Efficient Fluorescence Emission from Protonated 1,3,4-Oxadiazole Derivatives with Meta Dimethylamino Substitution

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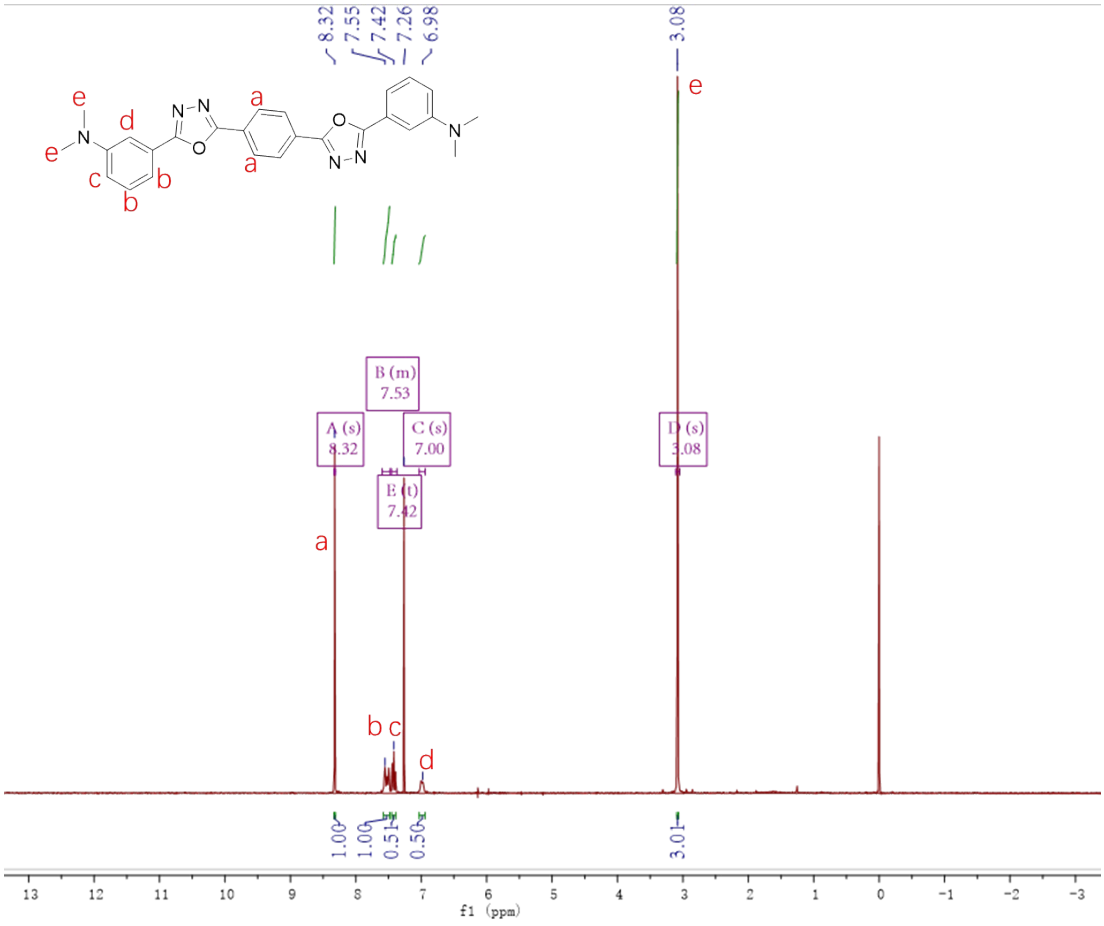
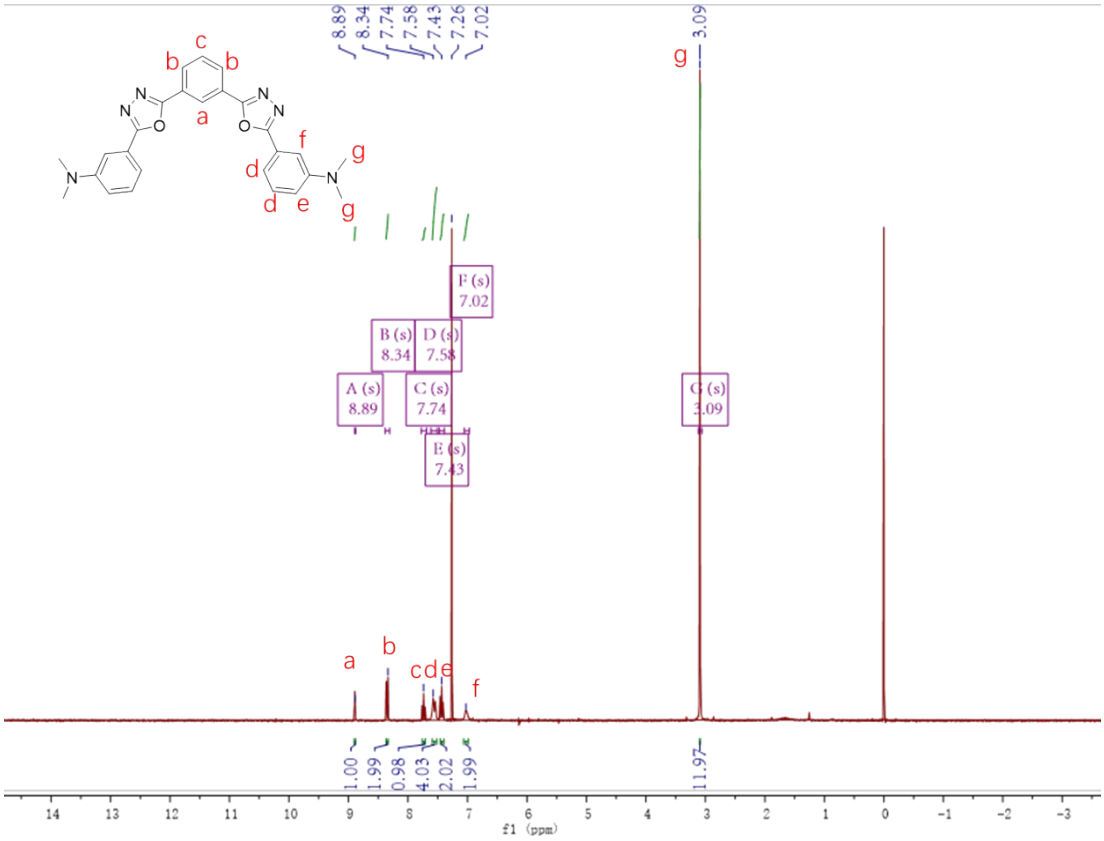
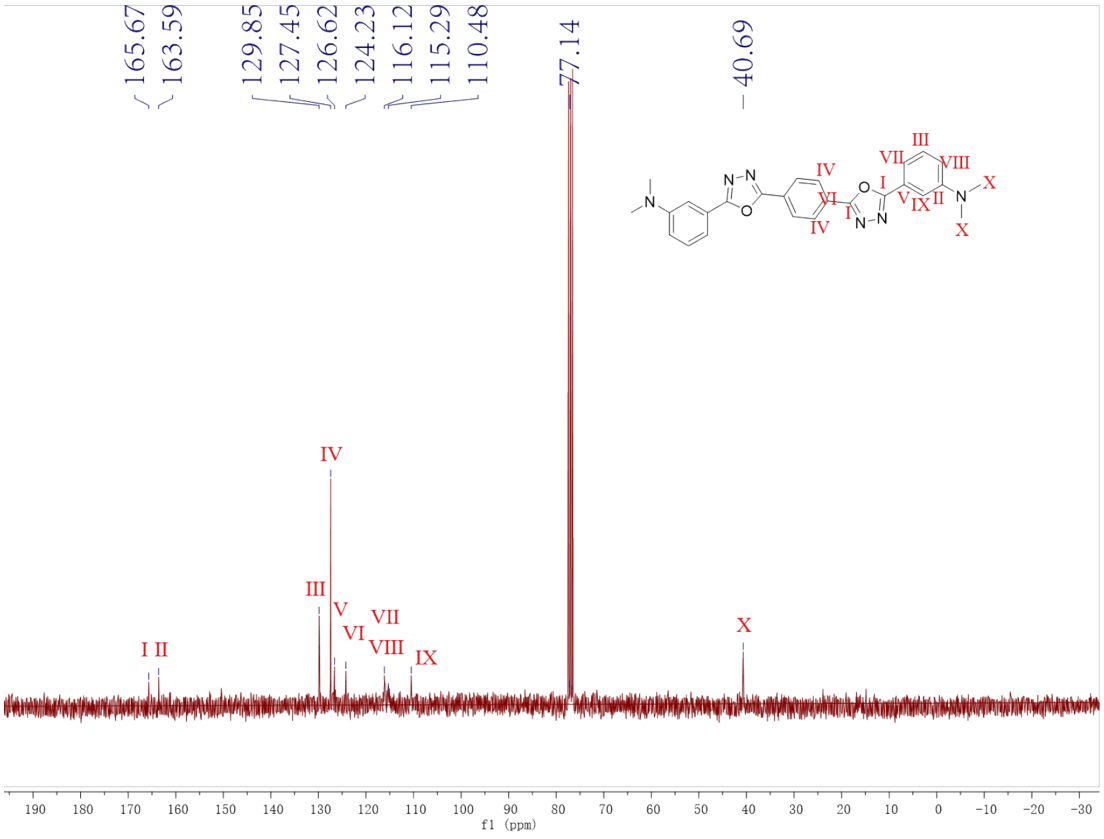


