Electronic Supplementary Material (ESI) for RSC Advances.

Table S1: Comparison of major experimental vibrational wave numbers (cm^{-1})

Compound	Vibrational modes (cm^{-1})								
	$\nu_{ass}(NH_2)$	$\nu_{ss}(NH_2)$	$\nu(C=N)_{py}$	$\nu_{ass}(SO_2)$	$\nu_{ss}(SO_2)$	$\nu(S-N)$	$\nu(C=N)_{bpy}$	$\nu(OH)_{HQ}$	$\nu(C=N)_{HQ}$
HL	3422	3258	1652	1331	1157	945			
NaL	3425	3355	1641	1295	1135	984			
bpy							1661		
HQ								3432	1625
Cu-bpy							1630		
Cu-Q									1605
1	3454	3360	1625 1591		1135	979			
2	3469	3354	1625			972	1638		
3	3440	3373	1630			1000			1593

HL: sulfamethazine, ss: symmetric, ass: asymmetric, py: pyrimidic, bpy: bipyridine, HQ: 8-hydroxyquinoline

Table S2: Selected bond lengths (Å), and angles (º) for complexes **1-3**

Bond lengths (Å)				**Angles (º)**			
1		**2**	**3**	**1**		**2**	**3**
Calcd.	**Exp***			**Calcd.**	**Exp***		
CuN12 = 2.098	2.043	CuN8 = 2.033	CuN5 = 2.818	N12CuN20 = 64.1	65.0	N8CuN9 = 60.3	N5CuN6 = 53.8
CuN20 = 2.104	2.035	CuN9 = 2.436	CuN6 = 1.988	N31CuN39 = 53.8	58.6	N10CuN11 = 60.3	O49CuO50 = 84.2
CuN31 = 2.051	2.021	CuN10 = 2.033	CuO49 = 1.970	N12CuN69 = 96.5	86.3	N12CuN13 = 80.0	N6CuO50 = 159.4
CuN39 = 2.818	2.509	CuN11 = 2.437	CuN50 = 2.003	N39CuN69 = 88.5	83.7	N11CuN13 = 103.8	O49CuO51 = 146.7
CuO40 = 2.184	1.982	CuN12 = 2.056	CuO51 = 2.037	N31CuO40 = 99.8	96.2	N9CuN12 = 103.8	N5CuN50 = 108.1
CuN69 = 2.039	2.698	CuN13 = 2.056				N10CuN13 = 163.8	
						N8CuN12 = 163.8	
						N9CuN13 = 87.5	
						N11CuN12 = 87.5	

* **[8]**

Table S3. Thermal stability (T_s) of rigid PVC thermally degraded at 180°C, in air, in presence of the studied compounds and reference stabilizers.

Compound	Induction time (min)
PVC Blank	0
DBLC (commercial reference)	6
Ca-Zn Stearate (commercial reference)	7
NaL	42
1	23
2	23
3	35

Table S4: Dehydrochlorination rate data of PVC blank, PVC stabilized with reference stabilizers and the investigated stabilizers.

DBLC								**Ca Zn Soap**							
Try 1		Try 2		Try 3		Average		Try 1		Try 2		Try 3		Average	
Induction period (min)	mV	Induction period (min)	mV	Induction period (min)	mV	Induction period (min)	mV	Induction period (min)	mV	Induction period (min)	mV	Induction period (min)	mV	Induction period (min)	mV
10	0	7	0	9	0	8.5	0	4	0	8	0	7	0	6	0
14	6	12	6	11.5	6	12.5	6	11	6	9.5	6	12	6	10.5	6
18	11.6	16	11.6	14.5	11.6	16.5	11.6	14.5	11.6	15	11.6	13	11.6	14.5	11.6
22	17.1	18.5	17.1	17	17.1	19.5	17.1	21	17.1	19	17.1	18	17.1	19.5	17.1
24	22.4	20	22.4	22.5	22.4	22.5	22.4	23	22.4	25	22.4	25	22.4	24	22.4
27	27.5	24	27.5	24	27.5	25.5	27.5	28.5	27.5	27	27.5	29	27.5	28.5	27.5
28.5	32.3	28.5	32.3	28.5	32.3	28.5	32.3	32	32.3	32	32.3	32	32.3	32	32.3
30	37	32	37	33	37	31.5	37	34.5	37	36	37	38	37	36	37

