Supplementary data

Design, synthesis, structural analysis and quantum chemical insight into the molecular structure of series of novel coumarin derivatives

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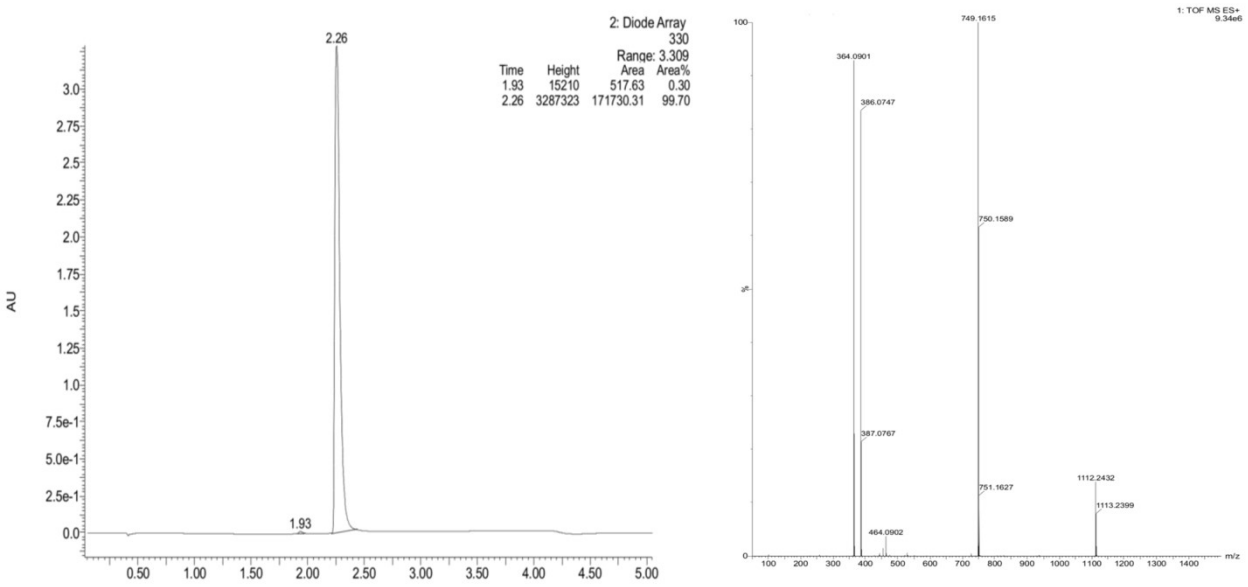

Figure S1 LC-MS spectra of compound **A**.

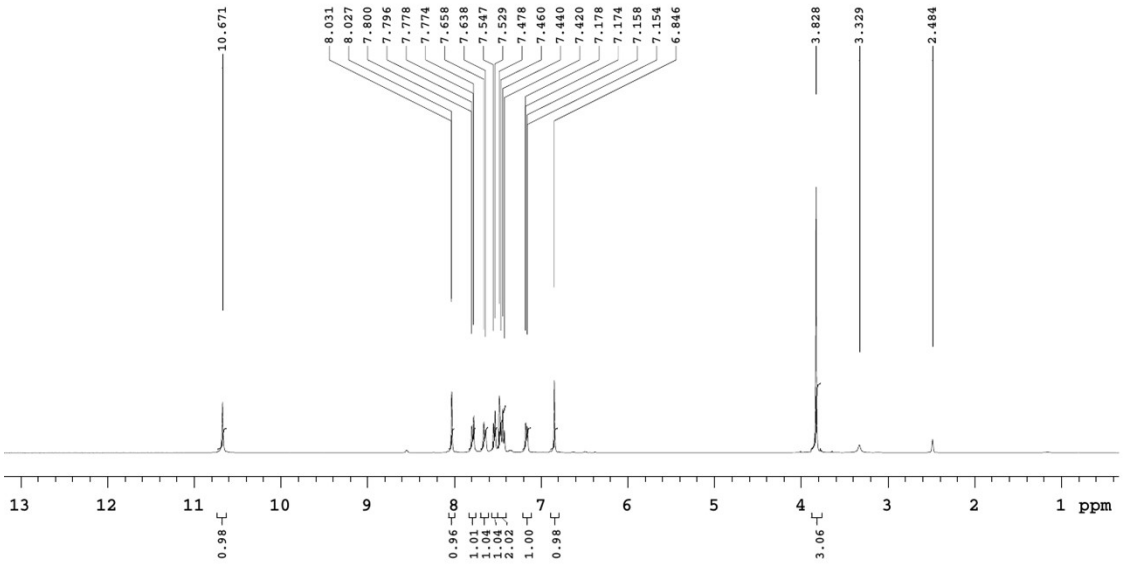

Figure S2 ^{1}H NMR of the compound **A**.

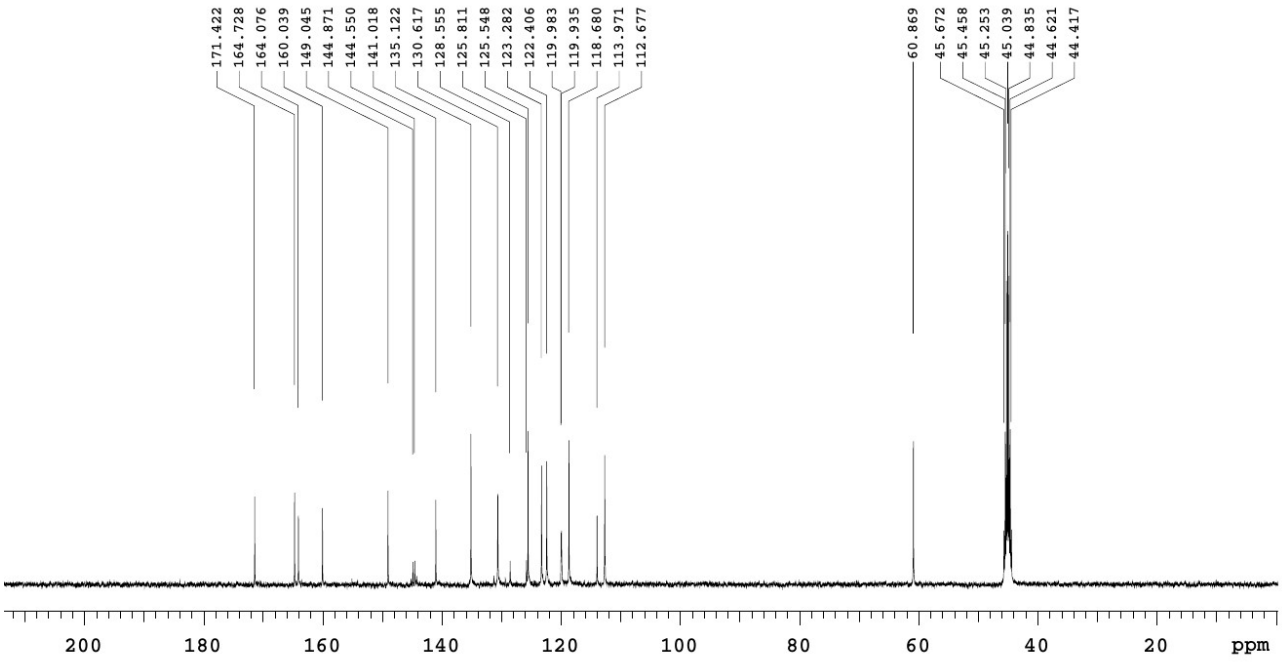

Figure S3 ^{13}H NMR of the compound **A**.

7-((3-methoxybenzoyl)amino)-2-oxo-4-(trifluromethyl)chromen-1-ide:(A)

LC-MS (m/z): 364.0901 ([M+H]$^{+}$, cal. 363.29). ^{1}H NMR (DMSO-d_6, δ ppm): 10.671 (s, 1H), 8.031-8.027 (d, J= 2 Hz, Ar-H), 7.800-7.774 (m, Ar-H), 7.658-7.638 (d, 10 Hz, Ar-H), 7.547-7.529 (d, 9 Hz, Ar-H), 7.478-7.420 (m, Ar-H), 7.178-7.154 (m, Ar-H), 6.846 (s, 1H, O-CH3). ^{13}C NMR (DMSO-d_6, δ ppm): 171.42, 164.72, 164.07, 160.03, 149.04, 135.12, 130.61, 128.55, 125.81, 125.54, 123.28, 122.40, 119.98, 119.93, 118.68, 113.97, 112.67, 60.86.

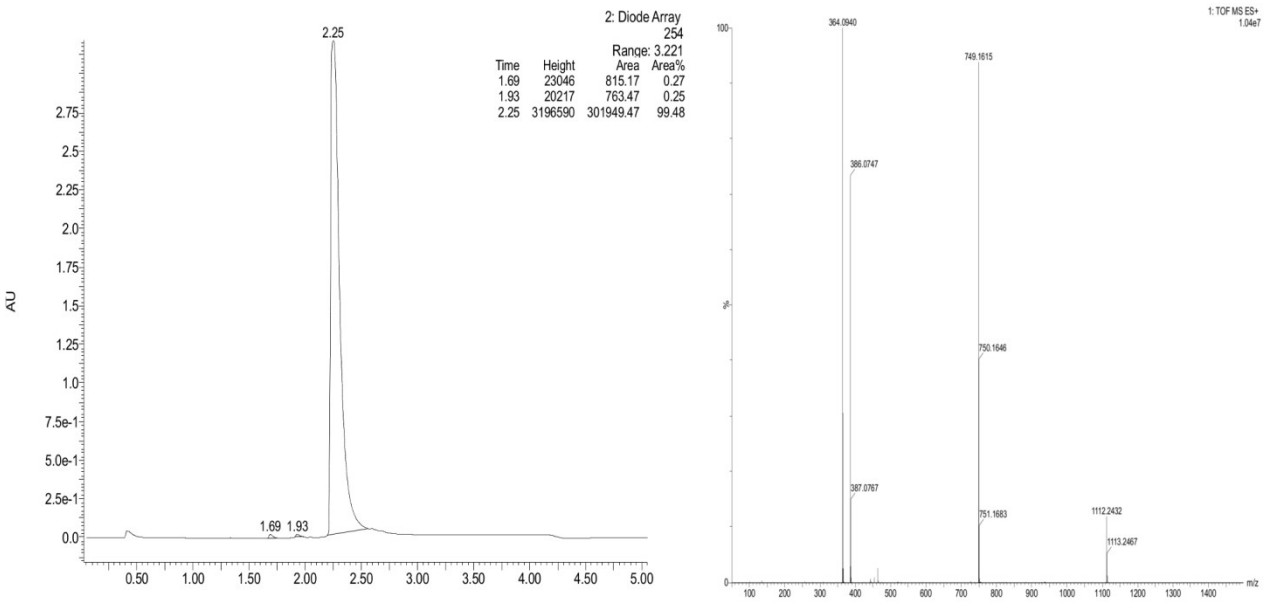

Figure S4 LC-MS spectra of compound **B**.

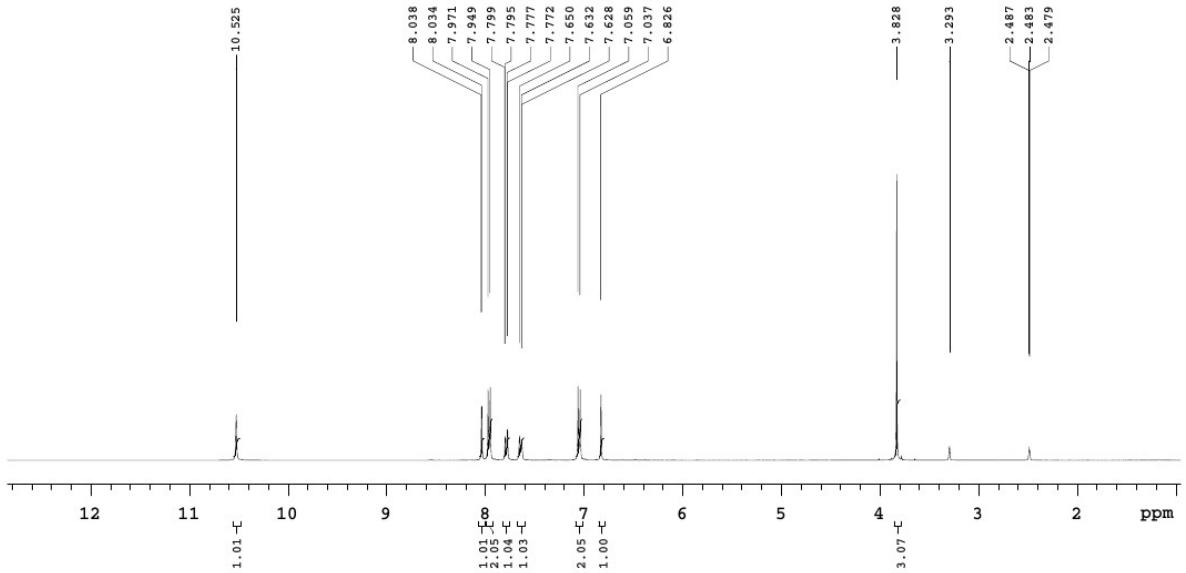

Figure S5 ^{1}H NMR of the compound **B**.

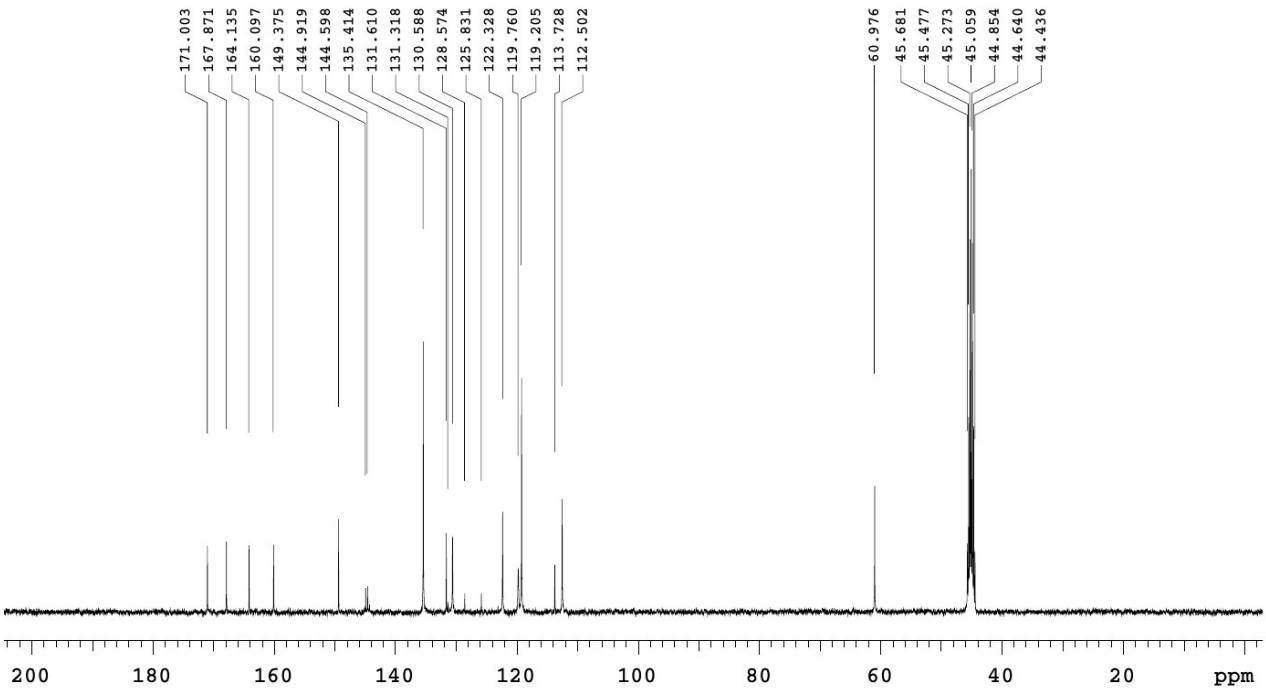

Figure S6 ^{13}H NMR of the compound **B**.

7-((4-methoxybenzoyl)amino)-2-oxo-4-(trifluromethyl)chromen-1-ide: (B)

LC-MS (m/z): 364.0940 ([M+H]$^+$, cal. 363.29). ^{1}H NMR (DMSO-d$_6$, δ ppm): 10.525 (s, 1H), 8.038-8.034 (d, J= 2 Hz, Ar-H), 7.971 (s, Ar-H), 7.949 (s, Ar-H), 7.799-7.795 (d, 2 Hz, Ar-H), 7.777-7.772 (d, 2.5 Hz, Ar-H), 7.650-7.628 (t, 11 Hz, Ar-H), 7.059-7.037 (d, 11 Hz, Ar-H), 6.826 (s, 1H, O-CH3). ^{13}C NMR (DMSO-d$_6$, δ ppm): 171.00, 167.87, 164.13, 160.09, 149.37, 144.59, 135.41, 131.61, 131.31, 130.58, 128.57, 125.83, 122.32, 119.76, 119.20, 113.72, 112.50, 60.97.

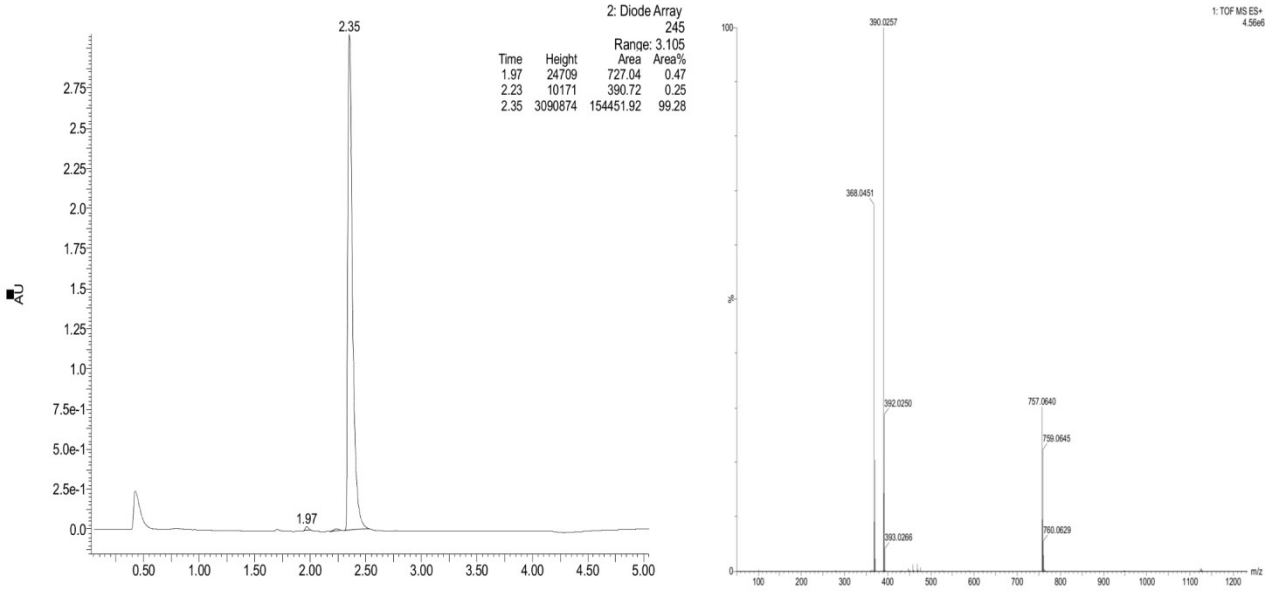

Figure S7 LC-MS spectra of compound **C**.

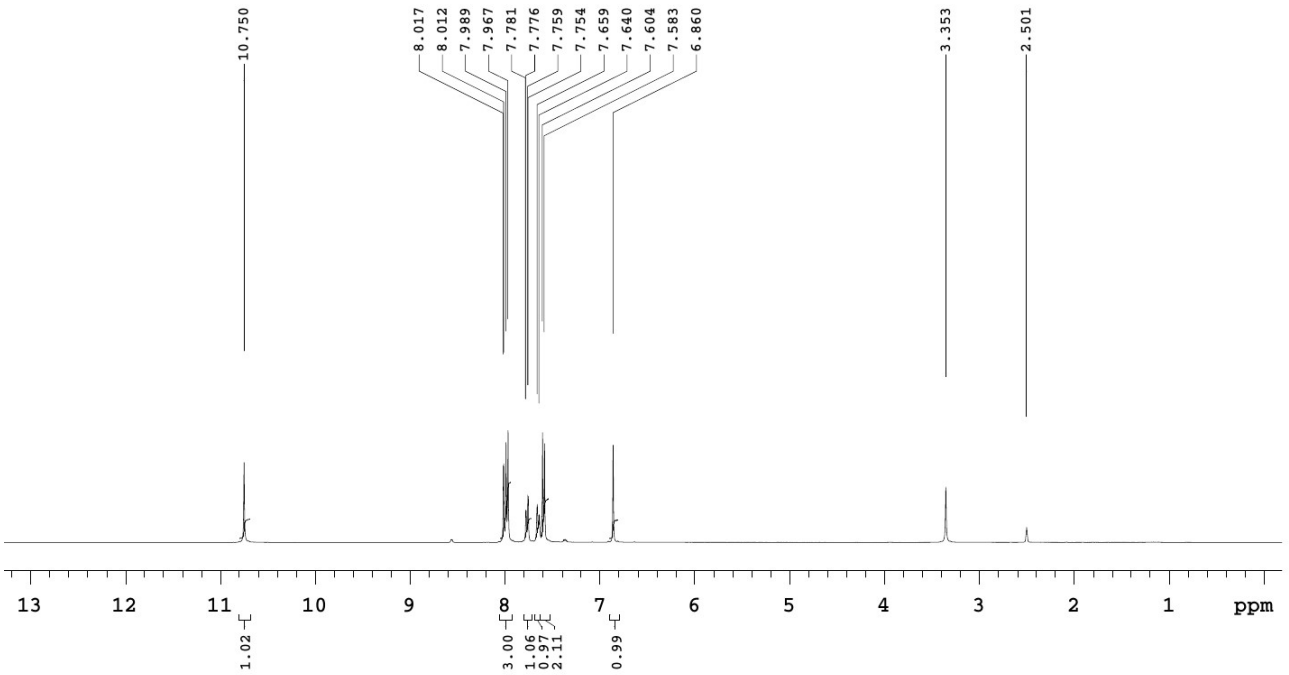

Figure S8 ^{1}H NMR of the compound **C**.

