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Supporting Information

A Combined Experimental and TD-DFT Investigation of Mono Azo Disperse Dyes.

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Table S1: Computed energy at B3LYP/6-31G(d) in vacuum and different solvent for dye **6c.**

6c						
Medium	**Azo**			**Hydrazone**		
	E/Hartree[a]	**ΔE/kJ[b] mol^{-1}**	**ΔG/Hartree[c]**	**E/Hartree[a]**	**ΔE/kJ[b] mol^{-1}**	**ΔG/Hartree[c]**
Gas	-1768.137	0	-1767.712	-1768.124	34.20	-1767.700
THF	-1768.152	0	-1767.729	-1768.141	30.19	-1767.718
DCM	-1768.153	0	-1767.729	-1768.141	29.99	-1767.719
Acetone	-1768.155	0	-1767.731	-1768.144	29.38	-1767.721
Ethanol	-1768.155	0	-1767.731	-1768.144	29.29	-1767.721
Methanol	-1768.155	0	-1767.732	-1768.144	29.18	-1767.721
Acetonitrile	-1768.155	0	-1767.732	-1768.144	29.16	-1767.722
DMF	-1768.155	0	-1767.732	-1768.144	29.14	-1767.722
DMSO	-1768.156	0	-1767.732	-1768.144	29.08	-1767.722

1 Hartree = 2625.5 kJ/mol
[a]Calculated energies, [b]Gibbs free energies, [c]relative energies.

Table S2: Computed energy at B3LYP/6-31G(d) in vacuum and different solvent for dye **6'b.**

6'b						
Medium	**Azo**			**Hydrazone**		
	E/Hartree[a]	**ΔE/kJ[b] mol^{-1}**	**ΔG/Hartree[c]**	**E/Hartree[a]**	**ΔE/kJ[b] mol^{-1}**	**ΔG/Hartree[c]**
Gas	-1653.624	0	-1653.227	-1653.601	59.68	-1653.206
THF	-1653.639	0	-1653.243	-1653.618	53.91	-1653.223
DCM	-1653.640	0	-1653.244	-1653.619	53.58	-1653.224
Acetone	-1653.641	0	-1653.246	-1653.621	52.56	-1653.226
Ethanol	-1653.642	0	-1653.246	-1653.622	52.40	-1653.226
Methanol	-1653.642	0	-1653.247	-1653.622	52.23	-1653.227
Acetonitrile	-1653.642	0	-1653.247	-1653.622	52.18	-1653.227
DMF	-1653.642	0	-1653.247	-1653.622	52.15	-1653.227
DMSO	-1653.642	0	-1653.247	-1653.623	52.05	-1653.227

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1 Hartree = 2625.5 kJ/mol
[a]Calculated energies, [b]Gibbs free energies, [c]relative energies.

Table S3: Computed energy at 6-31G(d) in vacuum and different solvent for dye **6'c.**

6'c						
Medium	**Azo**			**Hydrazone**		
	E/Hartree[a]	**ΔE/kJ[b] mol^{-1}**	**ΔG/Hartree[c]**	**E/Hartree[a]**	**ΔE/kJ[b] mol^{-1}**	**ΔG/Hartree[c]**
Gas	-1768.137	0	-1767.711	-1768.117	52.29	-1767.692
THF	-1768.152	0	-1767.727	-1768.135	46.38	-1767.710
DCM	-1768.153	0	-1767.728	-1768.135	46.09	-1767.710
Acetone	-1768.155	0	-1767.730	-1768.138	45.18	-1767.713
Ethanol	-1768.155	0	-1767.730	-1768.138	45.04	-1767.713
Methanol	-1768.155	0	-1767.730	-1768.138	44.89	-1767.714
Acetonitrile	-1768.156	0	-1767.731	-1768.138	44.84	-1767.714
DMF	-1768.156	0	-1767.731	-1768.139	44.83	-1767.714
DMSO	-1768.156	0	-1767.731	-1768.139	44.73	-1767.714

1 Hartree = 2625.5 kJ/mol
[a]Calculated energies, [b]Gibbs free energies, [c]relative energies.

Table S4: Energy of the frontier molecular orbitals in eV for dye **6a** in different solvents.

6a								
Solvent	**Energy**			Dipole moment **(μ Debye)**	**E_{HOMO}**	**E_{LUMO}**	**ΔE (Hartree)**	**ΔE (eV)**
	Hartree	**kcal/m**	**(eV)**					
THF	-1445.611	-907135.346	-39337.97	12.2621	-0.20191	-0.10257	0.0993	2.703
DCM	-1445.612	-907135.752	-39337.98	12.4064	-0.20198	-0.10302	0.0990	2.693
Acetone	-1445.614	-907136.958	-39338.04	12.8424	-0.20224	-0.10438	0.0979	2.663
Ethanol	-1445.614	-907137.131	-39338.04	12.9057	-0.20228	-0.10458	0.0977	2.659
Methanol	-1445.614	-907137.327	-39338.05	12.978	-0.20232	-0.10481	0.0975	2.653
Acetonitrile	-1445.614	-907137.382	-39338.05	12.9982	-0.20234	-0.10487	0.0975	2.652
DMF	-1445.614	-907137.406	-39338.06	13.007	-0.20234	-0.1049	0.0974	2.652
DMSO	-1445.614	-907137.522	-39338.06	13.0496	-0.20237	-0.10504	0.0973	2.649

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Table S5: Energy of the frontier molecular orbitals in eV for dye **6b** in different solvent.

6b								
Solvent	**Energy**			Dipole moment (μ Debye)	E_{HOMO}	E_{LUMO}	**ΔE (Hartree)**	**ΔE (eV)**
	Hartree	**kcal/m**	**(eV)**					
THF	-1653.643	-1037677.8	-44998.95	12.0989	-0.20558	-0.10856	0.097	2.640
DCM	-1653.644	-1037678.2	-44998.96	12.2427	-0.20562	-0.10883	0.097	2.634
Acetone	-1653.646	-1037679.4	-44999.02	12.6725	-0.20574	-0.10962	0.096	2.616
Ethanol	-1653.646	-1037679.6	-44999.02	12.7344	-0.20575	-0.10973	0.096	2.613
Methanol	-1653.647	-1037679.8	-44999.03	12.8047	-0.20577	-0.10986	0.096	2.610
Acetonitrile	-1653.647	-1037679.8	-44999.03	12.8242	-0.20578	-0.10989	0.096	2.609
DMF	-1653.647	-1037679.9	-44999.03	12.8328	-0.20578	-0.10991	0.096	2.609
DMSO	-1653.647	-1037680.0	-44999.04	12.874	-0.20579	-0.10998	0.096	2.607

Table S6: Energy of the frontier molecular orbitals in eV for dye **6c** in different solvent.

6c								
Solvent	**Energy**			Dipole moment (μ Debye)	E_{HOMO}	E_{LUMO}	**ΔE (Hartree)**	**ΔE (eV)**
	Hartree	**kcal/m**	**(eV)**					
THF	-1768.1523	-1109533.2	-48114.96	7.3628	-0.20618	-0.11158	0.0946	2.574
DCM	-1768.1529	-1109533.6	-48114.98	7.4537	-0.20621	-0.11177	0.0944	2.570
Acetone	-1768.1547	-1109534.8	-48115.03	7.7229	-0.20629	-0.11236	0.0939	2.556
Ethanol	-1768.1550	-1109534.9	-48115.03	7.7616	-0.2063	-0.11244	0.0939	2.554
Methanol	-1768.1553	-1109535.1	-48115.04	7.8055	-0.20631	-0.11253	0.0938	2.552
Acetonitrile	-1768.1553	-1109535.2	-48115.04	7.8177	-0.20632	-0.11256	0.0938	2.551
DMF	-1768.1554	-1109535.2	-48115.04	7.823	-0.20632	-0.11257	0.0938	2.551
DMSO	-1768.1555	-1109535.3	-48115.05	7.8487	-0.20633	-0.11263	0.0937	2.550

Table S7: Energy of the frontier molecular orbitals in eV for dye **6'a** in different solvent.

