Supporting Information

Effect of Donor Modification on Photo-Physical and Photo-Voltaic Properties of N-Alkyl /Aryl Amines Based Chromophores

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Synthesis:

2.3.1. Synthesis of aldehyde (1a-1f)

The aldehydes (1a-1f) were synthesized by using reported procedure given in literature [45,57], and were purified by using column chromatography and used for further synthesis.

*2.3.2. Synthesis of Compound **MD1-MD6***

Compounds 3a-3e were synthesized by condensing 0.1 mmol of aldehyde (1a-1f) with 0.105 mmol of rhodanine-3-acetic acid in ethanol in presence of catalytic amount of piperidine. The separated solid was filtered and dried under vacuum and the compounds were purified by silica gel column chromatography using dichloromethane: methanol [9:1] as the eluent. The compounds were confirmed by using ^{1}H-NMR and ^{13}C-NMR and elemental analysis (^{1}H-NMR spectra and ^{13}C-NMR spectra given in supporting information).

2.3.3. (Z)-2-(4-Oxo-5-((9-phenyl-9H-carbazol-3-yl) methylene)-2-thioxothiazolidin-3-yl) acetic acid (**MD1**)

^{1}H NMR (500 MHz, DMSO-*d6*) δ 7.65 (s, 1H), 7.48 (d, *J* = 8.9 Hz, 2H), 7.39 (t, *J* = 7.9 Hz, 3H), 7.21 – 7.14 (m, 5H), 6.94 – 6.89 (m, 2H), 4.36 (s, 2H). ^{13}C NMR (126 MHz, DMSO-*d6*) δ 193.28, 168.00, 167.37, 150.22, 146.10, 132.96, 132.89, 130.41, 130.18, 126.48, 126.24, 125.61, 125.41, 120.04, 118.94, 48.21. MS, m/z: cal.: 444.5, found: 445.1 [M^{+} + H]. CNH Analysis calculated (percent) for $C_{24}H_{16}N_2O_3S_2$: C, 64.85; H, 3.63; N, 6.30: O, 10.80; S, 14.43. Found: C, 64.87; H, 3.63; N, 6.31.

2.3.4. (Z)-2-(5-(4-(Diphenylamino) benzylidene)-4-oxo-2-thioxothiazolidin-3-yl) acetic acid **(MD2)**

^{1}H NMR (500 MHz, DMSO-*d6*) δ 9.33 (s, 1H), 7.66 (s, 1H), 7.50 (d, *J* = 8.7 Hz, 2H), 7.39 (t, *J* = 7.9 Hz, 4H), 7.22 – 7.14 (m, 6H), 6.92 (d, *J* = 8.8 Hz, 2H), 4.35 (s, 2H). ^{13}C NMR (126 MHz, DMSO-*d6*) δ 193.27, 167.70, 167.39, 150.21, 146.10, 132.99, 132.86, 130.42, 126.50, 125.62, 125.40, 120.04, 118.93, 48.28. MS, m/z: cal.: 446.5, found: 447.9 [M^{+} + H]. CNH Analysis calculated (percent) for $C_{24}H_{18}N_2O_3S_2$: C, 64.55; H, 4.06; N, 6.27: O, 10.75; S, 14.36. Found: C, 64.58; H, 4.05; N, 6.28.

2.3.5. (Z)-2-(5-(4-(9H-Carbazol-9-yl) benzylidene)-4-oxo-2-thioxothiazolidin-3-yl) acetic acid **(MD3)**

^{1}H NMR (500 MHz, DMSO-*d6*) δ 8.22 (d, *J* = 7.5 Hz, 2H), 7.95 (s, 1H), 7.90 (d, *J* = 7.8 Hz, 2H), 7.80 (d, *J* = 7.7 Hz, 2H), 7.48 (d, *J* = 8.0 Hz, 2H), 7.42 (t, *J* = 7.3 Hz, 2H), 7.30 (t, *J* = 7.1 Hz, 2H), 4.72 (s, 2H). ^{13}C NMR (126 MHz, DMSO-*d6*) δ 193.41, 167.72, 166.89, 139.94, 139.50, 133.12, 132.99, 131.88, 127.39, 126.90, 123.63, 122.67,

121.12, 121.05, 110.30, 45.96. MS, m/z: cal.: 444.5, found: 445.1 [M^++ H]. CNH Analysis calculated (percent) for $C_{24}H_{16}N_2O_3S_2$: C, 64.85; H, 3.63; N, 6.30: O, 10.80; S, 14.43. Found: C, 64.85; H, 3.63; N, 6.31.

2.3.6. (Z)-2-(5-((9-Hexyl-9H-carbazol-3-yl) methylene)-4-oxo-2-thioxothiazolidin-3-yl) acetic acid **(MD4)**

^{1}H NMR (500 MHz, DMSO-*d6*) δ 8.45 (s, 1H), 8.27 (d, *J* = 7.7 Hz, 1H), 7.99 (s, 1H), 7.77 (d, *J* = 8.5 Hz, 1H), 7.71 (d, *J* = 8.8 Hz, 1H), 7.66 (d, *J* = 8.2 Hz, 1H), 7.52 (t, *J* = 7.7 Hz, 1H), 7.28 (t, *J* = 7.4 Hz, 1H), 4.57 (s, 2H), 4.42 (t, *J* = 6.8 Hz, 2H), 2.98 – 2.93 (m, 2H), 1.31 – 1.17 (m, 6H), 0.79 (t, *J* = 6.7 Hz, 3H). ^{13}C NMR (126 MHz, DMSO-*d6*) δ 193.62, 167.64, 167.19, 141.82, 141.17, 135.43, 128.97, 127.25, 124.69, 124.22, 123.43, 122.33, 121.33, 120.44, 118.32, 111.01, 110.48, 46.99, 43.92, 31.36, 28.91, 26.51, 22.43, 14.28. MS, m/z: cal.: 452.6, found: 451.5 [M^+- H]. CNH Analysis calculated (percent) for $C_{24}H_{24}N_2O_3S_2$: C, 63.69; H, 5.34; N, 6.19: O, 10.61; S, 14.17. Found: C, 63.68; H, 5.34; N, 6.20

2.3.7. (Z)-2-(5-(4-(Hexyl(phenyl)amino) benzylidene)-4-oxo-2-thioxothiazolidin-3-yl) acetic acid **(MD5)**

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.70 (s, 1H), 7.45 (t, *J* = 7.7 Hz, 2H), 7.35 – 7.27 (m, 3H), 7.22 (d, *J* = 8.1 Hz, 2H), 6.73 (d, *J* = 8.8 Hz, 2H), 4.92 (s, 2H), 3.75 – 3.70 (m, 2H), 1.70 (dt, *J* = 15.2, 7.7 Hz, 2H), 1.37 – 1.28 (m, 6H), 0.89 (t, *J* = 6.5 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 192.83, 170.60, 167.27, 150.89, 145.53, 135.33, 133.13, 130.10, 127.35, 126.42, 121.90, 115.60, 114.33, 52.67, 44.27, 31.55, 27.27, 26.62, 22.62, 14.01. MS, m/z: cal.: 454.6, found: 456.2 [M^++ H]. CNH Analysis calculated (percent) for $C_{24}H_{26}N_2O_3S_2$: C, 63.41; H, 5.76; N, 6.16: O, 10.56; S, 14.11. Found: 63.43; H, 5.78; N, 6.15.

2.3.8. (Z)-2-(5-(4-(Dihexylamino) benzylidene)-4-oxo-2-thioxothiazolidin-3-yl) acetic acid **(MD6)**

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.71 (s, 1H), 7.39 (d, *J* = 8.8 Hz, 2H), 6.69 (d, *J* = 9.1 Hz, 2H), 4.93 (s, 2H), 3.36 – 3.32 (m, 4H), 1.65 – 1.59 (m, 4H), 1.34 (t, *J* = 6.8 Hz, 12H), 0.91 (t, *J* = 6.4 Hz, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 192.86, 169.88, 167.32, 135.70, 133.69, 114.07, 111.95, 111.88, 111.82, 51.25, 44.29, 31.62, 27.17, 26.71, 22.64, 14.03. MS, m/z: cal.: 462.7, found: 464.3 [M^++ H]. CNH Analysis calculated (percent) for C24H34N2O3S2: C, 62.30; H, 7.41; N, 6.05: O, 10.37; S, 13.86. Found: C, 62.30; H, 7.42; N, 6.06.

Table S1 Photophysical data of **MD1.**

Solvents	**λ_{abs}**		**λ_{ems}**		**ε_{max}**	**Stokes shift**		**FWHM**	**f**
	(nm)	(cm^{-1})	(nm)	(cm^{-1})	(M^{-1} cm^{-1})	(nm)	(cm^{-1})	(nm)	
MDC	446	22421.5	528	18939.4	25000	82	3482.13	66	0.465
THF	434	23041.5	491	20366.6	21400	57	2674.88	59	0.386
EA	433	23094.7	488	20491.8	14200	55	2602.88	60	0.261
1,4-Dioxane	434	23041.5	482	20746.9	20000	48	2294.59	60	0.367
Acetone	434	23041.5	513	19493.2	14800	79	3548.30	68	0.199
Acetonitrile	437	22883.3	523	19120.5	17200	86	3762.84	168	0.348
DMF	430	23255.8	505	19802.0	19400	75	3453.83	61	0.361
DMSO	442	22624.43	528	18939.4	21600	86	3685.04	62	0.386
Ethanol	434	23041.47	502	19920.3	14200	68	3121.16	66	0.263

Table S2 Photophysical properties of **MD2.**

Solvents	**λ_{abs}**		**λ_{ems}**		**ε_{max}**	**Stokes shift**		**FWHM**	**f**
	(nm)	(cm^{-1})	(nm)	(cm^{-1})	(M^{-1} cm^{-1})	(nm)	(cm^{-1})	(nm)	
MDC	479	20876.8	603	16583.7	26000	124	4293.08	71	0.440
THF	461	21692.0	549	18214.9	29400	88	3477.04	64	0.513
EA	465	21505.4	567	17636.7	26800	102	3868.69	65	0.477
1,4-Dioxane	467	21413.3	544	18382.4	29400	77	3030.92	64	0.519
Acetone	466	21459.2	593	16863.4	22600	127	4595.82	66	0.391
Acetonitrile	468	21367.5	523	19120.5	21600	55	2247.06	71	0.394
DMF	466	21459.2	597	16750.4	21000	131	4708.81	67	0.385
DMSO	475	21052.63	616	16233.8	23000	141	4818.87	72	0.381
Ethanol	469	21321.96	582	17182.1	18600	113	4139.83	67	0.328

Table S3 Photophysical properties of **MD3.**

Solvents	**λ_{abs}**		**λ_{ems}**		**ε_{max}**	**Stokes shift**		**FWHM**	**f**
	(nm)	(cm^{-1})	(nm)	(cm^{-1})	(M^{-1} cm^{-1})	(nm)	(cm^{-1})	(nm)	
MDC	427	23419.2	571	17513.1	21400	144	5906.07	69	0.486
THF	418	23923.4	533	18761.7	23200	115	5161.72	111	0.581
EA	417	23980.8	533	18761.7	22400	116	5219.09	110	0.564
Dioxane	419	23866.3	508	19685.0	24000	89	4181.31	110	0.588
Acetone	416	24038.5	582	17182.1	21200	166	6856.33	109	0.539
Acetonitrile	401	24937.7	586	17064.8	15200	185	7872.81	109	0.387
DMF	401	24937.7	566	17667.8	26200	165	7269.81	103	0.626
DMSO	423	23640.66	599	16694.5	21600	176	6946.17	118	0.569
Ethanol	401	24937.66	561	17825.3	26400	160	7112.34	103	0.632

Table S4 Photophysical properties of **MD4.**

Solvents	**λ_{abs}**		**λ_{ems}**		**ε_{max}**	**Stokes shift**		**FWHM**	**f**
	(nm)	(cm^{-1})	(nm)	(cm^{-1})	(M^{-1} cm^{-1})	(nm)	(cm^{-1})	(nm)	
MDC	451	22172.9	516	19379.8	31000	65	2793.10	63	0.517
THF	440	22727.3	495	20202.0	29400	55	2525.25	161	0.516
EA	439	22779.0	495	20202.0	29800	56	2577.02	59	0.529
Dioxane	438	22831.1	488	20491.8	28800	50	2339.25	58	0.493
Acetone	441	22675.7	516	19379.8	26000	75	3295.89	62	0.478
Acetonitrile	438	22831.1	524	19084.0	23600	86	3747.08	66	0.460
DMF	437	22883.3	515	19417.5	27600	78	3465.82	61	0.498
DMSO	452	22123.9	535	18691.6	28800	83	3432.31	66	0.545
Ethanol	431	23201.9	521	19193.9	26000	90	4008.00	64	0.495

Table S5 Photophysical properties of **MD5.**

Solvents	λ_{abs}		λ_{ems}		ε_{max}	Stokes shift		FWHM	f
	(nm)	(cm^{-1})	(nm)	(cm^{-1})	(M^{-1} cm^{-1})	(nm)	(cm^{-1})	(nm)	
MDC	478	20920.5	556	17985.6	75200	78	2934.89	60	1.418
THF	464	21551.7	542	18450.2	82800	78	3101.54	60	1.667
EA	462	21645.0	542	18450.2	66200	80	3194.84	60	1.317
Dioxane	462	21645.0	540	18518.5	64000	78	3126.50	60	1.288
Acetone	466	21459.2	551	18148.8	61200	85	3310.41	62	0.991
Acetonitrile	464	21551.7	559	17889.1	53400	95	3662.64	64	1.086
DMF	466	21459.2	554	18050.5	64600	88	3408.69	64	1.366
DMSO	480	20833.3	571	17513.1	57200	91	3320.20	66	1.199
Ethanol	462	21645.0	564	17730.5	61800	102	3914.53	66	1.339

Table S6 Photophysical properties of **MD6.**

Solvents	λ_{abs}		λ_{ems}		ε_{max}	Stokes shift		FWHM	f
	(nm)	(cm^{-1})	(nm)	(cm^{-1})	(M^{-1} cm^{-1})	(nm)	(cm^{-1})	(nm)	
MDC	488	20491.8	534	18726.6	65600	46	1765.21	60	1.157
THF	476	21008.4	512	19531.3	66400	36	1477.15	66	1.666
EA	474	21097.0	515	19417.5	68600	41	1679.57	66	1.520
Dioxane	472	21186.4	512	19531.3	56400	40	1655.19	56	0.925
Acetone	480	20833.3	553	18083.2	59800	73	2750.15	60	0.888
Acetonitrile	480	20833.3	561	17825.3	54200	81	3008.02	64	1.028
DMF	480	20833.3	553	18083.2	39800	73	2750.15	62	0.622
DMSO	496	20161.3	571	17513.1	50800	75	2648.16	64	0.731
Ethanol	470	21276.6	553	18083.2	53200	83	3193.41	66	1.032

Table S7: Comparison of experimental absorption and vertical excitation obtained by TD-DFT **for MD1**

Solvent	Absorption	Vertical Excitation	Oscillator Strength	Orbital Contribution
	nm	nm		
MDC	446	458	1.0176	99.3
THF	434	457	1.0133	99.2
EA	433	455	1.0048	99.2
1,4-Dioxane	434	447	1.0490	99.3
Acetone	434	459	0.9877	99.2
Acetonitrile	437	459	0.9799	99.2
DMF	430	462	1.0109	99.3
DMSO	442	462	1.0057	99.2
Ethanol	434	459	0.9877	99.2

Table S8: Comparison of experimental absorption and vertical excitation obtained by TD-DFT **for MD2**

Solvent	Absorption	Vertical Excitation	Oscillator Strength	Orbital Contribution
	nm	nm		
MDC	479	514	1.0508	99.5
THF	461	512	1.0450	99.5
EA	465	510	1.0352	99.5
1,4-Dioxane	467	501	1.0433	99.4
Acetone	466	514	1.0355	99.5
Acetonitrile	468	514	1.0325	99.5
DMF	466	517	1.0563	99.5
DMSO	475	517	1.0532	99.5
Ethanol	469	514	1.0366	99.5

Table S9: Comparison of experimental absorption and vertical excitation obtained by TD-DFT **for MD3**

Solvent	Absorption	Vertical Excitation	Oscillator Strength	Orbital Contribution
	nm	nm		
MDC	427	526	0.5536	99.2
THF	418	524	0.5463	99.2
EA	417	524	0.5383	99.2
1,4-Dioxane	419	526	0.5479	99.2

Acetone	**416**	**522**	**0.5383**	**99.2**
Acetonitrile	**401**	**521**	**0.5357**	**99.2**
DMF	**401**	**523**	**0.5554**	**99.2**
DMSO	**423**	**522**	**0.5529**	**99.2**
Ethanol	**401**	**521**	**0.5318**	**99.2**

