

Electronic Supplementary Information (ESI)

Novel thermally activated delayed fluorescence materials by high-throughput virtual screening: going beyond donor-acceptor design

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1. Calibration

We have constructed a large database of 100 singlet and triplet experimental excitation energies using data from the literature.¹ Through comparison between the calculated and experimental excited state energies, the calibration was established. The energy of the singlet excited state S_1 is calculated at M06-2X/def2-TZVP level. The energy of the triplet excited state T_1 is calculated by TDDFT and Δ SCF^{2,3} methods respectively. The comparison between experimental and computational data by two methods are shown in Fig. S1. It has been proved the calibration methodology is very useful for prediction the singlet fission molecules.³

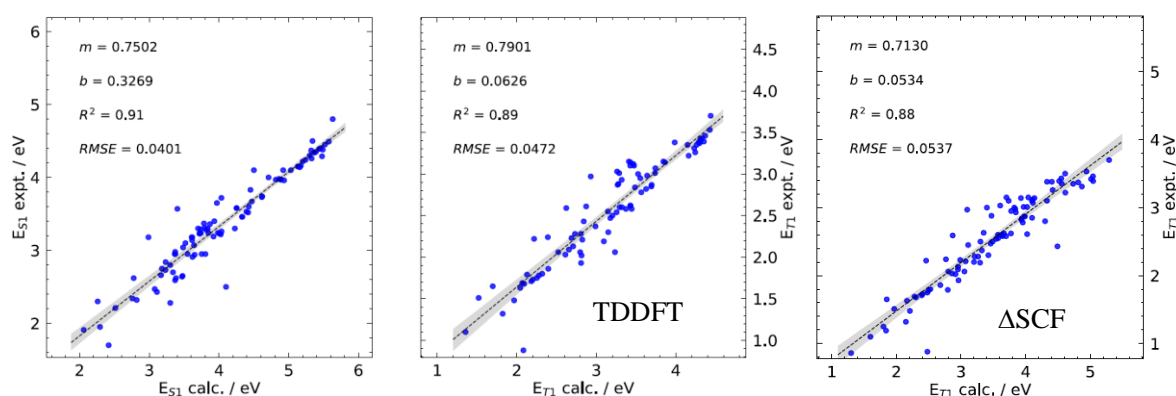


Fig. S1 Comparison between calculated (M06-2X/def2-TZVP) and experimental S_1 (left) and T_1 energies for TDDFT (middle) and Δ SCF (right) methods. Shade areas represent a 95% confidence interval. We calibrated the calculations to experimental data with a linear fit (*i.e.* $y=mx+b$), and we provide two metrics for the quality of the fit (squared correlation coefficient, R^2 , and root mean squared error, RMSE).

2. Convergence problem

Using Δ SCF method to calculate triplet energy should be slightly more accurate than TDDFT, but it has some convergence problems. When we calculate the singlet point energy of T_1 state for X-ray structure, it may occasionally converge on an excited state due to the poor orbital guess. We carefully examined some molecules calculation in the long-list and found the convergence problems. Several examples with T_1 energies calculated by Δ SCF and TDDFT are shown in Fig. S2. For these molecules, the calculated Δ SCF triplet energy $E_{x,scf}(T_1)$ is unreasonably high. We also noticed a number of instances where molecules formed by weakly interacting identical conjugated fragments, such as COXJAC and ANEWEX, had multi-configurational triplets that could not be studied accurately well within an unrestricted SCF calculation.

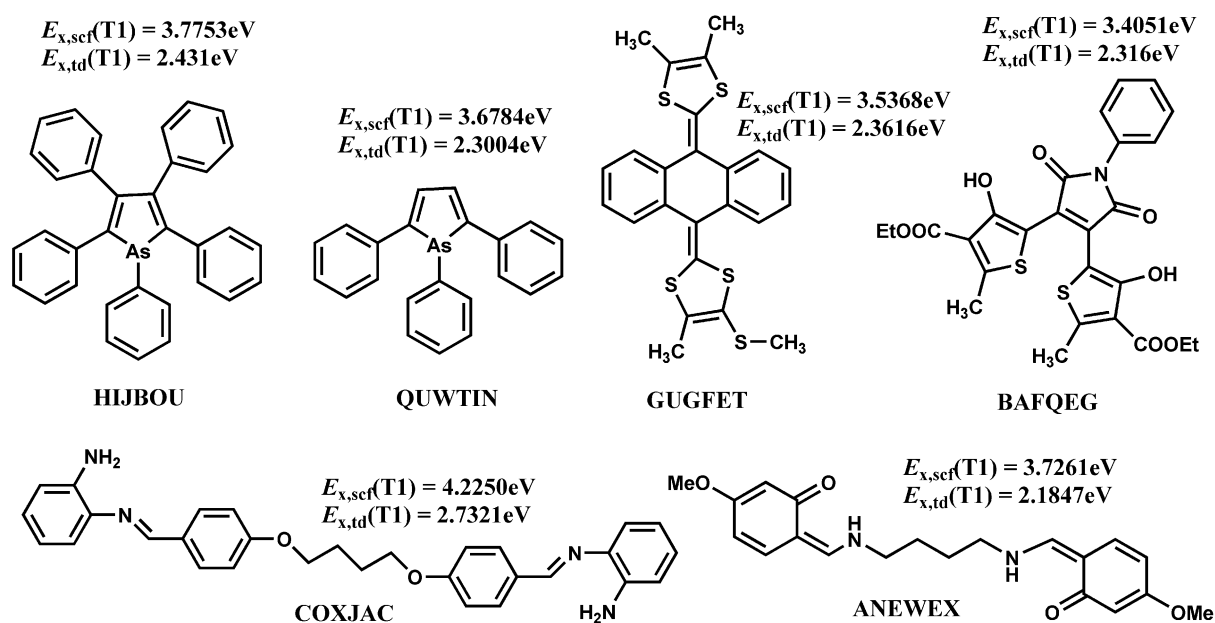


Fig. S2 The $E_{x,scf}(T_1)$ and $E_{x,td}(T_1)$ for the molecules having convergence problem.

3. Whole image of calculation

According to two strategies, we selected 698 molecules to perform accurate calculation. Fig. S3 gives the calibrated excitation energies of X-ray and optimized structures for all of the 698 molecules. Each point represents a series of calculation for one structure. From the Figure S3, we can see the whole S_1 and T_1 energy distribution and the energy changes before and after optimization for 698 molecules. From the 698 molecules, we identified 125 TADF candidates satisfying our energy criteria. The calibrated energies of the 125 candidates are plotted in Fig. S4. The red points, which denote the calibrated energies of optimized geometries are all located in the gray shaded area, that is, the range of $-0.4\text{ eV} < E(S_1)' - E(T_1)' < 0.4\text{ eV}$.

