Supporting Information

Unorthodox Synthesis, biological activity and DFT studies of novel and multifunctionalized naphthoxocine derivatives

Mohamed Ahmed Abozeid,[a] Aya Atef El-Sawi,[a] Mohamed Ramadan Elmorsy, Mohamed Abdelmoteleb,[b,c] Abdel-Rahman Hassan Abdel-Rahman[a] and El-Sayed Ibrahim El-Desoky*[a]

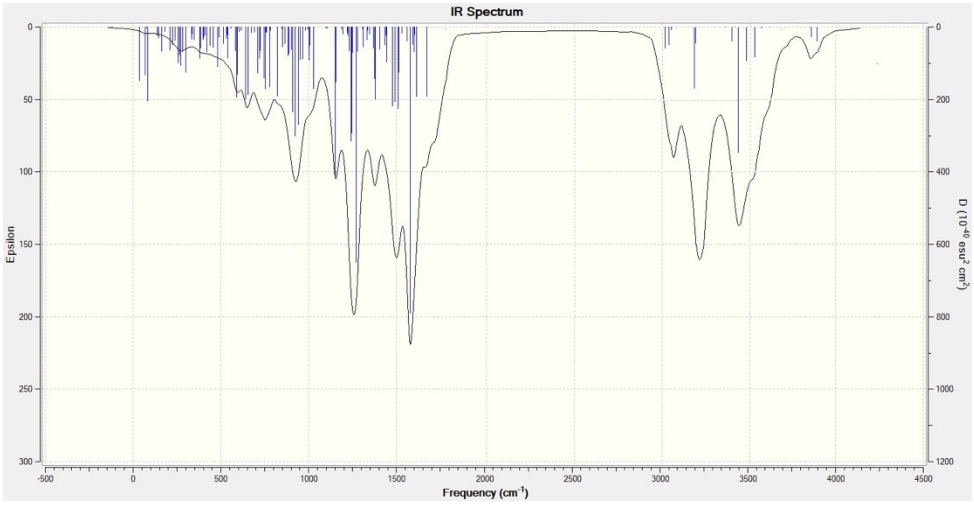
[a]*Department of Chemistry, Faculty of Science, Mansoura University, Mansoura-35516, Egypt*

[b]*Food Allergy Research & Resource Program (FARRP), Department of Food Science & Technology, University of Nebraska, Lincoln, NE, USA*

[c]*Department of Botany, Faculty of Science, Mansoura University, Mansoura-35516, Egypt*

Predicted IR spectrum of product 3a.

3450 cm^{-1} (OH), 3280 cm^{-1} (NH), 33105 cm^{-1} (Aromatic CH), 1608 cm^{-1} (C=N), 1530 cm^{-1} (C=C)



Cartesian coordinates for the optimized geometries of compounds 3a-e and 6

Table 1: Cartesian coordinates for the optimized geometry of **3a**.

Atom	**Cartesian Coordinates**		
C	-0.31114	0.450591	0.058856
C	0.515954	1.517585	-0.15121
H	-1.32387	0.715985	0.279849
C	1.131332	-1.85782	0.075498
C	7.624332	-1.45027	0.092224
C	6.712005	-0.64083	-0.50286
C	5.34797	-0.94042	-0.41004
C	4.935762	-2.05913	0.303191
C	5.888481	-2.88865	0.905657
C	7.207973	-2.58934	0.801677
H	4.713739	0.730412	-1.58769
H	8.666784	-1.22003	0.020241
H	7.035024	0.224446	-1.0431
C	4.396444	-0.12766	-1.03276
C	3.572575	-2.3415	0.414553
H	5.576938	-3.75668	1.448212
H	7.935405	-3.22407	1.263044
H	3.250727	-3.20449	0.959135
C	3.071594	-0.42239	-0.94658
C	2.621163	-1.49387	-0.17728
O	0.921362	-3.23155	0.412679
H	0.051186	-3.50511	0.113416
O	2.167603	0.35724	-1.67553
C	1.818979	1.48779	-0.9316
N	2.59572	2.522231	-0.9291
H	3.448874	2.508145	-1.45056
C	-1.31909	-1.95099	0.09151
H	-1.25295	-3.01878	0.110035
C	0.075958	2.87442	0.429313
C	-0.01609	5.174309	0.730335
C	-1.25286	4.854818	1.253141

C	0.393243	6.504812	0.636131
C	-2.17676	5.82814	1.624703
C	-0.50656	7.515132	1.033118
H	1.366299	6.75305	0.266752
C	-1.79529	7.178113	1.5128
H	-3.14596	5.557692	1.988571
H	-0.21462	8.542554	0.969293
H	-2.47987	7.951344	1.792743
N	0.766731	3.985819	0.289428
S	-1.42468	3.111188	1.351057
C	-0.03572	-1.10052	0.05594
N	-2.47709	-1.37445	0.098994
O	-3.61045	-2.12551	0.130401
H	-3.43699	-2.94726	0.595424

Table 2: Cartesian coordinates for the optimized geometry of **3b**.

