ADVANCED OPTICAL MATERIALS

Supporting Information

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Symmetric “Double Spiro” Wide Energy Gap Hosts for Blue Phosphorescent OLED Devices

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Jie Ma,[1] Muazzam Idris,[2] Tian Y. Li,[2] Daniel S. M. Ravinson,[2] Tyler Fleetham,[2] Jongchan Kim,[3] Peter I. Djurovich,[2] Stephen R. Forrest,[3,4,5] Mark E. Thompson[1,2,]*

[1] Department of Materials Science and Engineering, University of Southern California, Los Angeles, California 90089, USA
[2] Department of Chemistry, University of Southern California, Los Angeles, California 90089, USA
[3] Department of Electrical Engineering, University of Michigan, Ann Arbor, Michigan 48109, USA
[4] Department of Physics, University of Michigan, Ann Arbor, Michigan 48109, USA
[5] Department of Materials Science and Engineering, University of Michigan, Ann Arbor, Michigan 48109, USA

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Crystallographic Data of SAS and XAX

The X-ray diffraction images were recorded on a Bruker APEX DUO 3-circle platform diffractometer using Mo K_α radiation ($\lambda = 0.71073$ Å). The diffractometer was equipped with an APEX II CCD detector and an Oxford Cryosystems Cryostream 700 apparatus for low-temperature data collection adjusted to 100(2) K. A Cryo-Loop was used to mount the sample with Paratone oil. The frames were integrated using the SAINT algorithm to give the hkl files. Data were corrected for absorption effects using the multi-scan method (SADABS). The structures were solved by intrinsic phasing and refined with the Bruker SHELXTL Software Package.

Table S1. Crystallographic Data

Compound	SAS	XAX
Formula	$C_{38}H_{24}$	$C_{38}H_{24}O_2$
Formula weight	480.57	512.57
Temperature	100 K	100 K
Wavelength	0.71073 Å	0.71073 Å
Crystal system	orthorhombic	triclinic
Space group	*Pbca*	*P-1*
a (Å)	8.8755(15)	9.9792(18)
b (Å)	20.517(4)	10.6504(19)
c (Å)	27.081(5)	13.580(2)
α (deg)	90	73.536(3)
β (deg)	90	73.239(3)
γ (deg)	90	68.380(2)
Volume ($Å^3$)	4931.3(15)	1259.1(4)
Z	8	2
F (000)	2016.0	536.0
θ (deg) for collection	2.49 to 30.90	2.24 to 29.91
Index range	-12<=h<=12 -28<=k<=28 -38<=l<=38	-13<=h<=13 -14<=k<=14 -18<=l<=18
Reflections collected	115529	27353
Unique (R_{int})	5929 (0.0422)	5224 (0.0660)
data/restrain/parameter	7222/0/343	6509/0/361
Goodness of Fit	1.019	1.107
Final *R* indices [$I > 2\sigma$(I)]	R_1= 0.0422 wR_2= 0.1064	R_1= 0.0660 wR_2= 0.1836
R indices (all data)	R_1= 0.0552 wR_2= 0.1156	R_1= 0.0800 wR_2= 0.1939
CCDC number	1978365	1978366
$R_1 = \Sigma\|\|Fo\|-\|Fc\|\| / \Sigma\|Fo\|$, $wR_2 = [\Sigma[w(Fo^2-Fc^2)^2] / \Sigma w(Fo^2)^2]^{1/2}$		

Crystal Packing of SAS and XAX

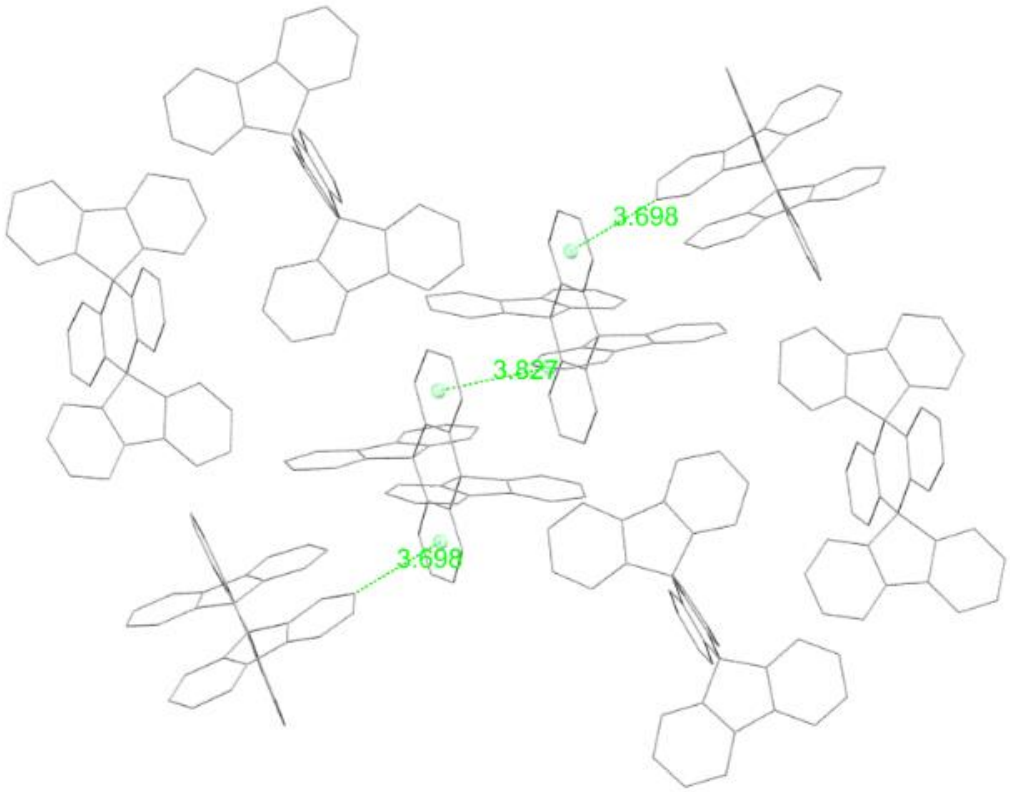


Figure S1. Crystal packing of SAS.

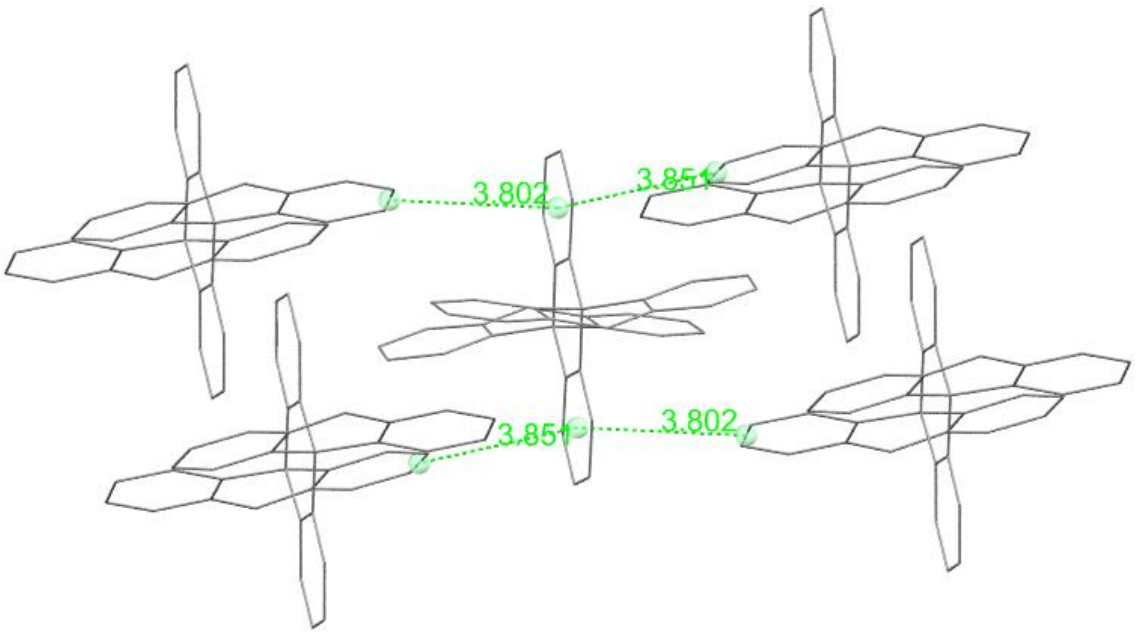


Figure S2. Crystal packing of XAX.

Electrochemical properties

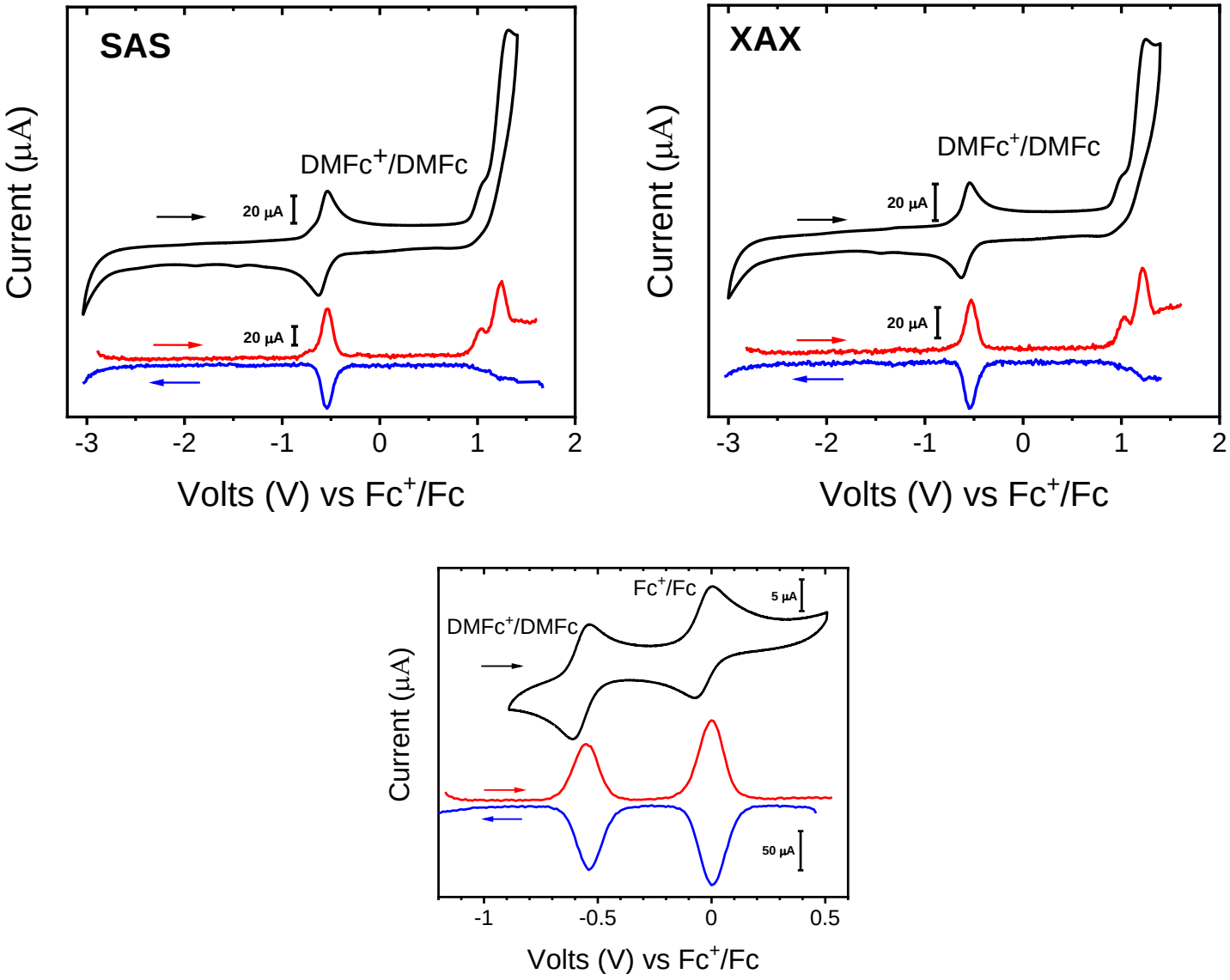


Figure S3. CV (black) and DPV curves (red: oxidation, blue: reduction) of compounds SAS, XAX and decamethylferrocene.
CV and DPV curves of SAS and XAX are recorded in MeCN (scan rate:0.1 V/s) with TBAF as electrolyte. Decamethylferrocene (DMFc) is used as internal reference. The average of the oxidation and reduction peak values of ferrocene is set to 0 V. CV and DPV curves of DMFc are recorded in MeCN with TBAF as electrolyte. Ferrrocence (Fc) is used as internal reference. The elelctrochemical plot at the bottom shows a comparison of Fc and DMFc

