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SUPPLEMENTARY INFORMATION

New Isomeric ancillary ligand and their Eu^{III} complexes: A single component white light emissive phosphor and their applications in Red/White smart LEDs, Electronic Noses and Temperature sensing

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General Information for synthesis:

All the reaction (ligands and complexes) was completed in the inert conditions. The required Solvent THF is distilled-dried by using Na Metal and benzophenone (indicator). All the commercially accessible components (Sigma Aldrich and Alpha Ezar) were castoff deprived of extra refinement unless otherwise needed. The reaction progress was checked by thin-layer chromatography (TLC) with silica gel 60 F254 Aluminium plates (Merck) at a regular interval of time. Further purification of crud, the reaction mass was carried out by the column chromatography using silica gel (Sigma-Aldrich).

Measurements:

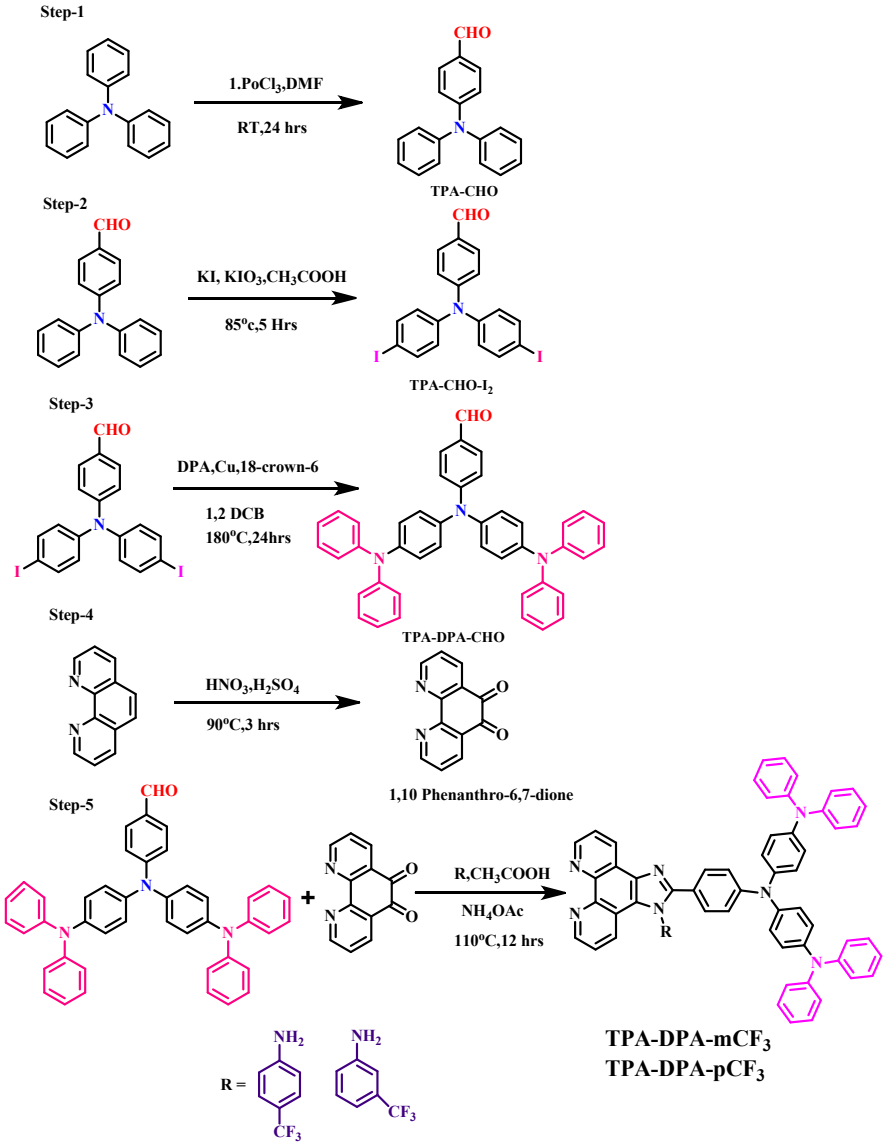
For the structural conformation ^{1}H and ^{13}C-NMR spectra were recorded by the help of the AV 400 Advance-III 400MHz Fourier transform nuclear magnetic resonance (FT-NMR) Spectrometer Bruker Biospin International, Switzerland. All the ^{1}H and ^{13}C-NMR spectra were recorded in deuterated chloroform/dimethyl sulfoxide solution and tetramethylsilane (TMS) was used as a standard reference for chemical shift measurement. The Fourier transform infrared spectroscopy (FTIR) was executed by PerkinElmer Spectrum Version 10.4.00, in the spectrum range of 400 – 4000 cm^{-1} making KBr pellets. Mass spectra of all the synthesized fluorophores were recorded on High Resolution Mass Spectrometer (HRMS) Waters, USA, XEVO G2-XS QTOF model .The PL emission and excitation spectra in the solution and solid were recorded by using the Edinburg spectrofluorometric FS–5 instruments associated with SC–10 modules and SC–5 modules respectively. The photoluminescence (excitation and emission) spectra, lifetime and quantum yield were monitored by using Edinburg Spectrofluorometer FS–5 instruments with attaching SC – 10 modules and SC – 30 integrating sphere module. The CIE color coordinate for all emission spectra is calculated by MATLAB software. The absorption spectra of all the synthesized compounds in solution form were utilizing UV-Visible spectrometer (Shimadzu Corporation, Japan or UV-2450

Perkin Elmer, USA/Lamda 25 and Lamda Perkin Elmer). The electrochemical properties of the ligands and their respective complex were estimated by utilizing cyclic voltammetry (CV), AUTOLAB 302N Modular potentiostat at RT in Dimethylformamide (DMF). The CV analysis is the set-up of mainly three electrode, the working (glass-carbon rod), auxiliary (counter, Pt wire) and reference (Ag/Agcl wire) electrodes. DMF containing 0.1 M Bu_4NClO_4 was used as an electrolyte and the sweep rate was kept as 100 mV s^{-1}. The ligand sub-atomic structures were optimized within density functional theory (DFT) frame work utilizing B3LYP/6-31G (d, p) level of theory. A UV-visible spectrum of the molecule is obtained by exciting molecule vertically after conformation of ground state geometry of the ligand. Further, to the depiction of PL emission and excitation mechanism of the Eu(III) complex, triplet energized condition of the ligand is additionally accessed by utilizing the same procedure specified previously. The Lifetime of the Eu(III) complex, as well as the ligand, were measured at 298 K with Edinburgh Instruments FLS 980 based on the time-correlated single photon counting technology upon the excitation at 380 nm. A pulsed xenon lamp was used as the excitation source, and the signals were detected with a photomultiplier. All the measurements were carried out at room temperature (RT). The optimization study of ligand is effectively accomplished by the G09W program.

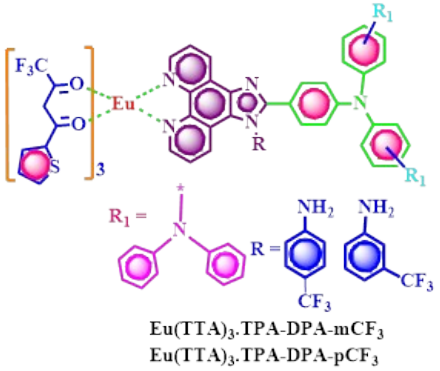
Materials:

The synthesis of Eu(III) chloride($EuCl_3.6H_2O$) from europium(III) oxide is done by the well-known process.[1]The resultant product ($EuCl_3.6H_2O$) was then treated with an alcoholic solution of DBM (3 eq.) in the presence of 1 N sodium hydroxide solution (3.1 eq.) to get $Eu(DBM)_3(H_2O)_2$. 1,10-Phenanthroline-5,6-dione was synthesized from 1,10-phenanthroline by a previously reported procedure.[2-3] All the ligands were successfully synthesized by a well-reported procedure .

General synthesis of ligands:



Scheme S1 Synthetic route of Triphenyl functional-DPA based ligand.



Scheme S2 Structure of complexes.

Synthesis of TPA-DPA-mCF_3:

TPA-DPA-CHO (0.725, 1.550 mmol) was added to a stirred solution of 1, 10 phenanthroline-6, 7 dione (0.325, 1.19mmol) in glacial acetic acid (30mL) at room temperature. To this reaction mixture,subsequently ammonium acetate (2.2g, 28.83mmol) and mCF_3-amine (0.19g, 1.54 mmol) was added. Then resulting mixture was stirred for 12 hrs at 110°C. The progress of the reaction was monitored by TLC (MeOH in Chloroform 1:9, Rf-0.3). The RM was pour into minimum amount of water and then ammonium hydroxide solution was added. Then the formed solid was filtered and dissolved in dichloromethane, followed by dried with anhydrous sodium sulphate and the solvent was evaporated to get 3g crude compound. The resultant compound was purified with column chromatography by using silica gel (100-200 mesh), eluent with 5% methanol in chloroform and the solvent was evaporated and dissolved in minimum amount of THF solution added excess of hexane solvent, the pale yellow color solid was formed. After settled of solid, decant and repeated this process three more times and get compound 1g (63.1%) as a pale yellow solid.[1 2]

^{1}H-NMR Data ($CDCl_3$, 400MHz):δ 9.24 (s, 1H), 9.18 (d, J = 7.7 Hz, 2H), 9.10 (s, 1H), 7.97 (d, J = 8.1 Hz, 1H), 7.81 (dd, J = 7.9, 4.5 Hz, 2H), 7.75 (d, J = 8.1 Hz, 2H), 7.58 (d, J = 8.6 Hz, 1H), 7.38 (m, J = 6.3 Hz, 3H), 7.28 (m, 6H), 7.13 (m, J = 7.7 Hz, 5H), 7.04 (m, J = 15.7, 8.2 Hz, 6H), 6.89 (d, J = 8.8 Hz, 1H).

