47877918	0.17232281
N	-2.79075657	0.12145698	-0.12062267
C	-1.66195927	-3.84903349	-0.45102625
H	-1.37271833	-4.88573624	-0.23566271
H	-1.66429584	-3.72281678	-1.54200729
C	-0.68658716	-2.85859241	0.19057818
H	0.28611207	-2.90028793	-0.31908900
H	-0.49021719	-3.15532105	1.23472548
C	-3.06007303	-3.56914799	0.08655186
H	-3.10557843	-3.80472700	1.16705152
H	-3.80995846	-4.19789322	-0.41135987
C	-4.80801593	-1.85494433	0.17343335
H	-5.44915464	-2.59902535	-0.31736417
H	-4.98370346	-1.95090712	1.26313260
C	-5.16691406	-0.44864680	-0.28351254
H	-6.17096331	-0.18419317	0.06996712
H	-5.16566777	-0.40156355	-1.37971375
C	-4.13762957	0.52747289	0.26950713
H	-4.23505127	0.59679678	1.37139911
H	-4.31188096	1.53436370	-0.12804380
C	-1.75940139	1.12556867	0.11113831
H	-0.85056298	0.85172395	-0.42534482
H	-2.12986795	2.08860982	-0.25770515
H	-1.50147135	1.22723200	1.17854903
H	-0.65997386	1.80906259	0.58164690
H	-2.88710762	2.84765933	0.78258303
H	-3.15756328	5.29277020	0.45443195
F	-1.16588051	6.95287416	-0.11247029

| H | 1.02852557 | 5.62050012 | -0.25061556 |

p-FP/MTBD(c')_Int2

O	1.66037827	-1.90776036	0.89874642
C	1.96023227	-0.73014536	0.15409342
O	1.13233627	-0.59878736	-0.90956358
H	2.72528127	-5.00530236	1.57486942
C	1.98600327	-4.20725136	1.46532842
H	1.22524927	-4.53824936	0.75175942
H	1.51327527	-4.01976236	2.43504642
C	2.65978327	-2.93866236	0.97158242
H	3.44039527	-2.63620836	1.69317642
C	3.42776827	-0.73537936	-0.32911558
H	4.08629727	-0.67680636	0.54818942
O	3.70598827	-1.98881836	-1.00565358
C	3.36548527	-3.13202036	-0.37519658
O	3.63828127	-4.20557136	-0.85034358
C	3.75830427	0.38075964	-1.30258258
H	3.12597327	0.30463364	-2.19038458
H	3.59186827	1.35587864	-0.83460458
H	4.80943427	0.30647664	-1.59900358
H	0.17696327	-0.79485536	-0.65250858
C	-1.07200600	5.61933900	0.07560300
C	0.17339600	5.01748100	-0.02696100
C	0.35581900	3.63724200	0.15487100
C	-0.77757600	2.86411900	0.44776000
C	-2.03885300	3.45935300	0.55632000
C	-2.19381000	4.83533700	0.37176100
H	-2.90087000	2.83773500	0.78625400
O	1.60716100	3.13464200	0.04071200
C	2.24642527	0.35941464	2.35419642
H	1.88093627	-0.51954036	2.89484542
H	1.88312727	1.26754964	2.84170542
H	3.34480827	0.37479164	2.36279942

O	1.71989127	0.39303564	1.02325742
H	1.61160300	2.17216400	0.21972800
H	-0.65804400	1.79174900	0.58384400
C	-2.40260550	-1.21906873	0.00797865
N	-3.42191629	-2.17361938	-0.15744936
N	-1.14906340	-1.47877918	0.17232281
N	-2.79075657	0.12145698	-0.12062267
C	-1.66195927	-3.84903349	-0.45102625
H	-1.37271833	-4.88573624	-0.23566271
H	-1.66429584	-3.72281678	-1.54200729
C	-0.68658716	-2.85859241	0.19057818
H	0.28611207	-2.90028793	-0.31908900
H	-0.49021719	-3.15532105	1.23472548
C	-3.06007303	-3.56914799	0.08655186
H	-3.10557843	-3.80472700	1.16705152
H	-3.80995846	-4.19789322	-0.41135987
C	-4.80801593	-1.85494433	0.17343335
H	-5.44915464	-2.59902535	-0.31736417
H	-4.98370346	-1.95090712	1.26313260
C	-5.16691406	-0.44864680	-0.28351254
H	-6.17096331	-0.18419317	0.06996712
H	-5.16566777	-0.40156355	-1.37971375
C	-4.13762957	0.52747289	0.26950713
H	-4.23505127	0.59679678	1.37139911
H	-4.31188096	1.53436370	-0.12804380
C	-1.75940139	1.12556867	0.11113831
H	-0.85056298	0.85172395	-0.42534482
H	-2.12986795	2.08860982	-0.25770515
H	-1.50147135	1.22723200	1.17854903
H	1.02852557	5.62050012	-0.25061556
H	-1.14641024	6.67628909	-0.07346250
F	-3.40976040	5.41247235	0.47606547

