

Supporting Material Information

Synthesis, Photophysical and Anticancer Activity of Isomeric Fluorinated Photosensitizers with a Known Iodinated Analog Derived from Chlorophyll-a in Bladder and Brain Tumor Models: Similarities and Differences

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Figure S1: ^1H NMR spectrum of 3

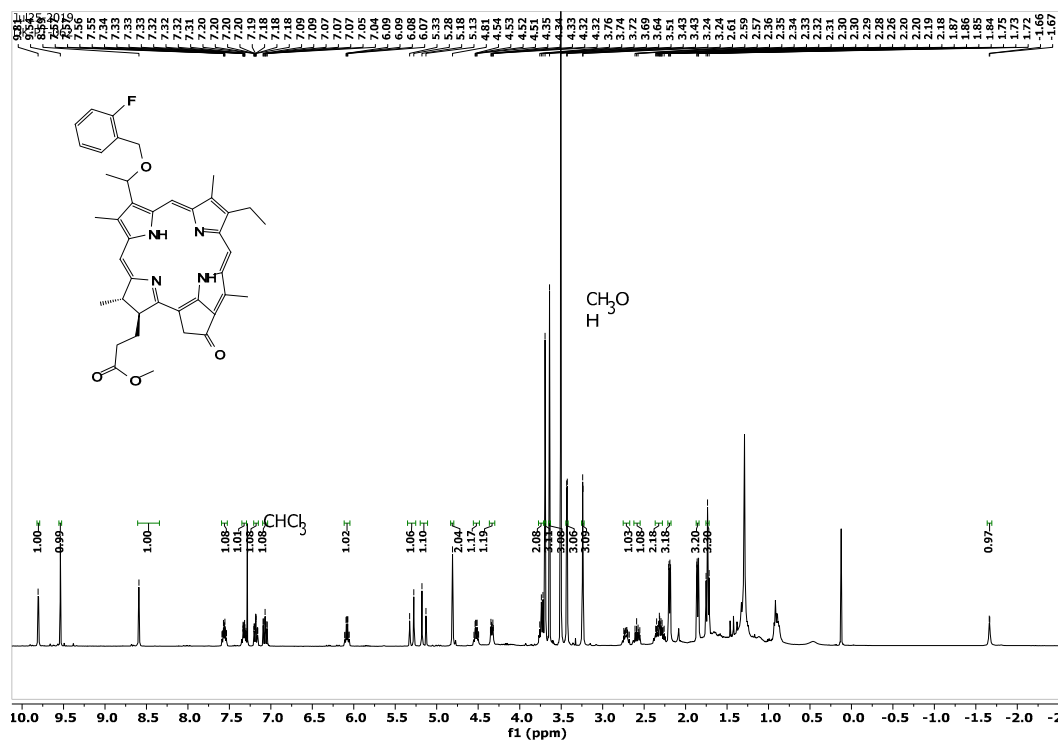


Figure S2: ^{13}C NMR spectrum of 3

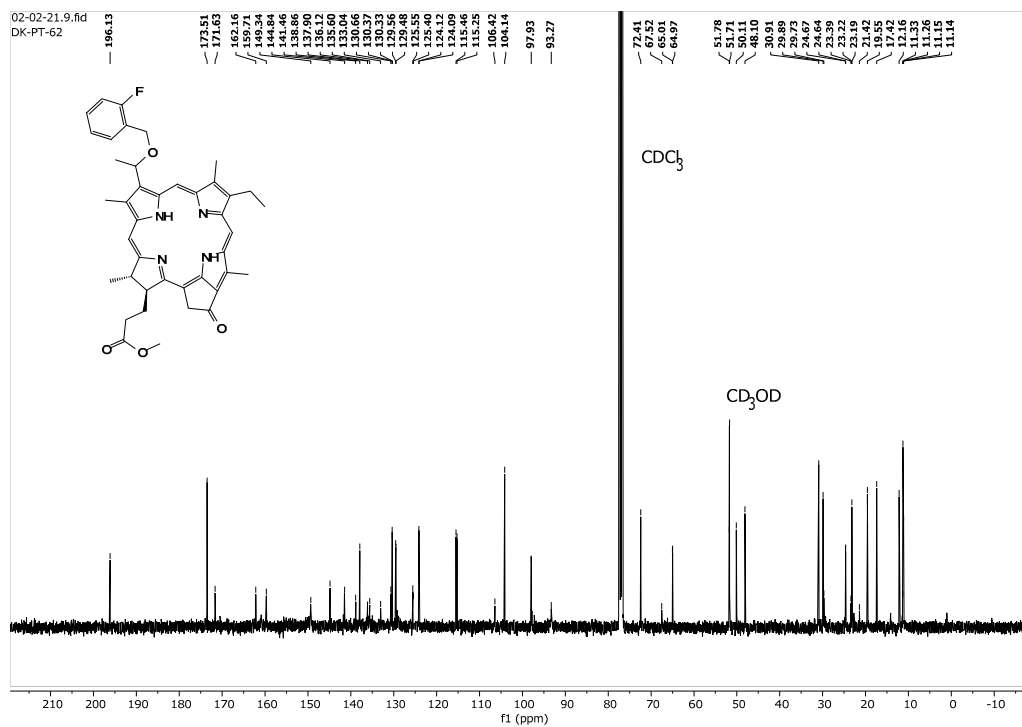


Figure S3: ^{19}F NMR spectrum of 3

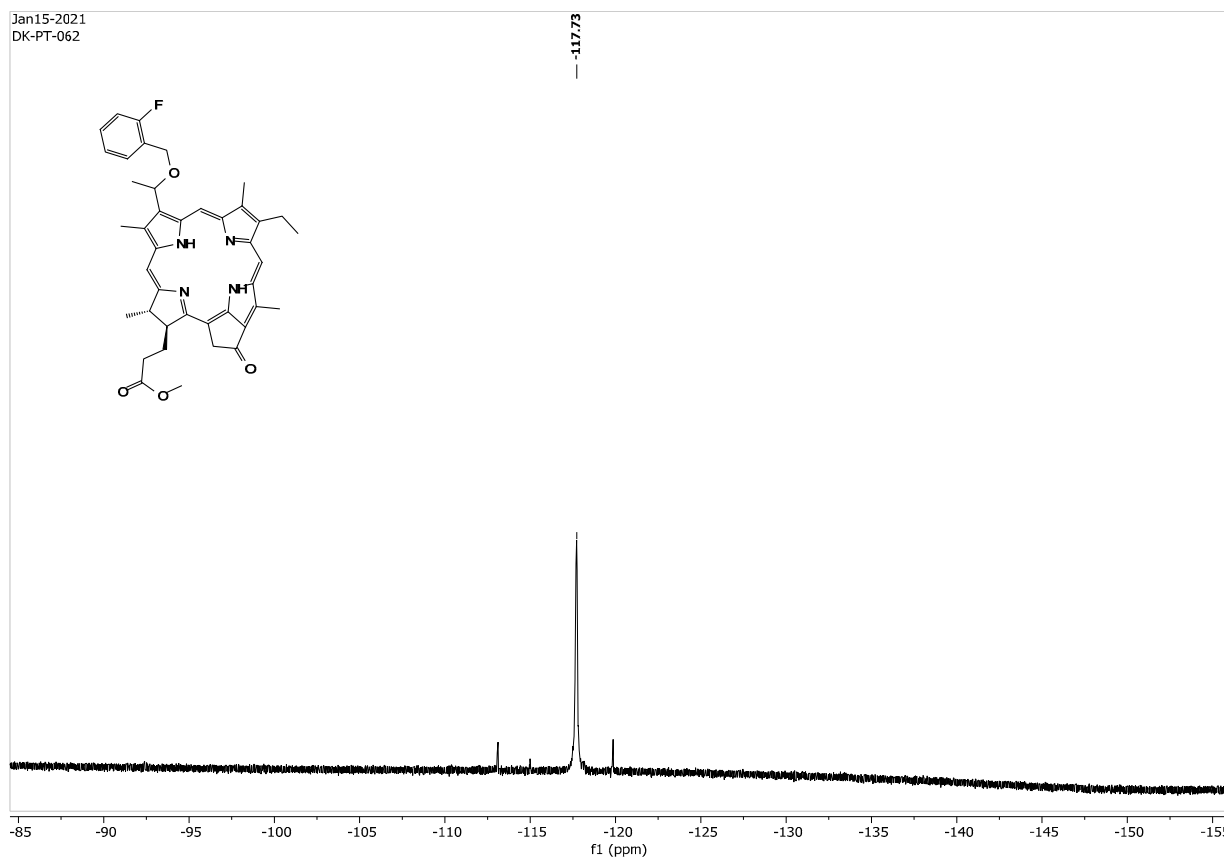
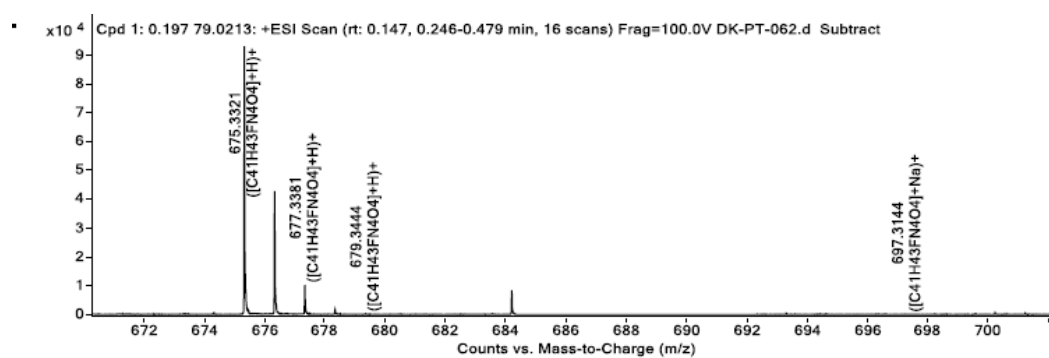