NaL								**1**							
Try 1		Try 2		Try 3		Average		Try 1		Try 2		Try 3		Average	
Induction period (min)	mV	Induction period (min)	mV	Induction period (min)	mV	Induction period (min)	mV	Induction period (min)	mV	Induction period (min)	mV	Induction period (min)	mV	Induction period (min)	mV
34.5	0	38	0	36.5	0	37	0	17	0	18	0	19	0	18	0
45	6	44.5	6	45	6	45	6	22	6	22	6	22	6	22	6
53	11.6	53	11.6	53	11.6	53	11.6	24	11.6	25.5	11.6	27	11.6	26	11.6
60	17.1	61	17.1	62	17.1	61	17.1	29	17.1	29.5	17.1	31	17.1	30	17.1
69	22.4	68.5	22.4	68.5	22.4	69	22.4	32	22.4	34	22.4	36	22.4	34	22.4
75	27.5	77	27.5	79	27.5	77	27.5	38	27.5	38	27.5	38	27.5	38	27.5
84	32.3	85.5	32.3	87	32.3	86	32.3	42	32.3	41.5	32.3	42	32.3	42	32.3
93	37	94	37	94.5	37	94	37	44	37	47	37	48	37	46	37

2								**3**							
Try 1		Try 2		Try 3		Average		Try 1		Try 2		Try 3		Average	
Induction period (min)	mV	Induction period (min)	mV	Induction period (min)	mV	Induction period (min)	mV	Induction period (min)	mV	Induction period (min)	mV	Induction period (min)	mV	Induction period (min)	mV
30	0	30	0	30	0	30	0	18	0	18	0	18	0	18	0
34	6	36	6	38	6	36	6	21	6	22.5	6	23	6	23	6

41	11.6	42	11.6	43	11.6	42	11.6	26	11.6	28	11.6	28	11.6	28	11.6
47	17.1	47.5	17.1	48	17.1	48	17.1	33	17.1	33	17.1	33	17.1	33	17.1
53	22.4	53.5	22.4	54	22.4	54	22.4	37	22.4	37.5	22.4	39	22.4	38	22.4
60	27.5	60	27.5	59	27.5	60	27.5	43	27.5	44	27.5	42	27.5	43	27.5
64	32.3	66	32.3	68	32.3	66	32.3	48	32.3	48	32.3	48	32.3	48	32.3
72	37	72	37	72	37	72	37	52	37	52.5	37	53	37	53	37

Table S5: Dehydrochlorination rate data of PVC blank, PVC stabilized with DBLC and the investigated stabilizer (NaL) in different ratios**.**

DBLC								**NaL**							
Try 1		Try 2		Try 3		Average		Try 1		Try 2		Try 3		Average	
Induction period (min)	mV	Induction period (min)	mV	Induction period (min)	mV	Induction period (min)	mV	Induction period (min)	mV	Induction period (min)	mV	Induction period (min)	mV	Induction period (min)	mV
10	0	7	0	9	0	8.5	0	34.5	0	38	0	36.5	0	37	0
14	6	12	6	11.5	6	12.5	6	45	6	44.5	6	45	6	45	6
18	11.6	16	11.6	14.5	11.6	16.5	11.6	53	11.6	53	11.6	53	11.6	53	11.6
22	17.1	18.5	17.1	17	17.1	19.5	17.1	60	17.1	61	17.1	62	17.1	61	17.1
24	22.4	20	22.4	22.5	22.4	22.5	22.4	69	22.4	68.5	22.4	68.5	22.4	69	22.4
27	27.5	24	27.5	24	27.5	25.5	27.5	75	27.5	77	27.5	79	27.5	77	27.5
28.5	32.3	28.5	32.3	28.5	32.3	28.5	32.3	84	32.3	85.5	32.3	87	32.3	86	32.3
30	37	32	37	33	37	31.5	37	93	37	94	37	94.5	37	94	37
NaL 25%: DBLC 75%								**NaL 50%: DBLC 50%**							
Try 1		Try 2		Try 3		Average		Try 1		Try 2		Try 3		Average	
Induction period (min)	mV	Induction period (min)	mV	Induction period (min)	mV	Induction period (min)	mV	Induction period (min)	mV	Induction period (min)	mV	Induction period (min)	mV	Induction period (min)	mV
55	0	55	0	55	0	55	0	69	0	69	0	69	0	69	0
61	6	63	6	65	6	63	6	75	6	77	6	79	6	77	6
70	11.6	71	11.6	71.5	11.6	71	11.6	84.5	11.6	85	11.6	84	11.6	85	11.6
78	17.1	79	17.1	80	17.1	79	17.1	92.5	17.1	93	17.1	94	17.1	93	17.1
86	22.4	86.5	22.4	87	22.4	87	22.4	101	22.4	101	22.4	101	22.4	101	22.4
93.5	27.5	95	27.5	97	27.5	95	27.5	108	27.5	109	27.5	110	27.5	109	27.5

