

IV. ELECTROCHEMISTRY

Apparatus

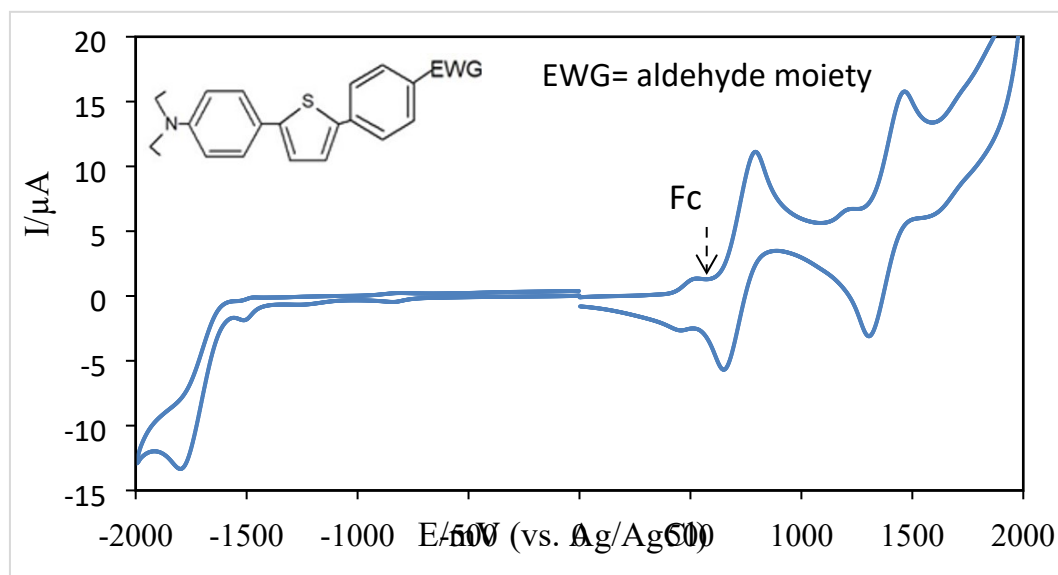
Swiss μ AUTOLAB, TYPE III (Metrohm, Herisau, Switzerland) operated the three-electrode electrochemical cell under the software GPES to collect the cyclic voltammetry (CV) data. A platinum wire with the area of 7.1 mm^2 served as the working electrode. A Pt-plate and Ag/AgCl/3M KCl-electrode were chosen as the counter and the reference electrode, respectively. The redox signals of 1 mM solutions of all synthesized molecular complexes were measured in dichloromethane (DCM) with 0.1 M tetrabutylammonium hexafluorophosphate (TBAPF₆) as the supporting electrolyte against the Ag/AgCl/3M KCl aqueous reference electrode separated from the main electrolytic compartment by a fritted junction containing the same supporting electrolyte (0.1M TBAPF₆ in DCM). The potential ranges from 0 V to -2V and from 0 V to + 2 V for the reduction and oxidation were used, respectively. As an internal redox standard Fc⁺/Fc (ferrocenium/ferrocene) couple and for the evaluation of HOMO, LUMO, gap energy the scan rate of 75 mV/s was chosen. All CV experiments were performed under argon atmosphere at constant room temperature (23 °C) and with repeatability of RSD $\leq 3.2 \%$.

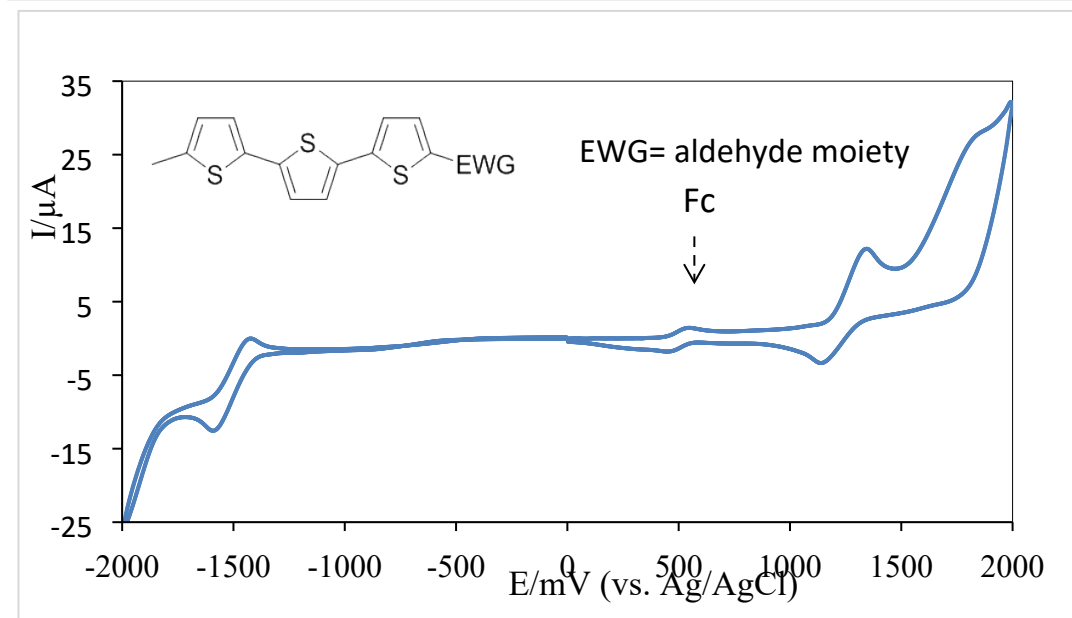
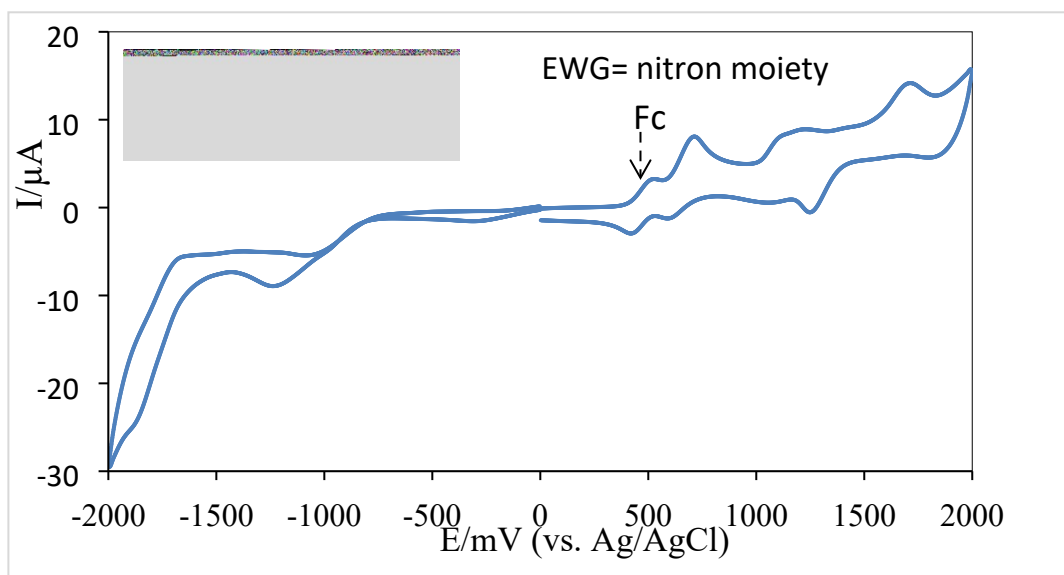
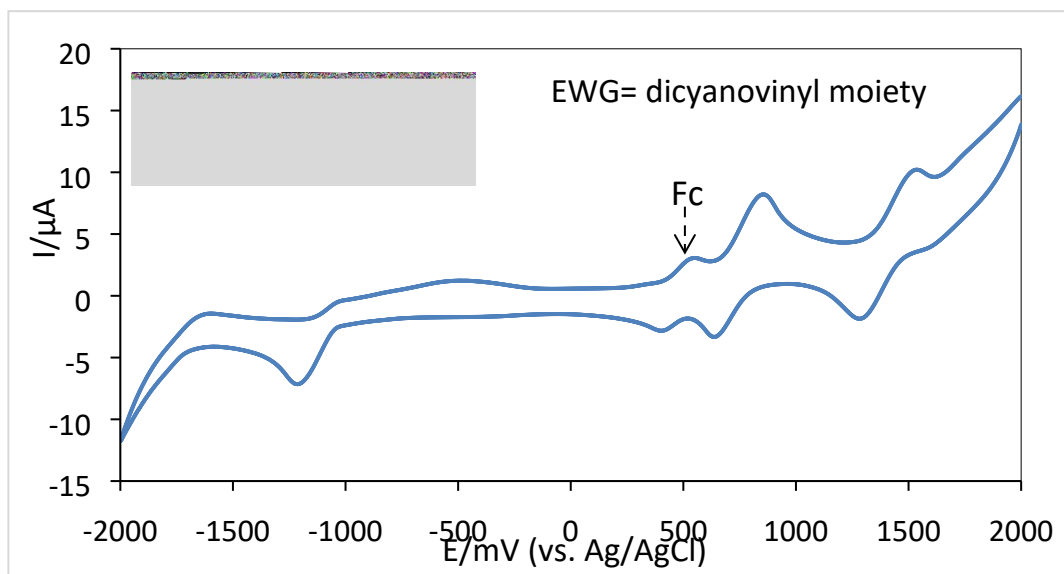
$$E_{\text{HOMO}} = -(E_{\text{onset, ox}} - E_{\text{Fc}^+/\text{Fc}}^0 + 4.89) \text{ (eV)} \quad (1)$$