Figure S4: Mass spectrum of 3



MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
675.3321	675.3341	2.99	1	93689.75	C ₄₁ H ₄₃ FN ₄ O ₄	(M+H) ⁺
676.3354	676.3373	2.86	1	42870.63	C ₄₁ H ₄₃ FN ₄ O ₄	(M+H) ⁺
677.3381	677.3403	3.23	1	10289.9	C ₄₁ H ₄₃ FN ₄ O ₄	(M+H) ⁺
678.3409	678.3433	3.45	1	1688.04	C ₄₁ H ₄₃ FN ₄ O ₄	(M+H) ⁺
679.3444	679.3461	2.45	1	252.69	C ₄₁ H ₄₃ FN ₄ O ₄	(M+H) ⁺
697.3144	697.3161	2.36	1	78.07	C ₄₁ H ₄₃ FN ₄ O ₄	(M+Na) ⁺

Figure S5: ^1H NMR spectrum of 5

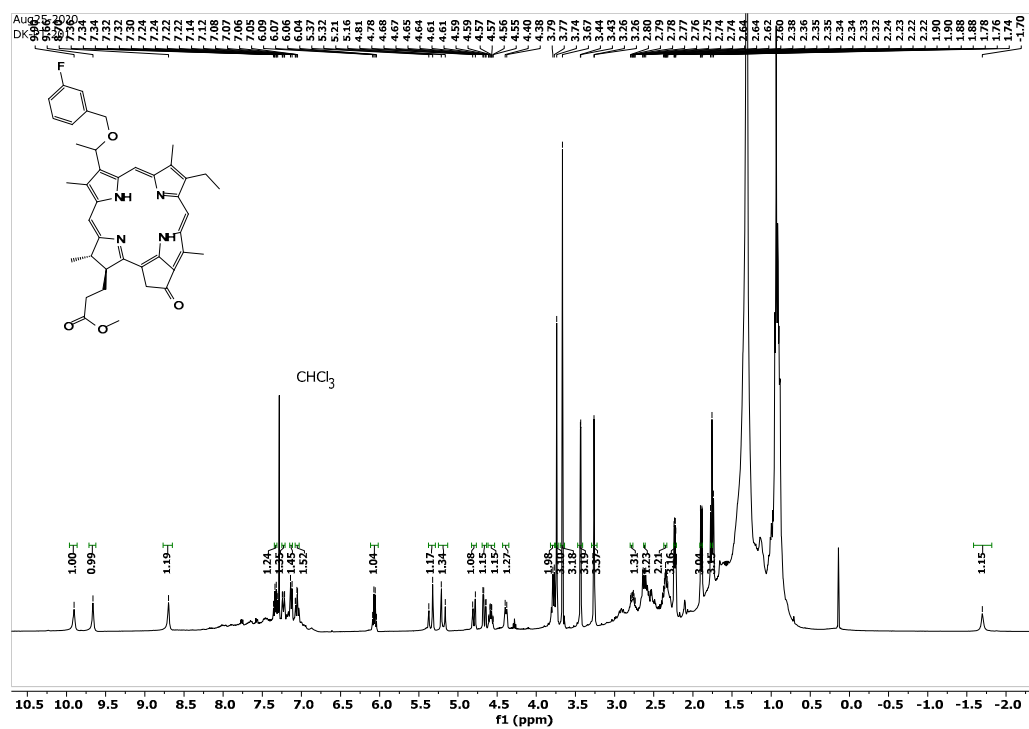


Figure S6: ^{13}C NMR spectrum of 5

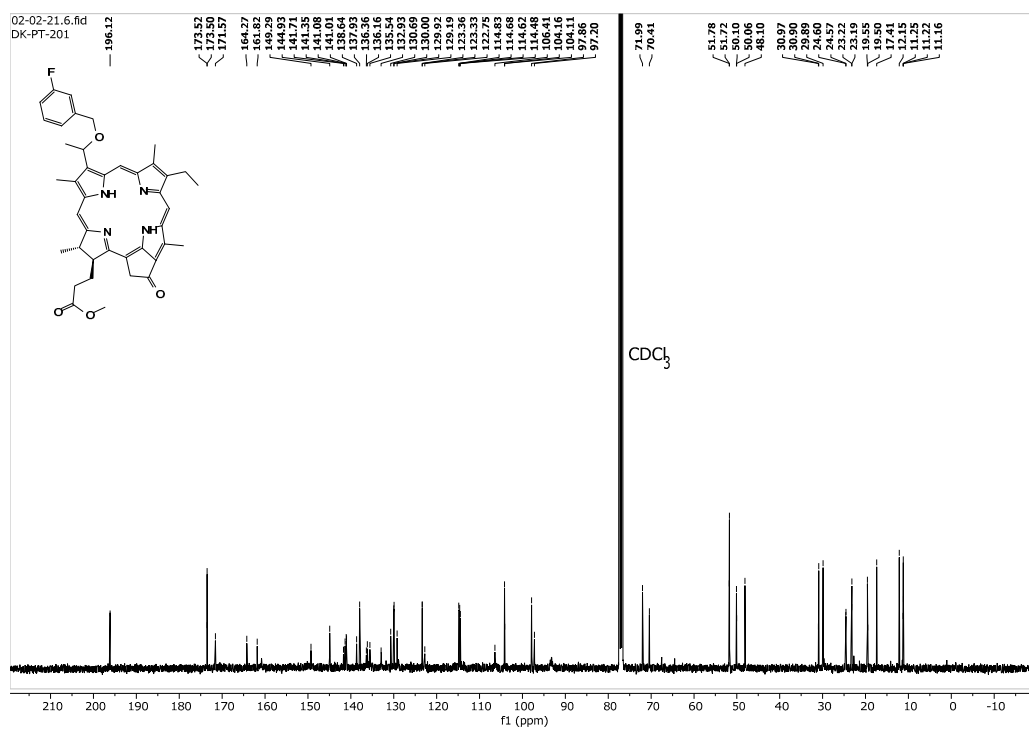


Figure S7: ^{19}F NMR spectrum of 5

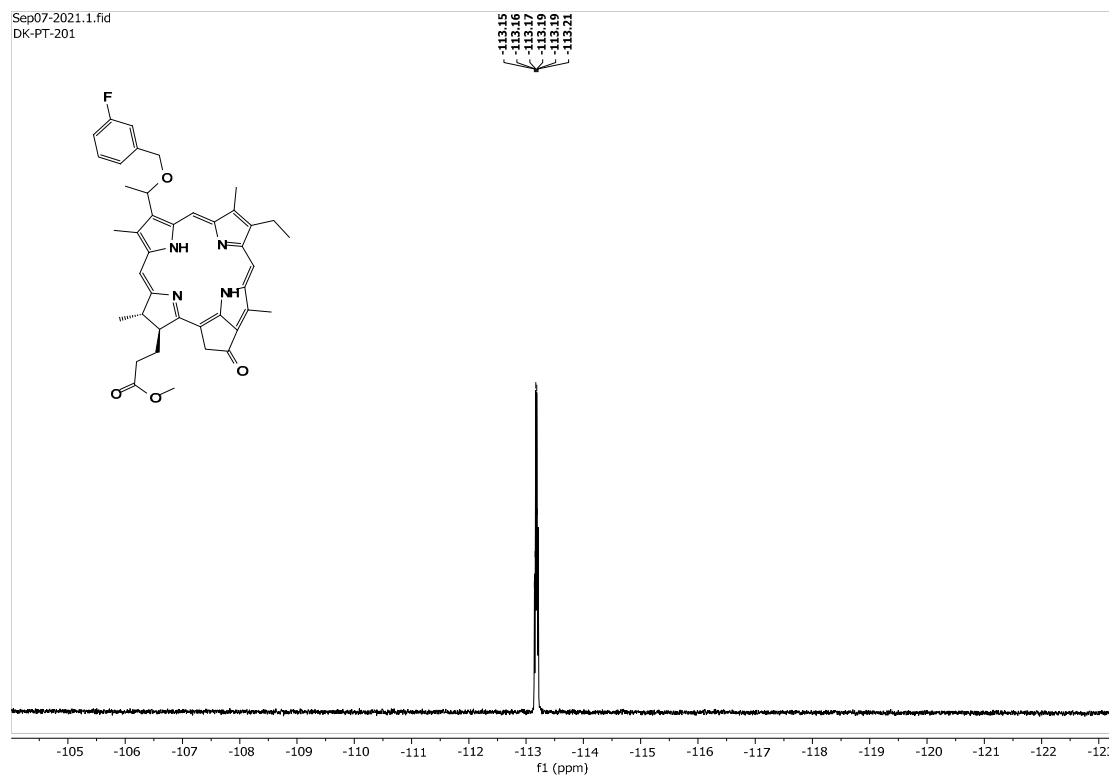
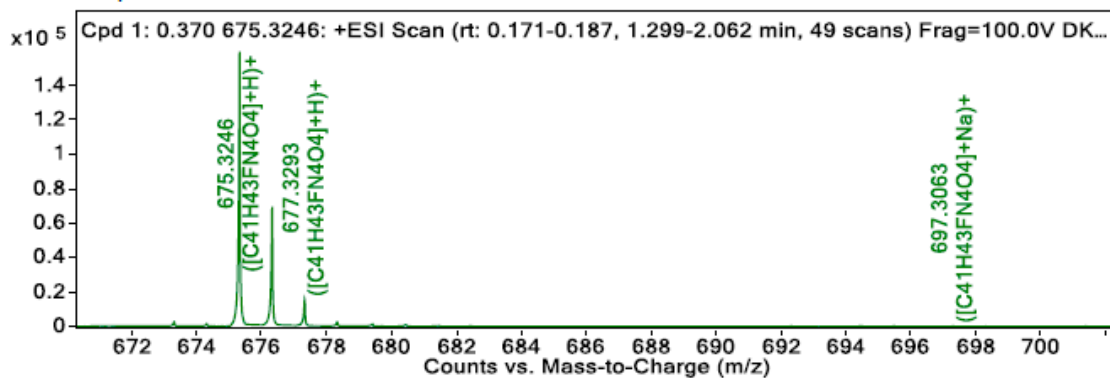