2,3-FP/MTBD(d')_Int2

O	1.39638200	1.93784100	0.94038200

C	0.13382800	2.01569600	0.28469600
O	-0.09352300	0.94384000	-0.51171300
H	4.62083000	2.73793500	0.54103200
C	3.78032900	2.11234700	0.85406700
H	3.88530500	1.12779500	0.38863000
H	3.80338400	1.99541600	1.94233800
C	2.46707500	2.75478900	0.44133300
H	2.39237500	3.75728500	0.90227900
C	0.04842100	3.30803600	-0.56018000
H	0.18904300	4.17524000	0.09956700
O	1.13651700	3.30162700	-1.52146000
C	2.36894700	2.98699300	-1.07100900
O	3.30915100	2.94921100	-1.82561900
C	-1.24098000	3.45089300	-1.34607400
H	-1.36587700	2.60079100	-2.02146500
H	-2.09539500	3.48850100	-0.66307400
H	-1.21578200	4.37490800	-1.93252600
H	0.27379000	0.05759700	-0.12599200
C	-5.91366700	-1.34373300	0.26007400
C	-5.11635300	-0.68952500	1.20122000
C	-3.88516700	-0.13412500	0.82332100
C	-3.45297600	-0.24034000	-0.50740800
C	-4.25159300	-0.89277900	-1.45276700
C	-5.46694500	-1.43304900	-1.05369000
O	-3.15243800	0.48970700	1.78923700
C	-0.74617200	2.93596600	2.39704800
H	0.24269000	2.87223400	2.86289000
H	-1.51323500	2.64784500	3.12030200
H	-0.94148700	3.96655200	2.07022400
O	-0.86189500	2.00526400	1.31509300
H	-2.34633700	0.89585900	1.41713800
C	1.78449500	-2.05520500	-0.05888700
N	2.62108100	-2.84101700	0.71752100
N	0.76760800	-1.37410600	0.40413600
N	2.06055200	-2.02237100	-1.41056100
C	1.53264700	-1.91006000	2.71075200
H	1.18817800	-2.15966900	3.72188600
H	2.19089400	-1.03474000	2.78476800
C	0.35510800	-1.58864400	1.79138600
H	-0.15973900	-0.68390400	2.13328600
H	-0.38800700	-2.40202500	1.83905900
C	2.30464200	-3.08643400	2.12461900
H	1.71553400	-4.01444500	2.22829700
H	3.25053400	-3.24245900	2.65991300

C	3.57068600	-3.73848100	0.07233300
H	4.25245000	-4.11417900	0.84327900
H	3.06458400	-4.61307600	-0.37396100
C	4.33178900	-2.95486600	-0.99076300
H	5.07123600	-3.58681500	-1.49620100
H	4.87115800	-2.13500700	-0.50082800
C	3.33779700	-2.41018600	-2.01392600
H	3.13043500	-3.17483100	-2.77919100
H	3.76875100	-1.54447600	-2.53982100
C	1.12411500	-1.38907800	-2.33175200
H	1.33207100	-0.32042000	-2.47500200
H	1.20289500	-1.89536200	-3.30163800
H	0.10570600	-1.49499500	-1.95517900
H	-5.43785100	-0.60045700	2.23525400
H	-6.87008000	-1.77830500	0.53664300
F	-2.25935385	0.27756799	-0.86732116
F	-3.85593392	-1.00584149	-2.73852388
H	-6.07682808	-1.93321952	-1.77671979

