

## *Supporting Information*

### **Rational Design of Cyclopenta[b]naphthalenes for Better Optoelectronic Applications and their Photophysical Properties Using DFT/TD-DFT Methods**

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## Supporting Information

### List of Figures

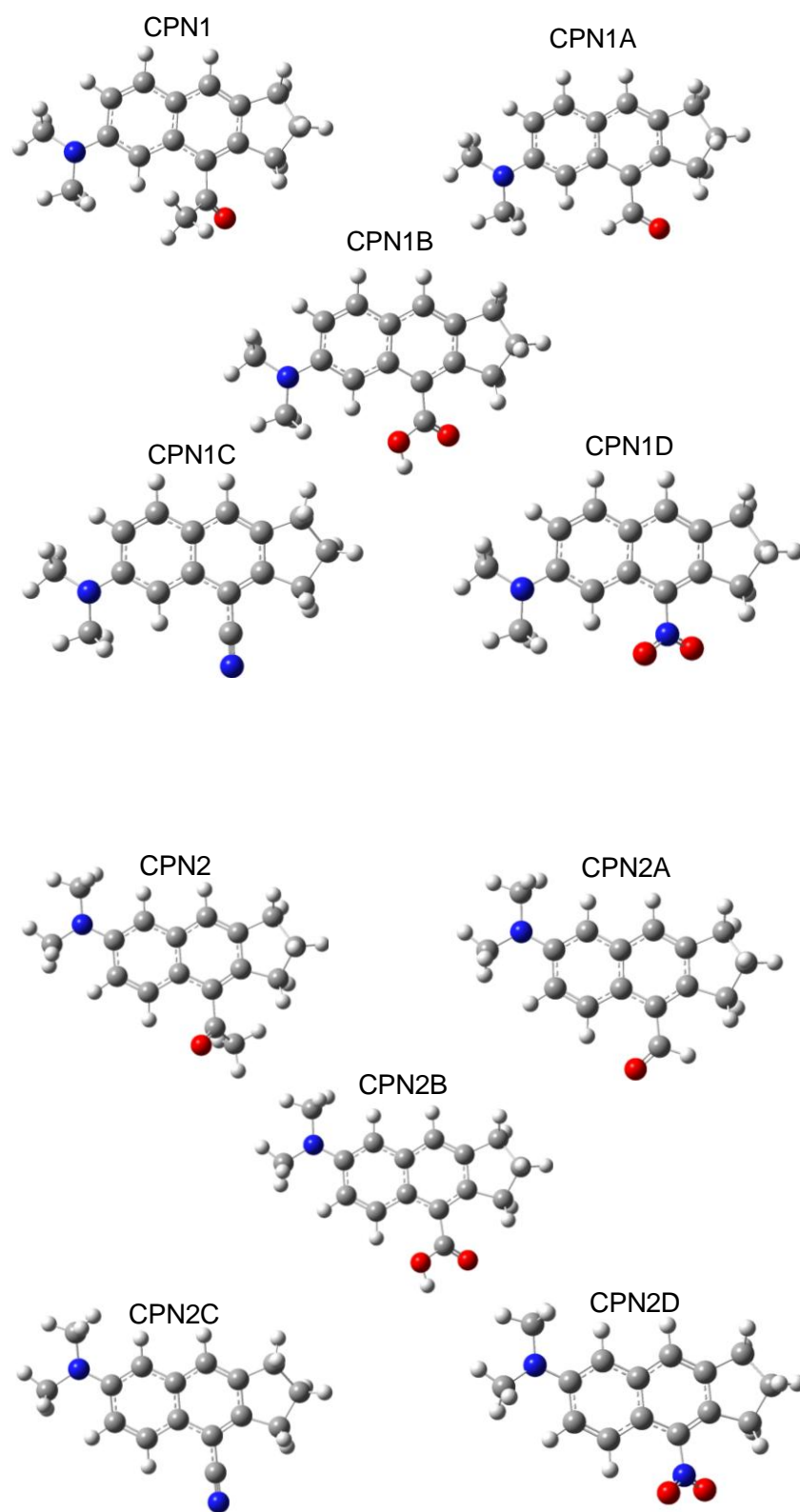
Figure No.	Title	Page No.
SIF1.	Optimized geometries of cyclopenta[b]naphthalene derivatives at B3LYP/6-311+G(d,p) level.	3
SIF2a.	SIF2a. Highest occupied molecular orbital and lowest unoccupied molecular orbitals of CPN1 and its derivatives computed at the B3LYP/6-311+G(d,p) level..	5
SIF2b.	SIF2b. Highest occupied molecular orbital and lowest unoccupied molecular orbitals of CPN2 and its derivatives computed at the B3LYP/6-311+G(d,p) level.	6
SIF2c.	SIF2c. Highest occupied molecular orbital and lowest unoccupied molecular orbitals of CPN3 and its derivatives computed at the B3LYP/6-311+G(d,p) level.	7

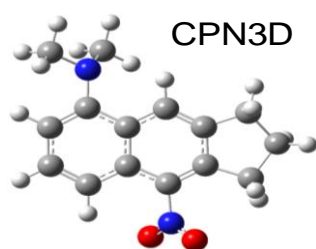
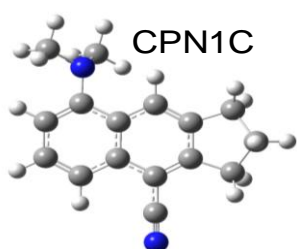
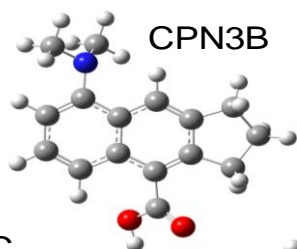
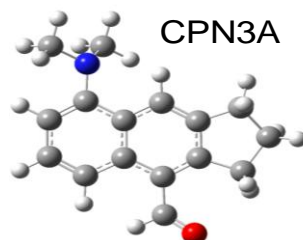
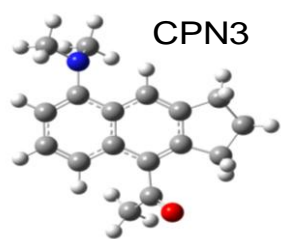
### List of Tables

Table No.	Title	Page No.
SIT1	SIT1. Computed absorption maxima ( $\lambda_{max}$ , nm) of experimental reported CPNs in DCM solution using TD-DFT method at the PBE1PBE with various basis set level.	8
SIT2.	SIT2. Molecular orbital composition (%) of various fragments in the ground state geometry of CPNs computed at the B3LYP/6-311+G(d,p) level.	9
SIT3.	SIT3. Computed bond parameters of optimized geometries of Cyclopenta[b]naphthalene derivatives computed at the B3LYP/6-311+G(d,p) level.	10
SIT4.	SIT4. Computed bond parameters of optimized geometries of Cyclopenta[b]naphthalene derivatives computed at the B3LYP/6-311+G(d,p) level.	11
SIT5.	SIT5. Frontier molecular orbital energies (eV) of CPN derivatives in ground state ( $S_0$ ) computed at the B3LYP/6-311+G(d,p) level.	12
SIT6.	SIT6. Frontier molecular orbital energies (eV) of excited state ( $S_1$ ) CPN derivatives computed at the PBE1PBE/6-311++G(d,p)level.	13