103	32.3	103	32.3	103	32.3	103	32.3	115.5	32.3	117	32.3	118	32.3	117	32.3
110	37	111	37	111	37	111	37	125	37	125	37	125	37	125	37
NaL 75%: DBLC 25%															
Try 1		Try 2		Try 3		Average									
Induction period (min)	mV	Induction period (min)	mV	Induction period (min)	mV	Induction period (min)	mV								
45	0	47	0	49	0	47	0								
55	6	55	6	55	6	55	6								
62.5	11.6	63	11.6	63	11.6	63	11.6								
70	17.1	71	17.1	71	17.1	71	17.1								
77.5	22.4	79	22.4	80.5	22.4	79	22.4								
87	27.5	87	27.5	87	27.5	87	27.5								
95.5	32.3	95	32.3	94	32.3	95	32.3								
102	37	103	37	104	37	103	37								

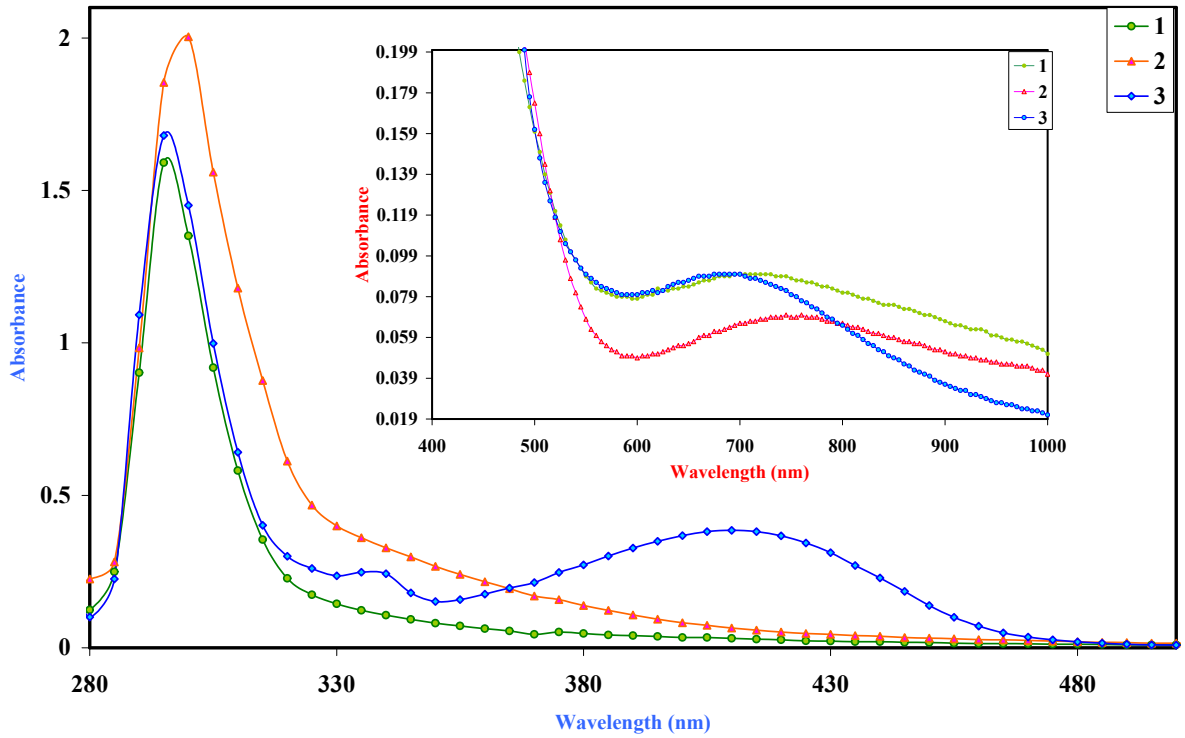
Table S6: Data of the thermal stability composition curve of NaL with the reference thermal stabilizers.