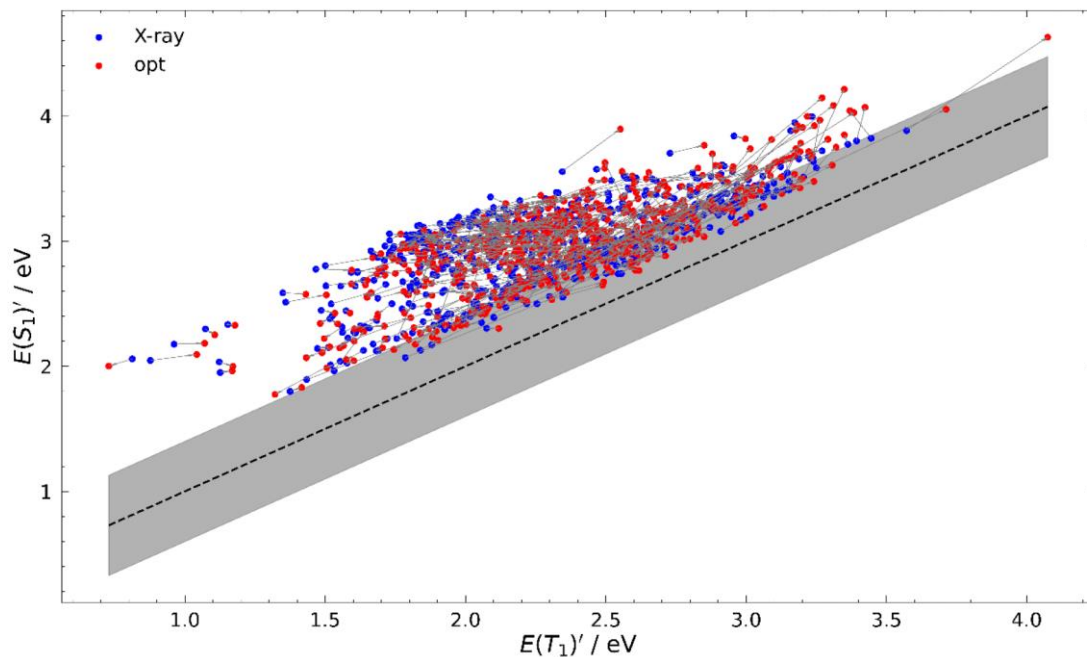


Fig. S3 The calibrated excitation energies of X-ray (blue points) and optimized structures (red points) for the 698 molecules. The gray shaded area identifies the range of $-0.4 \text{ eV} < E(S_1)' - E(T_1)' < 0.4 \text{ eV}$.

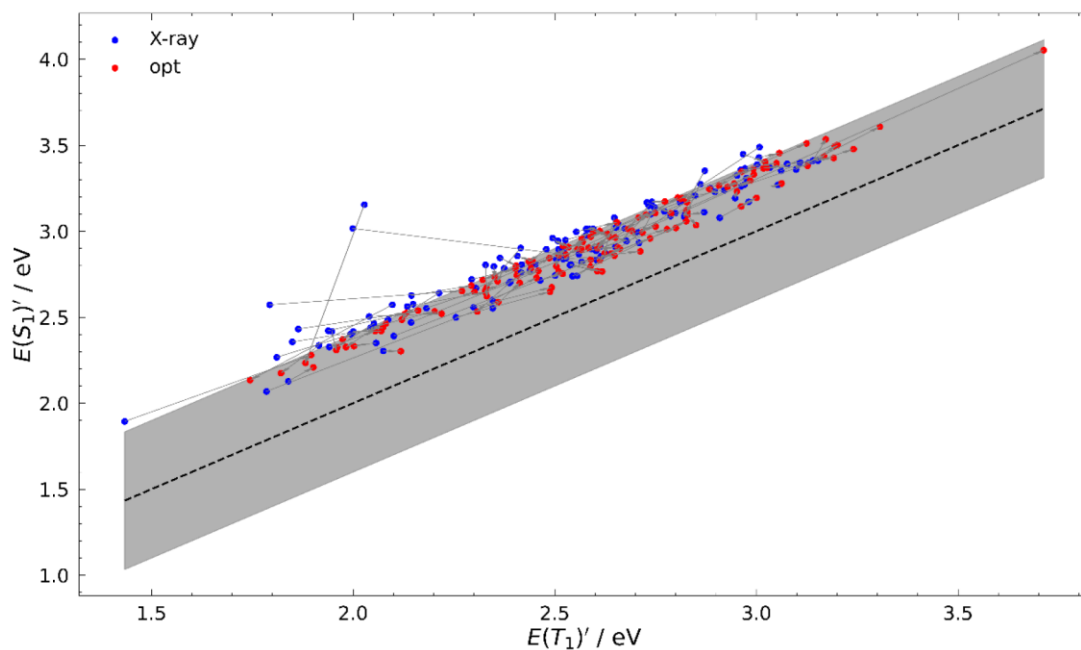


Fig. S4 The calibrated excitation energies of X-ray (blue points) and optimized structures (red points) for the 125 candidates. The gray shaded area identifies the range of $-0.4 \text{ eV} < E(S_1)' - E(T_1)' < 0.4 \text{ eV}$.

4. HOMO/LUMO orbitals of XOTCUF

The optimized geometry and the HOMO and LUMO orbitals are given in Fig. S5. From the side view, one can see that the molecule has a planar backbone. HOMO/LUMO distribution is

well separated and the small overlap localized on the central benzene ring. This indicates that the donor, acceptor and linker balance very well to obtain a small ΔE_{ST} in a coplanar molecule.

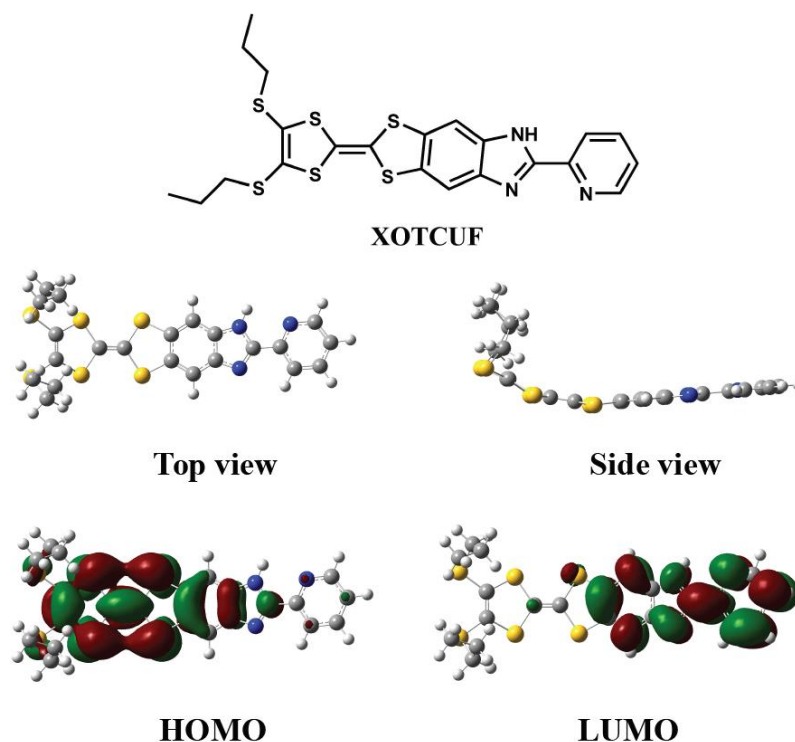


Fig. S5 The optimized geometry and HOMO/LUMO orbitals of XOTCUF molecule.