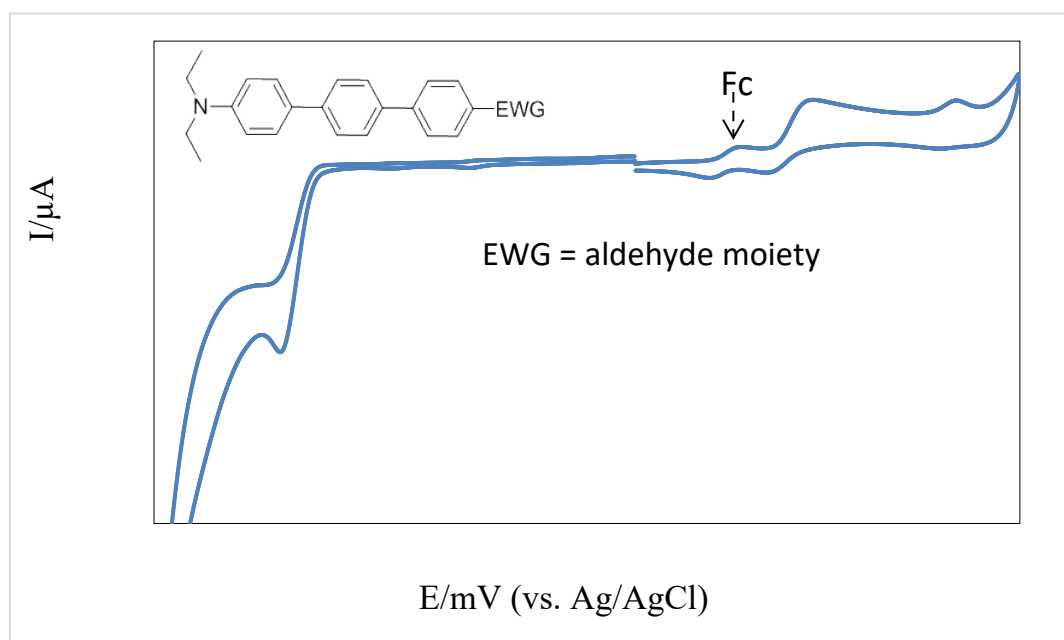
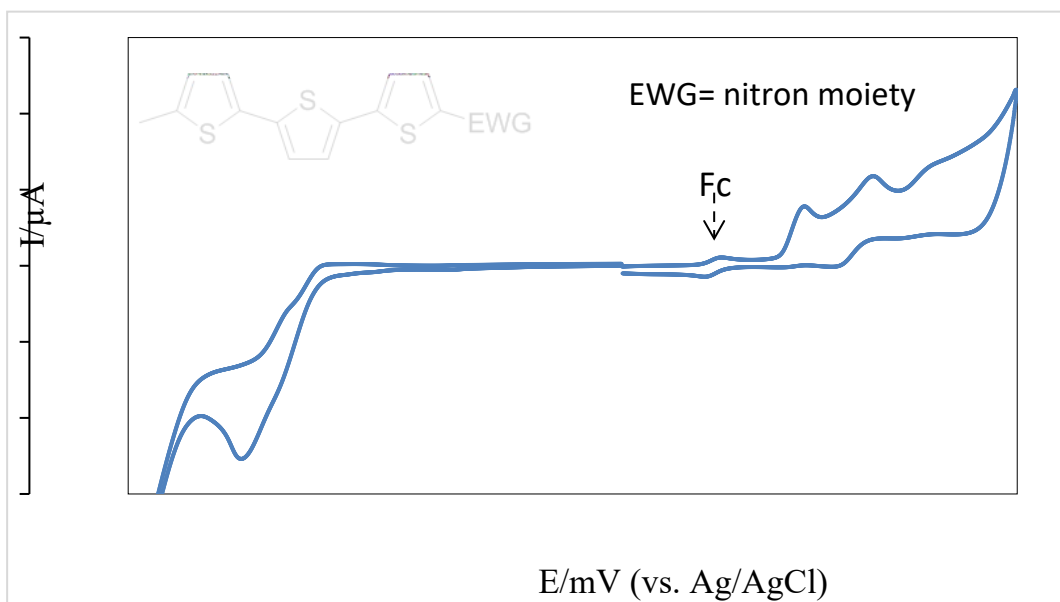
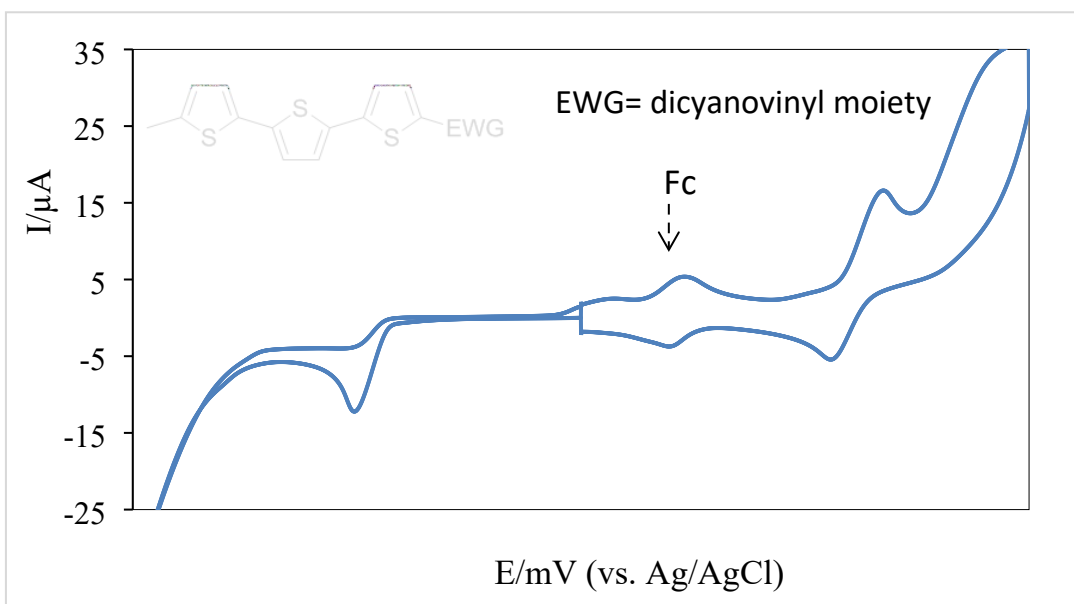
$$E_{\text{LUMO}} = -(E_{\text{onset, red}} - E_{\text{Fc}^+/\text{Fc}}^0 + 4.89) \text{ (eV)} \quad (2)$$

