Library of potential nucleobase analogue structures

Three lowest energy electronic transitions were predicted by TDDFT B3LYP/6-311+G(2d) calculations on either the B3LYP/6-31G** or AM1 optimized geometries. All spectra of nitro-aromatics have been predicted without solvation, while the transitions of most non-nitro compounds have been predicted with a CPCM solvation model for $\rm H_2O$ unless otherwise stated. f denotes oscillator strength.

ADENINE ANALOGUES

qA1	qA2	qA3	qA4	-qA5
NH NH	NH NH N	NH NH	N N N N N N N N N N N N N N N N N N N	NH N
350 nm f=0.060 330 nm f=0.20	359 nm f=0.20 341 nm f=0.083	360 nm f=0.041 337 nm f=0.22	359 nm f=0.035 324 nm f=0.18	355 nm f=0.30 347 nm f=0.003
283 nm f=0.10	281 nm f=0.091	277 nm f=0.22	279 nm f=0.18	283 nm f=0.10
qA6	qA7	qA8	qA9	qA10
N N N N N N N N N N N N N N N N N N N	N NH	NH NH NH	NH NH NN N	O NH
368 nm f=0.088	388 nm f=0.31	376 nm f=0.15	496 nm f=0.12	478 nm f=0.09
339 nm f=0.17 279 nm f=0.051	346 nm f=0.003 298 nm f=0.0045	346 nm f=0.14 287 nm f=0.0047	346 nm f=0.017 334 nm f=0.00	340 nm f=0.07 331 nm f=0.00
qA11	qA12	qA13	qA14	qA15
470 nm f=0.17 355 nm f=0.072	480 nm f=0.0971 354 nm f=0.1501	450 nm f=0.052 354 nm f=0.13	459 nm f=0.086 350 nm f=0.072	504 nm f=0.14 353 nm f=0.088
347 nm f=0.00	330 nm f=0.0000	342 nm f=0.000	347 nm f=0.000	334 nm f=0.000

GUANINE ANALOGUES

qG1	qG2	qG3	m qG4	qG5
NH NH ₂	NH NH ₂	N NH NH ₂	N NH NH ₂	N NH NH ₂
347 nm f=0.049	366 nm f = 0.20	373 nm f = 0.051	369 nm f=0.069	366 nm f=0.18
337 nm f = 0.17	351 nm f=0.035	340 nm f = 0.17	334 nm f = 0.11	351 nm f=0.078
308 nm f=0.18	303 nm f=0.17	302 nm f=0.18	299 nm f=0.18	305 nm f=0.17
qG6	qG7	qG8	m qG9	qG10
N N N N N N N N N N N N N N N N N N N	N NH NH ₂	N NH NH ₂	N N N N N N N N N N N N N N N N N N N	N NH NH ₂
386 nm f=0.11 353 nm f=0.085 295 nm f=0.16	408 nm f=0.2 356 nm f=0.035 313 nm f=0.004	393 nm f=0.099 356 nm f=0.14 295 nm f=0.004	494 nm f=0.054 348 nm f=0.005 334 nm f=0.000	474 nm f=0.14 344 nm f=0.031 333 nm f=0.000

CYTOSINE ANALOGUES

$tC^{c}1$	$\mathrm{tC^{c}2}$	tC ^c 3	$\mathrm{tC^{c}4}$	$\mathrm{tC}^{\mathrm{c}}5$
	N	N	N	N
NH	NH	NH	NH	NH
N	N		N	N
370 nm f = 0.35	370 nm f = 0.61	382 nm f = 0.23	353 nm f = 0.63	376 nm f = 0.55
342 nm f = 0.36	347 nm f = 0.00	356 nm f = 0.00	345 nm f = 0.00	352 nm f = 0.00
337 nm f=0.00	332 nm f = 0.11	344 nm f=0.39	334 nm f = 0.044	331 nm f=0.16