Ultraviolet Photoelectron Spectroscopy

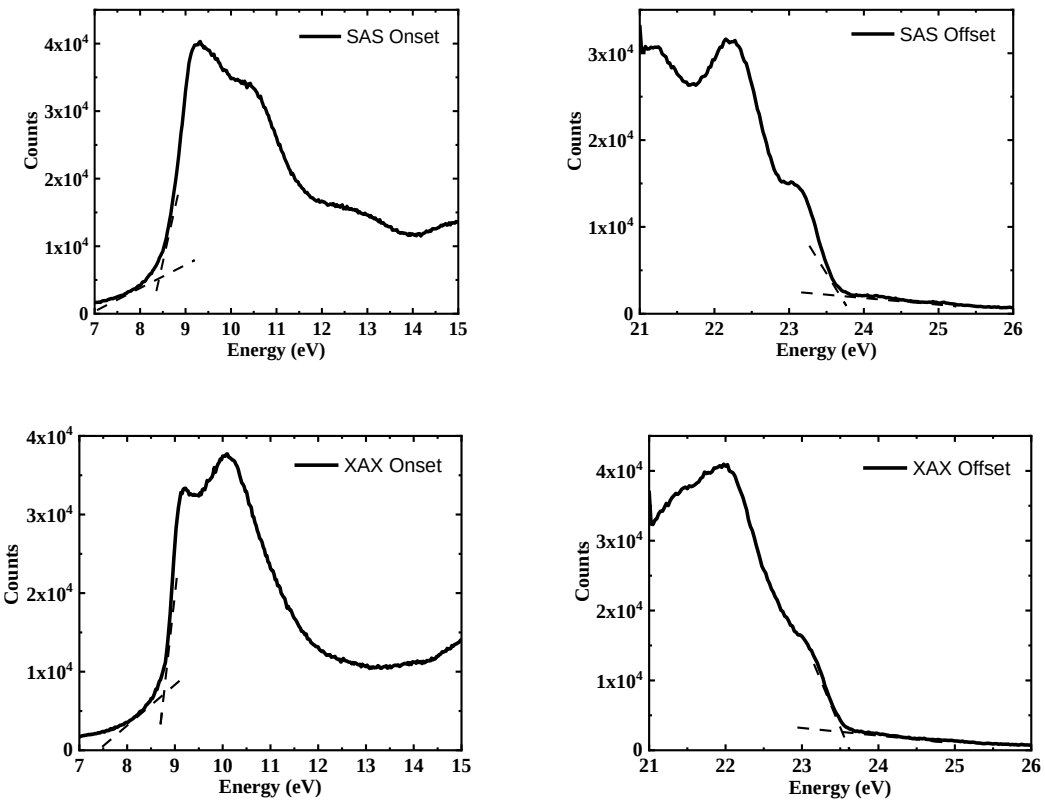


Figure S4. Ultraviolet photoelectron spectrum of SAS and XAX.

The HOMO energy is calculated using as: $E_{HOMO} = E_{UV} + E_{SE} - E_{HOMO-onset}$, where E_{UV} = 21.2 eV, E_{SE} is the secondary electron cutoff energy and $E_{HOMO\text{-}onset}$ is the HOMO onset energy. The E_{SE} is determined as the intersection of extended baseline and the linear part of the spectrum rising edge. It is the kinetic energy of the emitted photoelectrons with largest ionization energy. The $E_{HOMO\text{-}onset}$ is determined at the tail of the spectrum. It is the kinetic energy of the emitted photoelectrons with smallest ionization energy (HOMO electrons). According to the equation,

$$SAS_{HOMO} = 21.2 + 8.4 - 23.7 = 5.9 \text{ eV}$$

$$XAX_{HOMO} = 21.2 + 8.7 - 23.6 = 6.3 \text{ eV}$$

Thermal Measurements and Properties

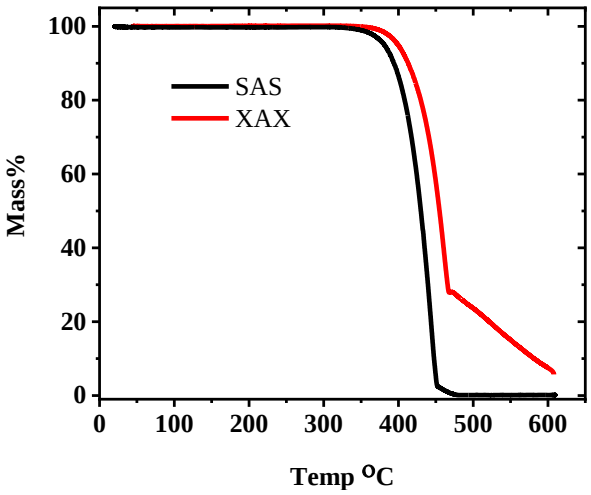


Figure S5. TGA curves (scan rate: 10K/min) of SAS and XAX.

Vacuum Deposited Films

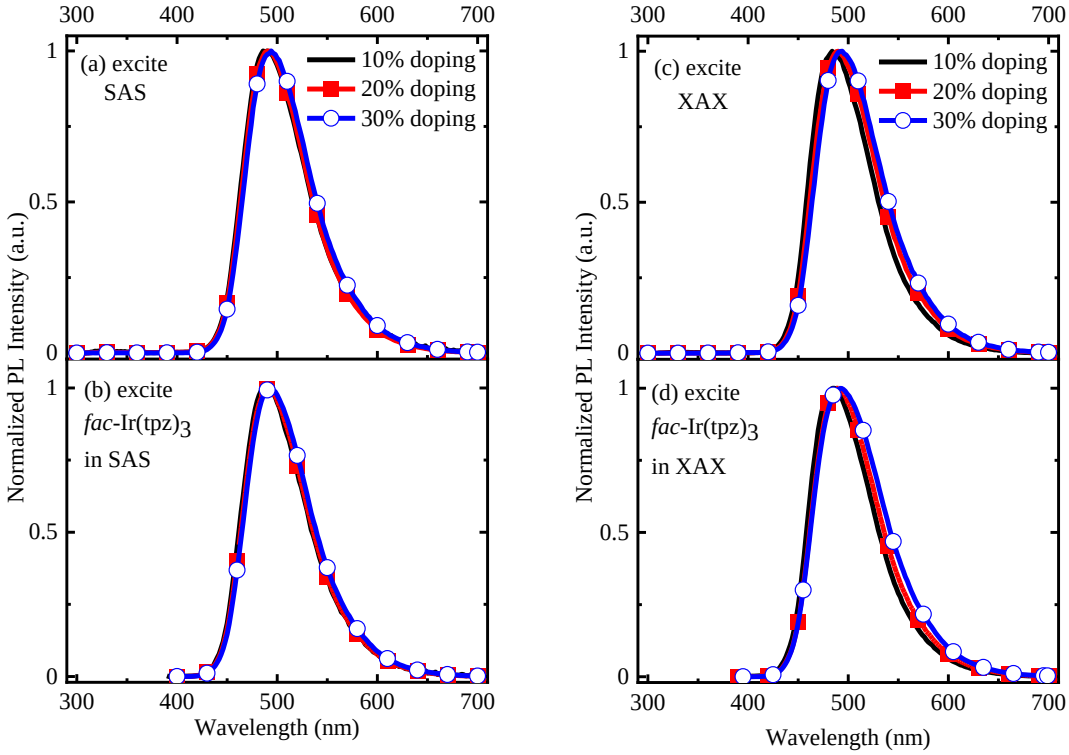


Figure S6. Normalized PL spectra of blend films of SAS or XAX hosts with different *fac*-Ir(tpz)$_3$ concentrations.
(a) SAS films excited at 310 nm (b) fac-Ir(tpz)$_3$ in SAS films excited at 380 nm, (c) XAX films excited at 290 nm and (d) fac-Ir(tpz)$_3$ in XAX films excited at 380nm.

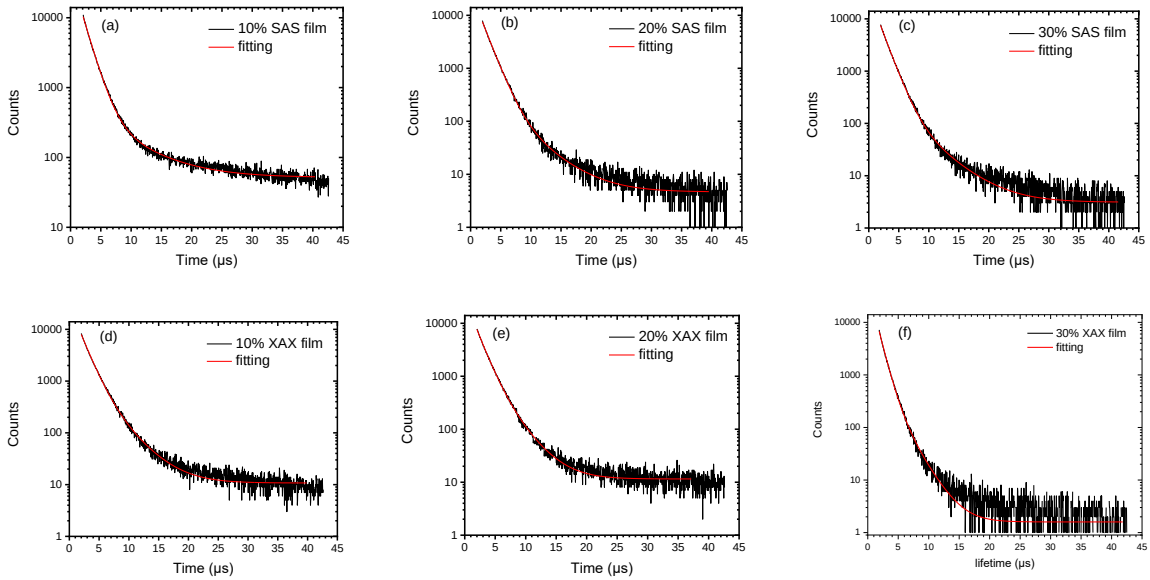


Figure S7. Time-resolved PL decays (excited at 370 nm) of SAS or XAX hosts with different *fac*-Ir(tpz)$_3$ concentrations. Lifetimes are calculated as weighted average lifetimes.