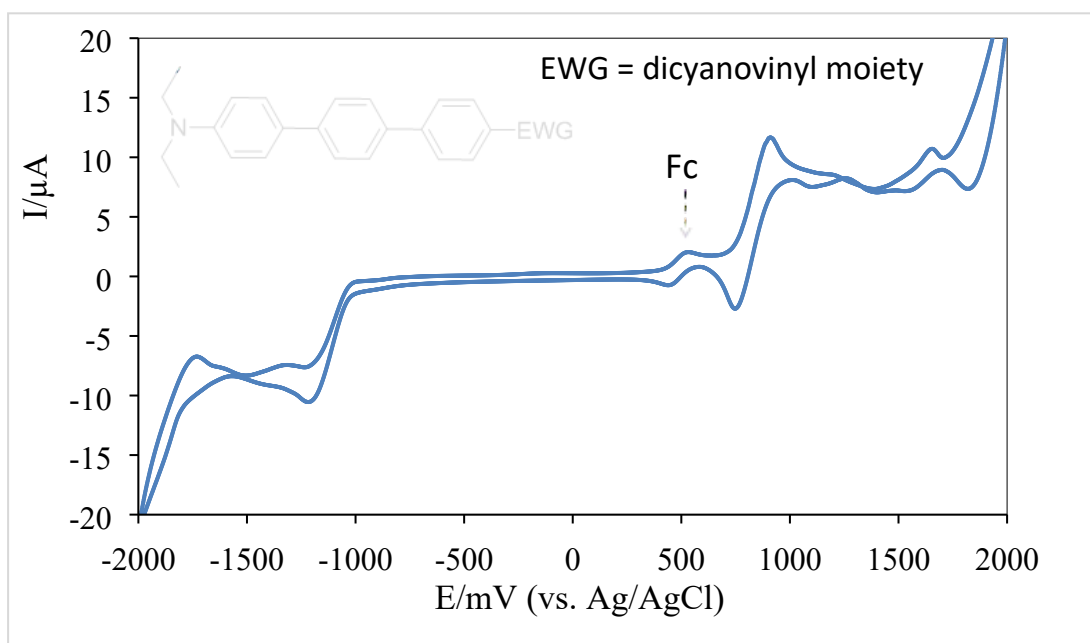
where $E_{\text{Fc}^+/\text{Fc}}^0$ is the formal redox potential of the Fc⁺/Fc, which is calculated from its anodic (E_{pa}) and cathodic (E_{pc}) potentials, i.e., $E_{\text{Fc}^+/\text{Fc}}^0 = (E_{\text{pa}} + E_{\text{pc}})/2$.