D+ DBLC								**D+ Ca-Zn soap**							
Try 1		Try 2		Try 3		Average		Try 1		Try 2		Try 3		Average	
Induction period (min)	mV	Induction period (min)	mV	Induction period (min)	mV	Induction period (min)	mV	Induction period (min)	mV	Induction period (min)	mV	Induction period (min)	mV	Induction period (min)	mV
0	10	0	7	0	9	0	8.5	0	4	0	8	0	7	0	6
25	53	25	55	25	57	25	55	25	50	25	51	25	51.5	25	51
50	69	50	69	50	69	50	69	50	54	50	55	50	56	50	55
75	46.5	75	47	75	46.5	75	47	75	46.5	75	46	75	47	75	47
100	34.5	100	38	100	36.5	100	37	100	34.5	100	38	100	36.5	100	37

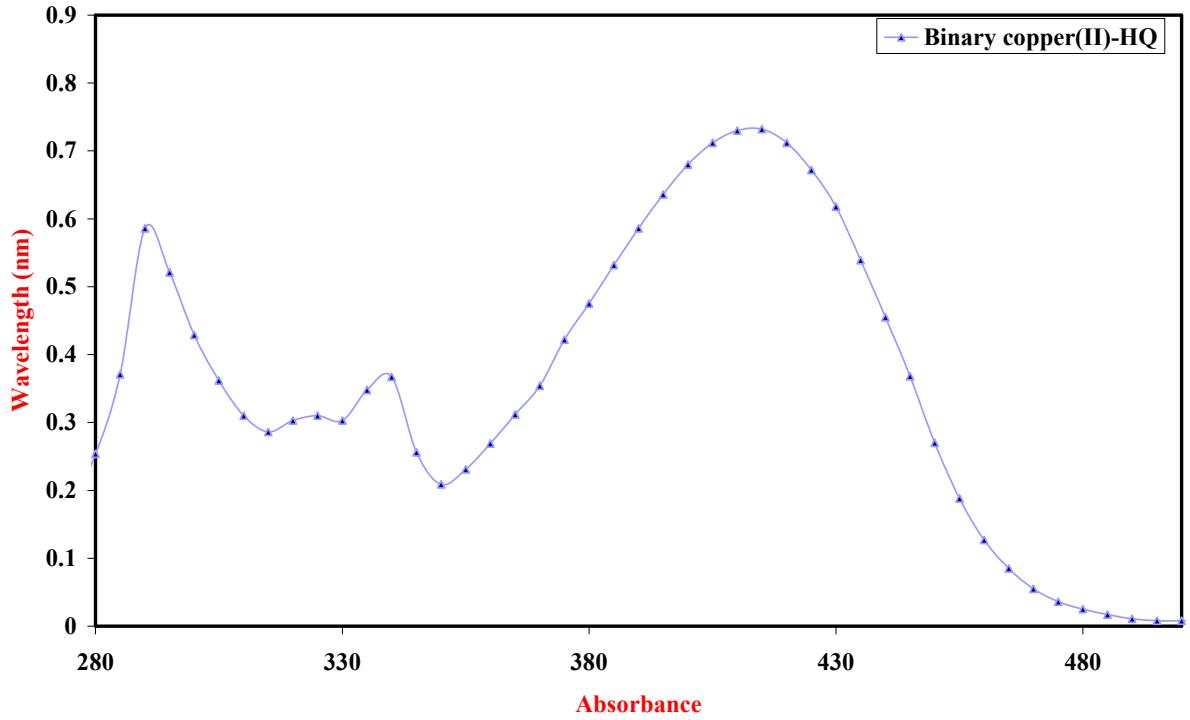
Table S7: Dehydrochlorination rate data of rigid PVC, in air, at 180 ^{o}C, in presence of 2 g of the investigated mixed stabilizer (NaL + Ca-Zn soap) per 100 g PVC