OLED Fabrication and Studies

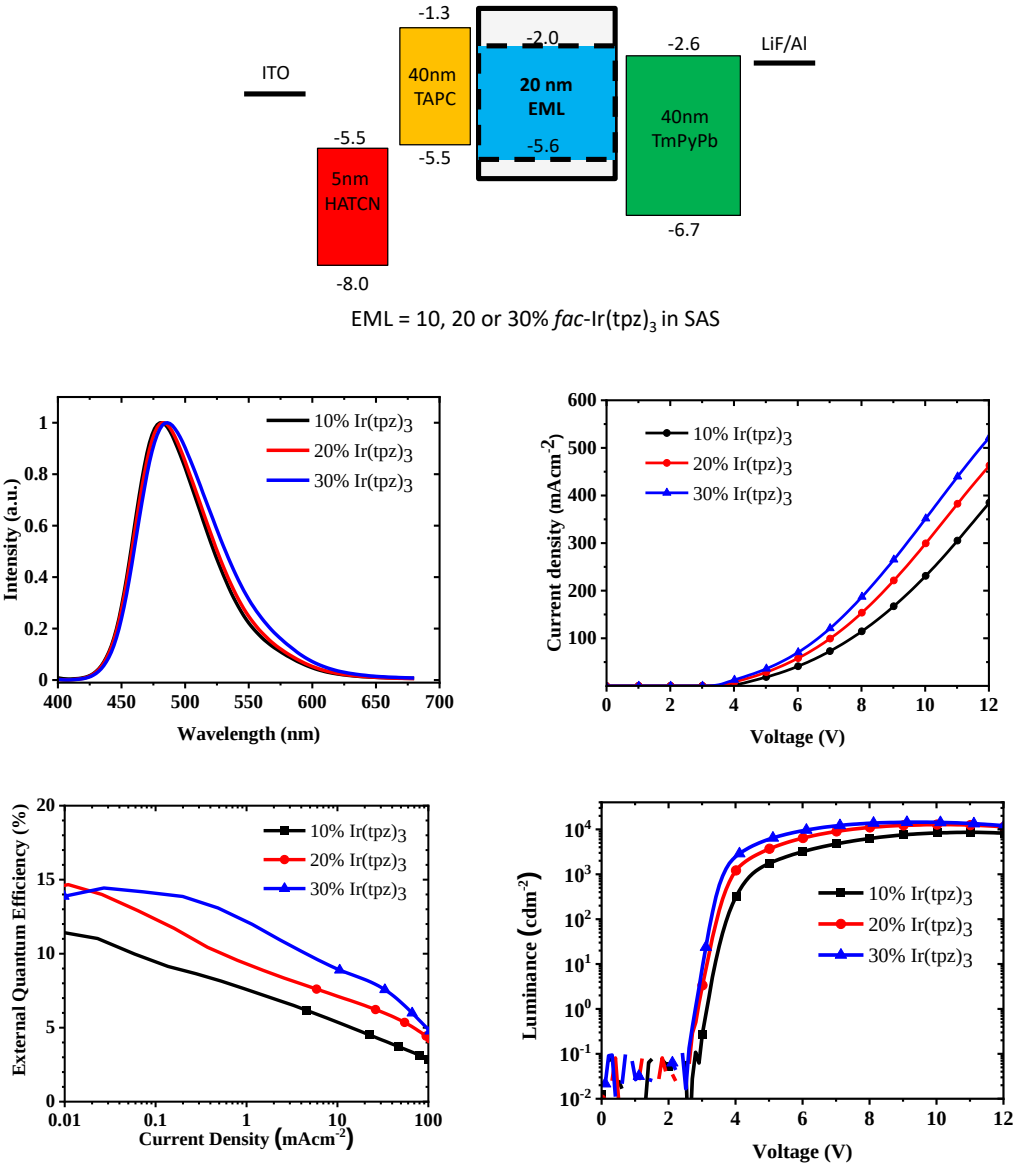
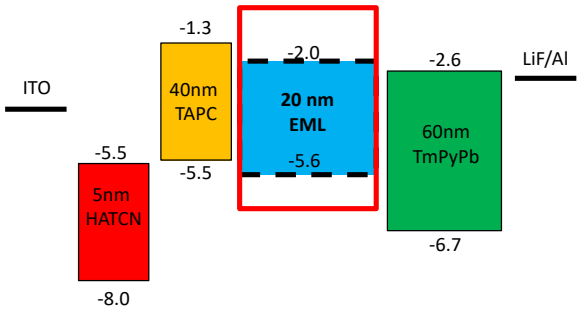


Figure S8. Doping concentration-controlled devices with SAS host material.



EML = 10, 20 or 30% *fac*-Ir(tpz)$_3$ in XAX

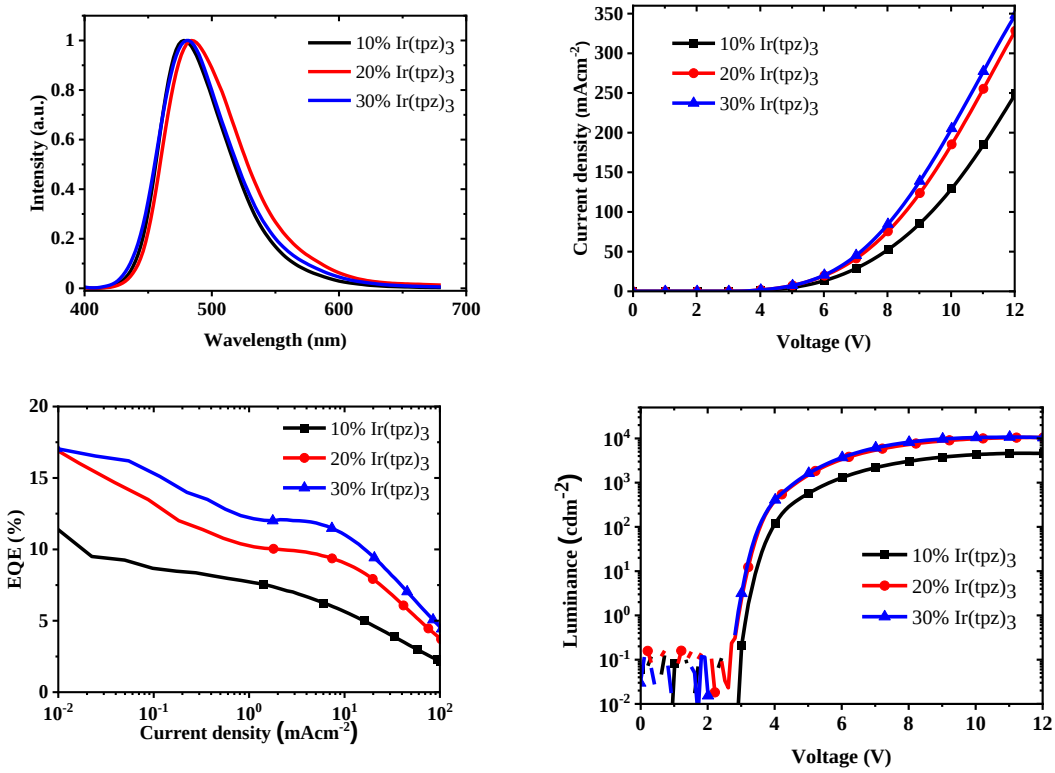


Figure S9. Doping concentration-controlled devices with XAX host material.

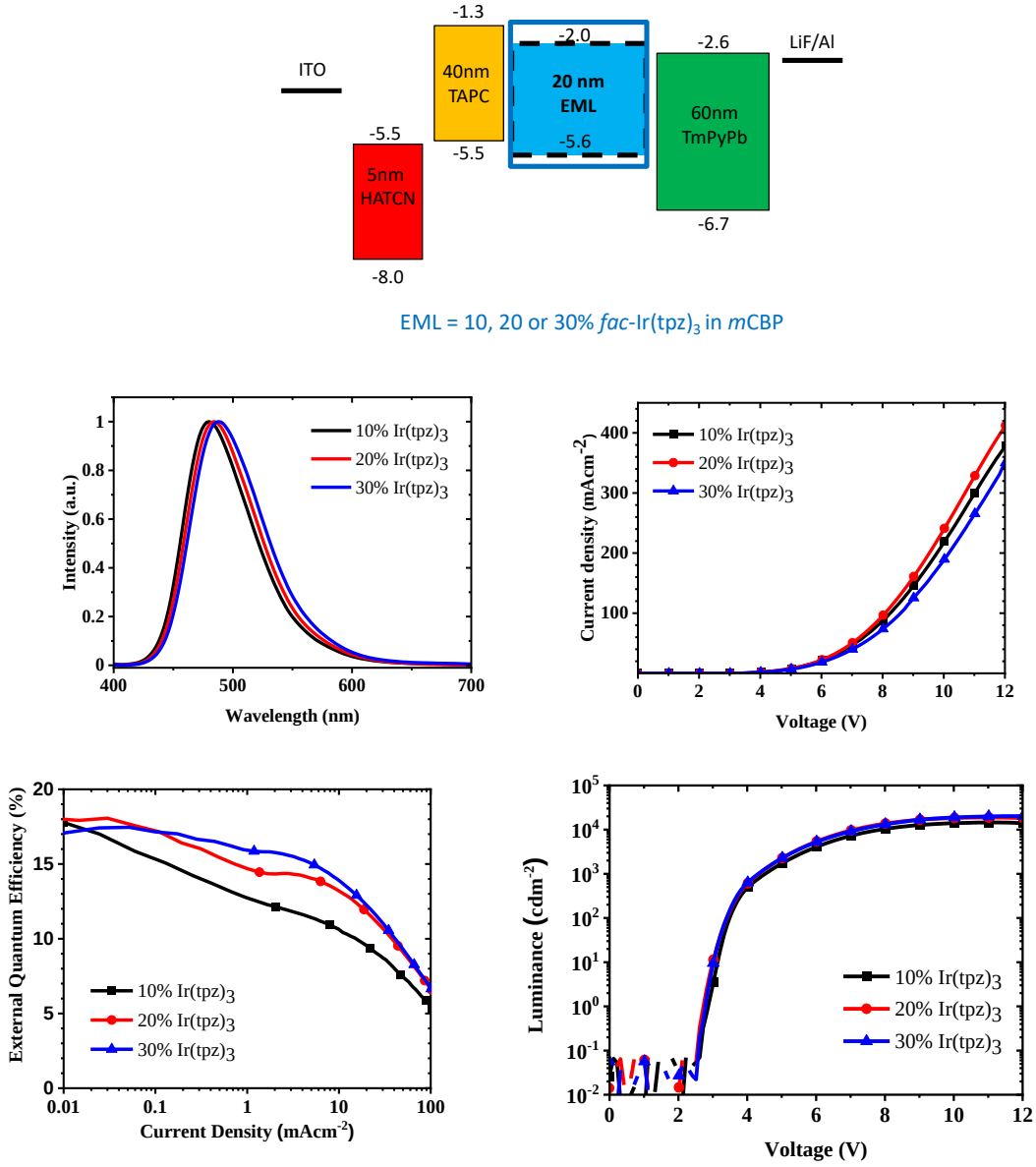
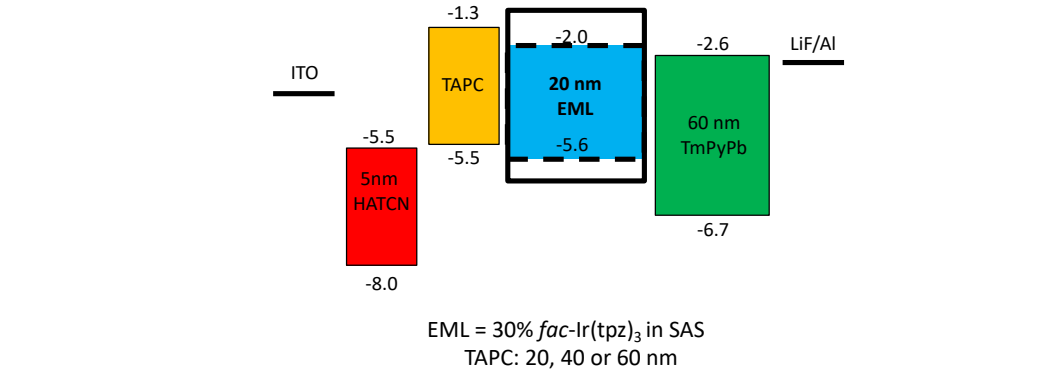


Figure S10. Doping concentration-controlled devices with *m*CBP host material.