2,4-FP/MTBD(e')_Int2

O	1.39638200	1.93784100	0.94038200
C	0.13382800	2.01569600	0.28469600
O	-0.09352300	0.94384000	-0.51171300
H	4.62083000	2.73793500	0.54103200
C	3.78032900	2.11234700	0.85406700
H	3.88530500	1.12779500	0.38863000
H	3.80338400	1.99541600	1.94233800
C	2.46707500	2.75478900	0.44133300
H	2.39237500	3.75728500	0.90227900
C	0.04842100	3.30803600	-0.56018000
H	0.18904300	4.17524000	0.09956700
O	1.13651700	3.30162700	-1.52146000
C	2.36894700	2.98699300	-1.07100900
O	3.30915100	2.94921100	-1.82561900
C	-1.24098000	3.45089300	-1.34607400

H	-1.36587700	2.60079100	-2.02146500
H	-2.09539500	3.48850100	-0.66307400
H	-1.21578200	4.37490800	-1.93252600
H	0.27379000	0.05759700	-0.12599200
C	-5.91366700	-1.34373300	0.26007400
C	-5.11635300	-0.68952500	1.20122000
C	-3.88516700	-0.13412500	0.82332100
C	-3.45297600	-0.24034000	-0.50740800
C	-4.25159300	-0.89277900	-1.45276700
C	-5.46694500	-1.43304900	-1.05369000
O	-3.15243800	0.48970700	1.78923700
C	-0.74617200	2.93596600	2.39704800
H	0.24269000	2.87223400	2.86289000
H	-1.51323500	2.64784500	3.12030200
H	-0.94148700	3.96655200	2.07022400
O	-0.86189500	2.00526400	1.31509300
H	-2.34633700	0.89585900	1.41713800
C	1.78449500	-2.05520500	-0.05888700
N	2.62108100	-2.84101700	0.71752100
N	0.76760800	-1.37410600	0.40413600
N	2.06055200	-2.02237100	-1.41056100
C	1.53264700	-1.91006000	2.71075200
H	1.18817800	-2.15966900	3.72188600
H	2.19089400	-1.03474000	2.78476800
C	0.35510800	-1.58864400	1.79138600
H	-0.15973900	-0.68390400	2.13328600
H	-0.38800700	-2.40202500	1.83905900
C	2.30464200	-3.08643400	2.12461900
H	1.71553400	-4.01444500	2.22829700
H	3.25053400	-3.24245900	2.65991300
C	3.57068600	-3.73848100	0.07233300
H	4.25245000	-4.11417900	0.84327900
H	3.06458400	-4.61307600	-0.37396100
C	4.33178900	-2.95486600	-0.99076300
H	5.07123600	-3.58681500	-1.49620100
H	4.87115800	-2.13500700	-0.50082800
C	3.33779700	-2.41018600	-2.01392600
H	3.13043500	-3.17483100	-2.77919100
H	3.76875100	-1.54447600	-2.53982100
C	1.12411500	-1.38907800	-2.33175200
H	1.33207100	-0.32042000	-2.47500200
H	1.20289500	-1.89536200	-3.30163800
H	0.10570600	-1.49499500	-1.95517900
H	-5.43785100	-0.60045700	2.23525400

H	-6.87008000	-1.77830500	0.53664300
F	-2.25935385	0.27756799	-0.86732116
F	-6.23642365	-2.06410526	-1.96592385
H	-3.93799654	-0.98239149	-2.47184838