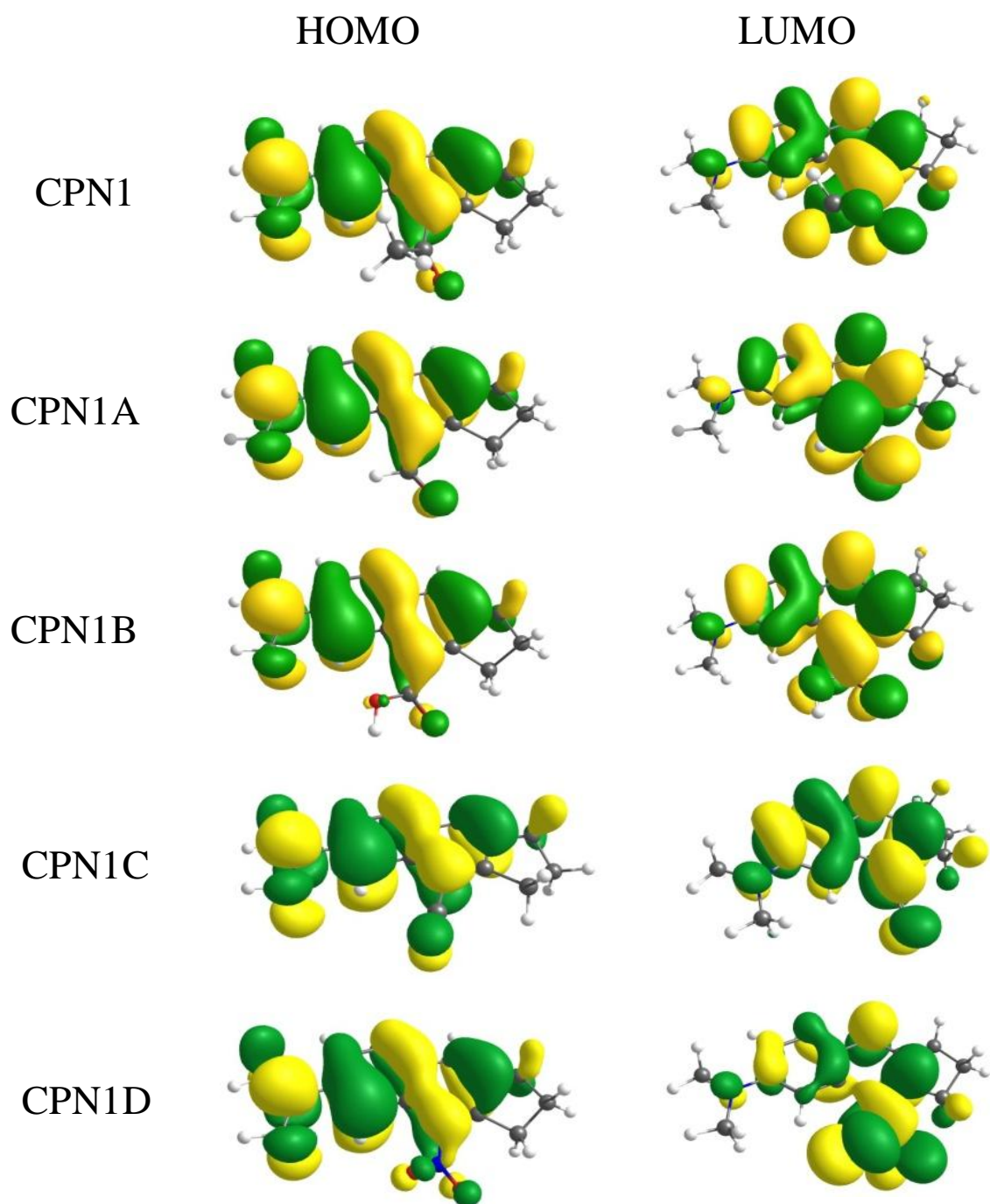
### Coordinates of the chosen molecules

SIF1. Optimized geometries of cyclopean[b]naphthalene derivatives at B3LYP/6-311+G(d,p) level.