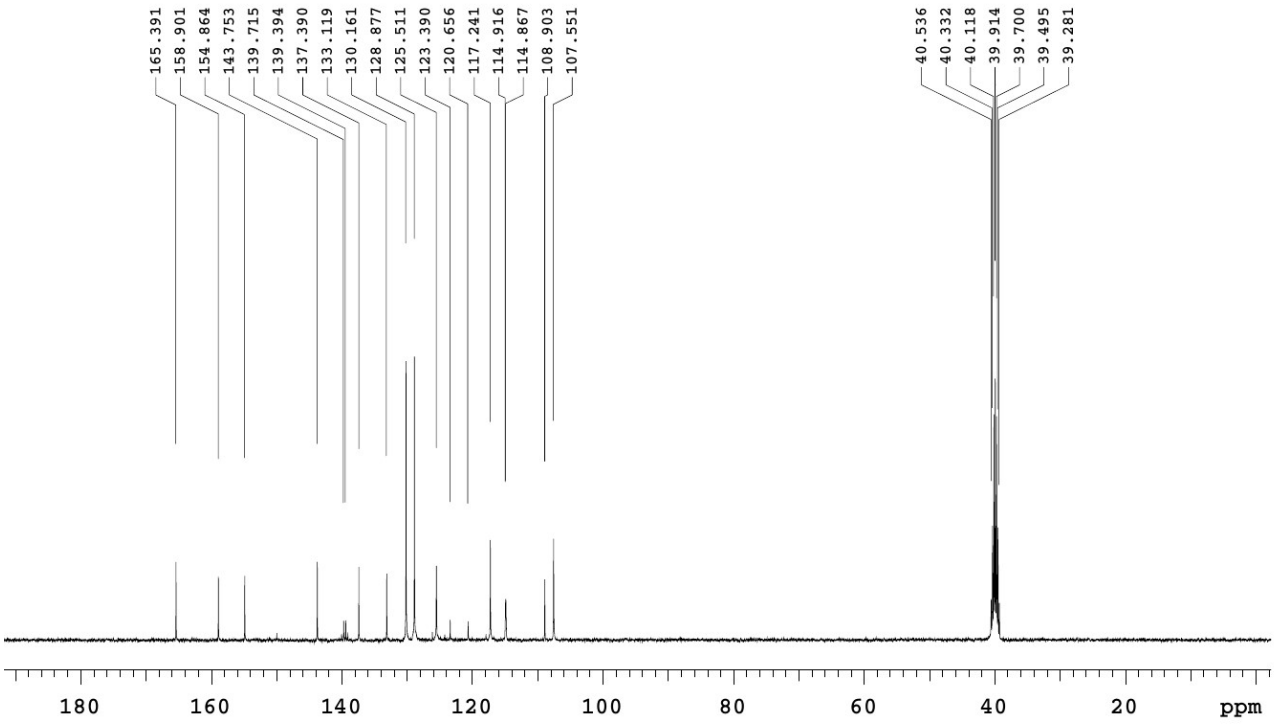

Figure S9 ^{13}H NMR of the compound **C**.

7-((4-chlorobenzoyl)amino)-2-oxo-4-(trifluromethyl)chromen-1-ide: (C)

LC-MS (m/z): 368.0451 ([M+H]$^+$, cal. 367.70) . ^{1}H NMR (DMSO-d$_6$, δ ppm): 10.750 (s, 1H), 8.017-8.012 (d, J= 2.5 Hz, Ar-H), 7.989 (s, Ar-H), 7.967 (s, Ar-H), 7.781-7.776 (d, 2.5 Hz, Ar-H), 7.759-7.754 (d, 2.5 Hz, Ar-H), 7.659 (s, Ar-H), 7.640 (s, Ar-H), 7.604 (s, Ar-H), 7.583 (s, Ar-H), 6.860 (s, 1H, O-CH3). ^{13}C NMR (DMSO-d$_6$, δ ppm): 165.39, 158.90, 154.86, 143.75, 139.39, 137.39, 133.11, 130.16, 128.87, 125.51, 123.39, 120.65, 117.24, 114.91, 114.86, 108.90, 107.55.

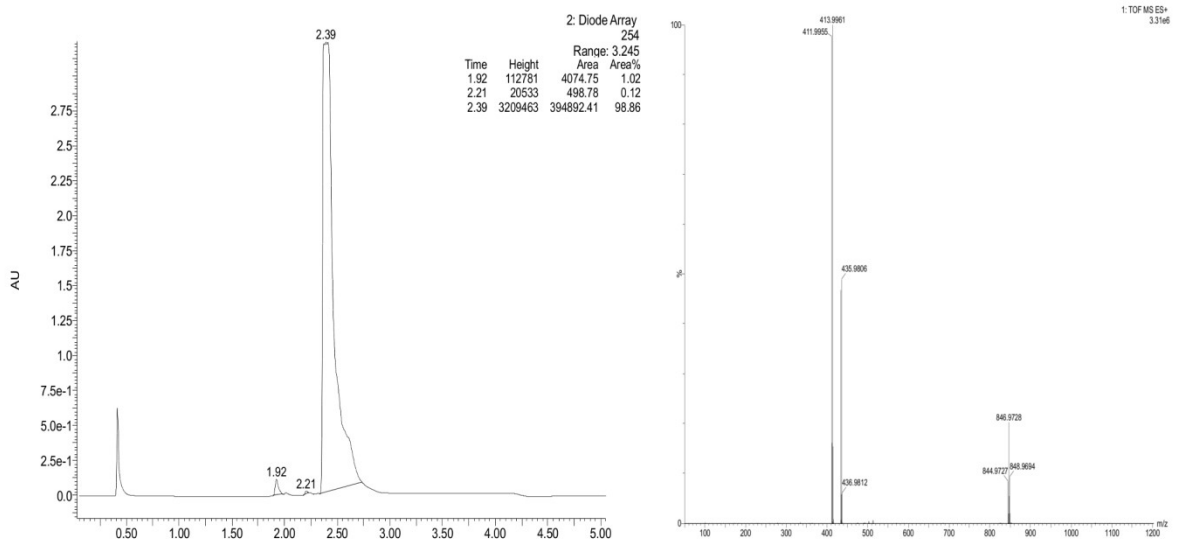

Figure S10 LC-MS spectra of compound **D**.

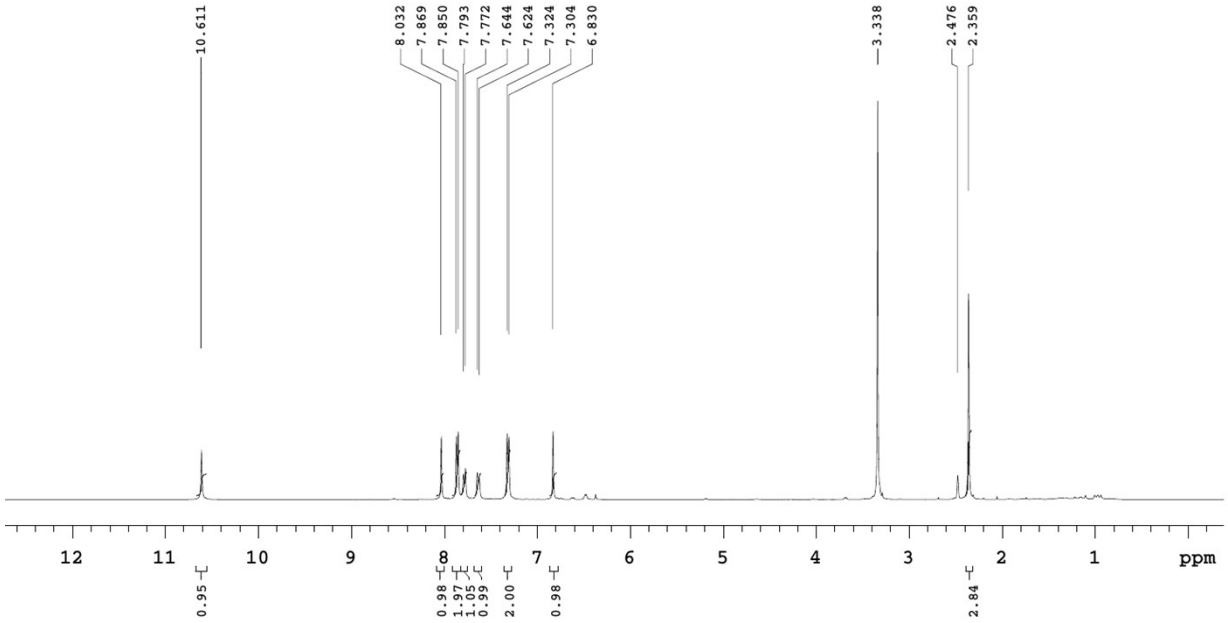

Figure S11 ^{1}H NMR of the compound **D**.

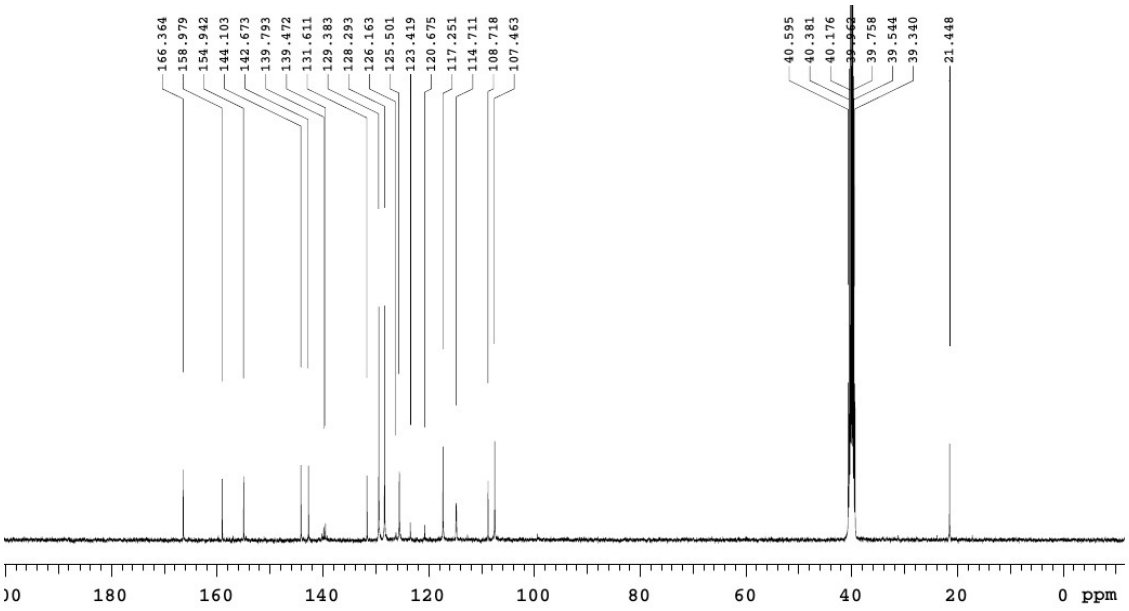

Figure S12 ^{13}H NMR of the compound **D**.

7-((4-methylbenzoyl)amino)-2-oxo-4-(trifluromethyl)chromen-1-ide: (D)

LC-MS (m/z): 348.1020 ([M+H]$^{+}$, cal. 347.29). ^{1}H NMR (DMSO-d_6, δ ppm): 10.611 (s, 1H), 8.032 (s, Ar-H), 7.869-7.850 (d, 9.5 Hz, Ar-H), 7.793-7.772 (d, 10.5 Hz, Ar-H), 7.644-7.624 (d, 10 Hz, Ar-H), 7.324-7.304 (d, 10 Hz, Ar-H), 6.830 (s, 1H, CH3). ^{13}C NMR (DMSO-d_6, δ ppm): 166.26, 158.97, 154.94, 144.10, 142.67, 139.79, 139.47, 131.61, 129.38, 128.29, 126.16, 125.50, 123.41, 120.67, 117.25, 114.71, 108.71, 107.46.

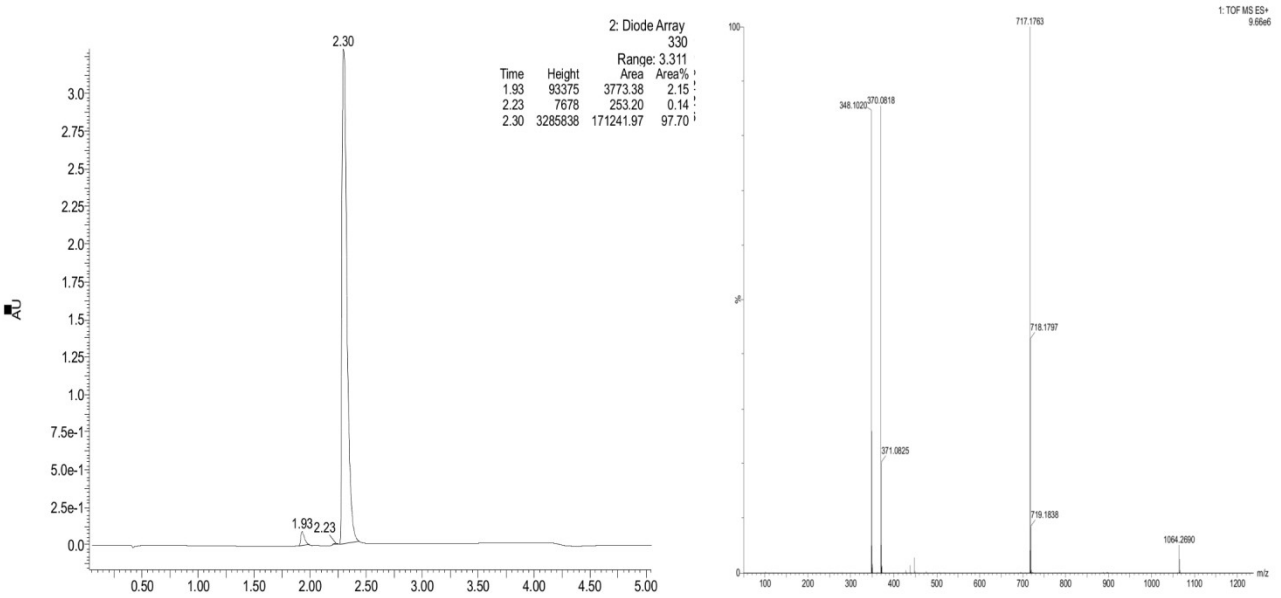

Figure S13 LC-MS spectra of compound **E**.

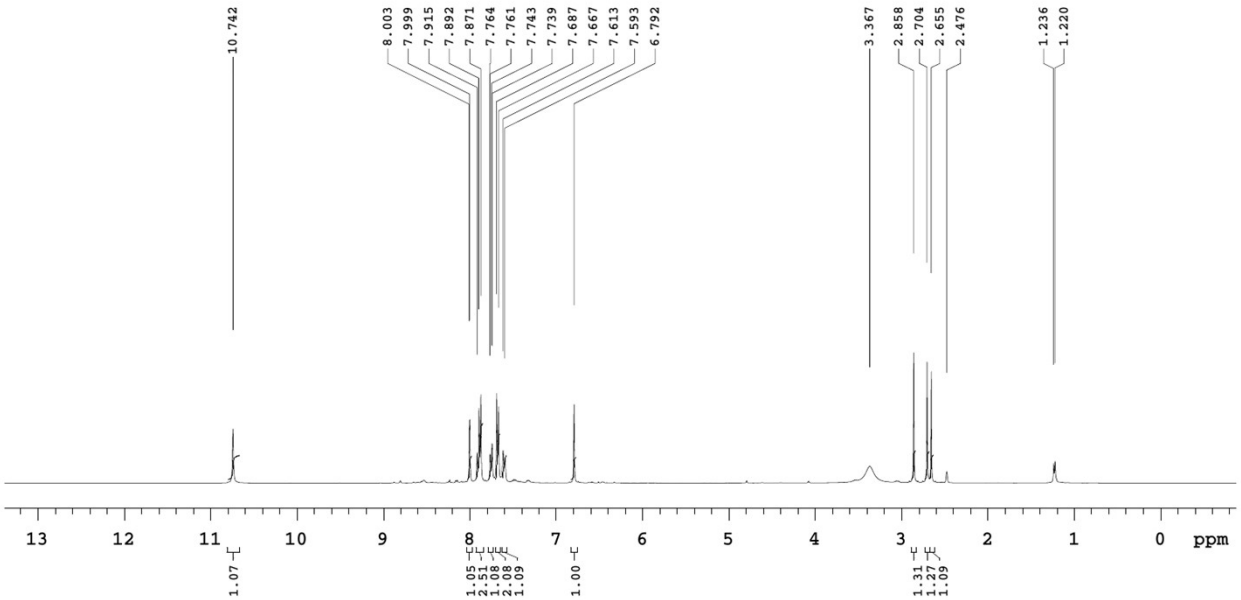

Figure S14 ^{1}H NMR of the compound **E**.

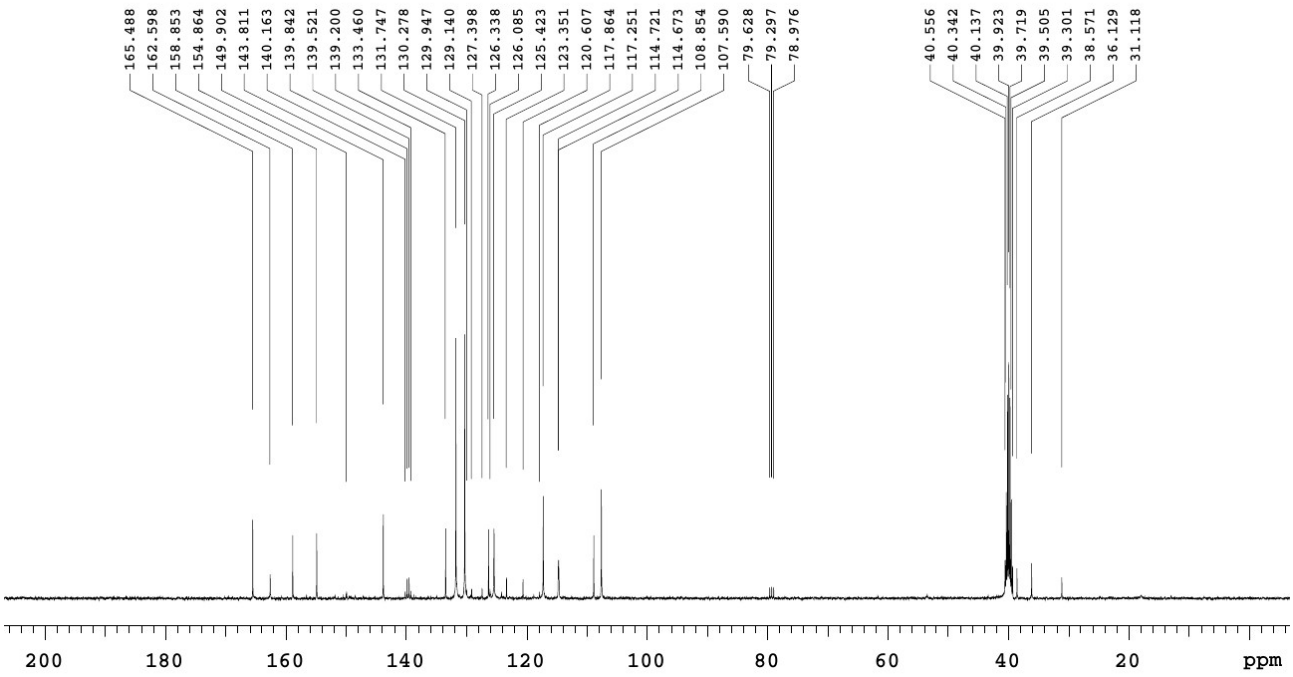

Figure S15 ^{13}H NMR of the compound **E**.

7-((4-bromobenzoyl)amino)-2-oxo-4-(trifluromethyl)chromen-1-ide: (E)

LC-MS (m/z): 411.9955 ([M+H]$^+$, cal. 412.16). ^{1}H NMR (DMSO-d$_6$, δ ppm): 10.742 (s, 1H, NH), 8.003-7.999 (d, 2 Hz, Ar-H), 7.915-7.871 (t, 22 Hz, Ar-H), 7.764-7.739 (m, Ar-H), 7.687-7.667 (d, 10 Hz, Ar-H), 7.613-7.593 (d, 10 Hz, Ar-H), 6.792 (s, 1H, Ar-H). ^{13}C NMR (DMSO-d$_6$, δ ppm): 165.48, 158.85, 154.86, 139.84, 133.46, 131.74, 130.27, 129.94, 129.14, 127.39, 126.33, 123.35, 117.86, 117.25, 114.72, 108.85, 107.59.

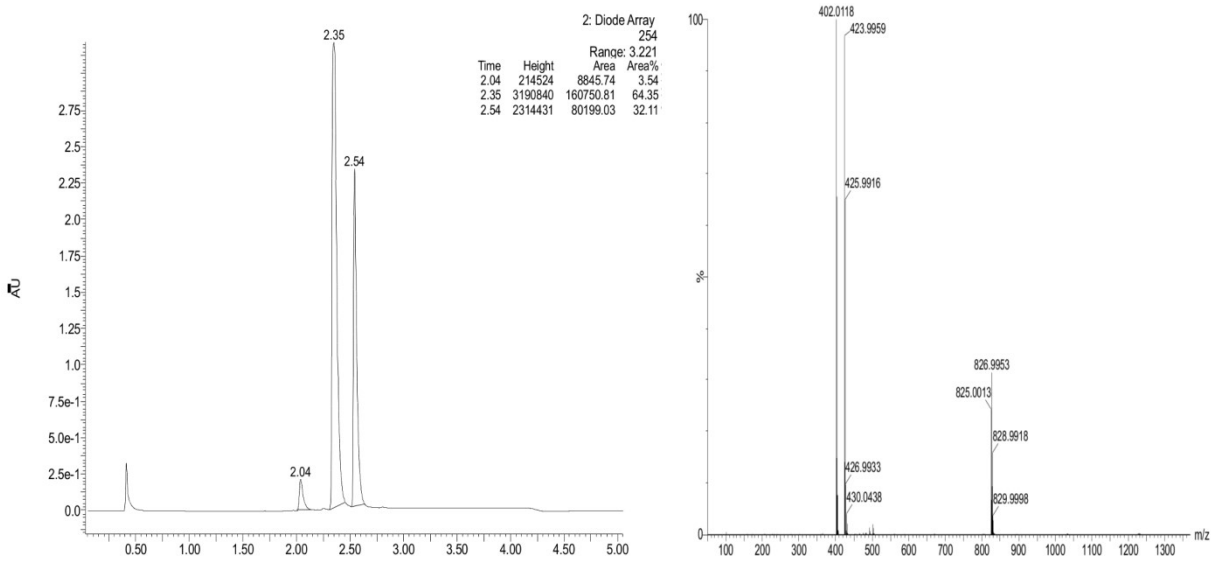

Figure S16 LC-MS spectra of compound **F**.