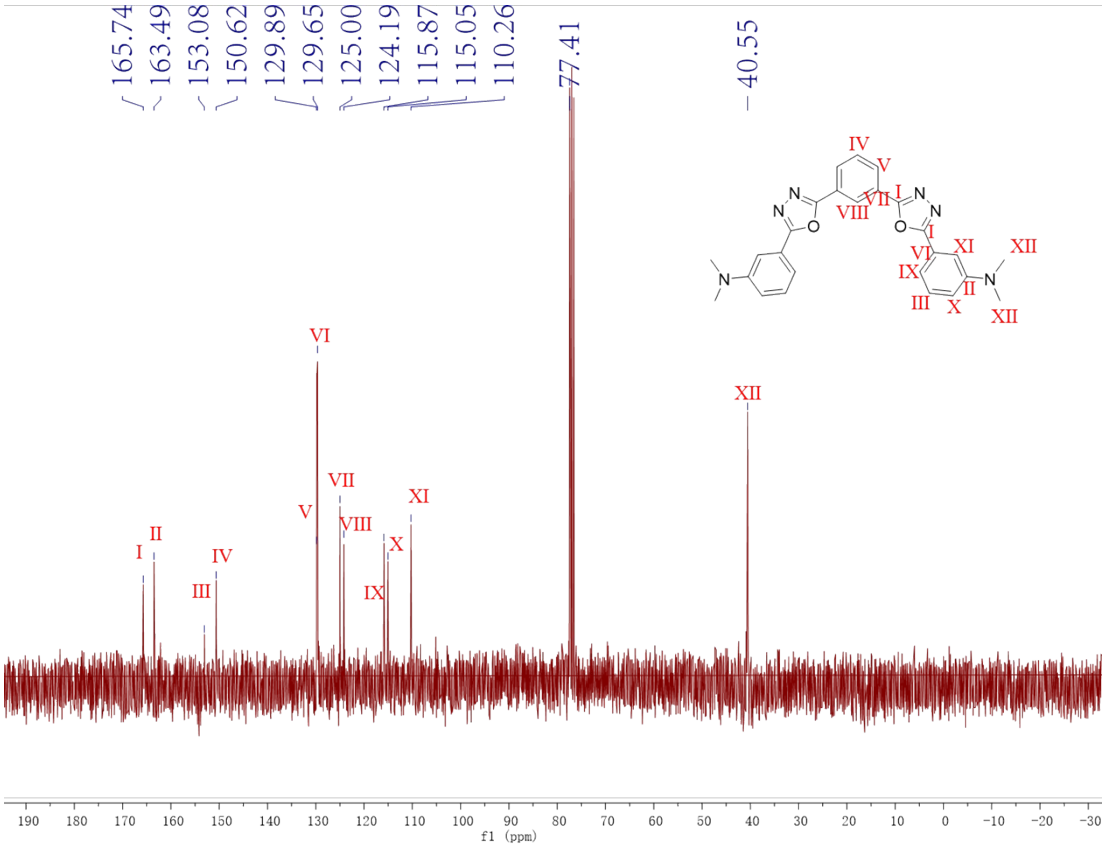
Spectrum S1. ^{1}H NMR spectrum of L-mDMAOXDBEN in $CDCl_3$.