VOLTAMMETRIC RECORDS

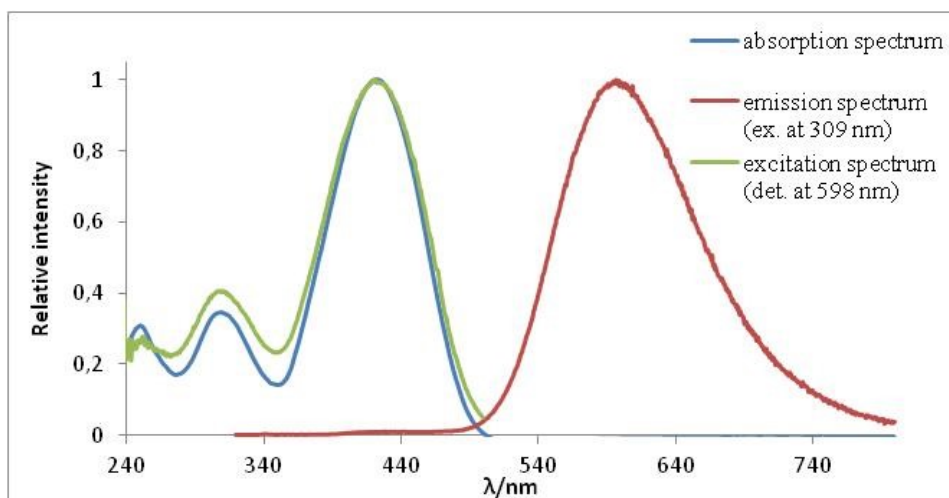






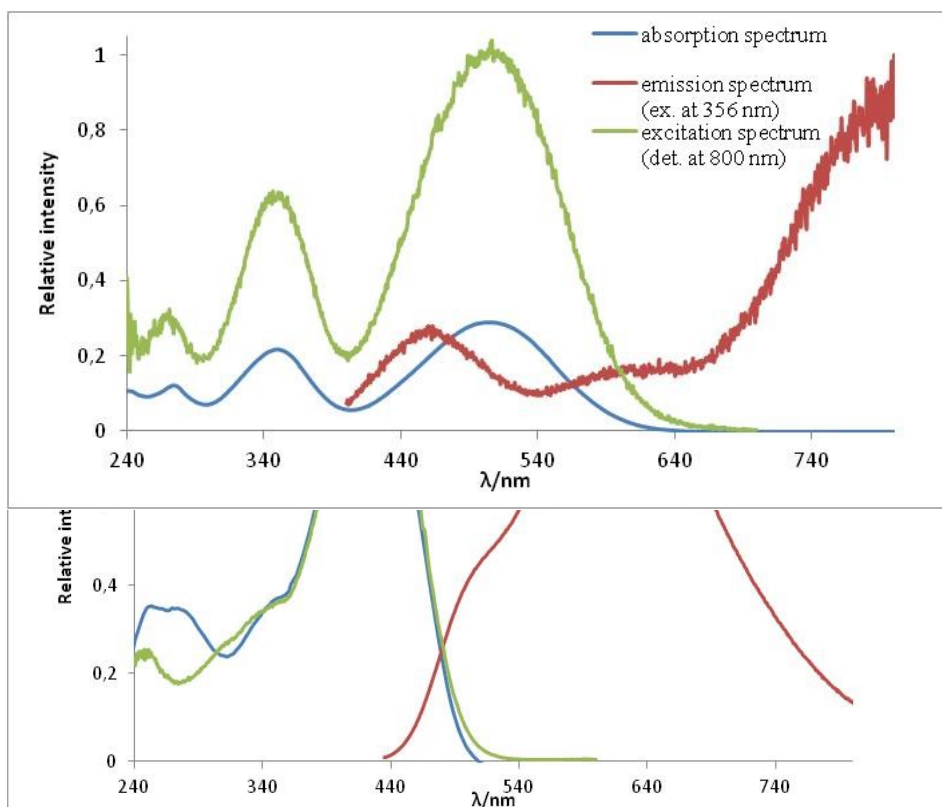


V. UV-VIS SPECTRA



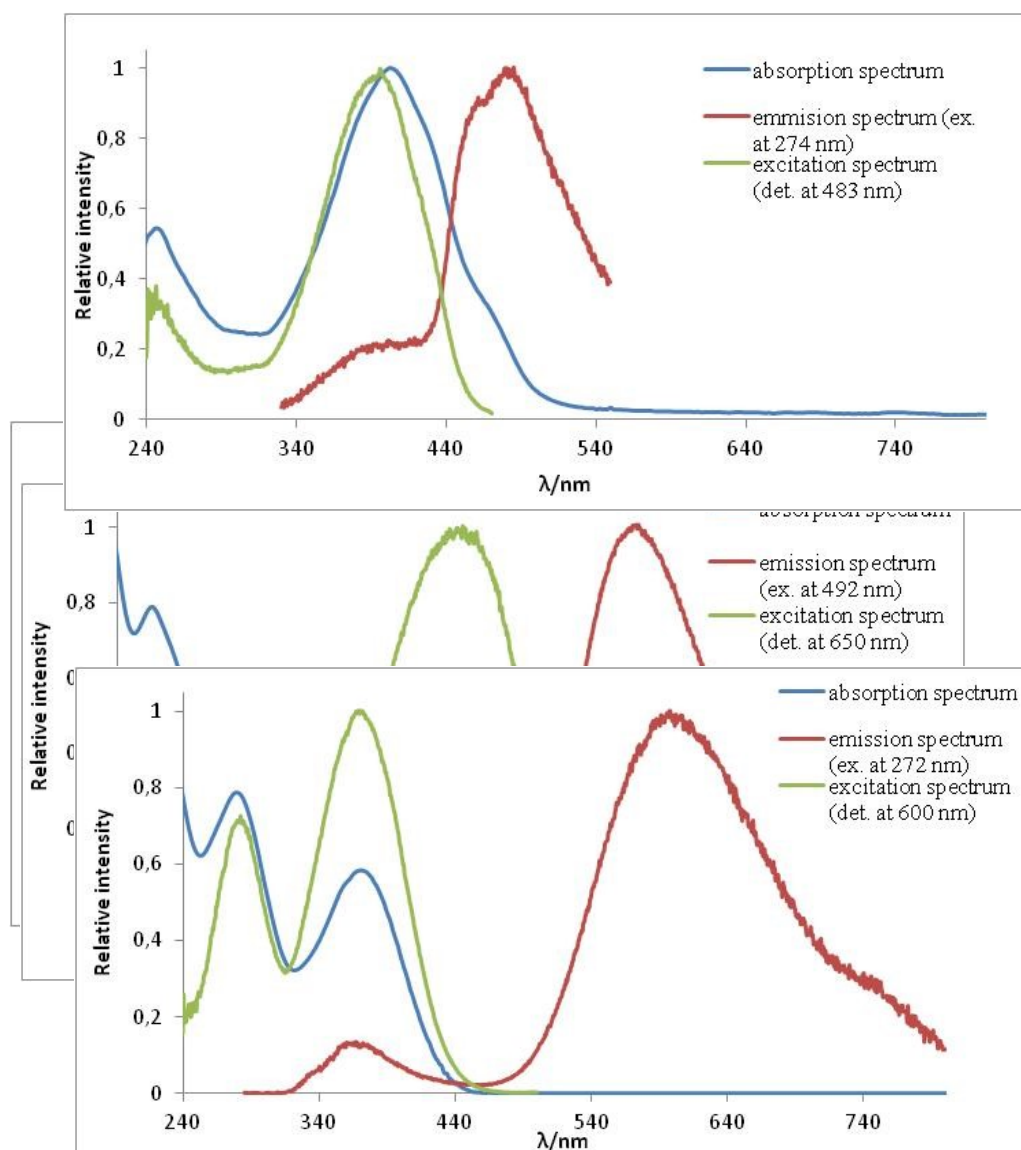
Compound 20

Compound 21



Compound 23

Compound 28

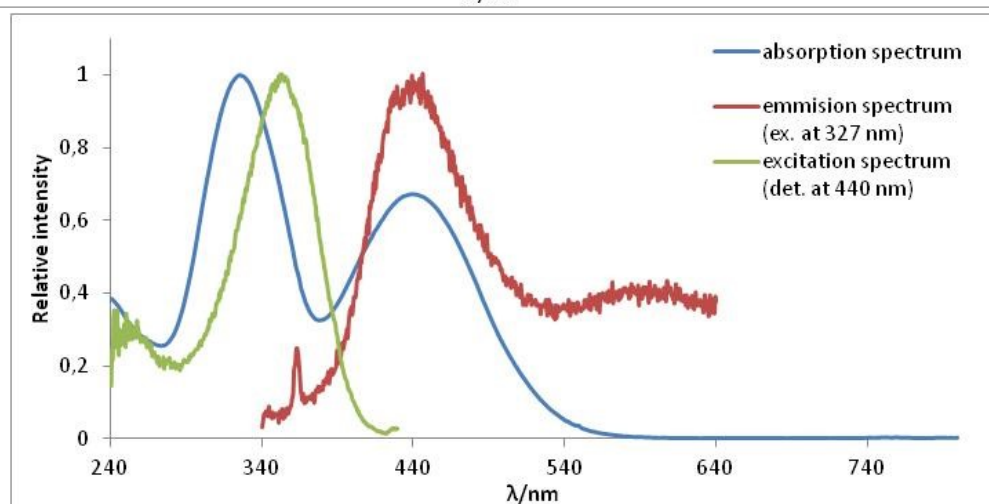
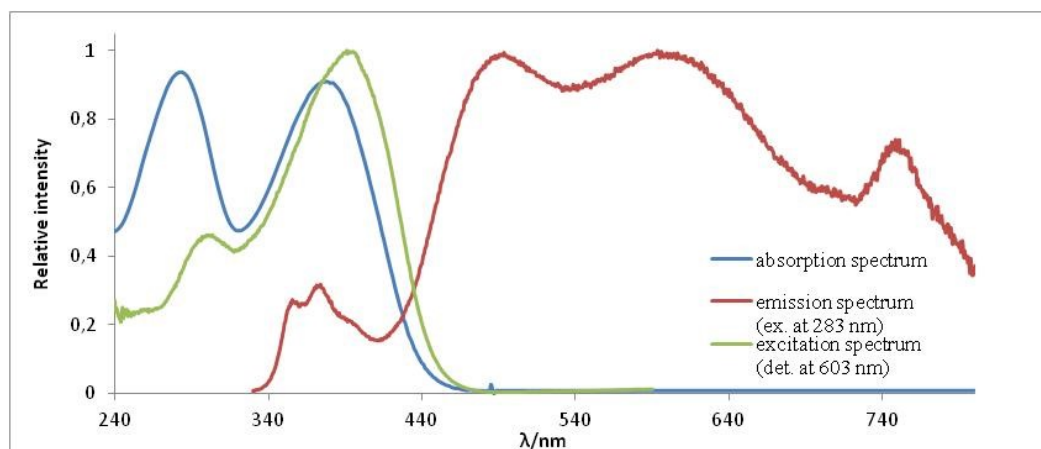


Compound 30

Compound 29

Compound 33

Compound 35



Compound 34

VI. THEORETICAL CALCULATIONS

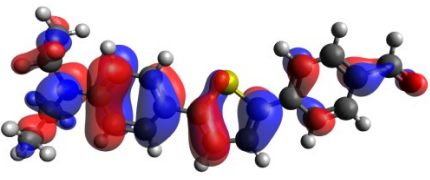
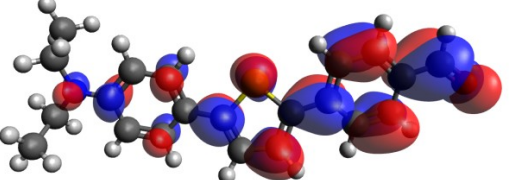
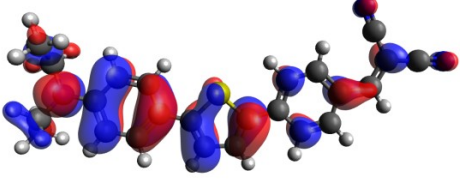
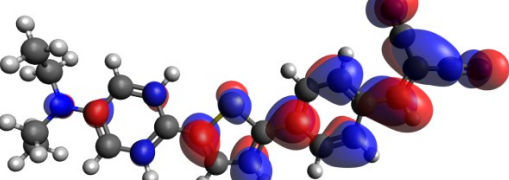
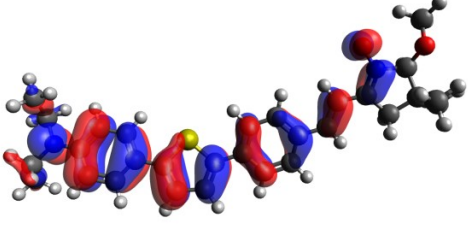
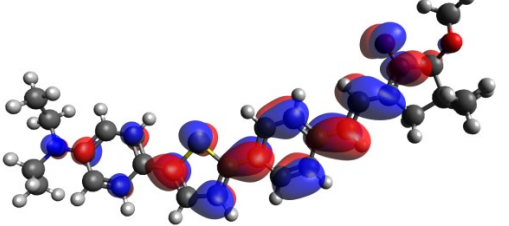
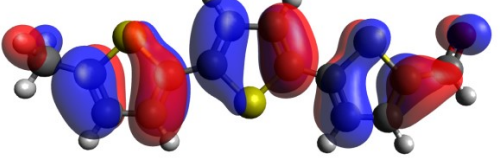
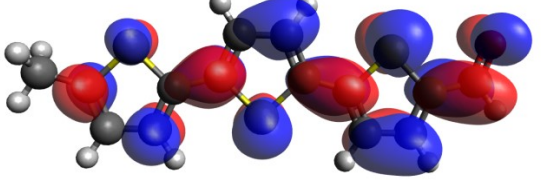
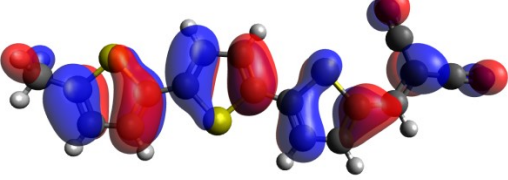
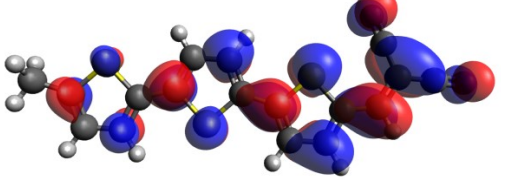
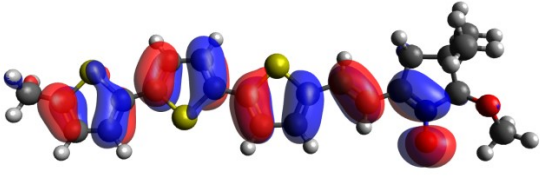
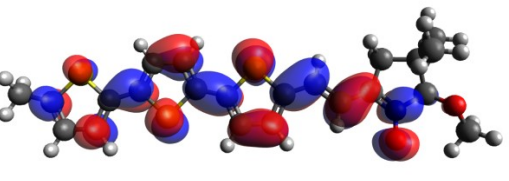
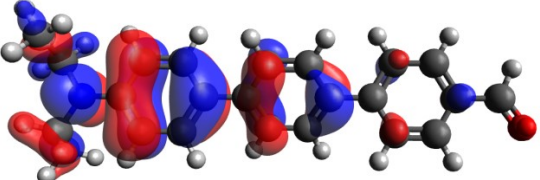
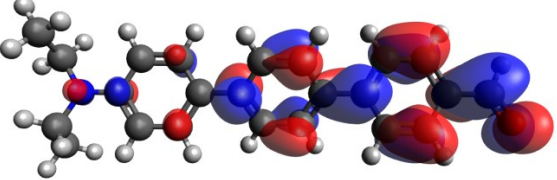
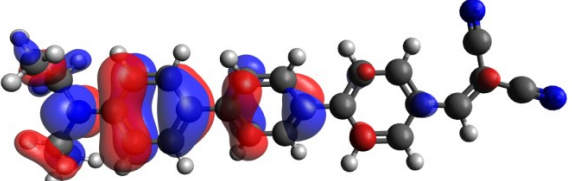
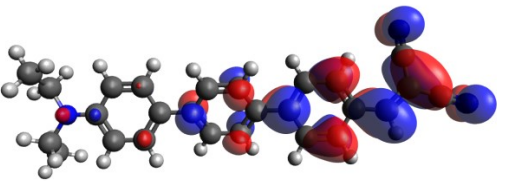
Structure	Torsion angles
20	$-18.2^{\circ}/14.4^{\circ}$
23	$13.6^{\circ}/-8.0^{\circ}$