NaL 25%: DBLC 75%								**NaL 50%: DBLC 50%**							
Try 1		Try 2		Try 3		Average		Try 1		Try 2		Try 3		Average	
Induction period (min)	mV	Induction period (min)	mV	Induction period (min)	mV	Induction period (min)	mV	Induction period (min)	mV	Induction period (min)	mV	Induction period (min)	mV	Induction period (min)	mV
50	0	51	0	51.5	0	51	0	54	0	55	0	56	0	55	0
58	6	58	6	58	6	58	6	63	6	62	6	64	6	63	6
64	11.6	65	11.6	66	11.6	65	11.6	71	11.6	70	11.6	72	11.6	71	11.6
71	17.1	71.5	17.1	72	17.1	72	17.1	78	17.1	78.5	17.1	80	17.1	79	17.1
78.5	22.4	78	22.4	79	22.4	79	22.4	87	22.4	87	22.4	87	22.4	87	22.4
85	27.5	86	27.5	87	27.5	86	27.5	94	27.5	94.5	27.5	96	27.5	95	27.5
93	32.3	93	32.3	93	32.3	93	32.3	103	32.3	103	32.3	103	32.3	103	32.3
99	37	99.5	37	101	37	100	37	111	37	111	37	111	37	111	37
NaL 75%: DBLC 25%															

Try 1		Try 2		Try 3		Average									
Induction period (min)	mV	Induction period (min)	mV	Induction period (min)	mV	Induction period (min)	mV								
46.5	0	46	0	47	0	47	0								
54	6	54	6	53.5	6	54	6								
61	11.6	61	11.6	61	11.6	61	11.6								
67	17.1	68	17.1	69	17.1	68	17.1								
73	22.4	75	22.4	77	22.4	75	22.4								
82	27.5	81.5	27.5	82.5	27.5	82	27.5								
88	32.3	89	32.3	88.5	32.3	89	32.3								
95	37	96	37	97	37	96	37								



(a)



(b)

Fig. S1: Electronic absorption spectra of **a)** complexes 1-3 and **b)** Binary copper(II)-HQ.