Spectrum S2. ^{1}H NMR spectrum of B-mDMAOXDBEN in $CDCl_3$.



Spectrum S3. ^{13}C NMR spectrum of L-mDMAOXDBEN in $CDCl_3$.



Spectrum S4. ^{13}C NMR spectrum of B-mDMAOXDBEN in $CDCl_3$.

Table S1 Bond length and dihedral angle optimization for ground and excited state geometries of L-mDMAOXDBEN and B-mDMAOXDBEN.

	L-mDMAOXDBEN		B-mDMAOXDBEN	
	Ground state	Excited state	Ground state	Excited state
l_1 (Å)	1.46	1.41	1.46	1.46
l_2 (Å)	1.46	1.43	1.46	1.46
θ_1 (°)	1.79	2.05	1.77	2.05
θ_2 (°)	0	0	0	0
θ_3 (°)	0	0	0	0

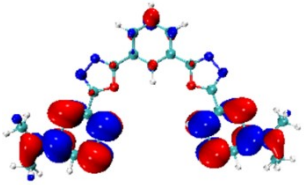
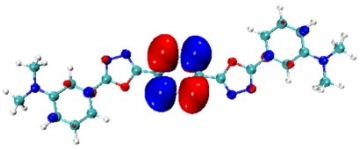
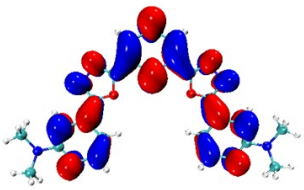
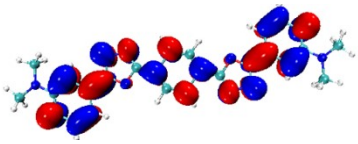
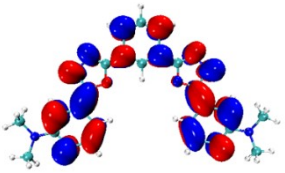
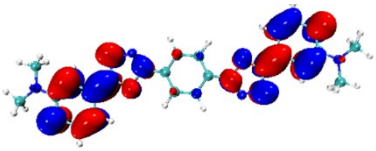
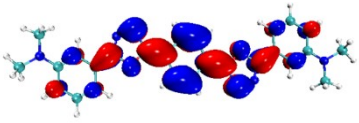
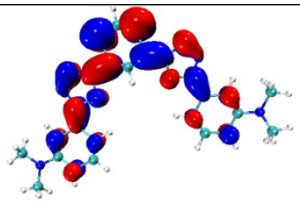
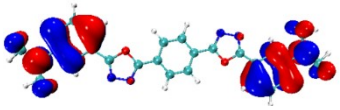
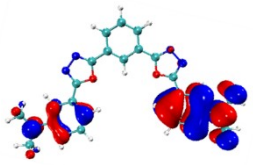
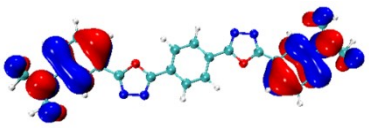
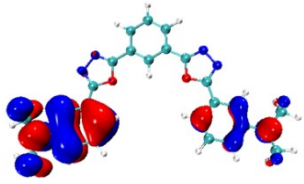
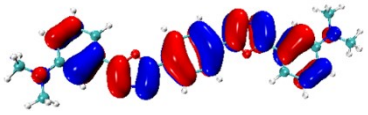
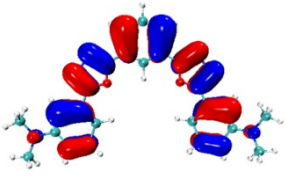