tC ^C 6	tCC7	tCC8	tC ^C 9	tCC10
358 nm f=0.69 357 nm f=0.0004 326 nm f=0.010	385 nm f=0.66 370 nm f=0.0001 348 nm f=0.0020	385 nm f=0.40 374 nm f=0.00 346 nm f=0.0020	464 nm f=0.00 445 nm f=0.24 382 nm f=0.17	426 nm f=0.00 391 nm f=0.21 369 nm f=0.17
tCC11	tCC12	tC ^c 13	tCC14	tC ^c 15
472 nm f=0.00 429 nm f=0.36 372 nm f=0.085	441 nm f=0.00 394 nm f=0.26 371 nm f=0.21	437 nm f=0.00 385 nm f=0.23 363 nm f=0.0083	449 nm f=0.00 407 nm f=0.33 357 nm f=0.00	480 nm f=0.00 449 nm f=0.30 379 nm f=0.11
tCC16	tCC17	tC ^c 18	tCC19	tCC20
443 nm f=0.00 390 nm f=0.46 362 nm f=0.037	456 nm f=0.00 395 nm f=0.43 364 nm f=0.0052	497 nm f=0.00 437 nm f=0.41 381 nm f=0.090	467 nm f=0.00 397 nm f=0.52 361 nm f=0.032	460 nm f=0.00 395 nm f=0.29 364 nm f=0.0074
tC ^N 1 406 nm f=0.28 385 nm f=0.0002	394 nm f=0.0025 394 nm f=0.56	tCN3 415 nm f=0.21 405 nm f=0.0001	393 nm f=0.0002 376 nm f=0.53	tCN5 403 nm f=0.53 400 nm f=0.0001
365 nm f=0.0002 365 nm f=0.43	356 nm f=0.0001	352 nm f=0.0001	361 nm f=0.33	354 nm f=0.0001

tC'N6	tC ^N 7	tC ^N 8	tC ^N 9	tC ^N 10
404 nm f=0.0001 374 nm f=0.68 373 nm f=0.0000	418 nm f=0.00 404 nm f=0.62 388 nm f=0.0002	423 nm f=0.00 410 nm f=0.37 375 nm f=0.0002	480nm f=0.00 435 nm f=0.23 393 nm f=0.0002	454 nm f=0.0001 388 nm f=0.34 375 nm f=0.0004
tC'N11	tC ^N 12	tC ^N 13	tC'N14	tC ^N 15
487 nm f=0.00 419 nm f=0.36 403 nm f=0.0001	462 nm f=0.00 389 nm f=0.0002 385 nm f=0.47	469 nm f=0.00 396 nm f=0.19 385 nm f=0.0003	471 nm f=0.00 396 nm f=0.32 388 nm f=0.0003	495 nm f=0.00 436 nm f=0.30 412 nm f=0.0001
tC'N16	tC ^N 17	tC ^N 18	tC ^N 19	tC ^N 20
469 nm f=0.0001 392 nm f=0.0002 391 nm f=0.43	476 nm f=0.0001 404 nm f=0.033 386 nm f=0.40	510 nm f=0.00 435 nm f=0.00 426 nm f=0.39	488 nm f=0.00 414 nm f=0.00 393 nm f=0.50	485 nm f=0.00 414 nm f=0.054 403 nm f=0.19
454 nm f=0.00 412 nm f=0.29	467 nm f=0.0001 374 nm f=0.31	349 nm f=0.014 344 nm f=0.12	346 nm f=0.21 342 nm f=0.07	
363 nm f=0.41	321 nm f=0.18	306 nm f=0.12	309 nm f=0.097	