2,6-FP/MTBD(f')_Int2

O	1.39638200	1.93784100	0.94038200
C	0.13382800	2.01569600	0.28469600
O	-0.09352300	0.94384000	-0.51171300
H	4.62083000	2.73793500	0.54103200
C	3.78032900	2.11234700	0.85406700
H	3.88530500	1.12779500	0.38863000
H	3.80338400	1.99541600	1.94233800
C	2.46707500	2.75478900	0.44133300
H	2.39237500	3.75728500	0.90227900
C	0.04842100	3.30803600	-0.56018000
H	0.18904300	4.17524000	0.09956700
O	1.13651700	3.30162700	-1.52146000
C	2.36894700	2.98699300	-1.07100900
O	3.30915100	2.94921100	-1.82561900
C	-1.24098000	3.45089300	-1.34607400
H	-1.36587700	2.60079100	-2.02146500
H	-2.09539500	3.48850100	-0.66307400
H	-1.21578200	4.37490800	-1.93252600
H	0.27379000	0.05759700	-0.12599200
C	-5.91366700	-1.34373300	0.26007400
C	-5.11635300	-0.68952500	1.20122000
C	-3.88516700	-0.13412500	0.82332100
C	-3.45297600	-0.24034000	-0.50740800
C	-4.25159300	-0.89277900	-1.45276700
C	-5.46694500	-1.43304900	-1.05369000
O	-3.15243800	0.48970700	1.78923700
C	-0.74617200	2.93596600	2.39704800
H	0.24269000	2.87223400	2.86289000
H	-1.51323500	2.64784500	3.12030200

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H	-0.94148700	3.96655200	2.07022400
O	-0.86189500	2.00526400	1.31509300
H	-2.34633700	0.89585900	1.41713800
C	1.78449500	-2.05520500	-0.05888700
N	2.62108100	-2.84101700	0.71752100
N	0.76760800	-1.37410600	0.40413600
N	2.06055200	-2.02237100	-1.41056100
C	1.53264700	-1.91006000	2.71075200
H	1.18817800	-2.15966900	3.72188600
H	2.19089400	-1.03474000	2.78476800
C	0.35510800	-1.58864400	1.79138600
H	-0.15973900	-0.68390400	2.13328600
H	-0.38800700	-2.40202500	1.83905900
C	2.30464200	-3.08643400	2.12461900
H	1.71553400	-4.01444500	2.22829700
H	3.25053400	-3.24245900	2.65991300
C	3.57068600	-3.73848100	0.07233300
H	4.25245000	-4.11417900	0.84327900
H	3.06458400	-4.61307600	-0.37396100
C	4.33178900	-2.95486600	-0.99076300
H	5.07123600	-3.58681500	-1.49620100
H	4.87115800	-2.13500700	-0.50082800
C	3.33779700	-2.41018600	-2.01392600
H	3.13043500	-3.17483100	-2.77919100
H	3.76875100	-1.54447600	-2.53982100
C	1.12411500	-1.38907800	-2.33175200
H	1.33207100	-0.32042000	-2.47500200
H	1.20289500	-1.89536200	-3.30163800
H	0.10570600	-1.49499500	-1.95517900
H	-6.87008000	-1.77830500	0.53664300
F	-2.25935385	0.27756799	-0.86732116
H	-3.93799654	-0.98239149	-2.47184838
F	-5.51581484	-0.57885785	2.48600910
H	-6.07682808	-1.93321952	-1.77671979

2,3,6-FP/MTBD(g')_Int2

O	1.39638200	1.93784100	0.94038200
C	0.13382800	2.01569600	0.28469600
O	-0.09352300	0.94384000	-0.51171300
H	4.62083000	2.73793500	0.54103200
C	3.78032900	2.11234700	0.85406700
H	3.88530500	1.12779500	0.38863000
H	3.80338400	1.99541600	1.94233800
C	2.46707500	2.75478900	0.44133300
H	2.39237500	3.75728500	0.90227900
C	0.04842100	3.30803600	-0.56018000
H	0.18904300	4.17524000	0.09956700
O	1.13651700	3.30162700	-1.52146000
C	2.36894700	2.98699300	-1.07100900
O	3.30915100	2.94921100	-1.82561900
C	-1.24098000	3.45089300	-1.34607400
H	-1.36587700	2.60079100	-2.02146500
H	-2.09539500	3.48850100	-0.66307400
H	-1.21578200	4.37490800	-1.93252600
H	0.27379000	0.05759700	-0.12599200
C	-5.91366700	-1.34373300	0.26007400
C	-5.11635300	-0.68952500	1.20122000
C	-3.88516700	-0.13412500	0.82332100
C	-3.45297600	-0.24034000	-0.50740800
C	-4.25159300	-0.89277900	-1.45276700
C	-5.46694500	-1.43304900	-1.05369000
O	-3.15243800	0.48970700	1.78923700
C	-0.74617200	2.93596600	2.39704800
H	0.24269000	2.87223400	2.86289000
H	-1.51323500	2.64784500	3.12030200
H	-0.94148700	3.96655200	2.07022400
O	-0.86189500	2.00526400	1.31509300
H	-2.34633700	0.89585900	1.41713800
C	1.78449500	-2.05520500	-0.05888700
N	2.62108100	-2.84101700	0.71752100
N	0.76760800	-1.37410600	0.40413600
N	2.06055200	-2.02237100	-1.41056100
C	1.53264700	-1.91006000	2.71075200
H	1.18817800	-2.15966900	3.72188600
H	2.19089400	-1.03474000	2.78476800
C	0.35510800	-1.58864400	1.79138600
H	-0.15973900	-0.68390400	2.13328600
H	-0.38800700	-2.40202500	1.83905900
C	2.30464200	-3.08643400	2.12461900
H	1.71553400	-4.01444500	2.22829700