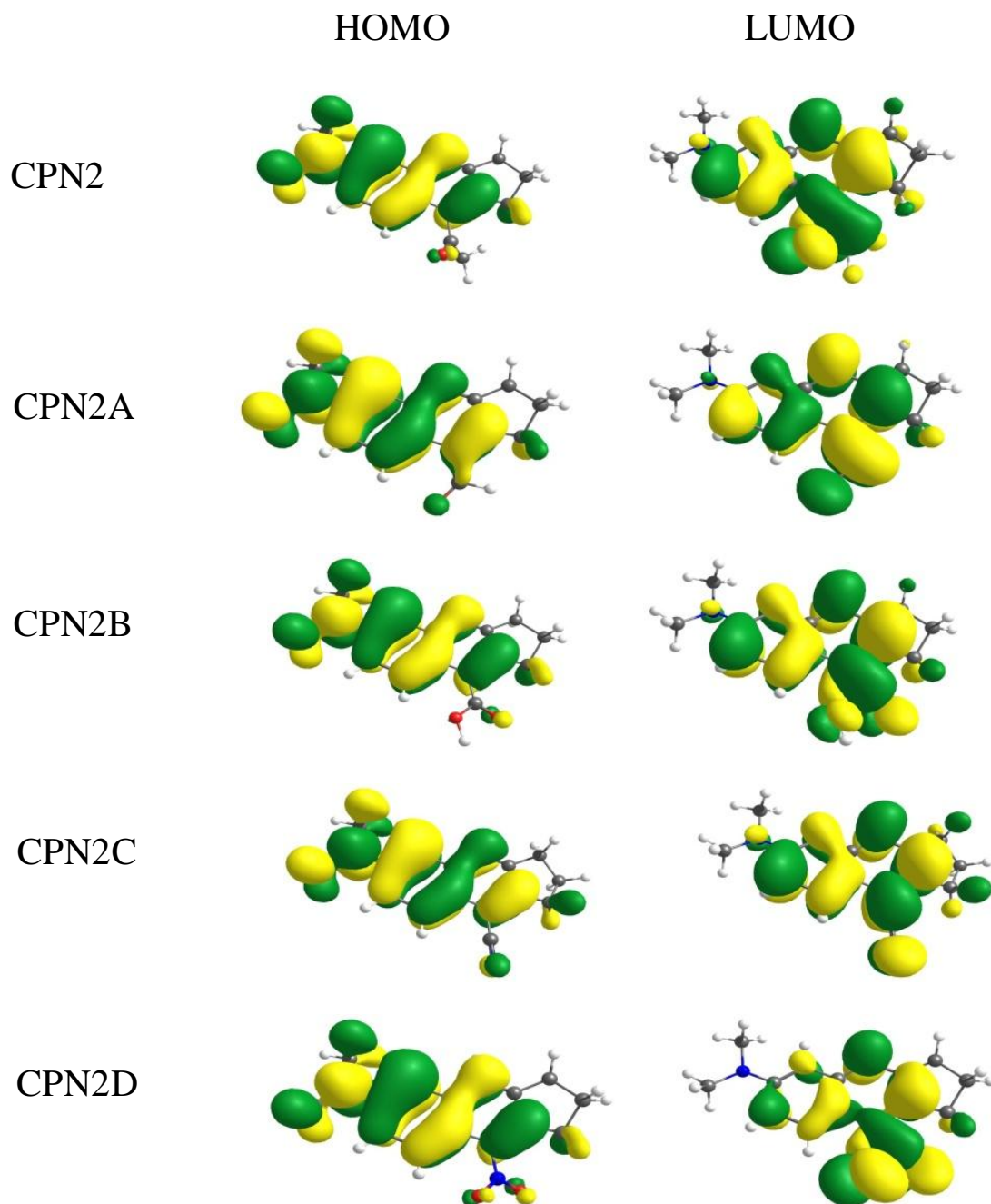




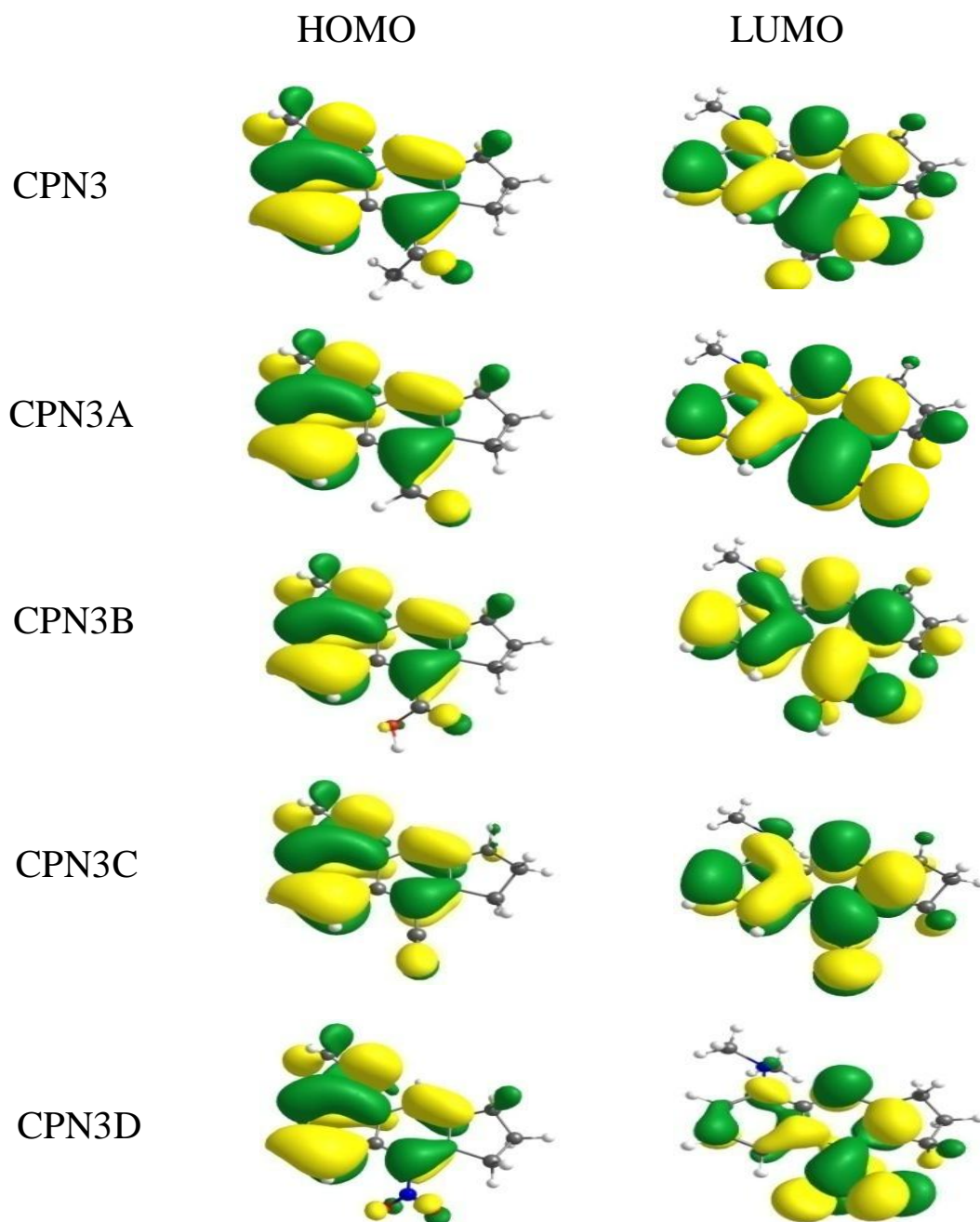
SIF2a. Highest occupied molecular orbital and lowest unoccupied molecular orbitals of CPN1 and its derivatives computed at the B3LYP/6-311+G(d,p) level..



SIF2b. Highest occupied molecular orbital and lowest unoccupied molecular orbitals of CPN2 and its derivatives computed at the B3LYP/6-311+G(d,p) level.



SIF2c. Highest occupied molecular orbital and lowest unoccupied molecular orbitals of CPN3 and its derivatives computed at the B3LYP/6-311+G(d,p) level.



SIT1. Computed absorption maxima ( $\lambda_{\text{max}}$ , nm) of experimental reported CPNs in DCM solution using TD-DFT method at the PBE1PBE with various basis set level.

<b>Molecule</b>	<b>EXP*</b>	<b>6-31+g(d)</b>	<b>6-31+g(d,p)</b>	<b>6-311g(d)</b>	<b>6-311g(d,p)</b>	<b>6-311+g(d,p)</b>
CPN1	377	388	389	383	384	390
CPN1A	437	422	424	414	416	425
CPN2	372	374	375	370	371	378
CPN3	334	368	369	364	365	372

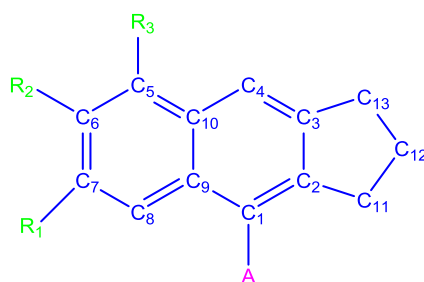
\*E. Benedetti, L. S. Kocsis and K. M. Brummond, *J. Am. Chem. Soc.*, 2012, **134**, 12418- 12421.



SIT2. Molecular orbital composition (%) of various fragments in the ground state geometry of CPNs computed at the B3LYP/6-311+G(d,p) level.

Fragments	CPN1		CPN1A		CPN1B		CPN1C		CPN1D	
	HOMO	LUMO	HOMO	LUMO	HOMO	LUMO	HOMO	LUMO	HOMO	LUMO
CPN	86	88	70	90	79	97	73	94	87	96
A	1	11	2	9	1	2	1	4	1	4
D	13	1	28	1	20	1	25	1	12	0
Fragment	CPN2		CPN2A		CPN2B		CPN2C		CPN2D	
	HOMO	LUMO	HOMO	LUMO	HOMO	LUMO	HOMO	LUMO	HOMO	LUMO
CPN	81	97	71	97	79	99	71	94	84	95
A	2	2	1	3	1	1	2	5	1	4
D	17	0	27	0	20	0%	27	1	14	0
Fragment	CPN3		CPN3A		CPN3B		CPN3C		CPN3D	
	HOMO	LUMO	HOMO	LUMO	HOMO	LUMO	HOMO	LUMO	HOMO	LUMO
CPN	89	95	89	97	90	99	82	89	90	89
A	2	5	1	3	1	1	2	10	1	10
D	8	0	10	0	9	0	16	1	9	1

SIT3. Computed bond parameters of optimized geometries of Cyclopenta[b]naphthalene derivatives computed at the B3LYP/6-311+G(d,p) level.



Molecule		C-Donor	C-Acceptor	C1-C2-C11-C12	C4-C3-C13-C12
CPN1	GS	1.391	1.499	-160.7	162.0
	ES	1.378	1.474	-162.0	163.6
CPN1A	GS	1.387	1.472	-163.5	162.4
	ES	1.382	1.454	-166.3	163.6
CPN1B	GS	1.390	1.486	-161.8	162.7
	ES	1.383	1.455	-164.9	162.8
CPN1C	GS	1.384	1.427	163.3	-163.0
	ES	1.383	1.411	166.3	-165.2
CPN1D	GS	1.383	1.468	-161.1	162.8
	ES	1.366	1.434	-164.9	164.1
CPN2	GS	1.392	1.508	-158.7	160.4
	ES	1.380	1.463	-160.5	161.5
CPN2A	GS	1.390	1.476	-163.5	162.4
	ES	1.383	1.446	-166.3	164.6
CPN2B	GS	1.392	1.488	-161.4	162.4
	ES	1.384	1.447	-166.8	164.3
CPN2C	GS	1.388	1.429	163.0	-162.7
	ES	1.386	1.407	166.6	-166.4
CPN2D	GS	1.392	1.508	-158.7	160.4
	ES	1.366	1.435	-165.1	164.1
CPN3	GS	1.421	1.502	162.6	-161.7
	ES	1.390	1.465	165.1	-162.7
CPN3A	GS	1.421	1.477	165.7	-161.8
	ES	1.389	1.448	168.1	-163.4
CPN3B	GS	1.423	1.489	163.2	-162.0
	ES	1.392	1.450	167.5	-163.3
CPN3C	GS	1.429	1.422	-160.9	163.0
	ES	1.394	1.406	-165.0	166.8
CPN3D	GS	1.422	1.474	162.9	-162.4
	ES	1.373	1.435	167.2	-164.1

SIT4. Computed bond parameters of optimized geometries of Cyclopenta[b]naphthalene derivatives computed at the B3LYP/6-311+G(d,p) level.