Table S10: Comparison of experimental absorption and vertical excitation obtained by TD-DFT for **MD4**

Solvent	**Absorption**	**Vertical Excitation**		
	nm	**nm**	**Oscillator Strength**	**Orbital Contribution**
MDC	**451**	**463**	**1.0035**	**99.3**
THF	**440**	**461**	**0.9990**	**99.3**
EA	**439**	**459**	**0.9903**	**99.2**
1,4-Dioxane	**438**	**449**	**1.0341**	**99.3**
Acetone	**441**	**464**	**0.9737**	**99.2**
Acetonitrile	**438**	**464**	**0.9659**	**99.2**
DMF	**437**	**467**	**0.9974**	**99.3**
DMSO	**452**	**467**	**0.9922**	**99.3**
Ethanol	**431**	**464**	**0.9739**	**99.2**

Table S11: Comparison of experimental absorption and vertical excitation obtained by TD-DFT for **MD5**

Solvent	**Absorption**	**Vertical Excitation**		
	nm	**nm**	**Oscillator Strength**	**Orbital Contribution**
MDC	**478**	**471**	**1.1507**	**99.5**
THF	**464**	**473**	**1.1414**	**99.5**
EA	**462**	**470**	**1.1332**	**99.5**
1,4-Dioxane	**462**	**462**	**1.1450**	**99.4**
Acetone	**466**	**475**	**1.1300**	**99.5**
Acetonitrile	**464**	**476**	**1.1261**	**99.5**
DMF	**466**	**479**	**1.1481**	**99.5**
DMSO	**480**	**479**	**1.1449**	**99.5**
Ethanol	**462**	**475**	**1.1218**	**99.5**

Table S12 Comparison of experimental absorption and vertical excitation obtained by TD-DFT for **MD6**

Solvent	Absorption	Vertical Excitation	Oscillator Strength	Orbital Contribution
	nm	nm		
MDC	488	474	0.8621	99.2
THF	476	473	0.8538	99.2
EA	474	471	0.8408	99.1
1,4-Dioxane	472	466	0.8346	98.8
Acetone	480	474	0.8554	99.3
Acetonitrile	480	474	0.8554	99.3
DMF	480	477	0.8794	99.4
DMSO	496	477	0.8771	99.4
Ethanol	470	475	0.8578	99.3

Table S13 Ratio of dipole moment for **MD1-MD6.**

Molecule		m1	m2	m1+m2	m2-m1	μe/μg
MD1	Bilot Kawski Function	1876.4	2257.0	4133.4	380.6	10.9
	Bakhshiev Function	1876.4	2261.2	4137.6	384.8	10.8
	Liptay Function	2231.0	2808.2	5039.2	577.2	8.7
MD2	Bilot Kawski Function	2302.7	2783.0	5085.7	480.3	10.6
	Bakhshiev Function	2302.7	2779.0	5081.7	476.3	10.7
	Liptay Function	2853.1	3434.1	6287.2	581.0	10.8
MD3	Bilot Kawski Function	Linearity Not Observed				
	Bakhshiev Function	4257.8	8688.8	12946.6	4431.0	2.9
	Liptay Function	Linearity Not Observed				
MD4	Bilot Kawski Function	1821.9	2357.4	4179.3	535.5	7.8
	Bakhshiev Function	1821.9	6315.4	8137.3	4493.5	1.8
	Liptay Function	2265.8	2724.5	4990.3	458.7	10.9
MD5	Bilot Kawski Function	1005.8	1394.3	2400.1	388.5	6.2
	Bakhshiev Function	1268.3	7074.0	8342.3	5805.7	1.4
	Liptay Function	Linearity Not Observed				
MD6	Bilot Kawski Function	2847.2	3977.9	6825.1	1130.7	6.0
	Bakhshiev Function	2847.2	11288.0	14135.2	8440.8	1.7
	Liptay Function	3779.6	4170.6	2617.1	801.3	3.3

Table S14: Estimated coefficients (y_0, a, b, c, d), their standard errors and correlation coefficients (r) for the multi-linear analysis of ($\bar{\upsilon}_{abs}$), ($\bar{\upsilon}_{emi}$) and ($\Delta\bar{\upsilon}$) of **MD1 to MD6** as a function of Kamlet-Taft and Catalan solvent scales.

MD1						
Kamlet-Taft	**$y_0 \times 10^3$**	**aα**	**bβ**	**cπ***	**r**	
$\nu_{abs}(cm^{-1})$	23.37 ± 0.35	(-0.35) ± 0.29	0.78 ± 0.36	(-1.09) ± 0.47	0.61	
$\nu_{emi}(cm^{-1})$	22.27 ± 0.50	(-1.27) ± 0.41	1.25 ± 0.51	(-4.18) ± 0.67	0.88	
$\nu_0(cm^{-1})$	1.09 ± 0.53	0.92 ± 0.44	(-0.45) ± 0.54	3.08 ± 0.71	0.79	
Catalan	**$y_0 \times 10^3$**	**aSA**	**bSB**	**cSPP**	**dSP**	**r**
$\nu_{abs}(cm^{-1})$	24.44 ± 0.84	(-0.79) ± 0.61	1.19 ± 0.43	(-0.61) ± 0.87	(-2.13) ± 1.16	0.74
$\nu_{emi}(cm^{-1})$	25.00 ± 0.91	(-1.12) ± 0.65	2.49 ± 0.47	(-6.94) ± 0.95	(-0.57) ± 1.26	0.95
$\nu_0(cm^{-1})$	(-0.56) ± 0.77	0.32 ± 0.55	(-1.31) ± 0.39	6.33 ± 0.80	(-1.56) ± 1.06	0.94
MD2						
Kamlet-Taft	**$y_0 \times 10^3$**	**aα**	**bβ**	**cπ***	**r**	
$\nu_{abs}(cm^{-1})$	21.99 ± 0.27	(-0.51) ± 0.23	0.65 ± 0.28	(-1.26) ± 0.36	0.74	
$\nu_{emi}(cm^{-1})$	20.20 ± 0.76	(-1.26) ± 0.63	0.60 ± 0.78	(-4.49) ± 1.02	0.79	
$\nu_0(cm^{-1})$	1.79 ± 0.88	0.74 ± 0.73	0.05 ± 0.91	3.23 ± 1.17	0.62	
Catalan	**$y_0 \times 10^3$**	**aSA**	**bSB**	**cSPP**	**dSP**	**r**
$\nu_{abs}(cm^{-1})$	23.08 ± 0.61	(-1.19) ± 0.44	1.08 ± 0.31	(-0.58) ± 0.64	(-2.38) ± 0.85	0.84
$\nu_{emi}(cm^{-1})$	23.02 ± 2.09	(-0.65) ± 1.50	1.49 ± 1.08	(-8.41) ± 2.19	0.97 ± 2.89	0.82
$\nu_0(cm^{-1})$	0.059 ± 1.66	(-0.54) ± 1.19	(-0.41) ± 0.85	7.83 ± 1.73	(-3.35) ± 2.29	0.83
MD3						
Kamlet-Taft	**$y_0 \times 10^3$**	**aα**	**bβ**	**cπ***	**r**	
$\nu_{abs}(cm^{-1})$	23.67 ± 1.03	0.84 ± 0.85	0.98 ± 1.06	(-0.13) ± 1.37	0.37	
$\nu_{emi}(cm^{-1})$	21.79 ± 1.03	(-1.68) ± 0.85	0.35 ± 1.06	(-5.41) ± 1.37	0.76	
$\nu_0(cm^{-1})$	1.87 ± 1.58	2.53 ± 1.31	0.64 ± 1.63	5.27 ± 2.11	0.65	
Catalan	**$y_0 \times 10^3$**	**aSA**	**bSB**	**cSPP**	**dSP**	**r**

$\nu_{abs}(cm^{-1})$	25.54 ± 2.71	0.92 ± 1.94	0.59 ± 1.39	2.23 ± 2.82	(-5.13) ± 3.73	0.48
$\nu_{emi}(cm^{-1})$	25.08 ± 1.46	(-0.81) ± 1.05	1.71 ± 0.75	(-11.71) ± 1.52	3.03 ± 2.01	0.94
$\nu_0(cm^{-1})$	0.46 ± 2.52	1.74 ± 1.81	(-1.11) ± 1.30	13.93 ± 2.63	(-8.16) ± 3.48	0.89
			MD4			
Kamlet-Taft	**$y_0 \times 10^3$**	**aα**	**bβ**	**cπ***	**r**	
$\nu_{abs}(cm^{-1})$	23.33± 0.44	0.07± 0.36	0.53± 0.45	(-1.32)± 0.58	0.6	
$\nu_{emi}(cm^{-1})$	22.16 ± 0.42	(-1.37) ± 0.35	(-0.02) ± 0.43	(-3.38)± 0.56	0.9	
$\nu_0(cm^{-1})$	1.18 ± 0.60	1.44 ± 0.50	0.56 ± 0.62	2.05± 0.80	0.76	
Catalan	**$y_0 \times 10^3$**	**aSA**	**bSB**	**cSPP**	**dSP**	**r**
$\nu_{abs}(cm^{-1})$	25.29 ± 1.09	0.04 ± 0.79	0.75 ± 0.56	(-1.09) ± 1.14	(-2.88) ± 1.51	0.7
$\nu_{emi}(cm^{-1})$	24.46 ± 1.03	(-1.80) ± 0.74	1.01 ± 0.53	(-6.34) ± 1.08	0.28 ± 1.42	0.93
$\nu_0(cm^{-1})$	0.83 ± 1.38	1.84 ± 0.99	(-0.27) ± 0.71	5.24 ± 1.44	(-3.15) ± 1.90	0.85
			MD5			
Kamlet-Taft	**$y_0 \times 10^3$**	**aα**	**bβ**	**cπ***	**r**	
$\nu_{abs}(cm^{-1})$	22.42 ± 0.36	(-0.16) ± 0.29	0.41 ± 0.37	(-1.68) ± 0.47	0.73	
$\nu_{emi}(cm^{-1})$	19.57 ± 0.19	(-0.88) ± 0.16	(-0.14) ± 0.20	(-1.83) ± 0.26	0.94	
$\nu_0(cm^{-1})$	2.85 ± 0.34	0.73 ± 0.28	0.55 ± 0.35	0.15 ± 0.45	0.74	
Catalan	**$y_0 \times 10^3$**	**aSA**	**bSB**	**cSPP**	**dSP**	**r**
$\nu_{abs}(cm^{-1})$	24.65 ± 0.76	(-0.43) ± 0.54	0.76 ± 0.39	(-1.61) ± 0.79	(-3.09) ± 1.04	0.85
$\nu_{emi}(cm^{-1})$	21.07 ± 0.63	(-1.64) ± 0.45	0.51 ± 0.33	(-2.89) ± 0.66	(-0.88) ± 0.87	0.92
$\nu_0(cm^{-1})$	3.57 ± 0.89	1.22 ± 0.64	0.26 ± 0.46	1.28 ± 0.92	(-2.20) ± 1.23	0.78
			MD6			
Kamlet-Taft	**$y_0 \times 10^3$**	**aα**	**bβ**	**cπ***	**r**	
$\nu_{abs}(cm^{-1})$	22.09 ± 0.28	0.05 ± 0.23	0.25 ± 0.29	(-1.93) ± 0.37	0.86	
$\nu_{emi}(cm^{-1})$	21.87 ± 0.73	(-1.53) ± 0.61	(-0.53) ± 0.75	(-4.03) ± 0.97	0.82	
$\nu_0(cm^{-1})$	0.23 ± 0.83	1.59 ± 0.69	0.78 ± 0.86	2.09 ± 1.12	0.67	

Catalan	$y_0 \times 10^3$	aSA	bSB	cSPP	dSP	r
$\nu_{abs}(cm^{-1})$	24.51 ± 0.68	0.29 ± 0.49	0.63 ± 0.35	(-2.68) ± 0.71	(-2.35) ± 0.94	0.91
$\nu_{emi}(cm^{-1})$	24.18 ± 2.23	(-1.65) ± 1.60	0.67 ± 1.15	(-8.17) ± 2.33	1.67 ± 3.07	0.8
$\nu_0(cm^{-1})$	0.33 ± 2.25	1.95 ± 1.62	(-0.04) ± 1.16	5.49 ± 2.35	(-4.02) ± 3.01	0.72

Table S15. Comparative study of the photovoltaic performance for the reported rhodanine 3-acetic acid anchoring group based dyes.

Dye	J_{sc} (mA cm^{-2})	V_{oc} (V)	FF (%)	PCE (%)	Ref.
JY04	5.89	0.582	0.72	2.47	S1
JY05	8.33	0.617	0.70	3.60	
CAR-R9	8.26	0.722	0.73	4.35	S2
TPA-R9	6.75	0.710	0.74	3.58	
J-R9	4.48	0.661	0.72	2.16	
3	3.94	0.53	0.74	1.59	S3
7a	2.06	0.47	0.47	0.72	
MD-153	13.5	0.72	0.42	4.0	S4
B18	5.40	0.669	0.71	2.56	S5
CPTD-R	3.87	0.657	0.71	1.82	
BYD-R	2.44	0.590	0.68	0.97	
DB-2	1.34	0.576	0.66	0.51	S6
SK2	7.1	0.534	0.53	2.0	S7
MC3	8.62	0.626	0.66	3.79	S8
MC4	11.18	0.637	0.65	4.60	
WHB-2	3.33	0.58	0.73	1.41	S9
WHB-4	4.03	0.60	0.73	1.77	
WHB-6	3.41	0.56	0.73	1.39	
C-RA	2.83	0.472	0.68	0.90	S10

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Table S16: Impedance spectroscopy fitting parameters of DSSCs sensitized with MD dye

Photovoltaic parameters	MD chromophore					
	MD1	MD2	MD3	MD4	MD5	MD6
RCT (Ω) b	22.81	23.64	23.22	24.63	23.10	23.28
CPE-P	0.81	0.78	0.77	0.79	0.75	0.77
C (F cm-2)	0.00257	0.00241	0.00344	0.00318	0.00324	0.00352

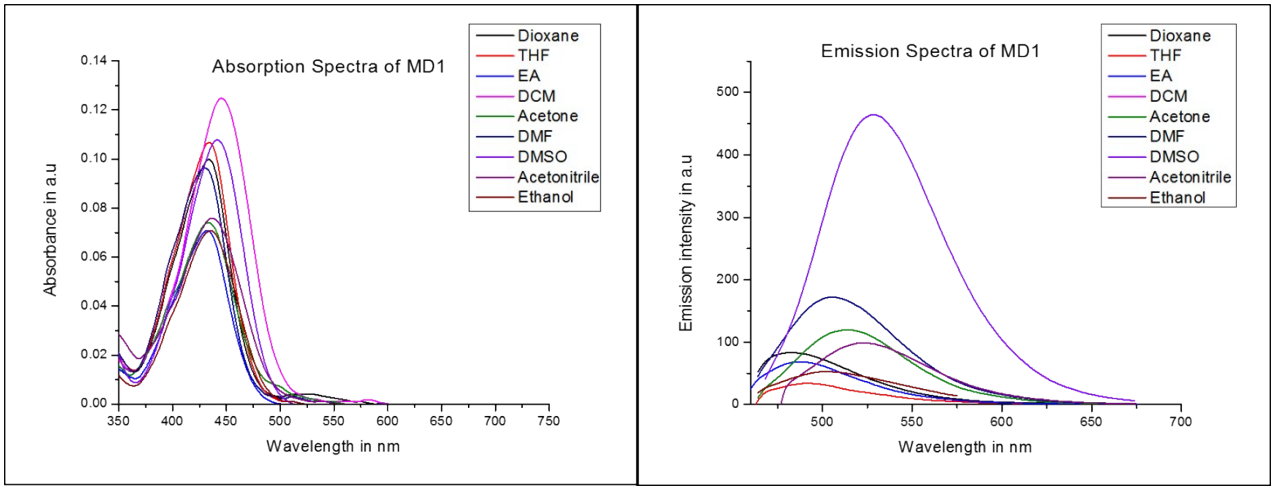

Fig. S1. Absorption and Emission spectra of MD1.