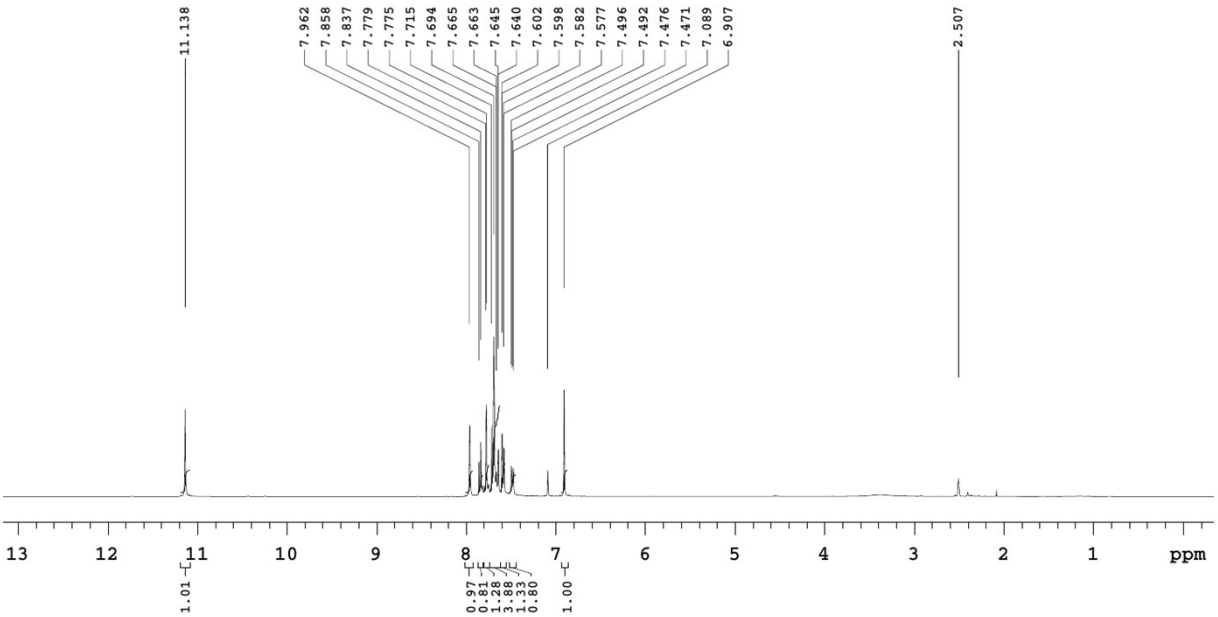

Figure S17 ^{1}H NMR of the compound **F**.

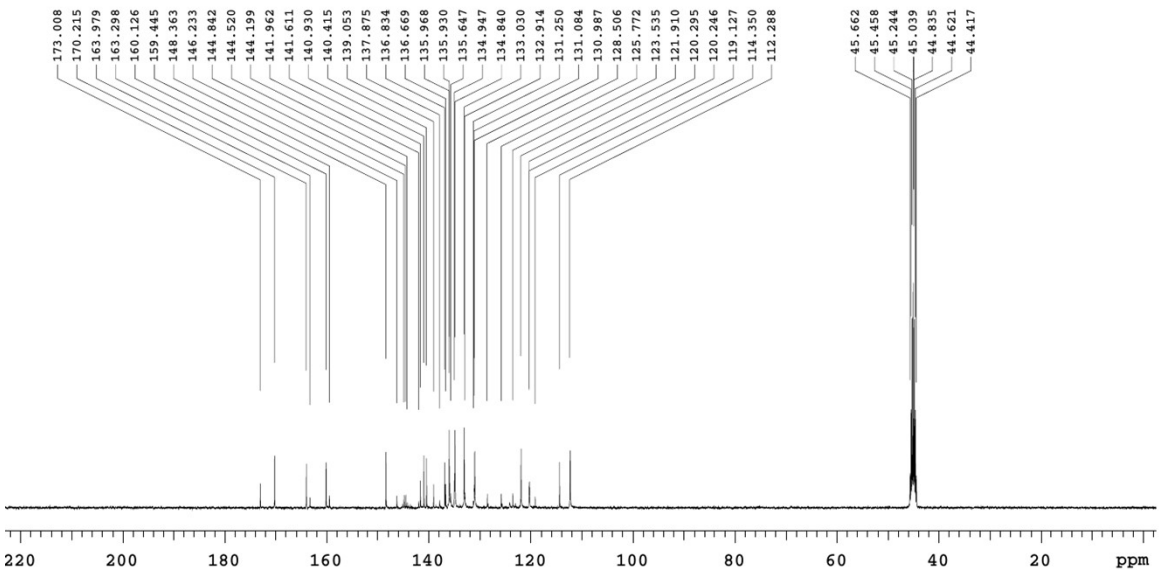

Figure S18 ^{13}H NMR of the compound **F**.

7-((2,4-dichlorobenzoyl)amino)-2-oxo-4-(trifluromethyl)chromen-1-ide: (F)

LC-MS (m/z): 402.0118 ([M+H]$^{+}$, cal. 402.14). ^{1}H NMR (DMSO-d_6, δ ppm): 11.138 (s, NH), 7.962 (s, Ar-H), 7.858-7.837 (d, 10.5 Hz, Ar-H), 7.779-7.775 (d, 2 Hz, Ar-H), 7.715 (s, Ar-H), 7.694 (s, Ar-H), 7.665-7.663 (d, 1Hz, Ar-H), 7.645-7.640 (d, 2.5 Hz, Ar-H), 7.602-7.598 (d, 2 Hz, Ar-H), 7.582-7.577 (d, 2.5 Hz, Ar-H), 7.496-7.492 (d, 2 Hz, Ar-H), 7.476-7.471 (d, 2.5 Hz, Ar-H), 7.089 (s, Ar-H), 6.907 (s, Ar-H). ^{13}C NMR (DMSO-d_6, δ ppm): 173.00, 163.97, 160.12, 159.44, 139.05, 136.83, 136.66, 135.96, 130.98, 128.50, 125.77, 123.53, 121.91, 120.29, 120.24, 119.12, 114.35.

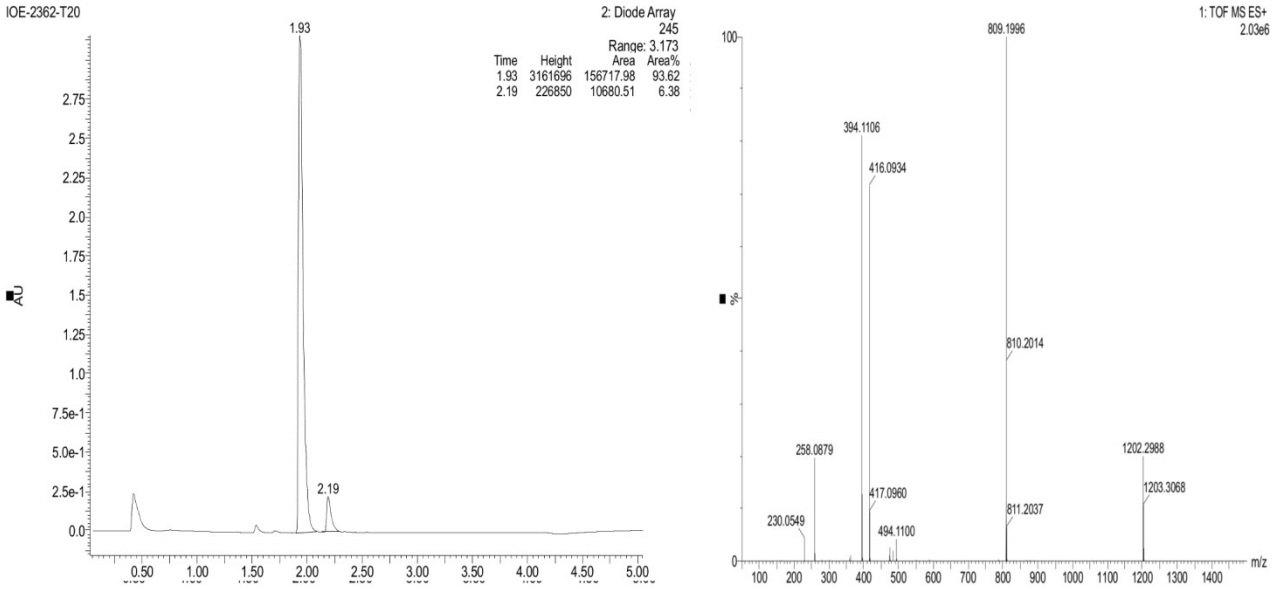

Figure S19 LC-MS spectra of compound **G**.

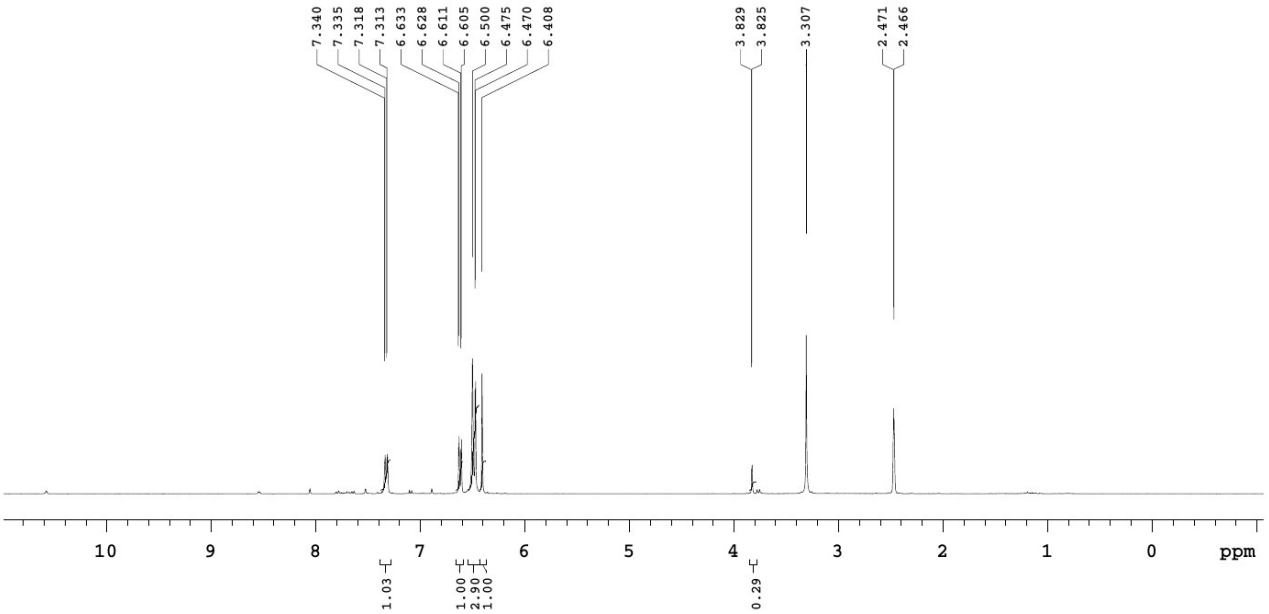

Figure S20 ^{1}H NMR of the compound **G**.

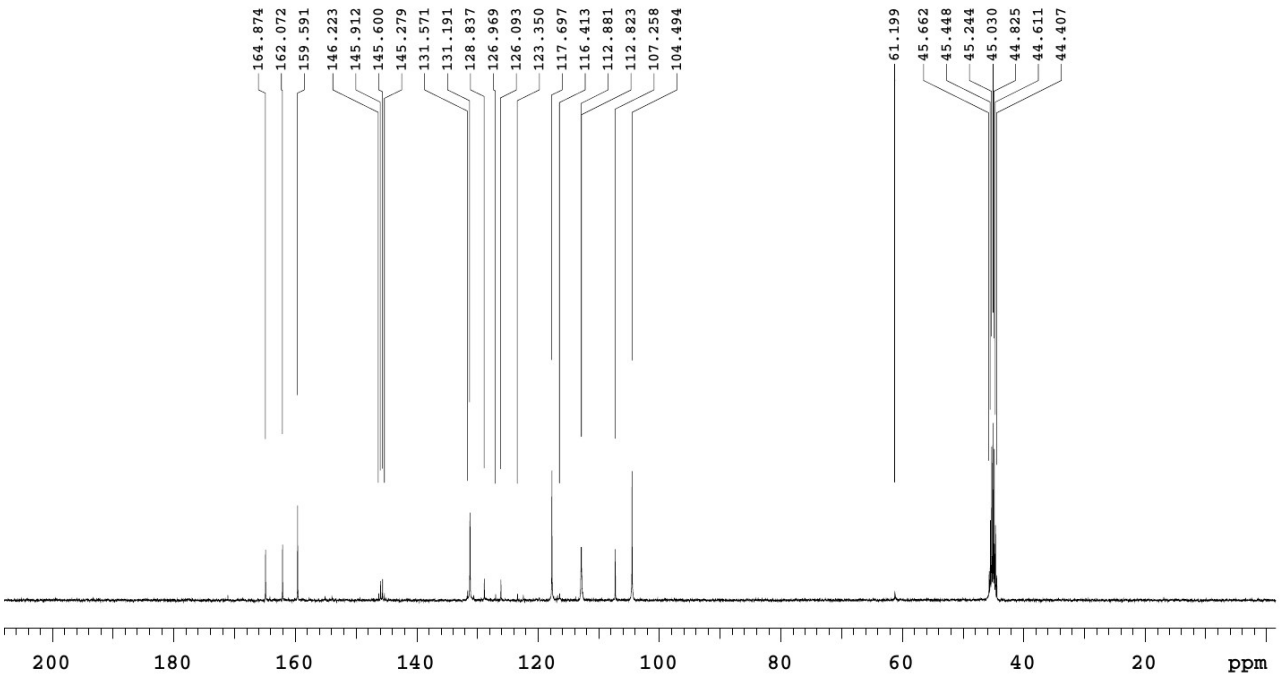

Figure S21 ^{13}H NMR of the compound **G**.

7-((3,4-dimethoxybenzoyl)amino)-2-oxo-4-(triflurомethyl)chromen-1-ide: (G)

LC-MS (m/z): 394.1106 ([M+H]$^+$, cal. 393.31). ^{1}H NMR (DMSO-d$_6$, δ ppm): 10.654 (s, NH), 7.340-7.335 (d, 2.5 Hz, Ar-H), 7.318-7.313 (d, 2.5 Hz, Ar-H), 6.633-6.628 (d, 2.5 Hz, Ar-H), 6.611-6.605 (d, 3 Hz, Ar-H), 6.500 (s, Ar-H), 6.475-6.470 (d, 2.5 Hz, Ar-H), 6.408 (s, Ar-H). ^{13}C NMR (DMSO-d$_6$, δ ppm): 164.87, 159.59, 146.22, 145.91, 145.60, 145.27, 131.57, 131.19, 128.83, 126.96, 126.09, 123.35, 117.69, 116.41, 112.88, 112.82, 107.25, 104.49, 61.19.

Table S1 Selected bond lengths, bond angles and torsion angles.

Atoms	Bond lengths (Å)		Atoms	Bond angles (°)		Atoms	Torsional angles (°)	
	XRD	DFT		XRD	DFT		XRD	DFT
A								
C10-O11	1.208(2)	1.2015	C2-C1-C15	120.8(2)	120.85	C15-C1-C2-C3	0.1(3)	0
O12-C13	1.382(2)	1.3650	C15-N16-C17	128.1(1)	128.82	C14-C15-N16-C17	-4.8(3)	-3.84
N16-C17	1.366(2)	1.3859	N16-C17-O18	122.1(2)	123.03	C2-C3-C13-O12	179.3(1)	179.97
C15-N16	1.403(2)	1.3993	O18-C17-C19	121.9(2)	122.07	C17-C19-C20-C21	-178.3(2)	179.14
C23-O25	1.363(2)	1.3593	C17-C19-C20	124.3(1)	123.59	C1-C2-C3-C4	179.2(2)	179.97
Correlation coefficient = 0.9858			Correlation coefficient = 0.9782			Correlation coefficient = 0.9999		
RMSD = 0.01228			RMSD = 0.6194			RMSD = 0.7391		
B								
C10-O12	1.363(2)	1.388	C2-C1-C15	120.9(2)	120.9	C2-C1-C15-N16	-179(2)	-179.42
C15-N16	1.394(2)	1.398	C4-C5-F8	113.0(2)	112.62	C2-C3-C13-O12	180(2)	179.98
N16-C17	1.375(2)	1.389	C1-C15-N16	116.6(2)	117.03	C4-C3-C13-C14	180.0(2)	179.96
C17-O18	1.220(2)	1.218	N16-C17-O18	121.8(2)	122.71	C13-C14-C15-N16	179.0(2)	179.32
C22-O25	1.358(2)	1.356	N16-C17-C19	116.1(2)	115.12	C15-N16-C17-O18	4.2(3)	3.48
Correlation coefficient = 0.9900			Correlation coefficient = 0.9904			Correlation coefficient = 0.9999		
RMSD = 0.01345			RMSD = 0.65081			RMSD = 0.3998		
C								
C1-C15	1.408(3)	1.411	C4-C5-F8	112.6(2)	112.6	C15-C1-C2-C3	0.3(4)	0.02
O12-C13	1.39(3)	1.364	C9-C10-C11	124.9(3)	125.68	C3-C4-C5-F7	-59.1(3)	-59.6
C15-N16	1.404(3)	1.4011	C1-C15-N16	117.3(2)	116.98	C15-N16-C17-O18	2.9(5)	2.69
N16-C17	1.362(3)	1.3855	C15-N16-C17	128.0(2)	128.73	C15-N16-C17-C19	-177.7(3)	-178.09
C17-O18	1.217(3)	1.2175	N16-C17-O18	122.3(3)	123.23	C22-C23-C24-C19	0.2(4)	0.2
Correlation coefficient = 0.9759			Correlation coefficient = 0.99862			Correlation coefficient = 0.9999		
RMSD = 0.01565			RMSD = 0.6494			RMSD = 0.32391		
D								
C1-C19	1.402(3)	1.412	C4-C5-F6	111.3(2)	111.37	C9-C4-C5-F6	120.5(2)	120.41
C7-F8	1.335(3)	1.353	C9-C10-O11	124.9(2)	125.66	C9-C4-C5-F7	-120.3(2)	-120.31
C17-C19	1.384(3)	1.395	C1-C15-N16	116.9(2)	117.02	C13-C14-C15-N16	179.8(2)	179.39
N20-C22	1.369(3)	1.388	C20-C19-C24	118.6(2)	118.63	C17-C19-C20-C21	-179.5(2)	-179.47
C22-O23	1.213(2)	1.218	C13-C14-C15	118.3(2)	118.81	C22-C23-C24-C19	0.1(4)	0.28
Correlation coefficient = 0.9978			Correlation coefficient = 0.9991			Correlation coefficient = 0.9999		
RMSD = 0.01392			RMSD = 0.41422			RMSD = 0.20414		
E								
C1-C15	1.398(5)	1.4116	C3-C4-C9	120.7(3)	120.87	C2-C3-C4-C9	-179.7(4)	-179.98
C3-C4	1.44(4)	1.4463	C4-C5-F8	112.8(3)	112.6	C13-C3-C4-C9	-0.2(5)	0
N16-C17	1.354(5)	1.3854	C4-C9-C10	121.4(4)	121.73	O11-C10-O12-C13	179.9(4)	179.97
C17-O18	1.217(4)	1.2175	N16-C17-O18	122.3(4)	123.26	C17-C19-C24-C23	-177.9(4)	-178.81
C20-C21	1.383(5)	1.3896	C15-N16-C17	128.1(3)	128.74	Br25-C22-C23-C24	179.5(3)	179.64
Correlation coefficient = 0.9914			Correlation coefficient = 0.9987			Correlation coefficient = 0.9999		
RMSD = 0.01584			RMSD = 0.54936			RMSD = 0.43594		
F								
C2-C3	1.401(4)	1.409	C1-C2-C3	121.1(3)	120.9	C1-C2-C3-C4	-179.6(3)	-179.9
C5-F6	1.327(7)	1.353	C4-C5-F8	112.4(3)	112.6	C2-C3-C13-O12	179.8(3)	179.99
C10-O11	1.201(4)	1.2008	N16-C17-O18	124.0(3)	124.33	C3-C4-C5-F6	-60.1(5)	-59.66
N16-C17	1.354(5)	1.3837	C19-C20-C21	120.9(3)	121.17	C10-O12-C13-C3	0.6(5)	0.02
C17-O18	1.221(5)	1.2125	C21-C22-Cl26	119.0(3)	119.05	C13-C14-C15-N16	-179.3(3)	-179.63
Correlation coefficient = 0.9923			Correlation coefficient = 0.9988			Correlation coefficient = 0.9999		

RMSD = 0.01861			RMSD = 0.22991			RMSD =0.39115		
G								
C1-C15	1.402(2)	1.412	C2-C1-C15	121.3(2)	120.91	C1-C2-C3-C4	179.5(2)	179.97
C4-C9	1.337(2)	1.3514	C3-C4-C9	120.8(2)	120.91	C2-C3-C13-O12	179.6(1)	180
C17-C19	1.492(2)	1.495	C4-C5-F7	111.9(2)	111.4	C9-C4-C5-F7	-120.0(2)	-120.43
C15-N16	1.397(2)	1.3976	C3-C13-O12	121.1(1)	121.5	C13-C14-C15-N16	-179.0(2)	-179.39
N16-C17	1.368(2)	1.3891	C14-C15-N16	123.8(1)	123.56	C1-C15-N16-C17	176.1(2)	176.6
Correlation coefficient = 0.9926			Correlation coefficient = 0.9975			Correlation coefficient = 0.9999		
RMSD =0.01248			RMSD = 0.35547			RMSD = 0.4399		

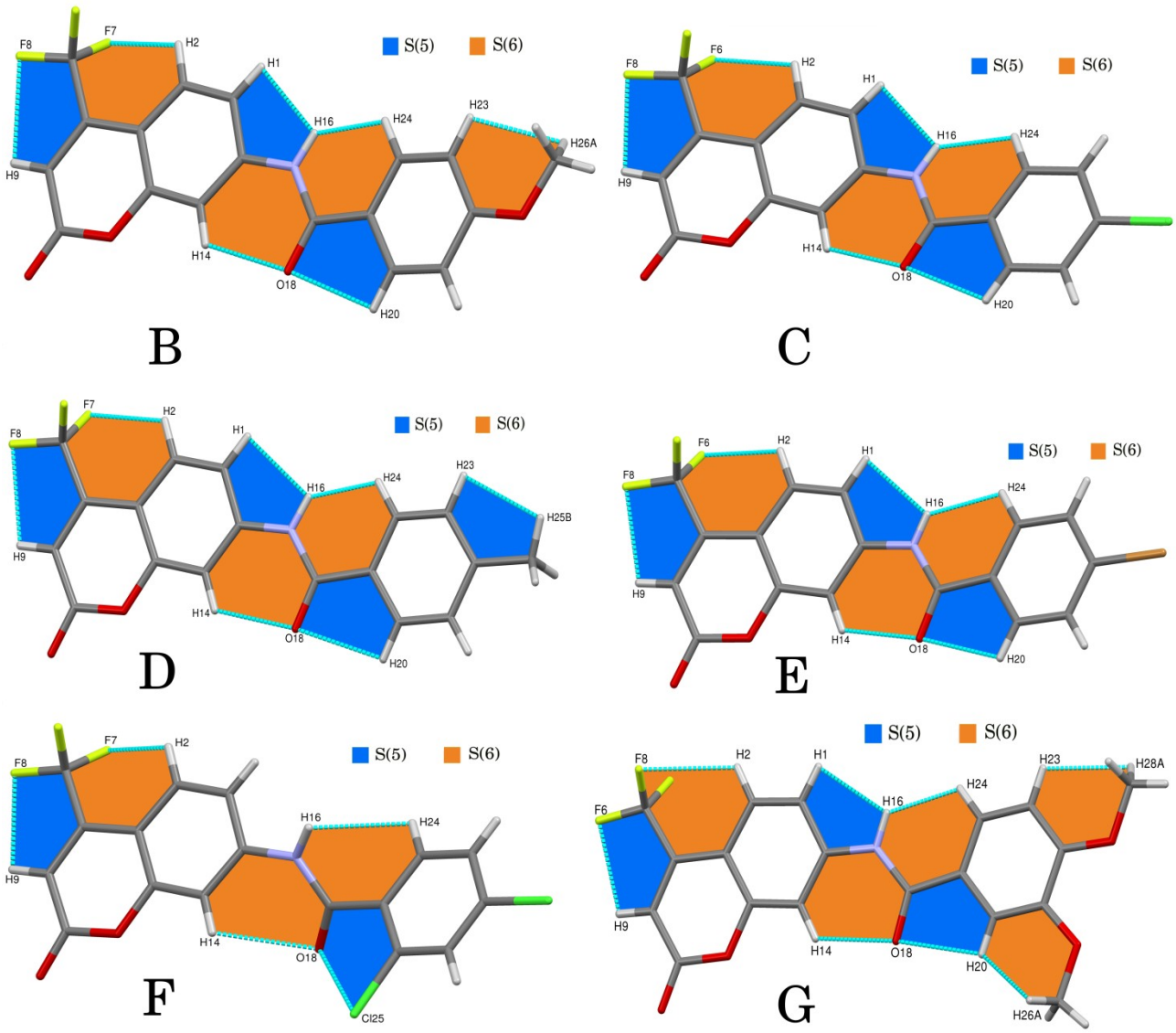

Figure S22 Various intramolecular interactions leading to the formation of five membered S(5) and six membered S(6) ring motifs (**B-G**).