Figure S8: Mass spectrum of 5



MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
675.3246	675.3341	14.11	1	159836.96	C41H43FN4O4	(M+H)+
676.3272	676.3373	14.91	1	69399.42	C41H43FN4O4	(M+H)+
677.3293	677.3403	16.34	1	15537.04	C41H43FN4O4	(M+H)+
678.3318	678.3433	16.88	1	2574.44	C41H43FN4O4	(M+H)+
697.3063	697.3161	14.05	1	122.01	C41H43FN4O4	(M+Na)+
698.308	698.3192	16.13	1	60.22	C41H43FN4O4	(M+Na)+

Figure S9: ^1H NMR spectrum of 7

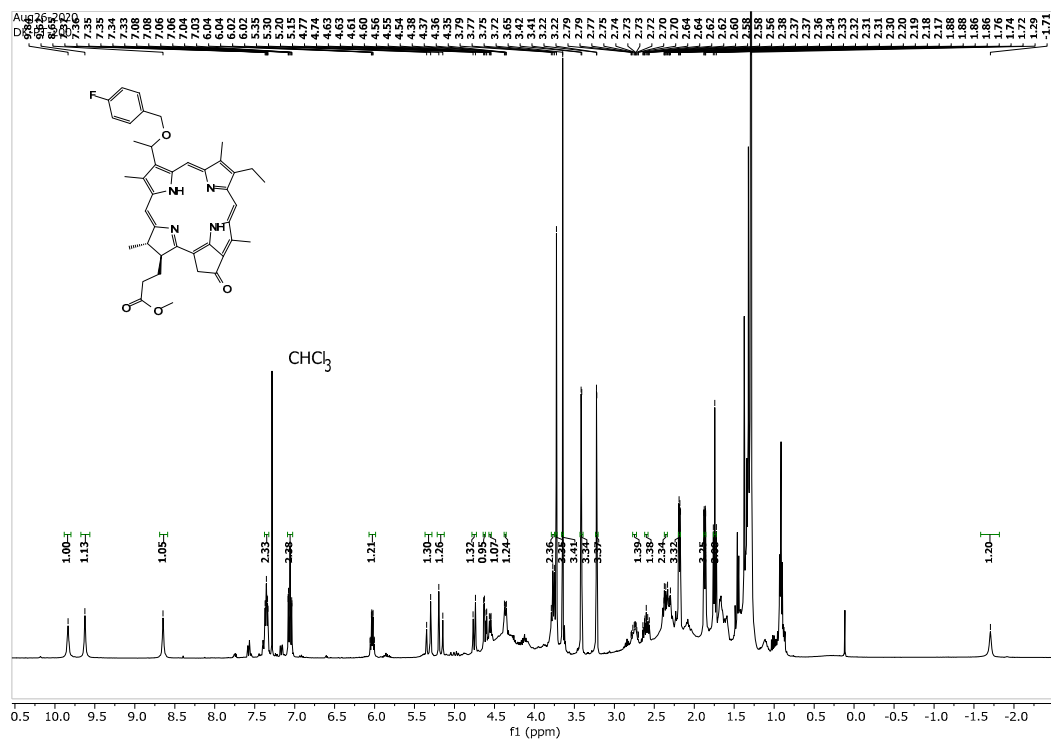


Figure S10: ^{13}C NMR spectrum of 7

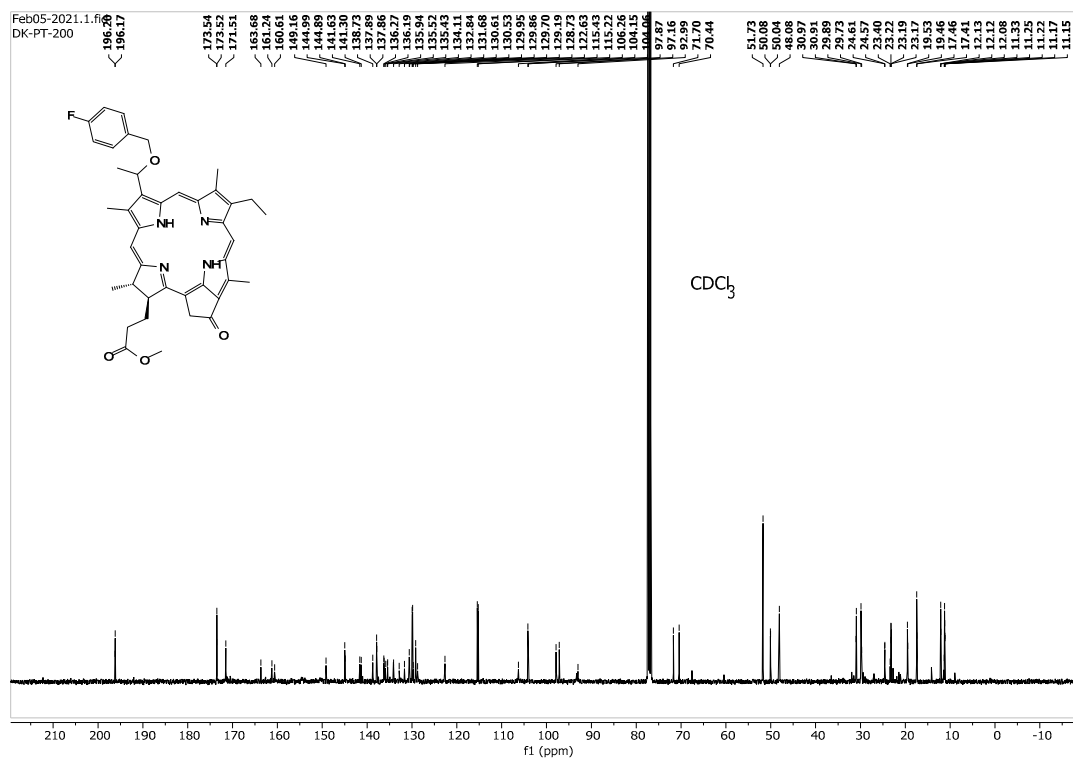


Figure S11: ^{19}F NMR spectrum of 7

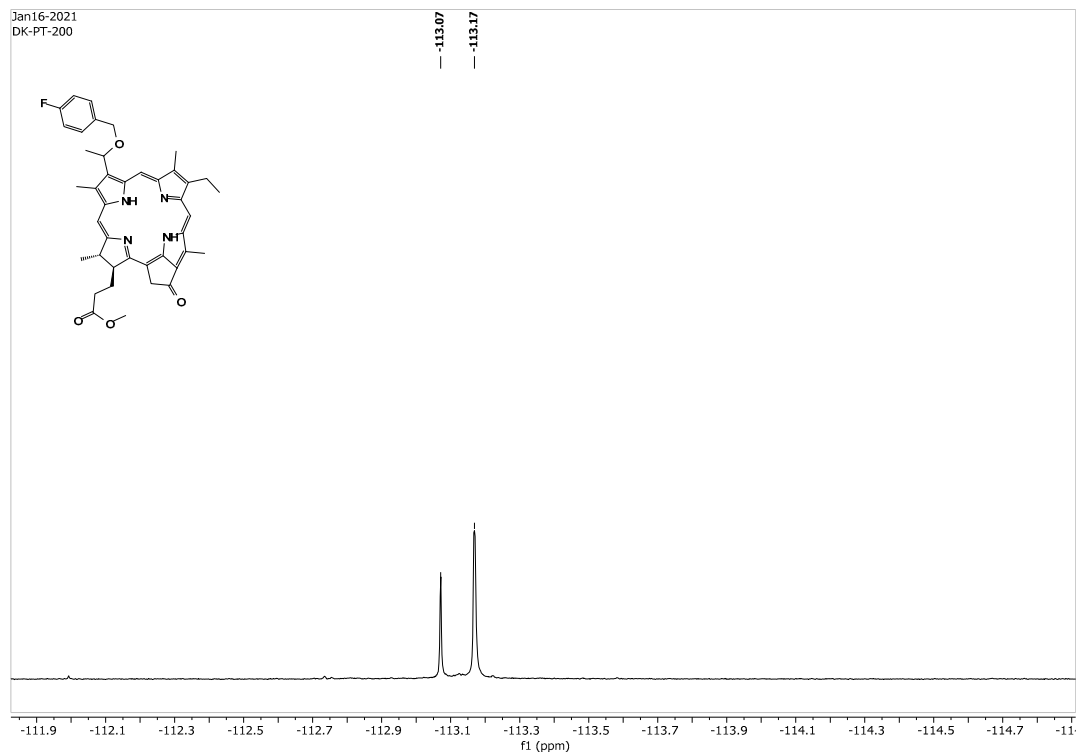
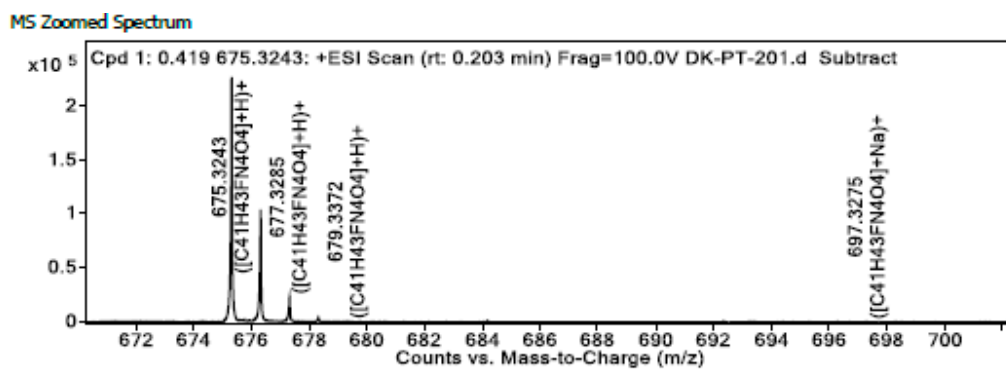