^{13}C-NMR Data ($CDCl_3$, 100MHz): δ 148.80, 147.98, 147.70, 138.78, 132.36, 131.29, 130.11, 129.27, 127.59, 127.08, 126.40, 126.23, 124.89, 124.25, 124.09, 123.74, 122.77, 122.77, 122.46, 119.57, 77.35, 77.24, 77.04, 76.72, 67.10 EI-MS: m/z = 942.35 $[M + H]^+$.

Synthesis of TPA-DPA-pCF_3:

Same procedure is followed as above for synthesis of ligand **TPA-DPA-pCF_3**; 1,10-phenanthroline-5,6-dione (phen-dione) (1.0 g, 4.762 mmol), 3-aminobenzonitrile (0.618 g, 5.238 mmol) and 4-(trifluoromethyl)benzaldehyde (0.910 g, 5.238 mmol).

^{1}H-NMR Data (400 MHz, $CDCl_3$): δ 9.33 (s, 1H), 9.26 (s, 2H), 9.14 (s, 1H), 8.99 (d, J = 7.9 Hz, 1H), 7.98 (d, J = 8.0 Hz, 1H), 7.76 (d, J = 7.4 Hz, 2H), 7.58 (d, J = 8.3 Hz, H), 7.40 (d, J = 9.0 Hz, 3H), 7.28 (s, 2H), 7.02 (d, J = 9.6 Hz, 7H).

^{13}C-NMR (100 MHz, $CDCl_3$, TMS, δ ppm):149.65, 148.62, 138.78, 134.78, 134.22, 133.35, 132.08, 131.85, 130.67, 129.67, 127.44, 125.72, 123.88, 123.73, 122.42, 77.01, 76.70, Calculated m/z ratio = 465.43 found m/z = 942.35 $[M + H]^+$.

Synthesis of $Eu(TTA)_3$TPA-DPA-mCF_3; The solution of $Eu(TTT)_3(H_2O)_2$ (0.100 g, 0.106mol) in dry THF (15 mL) was taken in round bottom flask and stirrer constantly unless a clear solution obtain, after 20 minutes a mixture of ligand1(0.09 mg, 0.1062 m in dry THF was added slowly drop by drop. The reaction mixture was then stirred for 6 hours at 60^{o}C in inert condition. The completion of the reaction is monitored by TLC then the mixture was concentrated by Rota evaporator and then dissolved in the least amount of THF.[3]To this solution, excess hexane was added by the wall of the round bottom flask; the precipitate was obtained. The upper solvent layer was then decanted slowly, and the residue was dried. The same procedure was repeated several times to achieve the final complex in pure powder form.found: **m/z** = 1918.001$[M + 2Na^+ + K^+]^+$.

Synthesis of $Eu(TTA)_3$TPA-DPA-pCF_3; The complex was synthesized by previously described procedure using **$_3$TPA-DPA-pCF_3** as the ligand instead of ligand1. **ESI-MS: m/z** = 1918.001 $[M + 2Na^+ + K^+]^+$.

1. **NMR Spectroscopy:**

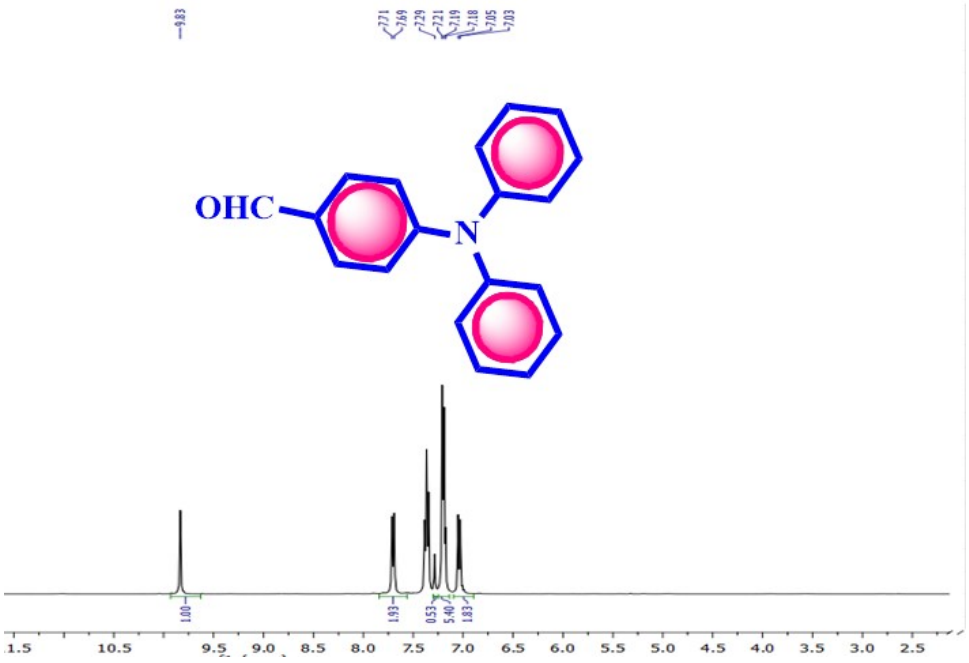


Fig S1. ^{1}H NMR spectroscopy of TPA-CHO

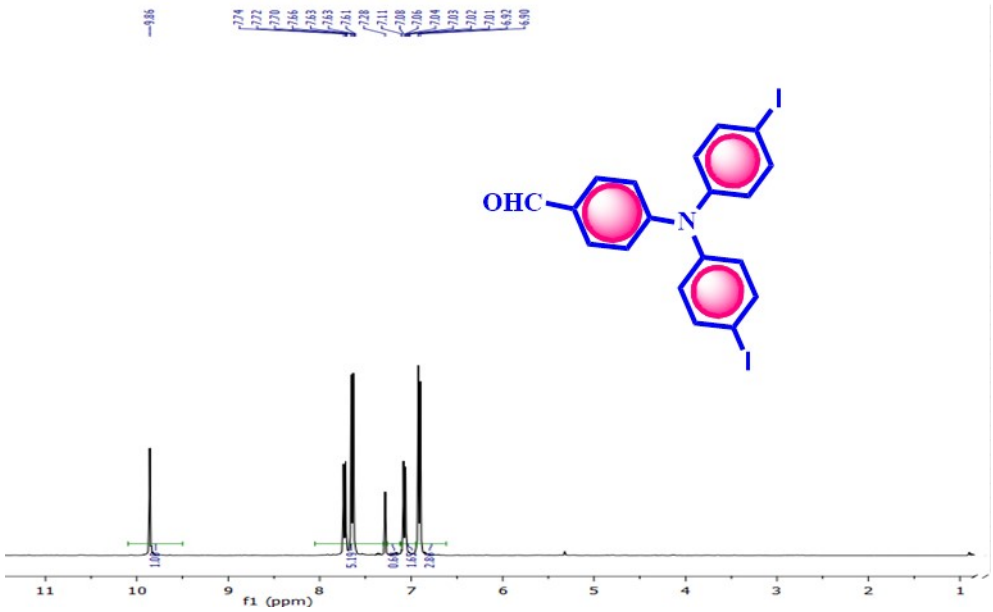


Fig S2. ^{1}H NMR spectroscopy of TPA-CHO-I2 in $CDCl_3$.