tC^{O} 1	tC°_{2}	tC^{o}_{3}	tC ^o 4	$\mathrm{tC}^{\mathrm{o}}5$
	N			N
o NH	NH	O NH	O NH	NH
N	N	N		
N - (0.10	261 6 0.21	0.50	202 5 0 12	256 6 0.21
362 nm f=0.19 294 nm f=0.091 290 nm f=0.003	361 nm f=0.21 308 nm f=0.10 288 nm f=0.084	352 nm f=0.12 300 nm f=0.20 281 nm f=0.009	363 nm f=0.12 290 nm f=0.074 286 nm f=0.049	356 nm f=0.21 310 nm f=0.14 288 nm f=0.057
1290 mm 1=0.003 tC ⁰ 6	tC ⁰ 7	tC ⁰ 8	tC ^o 9	tC ⁰ 10
	N N	N N	N*—O-	-O-N+
NH	O NH	NH		
	N	N	NH	NH
N		N——	N N	N N
365 nm f=0.13	358 nm f=0.30	350 nm f=0.094	438 nm f=0.097	452 nm f=0.072
304 nm f=0.072 287 nm f=0.14	332 nm f=0.037 283 nm f=0.086	315 nm f=0.26 283 nm f=0.051	349 nm f=0.037 333 nm f=0.25	333 nm f=0.21 332 nm f=0.00
tC ⁰ 11	tC ⁰ 12	tC ⁰ 13	tC ⁰ 14	tC ⁰ 15
N*0"	*O—N*	-0 — N	N==	N+—0-
N	N. N	*		N
	NA NA	NH	O' NH	O NH
N	N	N——(N	N——W	N
418 nm f=0.12	454 nm f=0.073	424 nm f=0.042	417 nm f=0.045	444 nm f=0.10
346 nm f=0.21 342 nm f=0.00	331 nm f=0.00 330 nm f=0.13	342 nm f=0.00 324 nm f=0.10	342 nm f=0.00 340 nm f=0.18	347 nm f=0.080 334 nm f=0.18
tC ⁰ 16	tC ⁰ 17	tC ⁰ 18	tC ⁰ 19	tC ^O 20
N	N — N		N. N	N,
Q NH	NH	NH NH	O, NH	NH
	N	N	N	, .
<u>)</u>	N	N——	\n	<u>)</u>
434 nm f=0.097 343 nm f=0.00	397 nm f = 0.043 354 nm f = 0.057	419 nm f=0.14 353 nm f=0.17	407 nm f = 0.058 357 nm f = 0.0055	407 nm f=0.058 357 nm f=0.0055
332 nm f=0.040	349 nm f=0.13	340 nm f=0.00	333 nm f=0.0047	333 nm f=0.0047

tC ^s 1 (tC)	$\mathrm{tC^s}2$	tC ^s 3	$\mathrm{tC^s}4$	$-$ t $C^{s}5$
	N N	N N	N N	N NH
S NH	S NH	S NH	N	N
369 nm f=0.092 309 nm f=0.077 297 nm f=0.029 tC ⁵ 6	370 nm f=0.084 320 nm f=0.11 306 nm f=0.098 tC ⁵ 7	370 nm f=0.044 312 nm f=0.19 298 nm f=0.024 tC ⁸ 8	373 nm f=0.051 308 nm f=0.076 297 nm f=0.052 tC ^s 9	372 nm f=0.082 326 nm f=0.17 306 nm f=0.060
NH NH	S NH	N NH	N'-O'	tCS10 (tC _{nitro})
380 nm f=0.049 323 nm f=0.060 304 nm f=0.14 tC*11	375 nm f=0.15 363 nm f=0.092 303 nm f=0.097 tC ^s 12	380 nm f=0.020 334 nm f=0.25 302 nm f=0.055 tC ^s 13	458 nm f=0.080 361 nm f=0.015 345 nm f=0.16 tC ^s 14	458 nm f=0.043 346 nm f=0.063 331 nm f=0.0042 tC ^s 15
NH S	466 nm f=0.046	437 nm f=0.023	NH NH NH 437 nm f=0.042	омт—о- мы 478 nm f=0.098
357 nm f=0.14 344 nm f=0.0007	347 nm f=0.016 330 nm f=0.0003	343 nm f=0.015 342 nm f=0.0015	350 nm f=0.11 344 nm f=0.0098	361 nm f=0.082 352 nm f=0.11
tC516	tCS17	tC ^s 18	tCs19	tCS20
457 nm f=0.066 360 nm f=0.0038 342 nm f=0.0011	416 nm f=0.038 364 nm f=0.12 351 nm f=0.0062	458 nm f=0.13 375 nm f=0.13 344 nm f=0.0033	462 nm f=0.077 371 nm f=0.018 341 nm f=0.0008	431 nm f=0.038 366 nm f=0.029 357 nm f=0.0038