Figure S12: Mass spectrum of 7



MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
675.3243	675.3341	14.57	1	228580.18	C41H43FN4O4	(M+H)+
676.3273	676.3373	14.86	1	103767.15	C41H43FN4O4	(M+H)+
677.3285	677.3403	17.43	1	23242.15	C41H43FN4O4	(M+H)+
678.3292	678.3433	20.79	1	4192.99	C41H43FN4O4	(M+H)+
679.3372	679.3461	13.04	1	623.11	C41H43FN4O4	(M+H)+
697.3275	697.3161	-16.4	1	116.86	C41H43FN4O4	(M+Na)+

Figure S13: ^1H NMR spectrum of 4

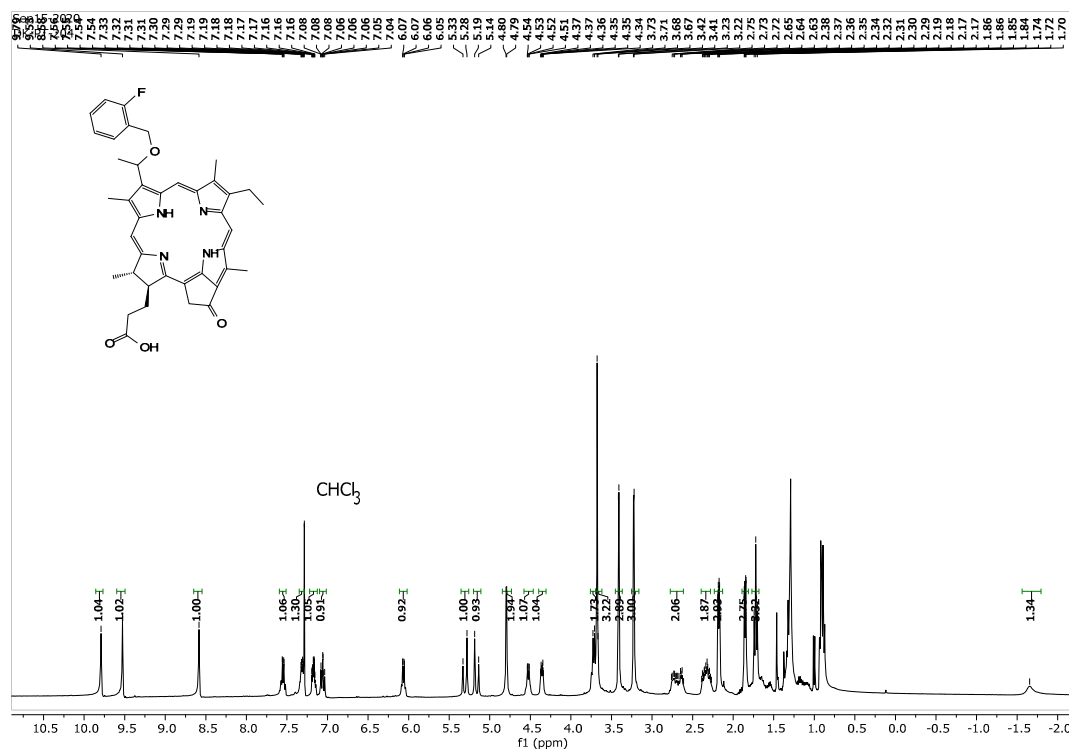


Figure S15: ^{19}F NMR spectrum of 4

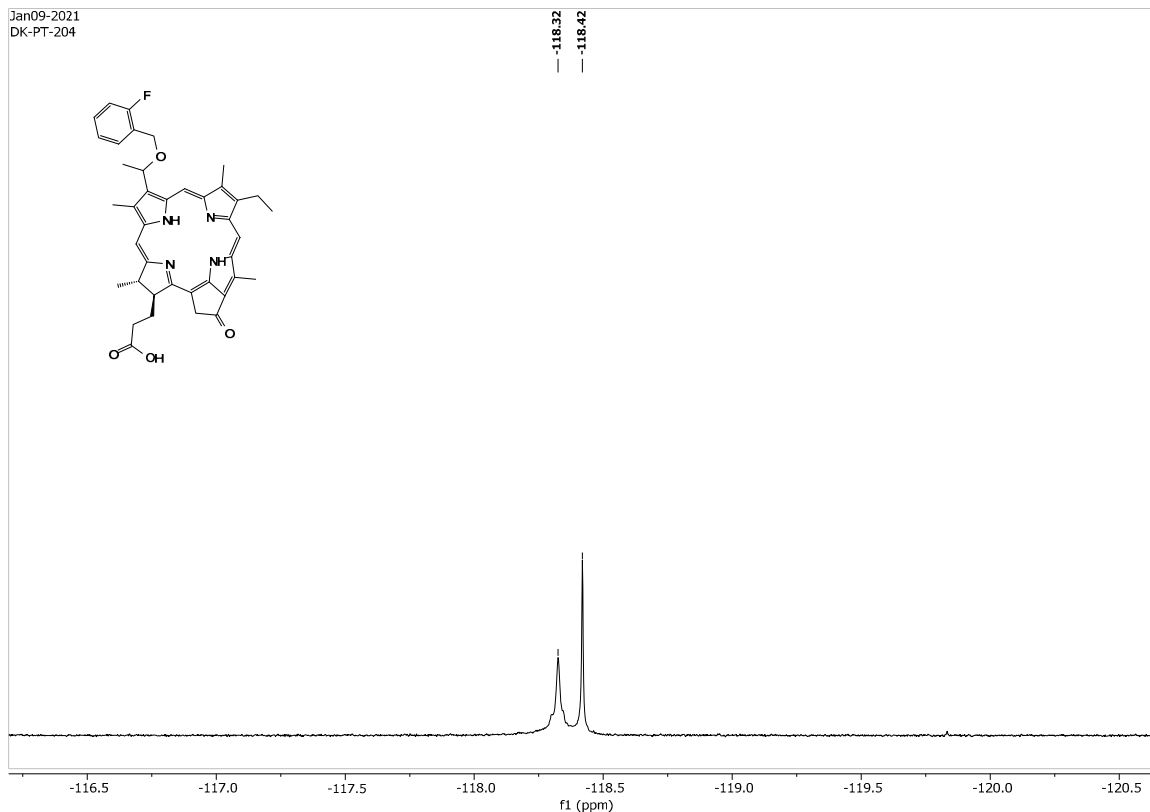
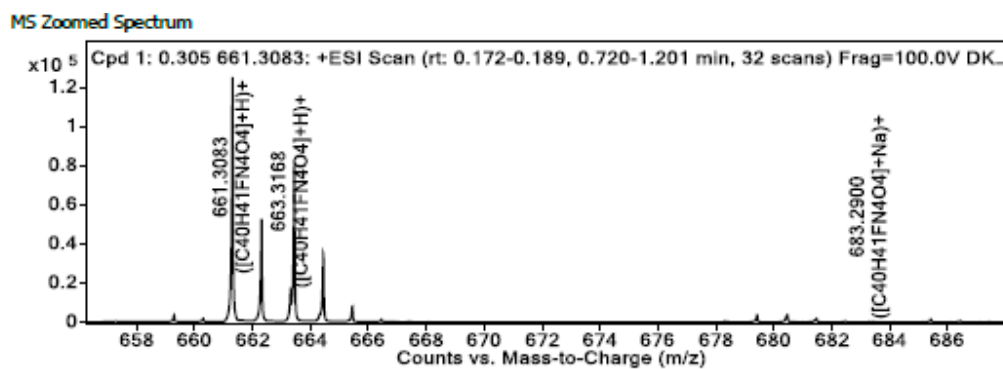


Figure S16: Mass spectrum of 4



MS Spectrum Peak List

<i>m/z</i>	<i>Calc m/z</i>	Diff(ppm)	z	Abund	Formula	Ion
661.3083	661.3185	15.3	1	125380.18	C40H41FN4O4	(M+H)+
662.3111	662.3216	15.95	1	53149.38	C40H41FN4O4	(M+H)+
663.3168	663.3247	11.93	1	15932.4	C40H41FN4O4	(M+H)+
683.29	683.3004	15.17	1	121.78	C40H41FN4O4	(M+Na)+
684.2936	684.3036	14.66	1	63.1	C40H41FN4O4	(M+Na)+