Table S2 Interaction energies (kJ/mol) from the energy framework calculation of the **A** molecule, using the energy B3LYP/6-31G(d,p) electron densities [Where, N refers to the number of molecules with an R molecular centroid to centroid distance (Å)].

	N	Symop	R	E_ele	E_pol	E_dis	E_rep	E_tot
	1	-x, -y, -z	7.02	-2.6	-2.2	-34	16.5	-23.8
	1	-x, -y, -z	4.01	-18	-3.2	-92.3	45	-73.9
	2	x, y, z	9.33	-37.9	-9.4	-17.9	35	-41.1
	1	-x, -y, -z	16.40	-0.4	-0.5	-13.2	5.8	-8.7
	2	x, y, z	15.48	-4.4	-0.5	-11.6	5.1	-12
	1	-x, -y, -z	4.35	-21.2	-3.9	-86.7	43.4	-74
	1	-x, -y, -z	13.68	-0.5	-0.2	-11.6	1.4	-9.9
	1	-x, -y, -z	13.54	-0.4	-0.1	-10.8	2.1	-8.6
	2	x, y, z	12.25	2.3	-0.9	-10.1	4.5	-4.3
	1	-x, -y, -z	8.76	-0.3	-3.3	-10.7	1.9	-10.9
	1	-x, -y, -z	12.37	-7.6	-3	-14.4	7.6	-18
	2	x, y, z	14.74	0.5	0	-2.5	0	-1.6

Table S3 Interaction energies (kJ/mol) from the energy framework calculation of the **B** molecule, using the energy B3LYP/6-31G(d,p) electron densities.

	N	Symop	R	E_ele	E_pol	E_dis	E_rep	E_tot
	2	x, y, z	9.3	-49.9	-12.4	-24.9	53.2	-50.8
	1	-x, -y, -z	5.62	-16	-5.9	-43.4	18.4	-47.8
	2	x, y, z	15.36	0	-0.2	-7.3	2.1	-5.2
	1	-x, -y, -z	6.53	-9.4	-3.9	-70	31.2	-54.5
	2	x, y, z	14.37	0.6	-0.1	-7.4	3.8	-3.6
	1	-x, -y, -z	14.64	-2.2	-0.4	-7.5	3.2	-7.2
	1	-x, -y, -z	3.69	-23.1	-3.8	-87.7	37.8	-80.3
	1	-x, -y, -z	19.80	-5.3	-0.8	-6.7	3.9	-9.6
	1	-x, -y, -z	10.92	-2.8	-0.4	-11.9	2.5	-12.1
	1	-x, -y, -z	9.13	0	-3	-21.8	9.3	-15.4

Table S4 Interaction energies (kJ/mol) from the energy framework calculation of the **C** molecule, using the energy B3LYP/6-31G(d,p) electron densities.

	N	Symop	R	E_ele	E_pol	E_dis	E_rep	E_tot
	2	x, -y+1/2, z+1/2	7.51	-2.4	-1.7	-41.8	19.9	-27.9
	2	-x, y+1/2, -z+1/2	14.19	-0.8	-0.1	-4.7	3.3	-3
	2	x, y, z	9.3	-40	-10.2	-19.6	39.2	-42.7
	1	-x, -y, -z	10.54	-3	-0.6	-9	1.7	-10.4
	1	-x, -y, -z	12.97	-1.3	0	-5.5	0.1	-6.1
	2	x, -y+1/2, z+1/2	4.87	-3.8	-3.7	-56.3	25	-40.3
	2	-x, y+1/2, -z+1/2	12.86	-1.4	-0.3	-6.8	2.3	-6.1
	1	-x, -y, -z	17.31	-3.4	-0.2	-7.4	6.8	-6
	1	-x, -y, -z	13.94	-1.9	-0.1	-11.8	2.9	-10.6
	1	x, -y+1/2, z+1/2	12.8	-7.6	-1.4	-10	7.2	-13.3

Table S5 Interaction energies (kJ/mol) from the energy framework calculation of the **D** molecule, using the energy B3LYP/6-31G(d,p) electron densities.

	N	Symop	R	E_ele	E_pol	E_dis	E_rep	E_tot
	1	-x, -y, -z	8.69	-6.4	-2.8	-43	14.4	-37.4
	2	-x, y+1/2, -z+1/2	12.83	-2.1	-0.3	-7.1	2	-7.4
	1	x, -y+1/2, z+1/2	14.28	0.7	-0.5	-7.9	4.5	-3.7
	1	-x, -y, -z	4.82	-13.5	-5.2	-61.9	30.8	-53
	0	-x, -y, -z	8.12	0.3	-1.9	-24.4	6	-18.6
	0	-x, y+1/2, -z+1/2	12.48	-2.5	-0.2	-9	3.4	-8.6
	1	x, y, z	9.24	-47.3	-11.4	-21	51.5	-44.9
	0	-x, -y, -z	3.84	-22.5	-4.8	-86.8	41.4	-77.3
	1	x, -y+1/2, z+1/2	11.12	-0.8	-0.3	-9.5	3	-7.5
	0	-x, -y, -z	11.59	6.5	-1.3	-2.2	0.1	4

Table S6 Interaction energies (kJ/mol) from the energy framework calculation of the **E** molecule, using the energy B3LYP/6-31G(d,p) electron densities.

	N	Symop	R	E_ele	E_pol	E_dis	E_rep	E_tot
	2	x, y, z	9.27	-46.6	-14.3	-20.9	30.3	-51.1
	1	-x, -y, -z	15.64	-3.1	-0.2	-12.2	1.4	-13.1
	2	x, -y+1/2, z+1/2	7.19	-4.4	-2.1	-44.7	17.9	-31.6
	2	x, -y+1/2, z+1/2	4.59	-1.5	-4.4	-56.7	20.8	-38.5
	1	-x, -y, -z	14.61	-1.5	-0.1	-5.8	0	-6.8
	2	-x, y+1/2, -z+1/2	13.23	-1.8	-0.4	-7.1	1.5	-7.4
	2	x, -y+1/2, z+1/2	12.74	-7.1	-1.5	-11.5	6.2	-13.5
	1	-x, -y, -z	11.88	-4.3	-0.7	-6.3	0.2	-10.4
	2	-x, y+1/2, -z+1/2	13.72	-1.7	-0.3	-6.4	3.3	-5
	1	-x, -y, -z	15.72	-2.2	-0.4	-9.9	5.7	-6.8

Table S7 Interaction energies (kJ/mol) from the energy framework calculation of the **F** molecule, using the energy B3LYP/6-31G(d,p) electron densities.

	N	Symop	R	E_ele	E_pol	E_dis	E_rep	E_tot
	2	x, y, z	9.16	-14.6	-5.8	-20.2	18.8	-25.8
	1	-x, -y, -z	15.32	-2.8	-0.2	-10	5.9	-8.2
	2	x, -y+1/2, z+1/2	7.2	4.2	-2.6	-48.1	24.3	-24.4
	2	-x, y+1/2, -z+1/2	13.66	-0.7	-0.1	-4.5	0.9	-4.2
	1	-x, -y, -z	16.31	-3.6	-0.2	-7.4	5.1	-7.4
	2	x, -y+1/2, z+1/2	4.68	-34.1	-10.1	-61	48.3	-66.8
	2	x, -y+1/2, z+1/2	12.64	-10.9	-2.2	-11.7	12.2	-15.7
	2	-x, y+1/2, -z+1/2	13.57	-0.7	-0.1	-3.8	1	-3.5
	1	-x, -y, -z	11.66	-3.3	-0.7	-17.2	7.4	-14.4
	2	-x, y+1/2, -z+1/2	14.13	-0.8	-0.1	-3.4	1.5	-2.9

Table S8 Interaction energies (kJ/mol) from the energy framework calculation of the **G** molecule, using the energy B3LYP/6-31G(d,p) electron densities.

	N	Symop	R	E_ele	E_pol	E_dis	E_rep	E_tot
	1	-x, -y, -z	6.16	-7.6	-3.5	-64.5	29.8	-48.4
	2	x, y, z	9.29	-47	-12.3	-25.8	50.2	-50.3
	1	-x, -y, -z	11.31	2.7	-2.8	-19	6.3	-11.8
	1	-x, -y, -z	4.68	-31.4	-5.5	-107.4	54.8	-96.9
	1	-x, -y, -z	16.87	-15.1	-3.5	-15	15.7	-21.9
	2	x, y, z	14.33	1.5	-0.1	-8	0.8	-5
	1	-x, -y, -z	5.40	-16.9	-6.4	-61.3	29.6	-57.7
	1	-x, -y, -z	11.61	-5.6	-0.7	-17.4	9.8	-15.5
	2	x, y, z	14.9	0	-0.1	-3.9	0.9	-3

Table S9 Experimental, calculated vibrational wave numbers and the PED assignments.

Experimental (cm^{-1})	Theoretical (cm^{-1}) (scaled values)	Vibrational assignment with PED (%)	Intensity
A			
3386.85	3502.6191	$\nu_{s\,(NH)}$ (100)	33.52
--	3144.5486	$\nu_{(CH)}$ (99)	18.19
--	3128.1096	$\nu_{(CH)}$ (100)	9.92
--	3114.8230	$\nu_{(CH)}$ (99)	5.66
--	3111.0711	$\nu_{(CH)}$ (97)	0.79
--	3092.4660	$\nu_{(CH)}$ (19), $\nu_{(CH)}$ (75)	5.17
--	3077.7676	$\nu_{(CH)}$ (77), $\nu_{as\,(CH)}$ (22)	9.7
--	3063.2433	$\nu_{as\,(CH)}$ (89)	4.94
--	3062.9048	$\nu_{(CH)}$ (92)	12.52
--	3037.2213	$\nu_{(CH)}$ (91)	22.09
--	2974.3760	$\nu_{(CH)}$ (100)	29.58
--	2913.7837	$\nu_{(CH)}$ (91)	39.42
--	1747.0209	$\nu_{as(OH)}$ (84)	726.79
1709.787	1682.2319	$\nu_{s(OC)}$ (80), $\rho_{(NH)}$	153.64
--	1612.2984	$\nu_{as(CC)}$ (58)	25.28
--	1599.3213	$\nu_{(CC)}$ (56)	260.56
--	1581.5575	$\nu_{as(CC)}$ (55)	100.23
1614.253	1570.4273	$\nu_{(CC)}$ (49) , $\delta_{(HCC)}$ (12)	12.32
1582.408	1542.8582	$\nu_{(CC)}$ (40), $\gamma_{(HNC)}$(16)	602.73
--	1492.2067	$\nu_{(CC)}$ (19) , $\nu_{(NC)}$ (11) $\delta_{(HCC)}$ (11)	225.79
1526.067	1480.3900	$\delta_{(HNC)}$ (26), $\delta_{(HCC)}$ (14)	233.16
--	1469.7530	$\delta_{(HCC)}$ (43), $\delta_{(HCH)}$ (10)	125.89
--	1453.7878	$\omega_{(CH2)}$(40), $\gamma_{(CH2)}$(17), $\tau_{(HCOC)}$(20)	78.34
--	1445.4813	$\chi_{(CH2)}$(37)	10.64
1487.853	1434.6219	$\delta_{(CH2)}$ (26),	2.41
1462.377	1407.8843	$\nu_{(CC)}$ (18)	58.35
--	1395.8258	$\nu_{(CC)}$ (37)	101.02
1411.425	1373.5171	$\nu_{as(CC)}$ (15), $\nu_{(CC)}$ (10), $\delta_{(CCC)}$ (18)	135.97
--	1331.5880	$\nu_{(CC)}$ (38)	89.23
1354.104	1319.4522	$\delta_{(HCC)}$ (18), $\nu_{(CC)}$ (50)	48.73

--	1272.8911	$\nu_{as(CC)}$ (17), $\delta_{(HCC)}$ (60)	3.03
--	1260.0203	$\delta_{(HCC)}$ (17),	287.86
1296.783	1251.6751	$\nu_{s(OC)}$ (16)	72.93
--	1240.1001	$\rho_{(HCC)}$(29)	9.31
--	1236.7447	$\nu_{s(OC)}$ (12), $\rho_{(HCC)}$(17)	437.98
1233.093	1196.0049	$\rho_{(NC)}$(12), $\nu_{s(CC)}$ (10), $\gamma_{(HNC)}$(13), $\tau_{(HCOC)}$(10)	362.24
--	1177.2355	$\delta_{(HCC)}$ (17), $\tau_{(HCOC)}$(12)	23.66
--	1167.4011	$\gamma_{(HCC)}$(12), $\delta_{(HCC)}$ (20)	39.42
--	1159.3943	$\delta_{(HCC)}$ (12), $\tau_{(HCOC)}$(41)	26.71
1182.142	1150.7397	$\nu_{s(CC)}$ (14), $\gamma_{(HCC)}$(64)	7.03
--	1130.6744	$\gamma_{(HCH)}$(14), $\delta_{(HCH)}$ (14), $\tau_{(HCOC)}$(10)	0.68
--	1128.1215	$\nu_{s(OC)}$ (15), $\gamma_{(HCC)}$(13)	369.07
1150.297	1112.9977	$\nu_{as(OC)}$ (14)	79.85
--	1099.0632	$\gamma_{(HCH)}$(14), $\delta_{(HCH)}$ (14)	154.84
--	1082.3631	$\nu_{s(NC)}$ (36), $\delta_{(HCC)}$ (12)	8.76
--	1078.9883	$\nu_{as(FC)}$ (80)	267.28
--	1069.5987	$\nu_{s(CC)}$ (38)	1.31
1042.024	1022.2834	$\nu_{s(OC)}$ (68)	70.2
--	983.9805	$\delta_{(HCC)}$ (14), $\delta_{(CCC)}$ (30)	29.27
997.441	974.9391	$\nu_{s(CC)}$ (20), $\gamma_{(CCC)}$(16), $\delta_{(CCC)}$ (39)	15.26
--	954.4193	$\tau_{(HCCC)}$(55), $\tau_{(CCCC)}$(13)	0.12
--	928.4554	$\nu_{s(FC)}$ (24)	29.66
959.227	926.6761	$\tau_{(HCCC)}$(80)	0.81
--	914.1148	$\nu_{s(OC)}$ (12)	5.12
--	880.0087	$\tau_{(HCCN)}$(88)	26.41
--	876.5952	$\tau_{(HCCC)}$(72)	1.62
--	871.1606	$\tau_{(HCCO)}$(73), $OUT_{(cccc)}$(13)	46.57
--	866.6931	$\tau_{(HCCC)}$(59), $\tau_{(CCCC)}$(20), $OUT_{(OCCC)}$(-10)	18.43
870.061	855.3695	$\nu_{as(OC)}$ (30), $\delta_{(OCC)}$ (13)	11.32
825.478	806.1009	$\tau_{(HCCC)}$(20), $\tau_{(HCCC)}$(-51)	91.41
--	790.1744	$\tau_{(HCCC)}$(73)	22.07
--	780.2143	$\tau_{(HCCC)}$(45), $out_{(OCNC)}$(13)	10.73
--	769.2002	$\nu_{s(CC)}$ (15), $\tau_{(HCCC)}$(10)	12.28

--	730.2010	$\tau_{(HCCC)}$(25), $out_{(OCNC)}$(-43)	36.95
--	725.9849	$out_{(CCCC)}$(28)	13.03
749.051	724.9502	$out_{(CCCC)}$(14)	15.07
--	696.4044	$\nu_{s(FC)}$ (19)	8.42
--	689.4517	$\tau_{(HCCO)}$(-14), $out_{(OCOC)}$(69)	1.75
--	669.5025	$\tau_{(HCCC)}$(30), $\tau_{(CCCC)}$(22), $out_{(OCCC)}$(-20)	15.32
685.361	659.0492	$\gamma_{(CCC)}$(45)	4.9
--	649.9691	$out_{(CCCC)}$(-49)	3.25
--	636.2086	$\delta_{(CCC)}$ (47), $\delta_{(CCO)}$ (12)	32.53
--	612.6622	$out_{(CCCC)}$(16), $\tau_{(CCCC)}$(39)	8.34
--	595.7397	$\delta_{(CCC)}$ (11), $out_{(FCFC)}$(-11)	0.21
--	568.4896	$\delta_{(CCC)}$ (16)	6.86
--	558.2201	$\tau_{(HNCC)}$(81)	34.25
--	536.3949	$\delta_{(CCC)}$ (14), $out_{(OCCC)}$(-20)	11.36
--	509.0481	$\delta_{(CNC)}$ (16), $out_{(FCFC)}$(16)	0.57
--	500.8770	$\delta_{(CCC)}$ (41)	3.32
--	497.4925	$\gamma_{(FCF)}$(67), $out_{(CCCC)}$(10)	0.45
--	444.8684	$\omega_{(CCCC)}$(60)	3.43
--	441.8416	$\delta_{(OCC)}$ (40)	2.1
--	438.3701	$\delta_{(COC)}$ (13)	2.67
--	413.0444	$\delta_{(CCN)}$ (10), $\tau_{(CCCC)}$(-11)	1.42
--	379.1994	$\delta_{(CCC)}$ (37)	1.89
--	345.8862	$\delta_{(CNC)}$ (38)	6.13
--	327.2715	$\delta_{(FCF)}$ (12), $out_{(OCCC)}$(36)	0.47
--	313.8882	$\gamma_{(CCC)}$(48)	2.07
--	286.3771	$\nu_{as(OC)}$ (22), $\delta_{(CCC)}$ (13), $\gamma_{(CCO)}$ (11)	2.39
--	264.6099	$out_{(CCCC)}$(37)	0.98
--	257.7829	$\tau_{(HCOC)}$(27), $\tau_{(CCCC)}$(27)	1.05
--	246.7107	$\gamma_{(CCC)}$(12)	7.68
--	239.1101	$out_{(CCCC)}$(62)	1.49
--	206.5512	$\tau_{(HCOC)}$(16), $\tau_{(CCCC)}$(27)	0.69
--	183.8170	$\tau_{(CCCC)}$(15)	0.14
--	166.0919	$\delta_{(CCC)}$ (20)	0.95
--	137.8459	$Out_{(CCCC)}$(23)	5.21