H	3.25053400	-3.24245900	2.65991300
C	3.57068600	-3.73848100	0.07233300
H	4.25245000	-4.11417900	0.84327900
H	3.06458400	-4.61307600	-0.37396100
C	4.33178900	-2.95486600	-0.99076300
H	5.07123600	-3.58681500	-1.49620100
H	4.87115800	-2.13500700	-0.50082800
C	3.33779700	-2.41018600	-2.01392600
H	3.13043500	-3.17483100	-2.77919100
H	3.76875100	-1.54447600	-2.53982100
C	1.12411500	-1.38907800	-2.33175200
H	1.33207100	-0.32042000	-2.47500200
H	1.20289500	-1.89536200	-3.30163800
H	0.10570600	-1.49499500	-1.95517900
H	-6.87008000	-1.77830500	0.53664300
F	-2.25935385	0.27756799	-0.86732116
F	-3.85593391	-1.00584149	-2.73852388
F	-5.51581484	-0.57885785	2.48600910
H	-6.07682808	-1.93321952	-1.77671979

3,4,5-FP/MTBD(h')_Int2

O	1.39638200	1.93784100	0.94038200
C	0.13382800	2.01569600	0.28469600
O	-0.09352300	0.94384000	-0.51171300
H	4.62083000	2.73793500	0.54103200
C	3.78032900	2.11234700	0.85406700
H	3.88530500	1.12779500	0.38863000
H	3.80338400	1.99541600	1.94233800
C	2.46707500	2.75478900	0.44133300
H	2.39237500	3.75728500	0.90227900
C	0.04842100	3.30803600	-0.56018000
H	0.18904300	4.17524000	0.09956700
O	1.13651700	3.30162700	-1.52146000
C	2.36894700	2.98699300	-1.07100900
O	3.30915100	2.94921100	-1.82561900

C	-1.24098000	3.45089300	-1.34607400
H	-1.36587700	2.60079100	-2.02146500
H	-2.09539500	3.48850100	-0.66307400
H	-1.21578200	4.37490800	-1.93252600
H	0.27379000	0.05759700	-0.12599200
C	-5.91366700	-1.34373300	0.26007400
C	-5.11635300	-0.68952500	1.20122000
C	-3.88516700	-0.13412500	0.82332100
C	-3.45297600	-0.24034000	-0.50740800
C	-4.25159300	-0.89277900	-1.45276700
C	-5.46694500	-1.43304900	-1.05369000
O	-3.15243800	0.48970700	1.78923700
C	-0.74617200	2.93596600	2.39704800
H	0.24269000	2.87223400	2.86289000
H	-1.51323500	2.64784500	3.12030200
H	-0.94148700	3.96655200	2.07022400
O	-0.86189500	2.00526400	1.31509300
H	-2.34633700	0.89585900	1.41713800
C	1.78449500	-2.05520500	-0.05888700
N	2.62108100	-2.84101700	0.71752100
N	0.76760800	-1.37410600	0.40413600
N	2.06055200	-2.02237100	-1.41056100
C	1.53264700	-1.91006000	2.71075200
H	1.18817800	-2.15966900	3.72188600
H	2.19089400	-1.03474000	2.78476800
C	0.35510800	-1.58864400	1.79138600
H	-0.15973900	-0.68390400	2.13328600
H	-0.38800700	-2.40202500	1.83905900
C	2.30464200	-3.08643400	2.12461900
H	1.71553400	-4.01444500	2.22829700
H	3.25053400	-3.24245900	2.65991300
C	3.57068600	-3.73848100	0.07233300
H	4.25245000	-4.11417900	0.84327900
H	3.06458400	-4.61307600	-0.37396100
C	4.33178900	-2.95486600	-0.99076300
H	5.07123600	-3.58681500	-1.49620100
H	4.87115800	-2.13500700	-0.50082800
C	3.33779700	-2.41018600	-2.01392600
H	3.13043500	-3.17483100	-2.77919100
H	3.76875100	-1.54447600	-2.53982100
C	1.12411500	-1.38907800	-2.33175200
H	1.33207100	-0.32042000	-2.47500200
H	1.20289500	-1.89536200	-3.30163800
H	0.10570600	-1.49499500	-1.95517900