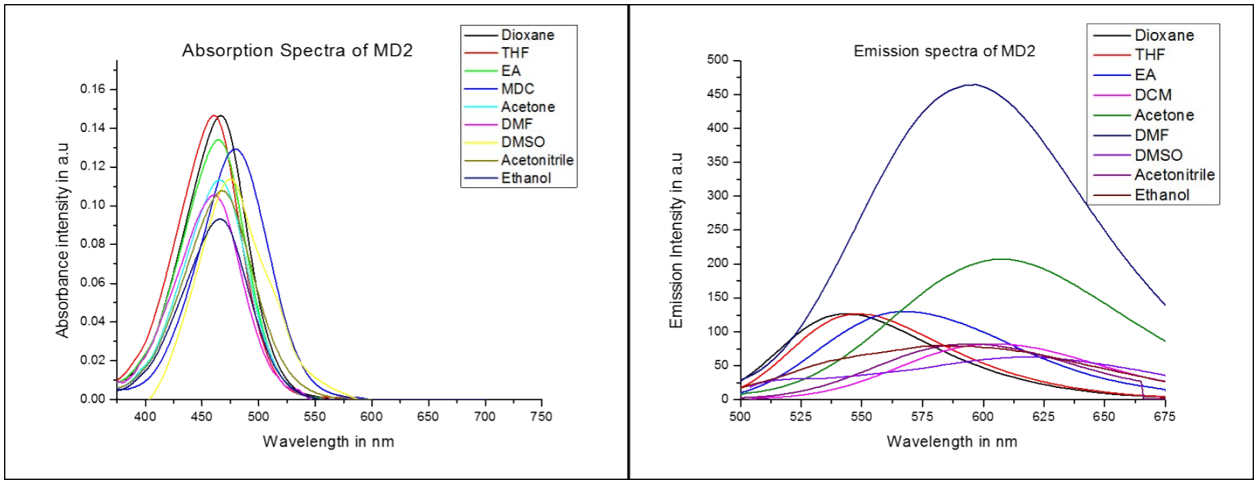

Fig. S2. Absorption and Emission spectra of **MD2.**

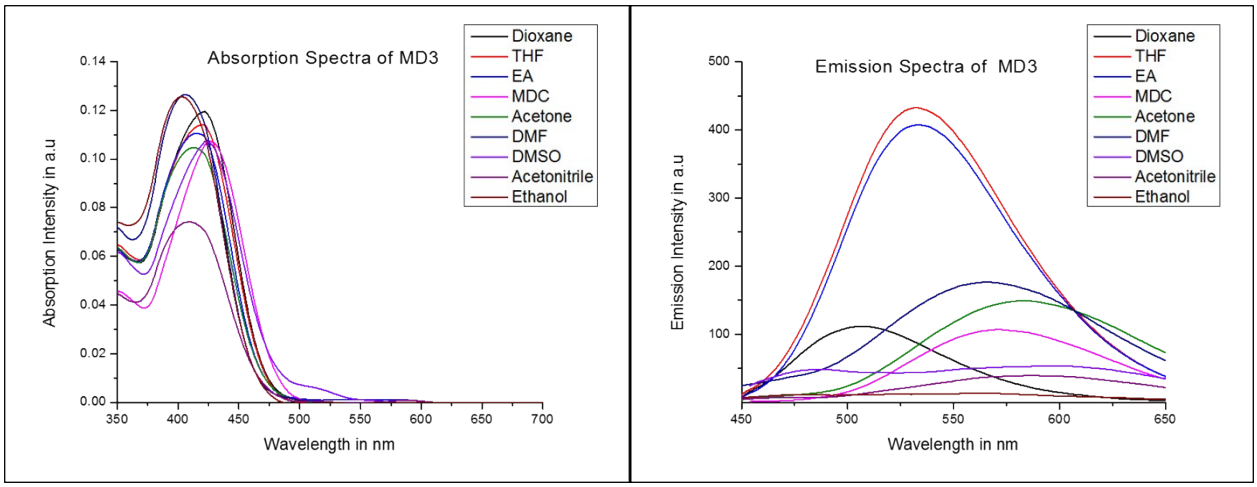

Fig. S3. Absorption and Emission spectra of **MD3.**

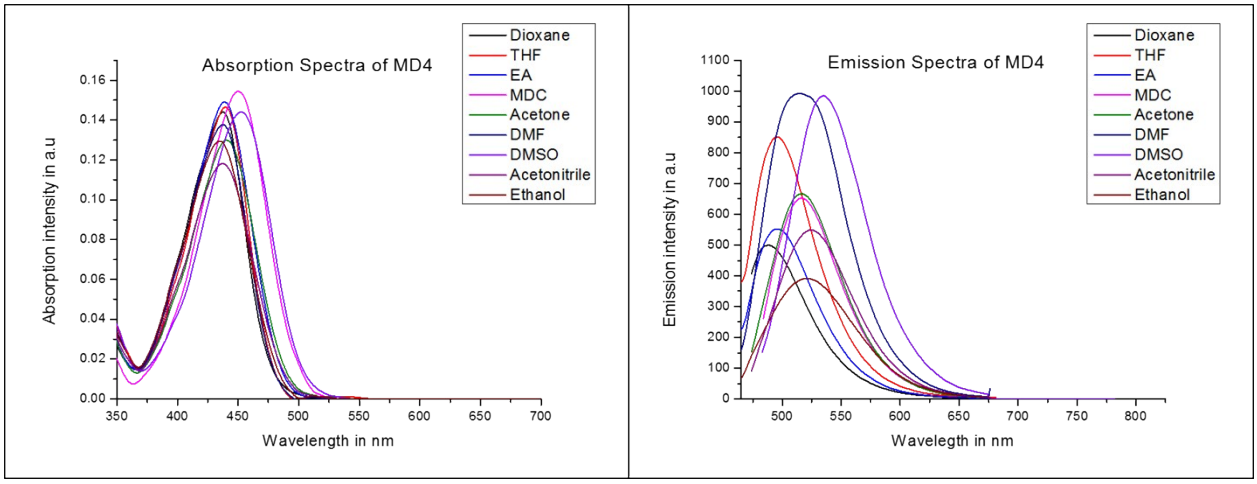

Fig. S4. Absorption and Emission spectra of **MD4.**

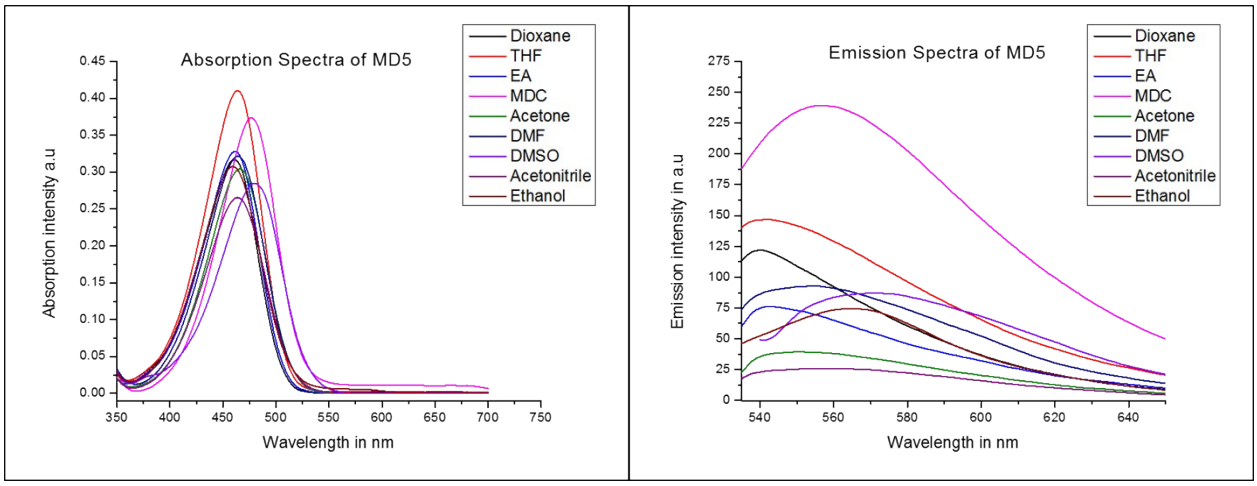

Fig. S5. Absorption and Emission spectra of **MD5.**

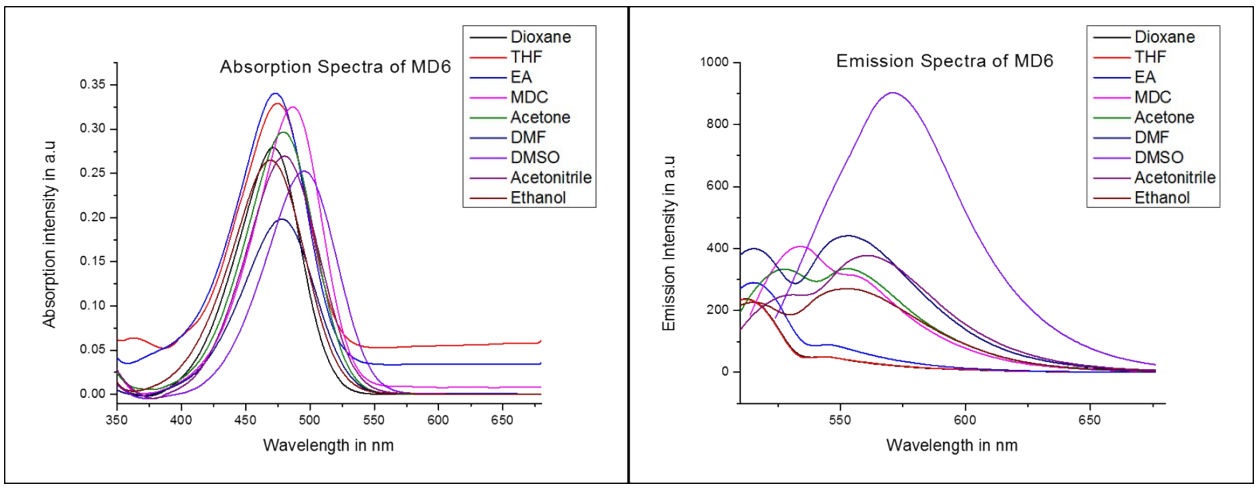

Fig. S6. Absorption and Emission spectra of **MD6.**

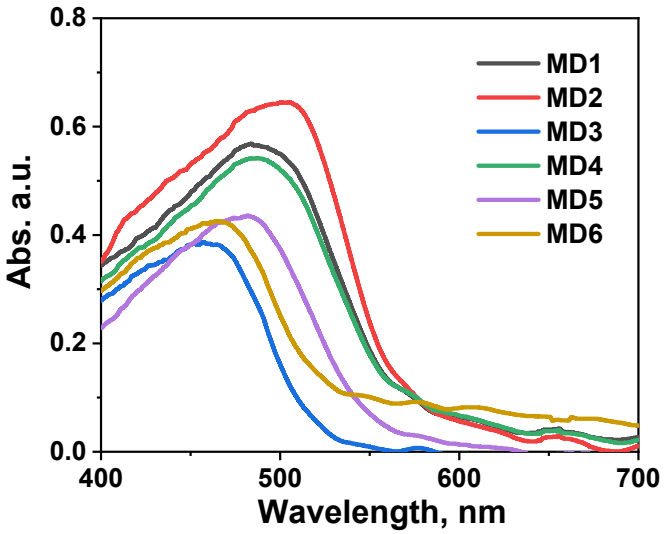