tCC22	tC ^{IN} 22	tC ^O 22	tCS22	
491 nm f=0.13	603 nm f=0.15	391 nm f=0.22	401 nm f=0.14	
412 nm f=0.00	389 nm f=0.54	335 nm f=0.084	342 nm f=0.061	
358 nm f=0.39	381 nm f=0.030	316 nm f=0.0099	332 nm f=0.020	
qCoal	qC°b1	qC°c1	qCsa1	qCSb1
409 nm f=0.060	360 nm f=0.35	406 nm f=0.14	404 nm f=0.049	362 nm f=0.17
351 nm f=0.22	333 nm f=0.026	348 nm f=0.091	344 nm f=0.16	346 nm f=0.0097
312 nm f=0.048	311 nm f=0.22	318 nm f=0.094	319 nm f=0.025	320 nm f=0.29
qCsc1	qC h	qC h (-O)	qC h imide	tC ^o p1
407 nm f=0.081	420 nm f=0.31	443 nm f=0.22	450 nm f=0.58	457 nm f=0.001
349 nm f=0.062	349 nm f=0.04	367 nm f=0.042	355 nm f=0.01	367 nm f=0.34
322 nm f=0.043	312 nm f=0.04	327 nm f=0.17	342 nm f=0.05	366 nm f=0.002
Coumarine	Ether	Amine	tCO-st2	tCO-st3
439 nm f=0.60	426 nm f=0.45	394 nm f=0.84	414 nm f=0.81	$\begin{array}{cccccccccccccccccccccccccccccccccccc$
346 nm f=0.29	351 nm f=0.033	349 nm f=0.054	346 nm f=0.030	
336 nm f=0.24	327 nm f=0.37	333 nm f=0.32	331 nm f=0.64	

THYMIN ANALOGUES

$$\begin{array}{c|c} & & & \\ & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ &$$

 sugar				
$\mathrm{tT^{c}1}$	${ m tT^{C}2}$	${ m tT^{C}3}$	${ m tT}^{ m C}4$	$\mathrm{tT}^{\mathrm{c}5}$
	N	N	N	N
N N	\(\)	N	N	N
NH	NH	NH	NH	NH
351 nm f=0.05 331 nm f=0.53	340 nm f=0.47	358 nm f=0.093	333 nm f=0.39 324 nm f=0.13	345 nm f = 0.45
331 mm 1=0.33	319 nm f=0.18 311 nm f=0.0002	322 nm f=0.46 317 nm f=0.0003	299 nm f=0.0001	329 nm f=0.0001 320 nm f=0.20
$\mathrm{tT^{c}6}$	$\mathrm{tT}^{\mathrm{c}}7$	$\mathrm{tT}^{\mathrm{c}}8$	$\mathrm{tT}^{\mathrm{c}}9$	$\mathrm{tT}^{\mathrm{c}}10$
N	N	N N	NO ₂	O ₂ N
/	N	N		
>			, N	N N
NН	NH	NH	NH	NH
335 nm f=0.56	376 nm f=0.0011	366 nm f=0.0008	392 nm f=0.040	363 nm f=0.096
332 nm f=0.0007 310 nm f=0.021	355 nm f=0.60 327 nm f=0.058	352 nm f = 0.32 321 nm f = 0.27	356 nm f=0.42 341 nm f=0.00	353 nm f=0.11 335 nm f=0.00
tT ^c 11	$tT^{c}12$	$tT^{c}13$	${ m tT}^{\rm C}14$	tT ^c 15
N+—O-	-ON+	-ON+	N+—O-	0
			N——	,
NN NN	, N	\(\)		N N
N	N	N		
NH	NH	NH NH	NH NH	NH
	/ \\	/ %		
374 nm f=0.25	364 nm f=0.26	354 nm f=0.14	359 nm f = 0.00	387 nm f = 0.20
367 nm f=0.00 338 nm f=0.00	348 nm f=0.00 334 nm f=0.00	349 nm f=0.00 324 nm f=0.0001	349 nm f=0.19 341 nm f=0.25	374 nm f=0.00 350 nm f=0.25
$\mathrm{tT^{c}16}$	$\mathrm{tT^{c}17}$	$\mathrm{tT^{c}18}$	$\mathrm{tT^{c}19}$	$\mathrm{tT^{c}20}$
-0-N*	N+—0-	N+—0-	-0-N+	-oN*
	N——			N N
N,	, N	N, N	, , , , , , , , , , , , , , , , , , ,	N N
N	N	N	N N	N
NH	NH	NH	NH	NH
360 nm f = 0.36	374 nm f=0.050	418 nm f=0.0002	405 nm f=0.0003	392 nm f=0.014
355 nm f = 0.0081	345 nm f = 0.35	384 nm f = 0.35	370 nm f = 0.40	355 nm f = 0.25
337 nm f=0.012	332 nm f=0.0078	355 nm f = 0.00	348 nm f=0.00	346 nm f=0.0095