Molecule		C <sub>1</sub> -C <sub>2</sub>	C <sub>2</sub> -C <sub>3</sub>	C <sub>3</sub> -C <sub>4</sub>	C <sub>5</sub> -C <sub>6</sub>	C <sub>6</sub> -C <sub>7</sub>	C <sub>7</sub> -C <sub>8</sub>	C <sub>8</sub> -C <sub>9</sub>	C <sub>9</sub> -C <sub>10</sub>	C <sub>1</sub> -C <sub>9</sub>	C <sub>10</sub> -C <sub>4</sub>	C <sub>10</sub> -C <sub>5</sub>	C <sub>2</sub> -C <sub>11</sub>	C <sub>11</sub> -C <sub>12</sub>	C <sub>12</sub> -C <sub>13</sub>	C <sub>3</sub> -C <sub>13</sub>
CPN1	GS	1.385	1.419	1.370	1.369	1.428	1.395	1.411	1.432	1.440	1.417	1.417	1.515	1.546	1.546	1.513
	ES	1.413	1.412	1.386	1.377	1.418	1.418	1.417	1.431	1.450	1.427	1.424	1.511	1.547	1.545	1.507
CPN1A	GS	1.393	1.415	1.372	1.368	1.428	1.396	1.416	1.433	1.448	1.415	1.417	1.513	1.546	1.545	1.513
	ES	1.416	1.413	1.382	1.379	1.419	1.418	1.418	1.426	1.453	1.436	1.424	1.512	1.548	1.546	1.510
CPN1B	GS	1.391	1.417	1.370	1.368	1.427	1.395	1.415	1.435	1.448	1.415	1.417	1.516	1.545	1.543	1.513
	ES	1.429	1.411	1.384	1.382	1.414	1.419	1.420	1.430	1.453	1.439	1.421	1.513	1.548	1.544	1.510
CPN1C	GS	1.384	1.415	1.374	1.370	1.431	1.396	1.409	1.431	1.439	1.417	1.418	1.511	1.548	1.548	1.514
	ES	1.425	1.402	1.395	1.388	1.416	1.419	1.413	1.428	1.441	1.438	1.419	1.505	1.551	1.549	1.511
CPN1D	GS	1.381	1.416	1.372	1.368	1.429	1.397	1.400	1.436	1.438	1.414	1.417	1.514	1.546	1.545	1.513
	ES	1.413	1.410	1.394	1.372	1.433	1.419	1.412	1.437	1.439	1.404	1.431	1.507	1.549	1.552	1.511
CPN2	GS	1.381	1.422	1.369	1.391	1.428	1.371	1.420	1.432	1.432	1.423	1.415	1.520	1.546	1.545	1.513
	ES	1.428	1.407	1.386	1.415	1.420	1.376	1.435	1.429	1.465	1.421	1.417	1.521	1.545	1.542	1.512
CPN2A	GS	1.392	1.418	1.370	1.392	1.427	1.374	1.419	1.431	1.442	1.423	1.415	1.522	1.547	1.544	1.512
	ES	1.419	1.403	1.390	1.413	1.422	1.376	1.432	1.428	1.457	1.422	1.418	1.513	1.548	1.547	1.513
CPN2B	GS	1.387	1.420	1.368	1.390	1.426	1.372	1.420	1.433	1.441	1.422	1.415	1.516	1.546	1.545	1.513
	ES	1.434	1.397	1.395	1.411	1.417	1.382	1.430	1.435	1.465	1.417	1.419	1.515	1.547	1.544	1.512
CPN2C	GS	1.382	1.417	1.371	1.394	1.430	1.372	1.415	1.429	1.434	1.425	1.415	1.510	1.548	1.548	1.514
	ES	1.425	1.390	1.408	1.415	1.419	1.387	1.417	1.432	1.453	1.416	1.420	1.506	1.549	1.550	1.512
CPN2D	GS	1.381	1.421	1.369	1.392	1.428	1.371	1.418	1.433	1.430	1.424	1.414	1.513	1.546	1.545	1.513
	ES	1.399	1.414	1.377	1.421	1.432	1.367	1.432	1.437	1.441	1.430	1.401	1.500	1.548	1.553	1.514
CPN3	GS	1.382	1.418	1.370	1.382	1.409	1.373	1.421	1.434	1.436	1.421	1.439	1.515	1.546	1.546	1.514
	ES	1.426	1.398	1.395	1.416	1.390	1.391	1.433	1.424	1.454	1.432	1.445	1.514	1.549	1.546	1.512
CPN3A	GS	1.389	1.415	1.371	1.382	1.408	1.373	1.422	1.435	1.445	1.420	1.439	1.513	1.547	1.545	1.513
	ES	1.424	1.399	1.391	1.414	1.390	1.389	1.435	1.420	1.455	1.437	1.445	1.514	1.549	1.546	1.513
CPN3B	GS	1.385	1.417	1.369	1.381	1.409	1.373	1.421	1.436	1.443	1.419	1.439	1.515	1.545	1.544	1.513
	ES	1.432	1.395	1.394	1.414	1.388	1.391	1.436	1.421	1.460	1.437	1.444	1.514	1.548	1.545	1.512
CPN3C	GS	1.382	1.415	1.372	1.383	1.410	1.373	1.417	1.431	1.437	1.422	1.438	1.510	1.548	1.548	1.514
	ES	1.426	1.388	1.404	1.417	1.389	1.392	1.425	1.418	1.451	1.439	1.442	1.506	1.550	1.549	1.512
CPN3D	GS	1.375	1.417	1.371	1.381	1.409	1.373	1.419	1.435	1.432	1.420	1.439	1.512	1.547	1.546	1.514
	ES	1.386	1.403	1.390	1.419	1.387	1.394	1.417	1.436	1.439	1.432	1.453	1.505	1.549	1.553	1.513

SIT5. Frontier molecular orbital energies (eV) of CPN derivatives in ground state ( $S_0$ ) computed at the B3LYP/6-311+G(d,p) level.

Molecule	HOMO-2	HOMO-1	HOMO	LUMO	LUMO+1	LUMO+2	Band gap
CPN	-7.81	-6.47	-5.93	-1.26	0.41	0.14	4.66
CPN1	-6.79	-6.21	-5.34	-1.61	-0.66	-0.26	3.73
CPN1A	-6.76	-6.33	-5.42	-1.94	-0.70	-0.34	3.48
CPN1B	-7.19	-6.25	-5.28	-1.63	-0.42	-0.19	3.65
CPN1C	-7.40	-6.44	-5.45	-1.77	-0.50	-0.23	3.68
CPN1D	-7.42	-6.55	-5.49	-2.39	-1.21	-0.51	3.10
CPN2	-6.84	-6.11	-5.25	-1.47	-0.61	-0.21	3.78
CPN2A	-6.77	-6.26	-5.37	-2.08	-0.38	-0.26	3.29
CPN2B	-7.21	-6.21	-5.32	-1.65	-0.34	-0.22	3.67
CPN2C	-7.39	-6.41	-5.50	-1.82	-0.52	-0.28	3.68
CPN2D	-7.49	-6.50	-5.55	-2.43	-1.22	-0.54	3.12
CPN3	-6.67	-6.56	-5.66	-1.77	-0.68	-0.55	3.89
CPN3A	-6.81	-6.70	-5.77	-2.12	-0.77	-0.65	3.65
CPN3B	-6.69	-6.61	-5.66	-1.77	-0.57	-0.36	3.89
CPN3C	-6.92	-6.83	-5.85	-1.97	-0.80	-0.32	3.88
CPN3D	-6.97	-6.93	-5.91	-2.53	-1.41	-0.88	3.38

SIT6. Frontier molecular orbital energies (eV) of excited state ( $S_1$ ) CPN derivatives computed at the PBE1PBE/6-311++G(d,p)level.