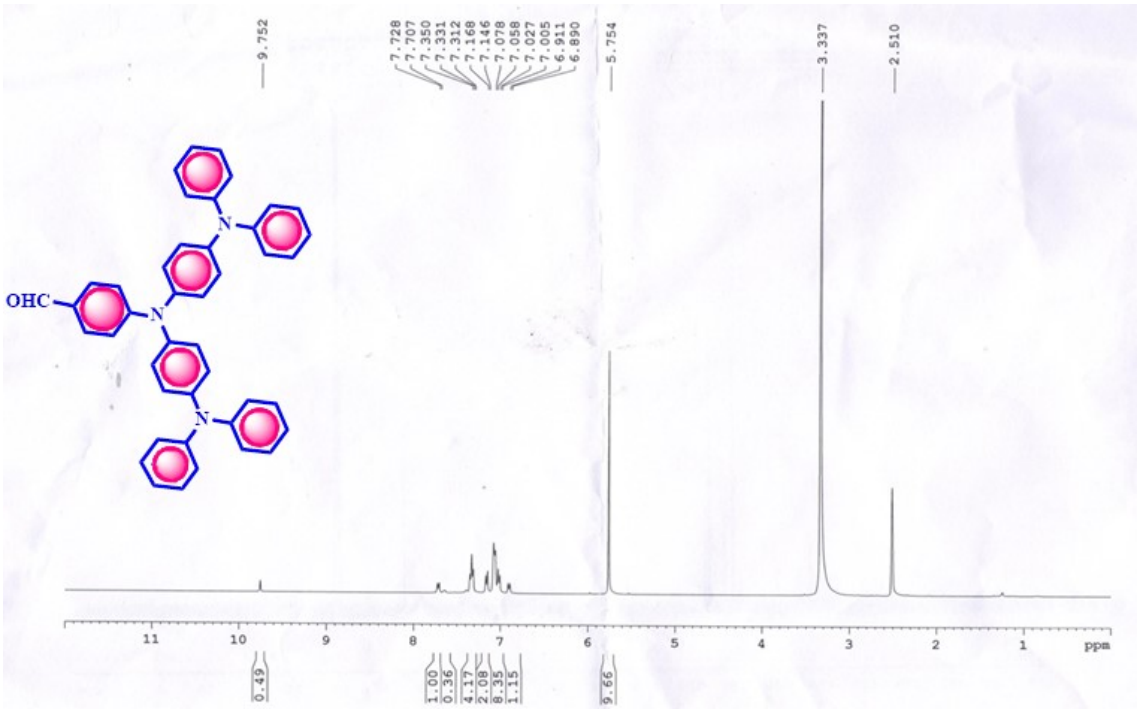


Fig S3. ^{1}H NMR spectroscopy of TPA-DPA-CHO in $CDCl_3$.