5. Design for improving property (acceptor number and isomerism effects)

WANTIQU has two isomers. One has a nearly linear backbone, and the other has a V-shaped conformation which corresponds to the X-ray structure. The calculated energy gap ΔE_{ST} and oscillator strength f of the two isomers are shown in Fig. S6. It is found that the linear structure has stronger oscillator strength due to the enhanced conjugation, but the ΔE_{ST} is larger than our criterion. Then we added more cyano units to modulate the charge transfer property. The results show that with the increase of cyano units, the ΔE_{ST} and the f decrease for both linear and V-shaped structures. The linear structure with three cyano units has a small ΔE_{ST} with a considerable f . It is expected that this structure could have better performance than the original WANTIQU molecule.

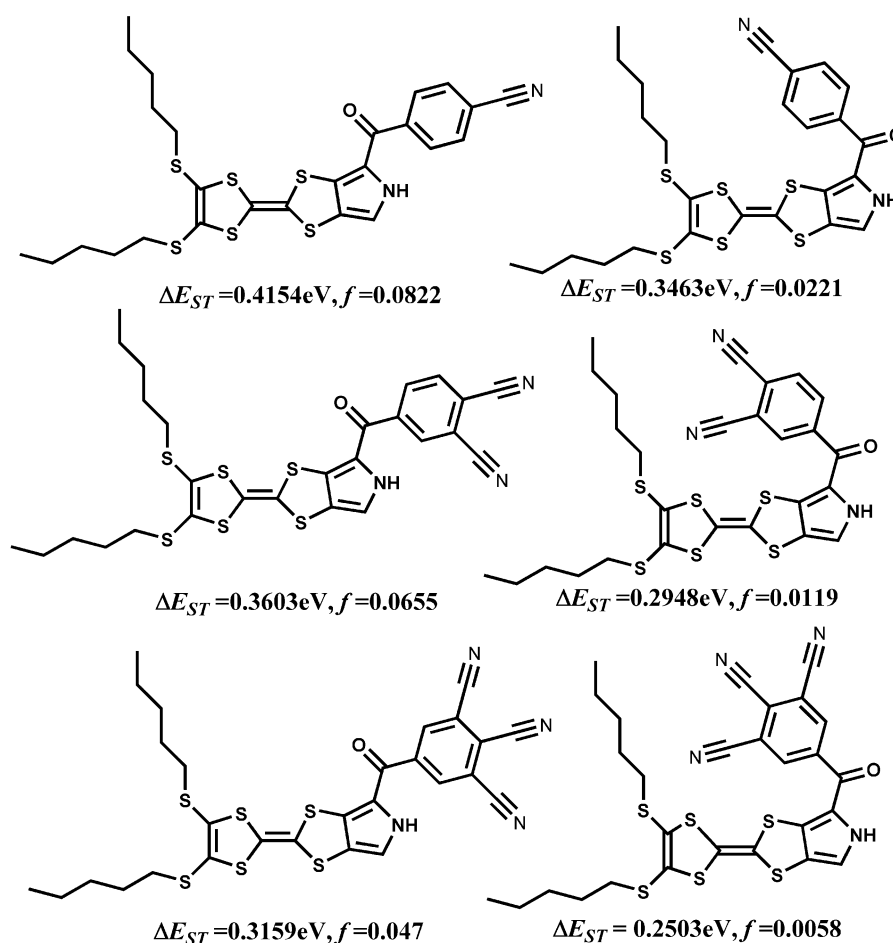


Fig. S6 Isomerism effects on the energy gap ΔE_{ST} and the oscillator strength f for the structures related to WANTIQ.

The calculated frontier orbitals of the ZERJEL02 and the corresponding designed molecules are presented in Fig. S7. In the designed molecules, the HOMO orbitals are more localized on the sulfur atoms and farther away from the central benzene ring, which makes the overlap of HOMO and LUMO orbitals smaller than that of the ZERJEL02 molecule. Therefore, both the energy gaps and the oscillator strengths of the designed structures decrease significantly, but their oscillator strengths are still larger than 0.02.

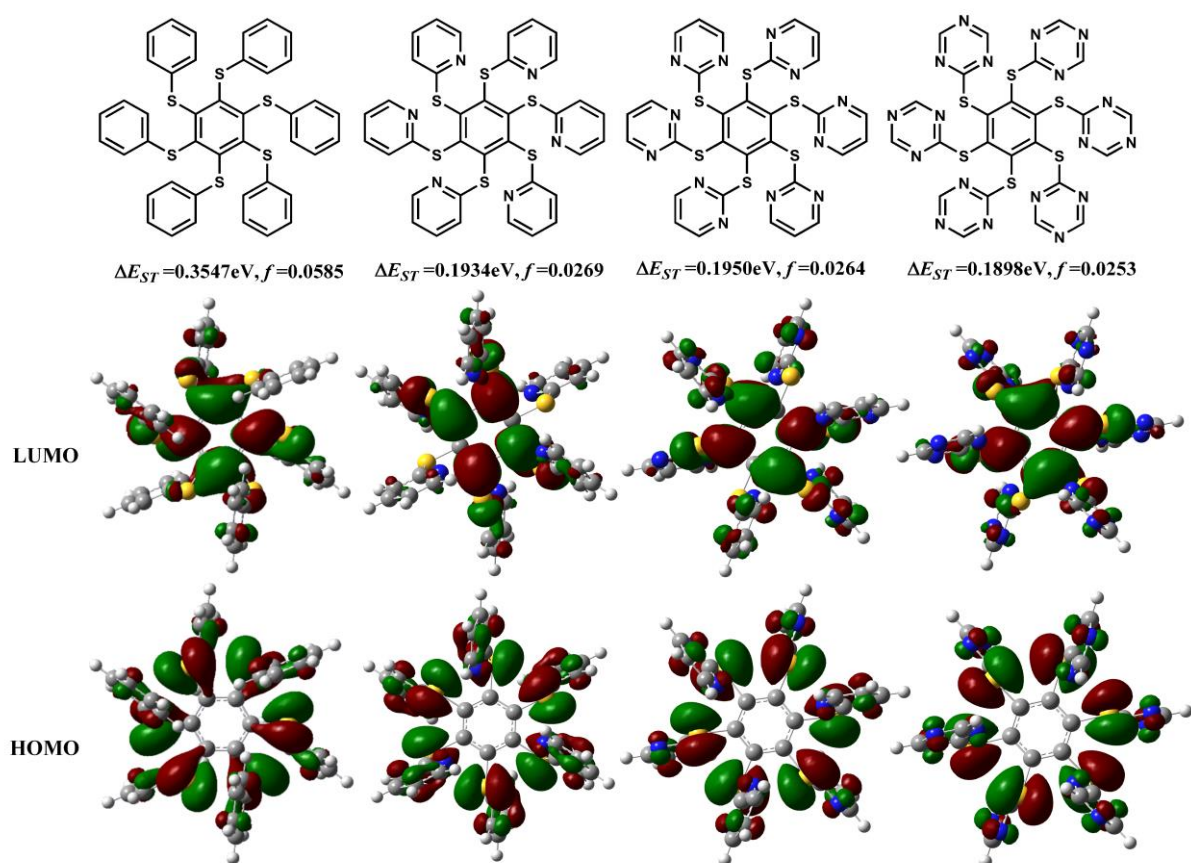


Fig. S7 Comparison of the HOMO/LUMO orbitals between the ZERJEL02 and the corresponding designed molecules.