Molecule	HOMO-2	HOMO-1	HOMO	LUMO	LUMO+1	LUMO+2	Band gap
CPN	-7.39	-6.31	-5.32	-1.22	0.01	0.93	4.10
CPN1	-6.30	-5.90	-4.91	-1.52	-0.15	0.29	3.39
CPN1A	-6.35	-6.01	-5.00	-1.72	-0.20	-0.20	3.28
CPN1B	-6.87	-5.92	-4.85	-1.54	0.09	0.39	3.31
CPN1C	-7.06	-6.06	-5.02	-1.61	0.02	0.27	3.41
CPN1D	-7.06	-6.09	-4.96	-3.24	-1.10	0.06	1.72
CPN2	-6.25	-5.82	-4.78	-1.73	0.12	0.41	3.05
CPN2A	-6.39	-5.94	-4.85	-1.92	0.06	0.33	2.93
CPN2B	-6.88	-5.91	-4.84	-1.67	0.19	0.40	3.17
CPN2C	-7.02	-6.05	-5.04	-1.69	0.01	0.33	3.35
CPN2D	-6.95	-6.11	-4.95	-3.31	1.11	0.04	1.64
CPN3	-6.37	-6.26	-4.88	-1.75	-0.10	0.03	3.13
CPN3A	-6.49	-6.41	-4.96	-1.93	-0.13	0.12	3.03
CPN3B	-6.46	-6.39	-4.84	-1.76	-0.03	-0.27	3.08
CPN3C	-6.67	-6.48	-5.02	-1.83	-0.23	-0.26	3.19
CPN3D	-6.62	-6.51	-4.90	-3.31	-1.18	-0.22	1.59

### Effect of electron donating groups (EDG) on CPNs

Among the reported CPNs the CPN1C shows better optoelectronic properties and hence we have chosen CPN1C as a reference molecule. In order to understand the influence of electron donating group, we have substituted different EDGs (based on reviewers suggestion) such as  $-\text{OCH}_3$ ,  $-\text{NHCOCH}_3$  and  $-\text{CH}_3$  in the place of  $-\text{N}(\text{CH}_3)_2$  in CPN1C. The molecules with  $-\text{OCH}_3$ ,  $-\text{NHCOCH}_3$  and  $-\text{CH}_3$  groups are denoted as CPN1CA, CPN1CB and CPN1CC respectively and  $-\text{CN}$  is common acceptor in all the cases. The computed results show that these groups do affect the energy gap, absorption and emission wavelengths. When the electron donating power decreases the energy gap of the molecules increases (see Table given below). Further the absorption wavelength for CPN1C, CPN1CA, CPN1CB, and CPN1CC's are predicted at 391, 341, 333 and 314 nm respectively and the emission wavelengths are predicted at 433, 384, 377 and 361 nm respectively. This clearly shows that when electron donating power decreases the absorption and emission wavelength of the molecules decreases.

SIT7. The computed HOMO (eV), LUMO (eV), band gap (eV), absorption ( $\lambda_{\text{max}}$ , nm) and emission wavelength ( $\lambda_{\text{max}}$ , nm) of the molecules in DCM medium.

Molecules	HOMO (eV)	LUMO (eV)	band gap (eV)	absorption wavelength(nm)	Emission wavelength(nm)
CPN1C	-5.45	-1.77	3.68	391	433
CPN1CA	-6.03	-1.99	4.04	341	384
CPN1CB	-6.15	-2.01	4.14	333	377
CPN1CC	-6.33	-2.00	4.33	314	361

### Effect of electron withdrawing groups (EWG) on CPNs

The effect of electron withdrawing groups has been discussed in Page14 of the supporting information. For example CPN1 derivatives such as CPN1, CPN1A, CPN1B, CPN1C and CPN1D have  $-\text{COCH}_3$ ,  $-\text{CHO}$ ,  $-\text{COOH}$ ,  $-\text{CN}$  and  $-\text{NO}_2$  acceptor groups respectively and  $-\text{N}(\text{CH}_3)_2$  is a common donor in all the molecules (please see figure1). This clearly shows that when the electron withdrawing power decreases, the band gap increases and the absorption and emission wavelength decreases.

## Coordinates of the chosen molecules

### CPN1

6	2.600388000	-0.422358000	0.053028000
6	1.465327000	0.384487000	-0.029775000
6	0.151541000	-0.143169000	0.026449000
6	-0.014883000	-1.563035000	0.108850000
6	1.147782000	-2.368974000	0.187602000
6	2.408147000	-1.833206000	0.165827000
1	1.584219000	1.447095000	-0.170839000
6	-1.025799000	0.681826000	-0.059138000
6	-1.312379000	-2.133359000	0.082465000
1	1.028686000	-3.445878000	0.252768000
1	3.259012000	-2.497167000	0.222489000
6	-2.415452000	-1.330580000	-0.048031000
6	-2.271368000	0.079131000	-0.131650000
1	-1.411027000	-3.212603000	0.157983000
6	-3.639333000	0.717266000	-0.266598000
6	-4.606254000	-0.394633000	0.201662000
6	-3.876330000	-1.717452000	-0.126111000
1	-3.812754000	0.975707000	-1.317374000
1	-3.745043000	1.647523000	0.293971000
1	-5.589633000	-0.324026000	-0.267746000
1	-4.751800000	-0.319331000	1.283958000
1	-4.141035000	-2.532747000	0.552044000
1	-4.121914000	-2.052674000	-1.142190000
6	-0.972403000	2.179512000	-0.031650000
8	-1.636688000	2.846732000	-0.804020000
6	-0.171810000	2.878918000	1.061187000
1	-0.878207000	3.479104000	1.641850000
1	0.351031000	2.193950000	1.726800000
1	0.540317000	3.575590000	0.610533000
7	3.884828000	0.111644000	0.037307000
6	4.053617000	1.527093000	-0.247848000
1	5.106924000	1.787053000	-0.147570000
1	3.723507000	1.802239000	-1.261161000
1	3.495562000	2.134178000	0.469426000
6	5.021083000	-0.755014000	-0.245729000
1	4.965071000	-1.221715000	-1.240051000
1	5.934328000	-0.162894000	-0.198063000
1	5.111225000	-1.547496000	0.500941000

### CPN1A

6	-2.605233000	-0.243194000	-0.078163000
6	-1.472257000	0.571920000	-0.038604000
6	-0.156624000	0.047952000	-0.026661000

6	0.006852000	-1.375887000	-0.013250000
6	-1.152853000	-2.190066000	-0.038245000
6	-2.413657000	-1.658656000	-0.070727000
1	-1.606561000	1.640211000	-0.003693000
6	1.032101000	0.874385000	-0.001340000
6	1.301592000	-1.945115000	0.042242000
1	-1.029093000	-3.268232000	-0.024257000
1	-3.263632000	-2.325927000	-0.085319000
6	2.415276000	-1.143903000	0.079605000
6	2.283376000	0.265043000	0.052934000
1	1.394276000	-3.027641000	0.054518000
6	3.656148000	0.901784000	0.080202000
6	4.609301000	-0.259877000	-0.287298000
6	3.872395000	-1.542674000	0.159120000
1	3.858440000	1.284943000	1.087938000
1	3.739942000	1.762987000	-0.582375000
1	5.595485000	-0.155873000	0.169506000
1	4.751294000	-0.281837000	-1.372223000
1	4.112868000	-2.412175000	-0.457946000
1	4.133786000	-1.801380000	1.193389000
6	0.934196000	2.341660000	-0.077611000
8	1.844838000	3.123201000	0.132992000
7	-3.885405000	0.289233000	-0.132609000
6	-4.065028000	1.724367000	0.012783000
1	-5.118183000	1.967136000	-0.122777000
1	-3.749033000	2.095228000	0.999159000
1	-3.501374000	2.266100000	-0.751878000
6	-5.037912000	-0.561094000	0.130749000
1	-5.027260000	-0.990931000	1.142565000
1	-5.944592000	0.032907000	0.023766000
1	-5.100612000	-1.380586000	-0.589981000
1	-0.052653000	2.744960000	-0.370470000

## CPN1B

6	-2.613487000	-0.420320000	-0.060651000
6	-1.483825000	0.397811000	-0.026066000
6	-0.166577000	-0.120481000	-0.027121000
6	-0.001513000	-1.546202000	-0.034762000
6	-1.159794000	-2.362203000	-0.058172000
6	-2.422325000	-1.834584000	-0.067985000
1	-1.606473000	1.465315000	-0.013305000
6	1.028064000	0.696450000	0.024452000
6	1.289776000	-2.123746000	-0.003678000
1	-1.031554000	-3.439912000	-0.059918000
1	-3.270672000	-2.504131000	-0.081291000
6	2.404198000	-1.328676000	0.047221000
6	2.274902000	0.082304000	0.071438000