--	133.4170	$Out_{(CCCC)}$(18)	3.43
--	113.9223	$\delta_{(CCC)}$ (28)	2.19
--	98.4309	$Out_{(CCCC)}$(40), $\tau_{(CCOC)}$(11)	0.73
--	90.2598	$\tau_{(CCCC)}$(11), $\tau_{(CCOC)}$(53)	3.76
--	86.2757	$\tau_{(CCCC)}$(54), $\tau_{(CCOC)}$(12)	0.96
--	56.0667	$\tau_{(CCCF)}$(29), $out_{(CCCC)}$(24)	4.18
--	47.7601	$\delta_{(CNC)}$ (15), $\tau_{(CCCF)}$(-50)	0.13
--	40.0822	$\gamma_{(CNC)}$(30), $out_{(CCCC)}$(19)	1.13
--	22.0089	$\tau_{(CCCN)}$(76)	0.04
--	14.6017	$\tau_{(CCNC)}$(-78)	0.1
B			
3382.31	3506.7200	$\nu_{s(NH)}$ (100)	28.29
--	3144.2779	$\nu_{s(CH)}$ (100)	18.76
--	3128.3417	$\nu_{s(CH)}$ (100)	9.97
--	3110.9164	$\nu_{s(CH)}$ (97)	0.87
--	3102.8322	$\nu_{s(CH)}$ (95)	7.32
--	3099.0319	$\nu_{s(CH)}$ (94)	2.91
--	3085.0394	$\nu_{as(CH)}$ (95)	1.28
--	3061.5027	$\nu_{s(CH)}$ (98)	9.34
--	3056.9578	$\nu_{s(CH)}$ (97)	15.18
--	3037.7338	$\nu_{s(CH)}$ (91)	20.33
--	2971.4266	$\nu_{s(CH)}$ (100)	32.27
--	2911.3662	$\nu_{s(CH)}$ (91)	55.28
--	1746.2763	$\nu_{s(OC)}$ (84)	732.28
1723.8819	1681.2746	$\nu_{s(OC)}$ (79)	199.3
1677.246	1612.0180	$\nu_{as(CC)}$ (55)	26.42
--	1599.4373	$\nu_{s(CC)}$ (49), $\delta_{(HCC)}$ (10)	166.86
--	1591.6723	$\nu_{s(CC)}$ (49), $\gamma_{(HCC)}$ (10)	320.22
1607.2924	1552.4992	$\nu_{s(CC)}$ (56), $\delta_{(HCC)}$ (11)	76.63
1578.145	1542.3167	$\nu_{s(CC)}$ (31), $\gamma_{(HNC)}$ (15), $\delta_{(CCO)}$ (10)	541.86
--	1493.8313	$\gamma_{(HCC)}$ (30)	44.22
--	1491.4234	$\nu_{as(CC)}$ (21), $\gamma_{(HCC)}$ (22)	164.24
--	1474.0271	$\nu_{s(CC)}$ (14), $\delta_{(HCC)}$ (11), $\delta_{(HNC)}$ (28)	412.02
1506.8460	1453.3913	$\gamma_{(HCH)}$ (60), $\delta_{(HCH)}$ (13), $\tau_{(HCOC)}$(21)	68.9

--	1445.7037	$\gamma_{(HCH)}$ (11), $\delta_{(HCH)}$ (10), $\delta_{(HCH)}$ (52),$\tau_{(HCOC)}$(18)	10.49
--	1427.3210	$\delta_{(HCH)}$ (72)	12.06
1454.3807	1401.2797	$\nu_{as(CC)}$ (35), $\nu_{as(CC)}$ (12), $\delta_{(HCC)}$ (13)	51.47
--	1394.8105	$\nu_{as(CC)}$ (11), $\nu_{as(CC)}$ (31), $\gamma_{(HCC)}$ (12)	85.43
1407.7449	1373.6719	$\nu_{s(CC)}$ (10), $\delta_{(CCC)}$ (18)	150.43
--	1331.7524	$\nu_{s(CC)}$ (45), $\nu_{s(NC)}$ (14)	95.59
--	1305.2759	$\nu_{s(CC)}$ (59)	32.68
--	1289.0303	$\delta_{(HCC)}$ (81)	1.89
1296.984	1258.4731	$\delta_{(HCC)}$ (44)	124.72
--	1245.4477		104.37
--	1242.4790	$\nu_{s(OC)}$ (32), $\gamma_{(HCC)}$ (14)	133.11
--	1238.5239	$\nu_{as(FC)}$ (35), $\nu_{s(CC)}$ (36), $\delta_{(HCC)}$ (46)	150.55
1255.730	1213.1595	$\nu_{as(NC)}$ (12), $\nu_{s(CC)}$ (22), $\gamma_{(HNC)}$ (15)	721.04
--	1180.1268	$\nu_{s(CC)}$ (11), $\delta_{(HCC)}$ (20), $\gamma_{(HCC)}$ (13)	123.94
--	1167.2560	$\gamma_{(HCC)}$ (14), $\delta_{(HCC)}$ (14)	56.61
--	1162.5177	$\gamma_{(HCH)}$ (19), $\tau_{(HCOC)}$(60)	13.15
--	1159.2880	$\delta_{(HCC)}$ (63)	224.91
--	1130.1909	$\delta_{(HCH)}$ (18), $\tau_{(HCOC)}$(37)	0.7
--	1127.9088	$\nu_{as(OC)}$ (11), $\delta_{(HCC)}$ (14), $\delta_{(FCF)}$ (13)	428.08
1155.2836	1113.0363	$\nu_{as(OC)}$ (48)	63.75
--	1101.1229	$\nu_{s(CC)}$ (25), $\delta_{(HCC)}$ (62)	59.26
--	1098.9472	$\nu_{as(CC)}$ (25)	151.32
--	1078.3501	$\nu_{s(FC)}$ (81)	267.67
--	1066.2432	$\nu_{as(NC)}$ (31)	44.68
--	1018.0866	$\nu_{as(CC)}$ (13), $\nu_{s(OC)}$ (70)	88.82
1027.0351	989.2700	$\delta_{(CCC)}$ (75)	4.8
--	982.4430	$\gamma_{(HNC)}$ (18), $\delta_{(CCC)}$ (25)	20.06
--	962.7549	$\tau_{(HCCC)}$(79)	3.64
962.91088	928.2136	$\nu_{s(FC)}$ (19), $\delta_{(CCO)}$ (15)	28.57
--	925.8542	$\tau_{(HCCC)}$(81)	0.7
--	914.0568	$\tau_{(HCCC)}$(70)	0.9

--	880.3761	$\tau_{(HCCN)}$(84)	26.2
--	873.0463	$\delta_{(OCN)}$ (21)	2.41
--	870.1840	$\tau_{(HCCO)}$(72), $out_{(OCOC)}$(12)	46.01
869.639	844.5488	$\nu_{as(OC)}$ (22), $\delta_{(CCC)}$ (18)	64.66
846.3213	834.3566	$\tau_{(HCCC)}$(61)	34.82
828.8328	791.7216	$\tau_{(HCCC)}$(-13), $\tau_{(HCCC)}$(-58)	11.83
--	789.4975	$\tau_{(HCCC)}$(48)	9.09
--	788.1243	$\nu_{s(CC)}$ (13), $\tau_{(HCCC)}$(-21)	7.22
--	772.4106		1.21
764.7086	744.5223	$Out_{(OCNC)}$(-61)	23.93
--	729.3598	$\nu_{s(CC)}$ (34)	7.64
741.3907	725.8786	$Out_{(OCCC)}$(12), $Out_{(FCFC)}$(52)	3.01
729.7317	696.5108	$\nu_{s(FC)}$ (28), $\delta_{(FCF)}$ (23)	10.68
--	689.5290	$\tau_{(HCCO)}$(14), $Out_{(OCNC)}$(70)	1.94
--	679.3949	$\tau_{(CCCC)}$(52)	6.48
--	650.4139	$Out_{(CCCC)}$(30)	4.92
--	636.1796	$\gamma_{(CCC)}$ (67)	40.38
--	629.3429	$\nu_{s(CC)}$ (13), $\delta_{(CCC)}$ (39)	3.38
--	616.1337	$\delta_{(CCC)}$ (30)	26.19
--	610.7959	$Out_{(OCCC)}$(54)	10.52
--	585.1897	$Out_{(FCFC)}$(-10)	15.09
--	544.2179	$\tau_{(HNCC)}$(85)	50.49
--	521.0389	$\gamma_{(CCN)}$ (24)	4.3
--	507.4526	$\delta_{(FCF)}$ (20), $\delta_{(CNC)}$ (12), $Out_{(FCFC)}$(10)	1.47
--	498.0437	$\delta_{(FCF)}$ (40), $Out_{(OCCC)}$(-16)	0.6
--	496.6609	$Out_{(OCCC)}$(-27)	3.09
--	471.4609	$\delta_{(COC)}$ (47)	1.25
--	455.4183	$\nu_{s(OC)}$ (17), $\delta_{(COC)}$ (27)	4.27
--	444.4429	$\tau_{(CCCC)}$(-69)	4.11
--	411.1394	$\gamma_{(CCN)}$ (12), $\gamma_{(CNC)}$ (10), $\tau_{(CCCC)}$(17)	4.95
--	409.6405	$\tau_{(HCCC)}$(12), $\tau_{(CCCC)}$(-58)	0.22
--	377.3331	$\gamma_{(OCN)}$ (17), $\gamma_{(CCO)}$ (10), $\delta_{(CCN)}$ (17)	1.02
--	343.8845	$\delta_{(FCF)}$ (37), $out_{(OCOC)}$(17)	9.68
--	330.0371	$\delta_{(FCF)}$ (11), $out_{(CCCC)}$(-41)	0.17

--	303.7347	$out_{(CCCC)}$(22)	2.25
--	295.7763	$\gamma_{(CNC)}$ (25)	6.91
--	274.5120	$\nu_{s(CC)}$ (17), $\delta_{(FCF)}$ (10)	6.63
--	255.1913	$\tau_{(CCCN)}$(-43)	2.05
--	242.3012	$\gamma_{(COC)}$ (36)	0.03
--	239.1875	$out_{(CCCC)}$(12), $\tau_{(CCCC)}$(45)	1.4
--	222.9032	$\tau_{(HCOC)}$(-20), $\tau_{(HCOC)}$(-12)	1.64
--	209.3652	$\delta_{(COC)}$ (12), $\tau_{(HCOC)}$(-14)	1.89
--	155.4453	$\tau_{(CCCC)}$(-45)	1.05
--	130.3033	$\tau_{(CCOC)}$(-41)	8.52
--	124.3659	$\delta_{(CCC)}$ (34)	0.05
--	119.3762	$\gamma_{(CCN)}$ (12), Out(CCCC)(-10)	4.35
--	98.1892	$\tau_{(CCCC)}$(-14), $\tau_{(CCNC)}$(-37), $\tau_{(CCCC)}$(14)	0.64
--	87.0880	$\tau_{(CCNC)}$(-52)	0.21
--	71.3453	$\tau_{(CCOC)}$(52)	0.45
--	59.0837	$\tau_{(FCCC)}$(19), $\tau_{(CCNC)}$(14), $\tau_{(CCCC)}$(17)	2.44
--	47.6634	$\tau_{(FCCC)}$(67)	0.21
--	37.0845	$\delta_{(CCN)}$ (56)	0.18
--	22.1927	$\tau_{(CCCN)}$(78)	1.1
--	17.5414	$\tau_{(CNCC)}$(-65)	0.17
C			
3380.67	3504.2500	$\nu_{s(NH)}$ (100)	28.35
--	3144.8291	$\nu_{s(CH)}$ (97)	18.17
--	3127.9646	$\nu_{s(CH)}$ (100)	10.24
--	3111.7286	$\nu_{s(CH)}$ (97)	0.7
--	3102.3971	$\nu_{s(CH)}$ (97)	1.87
--	3097.8522	$\nu_{s(CH)}$ (93)	0.91
--	3090.1355	$\nu_{s(CH)}$ (100)	0.11
--	3063.1272	$\nu_{s(CH)}$ (94)	9.06
--	3062.2763	$\nu_{s(CH)}$ (97)	10.12
--	1748.4520	$\nu_{s(OC)}$ (82)	733.93
1725.2703	1685.2876	$\nu_{s(OC)}$ (80)	178.83
1677.1211	1612.9753	$\nu_{s(CC)}$ (57)	20.98
--	1599.8822	$\nu_{s(CC)}$ (58), $\delta_{(HCC)}$ (10)	235.38

--	1576.4421	$\nu_{s(CC)}(55),\delta_{(CCC)}(14)$	116.37
1616.9345	1552.1220	$\nu_{s(CC)}(57)$	57.58
1574.8039	1544.2797	$\nu_{as(CC)}(33)$, $\delta_{(HNC)}(14)$	510.81
--	1491.8199	$\nu_{s(CC)}(14)$, $\nu_{s(NC)}(12)$, $\delta_{(HCC)}(19)$	240.85
--	1482.1983	$\nu_{s(CC)}(11)$, $\delta_{(HCC)}(13)$, $\delta_{(HNC)}(21)$	135.91
1520.6360	1465.4885	$\delta_{(HCC)}(37)$	184.26
1454.4308	1396.6574	$\nu_{as(CC)}(26)$, $\gamma_{(HCC)}(19)$	129.72
--	1378.6132	$\nu_{s(CC)}(36)$, $\delta_{(HCC)}(29)$	2.48
1406.2816	1372.9176	$\nu_{as(CC)}(14)$, $\nu_{s(CC)}(10)$, $\delta_{(CCC)}(17)$	134.24
1358.1323	1331.1722	$\nu_{s(CC)}(53)$	85.33
--	1285.3654	$\nu_{s(CC)}(19)$, $\nu_{s(CC)}(10)$, $\delta_{(HCC)}(32)$	2.24
--	1278.9542	$\nu_{as(CC)}(60)$, $\delta_{(HCC)}(14)$	8.83
1291.9271	1258.5118	$\gamma_{(HCC)}(46)$	103.41
--	1243.3976		21.78
--	1238.5046	$\nu_{s(CC)}(18)$, $\delta_{(HCC)}(46)$	162.04
1249.7965	1213.8268	$\nu_{as(CC)}(38)$,$\gamma_{(HNC)}(16)$	512.34
--	1179.3532	$\delta_{(HCC)}(20)$	68.72
1207.6659	1167.5848	$\delta_{(HCC)}(10)$	35.29
--	1163.8135	$\nu_{as(CC)}(12)$, $\delta_{(HCC)}(50)$	26.12
--	1128.4793	$\nu_{s(FC)}(23)$, $\gamma_{(HCC)}(13)$	368.41
1159.5167	1113.8099	$\nu_{s(OC)}(43)$	67.93
--	1099.3533	$\nu_{s(OC)}(50)$	172.15
1135.4420	1097.7964	$\nu_{as(CC)}(17)$, $\delta_{(HCC)}(42)$	11.43
--	1079.1720	$\nu_{s(FC)}(78)$	267.68
--	1072.6738	$\nu_{s(NC)}(33)$, $\delta_{(HCC)}(13)$	144.62
--	1062.8007	$\nu_{s(CC)}(70)$	19.73
--	995.3234	$\delta_{(CCC)}(77)$	58.73
1015.0689	983.2843	$\delta_{(CCO)}(31)$, $\delta_{(HCC)}(15)$	32.2
--	962.8129	$\tau_{(HCCC)}(-72)$, $\tau_{(CCCC)}(18)$	3.06
--	934.6055	$\tau_{(HCCC)}(68)$, $\tau_{(CCCC)}(12)$	0.52
954.8824	928.3103	$\nu_{as(OC)}(38)$	27.44
--	926.5987	$\tau_{(HCCC)}(63)$, $\tau_{(CCCC)}(-10)$	0.88
--	880.0377	$\tau_{(HCCN)}(-86)$	25.65

--	872.7465	$\gamma_{(NCO)}$ (45)	7.28
--	872.2050	$\tau_{(HCCO)}$(67), $Out_{(ococ)}$(11)	45.83
870.6212	843.2917	$\nu_{as(OC)}$ (21), $\delta_{(CCC)}$ (18)	76.32
--	832.0455	$\tau_{(HCCC)}$(62)	26.36
--	808.5764	$\tau_{(HCCC)}$(-75)	6.61
816.4533	789.7876	$\tau_{(HCCC)}$(-79)	19.27
--	780.4077	$\nu_{as(OC)}$ (17), $\nu_{as(OC)}$ (11), $\delta_{(CCO)}$ (14)	1.36
--	740.7510	$Out_{(OCNC)}$(-47)	23.94
--	736.5349	$\nu_{s(CC)}$ (14), $Out_{(OCNC)}$(-12)	12.8
750.2481	726.3427	$Out_{(OCCC)}$(12), $\tau_{(CCCC)}$(-43)	3.54
--	711.0448	$\nu_{s(CC)}$ (25), $\delta_{(CCC)}$ (24)	0.41
--	696.5204	$\nu_{s(FC)}$ (12), $\nu_{s(OC)}$ (14), $\delta_{(FCF)}$ (24)	11.05
--	689.2873	$\tau_{(HCCO)}$(14), $Out_{(OCNC)}$(-69)	1.99
--	677.2481	$\tau_{(CCCC)}$(-55)	6.26
--	649.8240	$Out_{(CCCC)}$(-40),	4.81
653.9496	635.8992	$\gamma_{(OCO)}$ (55)	34.23
--	622.6030	$\nu_{s(CC)}$ (14), $\gamma_{(CCC)}$ (65)	2.65
--	610.2447	$Out_{(OCCC)}$(-50), $\tau_{(CCCC)}$(10)	10.73
--	597.7801	$\gamma_{(CCC)}$ (53), $\delta_{(CCC)}$ (11)	3.05
--	547.9506	$\tau_{(HNCC)}$(84)	47.88
--	530.7766	$\delta_{(CCN)}$ (31)	8.52
--	508.0618	$\delta_{(FCF)}$ (27)	8.1
--	503.2848	$\nu_{s(CC)}$ (12)	12.59
--	497.4828	$\gamma_{(FCF)}$ (65)	0.43
--	471.2191	$\tau_{(CCCC)}$(34)	6.33
--	452.4110	$\nu_{as(OC)}$ (16), $\gamma_{(CCC)}$ (10), $\tau_{(CCCC)}$(10)	8.42
--	444.1431	$\tau_{(CCCC)}$(53)	3.84
--	404.6315	$\tau_{(HCCC)}$(13), $\tau_{(CCCC)}$(-69)	0.55
--	394.3329	$\gamma_{(CCN)}$ (13), $\delta_{(CCN)}$ (27)	3.74
--	372.6818	$\delta_{(CCC)}$ (11), $\delta_{(CNC)}$ (14)	0.55
--	342.5114	$\gamma_{(CCC)}$ (22), $\gamma_{(FCF)}$ (17), $\delta_{(FCF)}$ (12)	11.16
--	329.2442	$\delta_{(FCF)}$ (13), $\tau_{(CCCC)}$(-15),	0.37

		$Out_{(CCCC)}$(27)	
--	313.1436	$\delta_{(CCC)}$ (42)	1.28
--	291.5698	$\nu_{as(CC)}$ (17), $\delta_{(CCC)}$ (12), $\delta_{(FCF)}$ (13), $\delta_{(CNC)}$ (16)	3.04
--	277.6064	$\tau_{(CCCC)}$(-21), $\tau_{(CCOC)}$(-10)	1.7
--	256.9512	$\delta_{(CNC)}$ (21), $Out_{(CCCC)}$(-12)	3.5
--	240.1835	$Out_{(CCCC)}$(31), $Out_{(CCCC)}$(11)	1.17
--	238.5879	$\tau_{(CCOC)}$(41), $\tau_{(CCCC)}$(11)	1.52
--	208.0307	$\gamma_{(CNC)}$ (18)	1.01
--	152.8634	$\tau_{(CCCC)}$(11), $Out_{(CCCC)}$(22), $\tau_{(CCOC)}$(10)	3.72
--	129.0075	$\tau_{(CCCC)}$(11)	4.93
--	122.5382	$\delta_{(CCC)}$ (36)	0.27
--	101.6510	$Out_{(CCCC)}$(10), $\tau_{(CCOC)}$(25)	1
--	87.1654	$\tau_{(CCNC)}$(-69)	1.74
--	83.7712	$\tau_{(CCCC)}$(-11), $Out_{(CCCC)}$(-45)	1.42
--	59.4608	$\tau_{(CCCN)}$(-51), $\tau_{(FCCC)}$ (-11)	2.93
--	47.6924	$\tau_{(FCCC)}$ (64)	0.27
--	36.0111	$\delta_{(CNC)}$ (36), $\tau_{(CCCN)}$(10)	0.23
--	23.3627	$\tau_{(CCNC)}$(69)	0.43
--	18.2860	$\tau_{(CNCC)}$(-73)	0.15
D			
3377.65	3504.1700	$\nu_{s(NH)}$ (100)	28.46
--	3144.6066	$\nu_{s(CH)}$ (100)	18.29
--	3128.0613	$\nu_{s(CH)}$ (100)	10.34
--	3111.9027	$\nu_{s(CH)}$ (97)	0.68
--	3102.4358	$\nu_{s(CH)}$ (96)	1.15
--	3098.4034	$\nu_{s(CH)}$ (93)	0.74
--	3089.9421	$\nu_{s(CH)}$ (99)	0.22
--	3062.5277	$\nu_{s(CH)}$ (95)	4.42
--	3062.3633	$\nu_{s(CH)}$ (96)	15.1
--	1748.5584	$\nu_{s(OC)}$ (84)	736.83
1717.8385	1685.3843	$\nu_{s(OC)}$ (80)	180.45
1680.3813	1612.9947	$\nu_{as(CC)}$ (61)	21.11
--	1599.8822	$\nu_{s(CC)}$ (64)	239.34
1617.952	1571.5974	$\nu_{s(CC)}$ (52), $\delta_{(HCC)}$ (15), $\delta_{(CCC)}$ (16)	120.44

--	1549.2597	$\nu_{as(CC)}$ (62)	117.79
1574.252	1543.9896	$\nu_{s(CC)}$ (36), $\delta_{(CCC)}$ (16)6), $\gamma_{(HNC)}$ (15)	463.31
--	1491.8102	$\nu_{s(CC)}$ (17), $\nu_{s(NC)}$ (12), $\delta_{(HCC)}$ (20)	248.85
--	1481.5407	$\nu_{s(CC)}$ (14), $\delta_{(HCC)}$ (24), $\delta_{(HNC)}$ (24)	177.14
1518.066	1462.2781	$\delta_{(HCC)}$ (25)	142.44
1486.852	1396.6478	$\nu_{as(CC)}$ (30), $\gamma_{(HCC)}$ (18)	130.99
--	1374.3971	$\nu_{s(CC)}$ (36), $\delta_{(HCC)}$ (36), $\gamma_{(HCC)}$ (11)	3.55
1411.9380	1372.9176	$\nu_{as(CC)}$ (14), $\nu_{s(CC)}$ (10), $\delta_{(CCC)}$ (17)	137.5
--	1331.1722	$\nu_{s(CC)}$ (55)	86.63
1355.752	1285.1817	$\nu_{s(CC)}$ (12), $\delta_{(HCC)}$ (63)	0.99
--	1277.3103	$\nu_{as(CC)}$ (77), $\delta_{(HCC)}$ (11)	10.67
--	1258.5795	$\gamma_{(HCC)}$ (46)	102.07
--	1243.3589		20.27
1287.0807	1238.5433	$\nu_{s(CC)}$ (19), $\delta_{(HCC)}$ (45)	164.16
1249.6235	1213.8268	$\nu_{as(NC)}$ (16), $\nu_{s(CC)}$ (21), $\gamma_{(HNC)}$ (17)	513.96
1212.1663	1179.4016	$\delta_{(HCC)}$ (20)	73.94
--	1168.0683	$\delta_{(HCC)}$ (27)	32.07
--	1165.0996	$\nu_{as(NC)}$ (10), $\delta_{(HCC)}$ (44)	34.51
--	1128.5954	$\nu_{s(FC)}$ (25), $\gamma_{(HCC)}$ (14)	375.78
1143.4948	1113.8099	$\nu_{s(FC)}$ (44)	68.78
--	1099.2856	$\nu_{s(OC)}$ (52)	173.81
--	1098.0769	$\nu_{ss(CC)}$ (15), $\delta_{(HCC)}$ (53)	10.09
--	1079.1817	$\nu_{s(FC)}$ (77)	267.54
--	1070.0339	$\nu_{as(OC)}$ (11), $\nu_{s(NC)}$ (29), $\delta_{(HCC)}$ (11)	77.81
1093.5518	1046.7292	$\nu_{s(CC)}$ (73)	32.92
--	991.2234	$\delta_{(CCC)}$ (88)	79.76
1012.3946	983.2553	$\delta_{(CCC)}$ (34), $\delta_{(HCC)}$ (14)	35.48
--	962.3777	$\tau_{(HCCC)}$(73), $\tau_{(CCCC)}$(-17)	3.13
962.4516	933.7255	$\tau_{(HCCC)}$(66), $\tau_{(CCCC)}$(10)	0.55
--	928.2426	$\nu_{s(FC)}$ (36), $\delta_{(CCN)}$ (10)	27.37
--	926.5601	$\tau_{(HCCC)}$(65)	0.91