6. Information of candidates

125 TADF candidates are found by our high-throughput virtual screening process and we grouped them into seven types. Their key information is listed in Table S1 and their chemical structures are illustrated in Table S2.

Table S1. The key information of the 125 molecules.

Type	No.	CSD ID	$E_0(S_1)$ (eV)	$E_{0,td}(T_1)$ (eV)	ΔE_{ST} (eV)	f ($S_0 \rightarrow S_1$)	$\langle S_1 H_{so} T_1 \rangle$ (cm^{-1})	$\langle T_1 H_{so} S_0 \rangle$ (cm^{-1})
I	1	FARHEO	3.2509	3.2340	0.1479	0.0004	0.0498	0.5043
	2	HIFJOY	3.7558	3.6699	0.1823	0.0002	0.0669	1.9700
	3	EXAMUN	3.6110	3.5283	0.1856	0	0.0022	1.6440
	4	TEGVAF	3.2528	3.2183	0.1618	0	0.0494	1.7737
	5	IVETAG	3.3387	3.2267	0.2196	0	0.0031	1.0967
	6	VENXAQ	3.3436	3.1976	0.2462	0	0.0082	0.7674
	7	YUGDOV	3.2921	3.0897	0.2929	0.1017	0.1163	1.7923
	8	TESJEJ	2.9241	2.7296	0.3013	0.0001	0.0242	1.4939
	9	TURBOZ	3.4524	3.2238	0.3072	0.1602	0.0110	0.3300
	10	KETKAY	3.4394	3.1283	0.3729	0	0.0073	0.7529
	11	BICQEM	3.1010	2.7940	0.3831	0.0006	0.0128	1.2314
II	12	FECGOL	3.3742	3.2720	0.2104	0.0001	0.0155	2.2678
	13	ONAHIW	3.5822	3.3140	0.3333	0.0802	0.5233	1.2267
	14	IWOKUB	3.4499	3.1109	0.3945	0.0379	0.4789	2.61E-11
	15	SOHQAI	3.8146	3.4802	0.3763	0.0059	0.2017	0.4653
	16	XEXWIG	3.3814	3.1202	0.3358	0.0542	0.2370	0.8860
	17	TARNUW	3.2538	3.0969	0.2584	0.0891	0.1648	0.4789
	18	VIHGAU	2.9307	2.6193	0.3934	0.0832	0.9157	3.9921
	19	NUPIJR	2.8165	2.5459	0.3657	0.084	0.4324	1.8390
	20	RUPZIN	3.7938	3.4308	0.3997	0.0402	1.9308	13.1256
III	21	ILUBEY	3.8227	3.7179	0.1946	0.0447	0.1969	0.3050
	22	NEWKEH	3.4310	3.2187	0.2951	0.0264	0.6116	1.8428
	23	IKUZET	2.7886	2.5214	0.3642	0.0457	0.2244	0.6297
	24	DELJIQ	3.4073	3.3537	0.1707	0.0011	0.2917	1.3882
	25	HATXOP	3.7251	3.4982	0.2949	0.0409	1.3947	3.5427
	26	USINEQ	4.1440	3.9305	0.2676	0.0104	3.2622	3.3611