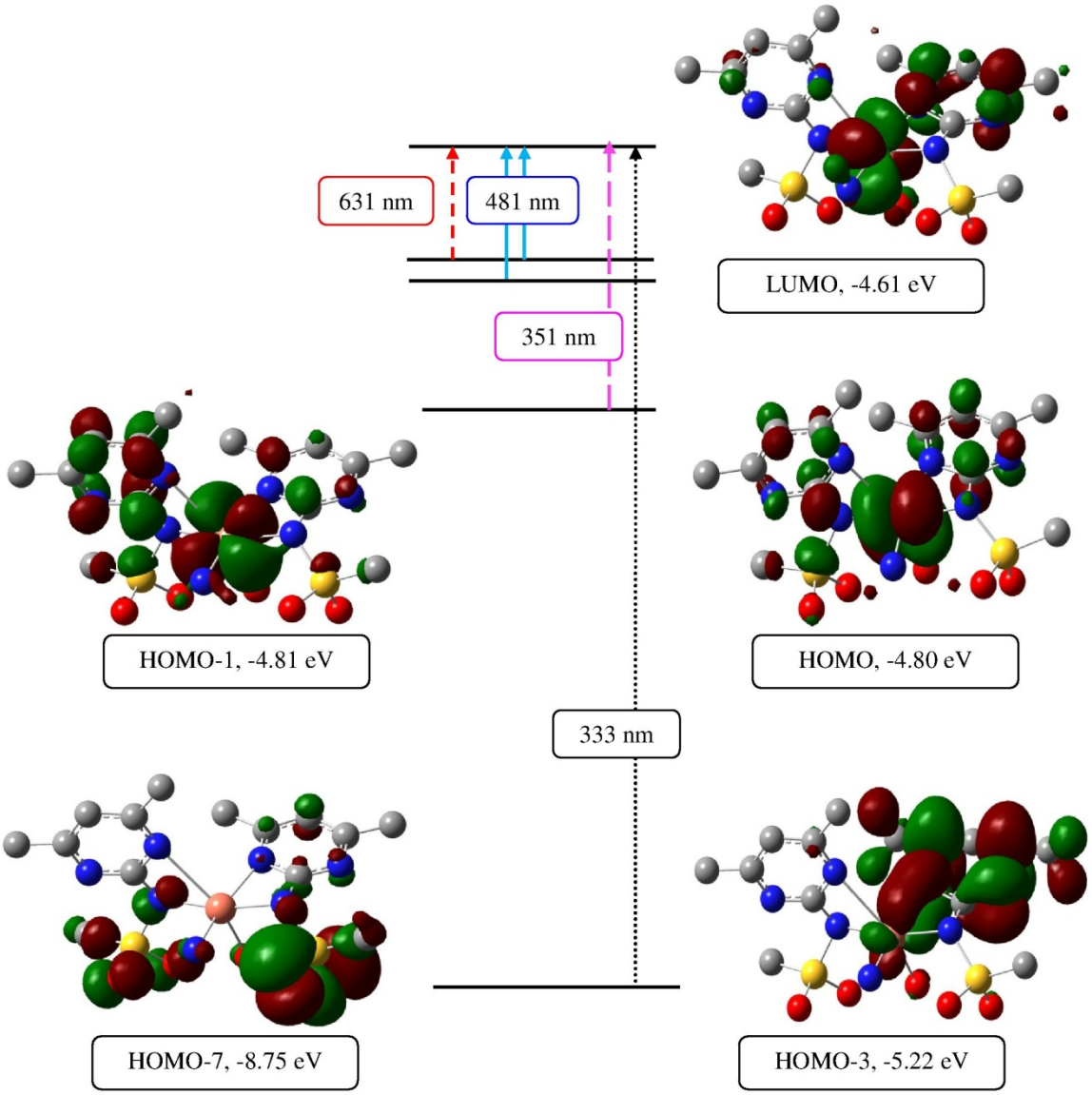


Fig. S2: TDDFT-calculated electronic transitions in complex **1**.

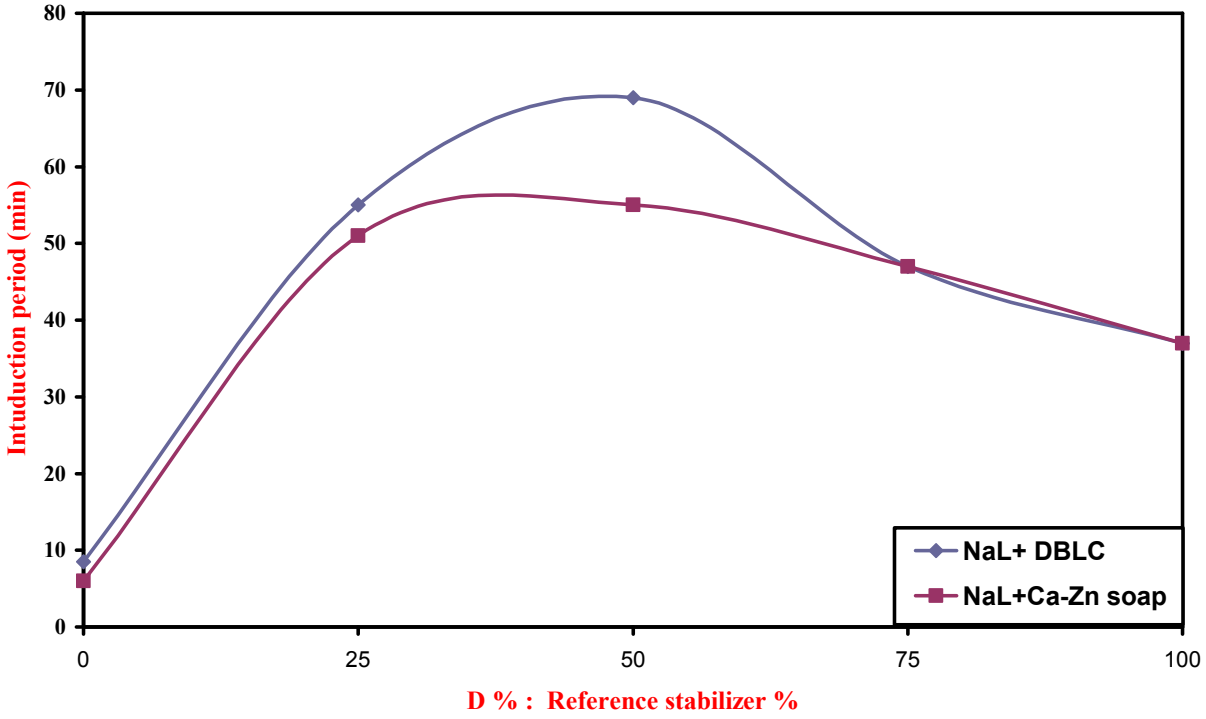


Fig. S3: Thermal stability composition curve of NaL with the reference thermal stabilizers. All experiments were carried out in triplicate and the mean results are given