Also, thickness-controlled experiments of hole transport layer TAPC and electron transport layer TmPyPb (Figure S11-14) have been done to optimize the device performance for SAS and XAX. Increasing TAPC layer thickness from 20 nm to 60 nm, decreases current density, but luminescence stays same. To further optimize SAS devices, TmPyPb thickness-controlled experiment was performed. As TmPyPb thickness increase from 20 nm to 60 nm, the current density slightly dropped whereas the highest luminescence increases dramatically from 8043 cdm^{-2} to 16712 cdm^{-2}. Hence the device maximum EQE increase from 10% to

18%. The thickness-controlled experiments performed on the ETL and HTL suggests that outcoupling is the major factor that determines the device efficiency instead of charge balance.



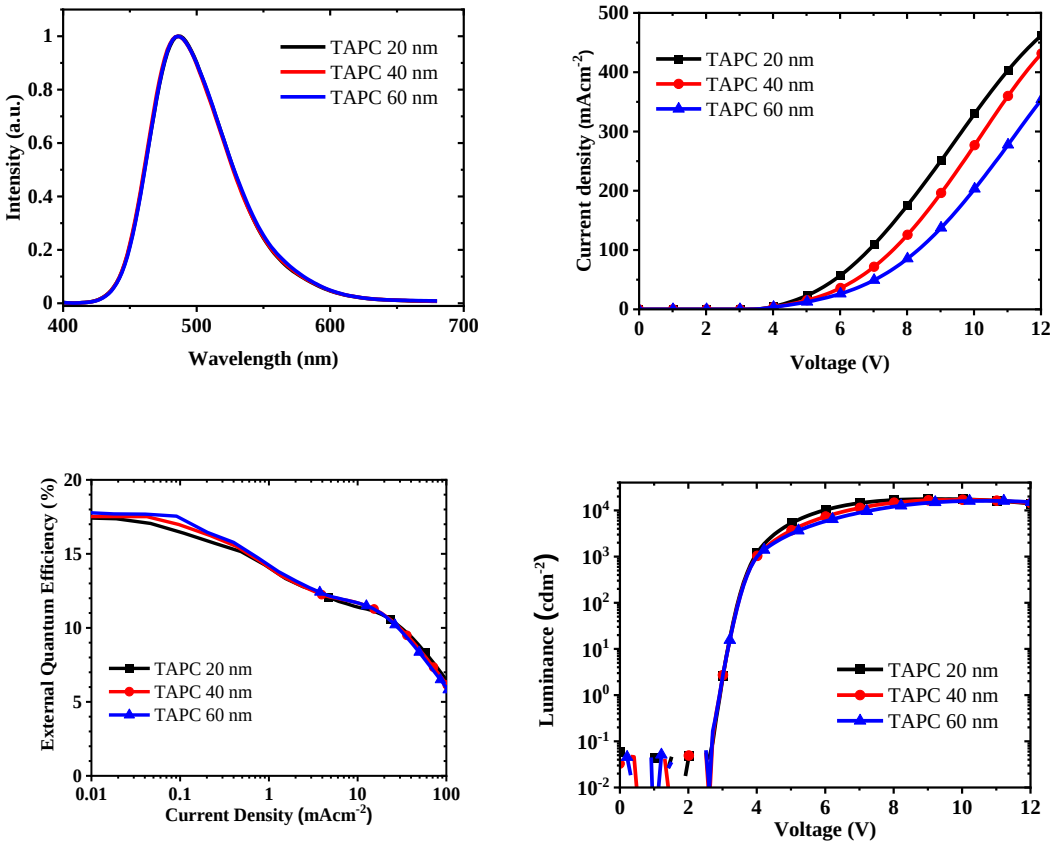
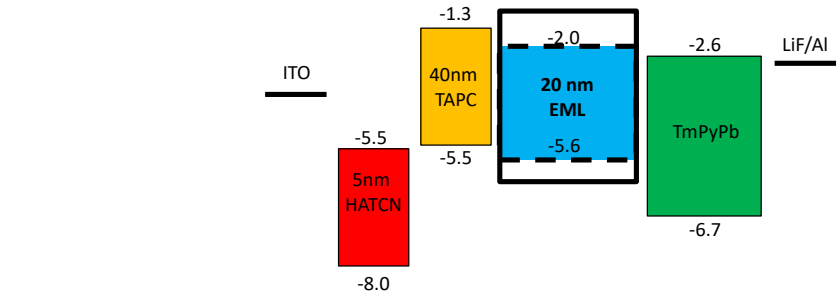


Figure S11. TAPC thickness-controlled devices with SAS host material.



EML = 30% *fac*-Ir(tpz)$_3$ in SAS
TmPyPb: 20, 40 or 60 nm

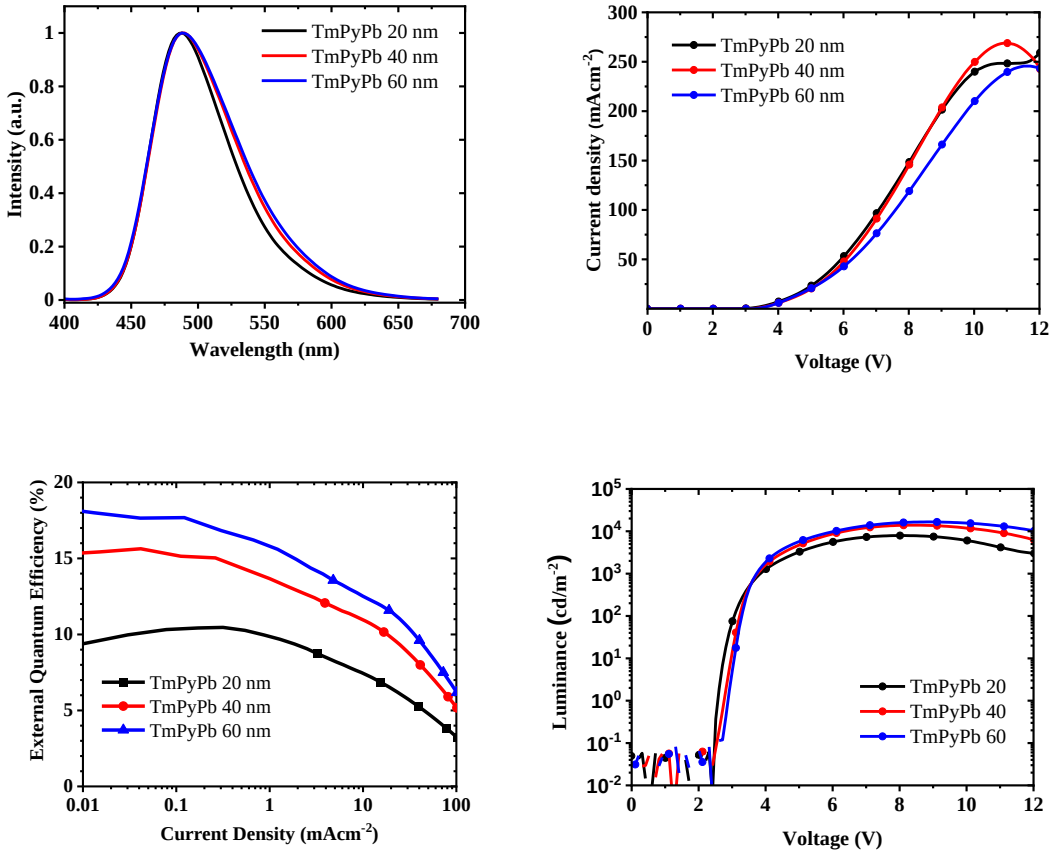
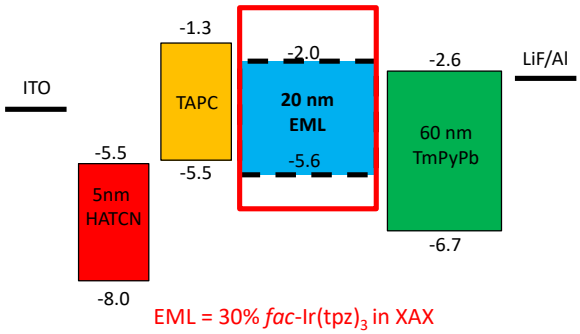


Figure S12. TmPyPb thickness-controlled devices with SAS host material.



EML = 30% *fac*-Ir(tpz)$_3$ in XAX
TAPC: 20, 40 or 60 nm

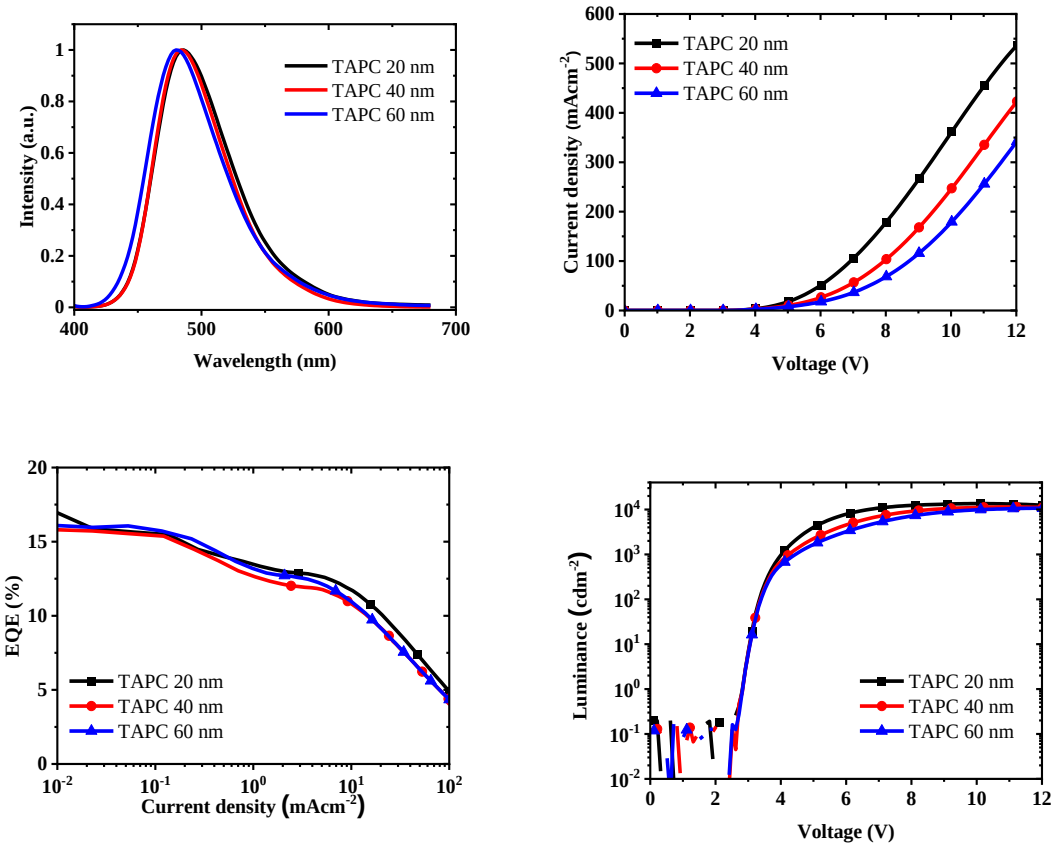


Figure S13. TAPC thickness-controlled devices with XAX host material.