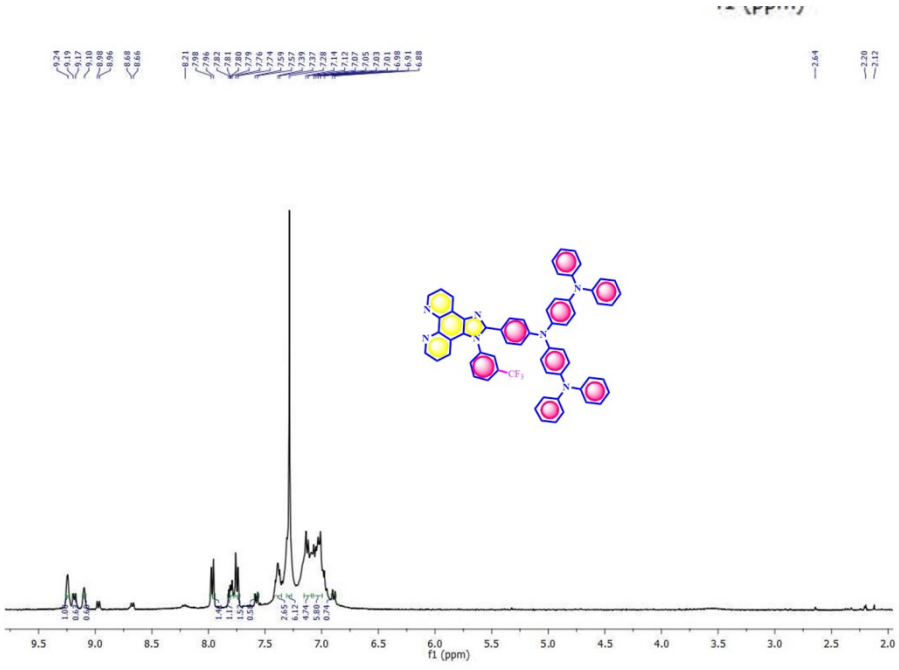


Fig S4. ^{1}H NMR spectroscopy of **TPA-DPA-mCF_3** in $CDCl_3$

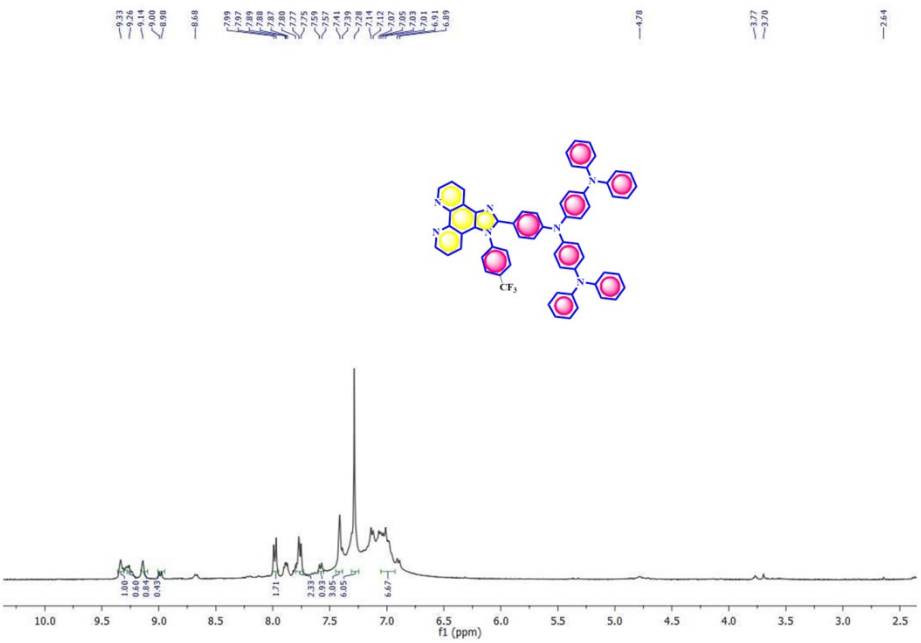


Fig S5. ^{1}H NMR spectroscopy of **TPA-DPA-PCF$_3$** in $CDCl_3$

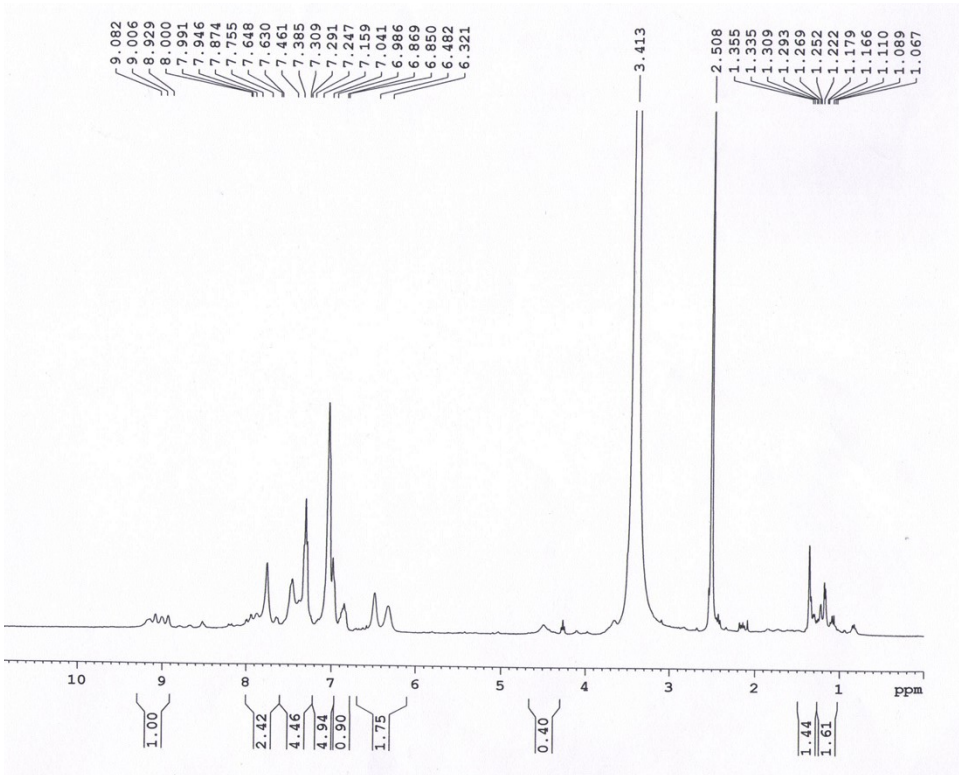


Fig S6. ^{1}H NMR spectroscopy of **Eu(TTA)$_3$TPA-DPA-pCF$_3$** in DMSO-d_6

Fig S7. ^{1}H NMR spectroscopy of **Eu (TTA)$_3$TPA-DPA-mCF$_3$** in DMSO-d$_6$

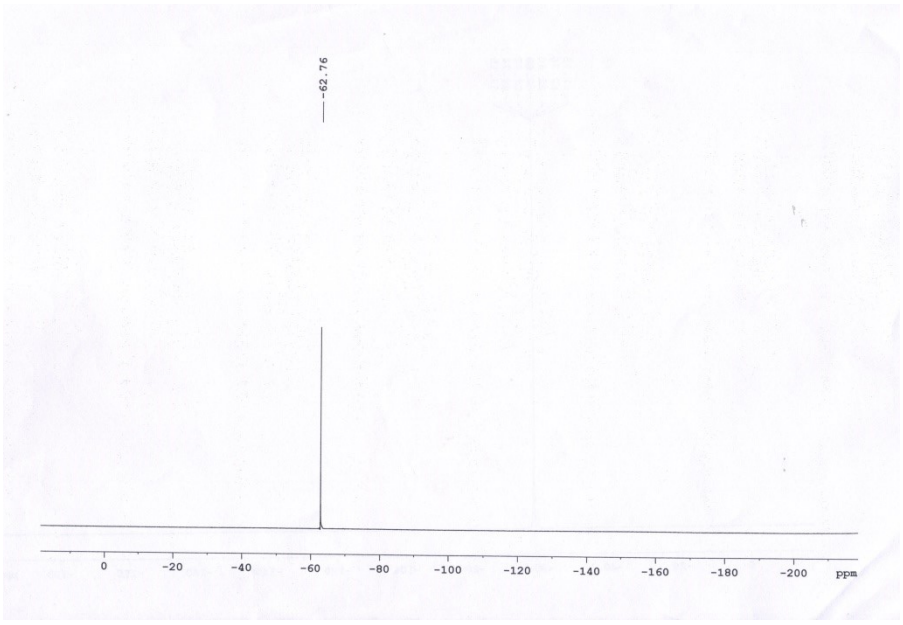


Fig S8. ^{19}F NMR spectroscopy of **TPA-DPA-mCF$_3$** in DMSO-d_6

2. Mass spectral analysis:

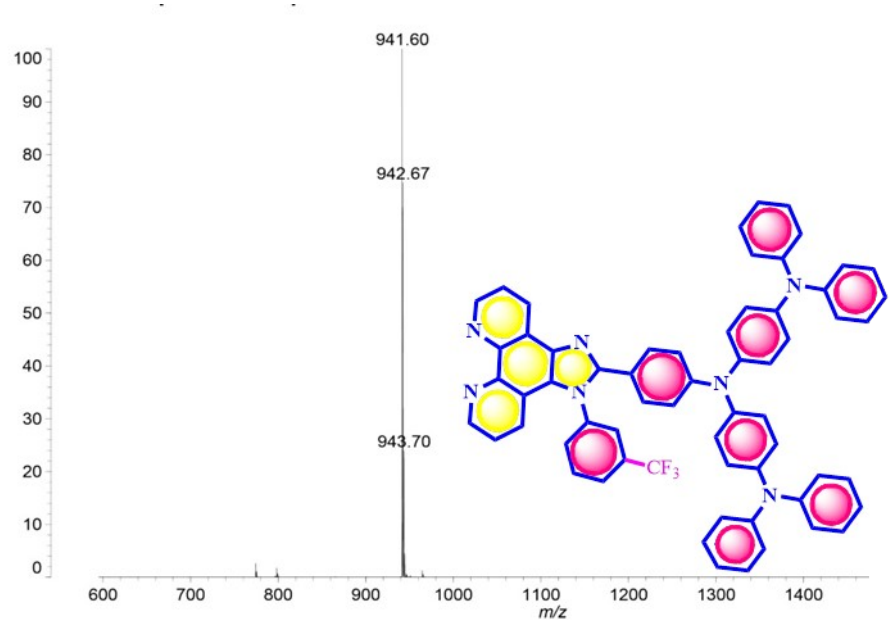


Figure S9. Mass spectral data of **TPA-DPA-mCF$_3$**

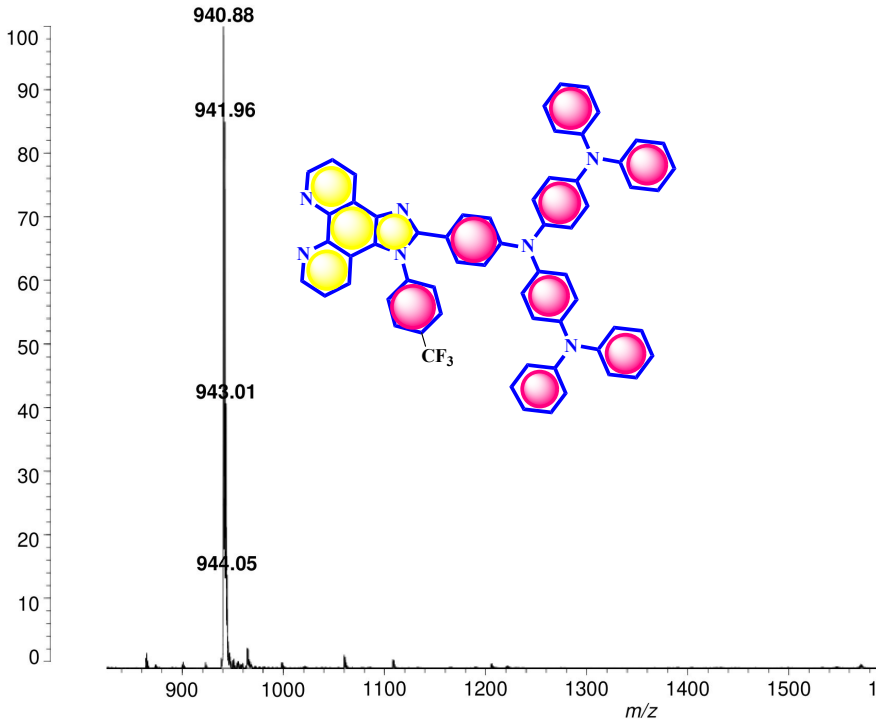


Figure S10. Mass spectral data of **TPA-DPA-pCF$_3$**

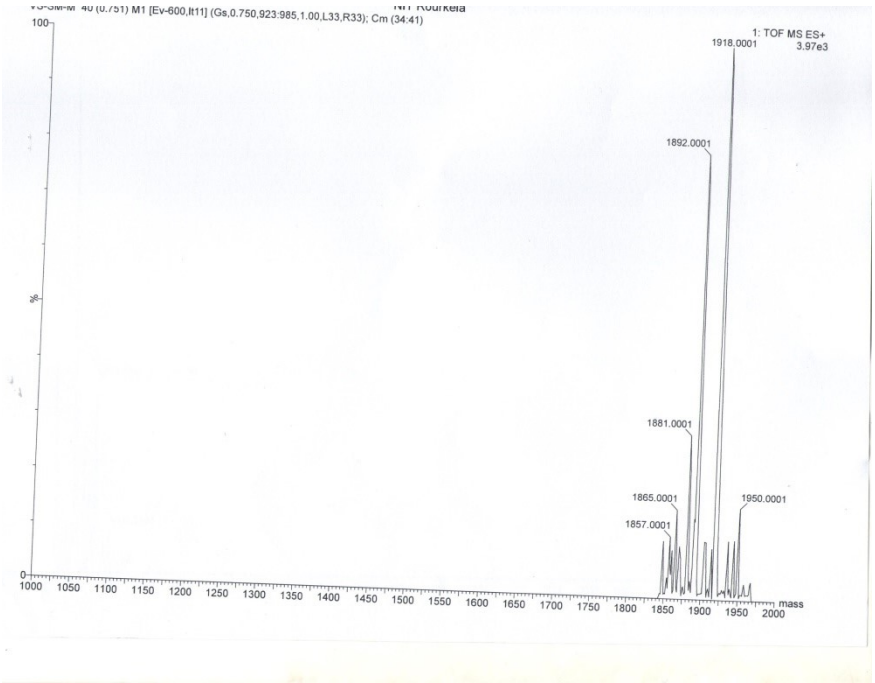


Fig S11. Mass spectral data of **Eu(TTA)$_3$TPA-DPA-mCF$_3$**

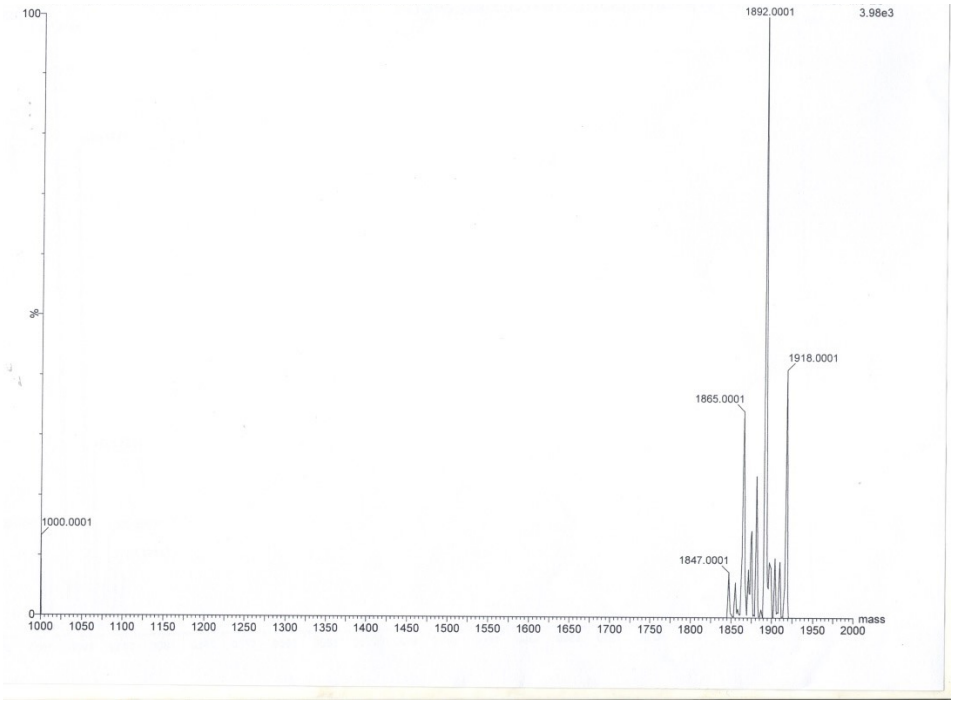


Fig S12. Mass spectral data of **Eu(TTA)$_3$TPA-DPA-pCF$_3$**

PL spectra:

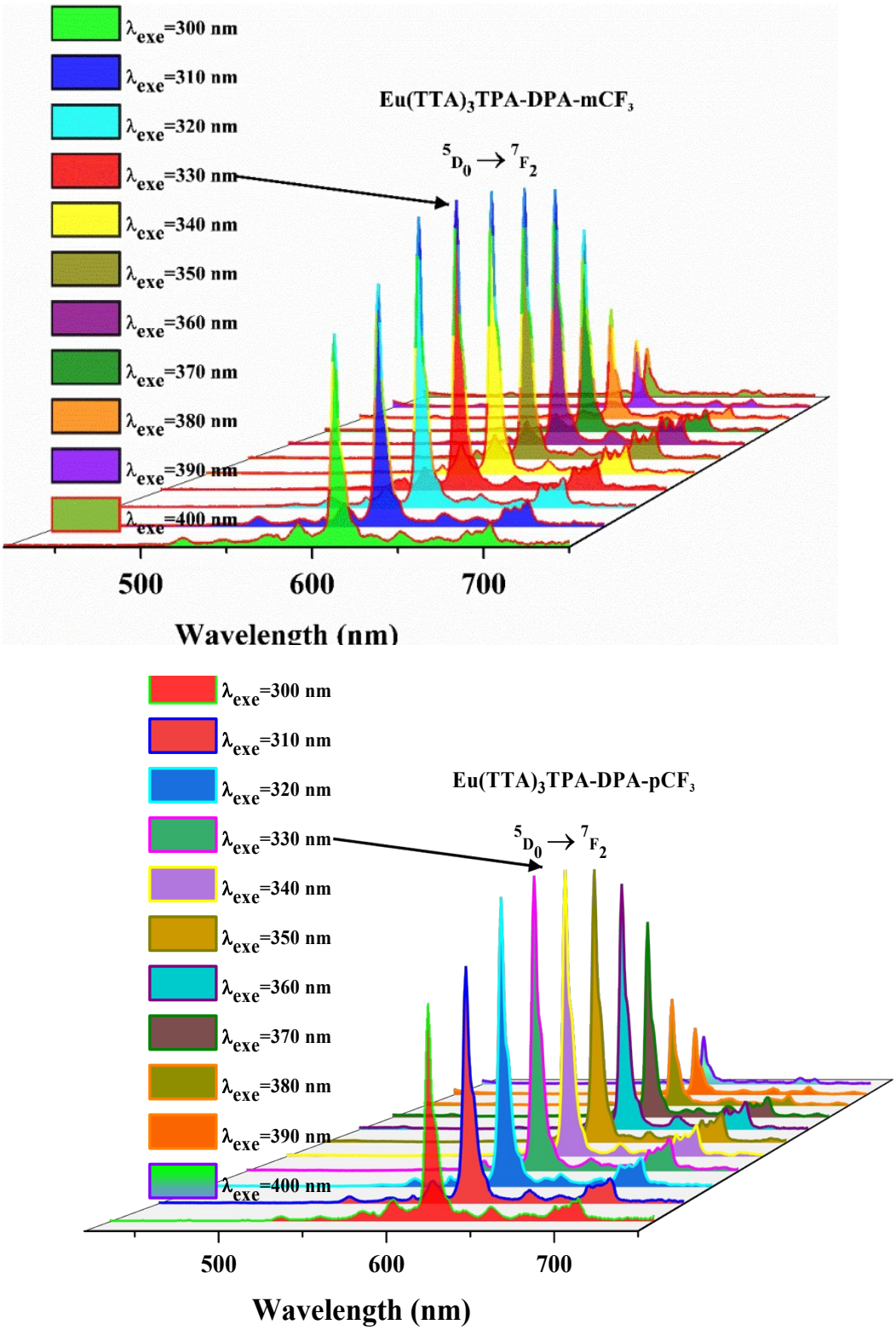


Fig S13. Different excitation spectral wavelength analysis of the **Eu (TTA)$_3$TPA-DPA-mCF$_3$** and **Eu(TTA)$_3$TPA-DPA-mCF$_3$** complex in solid state.

Table ST1. The Infrared frequencies (wavenumber in cm^{-1}) for free ligand and its corresponding Eu(III)-complexes.

Complex	ν (O-H)	ν (C=O)	ν (C=N)	ν (C=C)	ν (C-F)	ν (Eu-N)	ν (Eu-O)
Eu $(TTA)_3$TPA-DPA-mCF_3	3420	1659	1538	1422	1153	578	448
Eu $(TTA)_3$TPA-DPA-pCF_3	3411	1649	1510	1404	1130	583	449
TPA-DPA-mCF_3		-	1477	1330	1120	-	-
TPA-DPA-pCF_3		-	1793	1329	1122	-	-

Table ST2. The calculated CIE from the PL emission data of Eu(III) complexes in different solvents .

Eu$(TTA)_3$-TPA-DPA-pCF_3		**Solvents**	**Eu$(TTA)_3$-TPA-DPA-mCF_3**	
x	**y**		**x**	**y**
0.4601	0.3154	Hexane	0.5711	0.3154
0.5625	0.3726	Toluene	0.4311	0.3482
0.6763	0.3140	$CHCl_3$	0.3763	0.3940
0.5898	0.3879	THF	0.4257	0.4562
0.6348	0.3220	DCM	0.5030	0.3061
0.6666	0.3264	DMSO	0.4634	0.3266
0.6569	0.3294	DMF	0.5410	0.3260
0.5579	0.3268	ACN	0.3563	0.3261
0.5890	0.2794	MeOH	0.3775	0.3133

Table ST3. Intensity ratios as well as CIE Color Coordinates for the Eu (III) Complexes in different concentration ratio doped PMMA

%	$Eu(TTA)_3$-TPA-DPA-mCF_3			Color Purity	$Eu(TTA)_3$-TPA-DPA-pCF_3			Color Purity
	I_2/I_1	CIE			I_2/I_1	CIE		
		x	y			x	y	
1 :99	15.81	0.6473	0.3269	90.71	21.03	0.6490	0.3291	91.16
2:98	15.83	0.6661	0.3302	95.83	21.23	0.6480	0.3290	90.92
3:97	15.69	0.6656	0.3312	95.57	21.02	0.6430	0.3211	89.95
4:96	15.84	0.6671	0.3303	96.07	21.66	0.6430	0.3280	89.57

Table ST4. Electrochemical properties of the ligands and respective Eu(III)-complexes.

Sl. No.	Compound name	$Volatage_{oxi}^{onset}$[V] (E_{HOMO} [eV])	$Volatage_{red}^{onset}$ [V] (E_{HOMO} [eV])	λ_{onset}^{d} [nm]	Energy gap [eV]
1	**TPA-DPA-mCF_3**	1.30 (-5.875)	-1.44(-2.96)	426	2.91
2	**TPA-DPA-pCF_3**	1.35 (-5.75)	-1.53(-2.87)	386	3.21
3	**$Eu(TTA)_3$-TPA-DPA-pCF_3**	1.83(-6.23)	-1.14(-3.26)	417	2.97
4	**$Eu(TTA)_3$-TPA-DPA-mCF_3**	1.19(-5.59)	-1.31(-3.09)	495	2.5

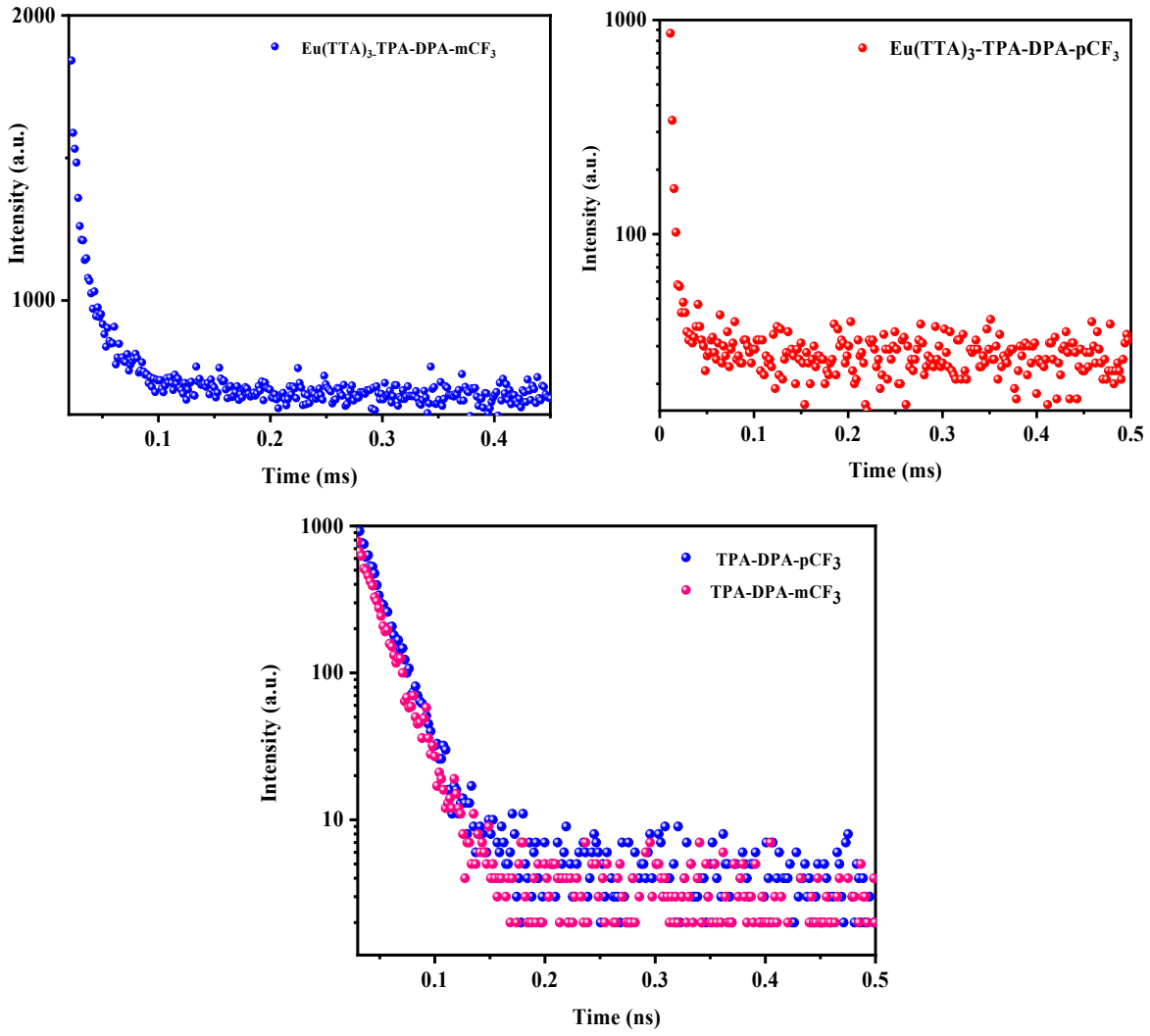


Fig S14. The photoluminescence lifetime decay curves for ligands and complexes in solution ($CHCl_3$)

Table ST5. Experimental Lifetime data of ligands and complexes in solid and solution($CHCl_3$).

Complex/ Ligands Name	Solid(ns/ms)	Solution(ns/ms)
TPA-DPA-mCF_3	6.88 ns	5.22 ms
TPA-DPA-pCF_3	6.90 ns	1.32 ms
$Eu(TTA)_3$-TPA-DPA- pCF_3	0.938ms	0.522 ms
$Eu(TTA)_3$-TPA-DPA- mCF_3	0.909ms	0. 411 ms

PLQY:

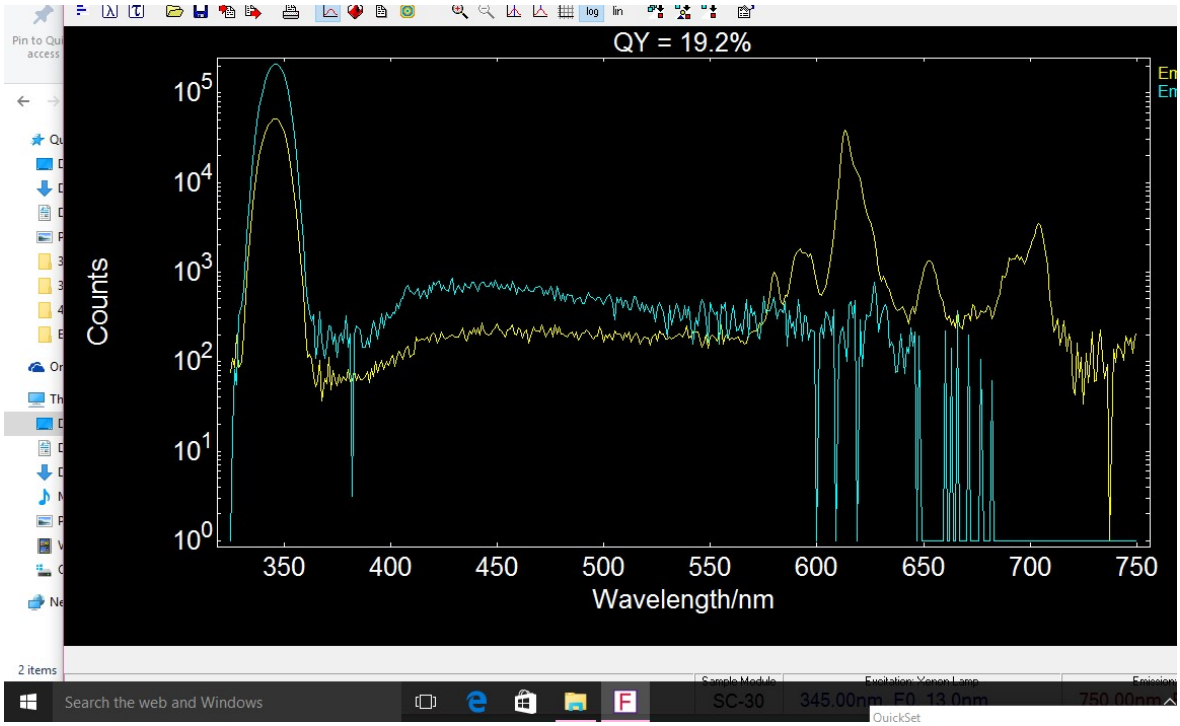


Fig S15. The photoluminescence quantum yield of $Eu(TTA)_3$-TPA-DPA- mCF_3 in solid.

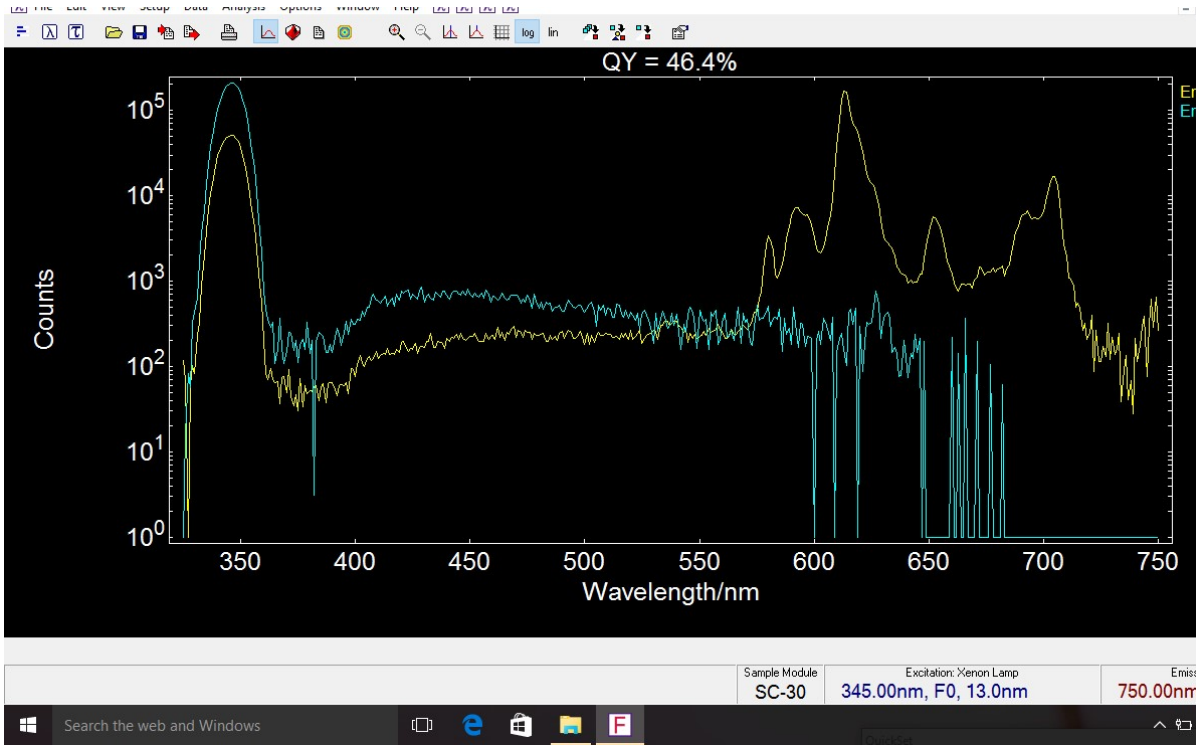


Fig S16. The photoluminescence quantum yield of $Eu(TTA)_3$-TPA-DPA- pCF_3 in solid.

To understand further, the overall quantum yield ($\Phi_{overall}$) (Eqn. 1) was calculated and other lifetime parameters also been calculated for Eu^{III} complexes. The $\Phi_{overall}$ obtained under ligand excitation and it depends on two essential parameters. The primary one, the efficiency of energy transfer from the ligand to the Eu^{III} ion (Φ_{sens}), and another one is the intrinsic quantum yield (Φ upon direct excitation into the f level).[4-6,]

$$\Phi_{QY} = \Phi_{sens}\Phi_{Ln} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (1)$$

The intrinsic quantum yield (Φ_{Ln}) of the Eu^{3+} ion can calculate with τ_{obs} and τ_{rad} life time, the equation (2) followed as

$$\Phi_{Ln} = \left(\frac{A_{RAD}}{A_{RAD} + A_{NR}}\right) = \frac{\tau_{obs}}{\tau_{RAD}} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (2)$$

The radiative lifetime (τ_{RAD}) can be calculated by corrected emission spectrum according to using equation 2. It is assuming that the energy of the $^5D_0 \rightarrow {}^7F_1$ transition (MD) and its oscillator strength are constant. Here, I_{TOT}/I_{MD} is the ratio of the total area of the corrected Eu^{3+} emission spectrum to the area of the $^5D_0$ - $^7F_1$ band, $A_{MD,0}$ (14.65 s^{-1}) represents the spontaneous emission probability of the $^5D_0 \rightarrow {}^7F_1$ transition (in vacuo), and n is the refractive index of the medium. An average index of refraction (1.5) was employed in the calculation.[1,2,3]

$$A_{RAD} = \left(\frac{1}{\tau_{RAD}}\right) = A_{MD,0} n^3 \left(\frac{I_{TOT}}{I_{MD}}\right) \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (3)$$

From the relative areas of the $^5D_0$–^7F_J emission transitions (which associates with the already predicted J–O theory) of Eu^{3+} ion is used to determine the experimental branching ratio ($\beta_{1\text{-}3}$). In general, the efficiency of the energy transfer from the ligand to Eu^{III} ion can be predicated by the obtained intrinsic quantum yield (Φ_{Ln}) and energy transfer efficiency (Φsen).

Table ST6: Lifetimes (τ_{obs}), overall quantum yields (QYs) and the calculated photoluminescence parameters: radiative lifetimes (τ_{rad}), intrinsic quantum yield (ϕLn) and sensitization efficiency (Φ_{sens} sens) of compound.

Sample Name	$\tau_{obs}{}_{ms}$	QY(%)	$\tau_{Rad}\ ms$	Φ_{Ln} (%)	Φ_{sens}
$Eu(TTA)_3$-TPA-DPA- pCF_3	0.938 ms	46.4	1.020	91.9	50.8
$Eu(TTA)_3$-TPA-DPA- mCF_3	0.909 ms	19.2	1.419	64.0	30.0

77K spectra of all the ligands

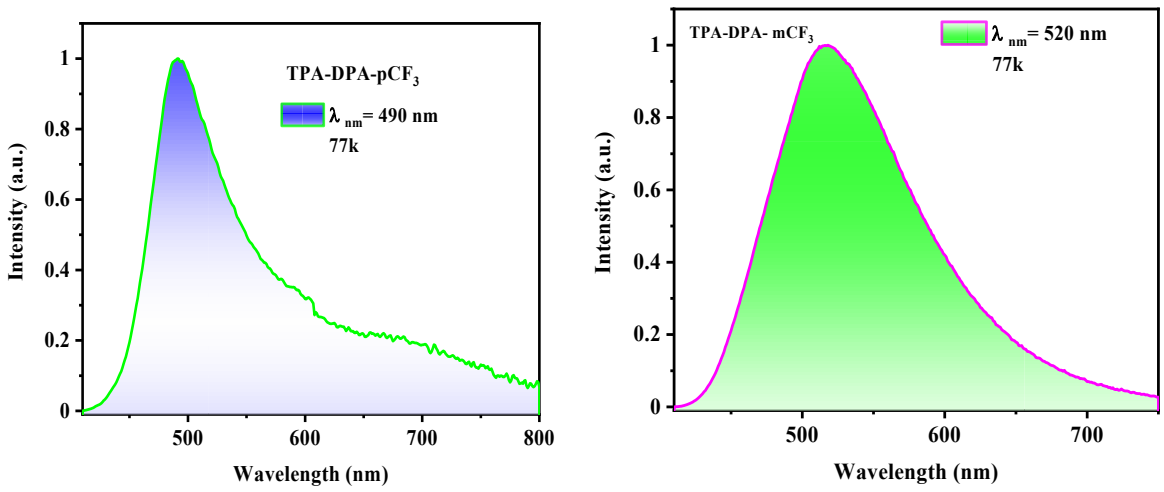


Fig S17. Phosphorescence spectra of TPA-DPA-pCF_3 and TPA-DPA-mCF_3 at 77K**.**

DFT Analysis:

Table ST7. The computed vertical transitions and there oscillator strengths (*f*) and configuration of the ligands.

Luminophores	State	Energy (eV)	λ_{max} nm	*f*	Configuration
TPA-DPA-mCF$_3$ Singlet	Gas	2.636	470.2	0.053	HOMO→LUMO (69.63%)
		2.858	433.7	0.366	HOMO→LUMO+ (68.95%)
		3.011	411.8	0.232	HOMO→LUMO+2 (63.87%) HOMO→LUMO+3 (26.78%)
Triplet	Gas	2.412	513.9	0	HOMO→LUMO (30.74%) HOMO-2→LUMO+1(22.88%) HOMO-2→LUMO (12.55%) HOMO→LUMO+1(42.06%)
		2.645	468.7	0	HOMO→LUMO (60.99%) HOMO→LUMO+3 (11.12%)
		2.806	441.7	0	HOMO-2→LUMO+1 (11.23%) HOMO-1→LUMO+9 (14.03%) HOMO→LUMO+4 (12.07%) HOMO→LUMO+6 (52.834%) HOMO→LUMO+9 (11.89%)
TPA-DPA-pCF$_3$ Singlet	Gas	2.719	455.9	0.082	HOMO-2→LUMO (10.59%) HOMO→LUMO (69.59%)
		3.009	412.0	0.372	HOMO→LUMO+2 (66.26%)
		3.017	410.8	0.244	HOMO-2→LUMO+1 (10.02%) HOMO→LUMO+1 (64.91%) HOMO→LUMO+2 (19.36%) HOMO→LUMO+3 (13.87%)
Triplet	Gas	2.474	501.1	0	HOMO-2→LUMO (17.61%) HOMO-2→LUMO+2 (21.39%) HOMO→LUMO (38.68%) HOMO→LUMO+1 (13.79%) HOMO→LUMO+2 (38.59%) HOMO→LUMO+3 (10.57%) HOMO→LUMO+4 (17.34%)
		2.753	450.2	0	HOMO→LUMO (51.82%) HOMO→LUMO+5 (11.98%)
		2.786	445.1	0	HOMO→LUMO (13.91%) HOMO→LUMO+2 (49.53%)

Table ST8. xyz coordinates of ligands

TPA-DPA-mCF$_3$:

6 -9.373033 -0.130327 0.503784

6	-7.998473	-0.233321	0.488381
6	-7.392653	-1.482551	0.237634
6	-8.264519	-2.590751	-0.021970
6	-10.134435	-1.283089	0.265714
6	-5.981663	-1.743431	0.190340
6	-7.719639	-3.915834	-0.350139
6	-6.316698	-4.102764	-0.428402
6	-5.465046	-2.984239	-0.153186
6	-5.824371	-5.376309	-0.762899
1	-4.753434	-5.527406	-0.823238
6	-6.723108	-6.393449	-0.998855
6	-8.096757	-6.110934	-0.892094
1	-9.858766	0.820083	0.691325
1	-7.393964	0.644907	0.660744
1	-11.220668	-1.236776	0.279779
1	-6.390759	-7.391655	-1.258927
1	-8.827737	-6.896355	-1.069785
6	-3.738938	-1.740862	0.158644
7	-4.099152	-2.964863	-0.172832
7	-4.859218	-0.935853	0.397829
6	-2.333006	-1.320435	0.210824
6	-1.839197	-0.227139	0.939529
6	-1.401626	-2.092781	-0.508629
6	-0.491814	0.101301	0.917327
1	-2.494640	0.368951	1.557012
6	-0.056181	-1.770318	-0.532703
1	-1.764172	-2.946623	-1.065809
6	0.425122	-0.651303	0.168907
1	-0.139096	0.949196	1.490766
7	-9.603715	-2.464820	0.006633
7	-8.585783	-4.923225	-0.581264
1	0.630059	-2.372382	-1.115017