1	1.376939000	-3.206601000	-0.018833000
6	3.655568000	0.706139000	0.134495000
6	4.596220000	-0.439307000	-0.303740000
6	3.860390000	-1.734342000	0.104116000
1	3.862457000	1.019938000	1.164014000
1	3.754085000	1.603826000	-0.476183000
1	5.591881000	-0.357805000	0.137065000
1	4.714894000	-0.416454000	-1.391580000
1	4.093957000	-2.583297000	-0.543451000
1	4.129147000	-2.027410000	1.127345000
6	1.024360000	2.182013000	0.049367000
8	1.873514000	2.867484000	0.577666000
7	-3.896232000	0.113501000	-0.106983000
6	-4.069665000	1.548548000	0.049450000
1	-5.120484000	1.797116000	-0.096531000
1	-3.762015000	1.910299000	1.042412000
1	-3.493259000	2.091038000	-0.703685000
6	-5.040376000	-0.729269000	0.210530000
1	-5.005633000	-1.128126000	1.234981000
1	-5.950629000	-0.139916000	0.105781000
1	-5.118978000	-1.570555000	-0.482547000
8	-0.008858000	2.772612000	-0.617669000
1	0.137203000	3.726590000	-0.528736000

## CPN1C

6	-2.519681000	-0.293561000	-0.051804000
6	-1.408383000	0.551258000	-0.045521000
6	-0.092043000	0.046473000	-0.053276000
6	0.130458000	-1.366771000	-0.052618000
6	-1.009900000	-2.209063000	-0.039294000
6	-2.283569000	-1.704909000	-0.036479000
1	-1.536126000	1.624043000	-0.035222000
6	1.061322000	0.907635000	-0.051544000
6	1.450459000	-1.883080000	-0.055216000
1	-0.862706000	-3.284238000	-0.029486000
1	-3.116174000	-2.394077000	-0.024222000
6	2.530845000	-1.034355000	-0.054925000
6	2.335707000	0.366758000	-0.050729000
1	1.588657000	-2.960520000	-0.053219000
6	3.666687000	1.081143000	-0.060131000
6	4.662214000	-0.020738000	0.377090000
6	4.011186000	-1.351170000	-0.073489000
1	3.684879000	1.961995000	0.585337000
1	3.889014000	1.430696000	-1.076544000
1	4.753366000	-0.012656000	1.467212000
1	5.661214000	0.125278000	-0.037821000
1	4.327709000	-1.612171000	-1.091422000

1	4.277720000	-2.193441000	0.569812000
7	-3.811628000	0.202289000	-0.085063000
6	-4.024239000	1.635950000	0.044730000
1	-5.084891000	1.850931000	-0.078051000
1	-3.701398000	2.024872000	1.021127000
1	-3.483308000	2.180777000	-0.733363000
6	-4.938983000	-0.677041000	0.189552000
1	-4.906218000	-1.106766000	1.200840000
1	-5.861268000	-0.105878000	0.093545000
1	-4.988793000	-1.497582000	-0.531292000
6	0.891751000	2.324544000	-0.046118000
7	0.750963000	3.473469000	-0.041879000

**CPN1D**

6	-2.619602000	-0.391831000	-0.044857000
6	-1.489135000	0.428742000	-0.041192000
6	-0.180364000	-0.099934000	-0.025230000
6	-0.005988000	-1.525135000	-0.002688000
6	-1.166649000	-2.338966000	-0.000201000
6	-2.427154000	-1.807650000	-0.015318000
1	-1.605690000	1.497472000	-0.074615000
6	1.022220000	0.687689000	0.017223000
6	1.287975000	-2.096034000	0.023305000
1	-1.041294000	-3.416546000	0.022536000
1	-3.277264000	-2.475027000	-0.006455000
6	2.404751000	-1.299098000	0.045697000
6	2.276758000	0.110867000	0.059330000
1	1.378209000	-3.178395000	0.022869000
6	3.650056000	0.746316000	0.097069000
6	4.586416000	-0.399122000	-0.352639000
6	3.864746000	-1.695720000	0.077969000
1	3.870159000	1.063954000	1.122056000
1	3.731778000	1.640958000	-0.521933000
1	5.589045000	-0.309352000	0.069594000
1	4.684381000	-0.382305000	-1.442288000
1	4.090456000	-2.546354000	-0.569755000
1	4.154203000	-1.981829000	1.097264000
7	-3.895152000	0.139661000	-0.093160000
6	-4.073513000	1.581458000	-0.003980000
1	-5.128640000	1.817587000	-0.134328000
1	-3.743941000	1.987642000	0.962800000
1	-3.517808000	2.092540000	-0.794317000
6	-5.052160000	-0.708980000	0.151984000
1	-5.044132000	-1.156215000	1.155819000
1	-5.955392000	-0.108311000	0.056728000
1	-5.118822000	-1.516161000	-0.583227000
7	0.956396000	2.154448000	0.016419000

8	1.771835000	2.760080000	0.707850000
8	0.107654000	2.709415000	-0.678397000

**CPN2**

6	-2.303413000	1.298066000	-0.002863000
6	-0.956332000	1.551690000	-0.044225000
6	0.007078000	0.510069000	0.004197000
6	-0.491086000	-0.829726000	0.083411000
6	-1.885911000	-1.069079000	0.118303000
6	-2.813846000	-0.032778000	0.093568000
1	-0.625424000	2.577218000	-0.139188000
6	1.423805000	0.739748000	-0.008273000
6	0.433549000	-1.911034000	0.103034000
1	-2.209318000	-2.100016000	0.165703000
6	1.780083000	-1.667814000	0.065234000
6	2.285204000	-0.339416000	0.027087000
1	0.052260000	-2.927521000	0.135539000
6	3.803437000	-0.381536000	-0.027963000
6	4.101606000	-1.825468000	-0.494752000
6	2.921917000	-2.660945000	0.050161000
1	4.226884000	-0.219006000	0.972162000
1	4.239342000	0.371193000	-0.688769000
1	5.075123000	-2.186288000	-0.156218000
1	4.096017000	-1.860250000	-1.588309000
1	2.710335000	-3.547622000	-0.552269000
1	3.133421000	-3.007243000	1.070258000
6	1.951911000	2.149219000	-0.099675000
8	1.625867000	2.889861000	-1.006280000
6	2.849200000	2.638324000	1.020407000
1	2.233192000	2.767512000	1.917978000
1	3.628223000	1.918829000	1.273852000
1	3.290784000	3.596989000	0.748005000
1	-2.983626000	2.136928000	-0.050574000
7	-4.184957000	-0.260480000	0.175591000
6	-4.668997000	-1.627992000	0.088369000
1	-5.747974000	-1.634146000	0.241041000
1	-4.452932000	-2.098213000	-0.883619000
1	-4.222195000	-2.245709000	0.871567000
6	-5.111450000	0.787534000	-0.230996000
1	-5.002185000	1.068559000	-1.288954000
1	-6.130499000	0.434621000	-0.074780000
1	-4.984214000	1.685469000	0.377532000

**CPN2A**

6	2.239729000	1.269531000	-0.024404000
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6	0.919596000	1.648885000	-0.015190000
6	-0.131921000	0.696996000	-0.043695000
6	0.249785000	-0.682401000	-0.073164000
6	1.615579000	-1.050991000	-0.078057000
6	2.633498000	-0.101240000	-0.069832000
1	0.670665000	2.698781000	0.015927000
6	-1.531546000	1.042953000	-0.032261000
6	-0.762280000	-1.682577000	-0.090907000
1	1.843390000	-2.108255000	-0.090533000
6	-2.087765000	-1.337043000	-0.073477000
6	-2.480170000	0.024832000	-0.035971000
1	-0.463375000	-2.726786000	-0.114888000
6	-3.999870000	0.106330000	-0.027633000
6	-4.435660000	-1.318597000	0.388875000
6	-3.299893000	-2.241579000	-0.103499000
1	-4.367502000	0.341957000	-1.034610000
1	-4.400564000	0.868413000	0.642485000
1	-5.413639000	-1.592439000	-0.011668000
1	-4.498999000	-1.371480000	1.479895000
1	-3.180809000	-3.137863000	0.510054000
1	-3.490772000	-2.577867000	-1.130619000
6	-2.028403000	2.432827000	-0.024078000
8	-1.369595000	3.456182000	-0.032122000
1	2.991601000	2.046037000	0.002815000
7	3.977922000	-0.452453000	-0.120748000
6	4.339009000	-1.853153000	0.017607000
1	5.415512000	-1.958093000	-0.113888000
1	4.066879000	-2.270107000	0.999577000
1	3.852934000	-2.455265000	-0.754496000
6	4.992165000	0.528308000	0.241432000
1	4.905017000	0.868445000	1.283870000
1	5.976444000	0.079935000	0.109692000
1	4.945779000	1.403890000	-0.409909000
1	-3.132371000	2.509937000	-0.015962000