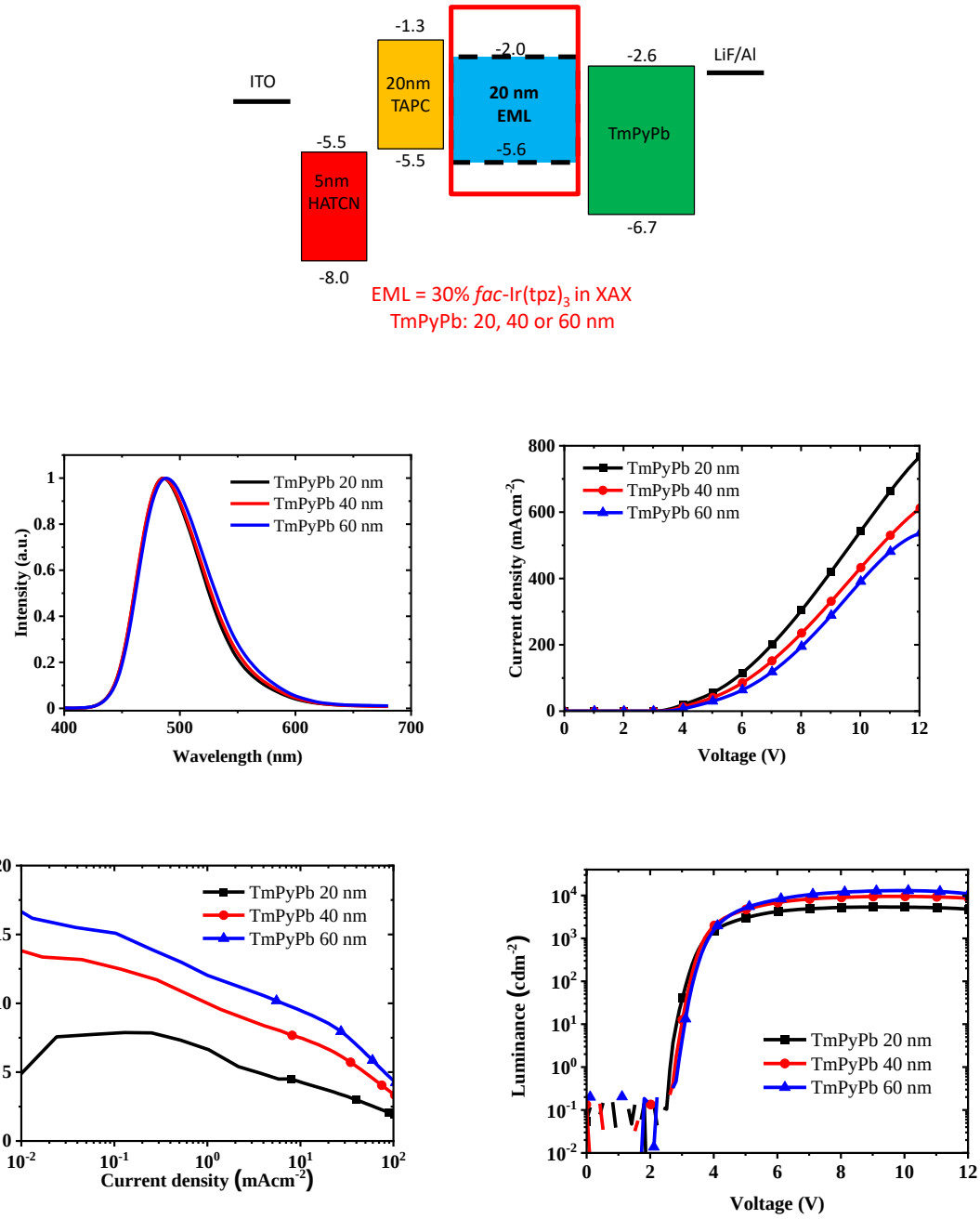


Figure S14. TmPyPb thickness-controlled devices with XAX host material.

NMR Spectra

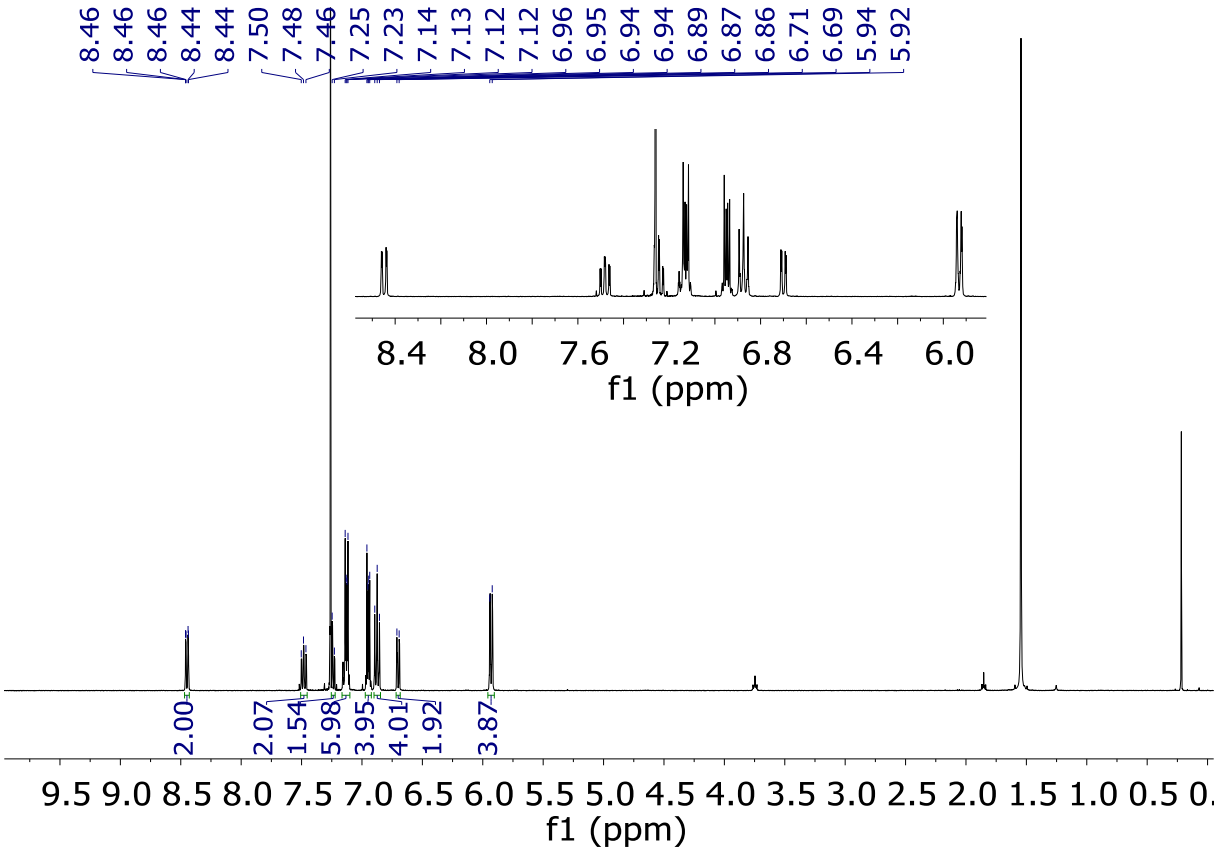


Figure S15. ^{1}H NMR of 1a in $CDCl_3$.

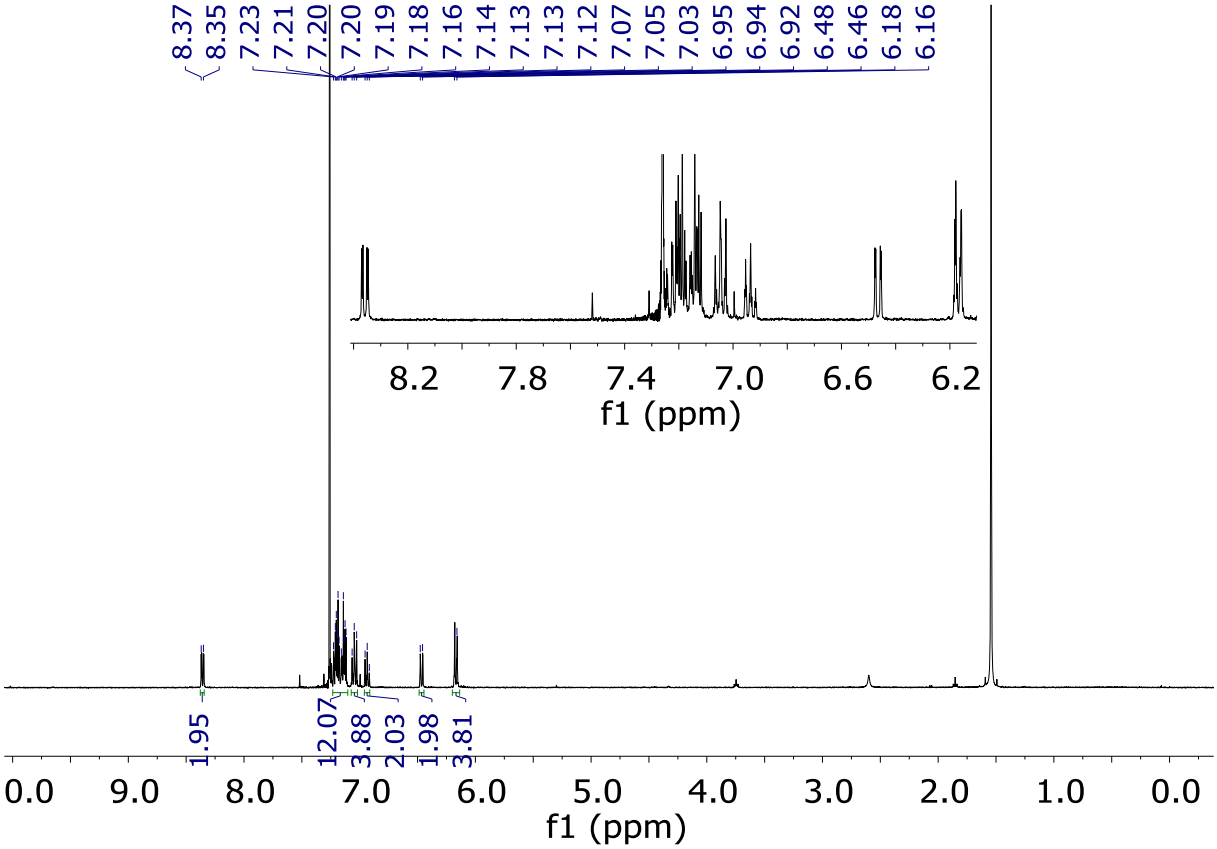


Figure S16. ^{1}H NMR of 1b in $CDCl_3$.