Table 5: Torsion angles of synthesised molecules

Structure	Torsion angles
20	$-18.2^{\circ}/14.4^{\circ}$

23	13.6°/−8.0°
21	8.7°/12.7°
28	−0.5°/0.1°
30	−8.0°/0.0°
29	−10.5°/7.9°
33	29.9°/−32.5°
35	28.6°/−29.2°
34	30.7°/−32.6°
39	34.7°/−34.8°

Follows frontier orbitals of D- π -A derivatives

	HOMO	LUMO
20		
23		
21		
28		
30		
29		
33		
35		

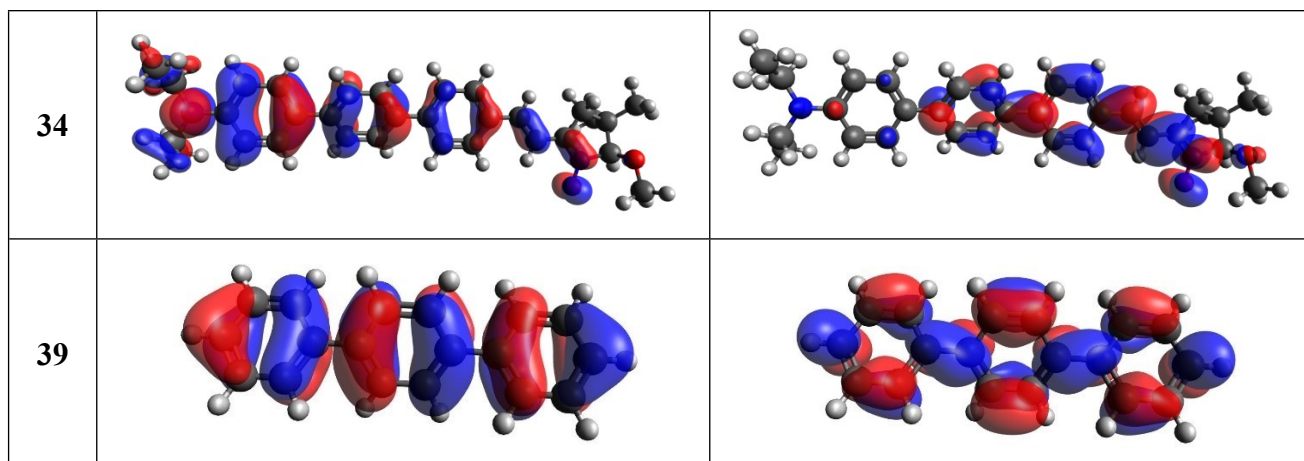


Table 6: Cartesian coordinates of related structures

20	x	y	z
C	-3.5818463631	0.5562174440	-0.0137209529
C	-2.9618374851	-0.6795348685	-0.0342920576
S	-2.3716748949	1.8296858724	-0.0087526488
C	-1.0443842336	0.6727236541	-0.0134873739
C	-1.5482090698	-0.6128039610	-0.0359334093
H	-3.5129386321	-1.6128385882	-0.0195586057
H	-0.9160612794	-1.4937268101	-0.0217259234
C	-5.0055349239	0.8639227985	-0.0131251757
C	0.3457364368	1.1050803460	0.0066494816
C	0.7042574985	2.4315417655	0.3247866863
C	1.3808348856	0.1890922254	-0.2988706484
C	2.0351179999	2.8251685015	0.3379668808
C	2.7068331586	0.5821605630	-0.2766237978
C	3.0530568723	1.9076021204	0.0413258643
C	-5.5073715779	2.1182724619	0.3811304475
C	-5.9538009757	-0.0986125982	-0.4123408546
C	-7.3133281336	0.1660766353	-0.4116360551
C	-7.8200412402	1.4321006740	-0.0162243405
C	-6.8635731216	2.4029565599	0.3787537486

H	-4.8222438990	2.8952603723	0.7108338271
H	-7.1805048131	3.3931632446	0.6808158849
H	-5.6181083647	-1.0776193034	-0.7412014973
H	-7.9893797990	-0.6225316668	-0.7174845474
H	1.1300373169	-0.8311910185	-0.5685857600
H	-0.0649643183	3.1548686569	0.5781728846
H	2.2947341639	3.8512968781	0.5872554811
H	3.4968087764	-0.1240717561	-0.5128674868
C	4.4559655121	2.3388868263	0.0640163978
O	5.4144446205	1.6184544496	-0.1789111813
H	4.6066942472	3.4070363183	0.3266897118
N	-9.1673048750	1.7038422934	-0.0168128161
C	-9.6978193142	2.9633995368	0.4998261394
C	-9.7213659007	4.0830686900	-0.5426439374
H	-9.1227488950	3.2668190111	1.3801588988
H	-10.7145617751	2.7657161142	0.8534874292
H	-8.7129967694	4.3084698803	-0.9051804594
H	-10.1444425496	4.9981101126	-0.1113744808
H	-10.3348444780	3.7961150302	-1.4044091905
C	-10.1465876752	0.7475995884	-0.5282657043
C	-10.6084819594	-0.2648289564	0.5217944279
H	-9.7332894274	0.2359984106	-1.4026710233
H	-11.0039488933	1.3241596732	-0.8898977634
H	-9.7687525026	-0.8627776008	0.8912625432
H	-11.3541732396	-0.9458392980	0.0946136267
H	-11.0633600947	0.2461384238	1.3781103321

23

x

y

z

S	-0.0900996689	-0.0006664822	-0.1180806330
C	1.2499882378	-0.9965857730	0.4242067915
C	-1.2848022824	-1.1656769097	0.4487491482
C	0.7668683858	-2.1641015312	0.9954547414
C	-0.6401675345	-2.2567113475	1.0070633230