6b								
Solvent	**Energy**			Dipole moment (μ Debye)	E_{HOMO}	E_{LUMO}	**ΔE (Hartree)**	**ΔE (eV)**
	Hartree	**kcal/m**	**(eV)**					
THF	-1445.610	-907134.47	-39337.93	9.0075	-0.2015	-0.09955	0.1020	2.774
DCM	-1445.610	-907134.88	-39337.95	9.131	-0.20156	-0.09992	0.1016	2.766
Acetone	-1445.612	-907136.11	-39338.00	9.5	-0.20179	-0.10104	0.1008	2.742
Ethanol	-1445.612	-907136.29	-39338.01	9.5543	-0.20183	-0.10121	0.1006	2.738
Methanol	-1445.613	-907136.49	-39338.02	9.6163	-0.20187	-0.1014	0.1005	2.734

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Acetonitrile	-1445.613	-907136.54	-39338.02	9.6336	-0.20188	-0.10146	0.1004	2.733
DMF	-1445.613	-907136.57	-39338.02	9.6412	-0.20189	-0.10189	0.1000	2.721
DMSO	-1445.613	-907136.68	-39338.02	9.6778	-0.20191	-0.10159	0.1003	2.730

Table S8: Energy of the frontier molecular orbitals in eV for dye **6'b** in different solvent.

6'b								
Solvent	**Energy**			Dipole moment **(μ Debye)**	**E_{HOMO}**	**E_{LUMO}**	**ΔE (Hartree)**	**ΔE (eV)**
	Hartree	**kcal/m**	**(eV)**					
THF	-1768.152	-1109533.32	-48114.96	7.9529	-0.19595	-0.10371	0.0922	2.510
DCM	-1768.153	-1109533.72	-48114.98	8.0699	-0.19602	-0.10401	0.0920	2.504
Acetone	-1768.155	-1109534.89	-48115.03	8.4192	-0.19624	-0.10492	0.0913	2.485
Ethanol	-1768.155	-1109535.06	-48115.04	8.4695	-0.19627	-0.10505	0.0912	2.482
Methanol	-1768.155	-1109535.25	-48115.05	8.5269	-0.19631	-0.10521	0.0911	2.479
Acetonitrile	-1768.156	-1109535.30	-48115.05	8.5428	-0.19632	-0.10525	0.0911	2.478
DMF	-1768.156	-1109535.33	-48115.05	8.5498	-0.19632	-0.10527	0.0911	2.478
DMSO	-1768.156	-1109535.44	-48115.06	8.5837	-0.19635	-0.10537	0.0910	2.476

Table S9: Energy of the frontier molecular orbitals in eV for dye **6'c** in different solvent.

6'c								
Solvent	**Energy**			Dipole moment **(μ Debye)**	**E_{HOMO}**	**E_{LUMO}**	**ΔE (Hartree)**	**ΔE (eV)**
	Hartree	**kcal/m**	**(eV)**					
THF	-1653.639	-1037674.99	-44998.82	7.7198	-0.20517	-0.10282	0.1024	2.785
DCM	-1653.640	-1037675.38	-44998.84	7.8294	-0.20524	-0.10314	0.1021	2.778
Acetone	-1653.641	-1037676.55	-44998.89	8.1586	-0.20545	-0.1041	0.1014	2.758
Ethanol	-1653.642	-1037676.72	-44998.90	8.2061	-0.20548	-0.10424	0.1012	2.755
Methanol	-1653.642	-1037676.91	-44998.91	8.2598	-0.20552	-0.1044	0.1011	2.752
Acetonitrile	-1653.642	-1037676.97	-44998.91	8.2749	-0.20553	-0.10444	0.1011	2.751
DMF	-1653.642	-1037676.99	-44998.91	8.2816	-0.20553	-0.10446	0.1011	2.750
DMSO	-1653.642	-1037677.10	-44998.92	8.3088	-0.20555	-0.10455	0.1010	2.748

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Cartesian coordinates 1. Ground state optimized geometry for dye **7a** in vacuum [B3LYP/6-31G(d)]**.**

(Total Energy = -1445.59547882 Hartree)

0 1

C	2.14520500	0.98153000	0.17690300
C	3.51083500	0.70279600	0.12888600
C	3.94364100	-0.63911100	0.14765700
C	2.99646400	-1.65491500	0.28160600
C	1.64130700	-1.35769100	0.35514300
C	1.17758700	-0.03017200	0.25641000
H	1.79614200	2.00670300	0.14611100
H	3.32207000	-2.68736300	0.33720300
C	5.37388200	-1.07065800	0.01707300
C	7.39852900	-0.72572700	-1.12568100
H	7.73020800	-0.16079400	-1.99710900
H	7.94125600	-0.40706000	-0.23196800
H	7.54827100	-1.79729100	-1.27859200
C	4.49482500	1.83029900	0.19725000
C	4.87154600	4.10214300	-0.28708600
H	4.33573200	4.90554000	-0.79289900
H	5.05663400	4.35884800	0.75928000
H	5.82704100	3.90535700	-0.77979900
C	-2.29903400	-0.12439700	-0.28965800
C	-3.16759100	-1.05196400	-0.88970600
C	-2.85279100	1.05212200	0.25614800
C	-4.53029700	-0.82578600	-0.95578100
H	-2.74045000	-1.96322400	-1.29733800
C	-4.21026700	1.28808300	0.19533800
H	-2.19219600	1.76832100	0.73269100
C	-5.10135600	0.36230500	-0.42508400
H	-5.15570200	-1.57832300	-1.41811100
H	-4.59209900	2.19765200	0.64143700

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N	0.74315500	-2.49373500	0.62895300
O	0.88310000	-3.49445700	-0.07082300
O	-0.02208500	-2.38999300	1.58212900
N	-0.95030800	-0.46674900	-0.27469400
N	-0.16215800	0.39268200	0.22883400
O	5.87357000	-1.95311100	0.68153200
O	5.57532800	1.76670700	0.74429500
O	4.01410900	2.95189500	-0.38023200
O	6.00000300	-0.42577400	-0.98417700
N	-6.45266300	0.61751500	-0.51598200
C	-7.36815200	-0.36441300	-1.10376100
C	-7.75776800	-1.52092000	-0.17278800
H	-6.92505500	-0.75541200	-2.02655500
H	-8.26823800	0.17791100	-1.40958700
H	-8.41194000	-2.22385200	-0.70164000
H	-6.87660800	-2.06947700	0.17361200
H	-8.29469400	-1.15545000	0.70824900
C	-7.03643400	1.83658700	0.04899000
C	-7.30467300	1.78523700	1.55941900
H	-7.97568400	2.01950400	-0.48253200
H	-6.38687100	2.68526800	-0.19089800
H	-7.70695600	2.74584900	1.90194900
H	-8.03335700	1.00633800	1.80573700
H	-6.38865700	1.57874300	2.12151700

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Cartesian coordinates 2. Ground state optimized geometry for dye **7b** in vacuum [B3LYP/6-31G(d)]**.**

(Total Energy = -1653.62815346 Hartree)

0 1

C	2.23372600	-0.78001400	0.08596900
C	3.62291100	-0.83555900	0.10372500
C	4.37586300	0.35817000	0.18786500
C	3.70083300	1.56917200	0.30791700
C	2.30978400	1.60549700	0.32860300
C	1.53145600	0.43605400	0.19487700
H	1.65184100	-1.68791700	-0.00515100
H	4.26007100	2.49338000	0.38781000
C	5.87076500	0.42833500	0.11974900
C	7.80342600	-0.42916600	-0.90862500
H	8.02837700	-1.09209500	-1.74431900
H	8.20904100	0.56980600	-1.08616700
H	8.21722000	-0.82864000	0.02086400
C	4.29474400	-2.17574500	0.17184300
C	4.16946300	-4.43767700	-0.46265400
H	3.51981900	-5.05212900	-1.08610600
H	5.19503800	-4.45412400	-0.83991000
H	4.16419800	-4.79343300	0.57096900
C	-1.83317000	-0.62193100	0.03653400
C	-2.38788600	-1.92111300	0.14300200
C	-2.74669900	0.47250600	-0.19354000
C	-3.72927300	-2.17908800	0.01725800
H	-1.68775100	-2.72898700	0.33136500
C	-4.10744900	0.20587500	-0.32412000
C	-4.63471100	-1.10592900	-0.24114200
H	-4.07994100	-3.19745300	0.11738600
H	-4.74972800	1.05517000	-0.48231400
N	1.69026600	2.92403300	0.50128400