--	879.9990	$\tau_{(HCCN)}$(85)	25.57
--	872.3114	$\tau_{(HCCO)}$(42)	27.47
--	872.1470	$\tau_{(HCCO)}$(29)	26.84
868.8086	842.8372	$\nu_{as(OC)}$ (19), $\delta_{(CCC)}$ (16), $\gamma_{(NCC)}$ (13)	82.33
--	830.1888	$\tau_{(HCCC)}$(64)	21.61
--	808.8665	$\tau_{(HCCC)}$(13), $\tau_{(HCCC)}$(77)	7.23
818.8657	789.7586	$\tau_{(HCCC)}$(82)	19.31
--	779.9919	$\nu_{s(FC)}$ (15), $\nu_{s(OC)}$ (10),$\gamma_{(CCC)}$ (10)	1.16
--	735.6066	$\nu_{as(CC)}$ (10), $out_{(OCNC)}$(20)	23.11
--	733.6822	$out_{(OCNC)}$(26)	15.69
743.9513	726.1590	$out_{(CCCC)}$(49)	4.58
718.9798	696.9846	$\nu_{s(CC)}$ (10), $\delta_{(CCC)}$ (28)	0.81
--	696.4721	$\nu_{s(FC)}$ (12), $\nu_{s(FC)}$ (15), $\delta_{(CCC)}$ (25)	10.54
--	689.2486	$\tau_{(HCCO)}$(-16), $out_{(OCOC)}$(71)	1.9
--	670.0827	$\tau_{(HCCC)}$(50)	4.2
--	649.6499	$\tau_{(CCCC)}$(-34), $\tau_{(CCCC)}$(18)	4.76
656.551	635.8412	$\gamma_{(CCC)}$ (15), $\delta_{(FCF)}$ (12), $\delta_{(OCO)}$ (35)	34.75
--	620.7753	$\nu_{s(CC)}$ (10), $\gamma_{(CCC)}$ (75)	2.68
--	610.0320	$out_{(OCCC)}$(-42)	10.28
619.094	595.3819	$\delta_{(CCC)}$ (16)	2.06
--	548.2407	$\tau_{(CCCC)}$(-86)	48.19
--	524.6362	$\delta_{(CCN)}$ (31)	2.12
--	506.8917	$\gamma_{(FCF)}$ (47)	1.87
--	497.4828	$\delta_{(FCF)}$ (63)	0.46
--	482.8908	$\nu_{as(CC)}$ (12), $\tau_{(CCCC)}$(13)	9.84
--	455.1379	$\nu_{s(OC)}$ (15)	0.41
--	448.1562	$\tau_{(CCCC)}$(-38)	13.66
--	442.3638	$\tau_{(CCCC)}$(-56)	5.63
--	401.7015	$\tau_{(HCCC)}$(-14), $\tau_{(CCCC)}$(71)	0.46
--	384.0441	$\gamma_{(CCN)}$ (44)	3.52
--	358.6313	$\delta_{(CCN)}$ (20)	0.09
--	334.5337	$\delta_{(CNC)}$ (20), $out_{(CCCC)}$(13)	11.65
--	325.7533	$out_{(CCCC)}$(17)	5.09

--	291.7342	$\nu_{as(CC)}$ (15), $\delta_{(CCC)}$ (12), $\delta_{(FCF)}$ (19)	1.74
--	284.2110	$\delta_{(BrCC)}$ (10), $out_{(CCCC)}$(-21)	1.83
--	263.5559	$\nu_{s(CC)}$ (12)	2.11
--	246.7784	$\delta_{(BrCC)}$ (18)	2.15
--	238.8877	$out_{(CCCC)}$(60)	1.37
--	230.6102	$out_{(CCCC)}$(33)	0.54
--	186.8437	$\gamma_{(CCC)}$ (11), $\delta_{(BrCC)}$ (23)	0.66
--	149.3822	$\tau_{(CCNC)}$(15), $out_{(CCCC)}$(-12), $out_{(CCCC)}$(-23)	4.95
--	123.2055	$\delta_{(CCC)}$ (13), $\tau_{(CCOC)}$(-13)	3.79
--	114.6282	$\delta_{(CCC)}$ (22)	0.18
--	98.5083	$\tau_{(CCOC)}$(-26)	0.66
--	86.6625	$\tau_{(CCOC)}$(70)	0.84
--	77.9692	$\tau_{(CCNC)}$(-51)	2.36
--	58.5712	$\tau_{(CCCN)}$(-66), $\tau_{(FCCC)}$(-14)	2.89
--	47.2960	$\tau_{(FCCC)}$(64)	0.17
--	31.6112	$\delta_{(CNC)}$ (43), $\tau_{(CCOC)}$(11)	0.25
--	22.8405	$out_{(CCCC)}$(76)	0.42
--	16.2263	$out_{(CCCC)}$(77)	0.22
E			
3379.96	3504.7200	$\nu_{s(NH)}$ (100)	30.83
--	3144.6937	$\nu_{s(CH)}$ (99)	18.57
--	3128.3030	$\nu_{s(CH)}$ (100)	9.9
--	3111.2258	$\nu_{s(CH)}$ (97)	0.83
--	3094.1099	$\nu_{s(CH)}$ (95)	2.46
--	3068.8229	$\nu_{s(CH)}$ (95)	11.76
--	3062.2763	$\nu_{s(CH)}$ (97)	8.96
--	3059.5977	$\nu_{s(CH)}$ (94)	13.5
--	3051.1848	$\nu_{as(CH)}$ (96)	16.72
--	3004.2176	$\nu_{s(CH)}$ (96)	13.78
--	2977.2093	$\nu_{s(CH)}$ (95)	15.57
--	2924.7205	$\nu_{s(CH)}$ (98)	24.73
--	1746.7018	$\nu_{s(OC)}$ (84)	734.09
1722.4192	1683.9725	$\nu_{s(OC)}$ (79)	186.25
1679.1605	1612.2211	$\nu_{s(CC)}$ (59)	26.45

--	1599.5824	$\nu_{s(CC)}$ (49)	189.92
--	1594.5733	$\nu_{s(CC)}$ (57)	140.25
1617.3625	1552.5765	$\nu_{s(CC)}$ (59)	42.43
1580.2836	1542.5971	$\nu_{s(CC)}$ (37), $\delta_{(HNC)}$ (16)	545.03
--	1492.7676	$\delta_{(HCC)}$ (33)	104.28
--	1491.7329	$\nu_{as(CC)}$ (11), $\gamma_{(HCC)}$ (22)	134.65
1518.4855	1475.1198	$\nu_{s(CC)}$ (11), $\delta_{(HNC)}$ (25), $\delta_{(HCC)}$ (11)	302.49
--	1443.6730	$\gamma_{(HCH)}$ (64), $\tau_{(HCCC)}$(19)	9.48
1481.4067	1439.0314	$\delta_{(HCH)}$ (68), $\tau_{(HCCC)}$(-20)	7.77
--	1397.0056	$\nu_{s(CC)}$ (25), $\gamma_{(HCC)}$ (17)	116.67
--	1386.2622	$\nu_{as(CC)}$ (21), $\gamma_{(HCC)}$ (27)	6.65
--	1373.4785	$\nu_{as(CC)}$ (14), $\delta_{(CCC)}$ (16)	144.84
1413.4288	1368.6821	$\delta_{(HCH)}$ (88)	0.14
1357.8106	1331.5783	$\nu_{s(CC)}$ (53)	93.74
--	1295.4802	$\delta_{(HCC)}$ (57)	0.8
--	1288.9820	$\nu_{as(CC)}$ (67)	4.77
--	1258.1347	$\delta_{(HCC)}$ (45)	105.15
1289.8327	1244.0745	$\nu_{as(CC)}$ (16)	28.87
--	1238.3499	$\nu_{as(FC)}$ (11), $\nu_{s(CC)}$ (18), $\delta_{(HCC)}$ (46)	154.38
1252.7538	1215.3740	$\nu_{s(CC)}$ (34), $\gamma_{(HNC)}$ (15)	470.72
--	1190.3770	$\nu_{s(CC)}$ (56)	47.31
--	1180.1655	$\delta_{(HCC)}$ (20), $\gamma_{(HCC)}$ (13)	105.46
1203.3154	1169.6155	$\nu_{s(CC)}$ (10), $\delta_{(HCC)}$ (36)	52.55
--	1166.1246	$\nu_{s(NC)}$ (10), $\delta_{(HCC)}$ (10), $\gamma_{(HCC)}$ (12)	46.03
--	1127.9088	$\gamma_{(HCC)}$ (14)	385.3
--	1113.1717	$\nu_{as(OC)}$ (41)	61.93
1141.5173	1106.1030	$\nu_{s(CC)}$ (23), $\gamma_{(HCC)}$ (45)	32.88
--	1099.0535	$\nu_{as(OC)}$ (48)	157.73
--	1078.6885	$\nu_{as(FC)}$ (75), $Out_{(FCFC)}$(-11)	267.75
--	1068.1772	$\nu_{s(NC)}$ (50)	44.19
--	1025.8129	$\gamma_{(HCH)}$ (18), $\tau_{(HCCC)}$(60)	13.24
--	1001.0094	$\delta_{(CCC)}$ (66)	16.02
1011.7413	983.4003	$\delta_{(CCC)}$ (18), $\gamma_{(HCC)}$ (17)	23.01
--	974.5716	$\delta_{(HCC)}$ (17), $\tau_{(HCCC)}$(-51)	2.97

--	965.4238	$\tau_{(HCCC)}$(-71), $\tau_{(CCCC)}$(19)	3.59
--	933.7062	$\tau_{(HCCC)}$(64), $Out_{(OCNC)}$(-10)	1.38
--	928.0396	$\nu_{s(FC)}$ (18)	28.03
956.1231	926.2796	$\tau_{(HCCC)}$(79)	0.96
--	880.1827	$\tau_{(HCCN)}$(-85)	25.57
--	873.8779	$\nu_{s(CC)}$ (25), $\delta_{(CCN)}$ (21)	3.05
--	870.5514	$\tau_{(HCCO)}$(68), $Out_{(OCOC)}$(11)	46.08
869.60581	844.6648	$\nu_{as(OC)}$ (23), $\delta_{(CCC)}$ (18)	55.95
--	832.2679	$\tau_{(HCCC)}$(77)	9.27
--	811.2260	$\tau_{(HCCC)}$(-73)	14.42
820.1673	789.7586	$\tau_{(HCCC)}$(74)	18.38
--	786.9349	$\gamma_{(CCC)}$ (19)	10.78
--	772.2365	$\delta_{(CCC)}$ (18)	2.29
--	732.8410	$\tau_{(HCCC)}$(14), $\tau_{(HCCC)}$(-14), $Out_{(OCNC)}$(47)	26.58
--	729.5338	$\nu_{s(CC)}$ (34)	11.21
746.0096	725.7625	$Out_{(CCCC)}$(-18), $\tau_{(CCCC)}$(45), $\nu_{s(CBr)}$ (37)	4.69
--	696.4237	$\nu_{s(FC)}$ (28), $\delta_{(FCF)}$ (27)	10.49
--	689.4517	$\tau_{(HCCO)}$(15), $Out_{(OCOC)}$(-67)	1.88
--	679.5399	$\tau_{(OCOOC)}$(-71)	4.95
--	649.9691	$\tau_{(CCCC)}$(31), $Out_{(FCFC)}$(-10)	4.82
653.3125	636.0346	$\gamma_{(OCO)}$ (54)	32.47
--	630.9868	$\gamma_{(CCC)}$ (60), $\delta_{(CCC)}$ (14)	4.15
--	615.5342		5.56
--	610.7669	$Out_{(OCCC)}$(45)	10.2
591.5144	578.4207	$\gamma_{(CCN)}$ (15)	5.21
--	549.1980	$\tau_{(HNCC)}$(88)	48.97
--	521.0583	$\delta_{(NCC)}$ (20), $\delta_{(CCO)}$ (12)	1.96
--	506.6790	$\delta_{(FCF)}$ (39), $Out_{(FCFC)}$(-10)	1.49
--	497.4441	$\delta_{(FCF)}$ (60)	0.45
--	473.7333	$Out_{(CCCC)}$(42)	4.54
--	451.9758	$\nu_{s(OC)}$ (14), $\delta_{(COC)}$ (14), $Out_{(CCCC)}$(-16)	8.82
--	444.2011	$\tau_{(CCCC)}$(71)	3.25
--	413.3925	$\delta_{(COC)}$ (10), $\gamma_{(CCC)}$ (10)	0.6
--	401.6821	$\tau_{(HCCC)}$(14), $\tau_{(CCCC)}$(-68)	0.49

--	377.7779	$\delta_{(CCN)}$ (32)	1.51
--	349.1063	$\delta_{(CCC)}$ (45)	10.33
--	341.4477		0.3
--	326.9427	$\gamma_{(FCF)}$ (15), $Out_{(CCCC)}$(21), $Out_{(FCFC)}$(12)	0.41
--	295.1864	$\nu_{as(CC)}$ (15), $\delta_{(CCC)}$ (12)	5.4
--	281.7645	$Out_{(OCCC)}$(18)	2.56
--	265.8283	$\delta_{(CNC)}$ (10), $Out_{(OCCC)}$(16)	3.82
--	243.9548	$Out_{(OCCC)}$(17)	1.16
--	239.0231	$Out_{(CCCC)}$(56)	1.6
--	222.5841	$\delta_{(CCC)}$ (11)	0.82
--	157.7854	$\tau_{(CCNC)}$(33), $Out_{(CCCC)}$(-10)	4.07
--	134.5484	$\delta_{(CCC)}$ (10), $Out_{(CCCC)}$(-11)	3.97
--	125.7100	$\delta_{(CCC)}$ (43)	0.49
--	106.6891	$\tau_{(CCNC)}$(-10), $Out_{(CCCC)}$(-16)	1.21
--	91.2945	$\tau_{(CCNC)}$(-37), $\tau_{(CCNC)}$(12)	0.8
--	86.5949	$\tau_{(CCOC)}$(-61)	0.23
--	60.2344	$\tau_{(CCOC)}$(-13), $\tau_{(FCCC)}$(-15)	3.32
--	48.1953	$\tau_{(FCCC)}$(66)	0.31
--	40.7687	$\gamma_{(NCC)}$ (15), $\delta_{(CNC)}$ (10), $\tau_{(CCNC)}$(-10), $Out_{(CCCC)}$(-12)	0.46
--	29.6772	$\tau_{(HCCC)}$(84)	0.41
--	21.8252	$\tau_{(CCNC)}$(69)	0.34
--	20.1813	$\tau_{(CNCC)}$(-74)	0.03
F			
3379.88	3491.8900	$\nu_{s(NH)}$ (100)	28.49
--	3142.2955	$\nu_{s(CH)}$ (99)	18.45
--	3127.8389	$\nu_{s(CH)}$ (100)	10.08
--	3111.9220	$\nu_{s(CH)}$ (97)	0.66
--	3110.0557	$\nu_{s(CH)}$ (99)	1.2
--	3102.8709	$\nu_{s(CH)}$ (95)	0.14
--	3069.8285	$\nu_{s(CH)}$ (95)	3.26
--	3064.2973	$\nu_{s(CH)}$ (97)	8.06
--	1749.8058	$\nu_{s(OC)}$ (96)	735.92
1723.373	1704.0571	$\nu_{s(OC)}$ (84)	171.58
1681.905	1613.5749	$\nu_{s(CC)}$ (60)	17.77

--	1599.5921	$\nu_{s(CC)}$ (53), $\delta_{(HCC)}$ (12)	263.89
1616.7402	1565.8534	$\nu_{s(CC)}$ (67)	117.78
--	1544.1733	$\nu_{s(CC)}$ (26), $\gamma_{(HNC)}$ (13), $\delta_{(HCC)}$ (15)	495.22
1575.2718	1536.1955	$\nu_{s(CC)}$ (67)	17.2
--	1490.6982	$\nu_{s(CC)}$ (11), $\nu_{s(NC)}$ (10), $\delta_{(HCC)}$ (23)	186.07
1521.955	1476.2706	$\delta_{(HNC)}$ (34), $\delta_{(HCC)}$ (14)	283.51
1486.4107	1446.5933	$\delta_{(HCC)}$ (46), $\delta_{(CCC)}$ (20)	71.52
--	1395.5357	$\nu_{s(CC)}$ (44), $\delta_{(HCC)}$ (15)	131.08
--	1372.3277	$\nu_{as(CC)}$ (15), $\nu_{s(CC)}$ (10), $\delta_{(CCC)}$ (18)	119.6
1409.397	1355.7340	$\nu_{as(CC)}$ (52), $\gamma_{(HCC)}$ (24)	23.31
1356.081	1329.9828	$\nu_{s(CC)}$ (50)	72.77
--	1265.5419	$\nu_{as(CC)}$ (64)	31.25
1290.916	1257.9220	$\gamma_{(HCC)}$ (42)	76.72
--	1243.5523	$\gamma_{(HCC)}$ (28)	17.4
--	1239.6166	$\nu_{s(CC)}$ (11), $\delta_{(HCC)}$ (45)	71.62
--	1236.4352	$\gamma_{(HCC)}$ (31)	133.44
1249.448	1210.3842	$\nu_{s(CC)}$ (42), $\gamma_{(HNC)}$ (17)	370.09
--	1178.1445	$\nu_{as(CC)}$ (10), $\gamma_{(HCC)}$ (20), $\delta_{(HCC)}$ (12)	61.05
1207.979	1166.8015	$\nu_{as(NC)}$ (10), $\gamma_{(HCC)}$ (20)	39.06
--	1128.8371	$\nu_{s(FC)}$ (22), $\gamma_{(HCC)}$ (13)	295.47
--	1126.9902	$\nu_{s(CC)}$ (15), $\nu_{s(CC)}$ (10), $\delta_{(HCC)}$ (49)	86.74
1148.7389	1114.9220	$\nu_{s(FC)}$ (39)	74.1
--	1099.5080	$\nu_{s(OC)}$ (12), $\nu_{as(OC)}$ (21), $\gamma_{(CCC)}$ (15)	172.69
--	1086.8306	$\nu_{as(NC)}$ (45)	14.11
--	1079.5685	$\nu_{as(FC)}$ (79)	264.43
1100.8907	1077.1897	$\nu_{s(CC)}$ (42), $\delta_{(HCC)}$ (20), $\gamma_{(CCC)}$ (12)	127.94
--	1026.8766	$\gamma_{(CCC)}$ (46)	56.22
1017.9538	983.6904	$\delta_{(CCO)}$ (29), $\gamma_{(HCC)}$ (13)	33.22
--	939.8757	$\tau_{(HCCC)}$(-74), $\tau_{(CCCC)}$(-14)	0.48
--	928.5714	$\nu_{as(FC)}$ (13), $\gamma_{(CCC)}$ (11)	26.6
958.7131	927.7978	$\tau_{(HCCC)}$(67)	1.36

--	883.2675	$\tau_{(HCCN)}$(89)	22.94
--	874.7869	$\delta_{(CCO)}$ (44)	23.52
--	873.8296	$\tau_{(HCCO)}$(68), $out_{(OCOC)}$(77)	45.82
--	861.3746	$\tau_{(HCCC)}$(82)	13.75
869.8521	846.2797	$\nu_{as(OC)}$ (23), $\delta_{(CCC)}$ (17)	92.57
--	812.8119	$\tau_{(HCCC)}$(75)	30.38
--	791.2768	$\tau_{(HCCC)}$(-77)	19.94
816.5355	789.1590	$\delta_{(CCC)}$ (17)	20.34
--	767.6723	$\nu_{s(CC)}$ (12), $\delta_{(CCO)}$ (10), $\gamma_{(COC)}$ (10)	19.58
--	745.3539	$out_{(OCNC)}$(-46), $out_{(CCCC)}$(10)	9.99
750.4593	729.2050	$\nu_{as(CC)}$ (13), $\tau_{(CCCC)}$(-12)	2.55
--	727.7739	$\tau_{(CCCC)}$(52)	3.68
720.3833	702.2741	$\nu_{s(FC)}$ (14), $\delta_{(FCF)}$ (10), $\tau_{(CCCC)}$(15), $\nu_{s(CCl)}$ (42)	8.83
--	689.6354	$\tau_{(CCCC)}$(16)	1.95
--	689.3453	$\tau_{(HCCO)}$(-13), $out_{(OCOC)}$(60)	2.45
--	662.2306	$\delta_{(CCC)}$ (56)	4.43
--	651.3422	$\tau_{(CCCF)}$(48)	3.77
655.2186	635.4254	$\gamma_{(OCO)}$ (62)	36.3
--	611.8306	$\tau_{(CCCC)}$(57)	8.96
--	599.9171	$\delta_{(CCC)}$ (17), $out_{(FCFC)}$(-11)	2.97
--	573.2666	$out_{(CCCC)}$(31)	11.59
--	566.8747	$\tau_{(HNCC)}$(87)	33.64
--	515.2660	$\nu_{s(CC)}$ (13)	19.37
--	507.8877	$\delta_{(CCN)}$ (30)	1.37
--	498.4015	$\delta_{(FCF)}$ (22)	5.24
--	497.5795	$\gamma_{(FCF)}$ (51)	1.52
--	460.5821	$\delta_{(COC)}$ (26)	3.09
--	445.4292	$\tau_{(CCCC)}$(55)	3.34
--	428.5164	$\tau_{(CCCC)}$(-52)	6.92
--	409.5438	$\nu_{s(ClC)}$ (17), $\gamma_{(CCCl)}$ (16)	6.98
--	393.7334	$\nu_{s(ClC)}$ (23), $\gamma_{(CCCl)}$ (12)	2.47
--	382.2068	$\nu_{s(ClC)}$ (12), $\gamma_{(CCCl)}$ (42)	2.17
--	361.3679	$\gamma_{(CCCl)}$ (28)	1.98
--	335.8584	$out_{(FCFC)}$(-17)	5.4