H	1.4140432849	-2.9236934024	1.4178891332
H	-1.1699188630	-3.0983510017	1.4384870756
C	2.6293285947	-0.5756626849	0.2443026244
C	3.6919982503	-1.4886781897	0.4051196865
C	5.0136735001	-1.1113600973	0.2462255957
C	5.3670472234	0.2210921363	-0.0968006420
C	4.2964523664	1.1385892757	-0.2646006779
C	2.9797823975	0.7460648634	-0.0943433098
H	2.2039652441	1.4966846302	-0.2222839164
H	3.4789644288	-2.5236494667	0.6538470881
H	5.7820906976	-1.8585346082	0.3980475655
H	4.4943546462	2.1667428081	-0.5395351007
C	-2.7063546184	-0.9278659900	0.3136813258
C	-3.2151060574	0.3154693732	-0.1331071675
C	-3.6412142619	-1.9421388868	0.6277773211
C	-4.9974718826	-1.7156081888	0.5090264069
C	-4.5716547308	0.5429983115	-0.2539562127
C	-5.5074807472	-0.4689041931	0.0687125381
H	-3.2937582480	-2.9144741670	0.9581876958
H	-2.5314035056	1.1220427404	-0.3796752165
H	-4.9047678251	1.5136697158	-0.5975779875
H	-5.6952340378	-2.5110293523	0.7552937404
C	-6.9344495294	-0.3417128405	-0.0116114497
N	6.6757633678	0.6006391348	-0.2580718694
C	7.0517090074	1.9932672319	-0.4960734951
C	7.7717110625	-0.3649187089	-0.1964455147
C	-7.7332772922	0.7201701906	-0.3694627150
H	-7.4836406430	-1.2397319897	0.2608978572
C	-9.1524167918	0.5575139281	-0.3605503479
C	-7.2752444141	2.0132816929	-0.7575109770
N	-10.3095169455	0.4269224860	-0.3543799787
N	-6.9284274927	3.0781271718	-1.0767929614
C	8.2776761771	-0.6138404392	1.2257246002
H	8.5838121772	0.0288224671	-0.8154616176
H	7.4578284901	-1.3024358323	-0.6652390722
H	8.6347820497	0.3182686127	1.6782247401

H	9.1087520520	−1.3288969840	1.2152067216
H	7.4845145263	−1.0176439249	1.8636255152
C	7.0317020871	2.3791000025	−1.9763375301
H	8.0591631912	2.1298324491	−0.0905639616
H	6.3973145013	2.6504014630	0.0844713216
H	7.7192182180	1.7472609870	−2.5502100243
H	7.3409572694	3.4233591068	−2.1026331481
H	6.0295898413	2.2633275125	−2.4023454291

21	x	y	z
C	−2.7602779558	0.7281587450	0.3680325067
C	−2.3296189331	−0.5528203803	0.6563487998
S	−1.3703185946	1.7921009924	0.1910418396
C	−0.2300585435	0.4869420375	0.5054118165
C	−0.9209634554	−0.6855654196	0.7331506905
C	1.2094550416	0.7154234975	0.4941574248
C	1.7585739544	2.0158840276	0.5035767506
C	3.1281877749	2.2240431693	0.4902329747
C	2.1105867027	−0.3687070018	0.4716109985
C	3.4811008230	−0.1578959409	0.4656246835
C	4.0311042131	1.1404392898	0.4724872509
C	−4.1212315267	1.2275826208	0.2124847944
C	−4.4013098780	2.5222590694	−0.2628782097
C	−5.2332163177	0.4227258277	0.5307920613
C	−6.5350192699	0.8708749117	0.3757439648
C	−6.8161948278	2.1757811443	−0.1061981678
C	−5.6971509293	2.9900675492	−0.4155335241
H	−3.0092106406	−1.3846265991	0.8030075431
H	−0.4293237784	−1.6248620342	0.9612887642
H	1.7310861353	−1.3848716928	0.4442011315
H	1.1005254532	2.8799052690	0.5336333514
H	3.5037168356	3.2423995467	0.4996142473
H	4.1515918572	−1.0135520410	0.4459303186
H	−3.5859919638	3.1914661134	−0.5259373970
H	−5.8382664038	4.0032119704	−0.7700129949

H	-5.0790019399	-0.5825441635	0.9107863299
H	-7.3430975266	0.1938536582	0.6229147594
N	-8.1057074488	2.6276719525	-0.2641435788
C	-8.3959960733	3.9238966255	-0.8722684364
C	-8.3907499163	5.0781010633	0.1322189160
H	-9.3808016843	3.8480715642	-1.3439802755
H	-7.6844688970	4.1139361998	-1.6818376658
H	-9.1346797243	4.9093614273	0.9192785551
H	-8.6320137650	6.0228767522	-0.3693851598
H	-7.4107876526	5.1830664900	0.6095448855
C	-9.2572496014	1.8286488280	0.1475712152
C	-9.7261457997	0.8451225293	-0.9269057185
H	-10.0659670513	2.5253194494	0.3902635788
H	-9.0210985571	1.3009441135	1.0767345932
H	-10.0064924015	1.3777765800	-1.8428784243
H	-10.6005419200	0.2836491793	-0.5768070095
H	-8.9366738899	0.1295748519	-1.1796832462
C	5.4769884452	1.2967382342	0.4568585762
C	6.1654141787	2.4664554119	0.4553652350
H	6.0396206070	0.3646329982	0.4425774354
C	7.5913172509	2.5434929822	0.4352343693
H	5.6530887245	3.4243819164	0.4671815938
C	8.5842454675	1.4171617315	0.3906886187
C	9.9309712466	2.0841505916	0.7807490268
H	8.6327112205	0.9881867571	-0.6197271864
H	8.3181271179	0.6044435061	1.0744845211
C	9.7176164685	3.5329707888	0.3024861914
C	11.1322746838	1.4430430162	0.0850279795
C	10.1090211735	2.0401613497	2.3059392109
N	8.2174268119	3.7097961626	0.4124739109
O	7.7067463579	4.8802634173	0.4141496553
O	10.4009601429	4.4646416052	1.0625487492
H	9.9500138472	3.6480103049	-0.7662254091
C	10.6814196183	5.6980055505	0.3952095304
H	9.7592999689	6.2224477341	0.1345977438
H	11.2772638413	5.5218072147	-0.5113949215

H	11.2659102384	6.2986857653	1.0966147119
H	11.0153505983	1.4559794833	−1.0047478023
H	11.2491759088	0.4004081091	0.4021224030
H	12.0557040997	1.9777328063	0.3364361055
H	9.2525179105	2.4835528682	2.8252675846
H	11.0074167503	2.5826959803	2.6117757179
H	10.2043654654	0.9987291259	2.6325835954

28	x	y	z
S	−1.2851342512	1.2716641512	−0.0519889138
C	−2.5871483186	0.0947106672	0.0142319666
C	−2.0737267955	−1.1878611454	0.0809063093
C	−0.6615817909	−1.2353533870	0.0806225475
C	−0.0616295589	0.0077846934	0.0134687437
H	−2.6975533854	−2.0736867950	0.1288775022
H	−0.1006368222	−2.1625710184	0.1291848663
C	−3.9643723212	0.5206530366	−0.0044891923
C	1.3391240956	0.3375138262	−0.0060460728
S	−5.2734747544	−0.6567144137	0.0484266378
C	−6.4918876232	0.5999554378	−0.0069285517
C	−5.9023656390	1.8370352019	−0.0623214956
C	−4.4803925278	1.7980017205	−0.0610387658
H	−6.4784534014	2.7555058093	−0.1025238089
H	−3.8599682298	2.6875941539	−0.0992628369
S	2.5585841584	−0.9213486435	0.0562437298
C	3.8418060584	0.2695470084	−0.0065301899
C	1.9252822114	1.5958713836	−0.0713638535
C	3.3340495307	1.5534113422	−0.0713347678
H	1.3533589890	2.5160736970	−0.1170797959
H	3.9696469638	2.4315590273	−0.1166353352
C	−7.9476982037	0.2576857965	0.0090729115
H	−8.2288962516	−0.3635589595	−0.8501881152
H	−8.5408888676	1.1763977172	−0.0270237653
H	−8.2261238393	−0.2923356713	0.9163877288
C	5.2290533600	−0.1353342960	0.0124693170