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O	0.65867700	2.99544200	1.17242000
O	2.25415500	3.88643100	-0.01820400
N	-0.47069500	-0.59453400	0.18150100
N	0.13714800	0.53214200	0.09077700
O	6.53935400	1.18730300	0.78877900
O	5.28649200	-2.40947900	0.82852200
O	3.62876500	-3.10729100	-0.54088400
O	6.36867300	-0.38467100	-0.83032200
N	-5.97753700	-1.33037000	-0.41405200
C	-6.54769700	-2.67347000	-0.26781300
C	-6.78211500	-3.11515600	1.18312100
H	-5.90282500	-3.39330500	-0.78342200
H	-7.49768400	-2.67931700	-0.81028800
H	-7.18094500	-4.13606800	1.20436400
H	-5.85207100	-3.09917600	1.75954400
H	-7.50053000	-2.45924400	1.68465700
C	-6.90731800	-0.22411000	-0.68044100
C	-7.35931800	0.55177100	0.56329100
H	-7.77902200	-0.65563400	-1.18210600
H	-6.44590000	0.45775600	-1.40136200
H	-8.03544300	1.36193100	0.26775800
H	-7.89264300	-0.09726300	1.26564400
H	-6.50834300	0.99775900	1.08591500
C	-2.91907900	2.95323200	-0.48333700
C	-2.01461800	4.16942300	-0.57349700
H	-2.60698700	5.05777200	-0.34720900
H	-1.15231800	4.11106700	0.09696800
H	-1.63844600	4.26414700	-1.60020300
O	-4.13256400	3.03212700	-0.62602300
N	-2.23643100	1.76473900	-0.26605400
H	-1.22453300	1.80856500	-0.12471400

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Cartesian coordinates 3. Ground state optimized geometry for dye **7c** in vacuum [B3LYP/6-31G(d)]**.**
(Total Energy = -1768.13741628 Hartree)

0 1

C	-2.44594200	-0.71464600	0.01430500
C	-3.82951800	-0.83567000	0.06464200
C	-4.64239700	0.31855100	-0.00529900
C	-4.03124800	1.55663600	-0.19589300
C	-2.64848100	1.65523900	-0.30021000
C	-1.80992500	0.52662900	-0.17255500
H	-1.82376600	-1.59524100	0.11700200
H	-4.63925500	2.45057500	-0.26182200
C	-6.12555800	0.33938700	0.18429900
C	-7.95842300	-0.63695700	1.29115600
H	-8.11319100	-1.43872900	2.01331300
H	-8.29051700	0.32054100	1.69988300
H	-8.50400800	-0.83794500	0.36536700
C	-4.36292700	-2.23855300	0.14456000
C	-5.91279600	-3.76518400	-0.74807500
H	-6.66920300	-3.75984600	-1.53299700
H	-5.13957200	-4.50746200	-0.96128700
H	-6.36386200	-3.98807200	0.22256200
C	1.60774900	-0.36479400	-0.17328800
C	2.21582800	-1.63970700	-0.28415100
C	2.47021900	0.77734200	-0.02419200
C	3.57348500	-1.83279100	-0.22500800
H	1.56656800	-2.49452500	-0.43981300
C	3.85016100	0.56815400	0.05630300
C	4.44100100	-0.70938200	-0.01700100
H	4.46200200	1.44043300	0.21818900
N	-2.10115100	2.99370200	-0.54975600
O	-1.10463500	3.08491500	-1.26987200

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O	-2.68597800	3.94883200	-0.04095200
N	0.23613700	-0.40731300	-0.24920400
N	-0.41738100	0.68963400	-0.14129800
O	-6.86059700	1.16398300	-0.31800500
O	-3.90110000	-3.10121200	0.85888500
O	-5.35256500	-2.44104000	-0.74664200
O	-6.54209700	-0.61189300	1.04450400
N	5.82111000	-0.86054100	0.05591400
C	6.37305400	-1.90050900	0.94913900
C	6.50408800	-1.44944000	2.41001800
H	7.34996000	-2.20107300	0.55877100
H	5.72388300	-2.77172500	0.88554300
H	6.88977900	-2.27579000	3.01822100
H	7.19145500	-0.60400100	2.52470400
H	5.53100300	-1.15453200	2.81755900
C	6.65643400	0.33584000	-0.13583600
C	8.09149700	0.00925200	-0.55321100
H	6.66940200	0.96956700	0.76483700
H	6.19108800	0.92806800	-0.92772700
H	8.59913400	0.93850700	-0.83251200
H	8.67404900	-0.45106000	0.25079100
H	8.10588100	-0.66096000	-1.41958500
C	2.54660100	3.27079700	0.19369800
C	1.59317300	4.44730200	0.30351100
H	2.13027300	5.35419200	0.02025800
H	0.69880500	4.33097000	-0.31555000
H	1.27051600	4.55497600	1.34701100
O	3.76101500	3.40676300	0.25639500
N	1.90662500	2.04579800	0.05703800
H	0.88752100	2.04131100	-0.02053100
C	4.57487600	-3.39057700	-1.68994000

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H	4.91146400	-4.42974700	-1.67597200
H	3.79104400	-3.26964500	-2.44838400
H	5.41814600	-2.73289500	-1.93092200
O	4.05824700	-3.11864300	-0.38276500

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Cartesian coordinates 4. Ground state optimized geometry for dye **7'a** in vacuum [B3LYP/6-31G(d)]**.**

(Total Energy = -1445.59383522 Hartree)

0 1

C	1.99072600	0.38277600	0.07851800
C	3.35778700	0.09723200	0.06489300
C	3.75422300	-1.24755800	-0.04980200
C	2.77693100	-2.24620000	-0.19594300
C	1.42847700	-1.93870900	-0.20769400
C	1.00185100	-0.60812600	-0.05884600
H	3.11383300	-3.27158000	-0.30437800
C	5.17137700	-1.71938000	-0.00208100
C	7.37720900	-1.23452400	0.66656700
H	7.88656800	-0.41777800	1.17793300
H	7.46447800	-2.16215100	1.23754800
H	7.79495400	-1.38884500	-0.33176600
C	4.33760800	1.24059400	0.19506400
C	5.95062300	2.51321100	-0.93160600
H	6.40152100	2.52434000	-1.92402900
H	5.42287700	3.44966800	-0.73561900
H	6.71200400	2.36050000	-0.16192300
C	-2.51540000	-0.75436700	-0.14582700
C	-3.46597200	-1.78858100	-0.10514900
C	-2.97897100	0.57397100	-0.25816100
C	-4.82144100	-1.52757400	-0.19063600
H	-3.10892900	-2.80925400	-0.00368900
C	-4.32842300	0.84553600	-0.33885000
C	-5.30254800	-0.19702000	-0.32534000
H	-4.63855600	1.88066000	-0.40475300
N	-1.17971900	-1.13469400	-0.04781400
N	-0.33898600	-0.18606300	-0.13223000
O	5.53180400	-2.80953300	-0.39958900

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O	4.44885500	1.92108400	1.18770200
O	5.02308400	1.41432900	-0.94508500
O	6.00087700	-0.83017200	0.57828600
N	-6.64755600	0.07600200	-0.44823000
C	-7.64445200	-0.99585700	-0.38555200
C	-7.99325000	-1.47071300	1.03183300
H	-7.29683800	-1.83989700	-0.99184800
H	-8.54784200	-0.62394300	-0.87868200
H	-8.71864900	-2.29132400	0.98452300
H	-7.10617900	-1.82942500	1.56277500
H	-8.43472300	-0.66166400	1.62241800
C	-7.13702800	1.45268300	-0.56347700
C	-7.25193900	2.21084500	0.76615400
H	-8.12011700	1.40481400	-1.04229800
H	-6.49174400	2.00197500	-1.25751400
H	-7.59749700	3.23527500	0.58485200
H	-7.96775800	1.72574600	1.43750500
H	-6.28823700	2.26264600	1.28200700
H	0.67254000	-2.70441700	-0.33572700
N	1.56505900	1.79040700	0.21429000
O	0.79494000	2.06516700	1.12457300
O	2.02256700	2.58735900	-0.60496000
H	-5.51104900	-2.36047900	-0.14740800
H	-2.25359900	1.38025700	-0.26383400

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Cartesian coordinates 5. Ground state optimized geometry for dye **7'b** in vacuum [B3LYP/6-31G(d)]**.**

(Total Energy = -1653.62393449 Hartree)