Fig. S7: Absorption spectra of MD1-MD6 on titania film

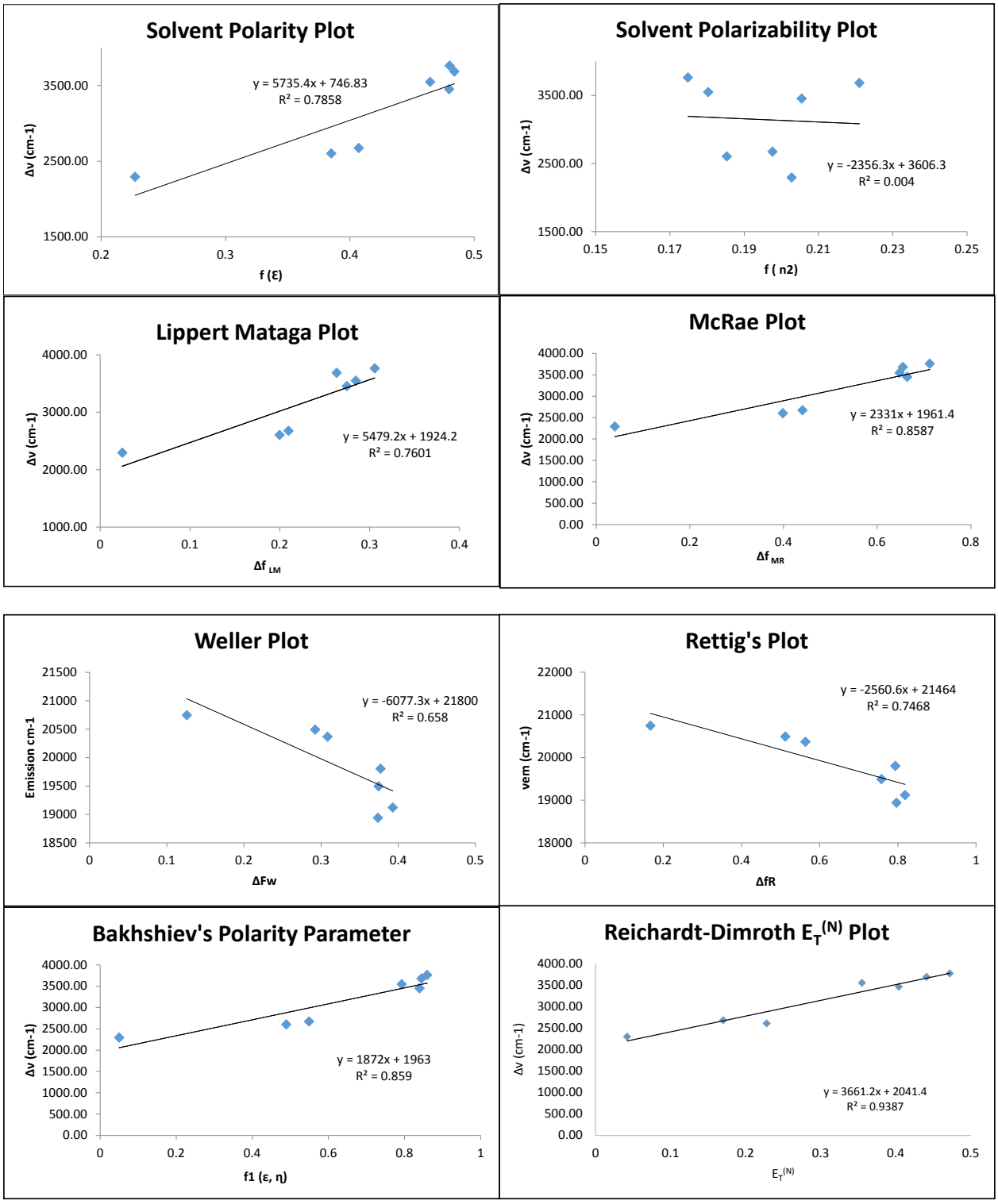

Fig. S8: Solvent polarity plots for MD1

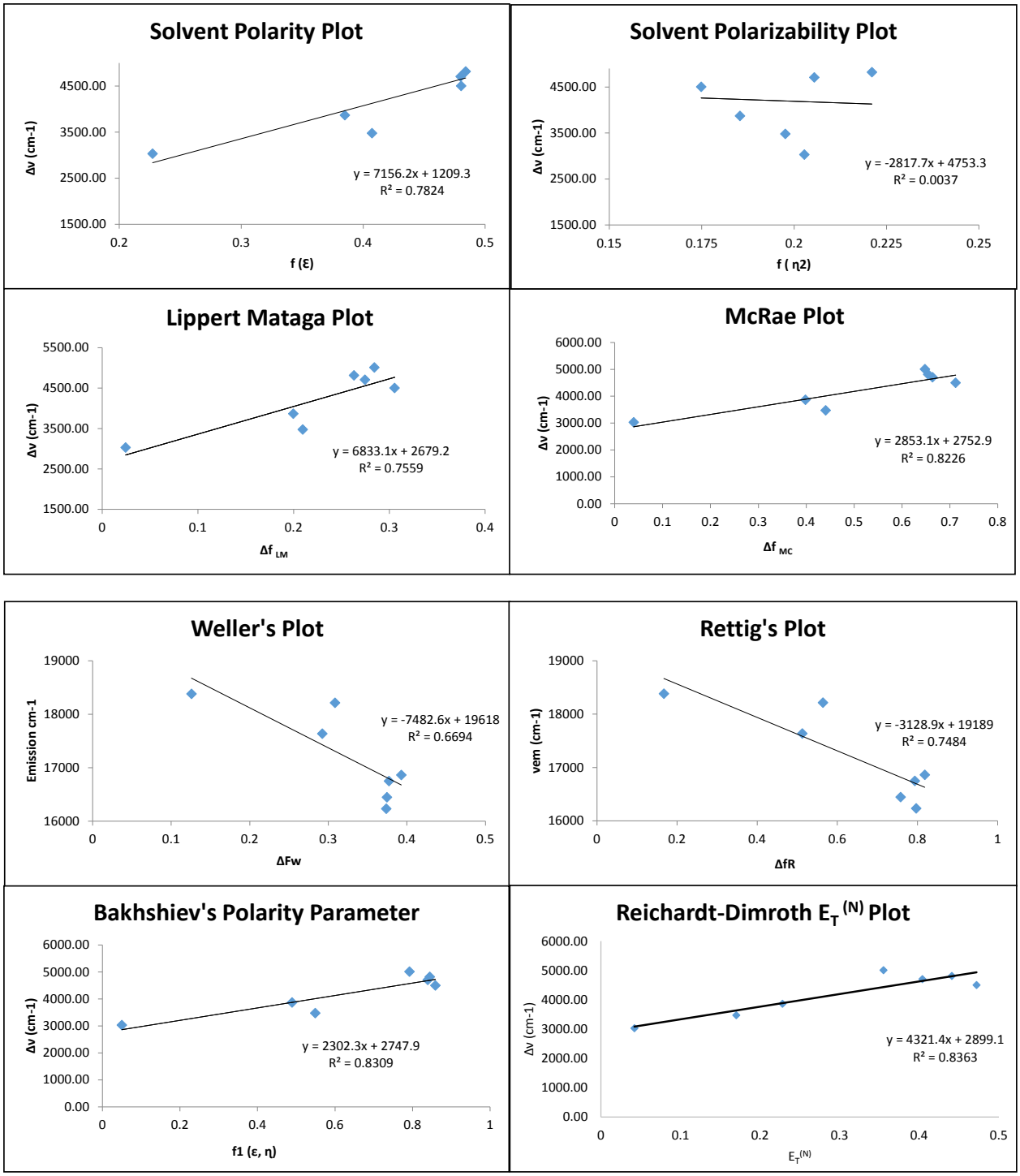

Fig. S9: Solvent polarity plots for MD2

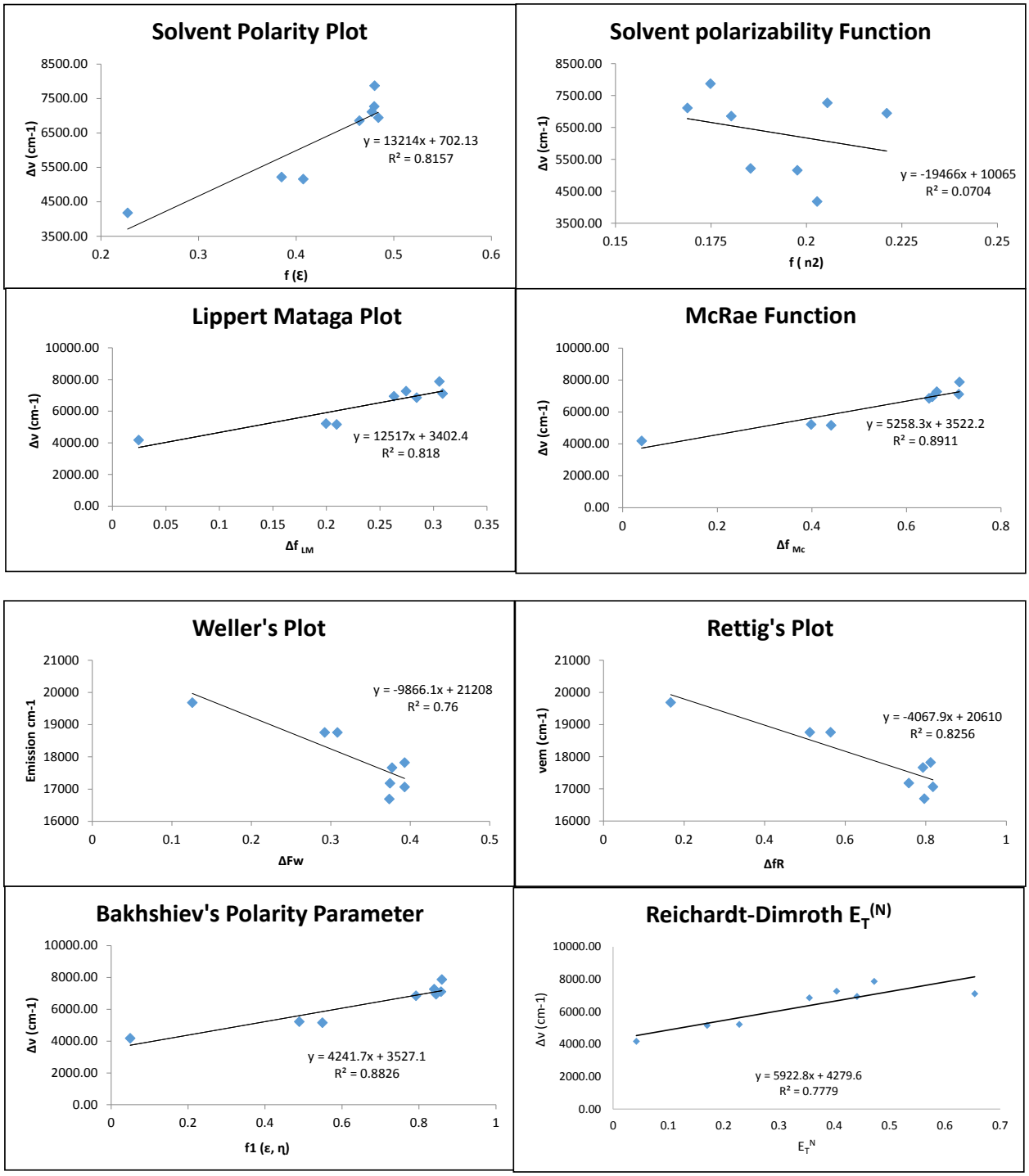

Fig. S10: Solvent polarity plots for MD3

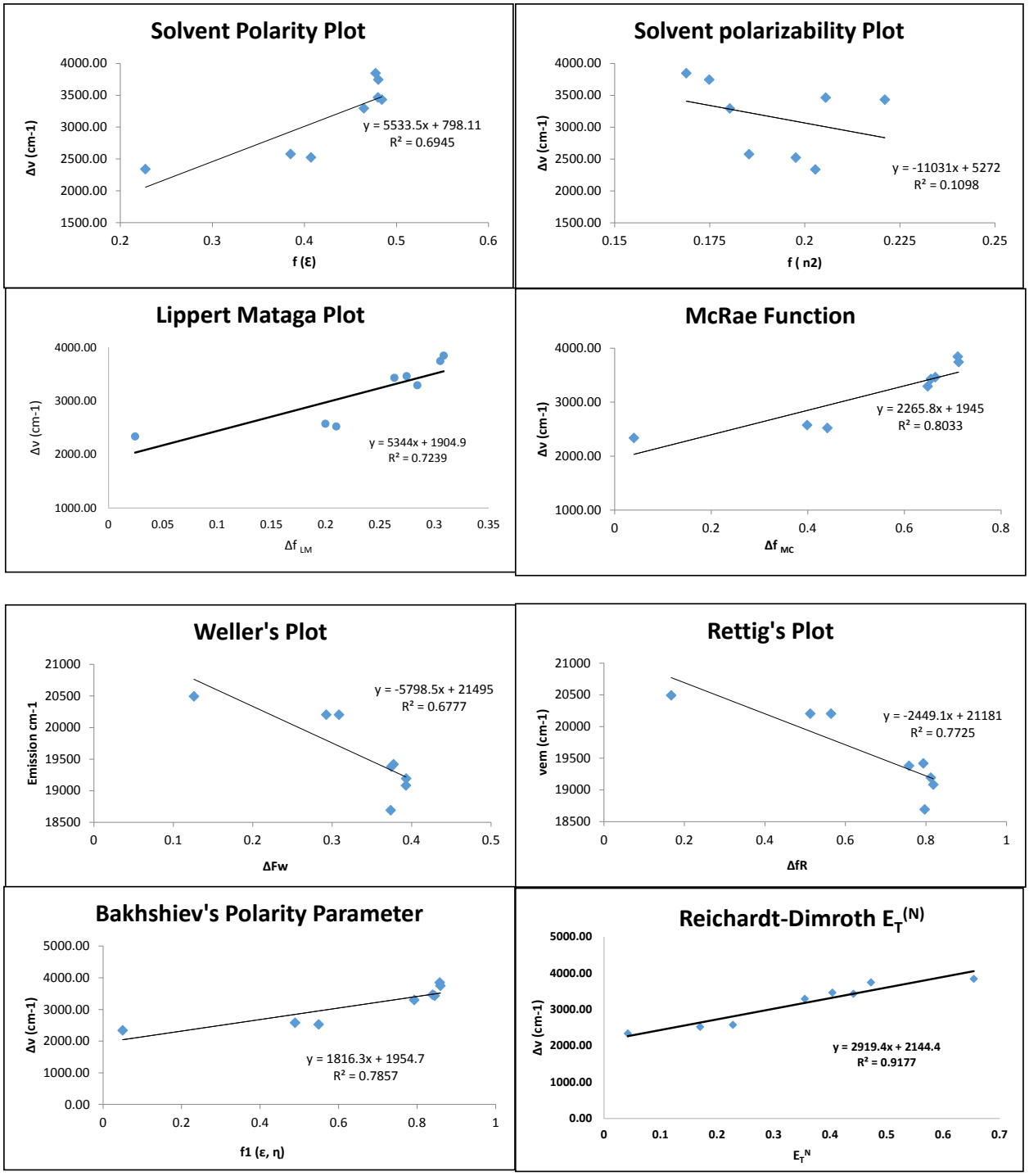

Fig. S11: Solvent polarity plots for MD4

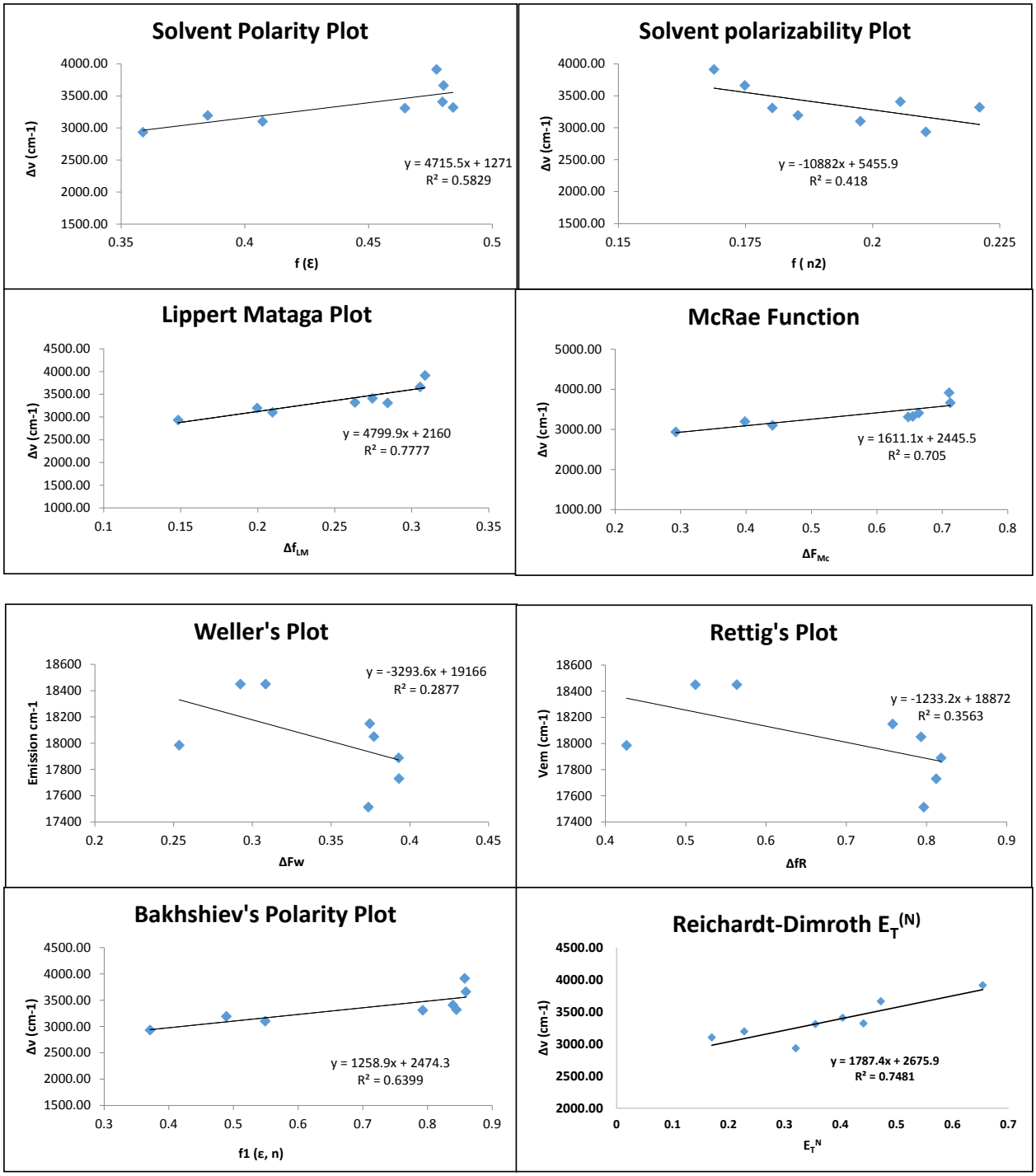

Fig. S12: Solvent polarity plots for MD5

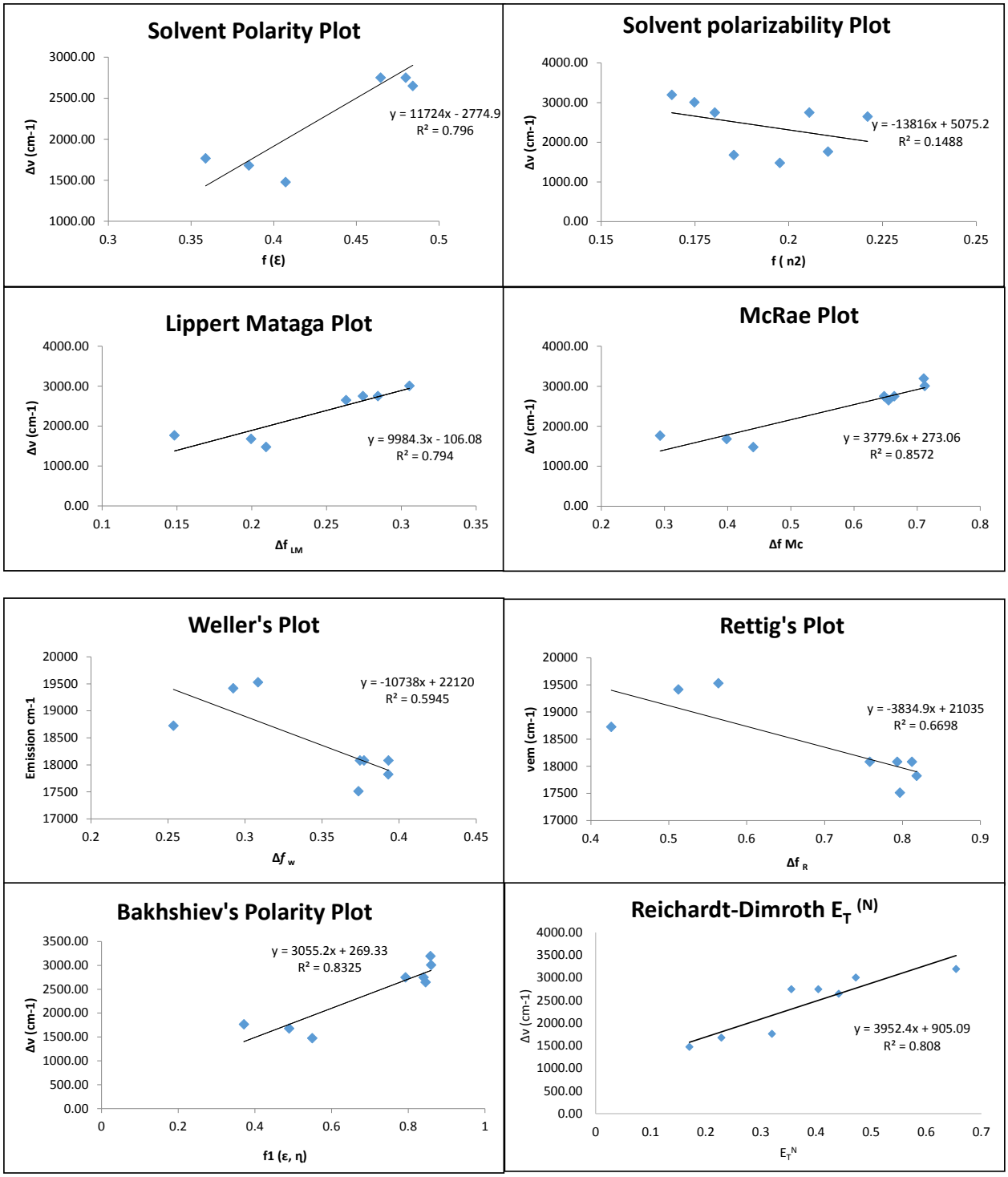