6	2.096750	1.123329	0.053316
6	2.942649	1.716524	0.994970
6	1.550349	1.924339	-0.954794
6	3.215824	3.077792	0.945219
1	3.370738	1.108763	1.783620
6	1.828686	3.282409	-1.014005
1	0.907532	1.473091	-1.701608
6	2.657583	3.886792	-0.056610
1	3.855066	3.523875	1.696782
1	1.403472	3.882473	-1.808342
6	2.826318	-1.227107	0.076601
6	3.961627	-1.014923	-0.717753
6	2.763696	-2.399091	0.844603
6	5.000414	-1.935624	-0.735124
1	4.035165	-0.113298	-1.313192
6	3.786688	-3.335761	0.797544
1	1.899671	-2.582307	1.471576
6	4.927548	-3.117561	0.013285
1	5.872988	-1.746999	-1.348763
1	3.712154	-4.239730	1.389813
6	-4.867566	0.432574	0.814393
6	-5.160797	0.747637	2.140670
6	-4.573256	1.441097	-0.102375
6	-5.162390	2.078198	2.552609
1	-5.384997	-0.050041	2.838529
6	-4.562777	2.766593	0.322424
1	-4.346286	1.187368	-1.128842
6	-4.859640	3.090041	1.648131
1	-5.393794	2.323717	3.582011
1	-4.854514	4.125226	1.966760
6	-4.213707	3.879018	-0.631095
9	-5.175949	4.827046	-0.662886

9	-4.033757	3.443877	-1.891056
9	-3.071021	4.504904	-0.255414
7	1.781234	-0.269004	0.116663
7	5.982938	-4.069249	-0.022501
7	2.919386	5.278121	-0.097978
6	6.571559	-4.420531	-1.266814
6	7.961360	-4.563270	-1.385244
6	5.771583	-4.622941	-2.400180
6	8.530681	-4.910840	-2.605830
1	8.588767	-4.401070	-0.517375
6	6.351429	-4.953513	-3.620543
1	4.696659	-4.518888	-2.317194
6	7.732519	-5.104482	-3.732076
1	9.607550	-5.016543	-2.678522
1	5.716464	-5.107205	-4.486142
1	8.180392	-5.368513	-4.682893
6	6.447621	-4.659168	1.182481
6	6.773321	-6.022391	1.230622
6	6.584628	-3.890040	2.346848
6	7.233870	-6.593956	2.411954
1	6.664436	-6.627170	0.338813
6	7.029916	-4.474682	3.527903
1	6.340708	-2.835202	2.318742
6	7.361818	-5.827607	3.569225
1	7.480585	-7.649848	2.429767
1	7.130308	-3.863337	4.418032
1	7.714302	-6.278298	4.489549
6	1.904692	6.191288	-0.499852
6	2.217633	7.280617	-1.324726
6	0.577391	6.018435	-0.082640
6	1.225576	8.174450	-1.714919
1	3.238758	7.421807	-1.656814

6	-0.412155	6.903763	-0.496948
1	0.321836	5.182347	0.556286
6	-0.095179	7.990084	-1.310653
1	1.486737	9.011052	-2.353601
1	-1.434986	6.741031	-0.177318
1	-0.867306	8.681333	-1.627369
6	4.207558	5.770874	0.256241
6	4.335013	6.878367	1.104594
6	5.365500	5.158547	-0.240740
6	5.594856	7.362863	1.441495
1	3.443541	7.355424	1.493277
6	6.621781	5.639008	0.114560
1	5.273883	4.306564	-0.903431
6	6.745146	6.745069	0.953674
1	5.676454	8.221094	2.099264
1	7.508060	5.153748	-0.278997
1	7.725058	7.121284	1.223200

TPA-DPA-pCF_3:

6	9.413442	0.587875	0.134717
6	8.049481	0.393220	0.091574
6	7.530136	-0.917444	0.039601
6	8.475070	-1.995440	0.063796
6	10.251392	-0.535893	0.127254
6	6.140112	-1.274386	-0.008032
6	8.021425	-3.393321	0.067141
6	6.634186	-3.685244	0.064717
6	5.708623	-2.592474	0.033437
6	6.229108	-5.031213	0.085350
1	5.170726	-5.261961	0.081861
6	7.194541	-6.013833	0.104479
6	8.546039	-5.624573	0.101206
1	9.832725	1.586251	0.176898

1	7.386769	1.245755	0.105523
1	11.331788	-0.415930	0.152166
1	6.930326	-7.064806	0.119390
1	9.328444	-6.379883	0.112937
6	3.904130	-1.428757	-0.024585
7	4.343331	-2.669765	0.028311
7	4.964884	-0.517739	-0.054074
6	2.476090	-1.090076	-0.025885
6	1.921027	0.033420	-0.656470
6	1.592155	-1.984942	0.602216
6	0.552484	0.260870	-0.649008
1	2.549588	0.728435	-1.195750
6	0.227447	-1.757838	0.624071
1	2.002297	-2.863346	1.083680
6	-0.324088	-0.624951	-0.001704
1	0.153545	1.126518	-1.161913
7	9.802441	-1.777969	0.099265
7	8.953667	-4.367619	0.083981
1	-0.423719	-2.456612	1.133498
6	-2.220550	0.943336	0.006011
6	-3.234454	1.312311	-0.885872
6	-1.735198	1.906884	0.898954
6	-3.757657	2.598193	-0.875898
1	-3.626854	0.577372	-1.578465
6	-2.232928	3.202579	0.886497
1	-0.950663	1.639529	1.596828
6	-3.259921	3.569302	0.004499
1	-4.550307	2.860645	-1.565765
1	-1.836932	3.936750	1.577318
6	-2.636967	-1.472000	0.017882
6	-3.723096	-1.476873	0.900779
6	-2.497594	-2.542041	-0.874263

6	-4.640734	-2.518727	0.893978
1	-3.841419	-0.660618	1.603288
6	-3.414706	-3.584511	-0.882410
1	-1.671435	-2.549331	-1.575162
6	-4.503609	-3.590583	0.000934
1	-5.468411	-2.508950	1.592408
1	-3.296493	-4.397238	-1.588455
6	4.864965	0.908903	-0.057485
6	5.143509	1.622250	-1.225403
6	4.482223	1.580194	1.101617
6	5.043776	3.007630	-1.229647
1	5.434389	1.086565	-2.120792
6	4.376449	2.967573	1.095017
1	4.265397	1.014616	1.998933
6	4.658032	3.680652	-0.068504
1	5.252279	3.564730	-2.134383
1	4.072780	3.493441	1.990713
6	4.598257	5.184987	-0.073047
9	5.826700	5.729698	0.084747
9	3.823619	5.667343	0.919716
9	4.108673	5.663336	-1.237304
7	-1.711149	-0.387960	0.016206
7	-3.782604	4.887945	0.004768
7	-5.444093	-4.653170	-0.009917
6	-4.010938	5.562290	1.235563
6	-4.593745	4.890531	2.318884
6	-3.656579	6.910192	1.384374
6	-4.806997	5.552538	3.523659
1	-4.877223	3.850776	2.209565
6	-3.889247	7.568616	2.587387
1	-3.201231	7.435588	0.553827
6	-4.460947	6.895182	3.665553

1	-5.259927	5.017829	4.351275
1	-3.608423	8.611427	2.685367
1	-4.634644	7.409747	4.603327
6	-4.078975	5.537226	-1.224782
6	-3.199983	5.440654	-2.312281
6	-5.255540	6.285588	-1.368338
6	-3.498177	6.072700	-3.515052
1	-2.285578	4.869652	-2.207786
6	-5.537222	6.927830	-2.569599
1	-5.942515	6.361910	-0.534467
6	-4.664903	6.822911	-3.651567
1	-2.806109	5.988609	-4.345674
1	-6.451745	7.503036	-2.663005
1	-4.890802	7.319357	-4.587980
6	-4.998284	-5.995680	-0.154330
6	-5.678652	-6.885116	-0.997393
6	-3.871865	-6.451392	0.544312
6	-5.243722	-8.199835	-1.128965
1	-6.547494	-6.540289	-1.544521
6	-3.434048	-7.763058	0.393029
1	-3.344330	-5.773318	1.203959
6	-4.117722	-8.647014	-0.439887
1	-5.781781	-8.874172	-1.786016
1	-2.560724	-8.098503	0.941410
1	-3.777757	-9.670000	-0.550500
6	-6.832637	-4.376038	0.114900
6	-7.649179	-5.180543	0.921809
6	-7.408833	-3.294897	-0.566586
6	-9.009451	-4.912123	1.033828
1	-7.212029	-6.014821	1.456681
6	-8.766761	-3.023860	-0.434582
1	-6.787318	-2.671049	-1.197189

6	-9.577254	-3.831218	0.361517
1	-9.625638	-5.545439	1.662492
1	-9.195307	-2.183826	-0.970058
1	-10.636113	-3.621161	0.456522

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