## CPN2B

6	2.320084000	1.278603000	-0.113658000
6	0.976242000	1.556353000	-0.090655000
6	-0.008737000	0.534239000	-0.048520000
6	0.478368000	-0.813693000	-0.039468000
6	1.869050000	-1.077567000	-0.050099000
6	2.814727000	-0.059361000	-0.099360000
1	0.668447000	2.590546000	-0.095696000
6	-1.431965000	0.762355000	-0.052020000
6	-0.449724000	-1.891143000	-0.019499000
1	2.173308000	-2.115187000	-0.028034000
6	-1.795936000	-1.648690000	-0.031413000

6	-2.297759000	-0.320820000	-0.059029000
1	-0.068810000	-2.908217000	0.001039000
6	-3.812837000	-0.356709000	-0.073918000
6	-4.146074000	-1.788737000	0.403655000
6	-2.936189000	-2.643213000	-0.034420000
1	-4.170488000	-0.186757000	-1.096015000
1	-4.272564000	0.420129000	0.537749000
1	-5.093669000	-2.156502000	0.004774000
1	-4.221516000	-1.799917000	1.495529000
1	-2.756181000	-3.502098000	0.616896000
1	-3.085330000	-3.034731000	-1.048981000
1	3.010003000	2.110396000	-0.145355000
7	4.181829000	-0.313404000	-0.156930000
6	4.644325000	-1.676091000	0.046113000
1	5.724398000	-1.710281000	-0.093805000
1	4.411317000	-2.061808000	1.050717000
1	4.196171000	-2.349316000	-0.689166000
6	5.123128000	0.752669000	0.157279000
1	5.016348000	1.128917000	1.185587000
1	6.137037000	0.372185000	0.036555000
1	5.010624000	1.594578000	-0.529486000
6	-2.055884000	2.113731000	-0.058875000
8	-3.115339000	2.382154000	-0.581039000
8	-1.361286000	3.066690000	0.622509000
1	-1.883826000	3.879587000	0.547763000

## CPN2C

6	2.228324000	1.334112000	-0.073357000
6	0.903170000	1.686272000	-0.039333000
6	-0.122178000	0.712053000	-0.002299000
6	0.265785000	-0.663141000	0.005301000
6	1.638177000	-1.004479000	-0.027567000
6	2.638362000	-0.035512000	-0.081336000
1	0.634112000	2.736605000	-0.037109000
6	-1.517033000	1.043149000	0.029427000
6	-0.745231000	-1.666156000	0.047975000
1	1.888353000	-2.056431000	-0.010421000
6	-2.071578000	-1.319164000	0.076543000
6	-2.469036000	0.041331000	0.065580000
1	-0.445079000	-2.709900000	0.051137000
6	-3.974822000	0.151522000	0.109069000
6	-4.441939000	-1.265386000	-0.304713000
6	-3.295406000	-2.208894000	0.132886000
1	-4.366666000	0.940471000	-0.536618000
1	-4.300555000	0.388421000	1.130151000
1	-4.550297000	-1.306569000	-1.392512000
1	-5.404607000	-1.536485000	0.132528000

1	-3.453289000	-2.560048000	1.160501000
1	-3.208228000	-3.096345000	-0.498628000
1	2.969169000	2.120761000	-0.095231000
7	3.984900000	-0.366283000	-0.156457000
6	4.376042000	-1.755761000	0.012287000
1	5.451059000	-1.844342000	-0.139831000
1	4.133293000	-2.148330000	1.011395000
1	3.884958000	-2.389115000	-0.731414000
6	4.996181000	0.647926000	0.108831000
1	4.937681000	1.052521000	1.129693000
1	5.981822000	0.203959000	-0.025654000
1	4.917087000	1.479594000	-0.595454000
6	-1.927028000	2.412037000	0.018669000
7	-2.264837000	3.518536000	0.010697000

**CPN2D**

6	2.326427000	1.280581000	-0.069073000
6	0.987178000	1.574178000	-0.040134000
6	0.001598000	0.554189000	-0.025518000
6	0.465035000	-0.801660000	-0.040163000
6	1.851889000	-1.077605000	-0.056683000
6	2.806403000	-0.064442000	-0.084731000
1	0.684494000	2.610636000	-0.012259000
6	-1.411755000	0.768996000	-0.035222000
6	-0.482616000	-1.864140000	-0.032067000
1	2.148427000	-2.117463000	-0.055267000
6	-1.826753000	-1.603942000	-0.037395000
6	-2.313740000	-0.270245000	-0.054408000
1	-0.117474000	-2.886728000	-0.022184000
6	-3.826296000	-0.273090000	-0.065096000
6	-4.179640000	-1.702491000	0.408713000
6	-2.986341000	-2.576736000	-0.039080000
1	-4.181861000	-0.093011000	-1.085652000
1	-4.267843000	0.508819000	0.554915000
1	-5.134742000	-2.051366000	0.011726000
1	-4.250591000	-1.716618000	1.500462000
1	-2.819219000	-3.440322000	0.608939000
1	-3.146473000	-2.961782000	-1.054156000
1	3.026394000	2.104158000	-0.076763000
7	4.166805000	-0.329103000	-0.142695000
6	4.622248000	-1.700139000	0.016892000
1	5.702967000	-1.734533000	-0.114842000
1	4.379642000	-2.116180000	1.006273000
1	4.176990000	-2.347495000	-0.743597000
6	5.125166000	0.732107000	0.135818000
1	5.032350000	1.133314000	1.155211000
1	6.132474000	0.335053000	0.016350000

1	5.017065000	1.558909000	-0.570391000
7	-1.954638000	2.138245000	-0.009932000
8	-2.925501000	2.373941000	-0.722323000
8	-1.427074000	2.963215000	0.729637000

**CPN3**

6	1.734986000	-2.609644000	-0.316562000
6	0.394316000	-2.323686000	-0.239643000
6	-0.054855000	-0.981671000	-0.110641000
6	0.921034000	0.069353000	-0.104775000
6	2.321100000	-0.262866000	-0.105021000
6	2.700283000	-1.586417000	-0.229832000
1	-0.323898000	-3.129176000	-0.317624000
6	-1.451611000	-0.643140000	-0.077954000
6	0.482622000	1.419744000	-0.154744000
6	-0.855480000	1.714794000	-0.176524000
6	-1.830219000	0.685192000	-0.133875000
1	1.224973000	2.205870000	-0.211463000
6	-3.216377000	1.295700000	-0.161850000
6	-2.967061000	2.771175000	0.227069000
6	-1.528935000	3.068158000	-0.256360000
1	-3.930159000	0.789897000	0.490805000
1	-3.623562000	1.217567000	-1.176022000
1	-3.012256000	2.874667000	1.315862000
1	-3.707709000	3.450893000	-0.198872000
1	-1.535772000	3.420246000	-1.295981000
1	-1.024039000	3.833995000	0.337454000
6	-2.531426000	-1.681122000	0.039267000
8	-3.518603000	-1.636259000	-0.670489000
6	-2.444929000	-2.726256000	1.144179000
1	-1.521319000	-2.681980000	1.718845000
1	-3.292404000	-2.555653000	1.814865000
1	-2.571664000	-3.725147000	0.718884000
1	2.062057000	-3.637014000	-0.433351000
1	3.749207000	-1.852400000	-0.254153000
7	3.268473000	0.793197000	-0.017422000
6	4.581823000	0.544949000	-0.595740000
1	5.115418000	1.495864000	-0.672835000
1	5.206320000	-0.138367000	0.004648000
1	4.475715000	0.129703000	-1.598923000
6	3.372847000	1.422467000	1.302865000
1	3.933236000	0.792071000	2.013118000
1	3.892385000	2.380342000	1.210742000
1	2.384277000	1.605939000	1.720711000