O	5.6161149013	−1.2980232458	0.0719523774
H	5.9465386006	0.7083252573	−0.0318899109

30	x	y	z
S	−1.2951042990	1.2871968410	0.3248649029
C	−2.5042472743	0.0389067509	0.0842895402
C	0.0167626284	0.1211330440	0.1802962884
C	−1.8988375752	−1.1937427331	−0.1036241736
C	−0.4915571967	−1.1469609755	−0.0494111843
H	−2.4573781336	−2.1087921252	−0.2661036269
H	0.1358108413	−2.0237127546	−0.1705227764
C	−3.9066126713	0.3649666397	0.0951059679
S	−5.1180530323	−0.8316918001	−0.3547256033
C	−6.4258265164	0.2996997199	−0.0866466913
C	−5.9348309253	1.5155775531	0.3189293312
C	−4.5183732482	1.5574709463	0.4228900382
H	−3.9692411167	2.4380905928	0.7397108104
H	−6.5795846164	2.3592633504	0.5410733977
C	1.3822098309	0.5353845628	0.2995290407
S	2.6866801484	−0.6249121917	0.1535016851
C	3.8961052334	0.6357517835	0.4084986095
C	1.8754770209	1.8190152098	0.5313275146
C	3.2706537043	1.8711355188	0.5910176348
H	1.2362531152	2.6861166276	0.6520523519
H	3.8388022951	2.7787724664	0.7636154753
C	−7.8487951951	−0.1063057865	−0.3021182142
H	−8.1333429348	−0.9468053375	0.3424997884
H	−8.0310978546	−0.4121111054	−1.3396631049
H	−8.5085221670	0.7362999987	−0.0745448557
C	5.2965870664	0.4603290193	0.4312871370
C	6.0524897734	−0.6837395096	0.2709050184
H	5.8558829247	1.3769288805	0.6032199902
C	7.4740229002	−0.6101920111	0.3333031209
C	5.4947636134	−1.9726860486	0.0417922877
N	5.0348548444	−3.0270109183	−0.1444800662

N	8.6363158169	−0.5516830621	0.3839081923
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29	x	y	z
S	−1.4155662834	1.7956680225	−0.2891763813
C	−2.2218538997	0.2338669144	−0.2101902169
C	0.1751121700	1.0459566995	−0.1995669416
C	−1.2893519628	−0.7824273705	−0.1390800197
C	0.0513272729	−0.3285949847	−0.1334977749
H	−1.5616087152	−1.8304867610	−0.0751221171
H	0.9039810951	−0.9960804035	−0.0663902207
C	−3.6618458917	0.1505288004	−0.2312792162
C	1.3669498895	1.8518555875	−0.2069332714
C	−4.5954319645	1.1576184934	−0.1135044661
S	−4.4719580781	−1.4002354111	−0.4394286416
C	−6.0572705190	−0.6576740501	−0.3539698843
C	−5.9410199174	0.6974439927	−0.1841056737
H	−4.3280110558	2.1992320450	0.0318870571
H	−6.8039056397	1.3507823616	−0.1062934064
C	−7.2989510239	−1.4847731900	−0.4612757729
H	−7.3676355796	−2.2233936043	0.3470657077
H	−7.3433407365	−2.0329619996	−1.4104318410
H	−8.1778309685	−0.8354325961	−0.4030157589
S	2.9545358186	1.1147461541	−0.3326246035
C	3.7600349609	2.6783741512	−0.2707020858
C	1.4872827441	3.2305432890	−0.1296660001
C	2.8202450103	3.6916168300	−0.1653610380
H	0.6315638698	3.8916352312	−0.0395434426
H	3.0924767378	4.7396181591	−0.1104605494
C	7.3503948274	3.9120242226	−0.3707531692
C	5.1957089621	2.7373479560	−0.3329404037
C	8.3033034355	2.7541183754	−0.4638589043
C	9.6421963865	3.4024612745	−0.9089095817
C	9.5164091649	4.8218057879	−0.3234845442
N	8.0195669245	5.0549467505	−0.3193886549
O	10.1816313775	5.7801434842	−1.0652191679

C	5.9275546858	3.8841711708	-0.3033644075
H	5.7172952239	1.7856703040	-0.4099100748
H	5.4429327697	4.8535239712	-0.2254507970
C	10.8662380921	2.6790858681	-0.3466547307
C	9.7084291055	3.4558695796	-2.4427694665
H	7.9618648596	1.9943696244	-1.1745223713
H	8.4071145627	2.2624164863	0.5131378667
H	10.8284062080	2.6231078679	0.7473736298
H	11.7877296610	3.2003134748	-0.6310128164
H	10.9223504028	1.6567742245	-0.7377568236
H	8.8330715760	3.9589672311	-2.8678186340
H	9.7435478980	2.4364196998	-2.8424619386
H	10.6012686920	3.9901506492	-2.7779800500
H	9.8221848483	4.8554636861	0.7322490096
C	10.5532349064	6.9542536689	-0.3378748087
H	11.1093861291	7.5833877951	-1.0372824426
H	11.2034547334	6.6956387875	0.5095599424
H	9.6714517368	7.4887071444	0.0229630248
O	7.5525257040	6.2377780507	-0.2165257709

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	<i>x</i>	<i>y</i>	<i>z</i>
C	-2.6401853583	-0.0357429581	-0.0992987405
C	-1.9309064972	1.0863988242	-0.5627114379
C	-0.5414245703	1.1013632148	-0.5848955095
H	-0.0316752894	1.9708221965	-0.9885155084
C	0.2120964614	0.0011696680	-0.1329606997
C	-0.5018471190	-1.1182291138	0.3359101944
C	-1.8913097596	-1.1390156972	0.3468104532
H	-2.4025815215	-2.0105166097	0.7447399095
C	-4.1180348413	-0.0544904207	-0.0804461399
C	-4.8286580347	-1.2521941077	-0.2851159924
C	-6.9372849667	-0.0851314374	-0.0374780032
C	-6.2385084211	1.1160395637	0.1653423040
H	-6.8000994268	2.0271102893	0.3477976936
C	-4.8525514864	1.1291327149	0.1450693003

H	-4.3232272938	2.0583272519	0.3302573081
C	1.6878187811	0.0204255594	-0.1491672512
C	2.4148801501	1.2151169626	-0.0034620787
H	1.8843310393	2.1514491423	0.1448635244
C	3.8022860302	1.2434433476	-0.0175822270
H	4.2986957815	2.1994053029	0.0934204893
C	4.5617379340	0.0569958451	-0.1783962273
C	3.8295356137	-1.1482627409	-0.3252103815
H	4.3476459962	-2.0913700187	-0.4464656115
C	2.4419315461	-1.1552944529	-0.3105584648
H	1.9323829652	-2.1047963028	-0.4482952179
H	0.0395411437	-1.9738854128	0.7276985566
H	-2.4735815556	1.9447141382	-0.9474943209
C	-6.2180578916	-1.2672782881	-0.2621094894
H	-4.2859425261	-2.1700305755	-0.4867393521
H	-6.7564196583	-2.1974082199	-0.4284944434
C	-8.4074394775	-0.1192090668	-0.0152989808
N	5.9387999131	0.0740282073	-0.1912403552
C	6.7193874668	-1.1281804817	-0.4703206857
C	6.9907126556	-1.9774293443	0.7735267528
H	7.6677329799	-0.8049115598	-0.9113977783
H	6.2129633968	-1.7210136282	-1.2385198246
H	7.5382086559	-1.3977304185	1.5256272156
H	7.5933407717	-2.8560949881	0.5140657900
H	6.0563211222	-2.3236328329	1.2276924515
C	6.6952629658	1.2941318459	0.0763915651
C	6.9286619182	2.1488975927	-1.1713015607
H	7.6573534335	0.9932274240	0.5034791444
H	6.1868008227	1.8755289808	0.8519072902
H	7.4778556778	1.5816385276	-1.9316084244
H	7.5149661346	3.0410989121	-0.9207828472
H	5.9798661812	2.4736292768	-1.6112832994
O	-9.1267457704	0.8508661605	0.1736820009
H	-8.8488671982	-1.1231976327	-0.1872570044

	x	y	z
C	-1.4568893029	-0.4469178337	-0.0243414603
C	-0.8268216923	0.6510440470	-0.6392383681
C	0.5571468167	0.7478996743	-0.6942565785
H	1.0046090838	1.5887228028	-1.2148959200
C	1.3871136102	-0.2387826648	-0.1261189411
C	0.7526515903	-1.3333521534	0.4936822189
C	-0.6311939008	-1.4386064368	0.5372524049
H	-1.0785655040	-2.2832032550	1.0521026800
C	-2.9254469580	-0.5547017587	0.0326111164
C	-3.5615942063	-1.8146236158	0.0640049856
C	-5.7575834957	-0.7779731378	0.1523581861
C	-5.1203579642	0.4839232715	0.1187576983
H	-5.7292676995	1.3831547033	0.1496119056
C	-3.7415723332	0.5932610762	0.0605407122
H	-3.2879181742	1.5784085146	0.0652865549
C	2.8562029720	-0.1285644865	-0.1795853123
C	3.5029677640	1.1195832624	-0.2295644693
H	2.9125882059	2.0310401868	-0.2052101662
C	4.8841090803	1.2358352928	-0.2844360298
H	5.3149918497	2.2283506665	-0.3268524523
C	5.7202154354	0.0900597822	-0.2923975655
C	5.0692224064	-1.1690241566	-0.2385092474
H	5.6479937005	-2.0841932010	-0.2334630633
C	3.6863751710	-1.2640756600	-0.1849122334
H	3.2417895218	-2.2549783556	-0.1679433820
H	1.3520747288	-2.0986341930	0.9766402109
H	-1.4262220602	1.4195486012	-1.1174744806
C	-4.9390937356	-1.9303436697	0.1228863537
H	-2.9620778374	-2.7172932457	0.0163856862
H	-5.3771454591	-2.9198135915	0.1373697957
C	-7.1961902605	-0.7767909189	0.2186274141
C	-8.1023411410	-1.8074974192	0.2459742042
H	-7.6445821649	0.2129219244	0.2528769526
N	7.0912667500	0.1941063657	-0.3498486025