--	326.0047	$\delta_{(FCF)}$ (15), $out_{(OCCC)}$(45)	0.47
--	291.6665	$\nu_{as(CC)}$ (21), $\delta_{(FCF)}$ (26)	4.06
--	271.7463	$out_{(FCFC)}$(-10)	1.83
--	261.3124	$\delta_{(COC)}$ (12)	4.43
--	239.6710	$out_{(FCFC)}$(-12)	1.66
--	239.0134	$\tau_{(CCCC)}$(-12), $out_{(CCCC)}$(-34)	1.42
--	200.8652	$\gamma_{(CCCl)}$ (63)	0.5
--	169.9212	$\delta_{(COC)}$ (19), $out_{(ClCCC)}$(11)	0.08
--	163.3166	$out_{(ClCCC)}$(-68)	0.24
--	151.9447	$\tau_{(CCCC)}$(13)	2.62
--	131.5120	$\delta_{(CCC)}$ (20), $\tau_{(CCCC)}$(-21), $\tau_{(CCCC)}$(-13)	6.84
--	113.2164	$\gamma_{(CCC)}$ (32)	0.13
--	98.1892	$\tau_{(CCNC)}$(42)	0.08
--	85.2217	$\delta_{(CCN)}$ (11), $\tau_{(CCCC)}$(16), $out_{(ClCCC)}$(12)	1.22
--	84.4384	$\tau_{(CCOC)}$(-15), $\tau_{(ClCCC)}$(-12)	0.2
--	51.4637	$out_{(ClCCC)}$(86)	2.22
--	36.6977	$\tau_{(CCNC)}$(-63)	1.43
--	31.4855	$\delta_{(CCN)}$ (38), $out_{(CCCC)}$(-30)	0.18
--	17.2610	$\tau_{(CNCC)}$(70)	0.08
--	13.2092	$\tau_{(CCCN)}$(74)	0.05
G			
3381.4274	3506.7400	$\nu_{s(NH)}$ (100)	30.13
--	3145.0805	$\nu_{s(CH)}$ (99)	18.7
--	3128.4481	$\nu_{s(CH)}$ (100)	10.09
--	3115.5676	$\nu_{s(CH)}$ (99)	6.68
--	3110.9937	$\nu_{s(CH)}$ (97)	0.88
--	3103.4801	$\nu_{s(CH)}$ (95)	6.76
--	3064.7808	$\nu_{s(CH)}$ (96)	13.63
--	3062.0829	$\nu_{s(CH)}$ (97)	10.07
--	3036.9602	$\nu_{s(CH)}$ (84)	29.37
--	3036.6991	$\nu_{s(CH)}$ (84)	12.39
--	2971.7844	$\nu_{s(CH)}$ (100)	31.49
--	2968.0421	$\nu_{as(CH)}$ (100)	31.65
--	2911.9948	$\nu_{s(CH)}$ (89)	32.51

--	2908.8037	$\nu_{s(CH)}$ (90)	72.84
--	1745.7058	$\nu_{s(OC)}$ (85)	731.08
1717.6989	1677.0681	$\nu_{s(OC)}$ (78)	182.86
1678.254	1611.7182	$\nu_{as(CC)}$ (65)	32.11
--	1598.9152	$\nu_{as(CC)}$ (57)	257.36
--	1577.7475	$\nu_{s(CC)}$ (51)	159.18
1611.369	1559.8580	$\nu_{as(CC)}$ (54), $\gamma_{(HCC)}$ (10), $\delta_{(CCO)}$ (10)	65.88
1577.9267	1541.8235	$\nu_{s(CC)}$ (26), $\gamma_{(HNC)}$ (16), $\delta_{(CCC)}$ (12)	536.72
--	1499.4592	$\delta_{(HCC)}$ (26)	45.57
--	1491.6749	$\nu_{as(CC)}$ (11), $\delta_{(HCC)}$ (10)	256.98
1522.1893	1475.9998	$\nu_{s(CC)}$ (16), $\delta_{(HNC)}$ (26), $\delta_{(HCC)}$ (11)	523.73
--	1454.0586	$\delta_{(HCH)}$ (73), $\tau_{(HCOC)}$(13)	62.3
--	1452.8305	$\delta_{(HCH)}$ (72), $\tau_{(HCOC)}$(13)	84.88
--	1445.1622	$\delta_{(HCH)}$ (68), $\tau_{(HCOC)}$(17)	14.45
--	1444.8527	$\delta_{(HCH)}$ (70), $\tau_{(HCOC)}$(17)	6.23
1482.3157	1434.9506	$\delta_{(HCH)}$ (70)	1.88
--	1427.0019	$\delta_{(HCH)}$ (81)	26.38
--	1399.2103	$\nu_{as(CC)}$ (12), $\nu_{s(CC)}$ (25)	183.13
--	1391.2616	$\nu_{as(CC)}$ (26), $\nu_{s(CC)}$ (11)	5.49
1409.8571	1373.9523	$\nu_{s(CC)}$ (17), $\gamma_{(CCC)}$ (10), $\gamma_{(HCC)}$ (15)	158.72
--	1332.0425	$\nu_{s(CC)}$ (49)	116.86
1359.693	1330.2729	$\nu_{s(CC)}$ (55)	16.04
--	1270.5316	$\nu_{as(CC)}$ (11), $\nu_{s(OC)}$ (10), $\delta_{(HCC)}$ (59)	80.01
--	1259.1210	$\delta_{(HCC)}$ (12)	366.02
--	1253.7639	$\delta_{(HCC)}$ (14), $\gamma_{(HCC)}$ (10)	141.64
1287.2348	1241.1155	$\nu_{s\,(CC)}$ (22)	57.98
--	1237.7407	$\nu_{as(CC)}$ (18), $\delta_{(HCC)}$ (34)	283.06
--	1229.0377	$\nu_{s(OC)}$ (20), $\nu_{s(OC)}$ (13), $\gamma_{(CCC)}$ (12)	215.07
1248.2187	1191.7598	$\nu_{s(NC)}$ (19), $\delta_{(HNC)}$ (12), $\tau_{(HCOC)}$(14)	602.72
--	1178.5216	$\delta_{(HCC)}$ (19)	35.06
1203.6288	1167.1980	$\delta_{(HCC)}$ (12), $\delta_{(HCC)}$ (21)	54.14

--	1166.0376	$\delta_{(HCH)}$(14), $\tau_{(HCOC)}$(63)	8.46
--	1153.8534	$\nu_{s(NC)}$(12), $\tau_{(HCOC)}$(40)	174.71
--	1136.6021	$\nu_{as(CC)}$(16), $\delta_{(HCC)}$(54)	104.28
--	1130.6454	$\delta_{(HCH)}$(25), $\tau_{(HCOC)}$(36)	0.98
--	1129.7751	$\delta_{(HCH)}$(25), $\tau_{(HCOC)}$(35)	0.58
--	1127.9475	$\nu_{s(FC)}$(21), $\gamma_{(HCC)}$(12)	416.71
--	1112.4368	$\nu_{s(FC)}$(37)	82.8
1136.7439	1098.9085	$\nu_{as(OC)}$(12), $\nu_{s(OC)}$(22)	143.17
--	1078.4758	$\nu_{s(FC)}$(78)	268.19
--	1077.1897	$\nu_{s(CC)}$(42),$\gamma_{(HCC)}$(17)	9.84
--	1023.1634	$\nu_{s(OC)}$(70)	37.33
--	1012.1492	$\nu_{s(OC)}$(54), $\delta_{(HCC)}$(20)	87.24
1014.1217	983.3326	$\delta_{(HCC)}$(15), $\delta_{(CCO)}$(34)	30.2
--	928.5231	$\nu_{s(FC)}$(12), $\delta_{(CCC)}$(12)	32.64
958.384	926.0766	$\tau_{(HCCC)}$(75)	0.93
--	922.8951	$\nu_{s(CC)}$(38)	5.26
--	891.1098	$\tau_{(HCCC)}$(76)	2.6
--	879.5542	$\tau_{(HCCN)}$(82)	26.59
--	870.3097	$\tau_{(HCCC)}$(60)	35.73
--	869.8745	$\tau_{(HCCC)}$(74), $Out_{(OCOC)}$(10)	32.01
874.7782	856.7620	$\nu_{as(OC)}$(26), $\delta_{(CCC)}$(11)	12.88
--	811.5934	$\delta_{(CCN)}$(23)	66.78
824.6146	791.4702	$\tau_{(HCCC)}$(58), $Out_{(OCOC)}$(12)	21.73
--	788.9753	$\tau_{(HCCC)}$(63)	13.74
--	774.1802	$\nu_{s(CC)}$(25)	0.69
--	757.3351	$\nu_{s(OC)}$(11), $\delta_{(CCC)}$(21)	34.12
--	741.2345	$\tau_{(HCCC)}$(-14), $Out_{(ONCC)}$(29), $Out_{(OCCC)}$(-14)	11.69
752.1560	725.1146	$Out_{(OCCC)}$(28)	13.03
--	724.3314	$Out_{(OCCC)}$(-22)	14.31
--	714.3713	$\tau_{(HCCC)}$(-28), $Out_{(OCCC)}$(28), $Out_{(OCCC)}$(21)	21.26
724.287	696.3657	$\nu_{s(FC)}$(20), $\delta_{(OCO)}$(17)	7.99
--	689.5097	$\tau_{(HCCC)}$(-10), $Out_{(OCOC)}$(-69)	1.66
--	650.1625	$\tau_{(HCCC)}$(-10), $Out_{(OCOC)}$(60)	4.4
--	636.8662	$\delta_{(CCO)}$(17), $\delta_{(OCO)}$(53)	44.13

651.8287	630.7258	$\gamma_{(CCC)}$ (16)	9.05
--	612.2754	$Out_{(OCCC)}$(55)	12.09
618.3863	608.3300	$\delta_{(OCC)}$ (10), $\gamma_{(COC)}$ (17), $Out_{(OCCC)}$(11)	0.85
--	577.6761	$\delta_{(OCC)}$ (11)	7.45
--	569.4663	$\tau_{(HNCC)}$(15), $Out_{(CCCC)}$(15), $Out_{(OCCC)}$(-11)	9.75
568.222	540.1952	$\tau_{(HNCC)}$(-74)	36.55
--	517.7705	$\delta_{(CCC)}$ (11)	0.86
--	505.0158	$\gamma_{(COC)}$ (13), $\gamma_{(FCF)}$ (22), $Out_{(FCFC)}$(14)	1.33
--	500.8963	$\gamma_{(CCO)}$ (11)	1.19
--	497.4248	$\delta_{(FCF)}$ (67)	0.43
--	462.1583	$Out_{(OCCC)}$(19), $Out_{(CCCC)}$(19)	1.05
--	454.6641	$\nu_{s(OC)}$ (10), $\delta_{(CCC)}$ (32)	5.49
--	444.2688	$\tau_{(CCCC)}$(-67)	4.14
--	421.6700	$\gamma_{(CCC)}$ (10), $\delta_{(CCC)}$ (13)	5.55
--	380.5532	$\gamma_{(CCN)}$ (53)	0.8
--	369.7421	$\gamma_{(CCO)}$ (12), $\delta_{(COC)}$ (45)	5.89
--	346.4374	$Out_{(OCCC)}$(-11), $\tau_{(CCCC)}$(29)	0.68
--	343.6428	$\gamma_{(COC)}$ (18), $\delta_{(FCF)}$ (10), $\gamma_{(CNC)}$ (11)	6.5
--	322.4365	$\gamma_{(FCF)}$ (12), $Out_{(CCCC)}$(-10), $\tau_{(CCCC)}$(-37)	0.11
--	302.1875	$\delta_{(CNC)}$ (17)	6.24
--	281.7935	$\nu_{as(CC)}$ (20)	2.53
--	264.6679	$\tau_{(CCCC)}$(32)	1.81
--	251.0912	$\tau_{(HCOC)}$(12), $\tau_{(CCCC)}$(14),	0.5
--	239.2455	$\tau_{(CCCC)}$(-14), $Out_{(OCCC)}$(36)	1.45
--	226.4231	$\tau_{(CCCC)}$(33), $\tau_{(HCOC)}$(19)	0.76
--	207.5666	$\gamma_{(CCO)}$ (42)	4.86
--	178.8467	$\gamma_{(CCO)}$ (10), $Out_{(CCCC)}$(16), $\tau_{(CCCC)}$(30)	1.81
--	169.8342	$\gamma_{(CCO)}$ (11), $\delta_{(OCC)}$ (25), $\delta_{(CCC)}$ (11)	1.7
--	153.3179	$Out_{(CCCC)}$(-11), $\tau_{(CCCF)}$(12), $\tau_{(CCOC)}$(10)	2.31
--	129.8778	$\tau_{(CCOC)}$(-22)	6.05

--	122.2191	$\delta_{(CNC)}$ (11), $\tau_{(CCOC)}$(32)	1.45
--	112.9843	$\delta_{(CCC)}$ (28)	1.41
--	98.6727	$\tau_{(COCC)}$(-11), $\tau_{(CCCF)}$(-12), $\tau_{(CCNC)}$(-26)	0.24
--	87.0977	$\tau_{(COCC)}$(52), $\tau_{(CCOC)}$(10)	0.36
--	84.8736	$\tau_{(CCOC)}$(53)	7.26
--	69.2082	$\tau_{(CCOC)}$(-52)	1.23
--	55.5445	$\tau_{(CCCF)}$(-41), $\tau_{(CCCF)}$(14), $\tau_{(CCNC)}$(-12)	4.45
--	46.2903	$\tau_{(CCCF)}$(-60)	0.07
--	34.4445	$\gamma_{(CNC)}$ (49)	0.61
--	17.9379	$\tau_{(CNCC)}$(65)	0.01
--	13.8378	$\tau_{(CCNC)}$(81)	0.02

v: stretching, *δ:* in plane bending, γ: out of plane bending, τ: twisting/torsion, v_s*:* symmetric, v_{as}*:* asymmetric.

Table S10 The major interaction energies calculated using the second-order perturbation theory analysis of the Fock matrix on NBO basis for all the seven novel compounds.

A								
Donor NBO (i)	Occupancy	Type	Acceptor NBO (j)	Occupancy	Type	$E^{(2)}$ kcal/mol	E(j)-E(i) a.u	F(i,j) a.u
C17-O18	0.27676	π*	C19-C20	0.38789	π*	148.18	0.02	0.073
N16	1.66294	LP(1)	C17-O18	0.27676	π*	56.89	0.3	0.117
O12	1.73761	LP(2)	C10-O11	0.26734	π*	39	0.35	0.105
N16	1.66294	LP(1)	C14-C15	0.36734	π*	36.89	0.3	0.095
O11	1.82818	LP(2)	C10-O12	0.12593	σ*	34.12	0.6	0.129
O25	1.83451	LP(2)	C23-C24	0.35926	π*	30.95	0.34	0.097
O12	1.73761	LP(2)	C3-C13	0.44799	π*	27.97	0.35	0.093
C14-C15	1.64783	π	C3-C13	0.44799	π*	26	0.28	0.078
C23-C24	1.64146	π	C19-C20	0.38798	π*	23.15	0.29	0.074
C21-C22	1.69413	π	C23-C24	0.35926	π*	21.45	0.29	0.071
C1-C3	1.73662	π	C14-C15	0.36734	π*	21.13	0.29	0.072
C3-C13	1.59784	π	C1-C5	0.29294	π*	20.86	0.3	0.072
C19-C20	1.68358	π	C21-C22	0.30763	π*	20.49	0.29	0.07
C4-C9	1.82645	π	C10-O11	0.26734	π*	20.28	0.32	0.074
C19-C20	1.68358	π	C17-O18	0.27676	π*	18.67	0.28	0.064

Table S11

B								
Donor NBO (i)	Occupancy	Type	Acceptor NBO (j)	Occupancy	Type	$E^{(2)}$ kcal/mol	E(j)-E(i) a.u	F(i,j) a.u
C3-C13	0.44950	π*	C1-C5	0.29371	π*	273.4	0.01	0.083
C19-C24	0.38593	π*	C20-C21	0.27315	π*	265.79	0.01	0.08
C17-O18	0.28135	π*	C19-C24	0.38593	π*	185.08	0.01	0.081
C22-C23	0.03048	π*	C20-C21	0.27315	π*	149.56	0.02	0.081
N16	1.66819	LP (1)	C17-O18	0.28135	π*	54.88	0.3	0.109
O12	1.73753	LP (2)	C10-O11	0.26793	π*	38.87	0.3	0.096
N16	1.66819	LP (1)	C14-C15	0.36762	π*	38.5	0.57	0.132
O11	1.66819	LP (2)	C10-O12	0.12574	σ*	33.88	0.35	0.099
O25	1.82705	LP (2)	C22-C23	0.38681	π*	32.9	0.34	0.1
O12	88.00000	LP (2)	C3-C13	0.44950	π*	28.04	0.35	0.097
C14-C15	1.64612	π	C3-C13	0.44950	π*	26.72	0.68	0.121
O18	1.86606	LP (2)	N16-C17	0.07908	σ*	25.53	0.28	0.077

Table S12

C								
Donor NBO (i)	Occupancy	Type	Acceptor NBO (j)	Occupancy	Type	$E^{(2)}$ kcal/mol	E(j)-E(i) a.u	F(i,j) a.u
C22-C23	0.38424	π*	C19-C24	0.37873	π*	334.2	0.01	0.085
C3-C13	0.44595	π*	C1-C5	0.29393	π*	261.29	0.01	0.08
C22-C23	0.38424	π*	C20-C21	0.28605	π*	139.27	0.02	0.08
N16	1.66509	LP(1)	C17-O18	0.27721	π*	49.89	0.3	0.11
O11	1.82766	LP(2)	C10-O12	0.12636	σ*	37.99	0.56	0.132
N16	1.66509	LP(1)	C14-C15	0.36664	π*	37.3	0.3	0.095
O12	1.73746	LP(2)	C10-O11	0.26566	π*	34.8	0.35	0.099
O12	1.73746	LP(2)	C3-C13	0.44595	π*	30.96	0.35	0.097
O18	1.86493	LP(2)	N16-C17	0.07789	σ*	26.11	0.69	0.121
C14-C15	1.65042	π	C3-C13	0.44595	π*	25.32	0.28	0.077
C20-C21	1.64703	π	C22-C23	0.38424	π*	22.85	0.27	0.07
C3-C13	1.59763	π	C1-C5	0.29393	π*	21.22	0.29	0.072

Table S13

D								
Donor NBO (i)	Occupancy	Type	Acceptor NBO (j)	Occupancy	Type	$E^{(2)}$ kcal/mol	E(j)-E(i) a.u	F(i,j) a.u
C19-C24	0.38295	π*	C14-C15	0.33259	π*	233.09	0.01	0.08
C17-O18	0.27638	π*	C20-C21	0.38295	π*	151.56	0.01	0.07
N16	1.66560	LP(1)	C1-C5	0.27638	π*	56.08	0.3	0.12
O12	1.73752	LP(2)	C17-O18	0.26744	π*	38.52	0.35	0.1
N16	1.66560	LP(1)	C14-C15	0.36724	π*	37.96	0.3	0.1
O11	1.82826	LP(2)	C10-O12	0.12583	σ*	33.67	0.6	0.13
O12	1.73752	LP(2)	C10-O11	0.44847	π*	27.97	0.35	0.09
C14-C15	1.64719	π	C3-C13	0.44847	π*	26.01	0.28	0.08
O18	1.86591	LP(2)	N16-C17	0.07865	σ*	25.72	0.71	0.12
C20-C21	1.65802	π	C3-C13	0.33259	π*	23.22	0.29	0.07
C22-C23	1.63289	π	C19-C24	0.38295	π*	22.69	0.29	0.07
C3-C13	1.59779	π	C22-C23	0.29345	π*	21	0.3	0.07
C1-C5	1.73740	π	C1-C5	0.36724	π*	20.81	0.3	0.07
C4-C9	1.82657	π	O12-C13	0.26744	π*	20.77	0.32	0.07
C20-C21	1.65802	π	C14-C15	0.38295	π*	20.29	0.28	0.07
C19-C24	1.66488	π	C10-O11	0.28516	π*	19.85	0.3	0.07
C19-C24	1.66488	π	C19-C24	0.27638	π*	19.45	0.28	0.07

Table S14

E								
Donor NBO (i)	Occupancy	Type	Acceptor NBO (j)	Occupancy	Type	$E^{(2)}$ kcal/mol	E(j)-E(i) a.u	F(i,j) a.u
C3-C13	0.44600	π*	C1-C5	0.29	π*	259.68	0.01	0.08
C22-C23	0.37972	π*	C20-C21	0.29	π*	147.88	0.02	0.08
N16	1.66494	LP(1)	C17-O18	0.28	π*	49.9	0.3	0.11
O11	1.82767	LP(2)	C10-O12	0.12	σ*	37.41	0.57	0.13
N16	1.66494	LP(1)	C14-C15	0.37	π*	37.35	0.3	0.1
O12	1.74000	LP(2)	C10-O11	0.27	π*	35.3	0.35	0.1
O12	1.74000	LP(2)	C3-C13	0.45	π*	30.71	0.35	0.1
O18	1.87000	LP(2)	N16-C17	0.08	σ*	26.02	0.68	0.12
C14-C15	1.65000	π	C3-C13	0.45	π*	25.34	0.28	0.08
C20-C21	1.64000	π	C22-C23	0.38	π*	22.66	0.27	0.07
C3-C13	1.60000	π	C1-C5	0.29	π*	21.14	0.29	0.07
C1-C5	1.74000	π	C14-C15	0.37	π*	20.76	0.29	0.07
C19-C24	1.66000	π	C22-C23	0.38	π*	20.51	0.28	0.07
C20-C21	1.64000	π	C19-C24	0.38	π*	20.11	0.28	0.07
C10-O12	0.12000	σ*	O12-C13	0.03	σ*	19.89	0.03	0.08