Atom	**Cartesian Coordinates**		
C	0.269375	-1.13531	-0.46637
C	-0.1024	0.265859	-0.32526
C	0.527165	1.461094	-0.19368
H	-1.19009	0.327466	-0.31592
C	1.47265	-1.82147	-0.57875
C	7.865862	-1.64772	0.655675
C	7.050176	-0.67901	0.115112
C	5.657382	-0.91305	-0.04517
C	5.11543	-2.17961	0.355275
C	5.988141	-3.15908	0.909464
C	7.330613	-2.8987	1.058805
H	5.167164	1.01374	-0.91784
H	8.925967	-1.45907	0.77661
H	7.458571	0.276709	-0.19412
C	4.775894	0.060977	-0.58378
C	3.735577	-2.42838	0.162227
H	5.57331	-4.11444	1.211546
H	7.988054	-3.64809	1.48272

H	3.338415	-3.40291	0.41026
C	3.437167	-0.20019	-0.72355
C	2.882926	-1.45604	-0.34245
O	1.443902	-3.19924	-0.84984
H	0.629513	-3.44473	-1.35628
O	2.545522	0.753301	-1.23352
C	1.988036	1.637105	-0.19737
N	2.655827	2.376639	0.562183
H	3.667516	2.363429	0.339209
C	-0.93902	-2.0074	-0.39846
H	-0.75183	-3.06056	-0.17107
C	-0.25434	2.686796	-0.03623
C	-0.78035	4.875491	0.064524
C	-2.10078	4.403437	0.248
C	-0.53971	6.254322	0.046584
C	-3.16933	5.276476	0.410146
C	-1.60503	7.133369	0.209171
H	0.473954	6.605185	-0.09366
C	-2.91102	6.648732	0.389854
H	-4.17718	4.906964	0.549673
H	-1.42779	8.201872	0.197015
H	-3.73005	7.346705	0.515593
N	0.199975	3.8942	-0.08826
S	-2.11916	2.590857	0.233615
C	-3.29794	-2.30624	-0.27191
C	-4.50541	-1.73462	-0.70859
C	-3.33962	-3.57334	0.340183
C	-5.71192	-2.40764	-0.56026
H	-4.45913	-0.75817	-1.17344
C	-4.54737	-4.24057	0.502764
H	-2.43305	-4.03005	0.719748
C	-5.74081	-3.66891	0.04603
H	-6.62979	-1.96329	-0.92429
H	-4.59207	-5.21131	0.979442
C	-8.00292	-3.73861	0.933836

H	-8.83721	-4.44019	0.911035
H	-7.70445	-3.54426	1.970735
H	-8.30244	-2.7958	0.462384
O	-6.91873	-4.40546	0.189928
N	-2.13252	-1.53631	-0.48317

Table 3: Cartesian coordinates for the optimized geometry of **3c**.

Atom	**Cartesian Coordinates**		
C	-0.21931	0.417366	-0.15099
C	-1.21901	0.81734	0.662981
H	-0.04225	1.021914	-1.03914
C	0.428102	-2.01934	0.168921
C	-5.38824	-4.74535	-0.88
C	-5.00635	-3.7855	0.029128
C	-3.65307	-3.35497	0.102158
C	-2.69042	-3.9383	-0.78938
C	-3.11965	-4.93069	-1.71447
C	-4.43691	-5.3244	-1.75917
H	-3.91407	-1.9816	1.766872
H	-6.42214	-5.06613	-0.92907
H	-5.73135	-3.34311	0.703319
C	-3.21637	-2.38832	1.045806
C	-1.34316	-3.50241	-0.72147
H	-2.38856	-5.36976	-2.38461
H	-4.75623	-6.07992	-2.46711
H	-0.60715	-3.93732	-1.38707
C	-1.90388	-1.99199	1.083434
C	-0.96203	-2.51294	0.161774
O	1.333544	-3.03738	0.22501
H	2.285581	-2.80795	0.461872
O	-1.43498	-1.17129	2.125718
C	-1.45991	0.245986	2.014152
N	-1.58827	0.969132	3.039453
H	-1.72091	0.424914	3.907785
C	2.114199	-0.39648	-0.31851