0 1

C	2.37619800	0.14352300	-0.02242500
C	3.72851600	-0.18159300	0.11600900
C	4.07814100	-1.53997100	0.20436600
C	3.06645400	-2.51302000	0.21083200
C	1.73094000	-2.16840100	0.10252300
C	1.34862500	-0.82162800	-0.02960000
H	3.36226700	-3.55238600	0.30746400
C	5.48460100	-2.04241700	0.27015200
C	7.73430700	-1.62364000	-0.28192300
H	8.28384800	-0.86789700	-0.84309900
H	8.06600400	-1.64710800	0.75911600
H	7.87116400	-2.61246800	-0.72653200
C	4.75919800	0.91221600	0.26156300
C	5.61665600	2.87163700	-0.71337800
H	5.51053900	3.39407600	-1.66390300
H	5.29537900	3.50729200	0.11554200
H	6.65173300	2.56063700	-0.55343100
C	-2.17208400	-1.00571300	-0.25926600
C	-3.01522100	-2.13307800	-0.41735400
C	-2.80735600	0.28617400	-0.15120300
C	-4.38359400	-2.04803700	-0.46579900
H	-2.52107700	-3.09644900	-0.49520800
C	-4.19638900	0.36928600	-0.20384600
C	-5.01774700	-0.77267900	-0.36851600
H	-4.62207700	1.35348000	-0.10822100
N	-0.83815200	-1.31930500	-0.22536800
N	0.01903800	-0.37524300	-0.08106900
O	5.79677800	-3.09872200	0.78124300

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O	5.46786700	1.04295500	1.23088500
O	4.75707100	1.72082200	-0.81169800
O	6.35433700	-1.22756300	-0.35652100
N	-6.38226700	-0.64537600	-0.44579700
C	-7.24887100	-1.82177500	-0.56973500
C	-7.52252300	-2.55856400	0.74825100
H	-6.81490300	-2.50848300	-1.30436500
H	-8.19435800	-1.47944300	-1.00091600
H	-8.15009400	-3.43804900	0.56254100
H	-6.59269000	-2.89493800	1.21709600
H	-8.04531800	-1.91333500	1.46124700
C	-7.03283200	0.66663600	-0.32269100
C	-7.19290700	1.17240200	1.11662200
H	-8.01684000	0.57811600	-0.79326000
H	-6.47392500	1.39550400	-0.91787300
H	-7.67130300	2.15827500	1.11111700
H	-7.81603500	0.49448500	1.70912900
H	-6.22380400	1.27151700	1.61357100
C	-2.38872700	2.73271500	0.18559300
C	-1.22435600	3.68071200	0.41067200
H	-0.32845900	3.40174000	-0.15145500
H	-1.54108900	4.68829900	0.13510300
H	-0.96365800	3.68575500	1.47660300
O	-3.55225300	3.11340100	0.20077100
N	-2.00499300	1.41165800	0.00545100
H	-1.00599600	1.19792900	-0.00983600
H	0.95011000	-2.91884400	0.12236000
N	1.99562000	1.56291000	-0.12613800
O	1.33346800	1.89989400	-1.10489200
O	2.35546400	2.31501700	0.77747200
H	-4.96216800	-2.95535500	-0.57549400

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Cartesian coordinates 6. Ground state optimized geometry for dye **7'c** in vacuum [B3LYP/6-31G(d)]**.**
(Total Energy = -1768.13724959 Hartree)

0 1

C	2.70283100	0.20785800	-0.03178500
C	4.03500200	-0.19112100	0.10788400
C	4.30434900	-1.56173400	0.26472000
C	3.23582900	-2.46963600	0.33655600
C	1.92216400	-2.05088500	0.22704400
C	1.61800800	-0.69195900	0.02696400
H	3.47065700	-3.51838300	0.48530600
C	5.67821700	-2.14534100	0.33830500
C	7.94242100	-1.88783900	-0.25246400
H	8.53028600	-1.18949600	-0.84812600
H	8.28334400	-1.89006800	0.78585400
H	8.01523100	-2.89998900	-0.65804900
C	5.13076400	0.84515600	0.18361200
C	6.09084800	2.69383600	-0.90490900
H	6.00615400	3.16824100	-1.88241200
H	5.81426100	3.39182000	-0.11072500
H	7.10776500	2.33262500	-0.73425200
C	-1.90967400	-0.67061500	-0.12241600
C	-2.82393500	-1.75717900	-0.19168200
C	-2.45265900	0.65787900	-0.07228400
C	-4.18719100	-1.59445500	-0.21455000
H	-2.37637300	-2.74264600	-0.19413800
C	-3.83851600	0.81489100	-0.11101000
C	-4.74131900	-0.26407700	-0.20154300
H	-4.20727100	1.82663100	-0.09592500
N	-0.59882200	-1.06724500	-0.09636000
N	0.31892000	-0.16960200	-0.03207100
O	5.93292700	-3.19581300	0.89197600

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O	5.85594200	0.98722400	1.13898400
O	5.16536200	1.59142900	-0.93345900
O	6.58805000	-1.41258600	-0.33155900
N	-6.09906800	-0.02976000	-0.22350100
C	-7.04405800	-0.86692900	-0.98457900
C	-8.07767000	-1.57253600	-0.10572700
H	-6.48317100	-1.59844300	-1.56124400
H	-7.55039600	-0.21066800	-1.70671700
H	-8.77448300	-2.14468600	-0.72969100
H	-7.58008400	-2.25862200	0.58457800
H	-8.66634600	-0.85745400	0.48037700
C	-6.62698800	1.28509700	0.17545600
C	-6.45512700	1.59453300	1.66463000
H	-7.69382500	1.27128400	-0.06275400
H	-6.18805000	2.08355300	-0.43879200
H	-6.90404100	2.56754500	1.89285700
H	-6.94902000	0.83143900	2.27522200
H	-5.40150800	1.63726300	1.95241500
C	-1.89077000	3.09003700	0.11884300
C	-0.67112700	3.98422900	0.25351400
H	-0.93676800	4.98477600	-0.09313100
H	-0.39260900	4.05587500	1.31247400
H	0.19797200	3.61453500	-0.29795900
O	-3.03148800	3.53355300	0.15780700
N	-1.58483600	1.74334900	-0.00902100
H	-0.60059200	1.47179600	-0.04357800
C	-4.55693500	-3.95759800	-0.12959000
H	-5.42499000	-4.61855400	-0.10243400
H	-3.94427800	-4.19691500	-1.00851300
H	-3.95737100	-4.10337000	0.77833900
O	-5.07677000	-2.63884600	-0.19966500

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H	1.09822300	-2.75028300	0.29818200
N	2.40732300	1.64038700	-0.20665800
O	1.74871000	1.96527500	-1.19202200
O	2.82925100	2.41634200	0.64871100