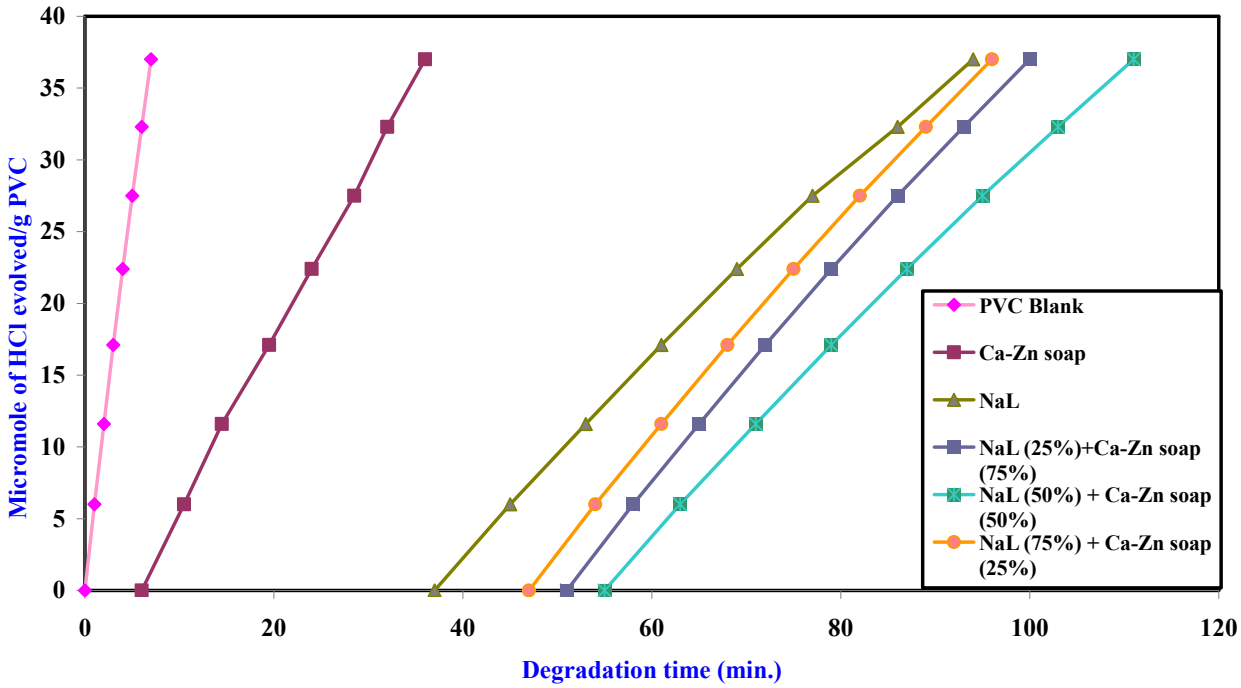


Fig. S4: Dehydrochlorination rate of rigid PVC, in air, at 180 ^{o}C, in presence of 2 g of the investigated mixed stabilizer (NaL + Ca-Zn soap) per 100 g PVC. All experiments were carried out in triplicate and the mean results are given

Table S4: Quantum chemical descriptors based on DFT calculations used for SAR studies				
	NaL	**1**	**2**	**3**
Total energy (a.u.)	-844.63	-2017.97	-2380.23	-1593.51
E_{HOMO} (eV)	-5.44	-5.86	-5.60	-5.32
E_{LUMO} (eV)	-0.789	-2.58	-3.09	-3.13
ΔE_{gap} (eV)	4.651	3.27	2.51	2.19
Total dipole moment (μ)	6.41	9.77	13.53	7.73
Ionization energy (I)	5.44	5.86	5.60	5.32
Electron affinity (A)	0.789	2.58	3.09	3.13
Mulliken electronegativity (χ)	3.11	4.22	4.34	4.22
Softness (*S*)	0.43	0.61	0.79	0.91
Hardness (η)	2.33	1.64	1.25	1.09
Electrophilicity index (ω)	11.28	14.61	11.87	9.76