Figure S17: ^1H NMR spectrum of 6

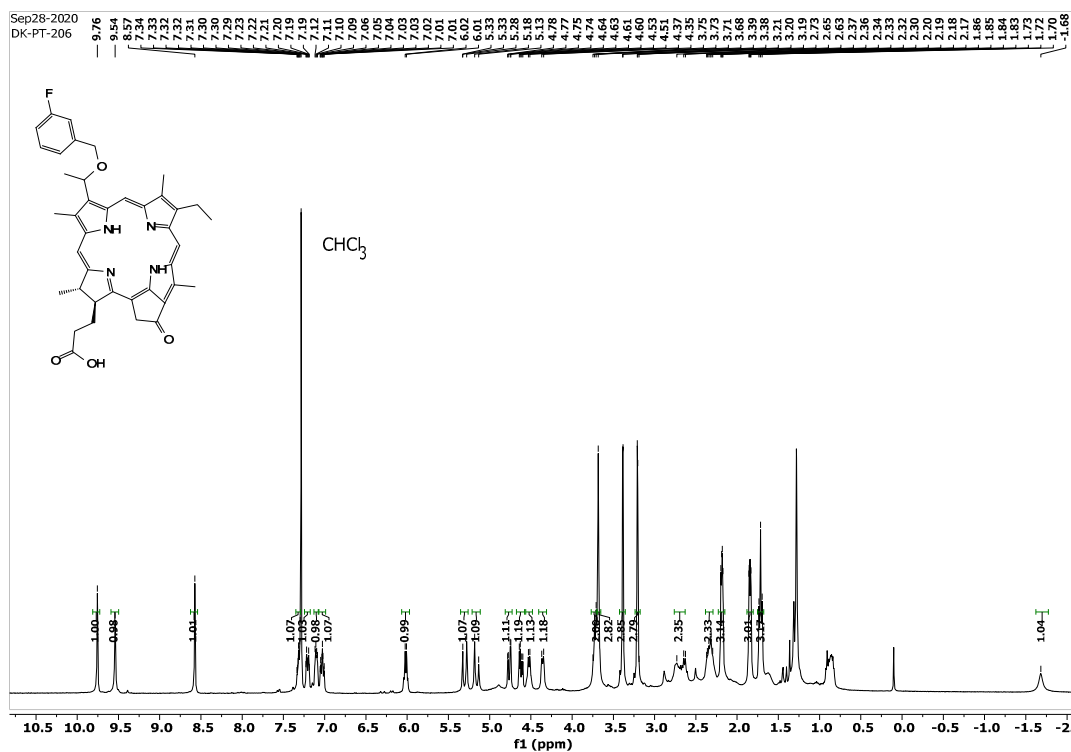


Figure S18: ^{13}C NMR spectrum of 6

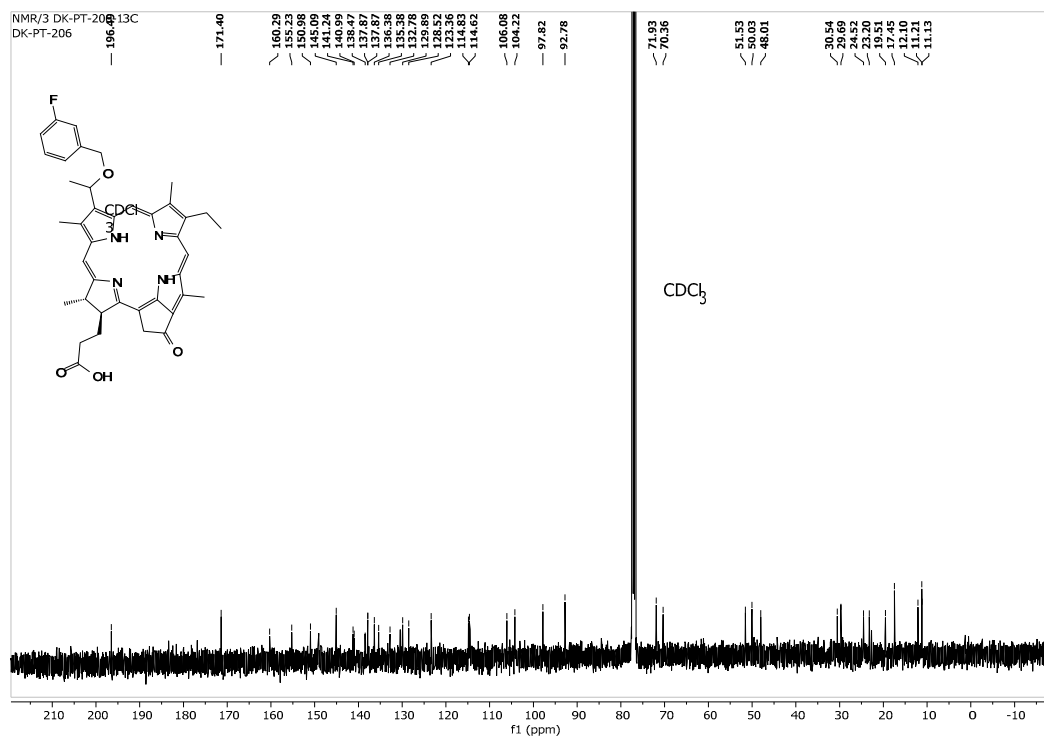


Figure S19: ^{19}F NMR spectrum of 6

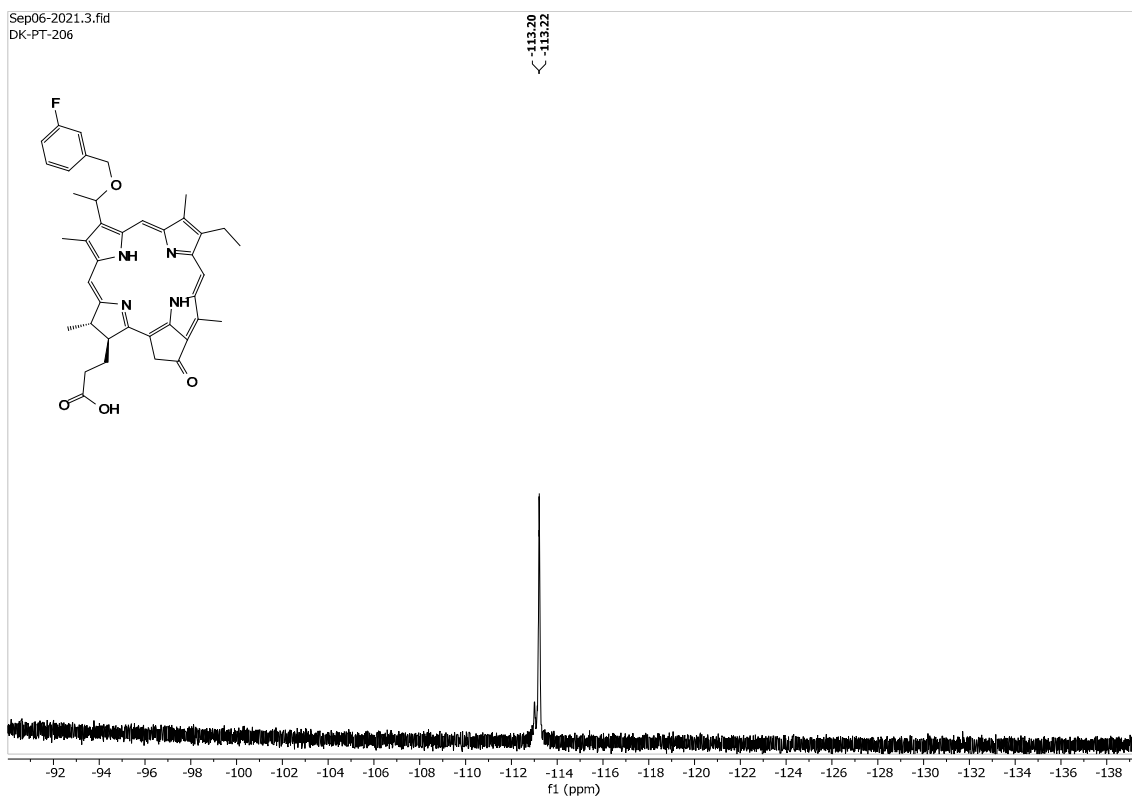
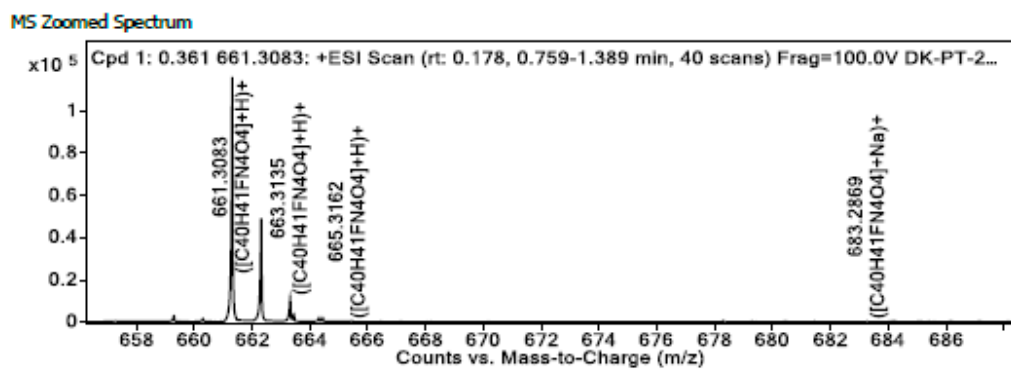