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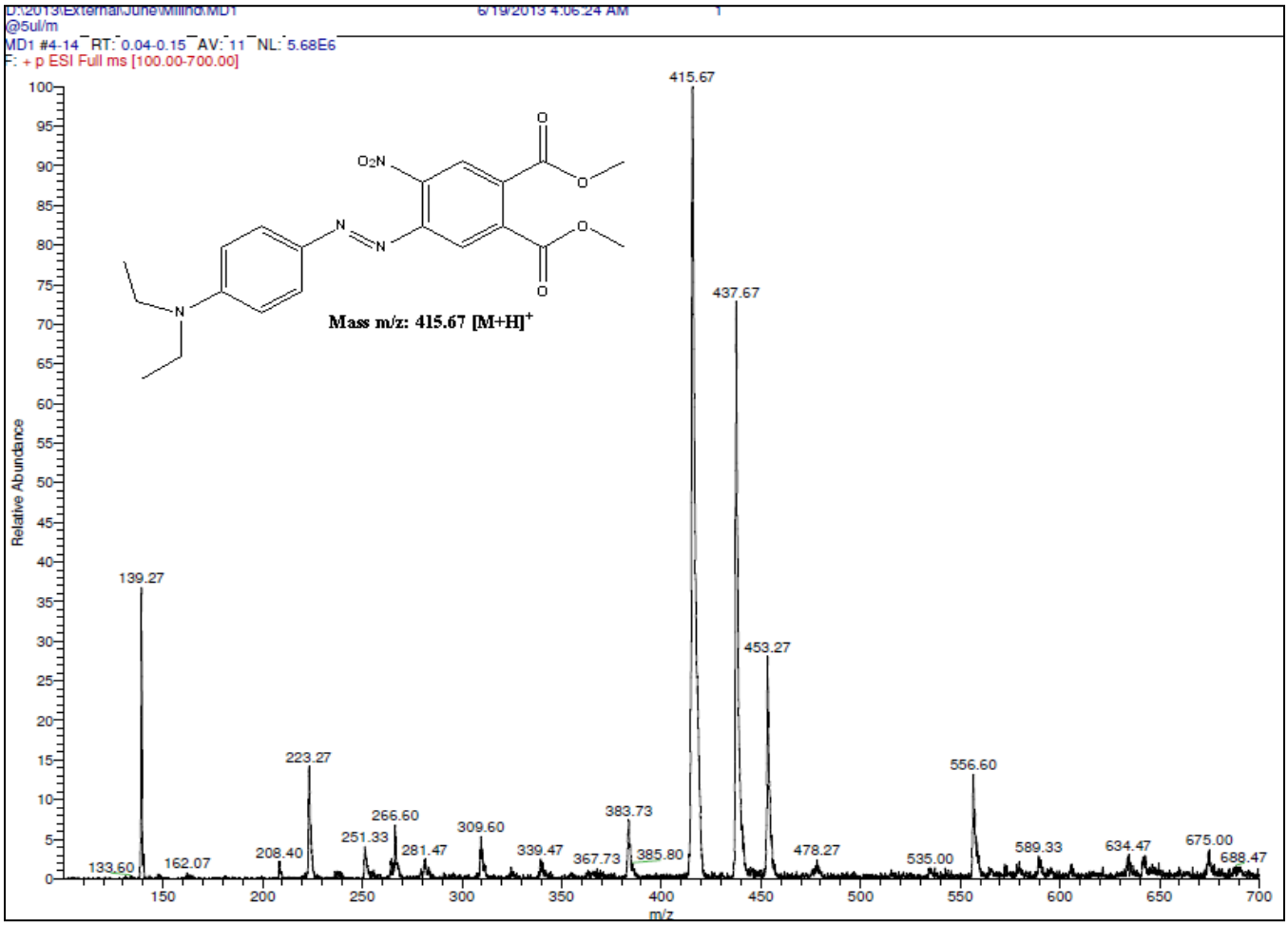
Spectrum 1: Mass spectra of dye **6a**.



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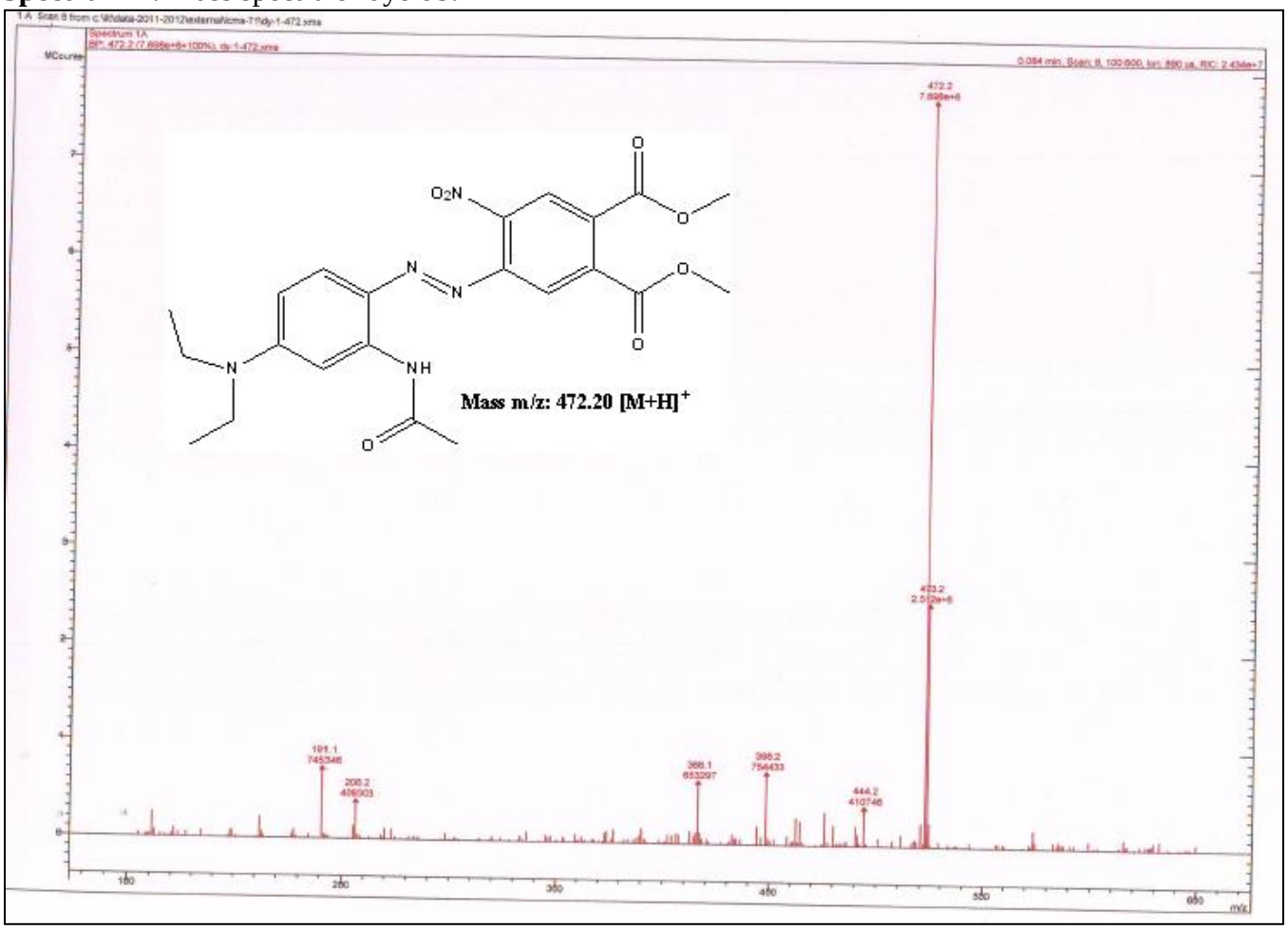
Spectrum 2: Mass spectra of dye **6b.**



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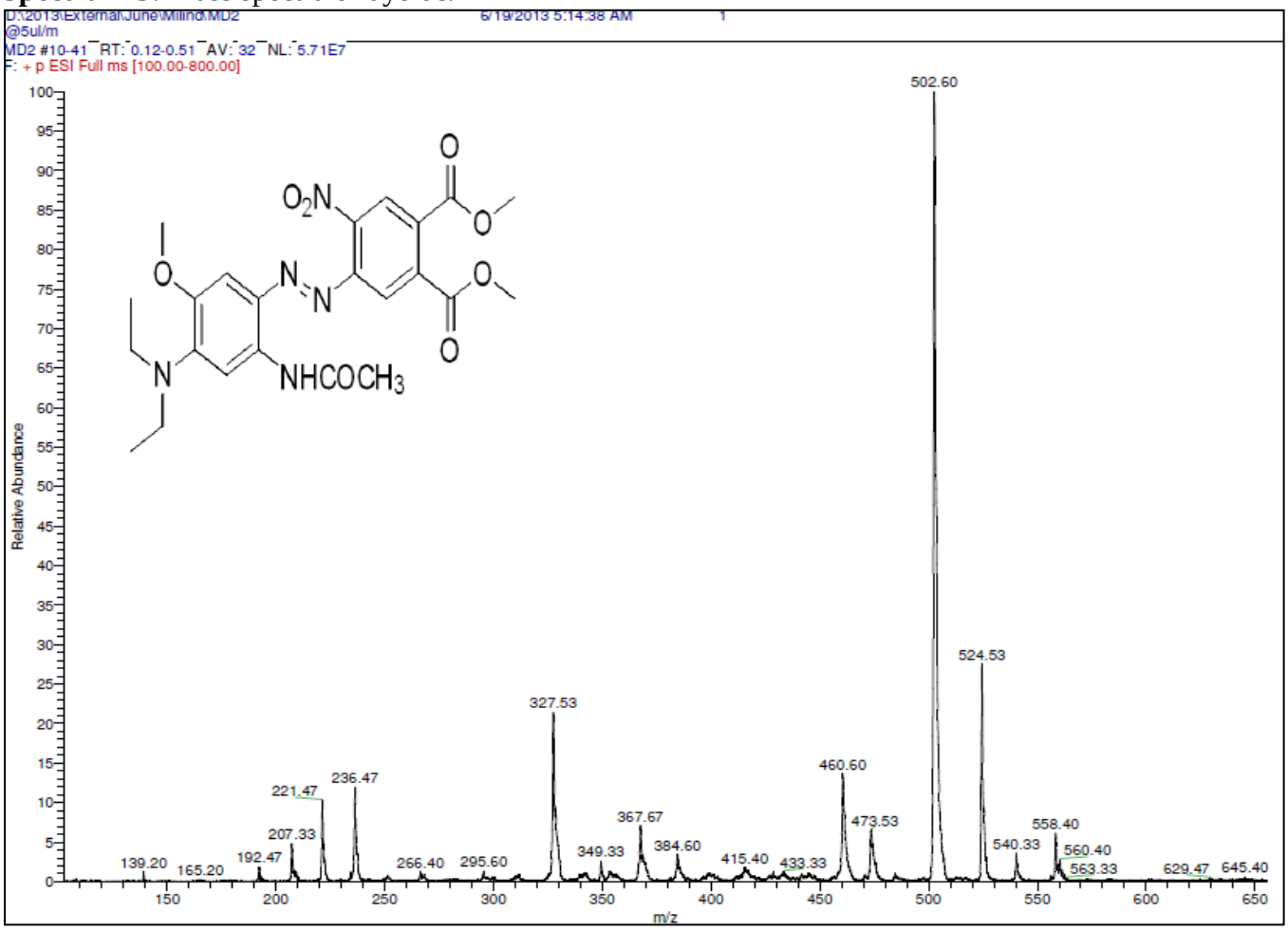
Spectrum 3: Mass spectra of dye **6c.**



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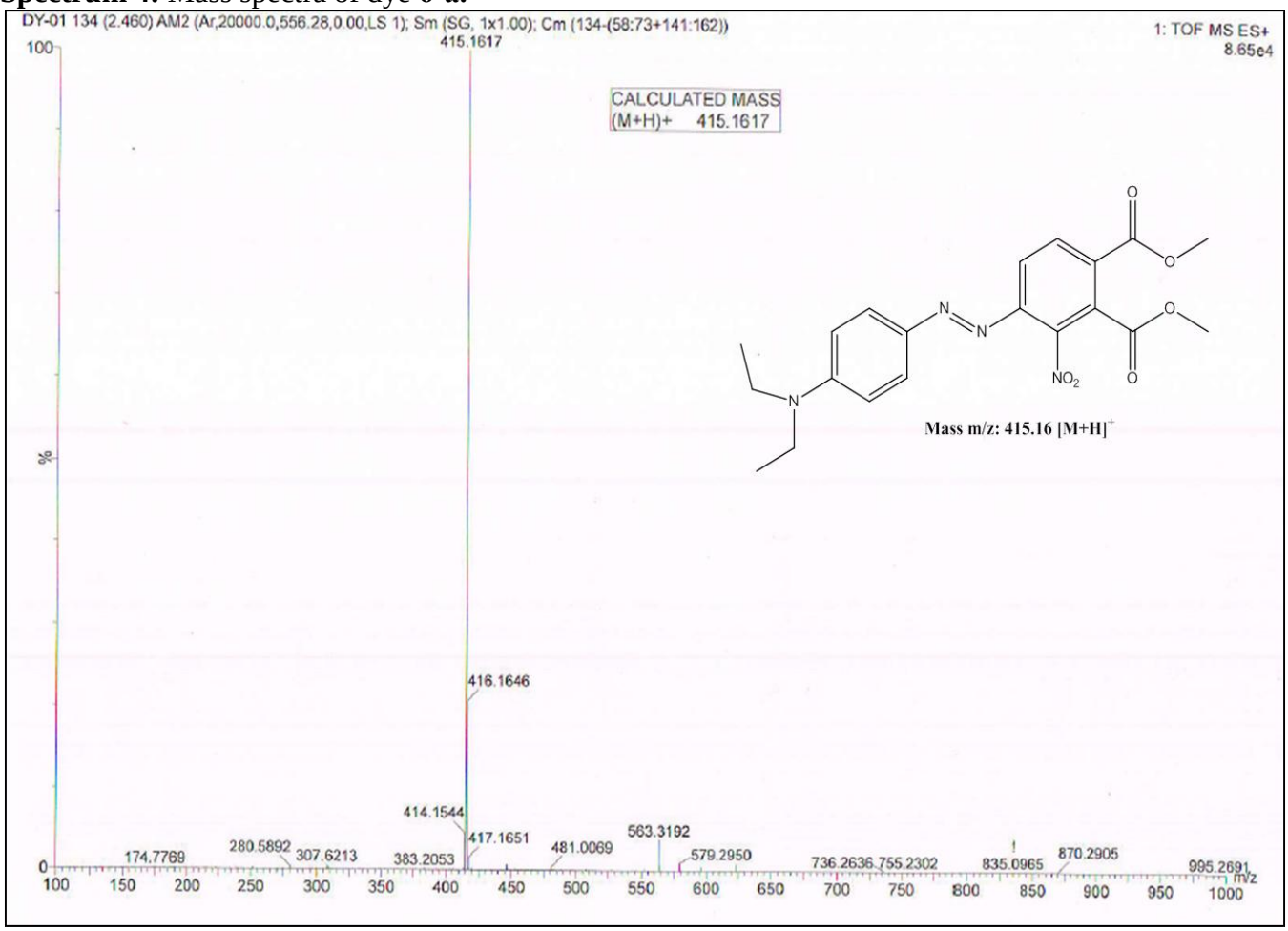
Spectrum 4: Mass spectra of dye **6'a.**



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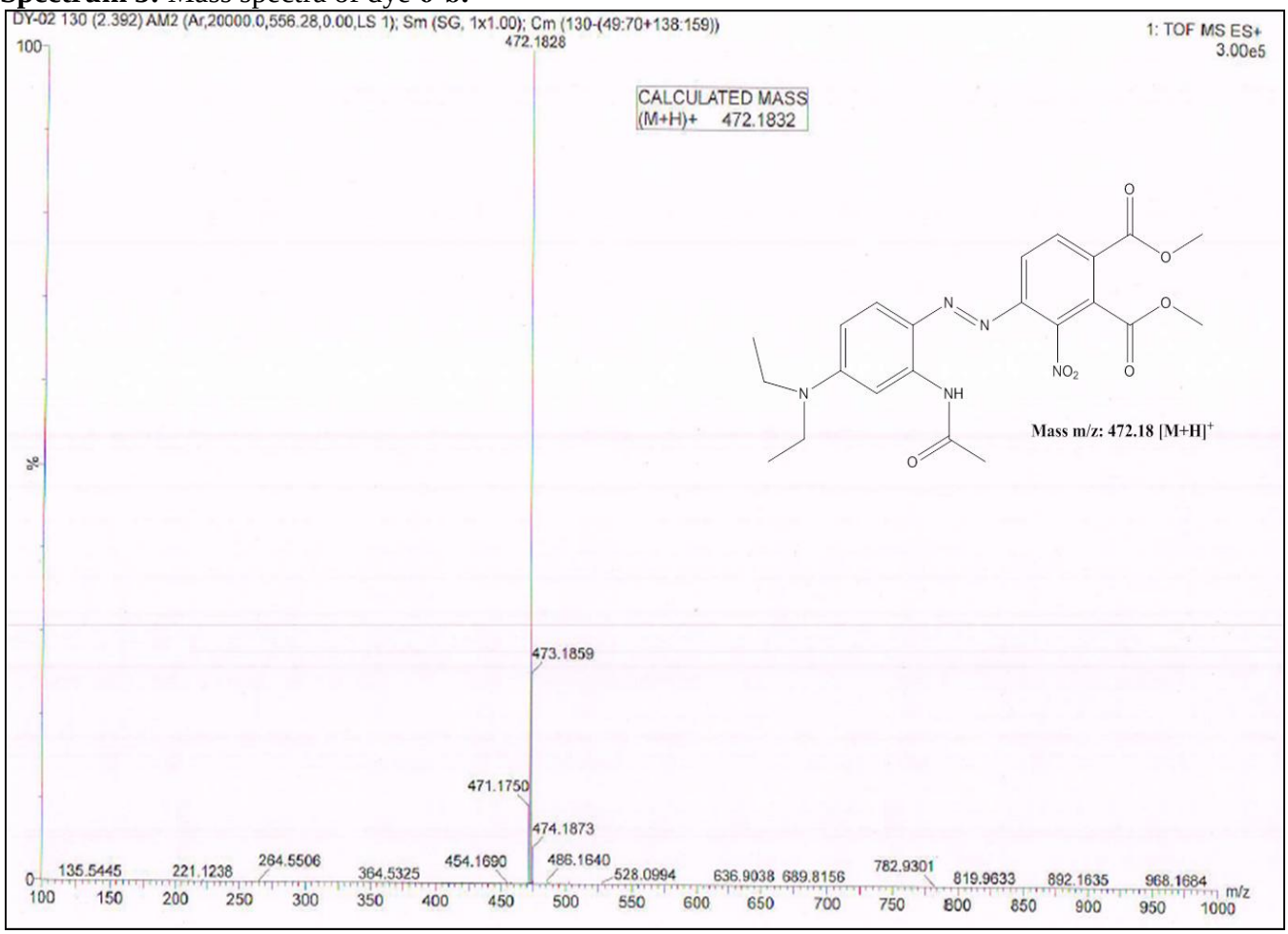
Spectrum 5: Mass spectra of dye **6'b.**