H	2.699748	-1.26132	-0.61406
C	-2.06716	1.961914	0.314161
C	-3.86459	3.293556	0.240585
C	-3.04544	4.01776	-0.66739
C	-5.1528	3.756414	0.533714
C	-3.50482	5.18785	-1.27475
C	-5.60837	4.920575	-0.07184
H	-5.76413	3.195892	1.228587
C	-4.79017	5.630776	-0.96927
H	-2.88139	5.741265	-1.96604
H	-6.6031	5.28851	0.148537
H	-5.1639	6.537199	-1.43062
N	-3.27509	2.144403	0.768655
S	-1.49763	3.225972	-0.83392
N	2.673011	0.783005	-0.28574
C	0.739419	-0.68813	-0.02402
C	4.048307	0.819873	-0.36921
N	4.735693	1.929579	-0.73258
H	4.347429	2.815548	-1.02874
C	5.028743	-0.14436	-0.01575
C	4.707393	-1.42098	0.453423
N	4.274817	-2.44936	0.81039
C	6.286734	0.504117	-0.21547
C	8.913004	1.217001	-0.35426
H	9.945578	0.889611	-0.21383
H	8.745115	1.511639	-1.39098
H	8.688485	2.058491	0.302585
S	7.854481	-0.21618	0.073547
N	6.1369	1.765599	-0.65645

Table 4: Cartesian coordinates for the optimized geometry of **3d**.

Atom	**Cartesian Coordinates**		
C	-0.48913	0.529743	0.62042
C	-0.54752	-0.79832	0.34638
H	-1.46126	1.014182	0.705476

C	1.927521	1.527028	0.879674
C	7.318478	-1.64397	-0.93953
C	6.151822	-2.13594	-0.39838
C	5.070777	-1.26408	-0.09582
C	5.217831	0.139654	-0.35303
C	6.438614	0.614241	-0.91212
C	7.463426	-0.25671	-1.20113
H	3.721044	-2.77935	0.676555
H	8.136087	-2.31677	-1.16952
H	6.040682	-3.19566	-0.19723
C	3.844456	-1.72796	0.448971
C	4.156747	1.014315	-0.01805
H	6.544309	1.676049	-1.10561
H	8.388566	0.111449	-1.62786
H	4.289623	2.078129	-0.15808
C	2.822866	-0.85714	0.728197
C	2.954763	0.541324	0.490548
O	2.602867	2.701192	1.250879
H	2.042734	3.260285	1.845558
O	1.596794	-1.2952	1.246953
C	0.628438	-1.67135	0.204692
N	0.803993	-2.55727	-0.6637
H	1.695333	-3.069	-0.53315
C	-0.07237	2.898967	0.932172
H	0.605638	3.740195	0.763239
C	-1.84294	-1.45374	0.172589
C	-3.39621	-3.07252	-0.03753
C	-4.3104	-1.99388	-0.06582
C	-3.87641	-4.38328	-0.14097
C	-5.67807	-2.20279	-0.19278
C	-5.2443	-4.59893	-0.2691
H	-3.16887	-5.20132	-0.11902
C	-6.1396	-3.51685	-0.29503
H	-6.37123	-1.3716	-0.2132
H	-5.6245	-5.60994	-0.35016

H	-7.20236	-3.70168	-0.39587
N	-2.05115	-2.72563	0.095953
S	-3.41975	-0.42186	0.080826
N	-1.23088	3.116165	-0.14078
C	-4.23568	4.53415	-1.32577
H	-5.30496	4.696577	-1.03915
N	-2.24562	5.355611	-0.13254
C	0.560382	1.499046	0.825188
C	-2.43041	3.886227	0.218426
N	-3.64373	3.370974	-0.54247
H	-3.99093	2.433263	-0.52998
N	-3.40783	5.774335	-1.02135

Table 5: Cartesian coordinates for the optimized geometry of **3e**.

Atom	**Cartesian Coordinates**		
C	0.071134	0.012107	-0.02395
C	-0.80693	0.688026	0.740077
H	0.438372	0.498007	-0.92564
C	-0.02092	-2.47961	0.242618
C	-6.34372	-3.44057	-0.93891
C	-5.72806	-2.63736	-0.00615
C	-4.31056	-2.60263	0.095706
C	-3.53099	-3.41948	-0.79088
C	-4.20055	-4.2407	-1.74087
C	-5.57417	-4.25065	-1.81364
H	-4.21048	-1.23104	1.777861
H	-7.42486	-3.45917	-1.01035
H	-6.31473	-2.01902	0.664142
C	-3.63957	-1.8076	1.061189
C	-2.11893	-3.37521	-0.69276
H	-3.60697	-4.85675	-2.40759
H	-6.07722	-4.87729	-2.54039
H	-1.51876	-3.98852	-1.35364
C	-2.2697	-1.78857	1.129778
C	-1.48828	-2.54265	0.21316