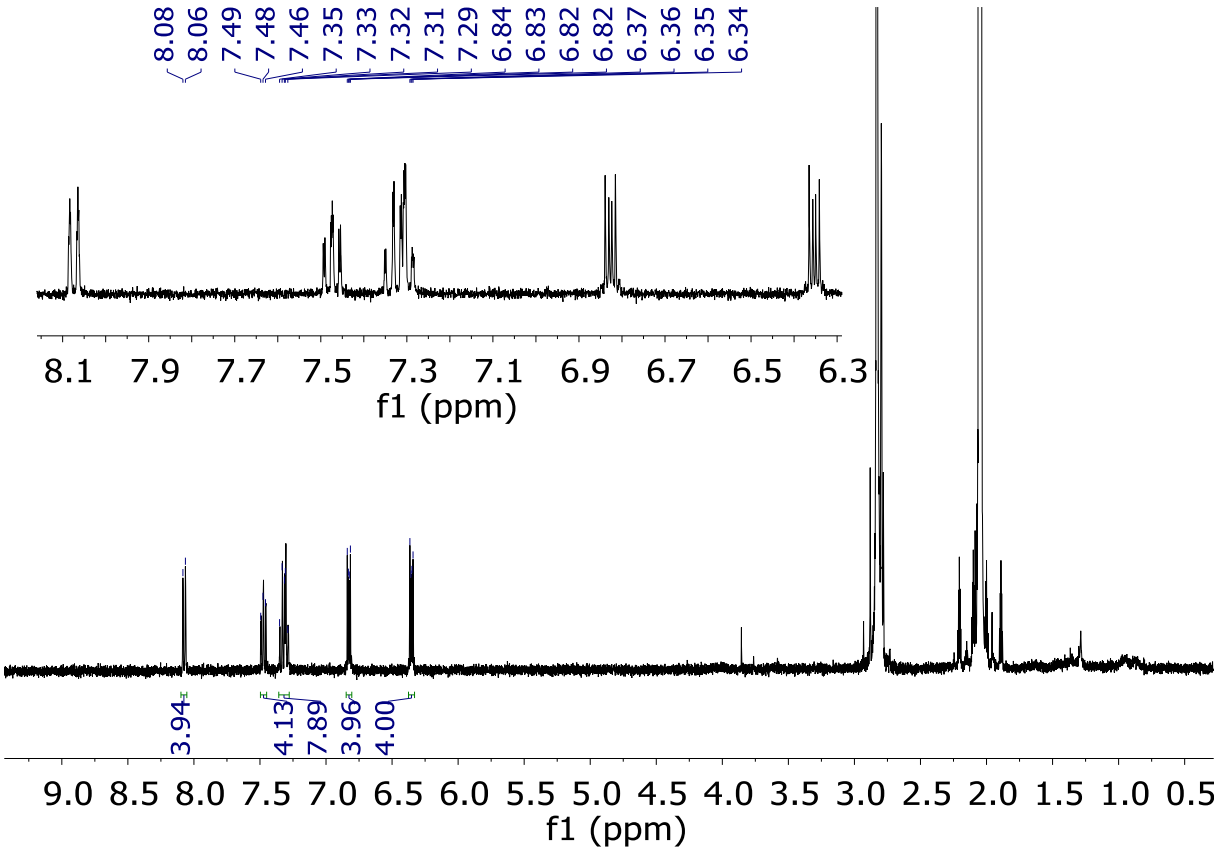


Figure S17. ^{1}H NMR of SAS in acetone-d_6.

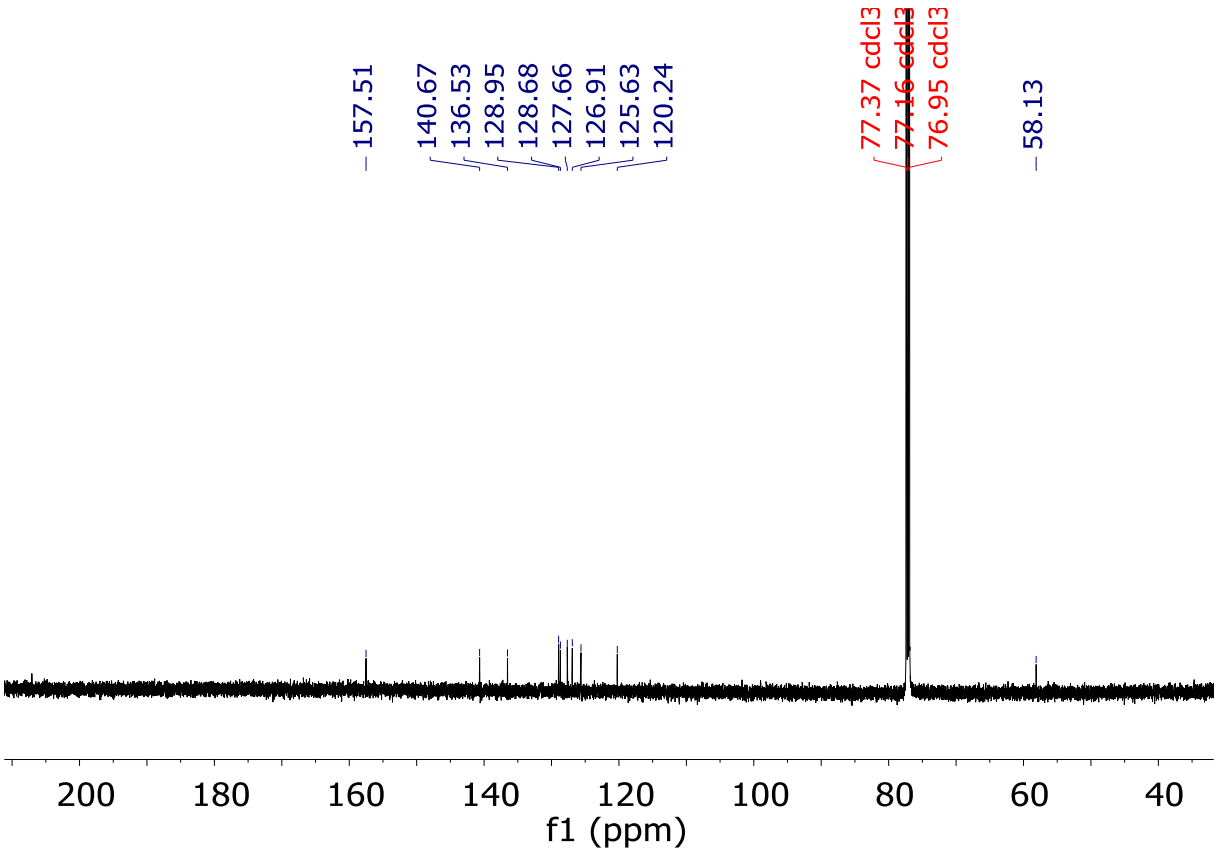


Figure S18. ^{13}C NMR of SAS in $CDCl_3$.

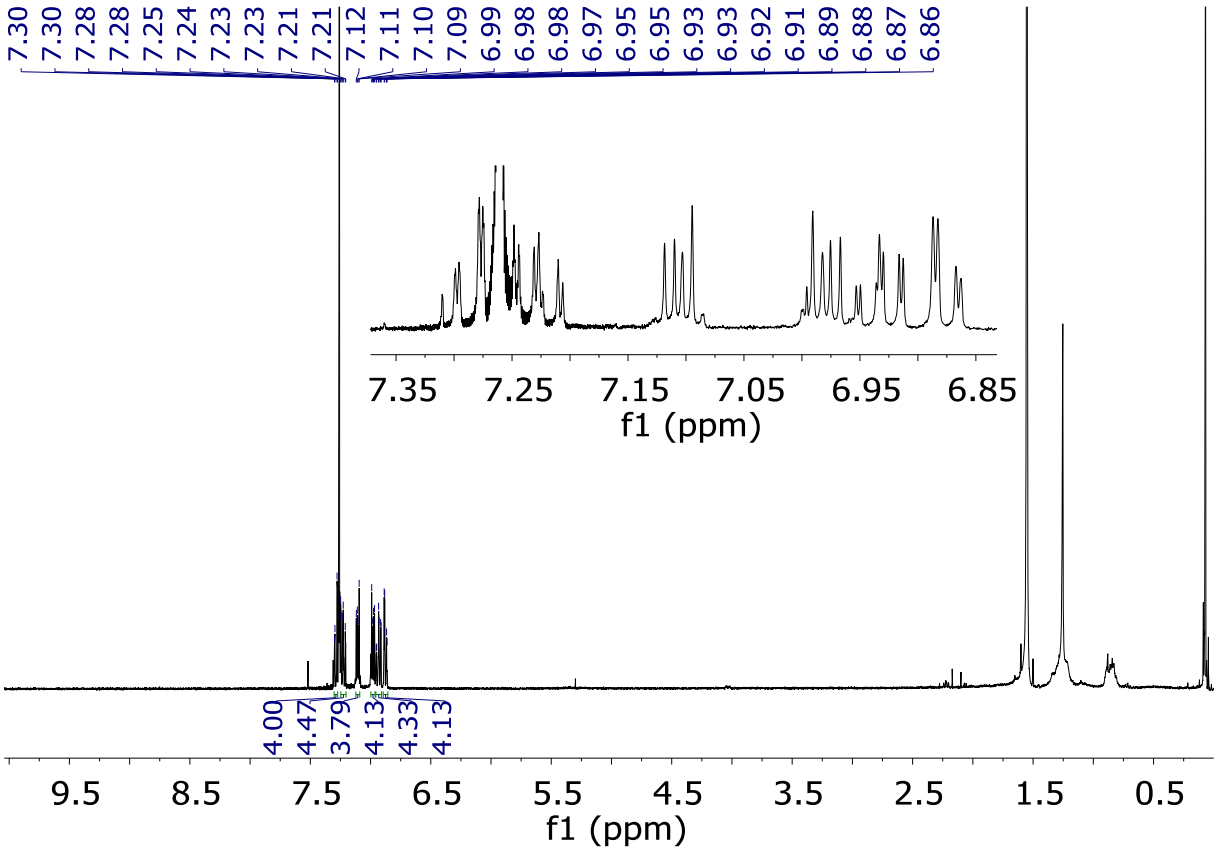


Figure S19. ^{1}H NMR of XAX in $CDCl_3$.

Mass Spectra

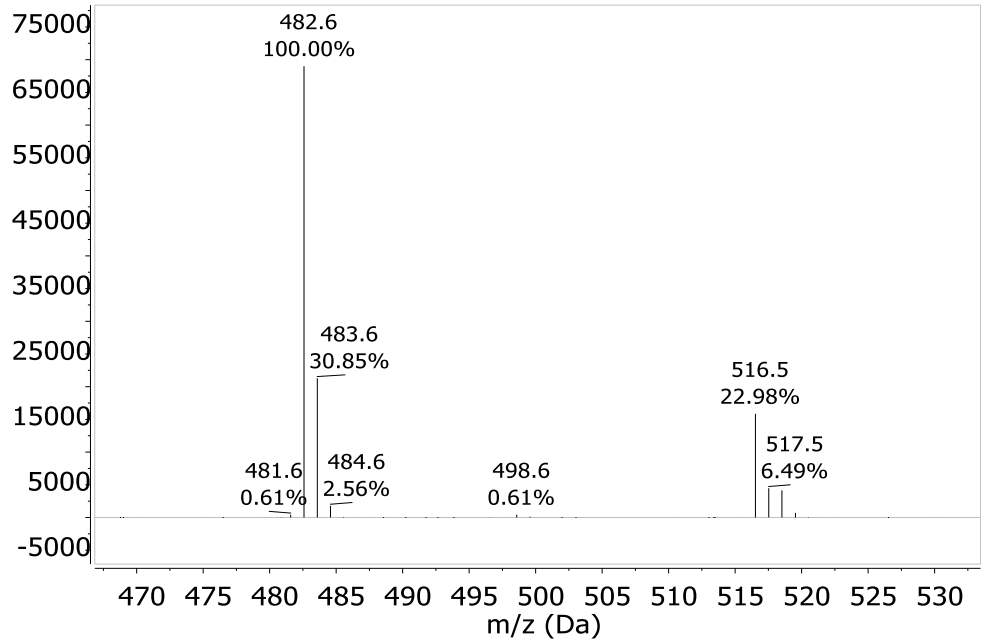


Figure S20. Mass spectrum of 1a.