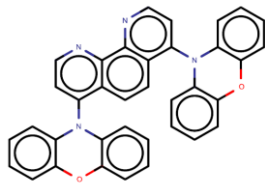
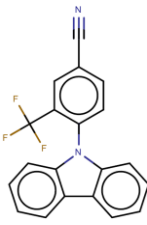
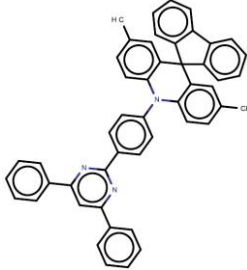
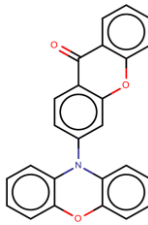
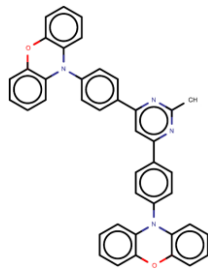
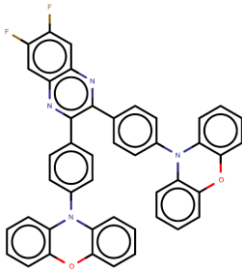
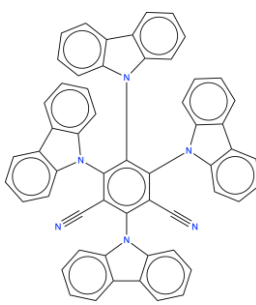
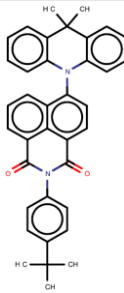
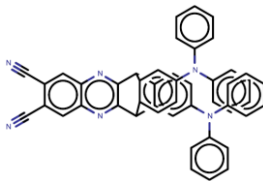
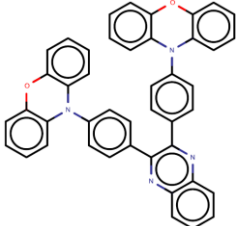
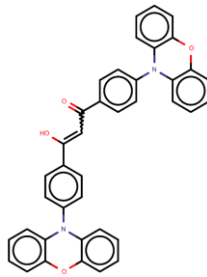
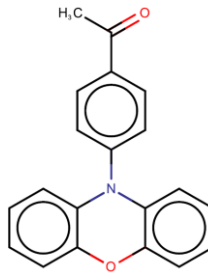
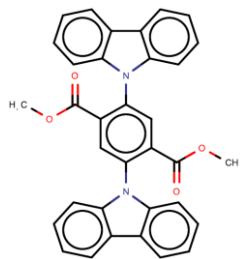
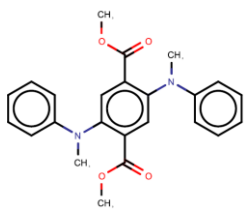
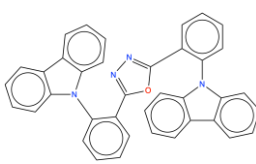
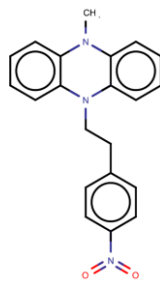
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	29	VALTOT	3.8907	3.5703	0.3622	0.0346	1.0914	2.4696
	30	NETZES	3.6700	3.3485	0.3719	0.0048	30.3455	48.3766
	31	YAXXOK	4.1015	3.7452	0.3822	0.0231	8.3677	5.1268
	32	OCUPEK	4.0257	3.6719	0.3832	0.0373	46.6174	421.5681
	33	PEHJUK	3.5994	3.4012	0.2773	0.0383	1.9866	3.2992
	34	KIRYEQ	4.0710	3.8782	0.2542	0.0235	2.1805	1.4262
	35	YOZFOI	3.7035	3.4501	0.3167	0.0162	8.6628	277.3763
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	53	LUBBAN	3.6900	3.5013	0.2662	0.0085	0.1008	0.6520
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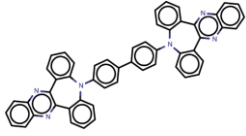
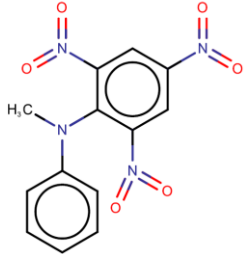
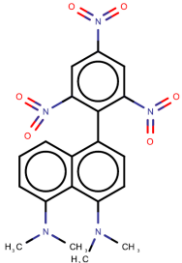
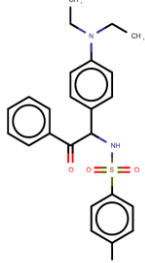
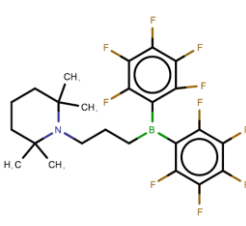
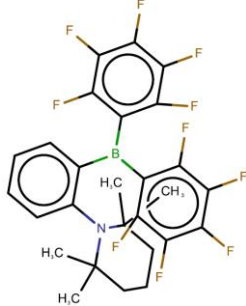
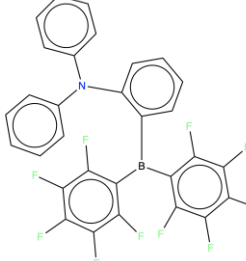
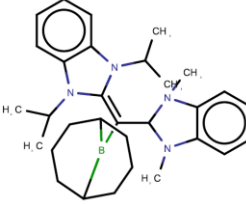
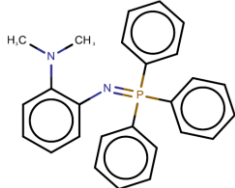
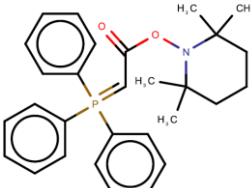
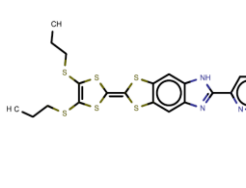
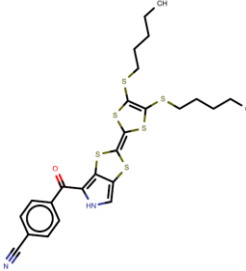
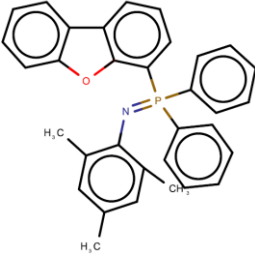
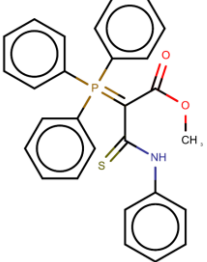
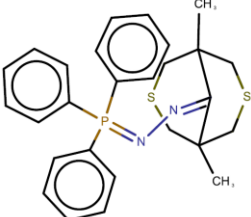
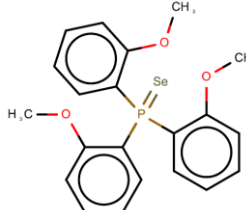
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	58	YOYVIR	2.5423	2.3024	0.3524	0.0006	7.3079	4.21608
	59	BARHEI	3.2695	2.9616	0.3771	0.0089	18.9907	32.4801
	60	EJINES	3.3311	3.0155	0.3807	0.0594	0.3633	3.4435
	61	CUTNOU	3.6324	3.2799	0.3979	0.0193	10.7455	57.6599
	62	CICGOK	3.2111	2.8964	0.3848	0.0401	5.3630	12.6641
	63	ZUBWAW	4.2448	3.8750	0.3871	0.0071	17.2435	38.6544
	64	LULSAM	3.3274	3.0038	0.3872	0.0199	40.7524	58.0128
	65	ZASLEK	3.5041	3.1691	0.3892	0.0071	0.2447	0.8969
	66	BARGOR	3.2970	2.9636	0.3962	0.0169	16.2726	30.4877
	67	JOFLAR	3.5527	3.2052	0.3971	0.02	56.5084	48.4960
	68	SIKTOV	3.5658	3.2261	0.3904	0.0368	2.3121	20.2008
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	72	SELDOE01	3.3564	3.0681	0.3582	0.0221	0.7282	3.8215
	73	HAXHAQ	3.5886	3.4649	0.2189	0.0252	4.4031	4.0549
	74	KEGZOM	3.6906	3.3719	0.3689	0.098	5.0645	22.4231
	75	BIDZUK	3.8246	3.4712	0.3909	0.0892	4.4078	17.3947
	76	TOZZOZ	3.2342	3.1099	0.2335	0.0205	1.2540	3.6035
	77	WAPLIJ	4.3731	4.1053	0.3014	0.033	0.2379	2.9255
	78	BACTIL	3.4348	3.1910	0.3199	0.0003	2.2589	41.7745
	79	YAXKAM	3.5078	3.3839	0.2222	0.0017	0.9484	41.2355
	80	HECLIK	2.9420	2.7082	0.3316	0.0025	51.8665	1.0565
	81	YETCAB	2.4092	2.129	0.3896	0.0007	15.5082	467.8790
	82	GUMLEG	4.2757	3.9357	0.3623	0.038	3.1518	35.7817
	83	FURVIZ	2.8473	2.5546	0.3820	0.0157	3.3980	16.1047
	84	DARQIZ	2.6036	2.3198	0.3846	0.0268	126.4642	11.8778