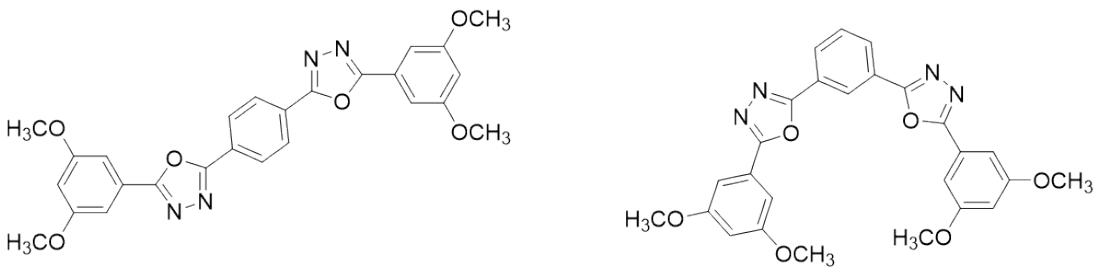
	L-mDMAOXDBEN	B-mDMAOXDBEN
L+4		
L+3		
L+2		
L+1		
LUMO		
HOMO		
H-1		
H-2		

Figure S1. Frontier molecular orbitals involved in the highest allowed transitions of L-mDMAOXDBEN and B-mDMAOXDBEN calculated in cyclohexane.



L-OXD **B-OXD**

Figure S2. Molecular structure of L-OXD and B-OXD.

Table S2 Calculated the atomic charges of each part in the molecule

	L-mDMADMAOXD			B-DMAOXDBEN			DMAOXDBEN$_{(previous)}$		
	S_0	S_1	S_1-S_0	S_0	S_1	S_1-S_0	S_0	S_1	S_1-S_0
DMA	-0.299	-0.189	0.110	-0.298	-0.176	0.122	-0.272	-0.192	0.080
BEN	0.533	0.592	0.059	0.531	0.527	-0.004	0.549	0.637	0.088
OXD	-0.385	-0.474	-0.089	-0.381	-0.475	-0.094	-0.413	-0.475	-0.062
c-BEN	0.150	0.071	-0.079	0.136	0.074	-0.062	0.136	0.030	-0.106

Table S3 The equilibrium Cartesian coordinates of atoms for the ground state of L-mDMAOXDBEN.

Atom	X	Y	Z
C	1.38995300	-0.09384900	-0.02709500
C	0.78473900	1.15027600	-0.02711400
C	-0.60847500	1.25150900	-0.02707700
C	-1.38995300	0.09384900	-0.02709500
C	-0.78473900	-1.15027600	-0.02711400
C	0.60847500	-1.25150900	-0.02707700