Table S15

F								
DonorNBO (i)	Occupancy	Type	Acceptor NBO (j)	Occupancy	Type	$E^{(2)}$ kcal/mol	E(j)-E(i) a.u	F(i,j) a.u
C3-C13	0.44366	π*	C1-C5	0.29348	π*	259.26	0.01	0.08
N16	1.66021	LP (1)	C17-O18	0.24954	π*	46.79	0.31	0.11
O11	1.82928	LP (2)	C10-O12	0.12464	σ*	37.5	0.57	0.13
N16	1.66021	LP (1)	C14-C15	0.36534	π*	36.74	0.3	0.09
C19-C23	0.36609	π*	C17-O18	0.24954	π*	36.66	0.02	0.04
O12	1.73709	LP (2)	C10-O11	0.26564	π*	35.23	0.35	0.1
O12	1.73709	LP (2)	C3-C13	0.44366	π*	30.82	0.35	0.1
O18	1.85347	LP (2)	N16-C17	0.08183	σ*	25.96	0.69	0.12
C14-C15	1.65326	π	C3-C13	0.44366	π*	25.05	0.28	0.08
C19-C23	1.66864	π	C20-C21	0.37057	π*	21.35	0.28	0.07
C3-C13	1.59875	π	C1-C5	0.29348	π*	21.11	0.29	0.07
C1-C5	1.73244	π	C14-C15	0.36534	π*	20.91	0.29	0.07
C22-C23	1.66430	π	C20-C21	0.37057	π*	20.84	0.29	0.07
C22-C23	1.66430	π	C19-C24	0.36609	π*	20.29	0.3	0.07
O18	1.85347	LP (2)	C17-C19	0.07173	σ*	20.08	0.65	0.1
C14-C15	1.65326	π	C3-C13	0.44366	π*	25.05	0.28	0.08
C19-C23	1.66864	π	C20-C21	0.37057	π*	21.35	0.28	0.07
C3-C13	1.59875	π	C1-C5	0.29348	π*	21.11	0.29	0.07
C1-C5	1.73244	π	C14-C15	0.36534	π*	20.91	0.29	0.07
C22-C23	1.66430	π	C20-C21	0.37057	π*	20.84	0.29	0.07

Table S16

G								
Donor NBO (i)	Occupancy	Type	Acceptor NBO (j)	Occupancy	Type	$E^{(2)}$ kcal/mol	E(j)-E(i) a.u	F(i,j) a.u
C3-C13	0.44989	π*	C14-C15	0.36806	π*	337.55	0.01	0.08
C3-C13	0.44989	π*	C1-C5	0.29270	π*	249.93	0.01	0.08
N16	1.66615	LP(1)	C17-O18	0.28501	π*	49.97	0.29	0.11
N16	1.66615	LP(1)	C14-C15	0.36806	π*	38.83	0.3	0.1
O11	1.83053	LP(2)	C10-O12	0.12363	σ*	37.21	0.57	0.13
O12	1.73747	LP(2)	C10-O11	0.26967	π*	35.5	0.35	0.1
O27	1.82465	LP(2)	C22-C22	0.37580	π*	32.94	0.34	0.1
O25	1.83338	LP(2)	C20-C21	0.34246	π*	31.61	0.34	0.1
O12	1.73747	LP(2)	C3-C13	0.44989	π*	30.52	0.35	0.1
O18	1.86748	LP(2)	N16-C17	0.07790	σ*	26.1	0.68	0.12
C14-C15	1.64509	π	C3-C13	0.44989	π*	25.93	0.28	0.08
C3-C13	1.59869	π	C1-C5	0.29270	π*	21.13	0.29	0.07
C10-O12	0.12363	σ*	O12-C13	0.03404	σ*	21	0.03	0.08
C1-C5	1.73915	π	C14-C15	0.36806	π*	20.55	0.29	0.07
C22-C22	1.68591	π	C19-C23	0.39078	π*	20.46	0.3	0.07
C4-C9	1.82623	π	C10-O11	0.26979	π*	19.71	0.31	0.07
C20-C21	1.69395	π	C19-C23	0.39078	π*	19	0.29	0.07
C19-C23	1.70402	π	C17-O18	0.28501	π*	18.93	0.28	0.07
C20-C21	1.69351	π	C22-C22	0.37580	π*	18.72	0.29	0.07

$E^{(2)}$: Energy of hyper conjugative interaction (stabilization energy).
E(i)-E(j): Energy difference between donor (i) and acceptor (j) NBO orbitals.
F(i,j) :Fock matrix element between (i) and (j) NBO orbitals.

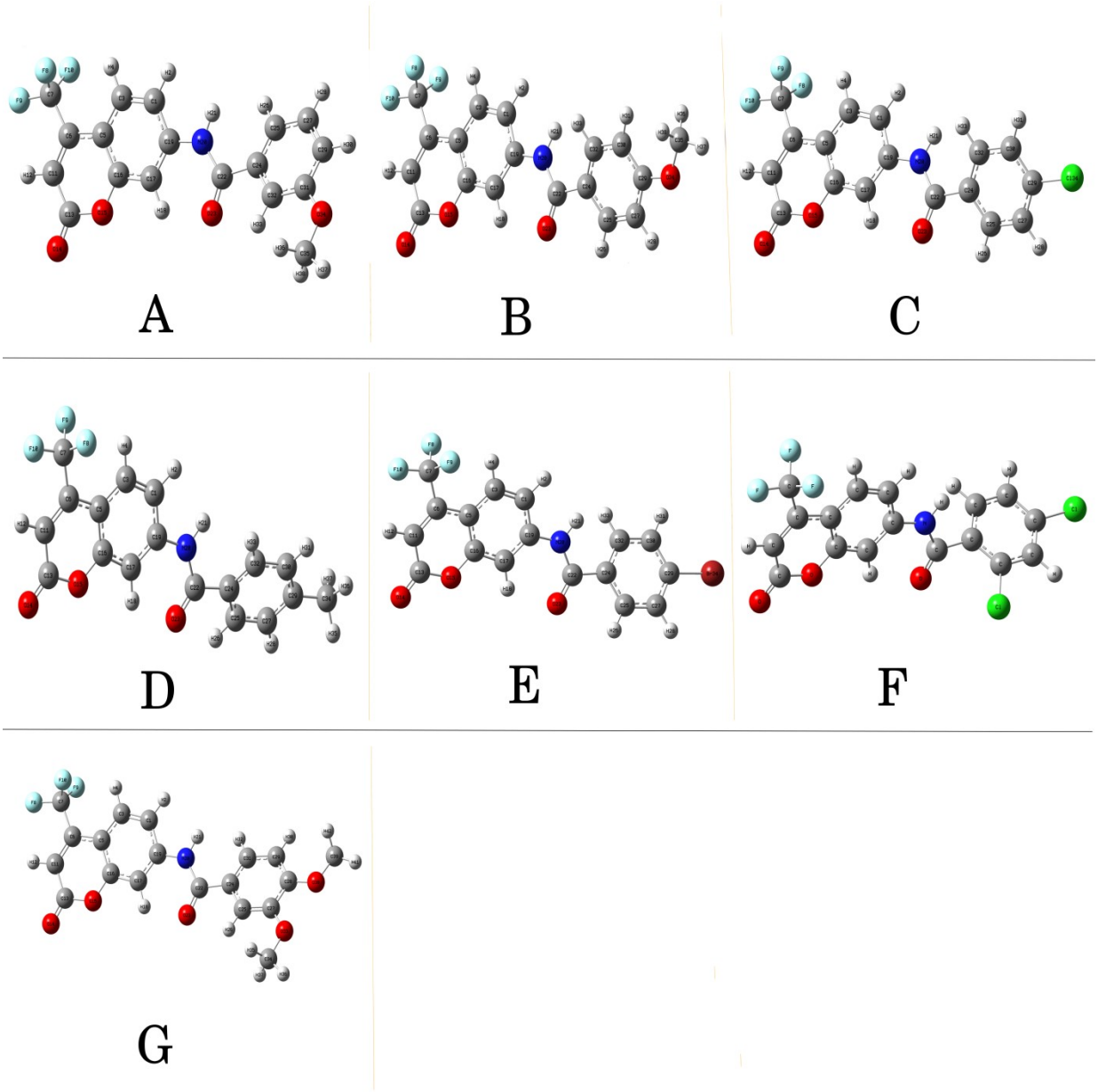

Figure S23 Theoretical optimized structure of the synthesized compound by the DFT/B3LYP method 6-311+G(d,p) basis set.

Fukui function analysis:

Table S17 Fukui function values all the molecules to identify the quantitative reactive atoms in the molecules.

Atom	A					B			
	f-	f+	fo	CDD		f-	f+	fo	CDD
C1	0.0444	0.0261	0.0353	-0.0183		0.0464	0.0269	0.0367	-0.0195
H4	0.0213	0.0206	0.0209	-0.0007		0.0224	0.0213	0.0218	-0.0012
C5	0.0264	0.0388	0.0326	0.0124		0.0278	0.04	0.0339	0.0122
H2	0.0191	0.0207	0.0199	0.0016		0.0199	0.0211	0.0205	0.0012
C3	0.0528	0.0159	0.0343	-0.0369		0.0558	0.0153	0.0355	-0.0405
C4	0.0188	0.0687	0.0438	0.0499		0.019	0.0721	0.0456	0.0531
C5	0.0049	0.0155	0.0102	0.0106		0.005	0.0163	0.0106	0.0113
F6	0.0114	0.0231	0.0172	0.0117		0.0117	0.024	0.0178	0.0124
F7	0.0154	0.0211	0.0182	0.0057		0.0117	0.0241	0.0179	0.0123
F8	0.0114	0.0231	0.0172	0.0117		0.0158	0.0217	0.0187	0.0059
C9	0.0566	0.0806	0.0686	0.024		0.0593	0.0832	0.0712	0.0239
H9	0.0244	0.0349	0.0296	0.0105		0.0253	0.0359	0.0306	0.0106
C10	0.02	0.0417	0.0309	0.0217		0.0205	0.0436	0.032	0.0231
O11	0.0676	0.0747	0.0711	0.0071		0.0687	0.0772	0.0729	0.0084
O12	0.0181	0.0312	0.0247	0.0132		0.0179	0.0326	0.0253	0.0147
C13	0.0237	0.0224	0.0231	-0.0013		0.0234	0.023	0.0232	-0.0005
C14	0.0231	0.0283	0.0257	0.0052		0.0268	0.0289	0.0279	0.0021
H14	0.014	0.0149	0.0145	0.0009		0.0155	0.0156	0.0156	0
C15	0.0311	0.0403	0.0357	0.0092		0.0335	0.0427	0.0381	0.0091
N16	0.0429	0.0122	0.0275	-0.0308		0.0505	0.0119	0.0312	-0.0386
H16	0.0153	0.0125	0.0139	-0.0028		0.0171	0.0126	0.0149	-0.0045
C17	0.0128	0.046	0.0294	0.0332		0.0121	0.044	0.0281	0.0319
O18	0.036	0.0531	0.0446	0.017		0.0328	0.0508	0.0418	0.0181
C19	0.0158	0.0123	0.014	-0.0035		0.0328	0.007	0.0199	-0.0258
C20	0.0469	0.0184	0.0327	-0.0285		0.0211	0.0178	0.0195	-0.0033
H20	0.0173	0.0092	0.0132	-0.0081		0.0155	0.0105	0.013	-0.005
C21	0.0262	0.0228	0.0245	-0.0034		0.0377	0.0206	0.0291	-0.017
H21	0.0208	0.0168	0.0188	-0.0041		0.0218	0.0159	0.0188	-0.006
C22	0.0481	0.0416	0.0448	-0.0066		0.037	0.032	0.0345	-0.0051
H22	0.0244	0.0217	0.0231	-0.0027		0.0317	0.0171	0.0244	-0.0147
C23	0.0347	0.0187	0.0267	-0.016		0.0182	0.0128	0.0155	-0.0054
C24	0.0232	0.021	0.0221	-0.0022		0.0208	0.0201	0.0204	-0.0007
H24	0.0136	0.01	0.0118	-0.0037		0.0119	0.0087	0.0103	-0.0033
O25	0.056	0.0142	0.0351	-0.0417		0.0522	0.0191	0.0356	-0.0332
C26	0.015	0.0065	0.0107	-0.0085		0.0143	0.008	0.0112	-0.0063
H26A	0.0143	0.0042	0.0092	-0.0101		0.0143	0.007	0.0106	-0.0073
H26B	0.0179	0.0121	0.015	-0.0057		0.017	0.0117	0.0143	-0.0053
H26C	0.0144	0.0043	0.0093	-0.0101		0.0145	0.0072	0.0109	-0.0073

Atom	C					Atom	D			
	f-	f+	fo	CDD			f-	f+	fo	CDD
C1	0.0577	0.0243	0.041	-0.0335		C1	0.0569	0.026	0.0415	-0.031
H4	0.0276	0.0191	0.0234	-0.0085		H4	0.0274	0.0205	0.0239	-0.0069
C5	0.0315	0.0366	0.0341	0.005		C5	0.0316	0.0387	0.0352	0.007
H2	0.0226	0.0198	0.0212	-0.0028		H2	0.0226	0.0206	0.0216	-0.002
C3	0.0654	0.0164	0.0409	-0.049		C3	0.0653	0.0156	0.0405	-0.0497
C4	0.0232	0.0629	0.043	0.0397		C4	0.0224	0.0688	0.0456	0.0464
C5	0.0058	0.0142	0.01	0.0083		C5	0.0057	0.0155	0.0106	0.0098
F6	0.0138	0.0214	0.0176	0.0076		F6	0.0136	0.0231	0.0183	0.0095
F7	0.0138	0.0213	0.0176	0.0075		F7	0.0136	0.0231	0.0184	0.0095
F8	0.0179	0.0199	0.0189	0.002		F8	0.0178	0.0211	0.0195	0.0033
C9	0.0686	0.0758	0.0722	0.0072		C9	0.0684	0.0805	0.0744	0.0121
H9	0.0288	0.0329	0.0309	0.0041		H9	0.0287	0.0348	0.0318	0.0061
C10	0.0241	0.0386	0.0313	0.0144		C10	0.0238	0.0418	0.0328	0.018
O11	0.0821	0.0702	0.0762	-0.0119		O11	0.0803	0.0747	0.0775	-0.0056
O12	0.0229	0.0288	0.0258	0.006		O12	0.0217	0.0313	0.0265	0.0095
C13	0.0292	0.0213	0.0253	-0.0079		C13	0.0281	0.0224	0.0252	-0.0057
C14	0.0298	0.0269	0.0283	-0.0029		C14	0.0312	0.0281	0.0296	-0.0031
H14	0.0184	0.0139	0.0162	-0.0044		H14	0.0185	0.0149	0.0167	-0.0036
C15	0.0442	0.0361	0.0401	-0.0081		C15	0.0429	0.0402	0.0415	-0.0028
N16	0.0584	0.0122	0.0353	-0.0462		N16	0.0616	0.012	0.0368	-0.0496
H16	0.0204	0.0123	0.0163	-0.0082		H16	0.0209	0.0125	0.0167	-0.0085
C17	0.0154	0.0469	0.0312	0.0315		C17	0.0148	0.0451	0.03	0.0303
O18	0.0379	0.0557	0.0468	0.0178		O18	0.0377	0.0529	0.0453	0.0152
C19	0.0121	0.0173	0.0147	0.0052		C19	0.0161	0.0115	0.0138	-0.0046
C20	0.017	0.025	0.021	0.0079		C20	0.0185	0.0212	0.0199	0.0027
H20	0.011	0.0134	0.0122	0.0025		H20	0.012	0.0118	0.0119	-0.0002
C21	0.0238	0.0251	0.0245	0.0013		C21	0.0264	0.0221	0.0242	-0.0043
H21	0.0161	0.0179	0.017	0.0018		H21	0.0177	0.0166	0.0172	-0.001
C22	0.0292	0.0386	0.0339	0.0094		C22	0.0381	0.0364	0.0373	-0.0017
C23	0.0211	0.0232	0.0222	0.0021		C23	0.023	0.02	0.0215	-0.0029
H23	0.0148	0.0169	0.0159	0.0022		H23	0.0162	0.0156	0.0159	-0.0006
C24	0.0112	0.0235	0.0174	0.0123		C24	0.0137	0.0206	0.0172	0.0069
H24	0.0059	0.0115	0.0087	0.0056		H24	0.0069	0.0097	0.0083	0.0027
Cl25	0.0784	0.0601	0.0692	-0.0183		C25	0.0123	0.011	0.0116	-0.0013
						H25A	0.0144	0.013	0.0137	-0.0014
						H25B	0.0121	0.0111	0.0116	-0.0009
						H25C	0.0169	0.0152	0.016	-0.0017

Atom	**E**					Atom	**F**			
	f-	f+	fo	CDD			f-	f+	fo	CDD
C1	0.0548	0.024	0.0394	-0.0308		C1	0.0583	0.0259	0.0421	-0.0324
H4	0.0262	0.0189	0.0226	-0.0073		H4	0.0278	0.0204	0.0241	-0.0074
C5	0.0303	0.0362	0.0332	0.0059		C5	0.031	0.0387	0.0349	0.0077
H2	0.0217	0.0196	0.0206	-0.0021		H2	0.0225	0.0205	0.0215	-0.0019
C3	0.0625	0.0163	0.0394	-0.0462		C3	0.0645	0.0158	0.0401	-0.0487
C4	0.0222	0.062	0.0421	0.0399		C4	0.0239	0.0681	0.046	0.0442
C5	0.0056	0.014	0.0098	0.0084		C5	0.006	0.0153	0.0106	0.0093
F6	0.0132	0.0211	0.0171	0.0079		F6	0.014	0.0228	0.0184	0.0088
F7	0.0132	0.0211	0.0172	0.0079		F7	0.014	0.0228	0.0184	0.0088
F8	0.0173	0.0197	0.0185	0.0025		F8	0.018	0.0209	0.0194	0.0029
C9	0.0658	0.075	0.0704	0.0092		C9	0.0681	0.0799	0.074	0.0118
H9	0.0277	0.0326	0.0301	0.0048		H9	0.0288	0.0345	0.0316	0.0057
C10	0.0231	0.038	0.0306	0.0149		C10	0.0245	0.0414	0.033	0.0169
O11	0.0787	0.0694	0.0741	-0.0093		O11	0.0842	0.0742	0.0792	-0.0101
O12	0.0218	0.0285	0.0251	0.0066		O12	0.0243	0.0309	0.0276	0.0065
C13	0.0279	0.0211	0.0245	-0.0068		C13	0.0308	0.0219	0.0264	-0.0089
C14	0.0283	0.0266	0.0274	-0.0016		C14	0.0269	0.0284	0.0276	0.0015
H14	0.0174	0.0138	0.0156	-0.0037		H14	0.0176	0.015	0.0163	-0.0026
C15	0.0417	0.0355	0.0386	-0.0061		C15	0.0441	0.0402	0.0422	-0.0039
N16	0.0547	0.0121	0.0334	-0.0426		N16	0.052	0.012	0.032	-0.0401
H16	0.0192	0.0121	0.0157	-0.0071		H16	0.0205	0.0128	0.0167	-0.0077
C17	0.0147	0.047	0.0308	0.0322		C17	0.0182	0.0395	0.0288	0.0213
O18	0.0363	0.0557	0.046	0.0195		O18	0.0463	0.0496	0.048	0.0033
C19	0.0144	0.0176	0.016	0.0032		C19	0.006	0.0144	0.0102	0.0084
C20	0.0174	0.0248	0.0211	0.0074		C20	0.0137	0.015	0.0144	0.0013
H20	0.0115	0.0133	0.0124	0.0018		H20	0.0152	0.021	0.0181	0.0058
C21	0.0237	0.0246	0.0242	0.0009		C21	0.0134	0.0153	0.0143	0.0019
H21	0.0157	0.0173	0.0165	0.0015		H21	0.0233	0.0337	0.0285	0.0104
C22	0.0262	0.0364	0.0313	0.0102		C22	0.0282	0.0211	0.0247	-0.007
C23	0.0212	0.0226	0.0219	0.0014		H23	0.0154	0.0154	0.0154	0
H23	0.0145	0.0164	0.0154	0.0019		C24	0.0064	0.0175	0.0119	0.011
C24	0.0119	0.0235	0.0177	0.0116		H24	0.0053	0.0091	0.0072	0.0038
H24	0.0066	0.0114	0.009	0.0048		Cl25	0.0415	0.0326	0.037	-0.0088
Br25	0.1125	0.0718	0.0922	-0.0407		Cl26	0.0655	0.0535	0.0595	-0.012

Atom	G			
	f-	f+	fo	CDD
C1	0.0344	0.0269	0.0307	-0.0075
H4	0.0167	0.0213	0.019	0.0046
C5	0.0228	0.0399	0.0314	0.0171
H2	0.0165	0.021	0.0188	0.0045
C3	0.0441	0.0151	0.0296	-0.0289
C4	0.015	0.0721	0.0435	0.0572
C5	0.004	0.0163	0.0102	0.0122
F6	0.0133	0.0217	0.0175	0.0084
F7	0.0094	0.024	0.0167	0.0146
F8	0.0094	0.0241	0.0167	0.0146
C9	0.048	0.083	0.0655	0.0351
H9	0.021	0.0358	0.0284	0.0148
C10	0.0165	0.0435	0.03	0.027
O11	0.0549	0.077	0.0659	0.0221
O12	0.0135	0.0326	0.023	0.0192
C13	0.0183	0.0229	0.0206	0.0047
C14	0.0209	0.0288	0.0248	0.0079
H14	0.0116	0.0155	0.0135	0.0039
C15	0.022	0.0429	0.0325	0.021
N16	0.0377	0.0117	0.0247	-0.0259
H16	0.0127	0.0124	0.0126	-0.0003
C17	0.0092	0.0442	0.0267	0.035
O18	0.0292	0.0499	0.0395	0.0208
C19	0.0358	0.0061	0.0209	-0.0296
C20	0.0218	0.0152	0.0185	-0.0066
H20	0.0156	0.008	0.0118	-0.0076
C21	0.0403	0.0153	0.0278	-0.025
C22	0.0436	0.0306	0.0371	-0.013
C23	0.0284	0.0156	0.022	-0.0128
H23	0.0199	0.0121	0.016	-0.0078
C24	0.0433	0.0182	0.0308	-0.0252
H24	0.0195	0.0079	0.0137	-0.0116
O25	0.0511	0.0127	0.0319	-0.0384
C26	0.0152	0.0058	0.0105	-0.0094
H26A	0.0149	0.0036	0.0092	-0.0112
H26B	0.0182	0.011	0.0146	-0.0073
H26C	0.0148	0.0037	0.0092	-0.0112
O27	0.0513	0.0186	0.0349	-0.0327
C28	0.0155	0.0078	0.0116	-0.0077
H28A	0.016	0.0071	0.0115	-0.0089
H28B	0.0182	0.0112	0.0147	-0.0069
H28C	0.0157	0.0069	0.0113	-0.0089