### CPN3A

6	-1.936455000	2.585447000	-0.083230000
6	-0.569409000	2.474136000	-0.011109000
6	0.055454000	1.197185000	0.005829000
6	-0.780637000	0.034371000	-0.078466000
6	-2.212525000	0.177129000	-0.070786000
6	-2.762216000	1.444462000	-0.097576000
1	0.024614000	3.376771000	0.003943000
6	1.489903000	1.027169000	0.046446000
6	-0.175530000	-1.241054000	-0.226823000
6	1.189284000	-1.375496000	-0.223739000
6	2.029834000	-0.248625000	-0.060750000
1	-0.815966000	-2.102059000	-0.372810000
6	3.477475000	-0.688144000	-0.053936000
6	3.396393000	-2.217869000	0.163745000
6	2.015844000	-2.631024000	-0.394405000
1	4.076426000	-0.170349000	0.695199000
1	3.936305000	-0.442092000	-1.019118000
1	3.434147000	-2.434357000	1.235853000
1	4.222299000	-2.754234000	-0.307255000
1	2.087515000	-2.885745000	-1.459598000
1	1.587327000	-3.498506000	0.113380000
6	2.381755000	2.188685000	0.237767000
8	3.590858000	2.171346000	0.100394000
1	-2.393692000	3.568440000	-0.111279000
1	-3.836677000	1.573863000	-0.112812000
7	-3.010312000	-0.998967000	-0.070494000
6	-4.346155000	-0.884011000	-0.640078000
1	-4.748854000	-1.888855000	-0.791179000
1	-5.054553000	-0.335728000	0.003772000
1	-4.297429000	-0.385556000	-1.609213000
6	-3.029502000	-1.732140000	1.199863000
1	-3.663944000	-1.232721000	1.950416000
1	-3.422319000	-2.738916000	1.033305000
1	-2.024497000	-1.817910000	1.609927000
1	1.893521000	3.128641000	0.551262000

### CPN3B

6	1.767117000	-2.614659000	-0.207436000
6	0.422867000	-2.349493000	-0.122249000
6	-0.049515000	-1.010483000	-0.053922000
6	0.916998000	0.051265000	-0.091338000
6	2.322036000	-0.258981000	-0.096672000
6	2.720715000	-1.578221000	-0.178729000
1	-0.280347000	-3.167149000	-0.111817000
6	-1.450783000	-0.667439000	-0.027504000



6	0.473016000	1.396975000	-0.172893000
6	-0.864327000	1.691395000	-0.176295000
6	-1.834728000	0.661931000	-0.097164000
1	1.214287000	2.180995000	-0.263866000
6	-3.221067000	1.273225000	-0.114392000
6	-2.966857000	2.757676000	0.232941000
6	-1.537127000	3.043245000	-0.278012000
1	-3.920801000	0.783144000	0.563547000
1	-3.648829000	1.167303000	-1.117677000
1	-2.996958000	2.888230000	1.319232000
1	-3.714889000	3.425155000	-0.199296000
1	-1.558193000	3.371626000	-1.325180000
1	-1.022561000	3.821283000	0.290986000
6	-2.546257000	-1.673390000	0.057123000
8	-3.631749000	-1.554782000	-0.466425000
1	2.106268000	-3.642631000	-0.274839000
1	3.773176000	-1.830084000	-0.205801000
7	3.253213000	0.816805000	-0.053054000
6	4.555473000	0.575762000	-0.659290000
1	5.073407000	1.532304000	-0.768005000
1	5.204784000	-0.086995000	-0.062166000
1	4.429934000	0.139344000	-1.651196000
6	3.381846000	1.462851000	1.257063000
1	3.961301000	0.845658000	1.963576000
1	3.892103000	2.423236000	1.141658000
1	2.400688000	1.644683000	1.693457000
8	-2.263821000	-2.754388000	0.833188000
1	-3.057741000	-3.310331000	0.817291000

### CPN3C

6	-1.854656000	2.563695000	-0.147133000
6	-0.490944000	2.451421000	-0.034606000
6	0.112174000	1.170538000	0.015913000
6	-0.707697000	-0.001312000	-0.046306000
6	-2.137336000	0.148204000	-0.091111000
6	-2.677917000	1.418687000	-0.165914000
1	0.133941000	3.335564000	0.002821000
6	1.538202000	1.007451000	0.087005000
6	-0.088313000	-1.279259000	-0.111406000
6	1.277704000	-1.399519000	-0.056658000
6	2.100514000	-0.254697000	0.059376000
1	-0.717148000	-2.151707000	-0.238551000
6	3.555348000	-0.654240000	0.113118000
6	3.542996000	-2.098814000	-0.443624000
6	2.134737000	-2.646897000	-0.105798000
1	3.902060000	-0.637901000	1.154290000
1	4.206725000	0.020496000	-0.446166000

1	4.346824000	-2.714170000	-0.035871000
1	3.669878000	-2.067963000	-1.529669000
1	1.777489000	-3.381983000	-0.830964000
1	2.134739000	-3.138351000	0.875314000
1	-2.313335000	3.544771000	-0.199638000
1	-3.751377000	1.548536000	-0.216332000
7	-2.940856000	-1.024463000	-0.083400000
6	-4.252073000	-0.921096000	-0.710591000
1	-4.653909000	-1.928279000	-0.847456000
1	-4.982768000	-0.350290000	-0.113106000
1	-4.160775000	-0.452659000	-1.691507000
6	-3.017806000	-1.709056000	1.211744000
1	-3.677947000	-1.177720000	1.916783000
1	-3.411404000	-2.718830000	1.067043000
1	-2.030978000	-1.785695000	1.665713000
6	2.386313000	2.154754000	0.166131000
7	3.083786000	3.075467000	0.230038000

**CPN3D**

6	1.810706000	-2.596359000	-0.147452000
6	0.461244000	-2.364509000	-0.052254000
6	-0.029842000	-1.033064000	-0.016946000
6	0.902804000	0.056380000	-0.081089000
6	2.314312000	-0.222886000	-0.094691000
6	2.738587000	-1.535803000	-0.154809000
1	-0.225842000	-3.195740000	-0.003225000
6	-1.421711000	-0.698323000	-0.000751000
6	0.419028000	1.388227000	-0.175654000
6	-0.926500000	1.650054000	-0.170883000
6	-1.871630000	0.598417000	-0.081767000
1	1.138082000	2.190648000	-0.280567000
6	-3.275572000	1.159896000	-0.099668000
6	-3.062581000	2.653738000	0.240390000
6	-1.641916000	2.980239000	-0.274175000
1	-3.955914000	0.651806000	0.585906000
1	-3.699188000	1.035133000	-1.102029000
1	-3.096272000	2.788681000	1.325620000
1	-3.830496000	3.295204000	-0.195430000
1	-1.673241000	3.305853000	-1.321645000
1	-1.150964000	3.773891000	0.293598000
1	2.175196000	-3.616612000	-0.190671000
1	3.796058000	-1.764407000	-0.188157000
7	3.220165000	0.872672000	-0.082303000
6	4.521111000	0.649858000	-0.699742000
1	5.014005000	1.616135000	-0.833949000
1	5.192487000	0.015523000	-0.096823000
1	4.394422000	0.190795000	-1.681152000

6	3.348542000	1.549339000	1.213181000
1	3.953691000	0.962268000	1.923206000
1	3.831164000	2.520090000	1.070751000
1	2.369150000	1.713830000	1.660225000
7	-2.436582000	-1.762034000	0.106531000
8	-3.425126000	-1.672399000	-0.614617000
8	-2.254489000	-2.661199000	0.919942000