Fig. S13: Solvent polarity plots for MD6

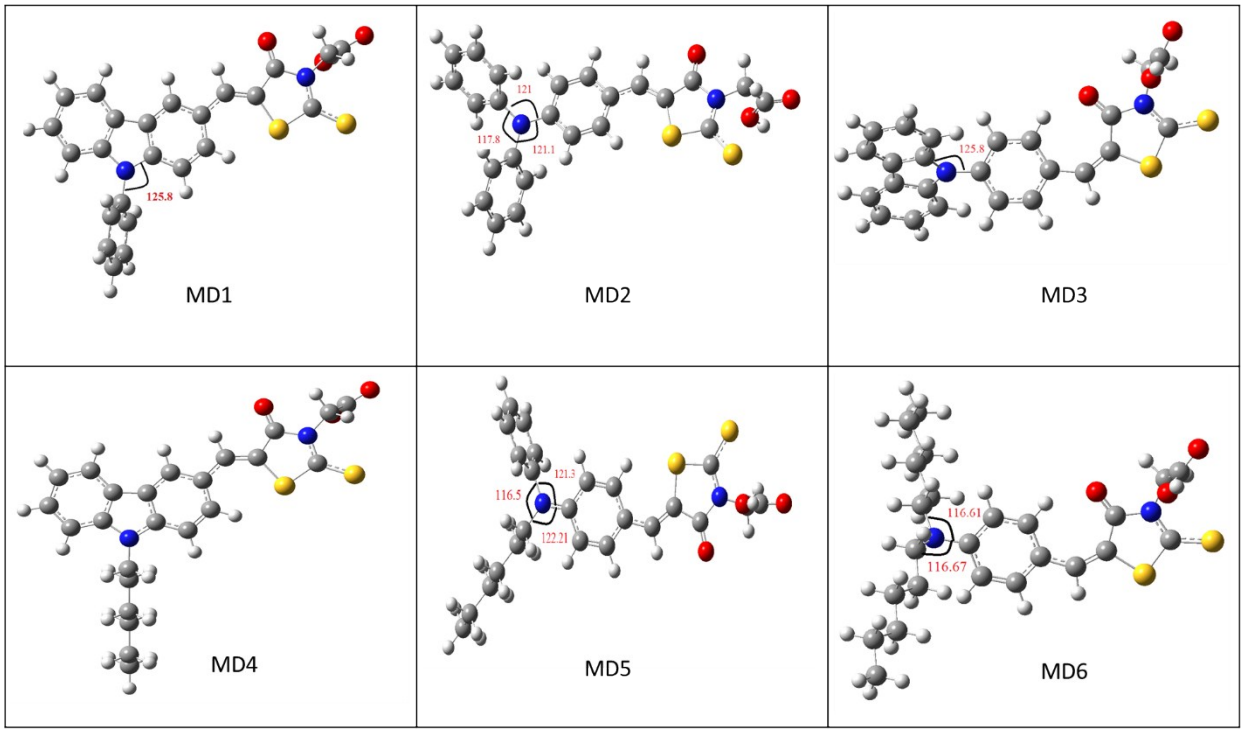

Figure S14. Optimised structures of **MD1** to **MD6** in acetonitrile

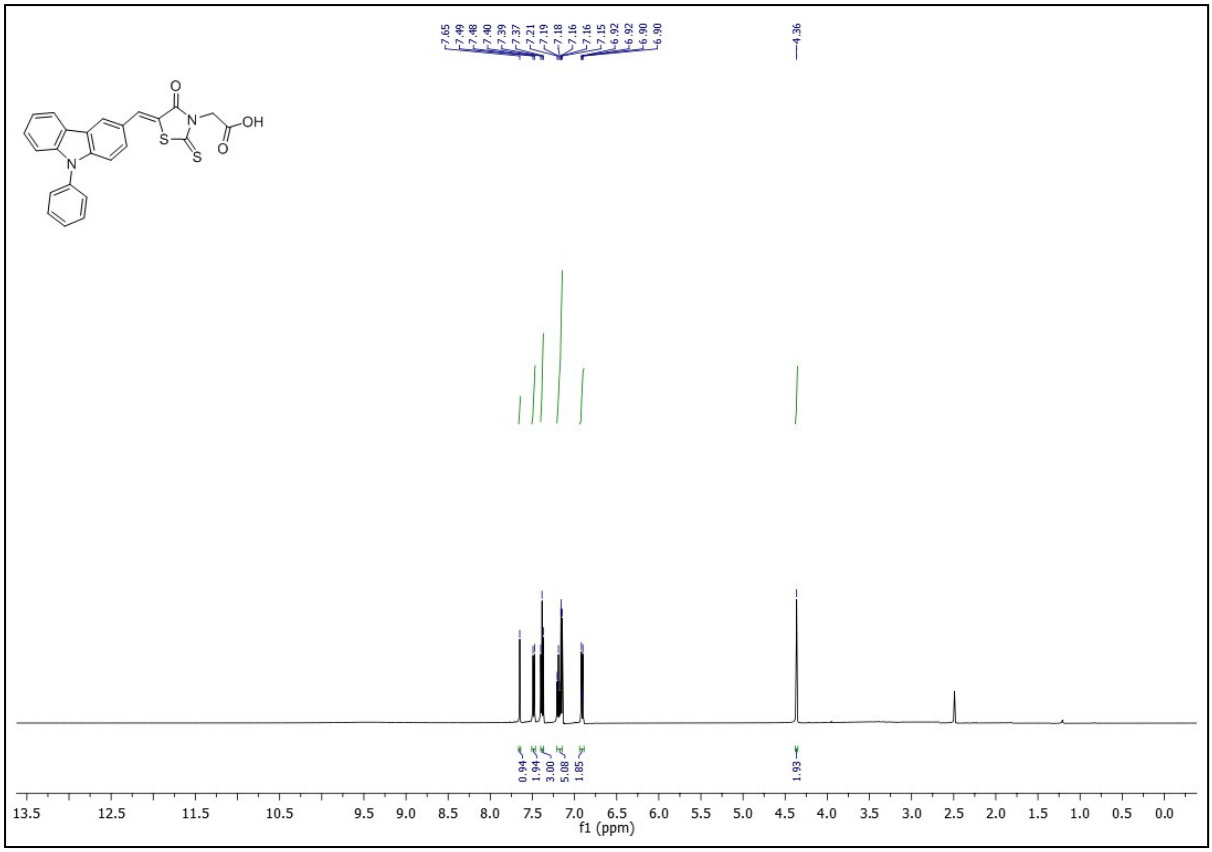

Fig. S15. ^{1}H NMR spectrum of chromophore **MD1**

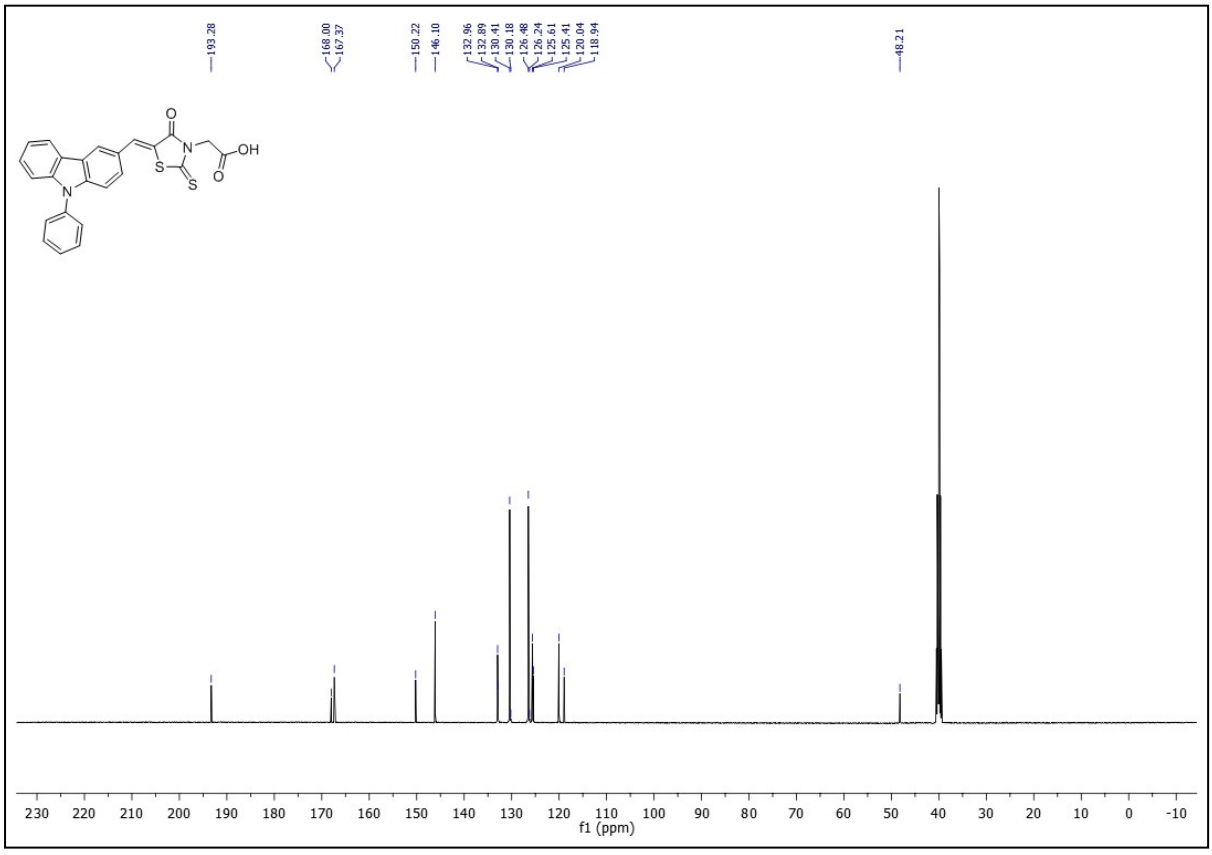

Fig. S16. ^{13}C NMR spectrum of chromophore **MD1**

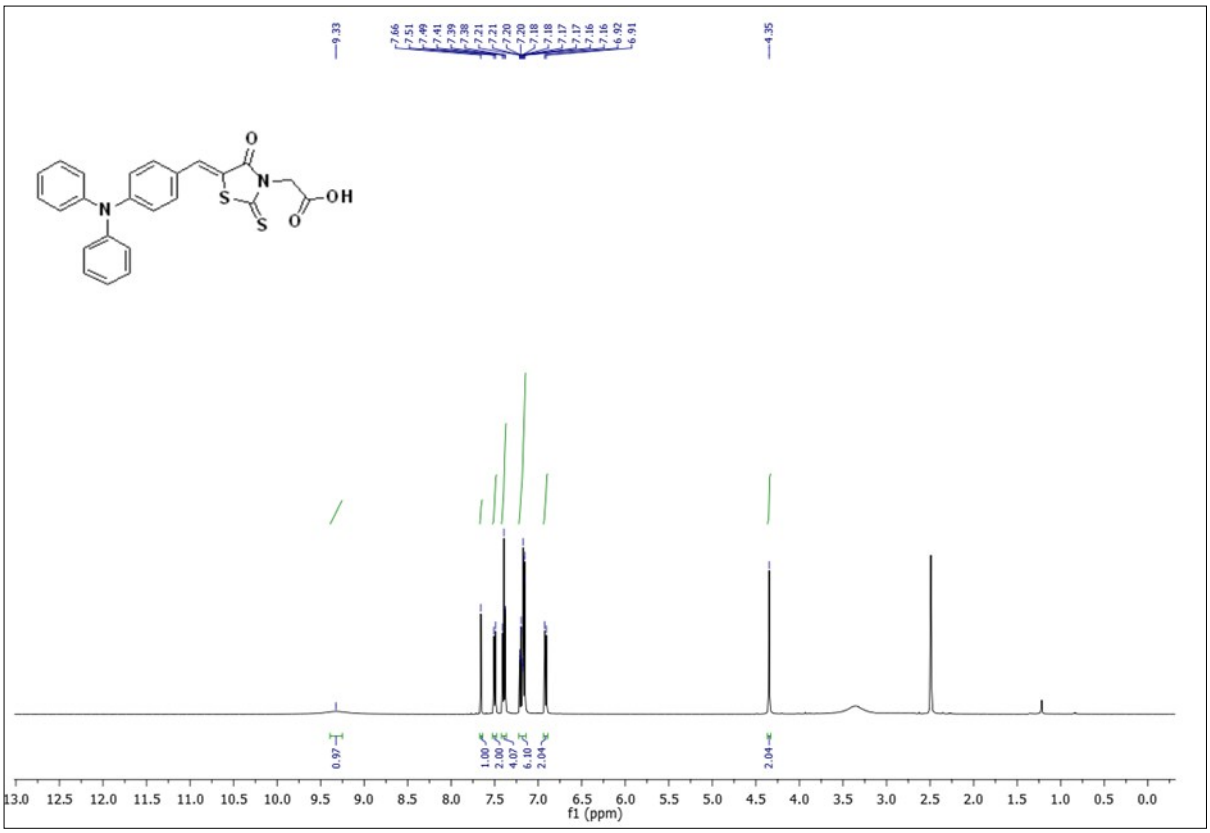

Fig. S17 ^{1}H NMR spectrum of chromophore **MD2**

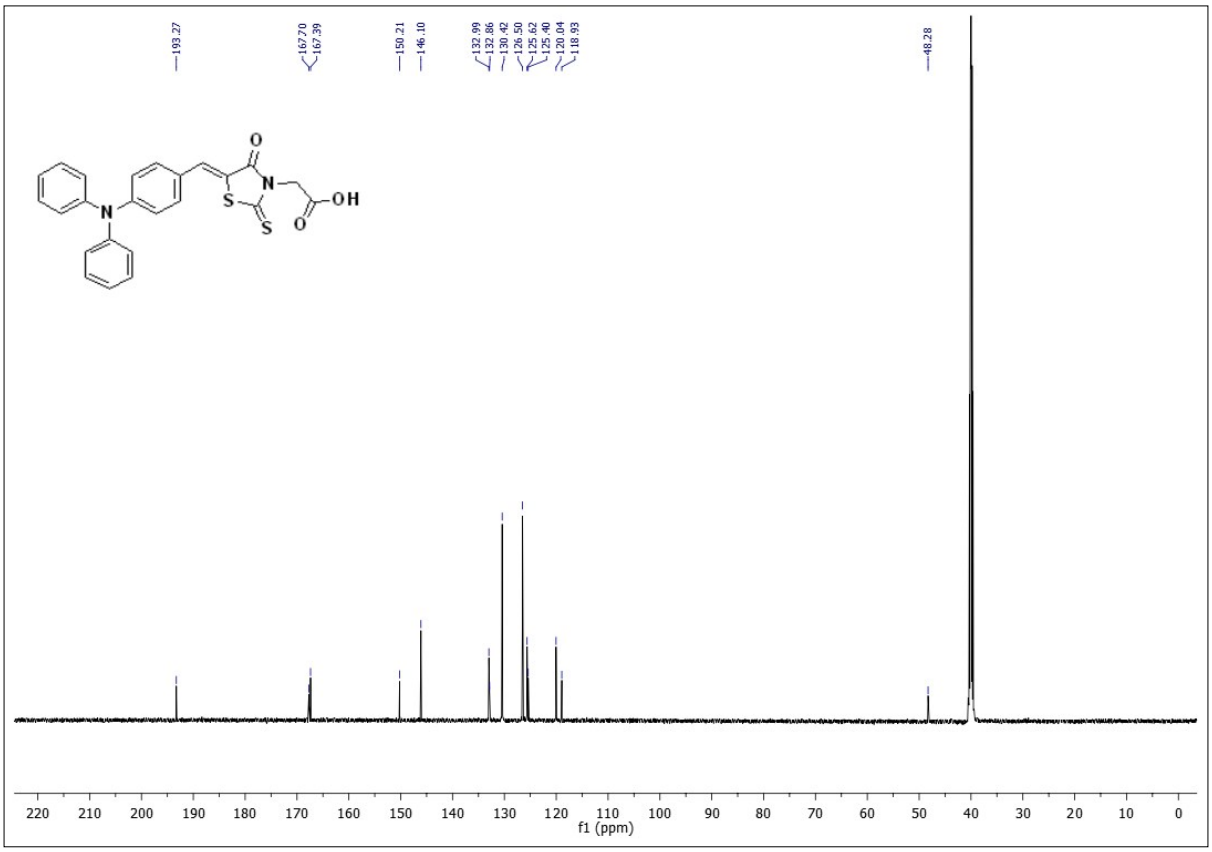

Fig. S18. ^{13}C NMR spectrum of chromophore **MD2**

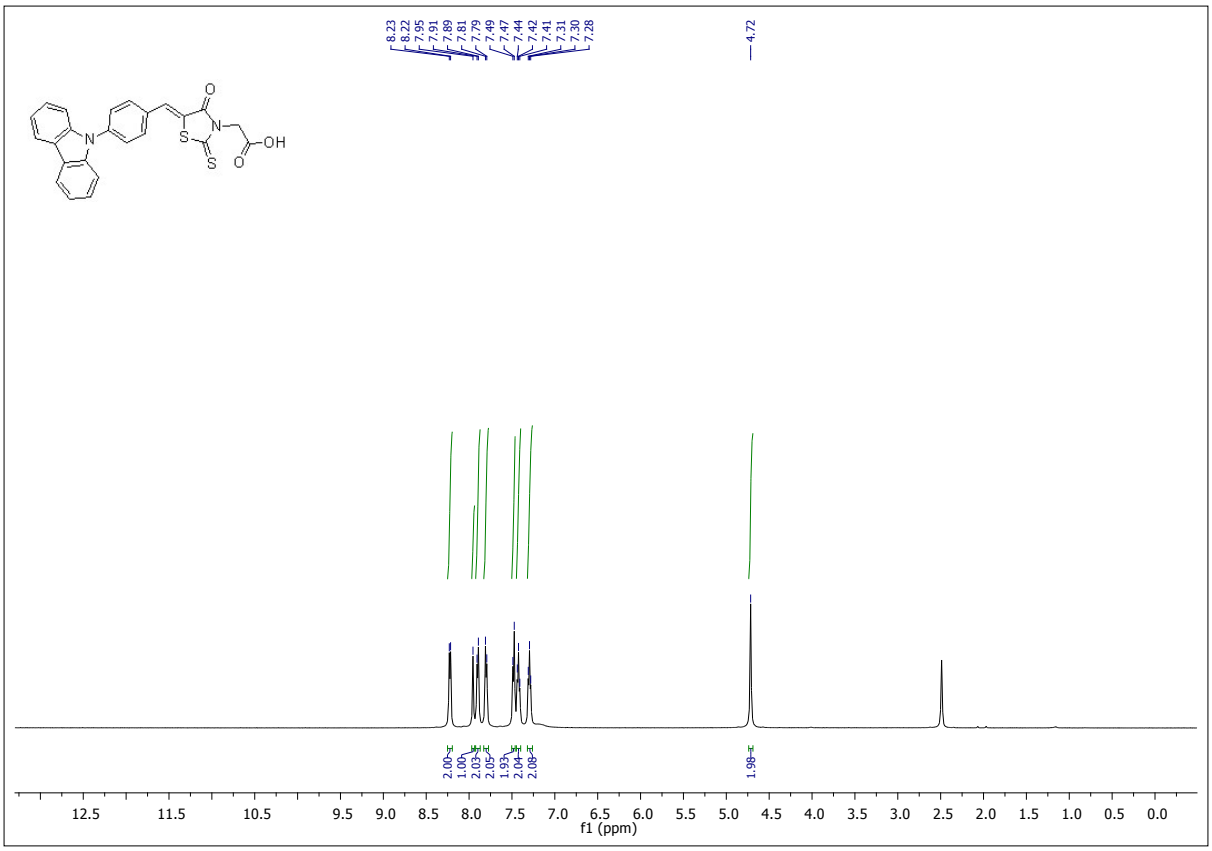

Fig. S19. ^{1}H NMR spectrum of chromophore **MD3**

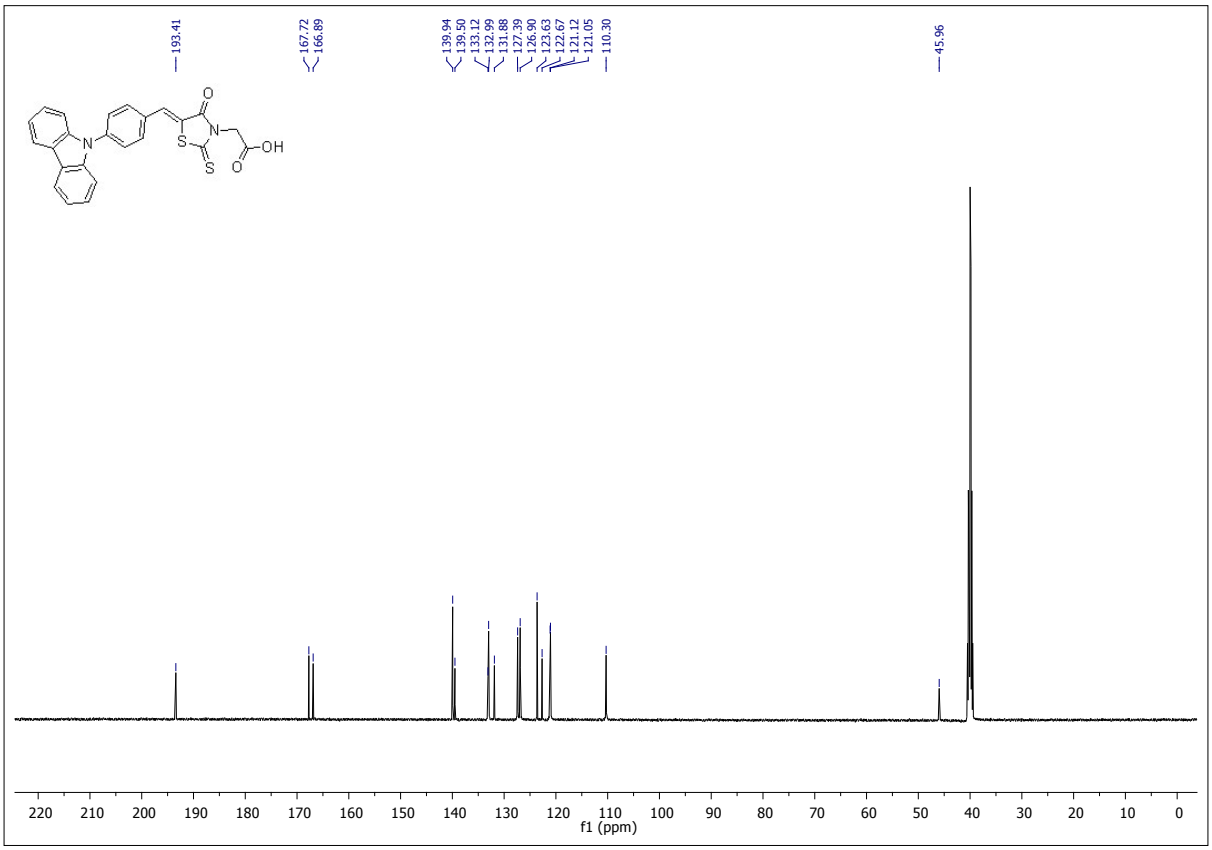

Fig. S20. ^{13}C NMR spectrum of chromophore **MD3**

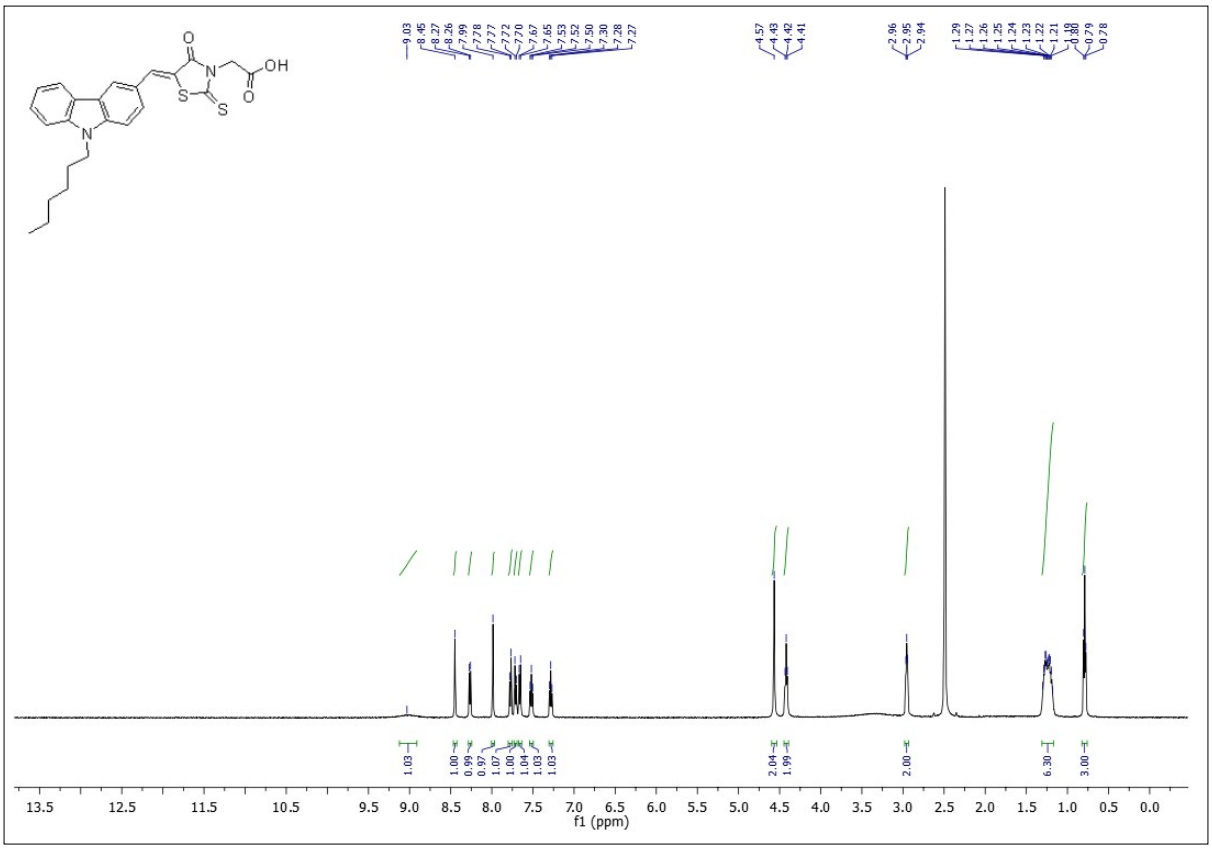

Fig. S21. ^{1}H NMR spectrum of chromophore **MD4**

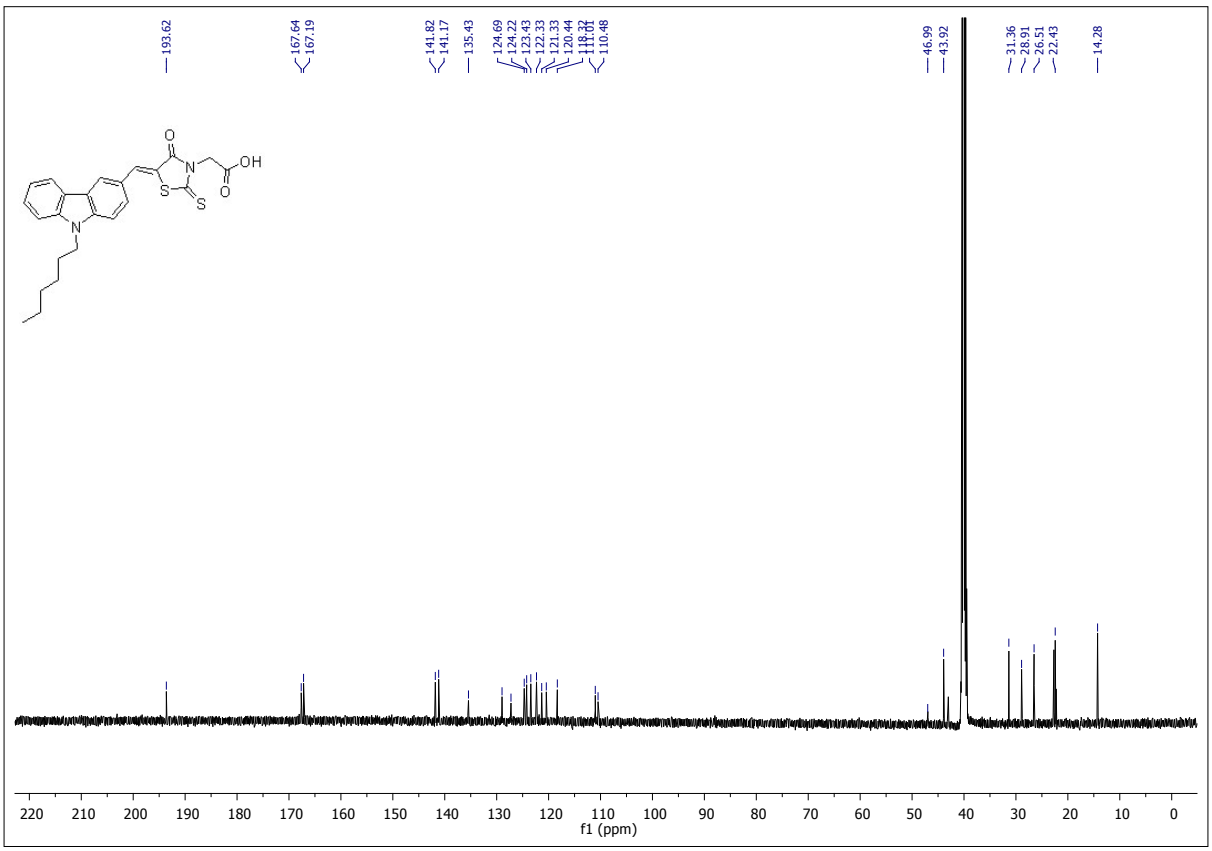

Fig. S22. ^{13}C NMR spectrum of chromophore **MD4**

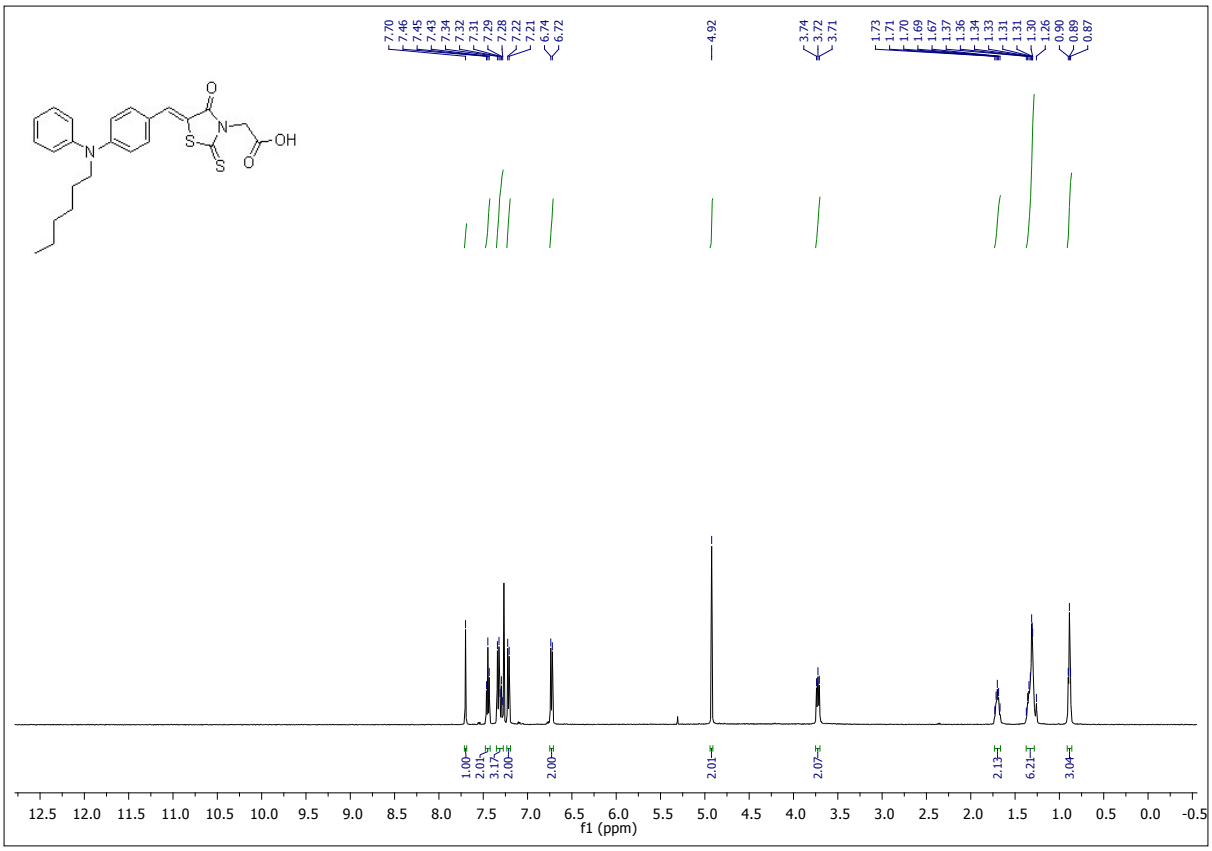

Fig. S23. ^{1}H NMR spectrum of chromophore **MD5**

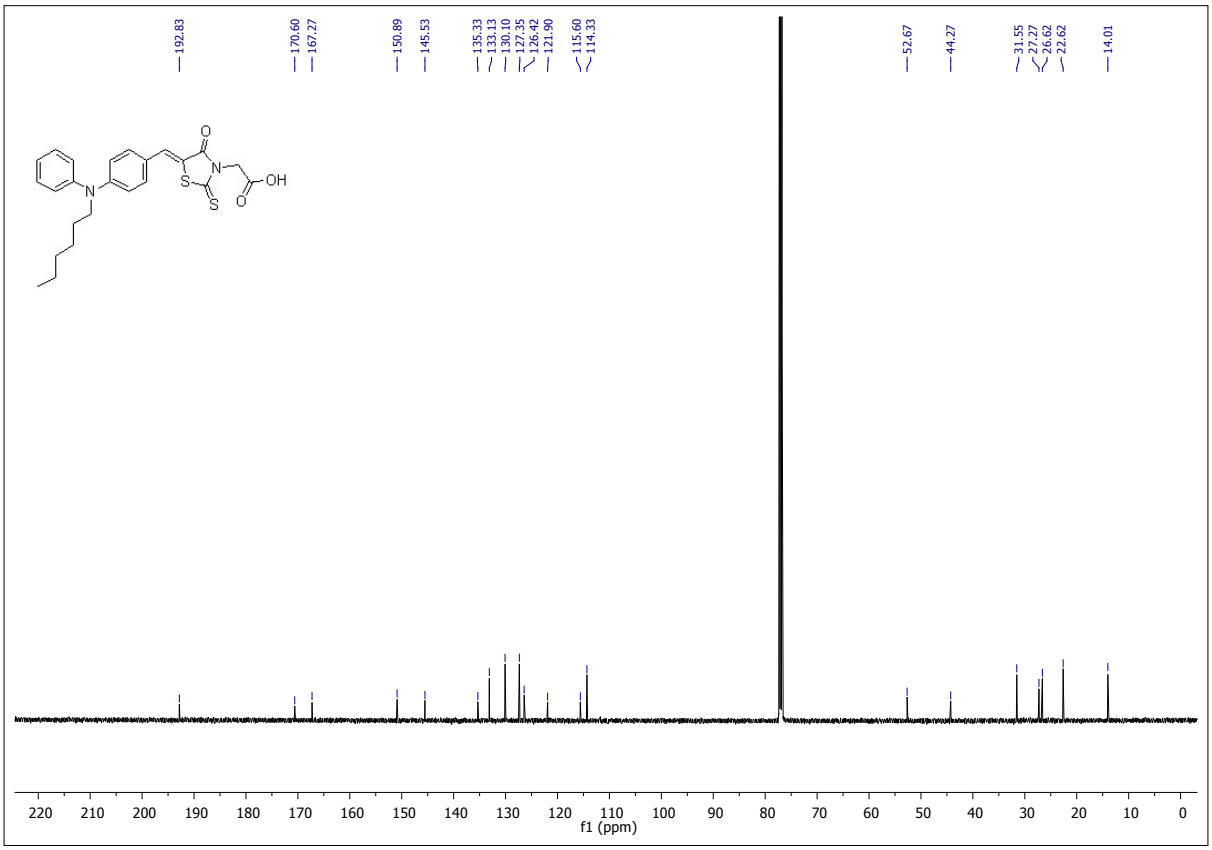

Fig. S24. ^{13}C NMR spectrum of chromophore **MD5**

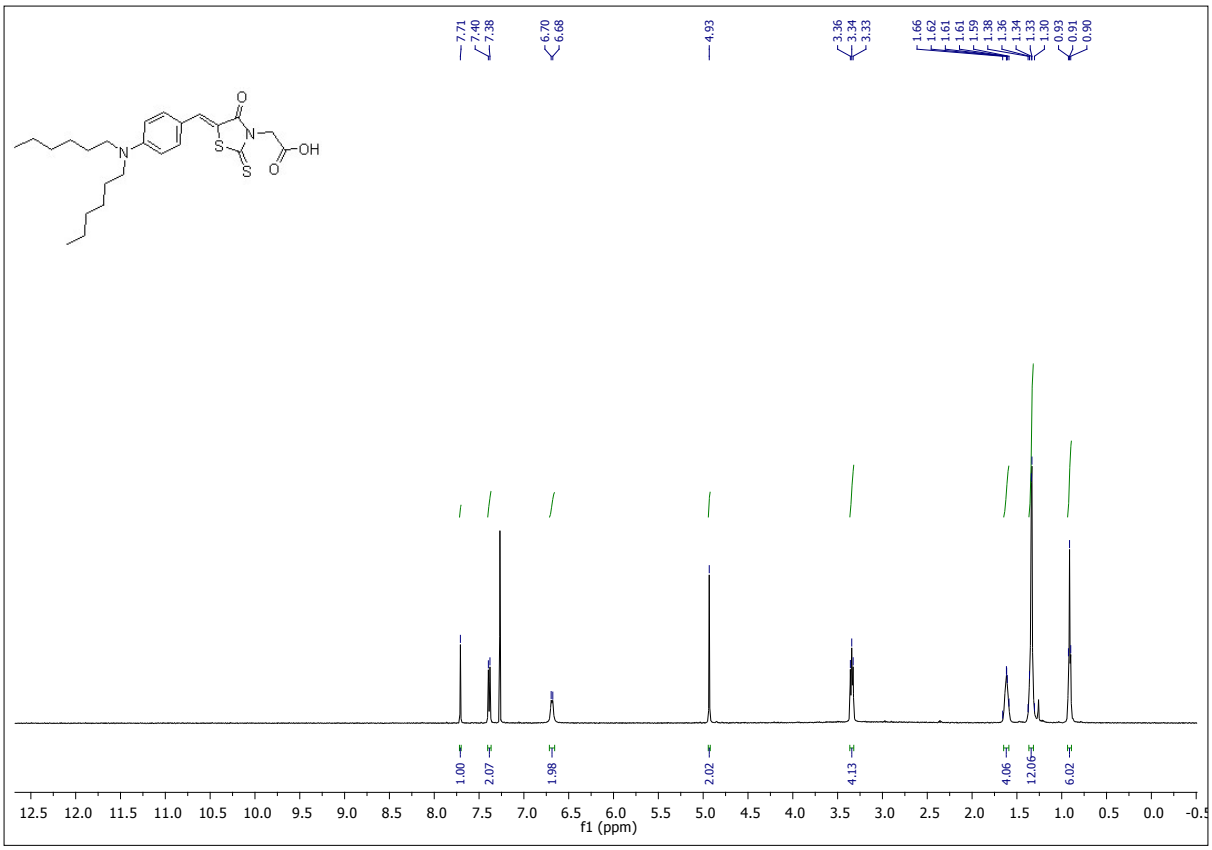

Fig. S25. ^{1}H NMR spectrum of chromophore **MD6**

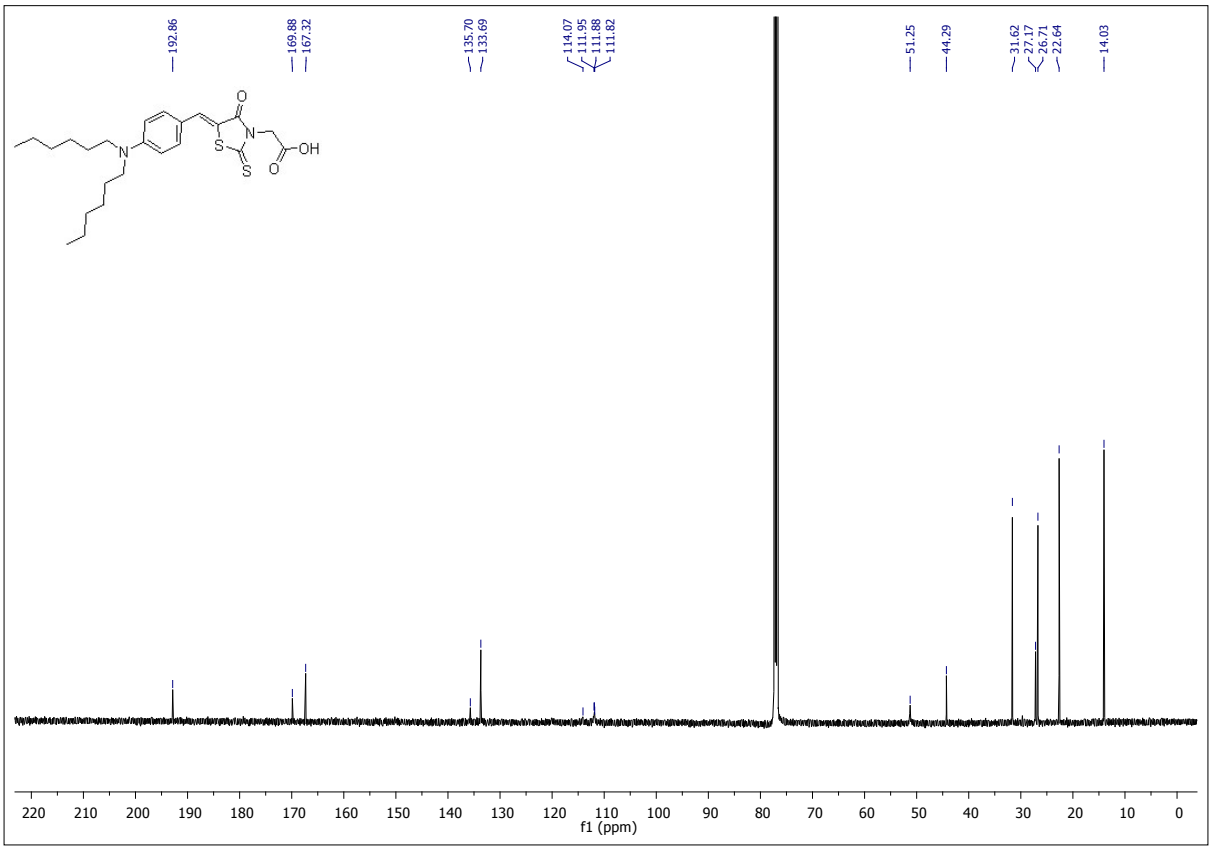

Fig. S26. ^{13}C NMR spectrum of chromophore **MD6**

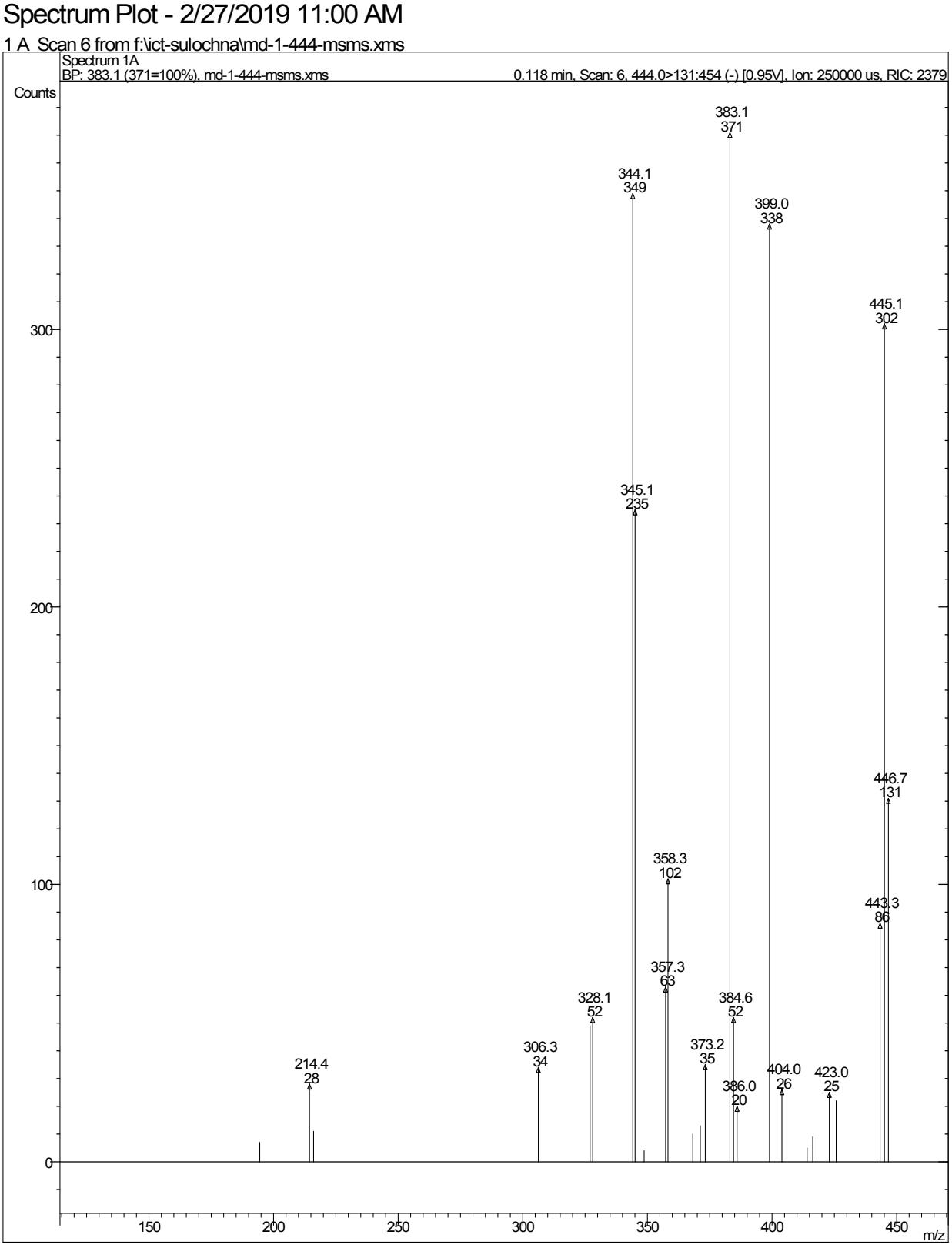

Fig. S27. Mass Spectra of MD1

Spectrum Plot - 2/27/2019 11:01 AM

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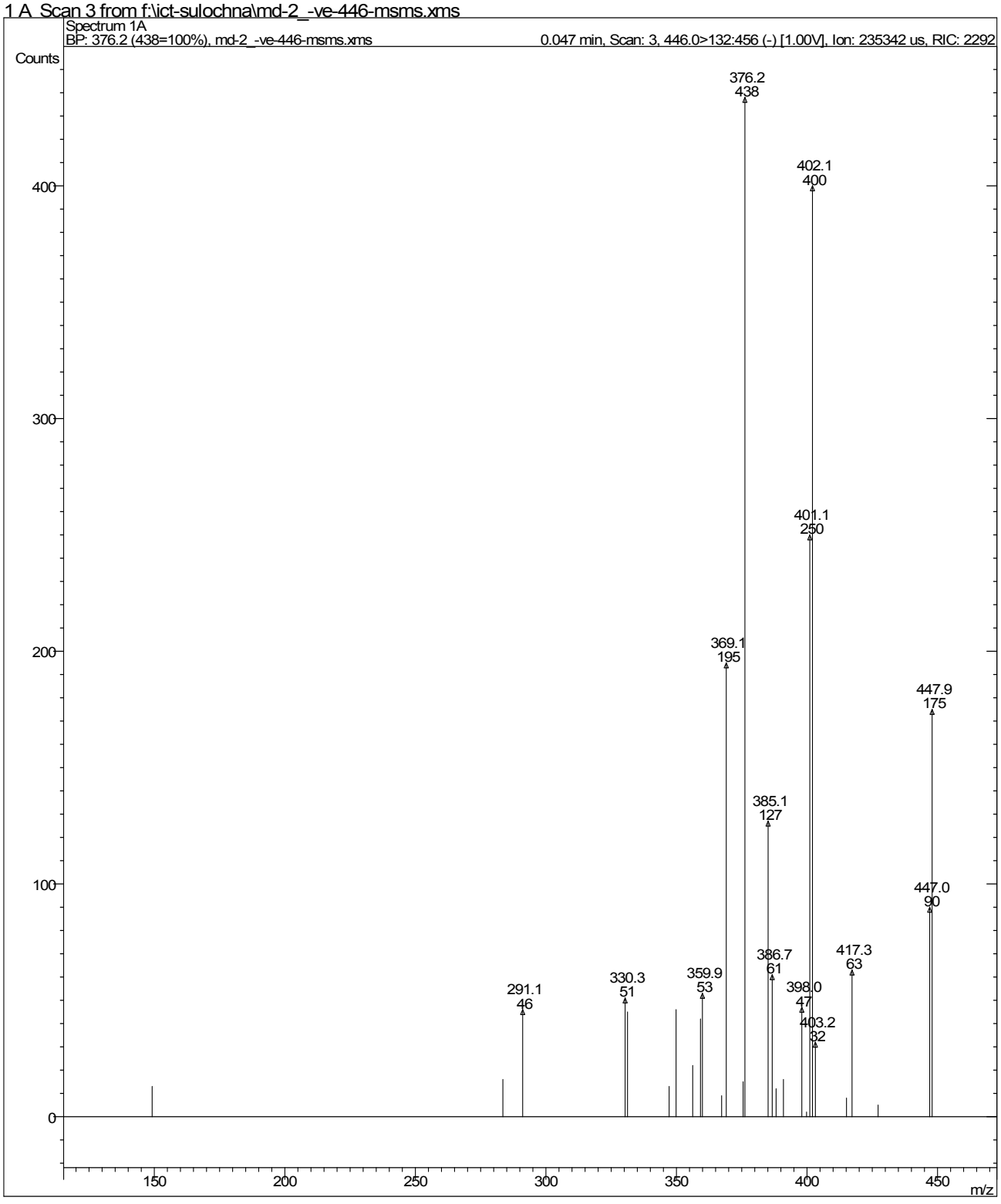

Fig. S28. Mass Spectra of MD2

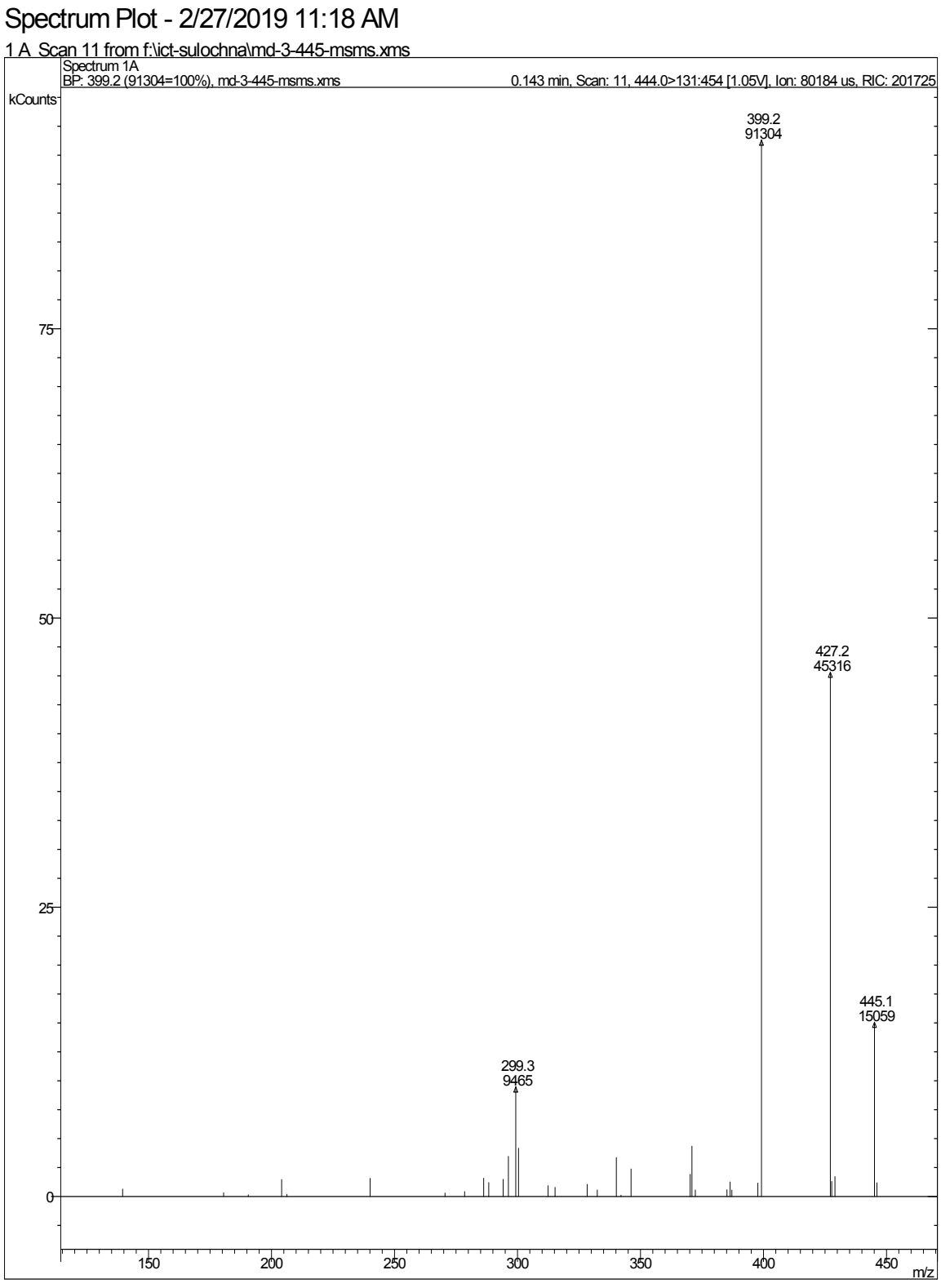

Fig. S29. Mass Spectra of MD3

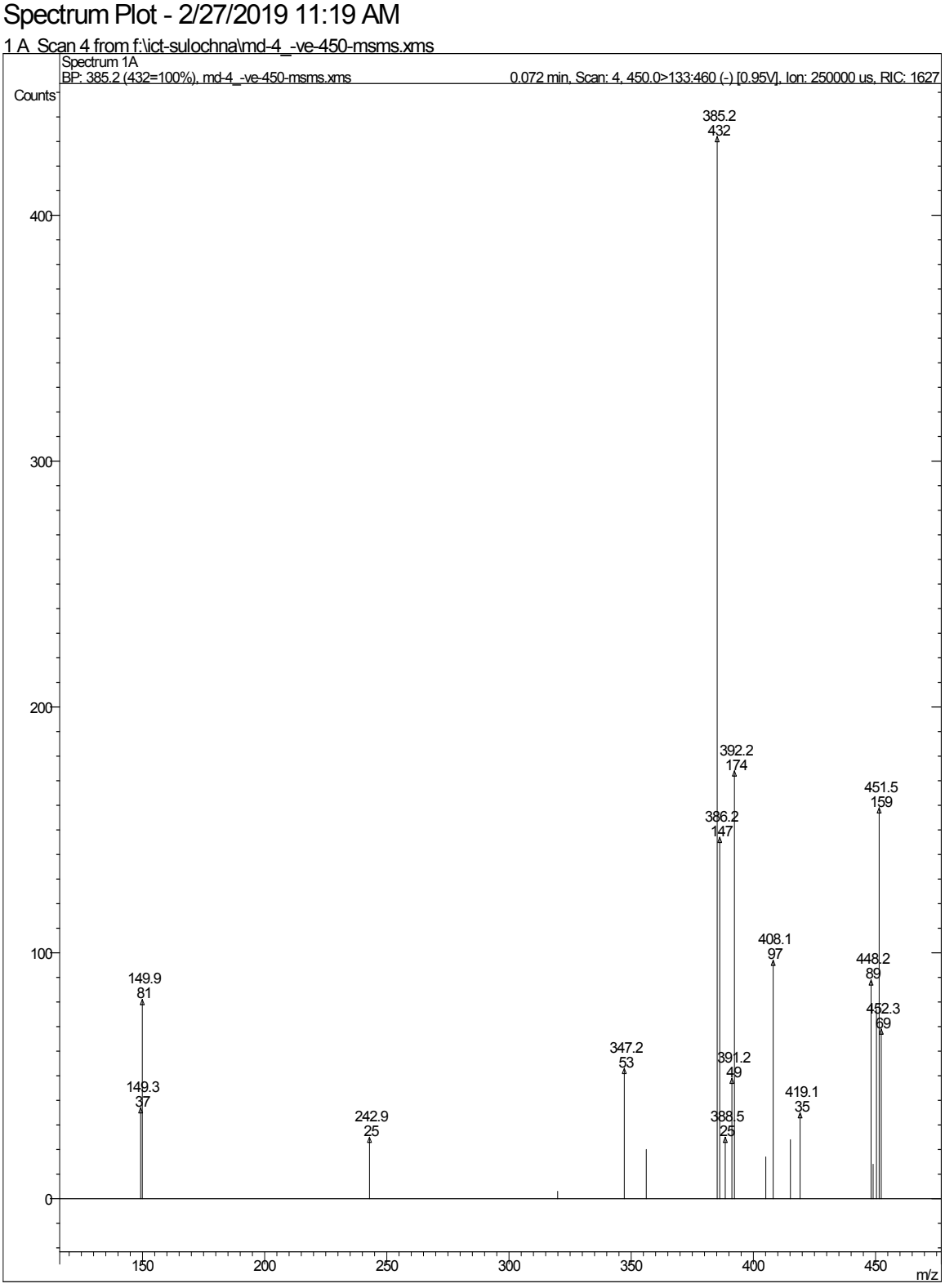

Fig. S30. Mass Spectra of MD4

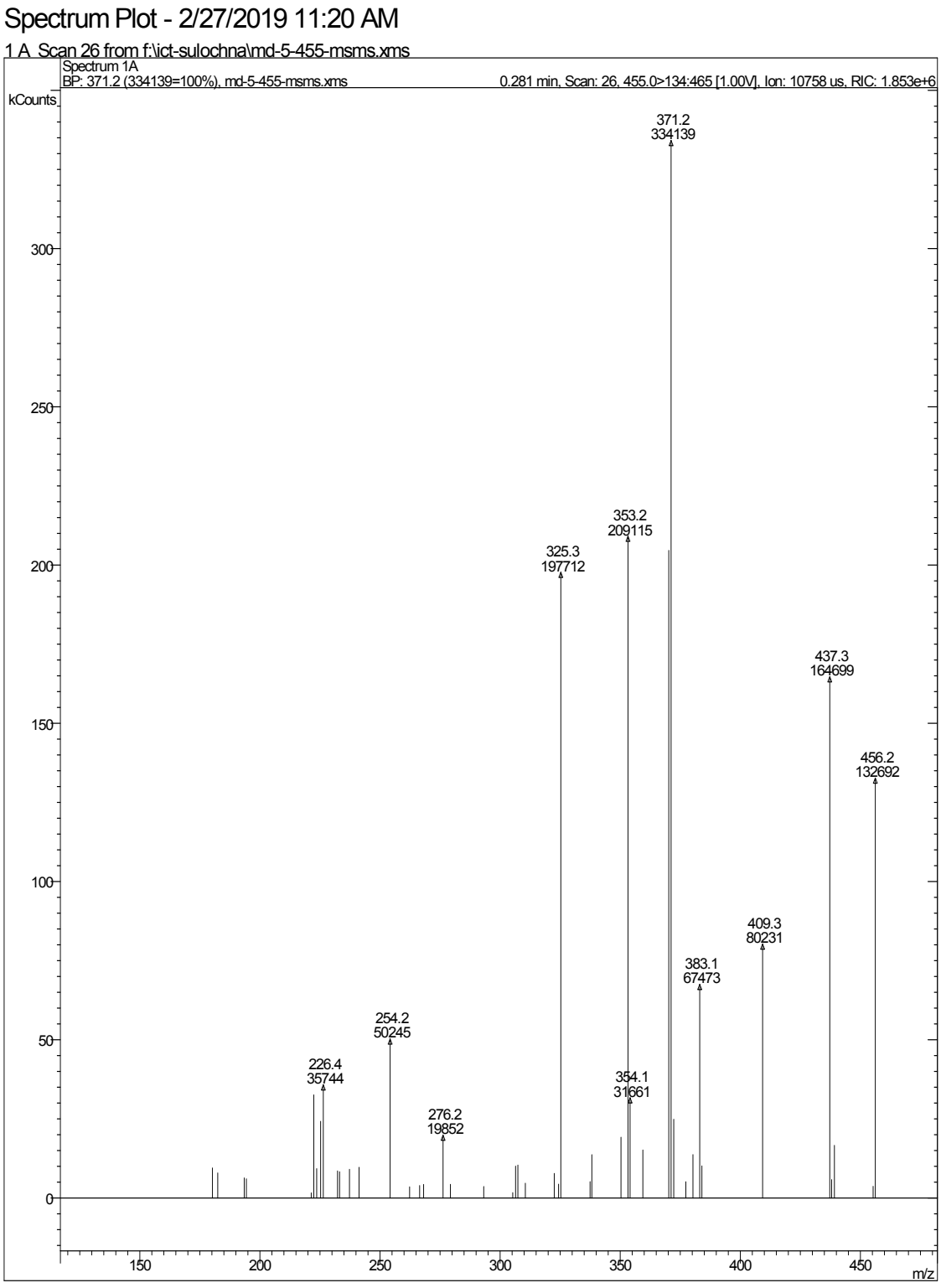

Fig. S31. Mass Spectra of MD5

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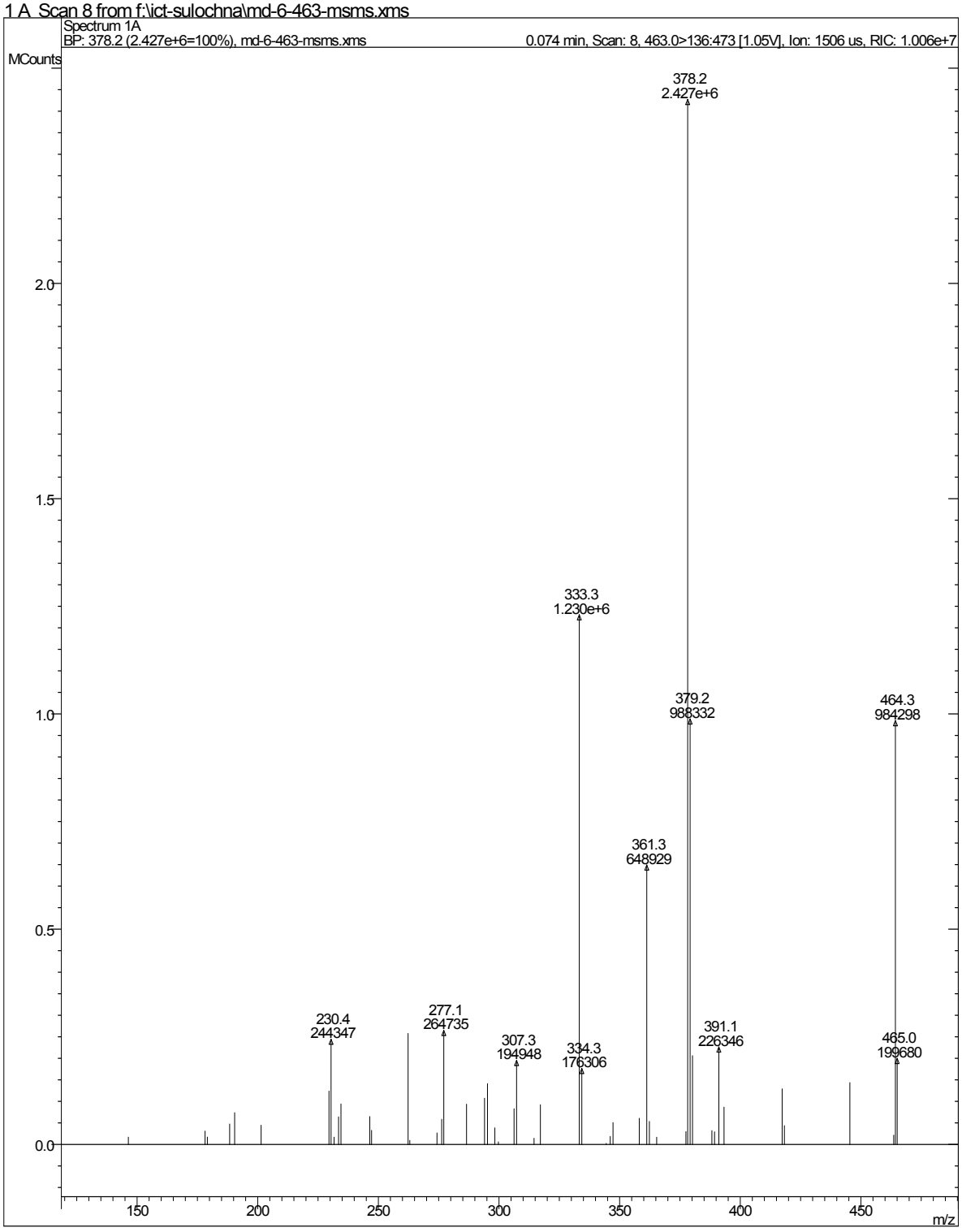

Fig. S32. Mass Spectra of MD6