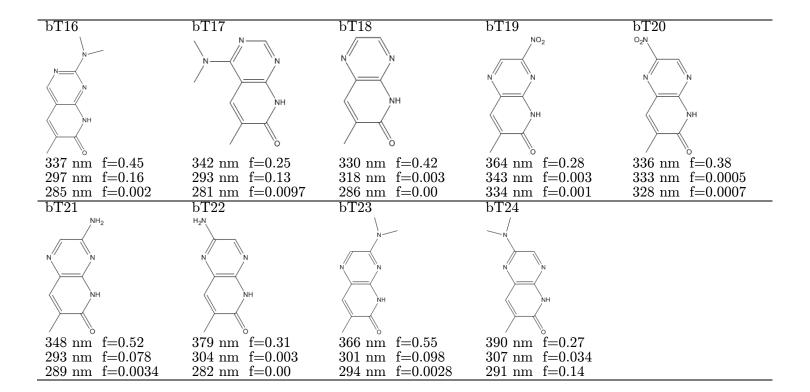
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$\mathrm{tT^c}21$	${ m tT^{c}22}$			
N N	V1 22			
358 nm f=0.032 357 nm f=0.0002	Gas: 460 nm f=0.080			
326 nm f=0.38	342 nm f = 0.27 303 nm f = 0.00			
$\mathrm{tT^{N}1}$	tT ^N 2	tT ^N 3	tTN4	tT ^N 5
N	N	N	N	N N
NH	NH	NH	NH	NH
373 nm f=0.12 348 nm f=0.54 344 nm f=0.0014	375 nm f=0.0002 360 nm f=0.59 308 nm f=0.00	379 nm f=0.20 365 nm f=0.0004 329 nm f=0.43	358 nm f=0.0006 350 nm f=0.39 343 nm f=0.24	378 nm f=0.0002 364 nm f=0.58 313 nm f=0.00
tT ^N 6	tT ^N 7	tT ^N 8	tT ^N 9	tT ^N 10
N	N N	N N	, -o-	
NH	NH	NH	N NH	NH
399 nm f=0.00 350 nm f=0.68 320 nm f=0.00	426 nm f=0.0001 370 nm f=0.68 322 nm f=0.00	408 nm f=0.00 369 nm f=0.45 324 nm f=0.0001	390 nm f=0.12 369 nm f=0.0007 351 nm f=0.37	364 nm f=0.30 358 nm f=0.0009 351 nm f=0.042
tT ^N 11	tT ^N 12	tT ^{IN} 13	tT ^N 14	tT ^N 15
N	N N	N N	N N	N N
NH	NH	NH	NH	NH
410 nm f=0.0001 375 nm f=0.39 353 nm f=0.0001	404 nm f=0.0001 363 nm f=0.48 330 nm f=0.00	378 nm f=0.0003 365 nm f=0.21 349 nm f=0.0001	383 nm f=0.0002 353 nm f=0.31 351 nm f=0.0003	420 nm f=0.0001 385 nm f=0.33 347 nm f=0.00
tT ^N 16	tT ^N 17	tT ^N 18	tT ^N 19	$\mathrm{tT}^{\scriptscriptstyle{\mathrm{N}}}20$
		N	N	N N
NH	N N	N NH	NH	NH NH
401 nm f=0.0001 362 nm f=0.50 350 nm f=0.0002	424 nm f=0.0064 357 nm f=0.38 343 nm f=0.020	470 nm f = 0.00 383 nm f = 0.47 362 nm f = 0.00	458 nm f=0.00 369 nm f=0.58 357 nm f=0.00	432 nm f=0.0051 368 nm f=0.30 348 nm f=0.030