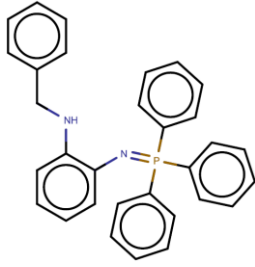
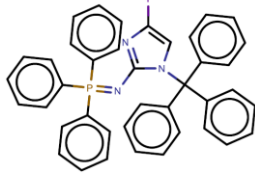
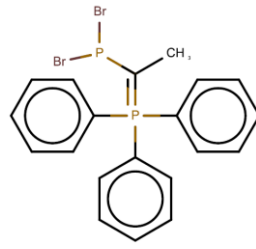
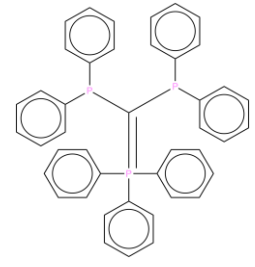
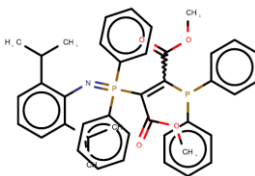
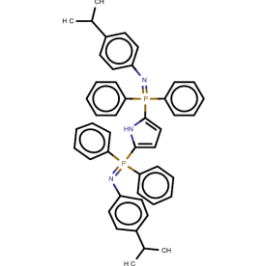
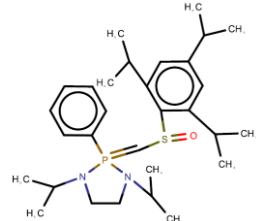
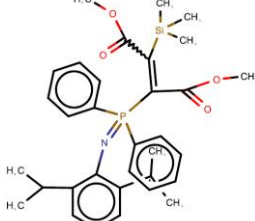
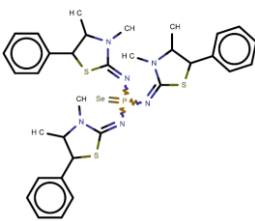
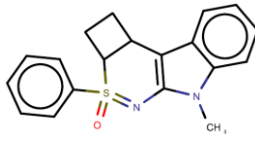
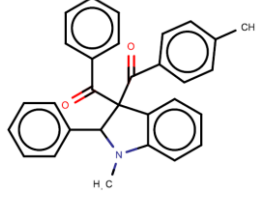
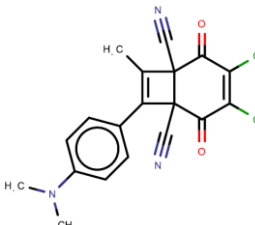
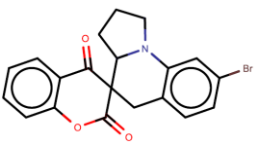
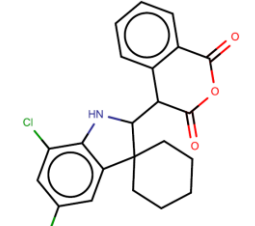
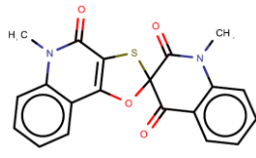
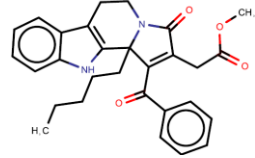
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	86	NACTEQ02	2.9413	2.8418	0.2256	0.0064	2.3325	7.3811
	87	LAHLAI	3.1287	3.0756	0.1814	0.0072	3.1282	10.4557
	88	BOCNEN	3.5787	3.437	0.2335	0.0096	1.1845	1.8193
	89	NOVXUT	2.6742	2.4546	0.3311	0.0435	1.8283	3.5292
	90	YAMVEQ	3.2032	3.0278	0.2751	0.0236	13.3261	3.71025
	91	PEQDEW	4.2214	3.9638	0.2994	0.016	0.6319	2.9695
	92	PEQDIA	4.2313	3.9729	0.2996	0.0339	0.8488	3.2459
	93	FEWBEO	3.7051	3.4001	0.3574	0.0391	7.1283	10.4074
	94	ZOXRIN	4.9668	4.6197	0.3404	0.0001	24.7212	14.5259
	95	TUCTAN	2.6339	2.6020	0.1844	0.0036	1.8356	10.8216
VI	96	VEBLIX	2.9198	2.6138	0.3896	0.066	1.1300	1.5207
	97	RIXDEH	2.7272	2.4190	0.3990	0.02	0.0044	0.0211
	98	HEXWIR	3.4219	3.1694	0.3273	0.0144	1.0740	0.0009
	99	GEHRIU	3.9560	3.6987	0.3097	0.0391	2.2480	2.9762
	100	NEYGIJ	4.1307	3.9605	0.2340	0.0114	3.2794	3.8390
	101	TOLPSO	4.1998	4.0228	0.2366	0.011	2.3883	4.7934
	102	RIXSIB	3.3903	3.2412	0.2468	0.0125	0.6319	2.9695
	103	UCOMIJ	4.0450	3.7081	0.3691	0.0182	7.9792	7.4403
	104	PEXZAY	3.1755	2.9055	0.3509	0.0279	2.4983	12.0160
	105	WAJPEC	3.3917	3.2628	0.2308	0.0183	0.4066	1.5145
	106	WAJPIG	3.5217	3.1975	0.3799	0.0297	3.6280	3.9100
VII	107	DEJMUC	3.9049	3.6270	0.3281	0.0279	1.0369	5.7383
	108	JUNQUE	4.0545	3.7507	0.3426	0.0016	10.2473	9.5414
	109	LAHWUN	3.6412	3.4976	0.2325	0.0208	0.4643	1.6552
	110	TUFWAS	2.4635	2.226	0.3537	0.0098	2.2871	0.0003
	111	SIFHIY	3.0596	2.8720	0.2904	0.0003	26.7783	2.41E-10
	112	MOPKEI	2.6661	2.4026	0.3661	0.0225	8.0335	3.76E-05
	113	GOBVUP	2.6660	2.4300	0.3444	0.0161	8.6444	7.76E-11

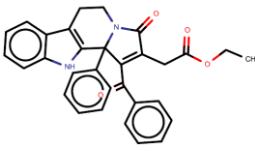
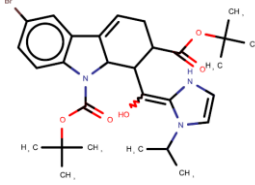
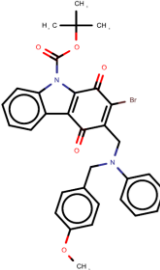
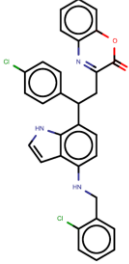
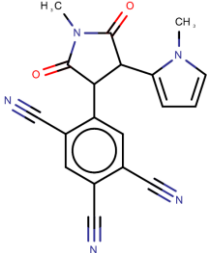
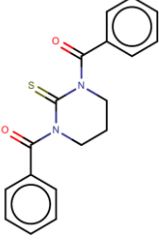
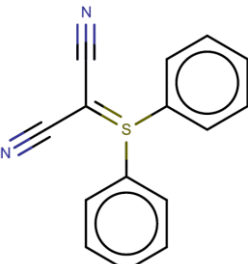
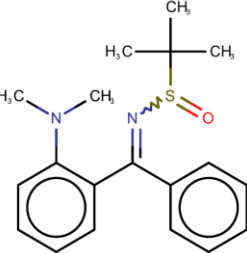
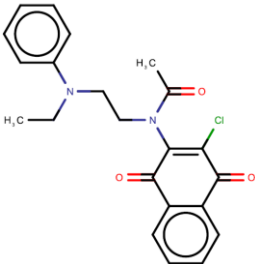
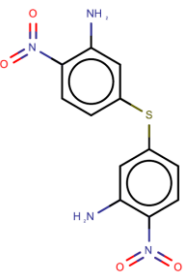
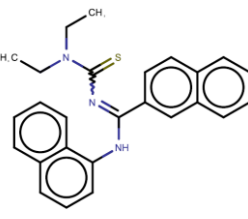
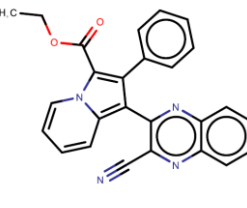
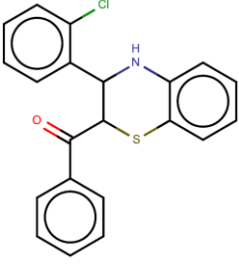
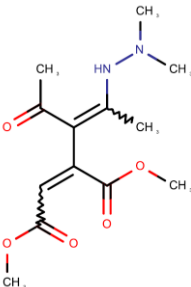
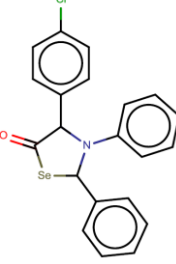
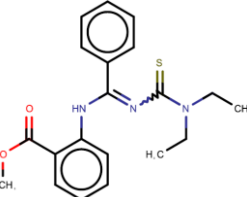
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	115	KUSLUF01	2.9482	2.6562	0.3774	0.0014	11.5847	18.6231
	116	HAKSIW	3.5654	3.3281	0.3095	0.0674	1.2344	0.0034
	117	HAKSOC	3.5154	3.2753	0.3137	0.0599	0.9688	0.0005
	118	MUHTOZ	3.2464	2.9679	0.3548	0.0298	28.2311	0.1021
	119	MUHTIT	3.4398	3.2822	0.2516	0.0359	5.3611	0.0175
	120	ZERJEL02	3.5431	3.2497	0.3547	0.0585	11.5277	0.0045
	121	YAFNOI	3.1863	2.8590	0.3958	0.0804	1.6614	18.7244
	122	KAGCAW	3.2807	3.0109	0.3466	0.1534	0.9249	0.0014
	123	RAPGEV	3.1416	2.8235	0.3903	0.0005	0.6207	14.4760
	124	WEWHOV	3.8210	3.4859	0.3766	0.0349	3.5853	0.0073
	125	HIBZEZ	3.9162	3.6005	0.3575	0.0544	1.0723	38.8420

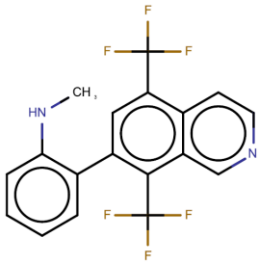
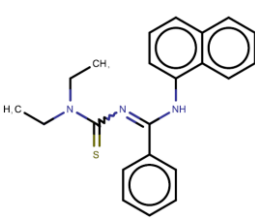
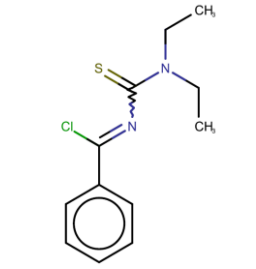
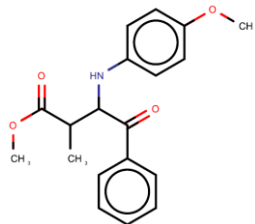
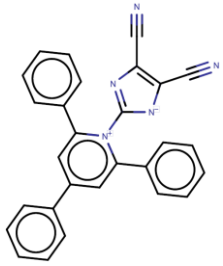
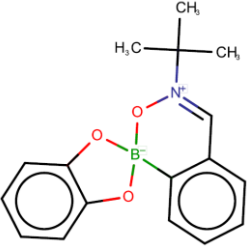
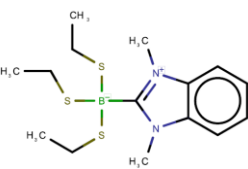
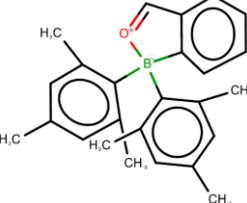
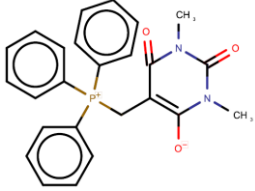
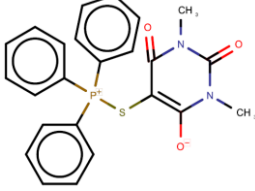
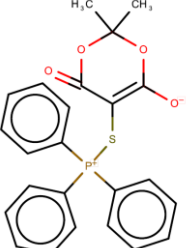
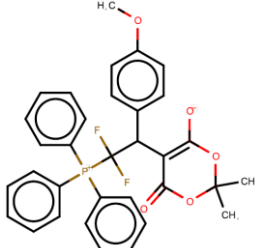
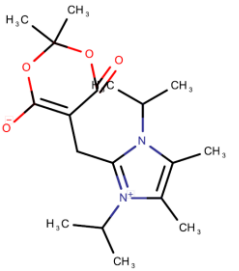
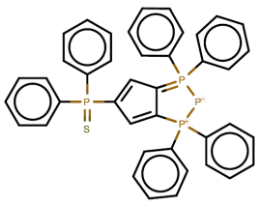
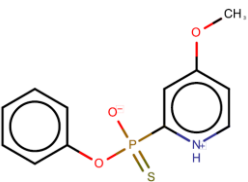
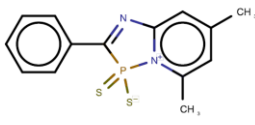
Table S2. The sketch of the 125 candidates. The structures are identified by their CSD ID.

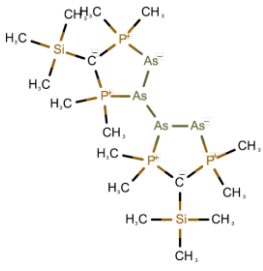
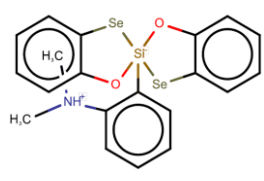
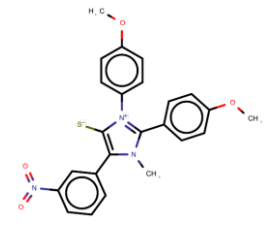
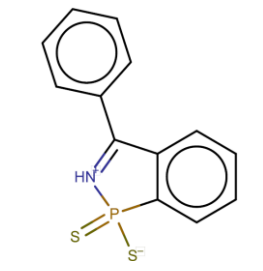
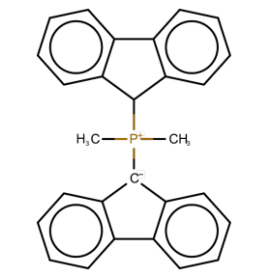
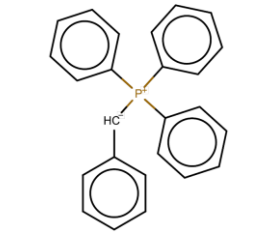
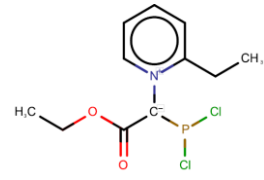
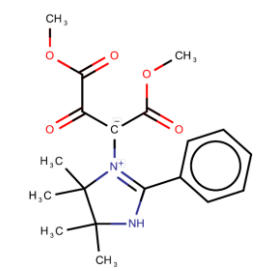
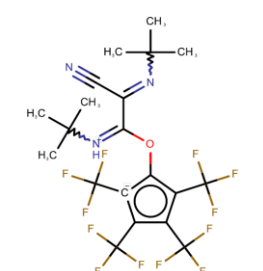
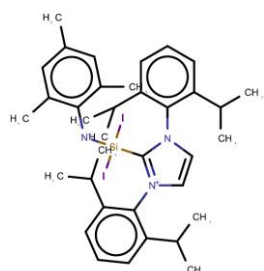
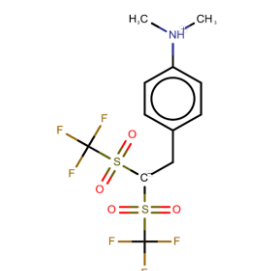
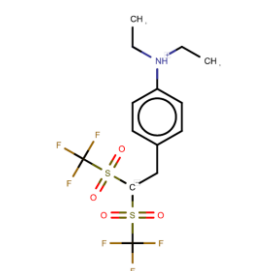
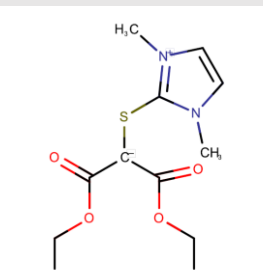
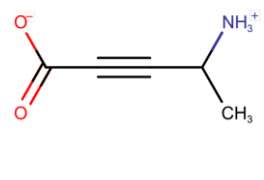
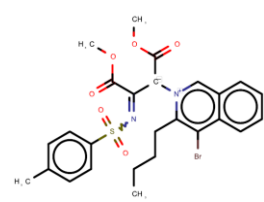
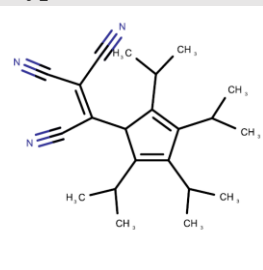
Type I	1	2	3	4
				