C	7.9472798362	−0.9836572118	−0.4681657993
C	8.3019326549	−1.6118839896	0.8813042642
H	8.8613914998	−0.6702575507	−0.9822527861
H	7.4674815290	−1.7189084766	−1.1217322775
H	8.8229954599	−0.8888152467	1.5192821322
H	8.9586488730	−2.4785626530	0.7398118462
H	7.4031361206	−1.9446068211	1.4110897088
C	7.7672526916	1.4881892246	−0.3031617623
C	−7.7865549594	−3.1985099383	0.2041939226
C	−9.4979460133	−1.5057182038	0.3206388106
N	−7.5579964968	−4.3394125650	0.1709895372
N	−10.6347071352	−1.2631105255	0.3818265071
H	8.7609795424	1.3201787260	0.1240560951
H	7.2439605159	2.1482055136	0.3956498625
C	7.9000706674	2.1520419531	−1.6755788223
H	8.4662945666	1.5115357505	−2.3615327004
H	8.4272150414	3.1096215819	−1.5883694447
H	6.9175358087	2.3399263950	−2.1211081850

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	<i>x</i>	<i>y</i>	<i>z</i>
C	2.4989925816	−0.7714319201	0.8532774358
C	1.6493241026	−1.7365041003	0.2842602615
C	0.6696993640	−1.3825602679	−0.6365549687
H	0.0459112075	−2.1600125631	−1.0675384934
C	0.4849620088	−0.0449433069	−1.0336339404
C	1.3354215326	0.9192039306	−0.4609834110
C	2.3178261873	0.5654322289	0.4568994578
H	2.9653312982	1.3378037032	0.8615384265
C	3.5430265687	−1.1475706670	1.8299000675
C	3.9068328619	−0.2786937359	2.8782151034
C	5.5555346944	−1.8630176547	3.7159172453
C	5.1916192373	−2.7297196442	2.6669168614
H	5.6985752098	−3.6869910803	2.5739669271
C	4.2098425413	−2.3825825548	1.7470463686
H	3.9743139787	−3.0671212172	0.9378335454

C	-0.5565798086	0.3307736612	-2.0109118363
C	-1.7674824410	-0.3761686952	-2.1117530040
H	-1.9592407352	-1.2094207298	-1.4414252156
C	-2.7510560322	-0.0323945025	-3.0291952719
H	-3.6575720978	-0.6243437601	-3.0566027724
C	-2.5809694656	1.0595706934	-3.9172317656
C	-1.3612663146	1.7748346122	-3.8141977827
H	-1.1691778350	2.6251967420	-4.4567440482
C	-0.3895567981	1.4144535295	-2.8906469842
H	0.5349375403	1.9847439175	-2.8689633872
H	1.2158799038	1.9651234765	-0.7272982129
H	1.7478737690	-2.7776879336	0.5772673248
C	4.8861386390	-0.6242323683	3.7974866576
H	3.3945293526	0.6726890723	2.9848632131
H	5.1300543428	0.0720642349	4.5938019929
N	-3.5503971076	1.4076720125	-4.8328605590
C	-3.3267539815	2.4507682340	-5.8297383426
C	-3.6628420943	3.8559770536	-5.3249706502
H	-3.9502957683	2.2110343213	-6.6971855725
H	-2.2902326651	2.4050995900	-6.1786884832
H	-4.7132907674	3.9155903319	-5.0176294384
H	-3.4955840063	4.5975979450	-6.1153134799
H	-3.0427530195	4.1259544069	-4.4636847258
C	-4.8538099280	0.7503288887	-4.8592764503
C	-4.8732824586	-0.5273540489	-5.7016404687
H	-5.5733219809	1.4698509007	-5.2633461915
H	-5.1768005344	0.5407389789	-3.8346709134
H	-4.5945363585	-0.3105360621	-6.7393020985
H	-5.8763825089	-0.9705335536	-5.7028668898
H	-4.1700346672	-1.2701887733	-5.3107152512
C	8.0549821092	-2.0584730508	6.6088517144
C	6.5899997764	-2.2811557731	4.6518329890
C	7.0309216037	-1.5881492382	5.7313262518
H	7.0347915295	-3.2524764619	4.4409981581
H	6.6166231051	-0.6174806175	5.9885578639
N	8.4405584035	-1.3432301668	7.6559658780

C	9.5937048626	−1.9805178977	8.3787678097
C	9.5083209029	−3.4522545373	7.9261445514
H	9.4160732503	−1.8205335145	9.4489082198
O	10.7931181846	−1.3940304802	7.9737428242
C	8.8433613210	−3.3327108553	6.5264234212
C	8.5699646151	−4.2029953851	8.8845860247
C	10.8712545862	−4.1412975508	7.8716883537
H	8.2068519991	−4.1960608353	6.3049692684
H	9.5956966327	−3.2700781447	5.7290714277
H	11.5577068592	−3.6178124847	7.2017485263
H	10.7505262457	−5.1693373313	7.5106823392
H	11.3303263450	−4.1846957969	8.8660675212
H	7.5835890412	−3.7281442922	8.9389295077
H	8.9891399579	−4.2308609256	9.8968479952
H	8.4298799250	−5.2351597580	8.5454425433
C	11.0287561916	−0.0825052965	8.4878372120
H	10.3586405716	0.6530324357	8.0328583214
H	12.0668461904	0.1589670564	8.2450549423
H	10.8942084413	−0.0602219750	9.5781550433
O	7.9982467981	−0.2050029965	8.0434740395

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x

y

z

C	−5.7699270303	0.5283542912	−0.3087464646
C	−5.0306175214	1.6932067417	−0.5259750067
C	−3.6375263254	1.6595815889	−0.4838828784
C	−2.9519571910	0.4598576674	−0.2258054277
C	−3.7089252428	−0.7047807595	−0.0101463772
C	−5.1020707112	−0.6707272907	−0.0503159078
C	−1.4706859053	0.4237362339	−0.1828958270
C	−0.6987019581	1.2390792126	−1.0276287845
C	0.6913426959	1.2050833182	−0.9880204155
C	1.3730730995	0.3542456507	−0.1017090167
C	0.6010891894	−0.4610974656	0.7430238090
C	−0.7889554646	−0.4271015564	0.7034154453
H	−3.2012379844	−1.6484288671	0.1662491048
H	−1.1923249986	1.8850619124	−1.7474636619

H	-5.6663067244	-1.5850717341	0.1122760665
H	-6.8555487843	0.5547463419	-0.3405919834
H	-5.5394958624	2.6335404431	-0.7200412142
H	-3.0751184977	2.5770988254	-0.6297090561
H	1.0947123040	-1.1070803978	1.4628584536
H	-1.3534785830	-1.0472112464	1.3933717022
H	1.2558658619	1.8251928404	-1.6779767994
C	2.8543443799	0.3181240007	-0.0587993974
C	3.6113125958	1.4827625229	-0.2744573606
C	5.0044580536	1.4487088266	-0.2342874367
C	5.6723140500	0.2496269552	0.0241425451
C	4.9330043770	-0.9152255393	0.2413701217
C	3.5399131969	-0.8816001801	0.1992775817
H	2.9775050517	-1.7991173107	0.3451032397
H	3.1036254168	2.4264107945	-0.4508522027
H	5.5686943791	2.3630532540	-0.3968785776
H	6.7579358568	0.2232347378	0.0559884489
H	5.4418826175	-1.8555593888	0.4354359392