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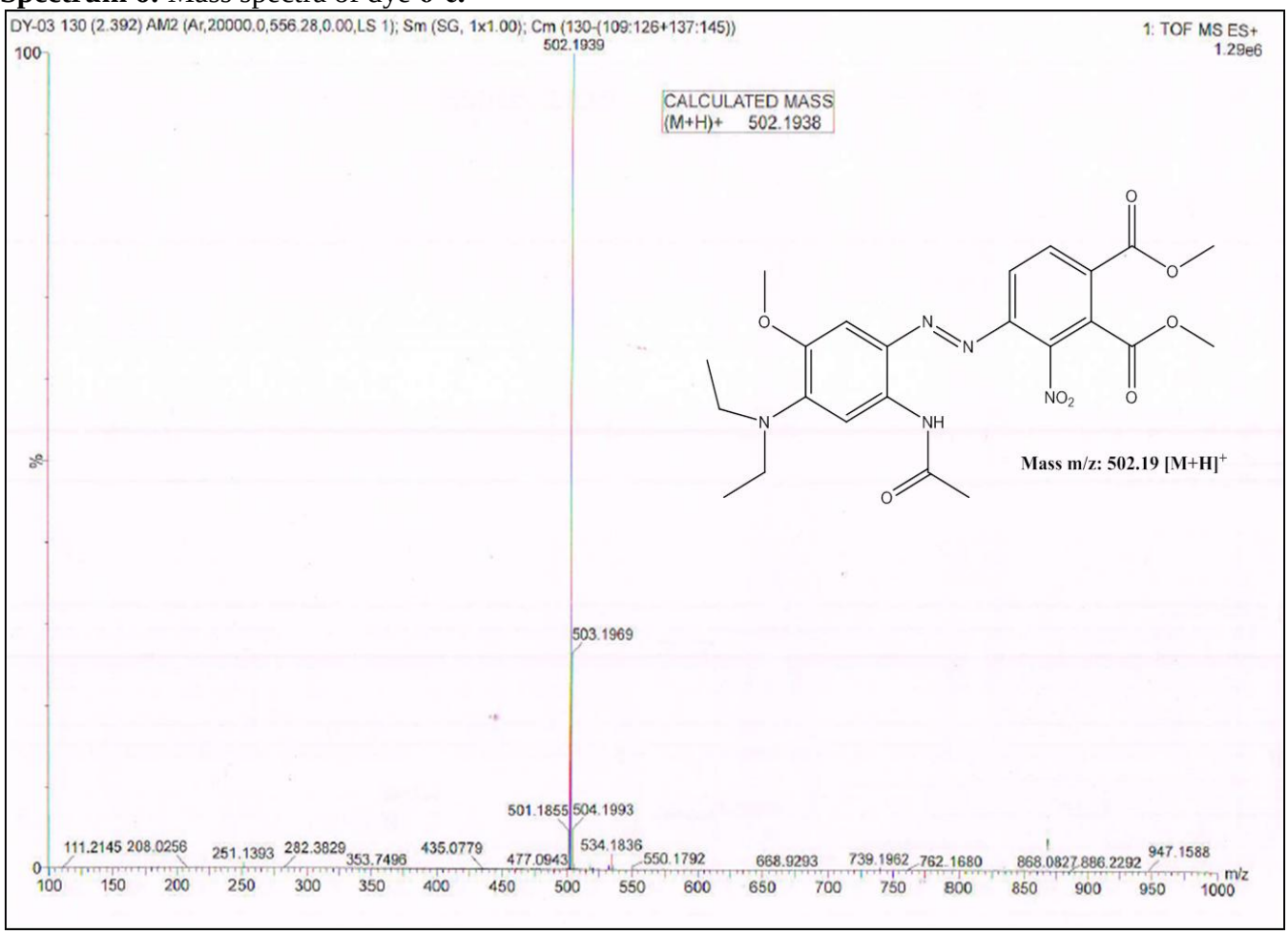
Spectrum 6: Mass spectra of dye **6'c.**



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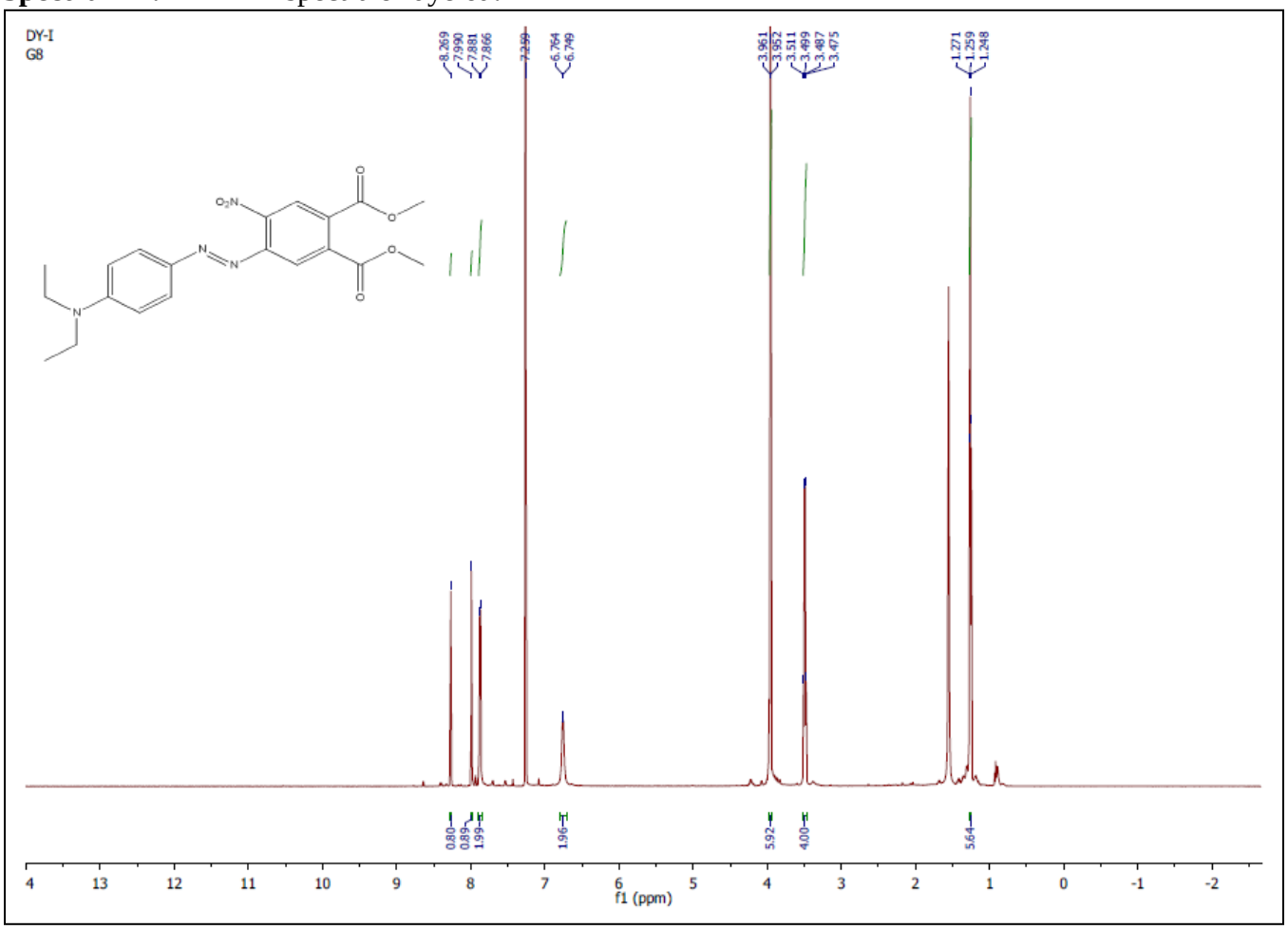
Spectrum 7: ^{1}H NMR spectra of dye **6a.**