H	2.46955700	-0.18834200	-0.02715100
H	1.38914200	2.04978000	-0.02720200
H	-2.46955700	0.18834200	-0.02715100
H	-1.38914200	-2.04978000	-0.02720200
C	-1.26827500	2.55049800	-0.02698300
C	-1.45848500	4.66677000	-0.02799800
O	-0.52093100	3.68339900	-0.02830600
N	-2.53518300	2.80813500	-0.02581500
N	-2.65914200	4.18352000	-0.02673300
C	1.26827500	-2.55049800	-0.02698300
C	1.45848500	-4.66677000	-0.02799800
O	0.52093100	-3.68339900	-0.02830600
N	2.65914200	-4.18352000	-0.02673300
N	2.53518300	-2.80813500	-0.02581500
C	-1.03711200	6.06353600	-0.02897600
C	-2.02535600	7.04495000	-0.02450100
C	0.31527400	6.40027300	-0.02908800
C	-1.68438300	8.40584700	-0.02869300
H	-3.05688400	6.72188900	-0.01719300
C	0.65569300	7.74519700	-0.02071600
H	1.07546600	5.62919200	-0.03054900
C	-0.31435000	8.73516300	-0.01636100
H	1.70165500	8.03436000	-0.01371900
H	-0.00217800	9.77093300	-0.00341700
C	1.03711200	-6.06353600	-0.02897600
C	2.02535600	-7.04495000	-0.02450100
C	-0.31527400	-6.40027300	-0.02908800
C	1.68438300	-8.40584700	-0.02869300
H	3.05688400	-6.72188900	-0.01719300
C	-0.65569300	-7.74519700	-0.02071600
H	-1.07546600	-5.62919200	-0.03054900
C	0.31435000	-8.73516300	-0.01636100
H	-1.70165500	-8.03436000	-0.01371900
H	0.00217800	-9.77093300	-0.00341700
N	2.65914200	-9.38538100	-0.04881900
N	-2.65914200	9.38538100	-0.04881900
C	4.04585200	-9.00844600	0.12635300
H	4.23557400	-8.52037500	1.09272100
H	4.66822500	-9.90093800	0.06702600
H	4.37277400	-8.32659400	-0.66495200
C	2.28174300	-10.76708100	0.15240900
H	3.17361100	-11.39116400	0.10370200
H	1.79631500	-10.93990800	1.12373200
H	1.59916800	-11.11080600	-0.63193800
C	-4.04585200	9.00844600	0.12635300
H	-4.23557400	8.52037500	1.09272100
H	-4.66822500	9.90093800	0.06702600
H	-4.37277400	8.32659400	-0.66495200
C	-2.28174300	10.76708100	0.15240900
H	-3.17361100	11.39116400	0.10370200

H	-1.79631500	10.93990800	1.12373200
H	-1.59916800	11.11080600	-0.63193800

Table S4 The equilibrium Cartesian coordinates of atoms for the ground state of B-mDMAOXDBEN.

Atom	X	Y	Z
C	3.79160700	-2.92379100	0.04926800
C	3.32116800	-1.61863100	0.04496000
C	4.25357300	-0.58285600	0.03533600
C	5.62168400	-0.84340100	0.03393800
C	6.10066900	-2.16202400	0.05083700
C	5.14948100	-3.20164400	0.04809000
H	3.08662500	-3.74887100	0.04994900
H	2.25970000	-1.40472500	0.04400200
H	6.29582400	0.00145200	0.01869600
H	5.47032800	-4.23484100	0.04539200
N	7.45655700	-2.42827000	0.07393900
C	3.82146300	0.81070500	0.02056800
O	2.49367100	1.10121000	0.01739500
C	2.47972700	2.45806300	0.00266900
N	4.54593400	1.88256200	0.00912500
N	3.67302800	2.95363300	-0.00290100
C	1.20467900	3.16622200	-0.00505900
C	0.00003600	2.46710000	0.00228100
C	1.20430300	4.56264900	-0.02011600
C	-1.20458300	3.16625900	-0.00548600
H	0.00001500	1.38408200	0.01401300
C	0.00008500	5.25176100	-0.02775000
H	2.15269200	5.08735400	-0.02557200
C	-1.20415600	4.56268700	-0.02054100
H	0.00010500	6.33612300	-0.03939100
H	-2.15252700	5.08741900	-0.02633100
C	-2.47965500	2.45813800	0.00179800
O	-2.49364700	1.10129400	0.01667800
C	-3.82145700	0.81082800	0.01941200
N	-3.67293800	2.95375000	-0.00422100
N	-4.54588200	1.88271000	0.00750100
C	-4.25362100	-0.58271300	0.03413700
C	-3.32124100	-1.61851400	0.04425500
C	-5.62173000	-0.84324400	0.03242200
H	-2.25977400	-1.40459500	0.04359900
C	-6.10062300	-2.16191200	0.04922700
H	-6.29601800	0.00150700	0.01722500
C	-5.14948600	-3.20161700	0.04720200
H	-5.47047100	-4.23476900	0.04448000
C	-3.79163400	-2.92370500	0.04874700