	FARHEO	HIFJOY	EXAMUN	TEGVAF
	5	6	7	8
				
	IVETAG	VENXAQ	YUGDOV	TESJEJ
	9	10	11	Type II 12
				
	TURBOZ	KETKAY	BICQEM	FECGOL
	13	14	15	16
				
	ONAHIW	IWOKUB	SOHQAI	XEXWIG

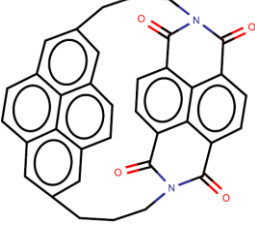
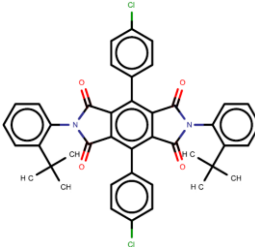
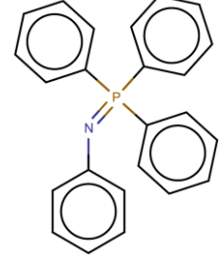
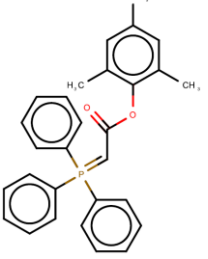
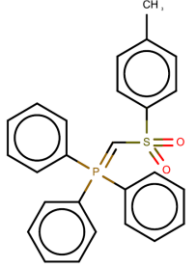
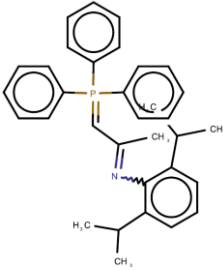
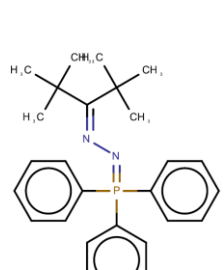
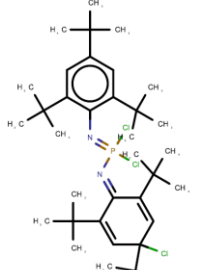
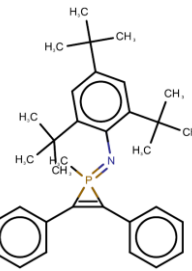
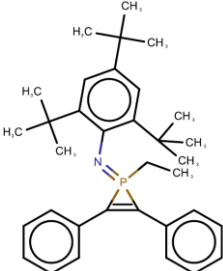
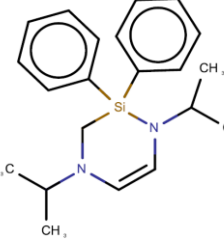
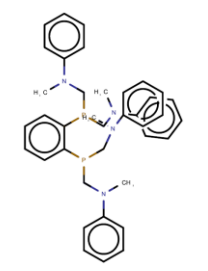
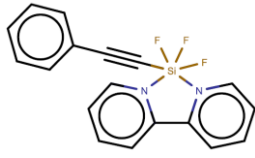
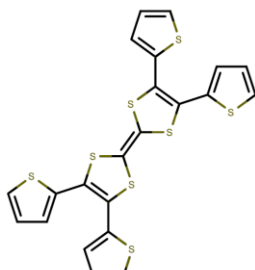
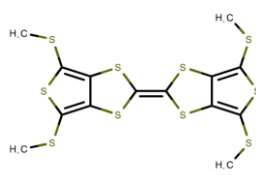
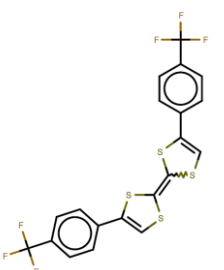
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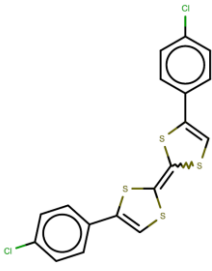
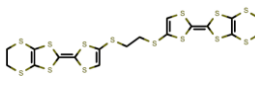
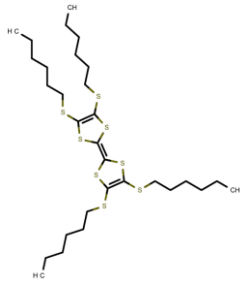
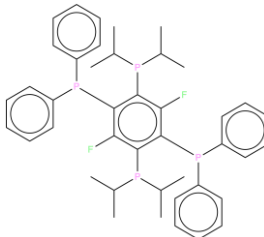
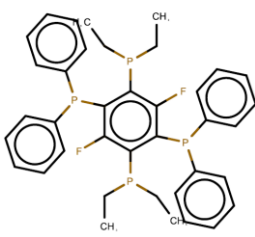
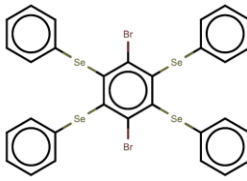
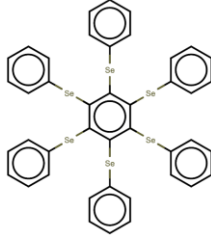
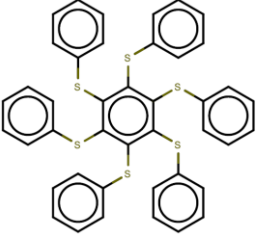
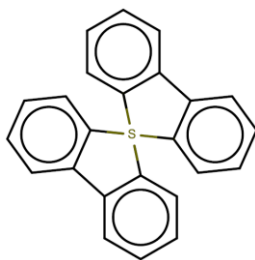
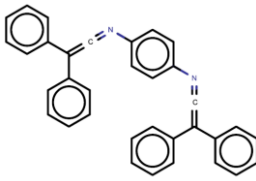
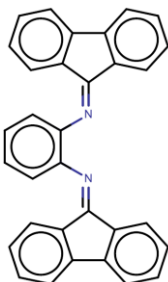
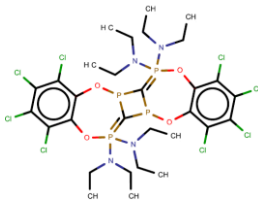
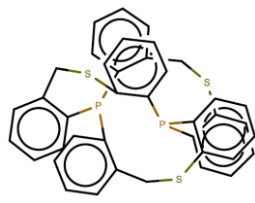
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References

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