F	-6.23642365	-2.06410526	-1.96592385
F	-3.85593391	-1.00584149	-2.73852388
F	-7.10223909	-1.88379273	0.60377718
H	-5.43296349	-0.60181104	2.21953432
H	-2.50691993	0.17015004	-0.79267250

2,3,5,6-FP/MTBD(I')_Int2

O	1.39638200	1.93784100	0.94038200
C	0.13382800	2.01569600	0.28469600
O	-0.09352300	0.94384000	-0.51171300
H	4.62083000	2.73793500	0.54103200
C	3.78032900	2.11234700	0.85406700
H	3.88530500	1.12779500	0.38863000
H	3.80338400	1.99541600	1.94233800
C	2.46707500	2.75478900	0.44133300
H	2.39237500	3.75728500	0.90227900
C	0.04842100	3.30803600	-0.56018000
H	0.18904300	4.17524000	0.09956700
O	1.13651700	3.30162700	-1.52146000
C	2.36894700	2.98699300	-1.07100900
O	3.30915100	2.94921100	-1.82561900
C	-1.24098000	3.45089300	-1.34607400
H	-1.36587700	2.60079100	-2.02146500
H	-2.09539500	3.48850100	-0.66307400
H	-1.21578200	4.37490800	-1.93252600
H	0.27379000	0.05759700	-0.12599200
C	-5.91366700	-1.34373300	0.26007400
C	-5.11635300	-0.68952500	1.20122000
C	-3.88516700	-0.13412500	0.82332100
C	-3.45297600	-0.24034000	-0.50740800
C	-4.25159300	-0.89277900	-1.45276700
C	-5.46694500	-1.43304900	-1.05369000
O	-3.15243800	0.48970700	1.78923700
C	-0.74617200	2.93596600	2.39704800
H	0.24269000	2.87223400	2.86289000

H	-1.51323500	2.64784500	3.12030200
H	-0.94148700	3.96655200	2.07022400
O	-0.86189500	2.00526400	1.31509300
H	-2.34633700	0.89585900	1.41713800
C	1.78449500	-2.05520500	-0.05888700
N	2.62108100	-2.84101700	0.71752100
N	0.76760800	-1.37410600	0.40413600
N	2.06055200	-2.02237100	-1.41056100
C	1.53264700	-1.91006000	2.71075200
H	1.18817800	-2.15966900	3.72188600
H	2.19089400	-1.03474000	2.78476800
C	0.35510800	-1.58864400	1.79138600
H	-0.15973900	-0.68390400	2.13328600
H	-0.38800700	-2.40202500	1.83905900
C	2.30464200	-3.08643400	2.12461900
H	1.71553400	-4.01444500	2.22829700
H	3.25053400	-3.24245900	2.65991300
C	3.57068600	-3.73848100	0.07233300
H	4.25245000	-4.11417900	0.84327900
H	3.06458400	-4.61307600	-0.37396100
C	4.33178900	-2.95486600	-0.99076300
H	5.07123600	-3.58681500	-1.49620100
H	4.87115800	-2.13500700	-0.50082800
C	3.33779700	-2.41018600	-2.01392600
H	3.13043500	-3.17483100	-2.77919100
H	3.76875100	-1.54447600	-2.53982100
C	1.12411500	-1.38907800	-2.33175200
H	1.33207100	-0.32042000	-2.47500200
H	1.20289500	-1.89536200	-3.30163800
H	0.10570600	-1.49499500	-1.95517900
F	-2.25935385	0.27756799	-0.86732116
F	-3.85593391	-1.00584149	-2.73852388
F	-5.51581484	-0.57885785	2.48600910
H	-6.07682808	-1.93321952	-1.77671979
F	-7.10223909	-1.88379273	0.60377718

2,3,4,5,6-FP/MTBD(j')_Int2

O	1.39638200	1.93784100	0.94038200
C	0.13382800	2.01569600	0.28469600
O	-0.09352300	0.94384000	-0.51171300
H	4.62083000	2.73793500	0.54103200
C	3.78032900	2.11234700	0.85406700
H	3.88530500	1.12779500	0.38863000
H	3.80338400	1.99541600	1.94233800
C	2.46707500	2.75478900	0.44133300
H	2.39237500	3.75728500	0.90227900
C	0.04842100	3.30803600	-0.56018000
H	0.18904300	4.17524000	0.09956700
O	1.13651700	3.30162700	-1.52146000
C	2.36894700	2.98699300	-1.07100900
O	3.30915100	2.94921100	-1.82561900
C	-1.24098000	3.45089300	-1.34607400
H	-1.36587700	2.60079100	-2.02146500
H	-2.09539500	3.48850100	-0.66307400
H	-1.21578200	4.37490800	-1.93252600
H	0.27379000	0.05759700	-0.12599200
C	-5.91366700	-1.34373300	0.26007400
C	-5.11635300	-0.68952500	1.20122000
C	-3.88516700	-0.13412500	0.82332100
C	-3.45297600	-0.24034000	-0.50740800
C	-4.25159300	-0.89277900	-1.45276700
C	-5.46694500	-1.43304900	-1.05369000
O	-3.15243800	0.48970700	1.78923700
C	-0.74617200	2.93596600	2.39704800
H	0.24269000	2.87223400	2.86289000
H	-1.51323500	2.64784500	3.12030200
H	-0.94148700	3.96655200	2.07022400
O	-0.86189500	2.00526400	1.31509300
H	-2.34633700	0.89585900	1.41713800
C	1.78449500	-2.05520500	-0.05888700
N	2.62108100	-2.84101700	0.71752100
N	0.76760800	-1.37410600	0.40413600

N	2.06055200	-2.02237100	-1.41056100
C	1.53264700	-1.91006000	2.71075200
H	1.18817800	-2.15966900	3.72188600
H	2.19089400	-1.03474000	2.78476800
C	0.35510800	-1.58864400	1.79138600
H	-0.15973900	-0.68390400	2.13328600
H	-0.38800700	-2.40202500	1.83905900
C	2.30464200	-3.08643400	2.12461900
H	1.71553400	-4.01444500	2.22829700
H	3.25053400	-3.24245900	2.65991300
C	3.57068600	-3.73848100	0.07233300
H	4.25245000	-4.11417900	0.84327900
H	3.06458400	-4.61307600	-0.37396100
C	4.33178900	-2.95486600	-0.99076300
H	5.07123600	-3.58681500	-1.49620100
H	4.87115800	-2.13500700	-0.50082800
C	3.33779700	-2.41018600	-2.01392600
H	3.13043500	-3.17483100	-2.77919100
H	3.76875100	-1.54447600	-2.53982100
C	1.12411500	-1.38907800	-2.33175200
H	1.33207100	-0.32042000	-2.47500200
H	1.20289500	-1.89536200	-3.30163800
H	0.10570600	-1.49499500	-1.95517900
F	-2.25935385	0.27756799	-0.86732116
F	-3.85593391	-1.00584149	-2.73852388
F	-5.51581484	-0.57885785	2.48600910
F	-7.10223909	-1.88379273	0.60377718
F	-6.23642365	-2.06410526	-1.96592385

Reference

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