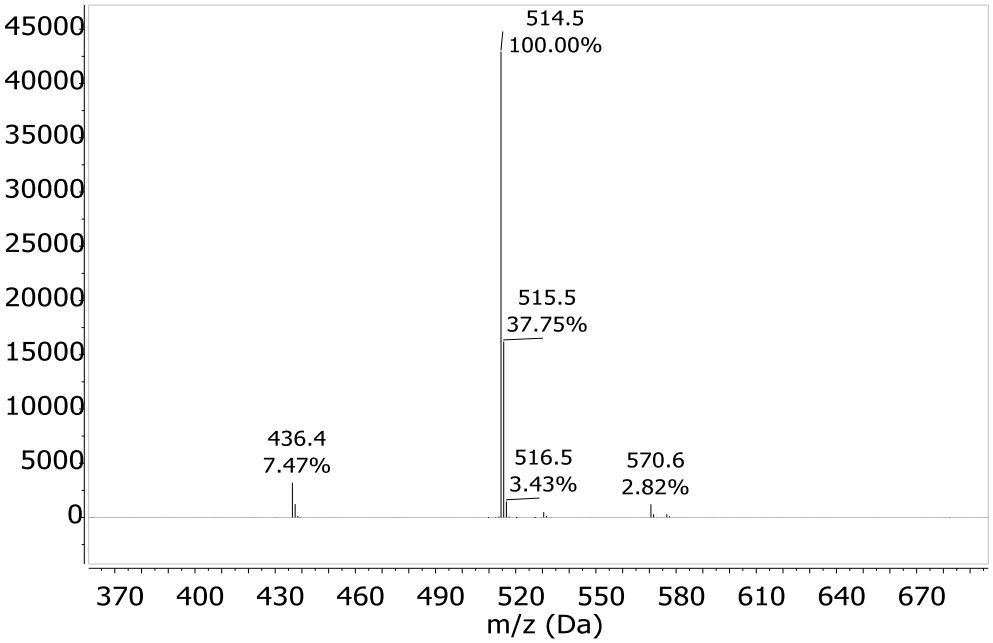


Figure S21. Mass spectrum of 1b

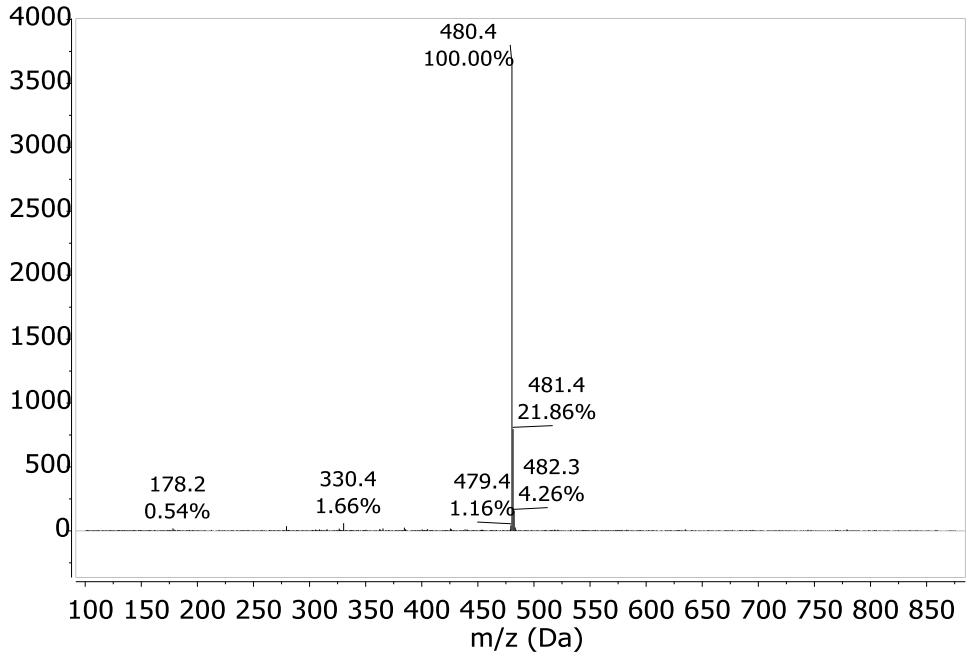


Figure S22. Mass spectrum of SAS.

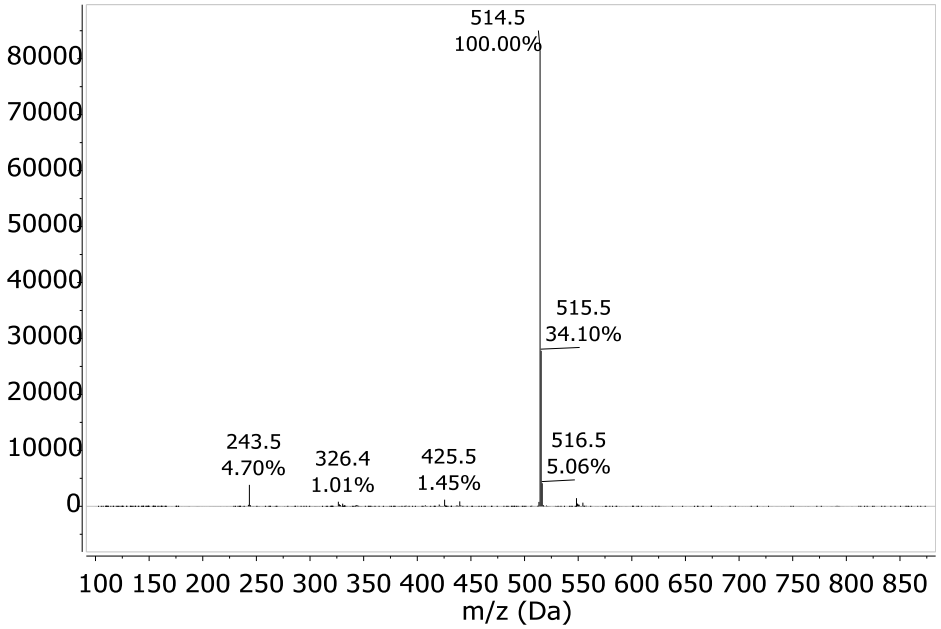


Figure S23. Mass spectrum of XAX.

Computational Results

Table S2. Cartesian coordinates of the optimized geometry of ground state of SAS

		Coordinates (Angstroms)		
ATOM		X	Y	Z
1	H	-1.2523799215	0.0000000000	4.6554948570
2	C	-0.6993110331	0.0000000000	3.7209042896
3	H	-2.4648298220	0.0000000000	2.5117711568
4	C	-1.3794993559	0.0000000000	2.5133581734
5	C	1.3794993559	0.0000000000	2.5133581734

6	C	-0.6995751843	0.0000000000	1.2800772248
7	C	0.6993110331	0.0000000000	3.7209042896
8	C	0.6995751843	0.0000000000	1.2800772248
9	C	-1.5427153221	0.0000000000	0.0000000000
10	H	1.2523799215	0.0000000000	4.6554948570
11	H	2.4648298220	0.0000000000	2.5117711568
12	C	-0.6995751843	0.0000000000	-1.2800772248
13	C	-1.3794993559	0.0000000000	-2.5133581734
14	C	0.6995751843	0.0000000000	-1.2800772248
15	H	2.4648298220	0.0000000000	-2.5117711568
16	C	1.5427153221	0.0000000000	0.0000000000
17	C	-0.6993110331	0.0000000000	-3.7209042896
18	H	-2.4648298220	0.0000000000	-2.5117711568
19	H	-1.2523799215	0.0000000000	-4.6554948570
20	C	0.6993110331	0.0000000000	-3.7209042896
21	H	1.2523799215	0.0000000000	-4.6554948570
22	C	1.3794993559	0.0000000000	-2.5133581734
23	C	2.5282089000	-1.1844143358	0.0000000000
24	C	4.6257585931	-3.0155116011	0.0000000000
25	C	3.8620143942	-0.7349030614	0.0000000000
26	C	2.2427309049	-2.5438358673	0.0000000000
27	C	3.2991866990	-3.4598710412	0.0000000000
28	C	4.9171278827	-1.6502331097	0.0000000000
29	H	1.2142031142	-2.8927766185	0.0000000000
30	H	3.0881871330	-4.5252923747	0.0000000000
31	H	5.9485369752	-1.3084451148	0.0000000000
32	H	5.4354530034	-3.7395094930	0.0000000000
33	C	2.5282089000	1.1844143358	0.0000000000
34	C	4.6257585931	3.0155116011	0.0000000000
35	C	2.2427309049	2.5438358673	0.0000000000
36	C	3.8620143942	0.7349030614	0.0000000000
37	C	4.9171278827	1.6502331097	0.0000000000
38	C	3.2991866990	3.4598710412	0.0000000000
39	H	1.2142031142	2.8927766185	0.0000000000
40	H	5.9485369752	1.3084451148	0.0000000000
41	H	3.0881871330	4.5252923747	0.0000000000
42	H	5.4354530034	3.7395094930	0.0000000000
43	C	-2.5282089000	-1.1844143358	0.0000000000
44	C	-4.6257585931	-3.0155116011	0.0000000000
45	C	-3.8620143942	-0.7349030614	0.0000000000
46	C	-2.2427309049	-2.5438358673	0.0000000000
47	C	-3.2991866990	-3.4598710412	0.0000000000
48	C	-4.9171278827	-1.6502331097	0.0000000000
49	H	-1.2142031142	-2.8927766185	0.0000000000
50	H	-3.0881871330	-4.5252923747	0.0000000000
51	H	-5.9485369752	-1.3084451148	0.0000000000
52	H	-5.4354530034	-3.7395094930	0.0000000000
53	C	-2.5282089000	1.1844143358	0.0000000000
54	C	-4.6257585931	3.0155116011	0.0000000000
55	C	-2.2427309049	2.5438358673	0.0000000000
56	C	-3.8620143942	0.7349030614	0.0000000000

57	C	-4.9171278827	1.6502331097	0.0000000000
58	C	-3.2991866990	3.4598710412	0.0000000000
59	H	-1.2142031142	2.8927766185	0.0000000000
60	H	-5.9485369752	1.3084451148	0.0000000000
61	H	-3.0881871330	4.5252923747	0.0000000000
62	H	-5.4354530034	3.7395094930	0.0000000000

The energy of SAS optimized ground state geometry is -1462.57440262579 hartree.