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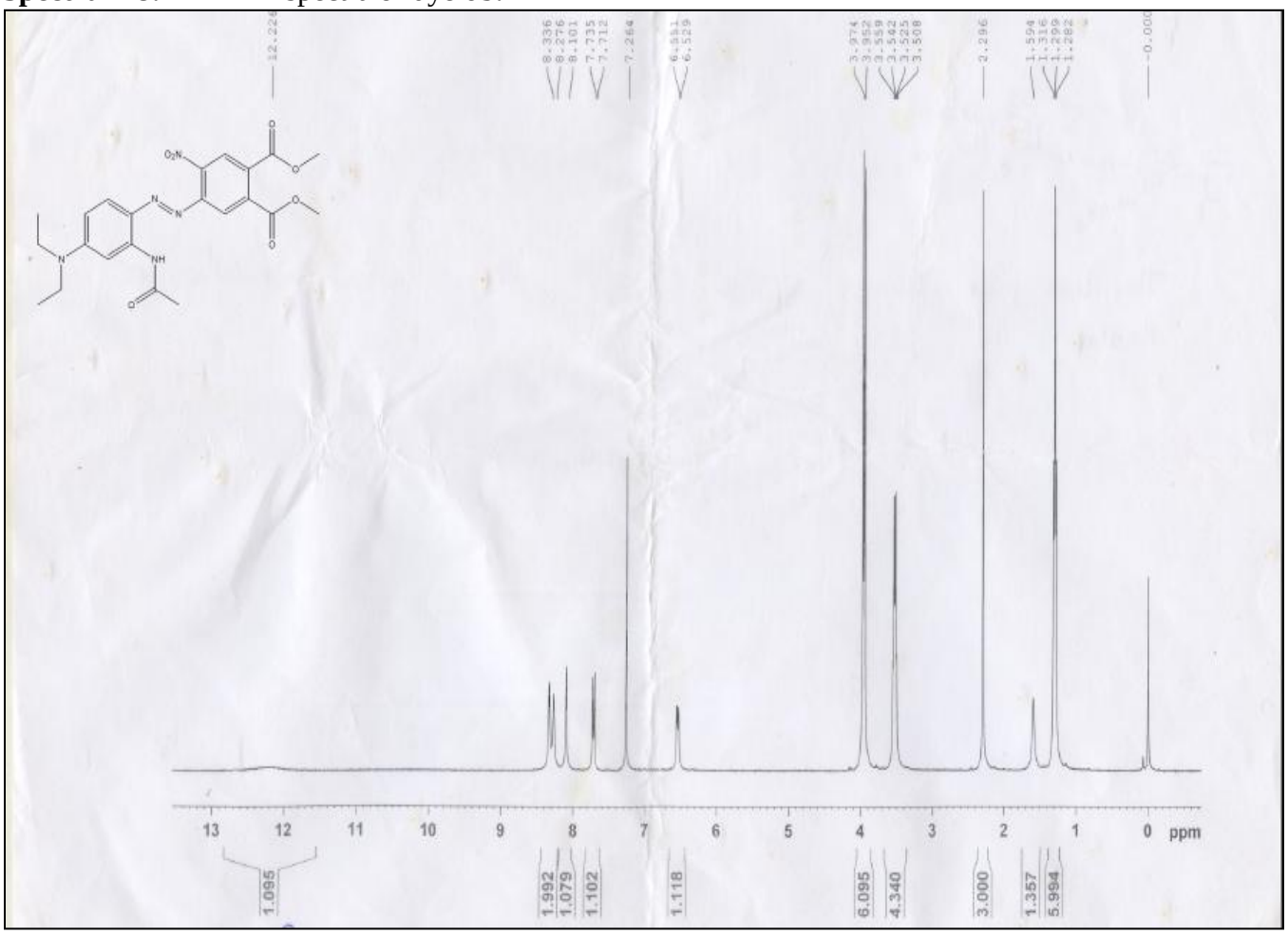
Spectrum 8: ^{1}H NMR spectra of dye **6b.**



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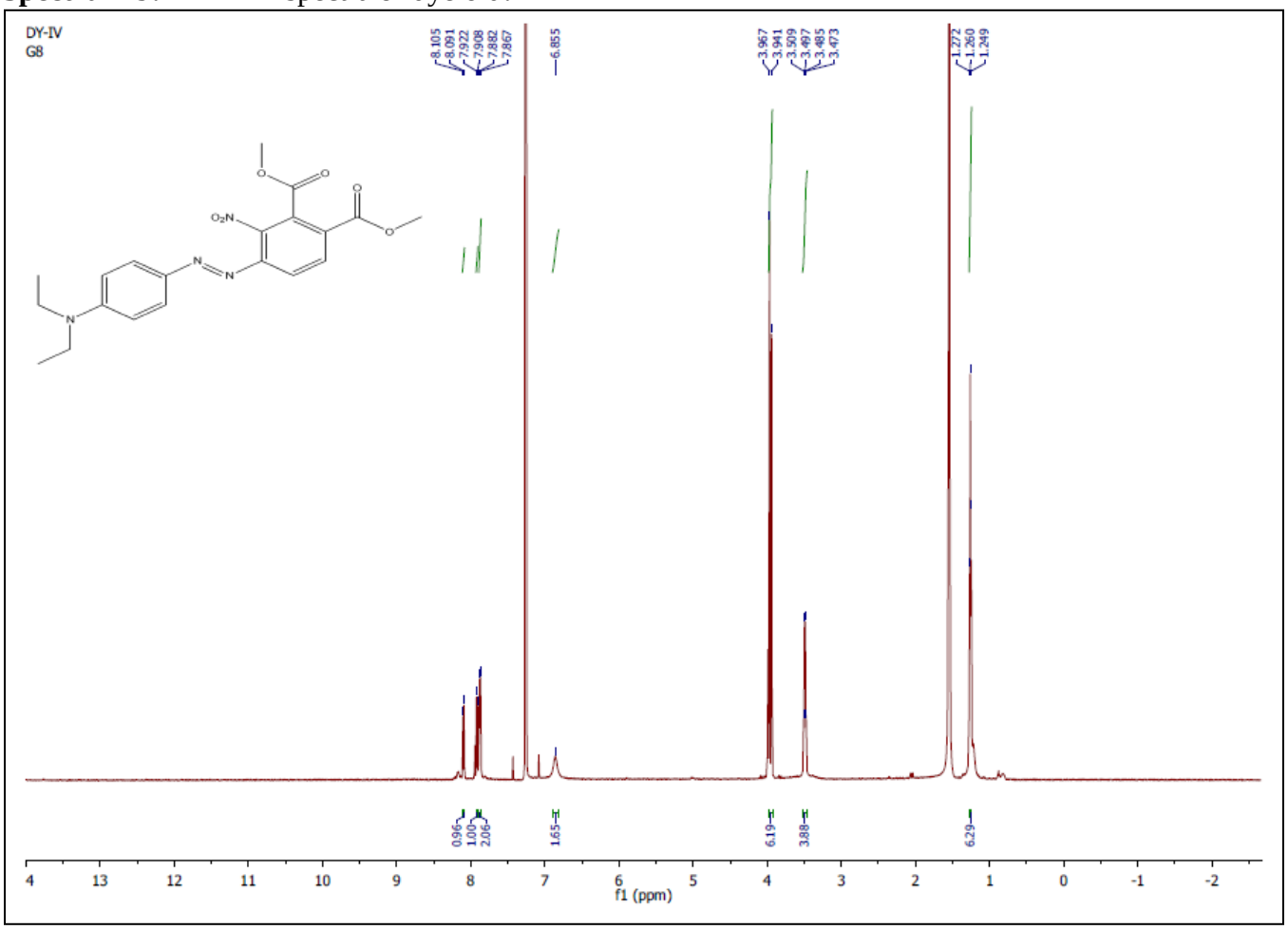
Spectrum 9: ^{1}H NMR spectra of dye **6'a.**



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Spectrum 10: ^{1}H NMR spectra of dye **6'b.**