O	0.534433	-3.73588	0.155061
H	1.518612	-3.69898	0.024809
O	-1.63545	-1.1334	2.198896
C	-1.22074	0.22374	2.091173
N	-1.13685	0.952349	3.11634
H	-1.44119	0.476301	3.981538
C	2.133806	-1.32691	0.152061
H	2.669847	-2.27192	0.297083
C	-1.33036	1.997047	0.340526
C	-2.71417	3.751791	0.214215
C	-1.75259	4.190264	-0.73586
C	-3.82785	4.55193	0.494712
C	-1.90026	5.410522	-1.39792
C	-3.97324	5.7658	-0.16503
H	-4.55022	4.205922	1.222208
C	-3.01645	6.191491	-1.10428
H	-1.16834	5.746283	-2.1221
H	-4.83071	6.393618	0.04488
H	-3.1478	7.141883	-1.60795
N	-2.4381	2.512967	0.794564
S	-0.47296	3.009017	-0.87579
N	2.823638	-0.24324	-0.05104
C	0.692293	-1.30856	0.210123
C	6.274417	-0.97652	-0.14132
C	6.290081	0.446785	-0.26755
C	7.481719	1.162629	-0.38062
C	8.668289	0.434126	-0.36702
C	8.667679	-0.97177	-0.24405
C	7.480245	-1.68511	-0.13128
C	4.198407	-0.33899	-0.1057
H	7.491638	2.241561	-0.47464
H	9.613127	0.957691	-0.45234
H	9.61351	-1.50028	-0.23712
H	7.470991	-2.76299	-0.03531
N	4.958285	-1.4336	-0.04334

N	4.956527	0.820337	-0.24425
H	4.56596	1.752827	-0.29577

Table 6: Cartesian coordinates for the optimized geometry of **6**.

Atom	**Cartesian Coordinates**		
C	-0.28768	0.29278	0.128571
C	0.490745	1.3897	-0.11546
H	-1.30625	0.518491	0.365733
C	1.254671	-1.95398	0.144129
C	7.724997	-1.25318	0.026201
C	6.765081	-0.49403	-0.55964
C	5.418374	-0.85837	-0.44114
C	5.071735	-1.98886	0.288351
C	6.073757	-2.76782	0.878204
C	7.375653	-2.40594	0.749636
H	4.686163	0.766365	-1.62446
H	8.753889	-0.97274	-0.06412
H	7.037061	0.381221	-1.11222
C	4.418849	-0.09828	-1.05414
C	3.724669	-2.33265	0.429058
H	5.814193	-3.64658	1.430572
H	8.140465	-3.0015	1.202569
H	3.453795	-3.20536	0.985444
C	3.110484	-0.45249	-0.93873
C	2.723178	-1.53247	-0.14828
O	1.109247	-3.33071	0.501918
H	0.244149	-3.64372	0.227393
O	2.158126	0.275306	-1.65831
C	1.778494	1.399732	-0.92105
N	2.513509	2.464259	-0.94481
H	3.358358	2.477229	-1.47967
C	-1.18732	-2.1531	0.234135
H	-1.07144	-3.216	0.273069
C	0.014693	2.742617	0.447544
C	-0.13698	5.044996	0.698956

C	-1.35327	4.703504	1.254789
C	0.233889	6.382957	0.565689
C	-2.29556	5.660445	1.624342
C	-0.68433	7.377523	0.958575
H	1.191912	6.648096	0.169994
C	-1.95305	7.017595	1.473458
H	-3.24934	5.37281	2.015247
H	-0.4221	8.410096	0.864771
H	-2.65171	7.77889	1.7504
N	0.669008	3.869965	0.268754
S	-1.47395	2.957489	1.394712
C	0.055336	-1.24593	0.144951
C	-2.42754	-1.60817	0.264376
H	-2.54788	-0.54632	0.214721
C	-5.85093	-2.16201	0.433968
C	-5.59713	-2.51614	-1.02066
H	-6.20574	-3.31147	-1.39808
H	-5.75902	-1.65359	-1.63228
N	-3.60817	-2.47835	0.367285
N	-4.7185	-1.85839	1.026019
O	-7.1348	-2.15737	1.064386
H	-7.69979	-2.81059	0.644827
C	-4.1276	-2.85846	-0.95887
N	-3.43964	-3.39984	-1.91177
H	-2.46785	-3.59486	-1.77866