Table S3. Cartesian coordinates of the optimized geometry of triplet state of SAS

		Coordinates (Angstroms)		
ATOM		X	Y	Z
1	H	-4.6565410346	0.0000000000	-1.2629274272
2	C	-3.7207153016	0.0000000000	-0.7119088178
3	H	-2.5158569187	0.0000000000	-2.4808869253
4	C	-2.5143380671	0.0000000000	-1.3955385829
5	C	-2.5098706895	0.0000000000	1.3648105271
6	C	-1.2801238463	0.0000000000	-0.7183782594
7	C	-3.7187713268	0.0000000000	0.6864792792
8	C	-1.2778145148	0.0000000000	0.6812026475
9	C	0.0000000000	0.0000000000	-1.5619268721
10	H	-4.6529247506	0.0000000000	1.2402654890
11	H	-2.5061478760	0.0000000000	2.4500853843
12	C	1.2801238435	0.0000000000	-0.7183782588
13	C	2.5143380680	0.0000000000	-1.3955385755
14	C	1.2778145171	0.0000000000	0.6812026481
15	H	2.5061478702	0.0000000000	2.4500853913
16	C	0.0000000000	0.0000000000	1.5233955415
17	C	3.7207153013	0.0000000000	-0.7119088088
18	H	2.5158569240	0.0000000000	-2.4808869179
19	H	4.6565410345	0.0000000000	-1.2629274179
20	C	3.7187713269	0.0000000000	0.6864792883
21	H	4.6529247504	0.0000000000	1.2402654986
22	C	2.5098706881	0.0000000000	1.3648105342
23	C	0.0000000000	-1.1848368654	2.5098193652
24	C	0.0000000000	-2.9892552762	4.6756084723
25	C	0.0000000000	-0.6898358200	3.8945487159
26	C	0.0000000000	-2.5264562760	2.2471103456
27	C	0.0000000000	-3.4522207281	3.3236827701
28	C	0.0000000000	-1.6546119696	4.9786564996
29	H	0.0000000000	-2.8899928825	1.2234167086
30	H	0.0000000000	-4.5179081259	3.1217645815
31	H	0.0000000000	-1.3135757640	6.0091546925
32	H	0.0000000000	-3.7227495036	5.4774168562
33	C	0.0000000000	1.1848368563	2.5098193562
34	C	0.0000000000	2.9892552710	4.6756084764
35	C	0.0000000000	2.5264562689	2.2471103524
36	C	0.0000000000	0.6898358105	3.8945487089
37	C	0.0000000000	1.6546119610	4.9786564882
38	C	0.0000000000	3.4522207260	3.3236827727
39	H	0.0000000000	2.8899928794	1.2234167165

40	H	0.0000000000	1.3135757498	6.0091546793
41	H	0.0000000000	4.5179081225	3.1217645806
42	H	0.0000000000	3.7227494949	5.4774168685
43	C	0.0000000000	-1.1843971454	-2.5469050341
44	C	0.0000000000	-3.0156798129	-4.6439985288
45	C	0.0000000000	-0.7348139367	-3.8808247045
46	C	0.0000000000	-2.5436672159	-2.2609938228
47	C	0.0000000000	-3.4598919574	-3.3175052479
48	C	0.0000000000	-1.6502911179	-4.9357014288
49	H	0.0000000000	-2.8924567988	-1.2324277851
50	H	0.0000000000	-4.5251994651	-3.1061230194
51	H	0.0000000000	-1.3091049380	-5.9672761245
52	H	0.0000000000	-3.7394725044	-5.4538381552
53	C	0.0000000000	1.1843971479	-2.5469050359
54	C	0.0000000000	3.0156798094	-4.6439985379
55	C	0.0000000000	2.5436672192	-2.2609938308
56	C	0.0000000000	0.7348139355	-3.8808247052
57	C	0.0000000000	1.6502911126	-4.9357014343
58	C	0.0000000000	3.4598919567	-3.3175052579
59	H	0.0000000000	2.8924568058	-1.2324277945
60	H	0.0000000000	1.3091049292	-5.9672761287
61	H	0.0000000000	4.5251994650	-3.1061230319
62	H	0.0000000000	3.7394724985	-5.4538381649

The energy of SAS optimized triplet state geometry is -1462.46543958210 hartree.

Table S4. Cartesian coordinates of the optimized ground state geometry of XAX

		Coordinates (Angstroms)		
ATOM		X	Y	Z
1	H	-1.5354353747	4.5698437445	0.0000000000
2	C	-0.9266760187	3.6705466371	0.0000000000
3	H	-2.6166239635	2.3645319339	0.0000000000
4	C	-1.5336287409	2.4241723559	0.0000000000
5	C	1.2195971923	2.5921969655	0.0000000000
6	C	-0.7813797136	1.2330738430	0.0000000000
7	C	0.4691607005	3.7570348248	0.0000000000
8	C	0.6150648406	1.3202020008	0.0000000000
9	C	-1.5489398163	-0.1049739416	0.0000000000
10	H	0.9633752275	4.7239316527	0.0000000000
11	H	2.3035204737	2.6522242238	0.0000000000
12	C	-0.6150648406	-1.3202020008	0.0000000000
13	C	-1.2195971923	-2.5921969655	0.0000000000
14	C	0.7813797136	-1.2330738430	0.0000000000
15	H	2.6166239635	-2.3645319339	0.0000000000
16	C	1.5489398163	0.1049739416	0.0000000000
17	C	-0.4691607005	-3.7570348248	0.0000000000
18	H	-2.3035204737	-2.6522242238	0.0000000000
19	H	-0.9633752275	-4.7239316527	0.0000000000
20	C	0.9266760187	-3.6705466371	0.0000000000
21	H	1.5354353747	-4.5698437445	0.0000000000
22	C	1.5336287409	-2.4241723559	0.0000000000

23	C	2.4453179884	0.1537481535	1.2534793776
24	C	4.0644924908	0.1089955571	3.5651413222
25	C	3.8070712172	-0.1543124989	1.1835504033
26	C	1.9198911307	0.4614712462	2.5168313491
27	C	2.7087896721	0.4376379835	3.6626003539
28	C	4.6162931056	-0.1807958177	2.3236999824
29	H	0.8724857249	0.7344149913	2.5922427085
30	H	2.2703164420	0.6778211760	4.6260956553
31	H	5.6672974734	-0.4228435099	2.2060270527
32	H	4.6908237354	0.0888024293	4.4517694228
33	C	2.4453179884	0.1537481535	-1.2534793776
34	C	4.0644924908	0.1089955571	-3.5651413222
35	C	1.9198911307	0.4614712462	-2.5168313491
36	C	3.8070712172	-0.1543124989	-1.1835504033
37	C	4.6162931056	-0.1807958177	-2.3236999824
38	C	2.7087896721	0.4376379835	-3.6626003539
39	H	0.8724857249	0.7344149913	-2.5922427085
40	H	5.6672974734	-0.4228435099	-2.2060270527
41	H	2.2703164420	0.6778211760	-4.6260956553
42	H	4.6908237354	0.0888024293	-4.4517694228
43	C	-2.4453179884	-0.1537481535	1.2534793776
44	C	-4.0644924908	-0.1089955571	3.5651413222
45	C	-3.8070712172	0.1543124989	1.1835504033
46	C	-1.9198911307	-0.4614712462	2.5168313491
47	C	-2.7087896721	-0.4376379835	3.6626003539
48	C	-4.6162931056	0.1807958177	2.3236999824
49	H	-0.8724857249	-0.7344149913	2.5922427085
50	H	-2.2703164420	-0.6778211760	4.6260956553
51	H	-5.6672974734	0.4228435099	2.2060270527
52	H	-4.6908237354	-0.0888024293	4.4517694228
53	C	-2.4453179884	-0.1537481535	-1.2534793776
54	C	-4.0644924908	-0.1089955571	-3.5651413222
55	C	-1.9198911307	-0.4614712462	-2.5168313491
56	C	-3.8070712172	0.1543124989	-1.1835504033
57	C	-4.6162931056	0.1807958177	-2.3236999824
58	C	-2.7087896721	-0.4376379835	-3.6626003539
59	H	-0.8724857249	-0.7344149913	-2.5922427085
60	H	-5.6672974734	0.4228435099	-2.2060270527
61	H	-2.2703164420	-0.6778211760	-4.6260956553
62	H	-4.6908237354	-0.0888024293	-4.4517694228
63	O	-4.4424355256	0.4560224928	0.0000000000
64	O	4.4424355256	-0.4560224928	0.0000000000

The energy of XAX optimized ground state geometry is -1612.99292887600 hartree.

Table S5. Cartesian coordinates of the optimized triplet state geometry of XAX

		Coordinates (Angstroms)		
ATOM		X	Y	Z
1	H	-4.4734553420	-0.0925756870	-1.6397408151
2	C	-3.5864288330	-0.0443782444	-1.0149815714
3	H	-2.2574277557	-0.2856335802	-2.6649990958
4	C	-2.3299397899	-0.1457315185	-1.5927096596

5	C	-2.5484402957	0.1473465313	1.1426111446
6	C	-1.1510075669	-0.0862172849	-0.8184020099
7	C	-3.7001584760	0.1117449163	0.3694887920
8	C	-1.2669883848	0.0506522881	0.5728566984
9	C	0.2108526451	-0.1002003322	-1.5470382721
10	H	-4.6754074890	0.1916190703	0.8399562501
11	H	-2.6306350142	0.2440122720	2.2209418772
12	C	1.4016353636	-0.1401150382	-0.5868501145
13	C	2.6839234391	-0.2277057034	-1.1622458118
14	C	1.2825815330	-0.0449914093	0.8031698214
15	H	2.3726977096	0.0251530201	2.6621086303
16	C	-0.0720953620	0.0385931595	1.5346825216
17	C	3.8314375904	-0.2286383024	-0.3843949493
18	H	2.7644042319	-0.2988838293	-2.2426487623
19	H	4.8081677961	-0.3004681567	-0.8533453154
20	C	3.7140020065	-0.1353079054	1.0064442990
21	H	4.5993441441	-0.1328085437	1.6353775296
22	C	2.4562287053	-0.0458783791	1.5828569917
23	C	-0.1881546696	-1.1960290170	2.4523139342
24	C	-0.2650663991	-3.4810185368	4.1075470061
25	C	0.0465184930	-1.1072274087	3.8271737464
26	C	-0.4792559706	-2.4647879442	1.9301185080
27	C	-0.5166762308	-3.5972718210	2.7366697285
28	C	0.0111067583	-2.2346440576	4.6544872558
29	H	-0.6884923997	-2.5546726146	0.8689705772
30	H	-0.7429905937	-4.5650458342	2.3001932422
31	H	0.1976675911	-2.1028572978	5.7151122537
32	H	-0.2924248854	-4.3570861678	4.7483460046
33	C	-0.0937154428	1.3111968627	2.4009034455
34	C	-0.0283612931	3.6572688107	3.9690348487
35	C	-0.2998462642	2.5753621011	1.8293646869
36	C	0.1287252903	1.2595349764	3.7799235140
37	C	0.1641376866	2.4173349848	4.5642003444
38	C	-0.2662887346	3.7374085322	2.5931812648
39	H	-0.4963686082	2.6381682095	0.7641689103
40	H	0.3369936543	2.3136506073	5.6302528435
41	H	-0.4278588867	4.7005291890	2.1191831262
42	H	-0.0017469012	4.5568217770	4.5764996982
43	C	0.2582655316	-1.3069500085	-2.4976004500
44	C	0.2680425583	-3.5263189372	-4.2462451598
45	C	-0.0216199473	-1.1649895476	-3.8640323104
46	C	0.5364613178	-2.5967048582	-2.0321872157
47	C	0.5468719060	-3.6985134361	-2.8858999319
48	C	-0.0179017818	-2.2598310490	-4.7380550498
49	H	0.7685639451	-2.7289318511	-0.9800845129
50	H	0.7798817039	-4.6834481074	-2.4941198930
51	H	-0.2422841163	-2.0881068275	-5.7854062947
52	H	0.2752073213	-4.3768412272	-4.9209033336
53	C	0.2929678242	1.1813699799	-2.3643306516
54	C	-0.5145962770	3.5846843126	-3.7392377828
55	C	0.6422411098	2.4599605557	-1.8414562163

56	C	-0.3308245104	1.1937634851	-3.7328513921
57	C	-0.7472848509	2.3649570312	-4.3544386595
58	C	0.2667752643	3.6116267381	-2.4756359351
59	H	1.2067934496	2.5122775972	-0.9154446157
60	H	-1.2082564827	2.2990550100	-5.3359735010
61	H	0.5617358803	4.5743459731	-2.0686237543
62	H	-0.8558382544	4.5129024137	-4.1804386479
63	O	-0.3542546511	0.0404990131	-4.4452151974
64	O	0.3323473105	0.0806860463	4.4606850875

The energy of XAX optimized triplet state geometry is -1612.86298083688 hartree.