H	-3.08658600	-3.74872700	0.04989200
N	-7.45634900	-2.42786900	0.07127400
C	-7.91731400	-3.78663100	-0.11048000
H	-7.54530500	-4.44239100	0.68390700
H	-7.61070300	-4.21561900	-1.07528700
H	-9.00576200	-3.80350700	-0.06317700
C	-8.39510600	-1.34073000	-0.10941900
H	-9.41020700	-1.73230500	-0.04962200
H	-8.28561800	-0.58880700	0.67849100
H	-8.27832200	-0.83456900	-1.07796100
C	7.91686700	-3.78588000	-0.11641200
H	7.54540600	-4.44618600	0.67437900
H	7.60937600	-4.20910800	-1.08350800
H	9.00536400	-3.80352100	-0.06990400
C	8.39516700	-1.34108900	-0.10954700
H	8.28043400	-0.83913500	-1.08057600
H	8.28302000	-0.58628600	0.67503600
H	9.41034800	-1.73180200	-0.04535400

Table S5 The distinct transition modes and oscillator strengths of L-mDMAOXDBEN and B-mDMAOXDBEN in chloroform.

Compound	energy	E(f)	Obital Component
L-mDMAOXDBEN	S1	3.94(0.79)	H-2->L 30.8% H-1->L+1 33.6% H->L 45.6%
	S2	4.00(0)	H-1->L 46.9% H-1->L+2 30.0% H->L+1 40.9%
	S3	4.15(1.29)	H-3->L+1 17.3% H-2->L 56.9% H-1->L+1 24.1%
	S1	4.06(1.98)	H-1->L+1 32.8% H->L 85.2%

L-mDMAOXDBEN(Proton)	S2	4.79(0)	H-1->L 41.2% H-1->L+2 12.8% H->L+1 52.8%
	S3	4.86(0.02)	H-2->L 55.5% H-2->L+2 27.3% H->L+5 30.1%
B-mDMAOXDBEN	S1	4.04(0.002)	H-1->L 34.5% H-1->L+1 18.9% H-1->L+2 25.8%
	S2	4.05(0.16)	H-1->L 20.3% H-1->L+1 42.7% H-1->L+2 18.5%
	S3	4.56(1.12)	H-3->L 38.9% H-3->L+2 15.3% H-2->L+1 55.7%
	S4	4.62(0.75)	H-3->L+1 32.4% H-2->L 57.3% H->L 12.6%
B-mDMAOXDBEN(Proton)	S1	4.43(1.05)	H-2->L+1 9.7% H-1->L 28.6% H->L+1 60.3%
	S2	4.55(0.93)	H-1->L+1 31.7% H->L 58.4% H->L+2 7.9%
	S3	4.81(0.08)	H-2->L 22.8% H-2->L+2 23.4% H-1->L 53.2%

	S4	5.18(0)	H-5->L 30.1%
			H-5->L+2 28.5%
			H-4->L+1 36.7%