tT ^N 21	tT ^N 22			
N	N. N.			
N NH	NH			
396 nm f=0.00 371 nm f=0.058	516 nm f=0.11 352 nm f=0.23			
341 nm f = 0.0009	349 nm f = 0.082	(TO)	, TDQ 4	(TDO)
$\operatorname{tT}^{\mathrm{o}}1$	tT ^O 2	tT ^o 3	tT ⁰ 4	tT°5
» N	o N	N	Q N	
NH	NH	NH	NH	NH
374 nm f=0.32	380 nm f=0.34	367 nm f=0.247	382 nm f=0.24	371 nm f=0.36
306 nm f=0.078 293 nm f=0.0045	308 nm f=0.12 301 nm f=0.040	310 nm f=0.218 289 nm f=0.0011	300 nm f=0.15 288 nm f=0.0055	313 nm f=0.14 300 nm f=0.018
tT ^o 6	tT ^o 7	tT ^o 8	$\mathrm{tT}^{0}9$	tT ⁰ 10
N N	N N	N N		
o N	, N	N N		N
N—————————————————————————————————————	N-N-N-N-N-N-N-N-N-N-N-N-N-N-N-N-N-N-N-	N——NH	NH N	N——NH
391 nm f=0.25 302 nm f=0.15	381 nm f=0.43 331 nm f=0.051	368 nm f=0.24 322 nm f=0.28	435 nm f=0.039 357 nm f=0.38	454 nm f=0.23 336 nm f=0.00
$\frac{295 \text{ nm f}}{\text{tT}^{\circ}11}$	$\frac{296 \text{ nm f}}{\text{tT}^{\circ}12}$	$\frac{294 \text{ nm f}}{\text{tT}^{\circ}13}$	$\frac{331 \text{ nm f}}{\text{tT}^{\circ}14}$	333 nm f=0.15 tT°15
N'0'	·0—N*	·	0.1.14	N*0-
N	N N	N N	N T	N
	N	N		N
N——NH	N-NH	NH NH	N NH	N-N-N-N-N-N-N-N-N-N-N-N-N-N-N-N-N-N-N-
407 nm f=0.049 365 nm f=0.45	455 nm f=0.24 335 nm f=0.00	430 nm f=0.20 349 nm f=0.00	412 nm f=0.0045 352 nm f=0.35	441 nm f=0.040 356 nm f=0.46
$\frac{344 \text{ nm f} = 0.00}{\text{tT}^{\circ}16}$	$\frac{334 \text{ nm f} = 0.00}{\text{tT}^{0}17}$	321 nm f=0.15 tT ⁰ 18	$\frac{343 \text{ nm f}=0.00}{\text{tT}^{\circ}19}$	$\frac{330 \text{ nm f} = 0.00}{\text{tT}^{\circ}20}$
0—N*	N*O-	N*—-O-	-ON*	-0N ⁺
N.	N N	N N	N	N N
N N	O N	NH	N	, N
N N	N N		NH NH	N NH
436 nm f=0.28 349 nm f=0.00	393 nm f=0.052 358 nm f=0.29	407 nm f = 0.050 368 nm f = 0.49	433 nm f = 0.32 354 nm f = 0.00	414 nm f = 0.23 363 nm f = 0.0007
327 nm f=0.082	345 nm f = 0.045	342 nm f=0.00	341 nm f=0.00	319 nm f=0.0099