Figure S20: Mass spectrum of 6



MS Spectrum Peak List

<i>m/z</i>	<i>Calc m/z</i>	Diff(ppm)	<i>z</i>	Abund	Formula	Ion
661.3083	661.3185	15.39	1	116156.56	C40H41FN4O4	(M+H)+
662.311	662.3216	16.15	1	49524.24	C40H41FN4O4	(M+H)+
663.3135	663.3247	16.76	1	11306.08	C40H41FN4O4	(M+H)+
664.3166	664.3276	16.58	1	1973.33	C40H41FN4O4	(M+H)+
665.3162	665.3304	21.37	1	240.83	C40H41FN4O4	(M+H)+
683.2869	683.3004	19.82	1	142.26	C40H41FN4O4	(M+Na)+
684.295	684.3036	12.57	1	66.94	C40H41FN4O4	(M+Na)+

Figure S21: ^1H NMR spectrum of 8

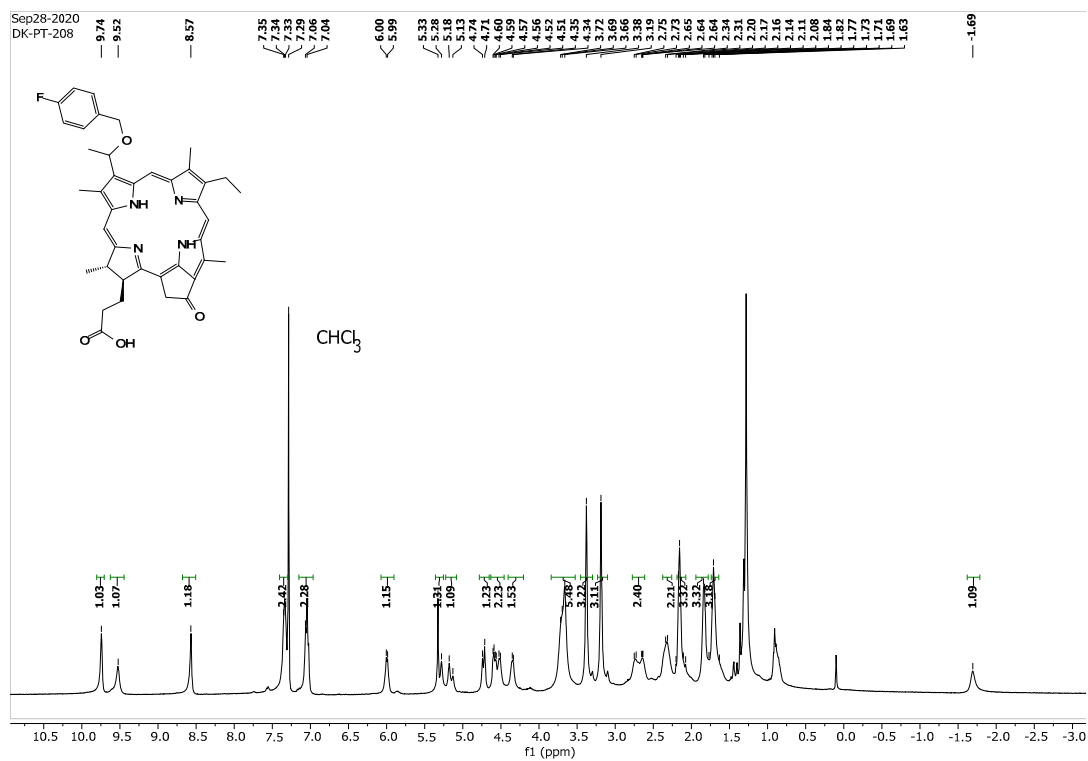


Figure S22: ^{13}C NMR spectrum of 8

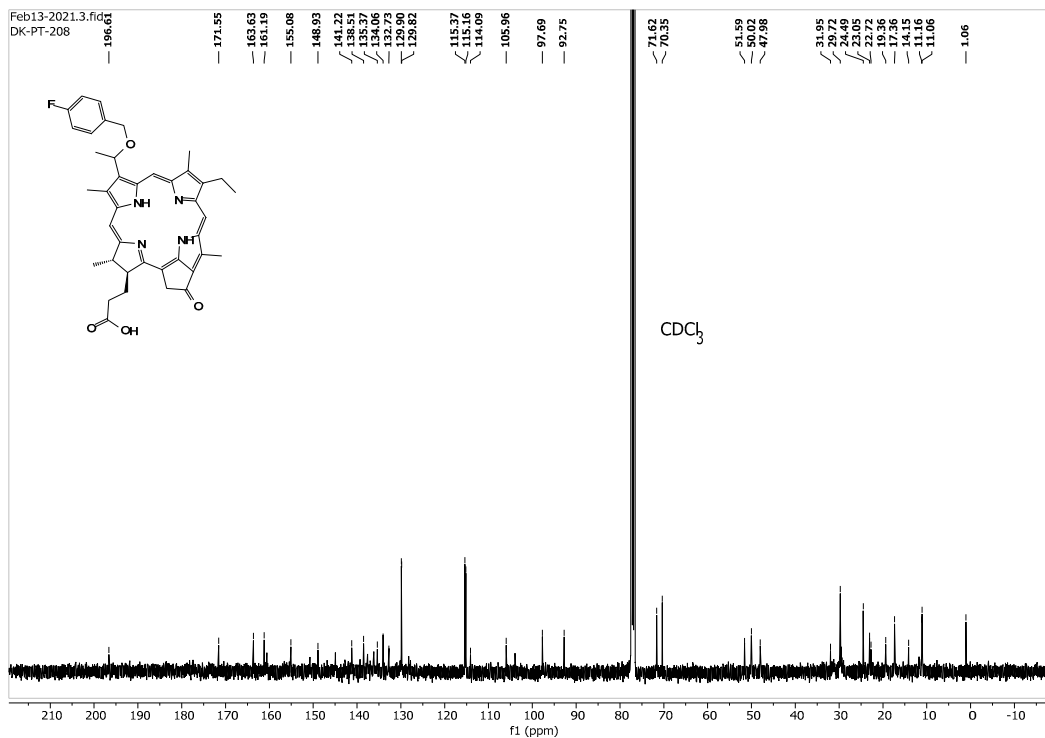


Figure S23: ^{19}F NMR spectrum of 8

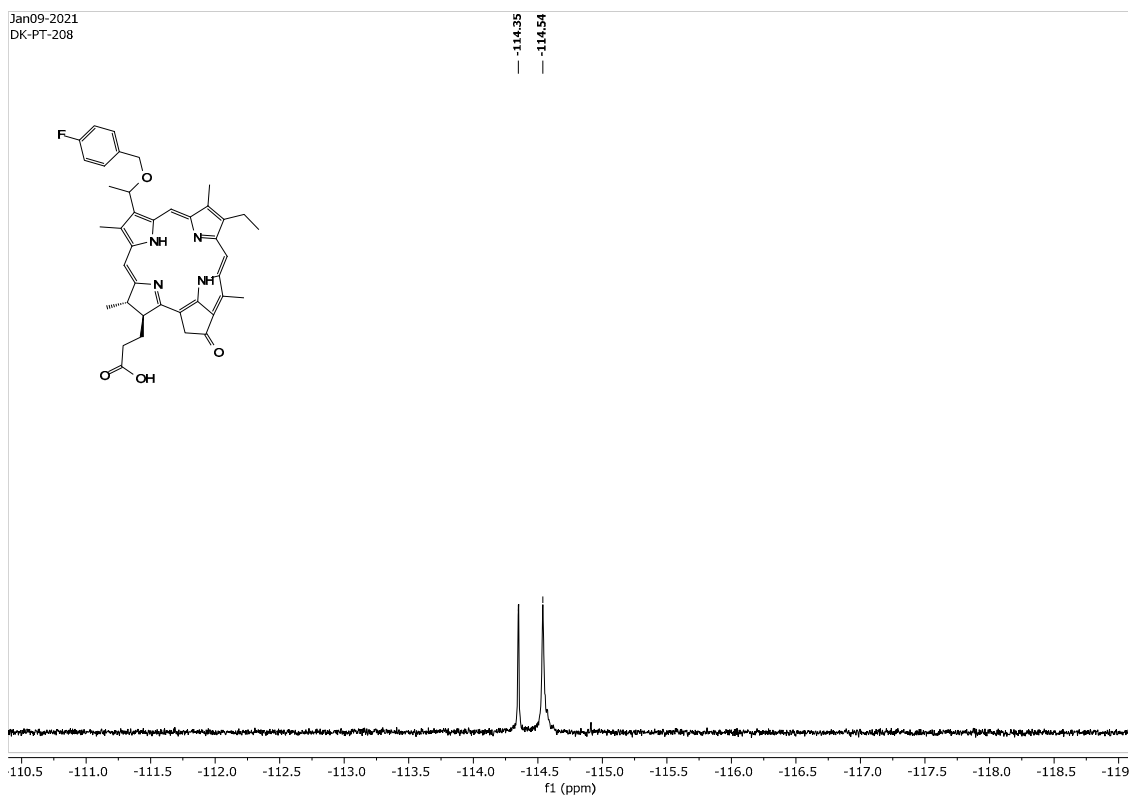
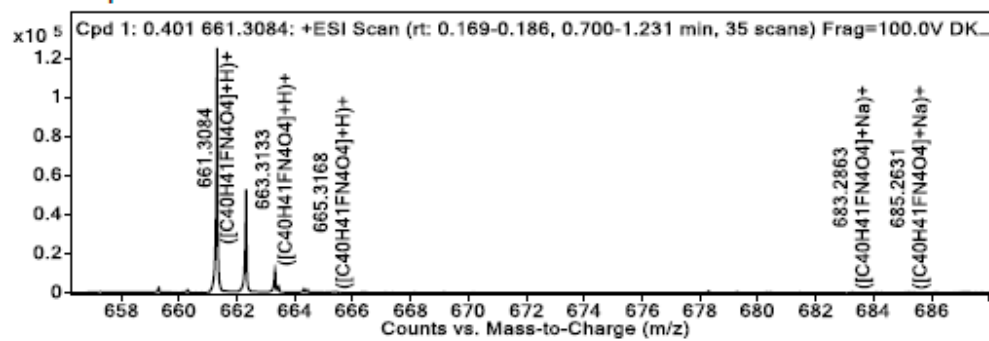


Figure S24: Mass spectrum of 8

MS Zoomed Spectrum



MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
661.3084	661.3185	15.18	1	125126.84	C ₄₀ H ₄₁ FN ₄ O ₄	(M+H) ⁺
662.3109	662.3216	16.18	1	53093.64	C ₄₀ H ₄₁ FN ₄ O ₄	(M+H) ⁺
663.3133	663.3247	17.13	1	12100.66	C ₄₀ H ₄₁ FN ₄ O ₄	(M+H) ⁺
664.3159	664.3276	17.64	1	2109.61	C ₄₀ H ₄₁ FN ₄ O ₄	(M+H) ⁺
665.3168	665.3304	20.46	1	342.14	C ₄₀ H ₄₁ FN ₄ O ₄	(M+H) ⁺
683.2863	683.3004	20.69	1	186.88	C ₄₀ H ₄₁ FN ₄ O ₄	(M+Na) ⁺
684.2862	684.3036	25.47	1	88.82	C ₄₀ H ₄₁ FN ₄ O ₄	(M+Na) ⁺
685.2631	685.3066	63.51	1	60.77	C ₄₀ H ₄₁ FN ₄ O ₄	(M+Na) ⁺

Figure S25: Molecular Formula Strings Spread sheet

Compound	Molecular Formula Strings
3a	<chem>O=C1CC(C2=N/C([C@@H](C)[C@@H]2CCC(OC)=O)=C\3)=C(C1=C/4C)NC4=C/C(C(CC)=C/5C)=NC5=C/C6=C(C(OCC7=CC=CC=C7F)C)C(C)=C3N6</chem>
3b	<chem>O=C1CC(C2=N/C([C@@H](C)[C@@H]2CCC(OC)=O)=C\3)=C(C1=C/4C)NC4=C/C(C(CC)=C/5C)=NC5=C/C6=C(C(OCC7=CC=CC(F)=C7)C)C(C)=C3N6</chem>
3c	<chem>O=C1CC(C2=N/C([C@@H](C)[C@@H]2CCC(OC)=O)=C\3)=C(C1=C/4C)NC4=C/C(C(CC)=C/5C)=NC5=C/C6=C(C(OCC7=CC=C(F)C=C7)C)C(C)=C3N6</chem>
4a	<chem>O=C1CC(C2=N/C([C@@H](C)[C@@H]2CCC(O)=O)=C\3)=C(C1=C/4C)NC4=C/C(C(CC)=C/5C)=NC5=C/C6=C(C(OCC7=CC=CC=C7F)C)C(C)=C3N6</chem>
4b	<chem>O=C1CC(C2=N/C([C@@H](C)[C@@H]2CCC(O)=O)=C\3)=C(C1=C/4C)NC4=C/C(C(CC)=C/5C)=NC5=C/C6=C(C(OCC7=CC=CC(F)=C7)C)C(C)=C3N6</chem>
4c	<chem>O=C1CC(C2=N/C([C@@H](C)[C@@H]2CCC(O)=O)=C\3)=C(C1=C/4C)NC4=C/C(C(CC)=C/5C)=NC5=C/C6=C(C(OCC7=CC=C(F)C=C7)C)C(C)=C3N6</chem>

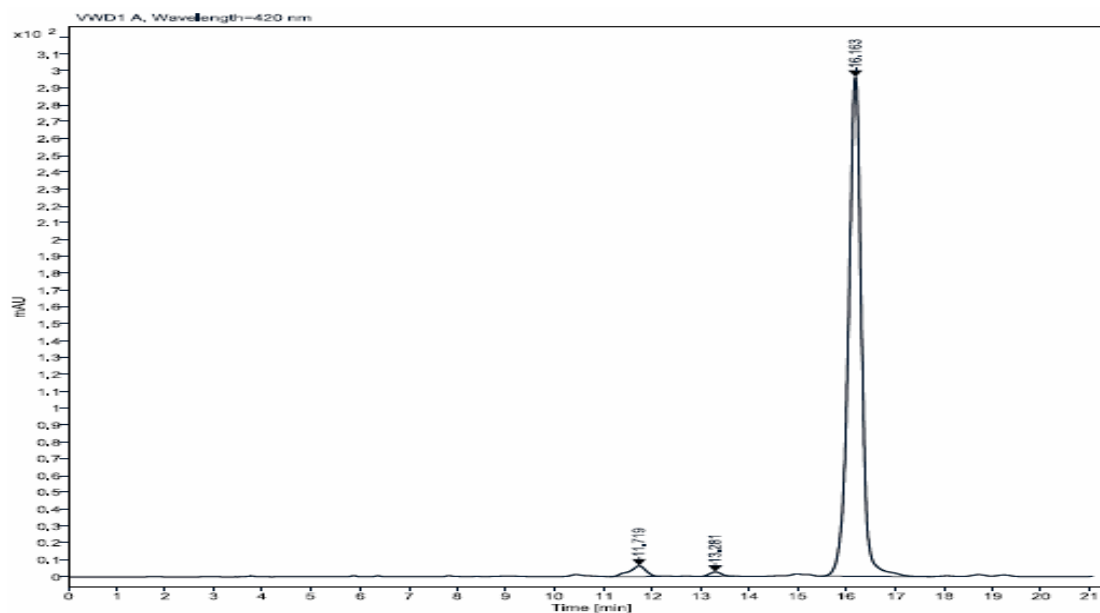
Figure S26: HPLC Analysis

Method(s) for HPLC analysis:

- A. Instrument: Agilent 1260 Infinity II system with diode array detector
- B. HPLC parameter: Solvent flow rate: 1.0 mL/min Mobile phase 0.1% (v/v) TFA in water/acetonitrile (5%) over 20 min, Data collected between 410 nm to 420 nm.
- C. HPLC Column: Sunfire C18 analytical column (5 μ m 4.6 \times 250 mm)

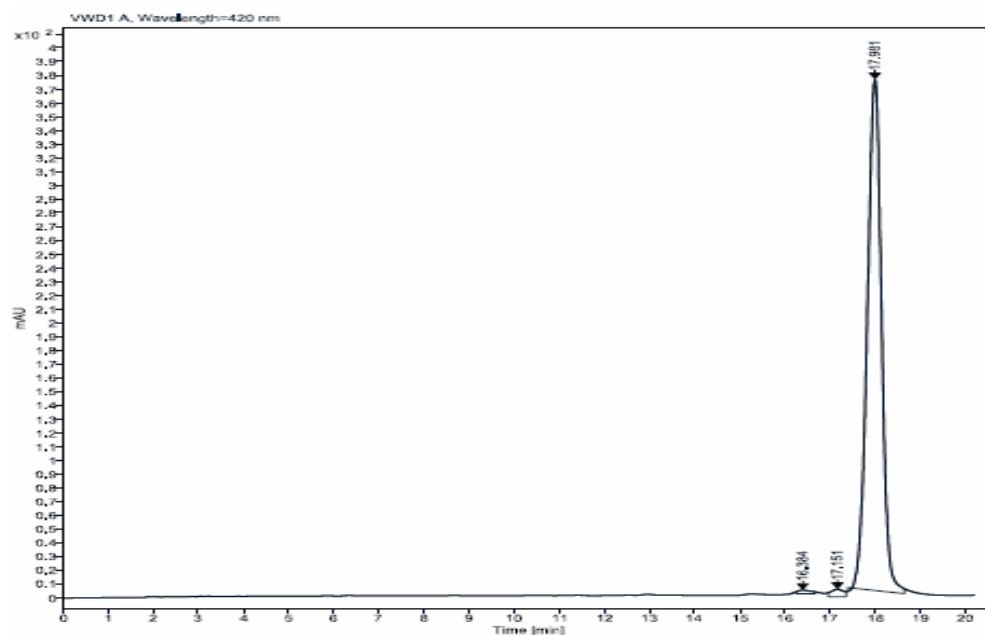
Compound	Retention times (min)	Purity (%)
3	16.163	96.63
5	17.799	99.01
7	18.059	97.79
4	12.605	99.32
6	14.927	97.89
8	12.081	97.84

Figure S27: HPLC chromatogram of 3



RT [min]	Type	Width [min]	Area	Height	Area%	Name
11.719	BB	0.3410	147.5701	6.2381	2.5915	
13.281	BB	0.2731	43.7973	2.5533	0.7691	
16.163	BB	0.2827	5503.0796	296.2810	96.6394	
Sum			5694.4471			

Figure S28: HPLC chromatogram of 5



RT [min]	Type	Width [min]	Area	Height	Area%	Name
16.384	MM	0.3623	52.4034	2.4106	0.6307	
17.151	MM	0.3239	102.7382	5.2870	1.2365	
17.981	MM	0.3656	8153.4653	371.7141	98.1328	
		Sum	8308.6069			

Figure S29. HPLC chromatogram of 7

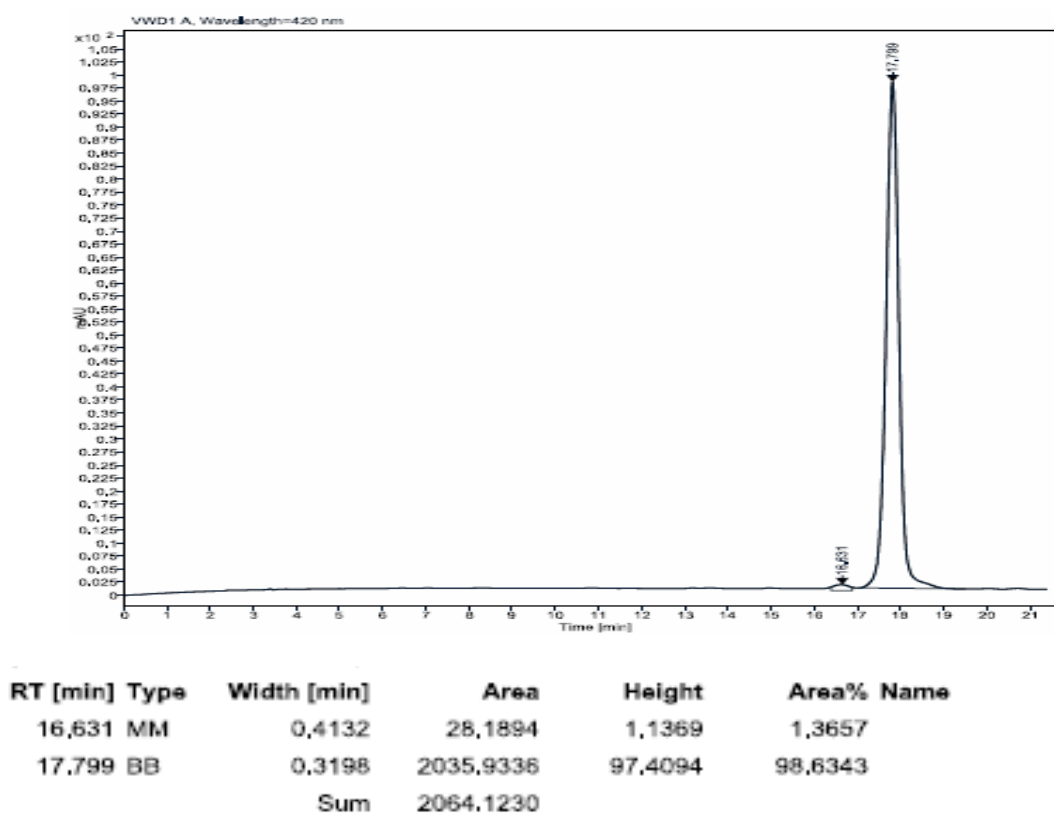
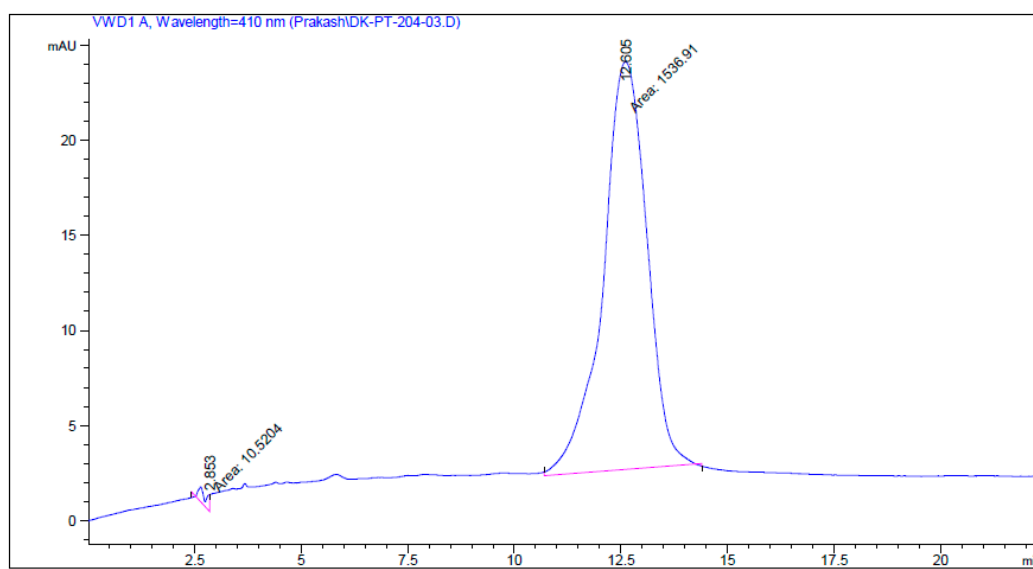


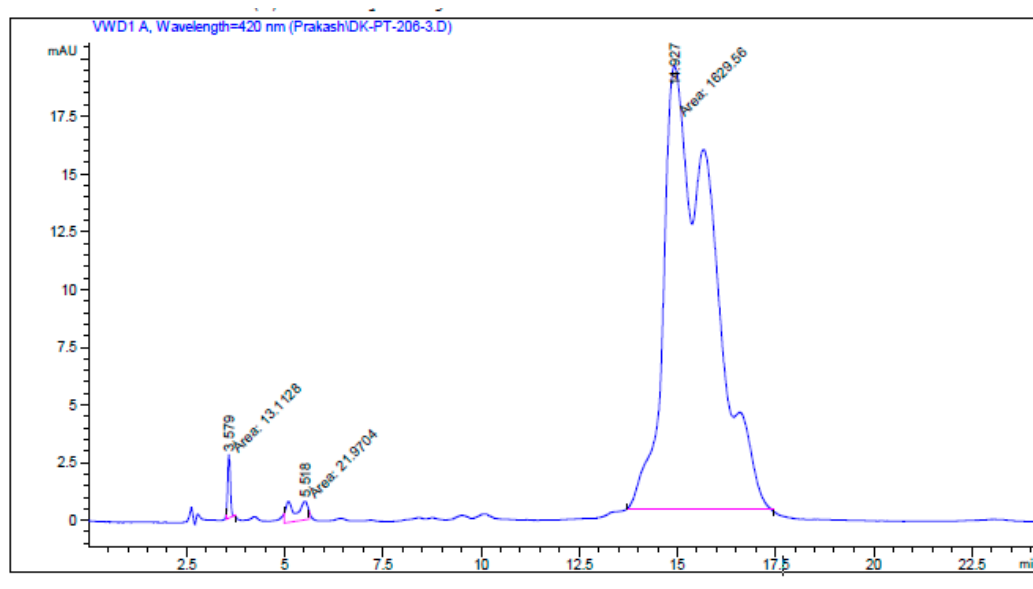
Figure S30. HPLC chromatogram of 4



Signal 1: VWD1 A, Wavelength=410 nm

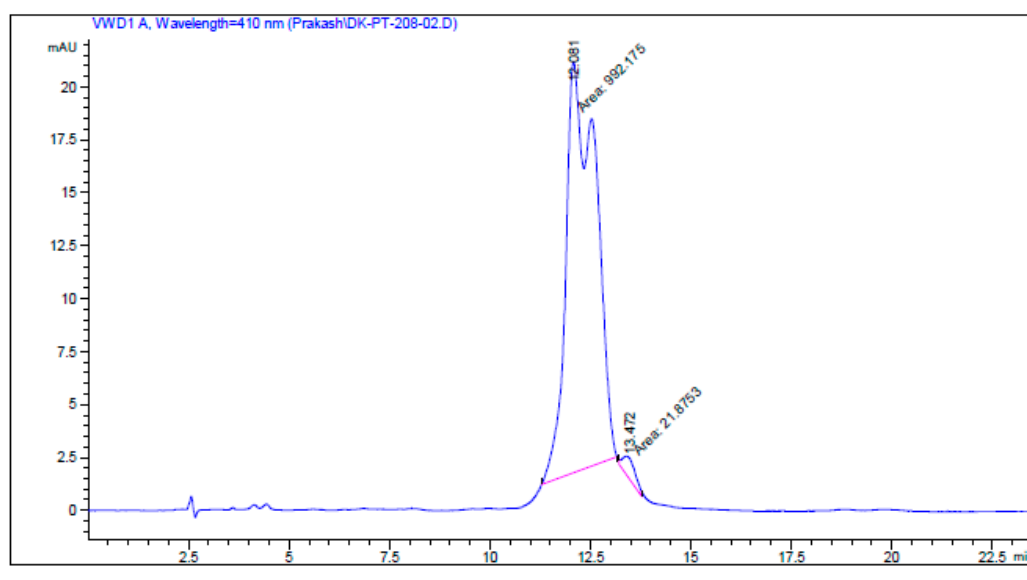
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.853	MM	0.1966	10.52040	8.91656e-1	0.6799
2	12.605	MM	1.1947	1536.90894	21.44054	99.3201

Figure S31. HPLC chromatogram of 6



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.579	MM	0.0800	13.11280	2.73324	0.7877
2	5.518	MM	0.4536	21.97040	8.07332e-1	1.3198

Figure S32: HPLC chromatogram of 8



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.081	MM	0.8530	992.17529	19.38589	97.8428
2	13.472	MM	0.3649	21.87533	9.99117e-1	2.1572