tT ^S 1 408 nm f=0.20 329 nm f=0.081 313 nm f=0.020 tT ^S 6	tT ^S 2 416 nm f=0.20 333 nm f=0.092 326 nm f=0.11 tT ^S 7	tT ^S 3 407 nm f=0.13 331 nm f=0.22 313 nm f=0.018 tT ^S 8	tT ^S 4 A24 nm f=0.14 326 nm f=0.099 311 nm f=0.019 tT ^S 9	tT ⁵ 5 406 nm f=0.21 337 nm f=0.17 322 nm f=0.042 tT ⁵ 10
437 nm f=0.14	416 nm f=0.26	410 nm f=0.11	472 nm f=0.038	499 nm f=0.15
330 nm f=0.14 323 nm f=0.14	366 nm f = 0.10	346 nm f=0.11 346 nm f=0.29 316 nm f=0.042	383 nm f = 0.28	364 nm f=0.066 336 nm f=0.00
$\frac{525 \text{ nm } 1=0.14}{\text{tT}^{8}11}$	$\frac{318 \text{ nm f}}{\text{tT}^{\text{s}}12}$	$tT^{s}13$	$\frac{333 \text{ nm f}=0.00}{\text{tT}^{\text{s}}14}$	$tT^{s}15$
N+O-	-0N+	~ON*	N+O-	N*O-
N NH	S NH	N NH	N NH	N N N N N N N N N N N N N N N N N N N
442 nm f=0.034 389 nm f=0.34	491 nm f=0.16 355 nm f=0.044	473 nm f=0.13 351 nm f=0.0001	449 nm f=0.012 372 nm f=0.23	483 nm f=0.041 384 nm f=0.34
346 nm f = 0.0003	342 nm f = 0.0011	350 nm f = 0.049	345 nm f = 0.0002	331 nm f = 0.00
tT ^s 16	tT ^s 17	tT ⁵ 18	tT ^s 19	tT ^s 20
S N	N NH	N N NH	N N N N N N N N N N N N N N N N N N N	N N N N N N N N N N N N N N N N N N N
480 nm f=0.20 362 nm f=0.0089 350 nm f=0.00	432 nm f=0.041 373 nm f=0.25 350 nm f=0.0012	450 nm f=0.040 398 nm f=0.39 350 nm f=0.0003	482 nm f=0.22 364 nm f=0.00 359 nm f=0.0023	456 nm f=0.15 370 nm f=0.0019 356 nm f=0.012

${ m tT}^{ m s}22_{}$	qT h	qT h (-O)	qT h2	${ m tT}^{\circ}22$
S N NH NH	N N N N N N N N N N N N N N N N N N N	N N N N N N N N N N N N N N N N N N N	N N N N N N N N N N N N N N N N N N N	N NH
430 nm f=0.31 359 nm f=0.0077 342 nm f=0.030	452 nm f=0.38 349 nm f=0.01 319 nm f=0.02	524 nm f=0.28 383 nm f=0.04 339 nm f=0.14	430 nm f=0.39 334 nm f=0.026 312 nm f=0.032	407 nm f=0.39 332 nm f=0.017 327 nm f=0.034
tTS (-O)	tTO (-O)			
423 nm f=0.26 402 nm f=0.032 335 nm f=0.11 bT1	390 nm f=0.38 369 nm f=0.033 317 nm f=0.084 bT2	bT3	bT4	bT5
NH NH	NO ₂	D13 O2N NH	0 ₂ N NH	NH ₂
310 nm f=0.36 270 nm f=0.00 263 nm f=0.01	350 nm f=0.23 315 nm f=0.00 308 nm f=0.01	333 nm f=0.20 319 nm f=0.00 303 nm f=0.00	393 nm f=0.12 341 nm f=0.003 328 nm f=0.01	327 nm f=0.54 287 nm f=0.029 260 nm f=0.00
bT6 H ₂ N NH	bT7	bT8	bT9	bT10
371 nm f=0.18 281 nm f=0.002 275 nm f=0.099 bT11	320 nm f=0.14 304 nm f=0.26 265 nm f=0.00 bT12	341 nm f=0.58 294 nm f=0.03 262 nm f=0.00 bT13	386 nm f=0.14 287 nm f=0.0077 281 nm f=0.13 bT14	342 nm f=0.16 311 nm f=0.23 270 nm f=0.003 bT15
N NH	NO ₂	O ₂ N N	NH2	H ₂ N N
299 nm f=0.39 288 nm f=0.0014 274 nm f=0.00	302 nm f=0.00 296 nm f=0.00 285 nm f=0.00	333 nm f=0.10 312 nm f=0.00 304 nm f=0.00	321 nm f=0.45 287 nm f=0.12 275 nm f=0.002	316 nm f=0.34 280 nm f=0.043 269 nm f=0.00



STRUCTURES BASED ON KNOWN DYES:

