

Supplementary Material

A Quantum Theory of Atoms-in-Molecules Perspective and DFT Study of Two Natural Products: Trans-Communic and Imbricatolic Acid

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Table S1. Geometrical parameters of optimized geometries of Trans-communic Acid and Imbricatolic Acid at B3LYP/cc-pVTZ level

Trans-communic Acid

R1	R(1,2)	1.5262	A25	A(4,5,6)	110.0117
R2	R(1,6)	1.5265	A26	A(4,5,10)	112.205
R3	R(1,23)	1.0921	A27	A(4,5,14)	106.6858
R4	R(1,24)	1.0912	A28	A(6,5,10)	109.7161
R5	R(2,3)	1.5506	A29	A(6,5,14)	105.9795
R6	R(2,25)	1.0917	A30	A(10,5,14)	112.0224
R7	R(2,26)	1.0952	A31	A(1,6,5)	115.167
R8	R(3,4)	1.5766	A32	A(1,6,28)	107.9313
R9	R(3,16)	1.5348	A33	A(1,6,29)	110.2296
R10	R(3,20)	1.5471	A34	A(5,6,28)	108.0836
R11	R(4,5)	1.5655	A35	A(5,6,29)	109.2819
R12	R(4,7)	1.5568	A36	A(28,6,29)	105.6928
R13	R(4,27)	1.0936	A37	A(4,7,8)	115.0825
R14	R(5,6)	1.5484	A38	A(4,7,30)	109.3482
R15	R(5,10)	1.5745	A39	A(4,7,31)	109.1446
R16	R(5,14)	1.5485	A40	A(8,7,30)	108.7058
R17	R(6,28)	1.0952	A41	A(8,7,31)	108.5213
R18	R(6,29)	1.0926	A42	A(30,7,31)	105.6154
R19	R(7,8)	1.5457	A43	A(7,8,9)	112.0321
R20	R(7,30)	1.0905	A44	A(7,8,32)	109.6584
R21	R(7,31)	1.0891	A45	A(7,8,33)	109.4851
R22	R(8,9)	1.5014	A46	A(9,8,32)	110.0587
R23	R(8,32)	1.0899	A47	A(9,8,33)	109.3624
R24	R(8,33)	1.093	A48	A(32,8,33)	106.0654
R25	R(9,10)	1.5215	A49	A(8,9,10)	115.9069
R26	R(9,15)	1.3301	A50	A(8,9,15)	121.8013
R27	R(10,11)	1.5615	A51	A(10,9,15)	122.2838
R28	R(10,34)	1.0909	A52	A(5,10,9)	113.32
R29	R(11,12)	1.4955	A53	A(5,10,11)	112.456
R30	R(11,35)	1.0942	A54	A(5,10,34)	106.9776
R31	R(11,36)	1.088	A55	A(9,10,11)	110.7158
R32	R(12,13)	1.344	A56	A(9,10,34)	107.1382
R33	R(12,37)	1.0876	A57	A(11,10,34)	105.7213
R34	R(13,17)	1.4644	A58	A(10,11,12)	113.8107
R35	R(13,19)	1.5041	A59	A(10,11,35)	108.0406
R36	R(14,38)	1.0912	A60	A(10,11,36)	109.6892
R37	R(14,39)	1.0874	A61	A(12,11,35)	107.1215
R38	R(14,40)	1.089	A62	A(12,11,36)	111.4433
R39	R(15,41)	1.0815	A63	A(35,11,36)	106.3754
R40	R(15,42)	1.0828	A64	A(11,12,13)	129.2958
R41	R(16,43)	1.0852	A65	A(11,12,37)	114.156
R42	R(16,44)	1.0852	A66	A(13,12,37)	116.5359

R43	R(16,45)	1.0891	A67	A(12,13,17)	118.195
R44	R(17,18)	1.3346	A68	A(12,13,19)	124.2685
R45	R(17,46)	1.0858	A69	A(17,13,19)	117.5366
R46	R(18,47)	1.0811	A70	A(5,14,38)	109.6598
R47	R(18,48)	1.0814	A71	A(5,14,39)	113.5184
R48	R(19,49)	1.0859	A72	A(5,14,40)	111.4437
R49	R(19,50)	1.092	A73	A(38,14,39)	107.4239
R50	R(19,51)	1.0926	A74	A(38,14,40)	106.9588
R51	R(20,21)	1.1992	A75	A(39,14,40)	107.5478
R52	R(20,22)	1.3615	A76	A(9,15,41)	122.2215
R53	R(22,52)	0.9637	A77	A(9,15,42)	121.1795
A1	A(2,1,6)	110.5752	A78	A(41,15,42)	116.599
A2	A(2,1,23)	109.4247	A79	A(3,16,43)	111.7355
A3	A(2,1,24)	110.3451	A80	A(3,16,44)	112.0247
A4	A(6,1,23)	109.3764	A81	A(3,16,45)	109.4162
A5	A(6,1,24)	111.0605	A82	A(43,16,44)	108.0036
A6	A(23,1,24)	105.941	A83	A(43,16,45)	108.4491
A7	A(1,2,3)	112.3352	A84	A(44,16,45)	107.0399
A8	A(1,2,25)	110.8686	A85	A(13,17,18)	126.6613
A9	A(1,2,26)	107.5967	A86	A(13,17,46)	115.0683
A10	A(3,2,25)	109.1406	A87	A(18,17,46)	118.2702
A11	A(3,2,26)	110.6229	A88	A(17,18,47)	120.9055
A12	A(25,2,26)	106.0889	A89	A(17,18,48)	122.5709
A13	A(2,3,4)	109.466	A90	A(47,18,48)	116.5236
A14	A(2,3,16)	109.1721	A91	A(13,19,49)	112.546
A15	A(2,3,20)	108.6617	A92	A(13,19,50)	110.5257
A16	A(4,3,16)	115.3543	A93	A(13,19,51)	110.8165
A17	A(4,3,20)	107.4519	A94	A(49,19,50)	107.7353
A18	A(16,3,20)	106.5141	A95	A(49,19,51)	108.0453
A19	A(3,4,5)	116.6852	A96	A(50,19,51)	106.9513
A20	A(3,4,7)	112.8741	A97	A(3,20,21)	124.3985
A21	A(3,4,27)	104.1126	A98	A(3,20,22)	117.0765
A22	A(5,4,7)	112.4294	A99	A(21,20,22)	118.525
A23	A(5,4,27)	103.0976	A100	A(20,22,52)	110.7881
A24	A(7,4,27)	106.1621			

Imbricatolic Acid

R1	R(1,2)	1.5269	A29	A(6,5,11)	105.8237
R2	R(1,6)	1.5261	A30	A(10,5,11)	112.0217
R3	R(1,24)	1.0921	A31	A(1,6,5)	115.3106
R4	R(1,25)	1.0911	A32	A(1,6,29)	107.9131
R5	R(2,3)	1.5502	A33	A(1,6,30)	110.2148
R6	R(2,26)	1.0917	A34	A(5,6,29)	108.0527
R7	R(2,27)	1.0953	A35	A(5,6,30)	109.1946
R8	R(3,4)	1.5772	A36	A(29,6,30)	105.6897
R9	R(3,18)	1.535	A37	A(4,7,8)	115.047
R10	R(3,19)	1.5469	A38	A(4,7,31)	109.3771
R11	R(4,5)	1.5654	A39	A(4,7,32)	109.1616
R12	R(4,7)	1.5568	A40	A(8,7,31)	108.7292
R13	R(4,28)	1.0937	A41	A(8,7,32)	108.4282
R14	R(5,6)	1.5485	A42	A(31,7,32)	105.6831
R15	R(5,10)	1.5775	A43	A(7,8,9)	111.4918
R16	R(5,11)	1.5494	A44	A(7,8,33)	109.5972
R17	R(6,29)	1.0951	A45	A(7,8,34)	109.698
R18	R(6,30)	1.0922	A46	A(9,8,33)	110.1854
R19	R(7,8)	1.5463	A47	A(9,8,34)	109.5234
R20	R(7,31)	1.0904	A48	A(33,8,34)	106.2049
R21	R(7,32)	1.0892	A49	A(8,9,10)	115.7969
R22	R(8,9)	1.5012	A50	A(8,9,12)	121.5285
R23	R(8,33)	1.0899	A51	A(10,9,12)	122.6356
R24	R(8,34)	1.0926	A52	A(5,10,9)	112.8777
R25	R(9,10)	1.5226	A53	A(5,10,14)	112.3967
R26	R(9,12)	1.3309	A54	A(5,10,35)	106.8899
R27	R(10,14)	1.5523	A55	A(9,10,14)	111.3405
R28	R(10,35)	1.0918	A56	A(9,10,35)	106.9544
R29	R(11,36)	1.0913	A57	A(14,10,35)	105.8698
R30	R(11,37)	1.0873	A58	A(5,11,36)	109.5678
R31	R(11,38)	1.0886	A59	A(5,11,37)	113.6311
R32	R(12,39)	1.0821	A60	A(5,11,38)	111.4286
R33	R(12,40)	1.0828	A61	A(36,11,37)	107.4257
R34	R(13,14)	1.5297	A62	A(36,11,38)	107.0113
R35	R(13,15)	1.5401	A63	A(37,11,38)	107.4872
R36	R(13,41)	1.0911	A64	A(9,12,39)	122.271
R37	R(13,42)	1.0952	A65	A(9,12,40)	121.2356
R38	R(14,43)	1.0927	A66	A(39,12,40)	116.4831
R39	R(14,44)	1.0913	A67	A(14,13,15)	114.4981
R40	R(15,16)	1.5411	A68	A(14,13,41)	110.109
R41	R(15,17)	1.5338	A69	A(14,13,42)	108.6219
R42	R(15,45)	1.0958	A70	A(15,13,41)	109.5504
R43	R(16,22)	1.5208	A71	A(15,13,42)	107.7965
R44	R(16,46)	1.0929	A72	A(41,13,42)	105.88
R45	R(16,47)	1.0918	A73	A(10,14,13)	114.7303
R46	R(17,48)	1.0914	A74	A(10,14,43)	108.7161

R47	R(17,49)	1.0914	A75	A(10,14,44)	109.2978
R48	R(17,50)	1.0915	A76	A(13,14,43)	107.6147
R49	R(18,51)	1.0852	A77	A(13,14,44)	109.9596
R50	R(18,52)	1.0851	A78	A(43,14,44)	106.1563
R51	R(18,53)	1.0891	A79	A(13,15,16)	114.1797
R52	R(19,20)	1.1993	A80	A(13,15,17)	110.3964
R53	R(19,21)	1.3614	A81	A(13,15,45)	107.027
R54	R(21,54)	0.9637	A82	A(16,15,17)	112.0879
R55	R(22,23)	1.4289	A83	A(16,15,45)	105.7394
R56	R(22,55)	1.0954	A84	A(17,15,45)	106.9086
R57	R(22,56)	1.0955	A85	A(15,16,22)	116.1077
R58	R(23,57)	0.9609	A86	A(15,16,46)	108.7787
A1	A(2,1,6)	110.5551	A87	A(15,16,47)	110.0522
A2	A(2,1,24)	109.4551	A88	A(22,16,46)	107.7247
A3	A(2,1,25)	110.2602	A89	A(22,16,47)	107.6939
A4	A(6,1,24)	109.4009	A90	A(46,16,47)	105.999
A5	A(6,1,25)	111.0638	A91	A(15,17,48)	111.2348
A6	A(24,1,25)	105.9922	A92	A(15,17,49)	110.8235
A7	A(1,2,3)	112.2205	A93	A(15,17,50)	111.8619
A8	A(1,2,26)	110.9132	A94	A(48,17,49)	107.7499
A9	A(1,2,27)	107.6441	A95	A(48,17,50)	107.6981
A10	A(3,2,26)	109.1409	A96	A(49,17,50)	107.2753
A11	A(3,2,27)	110.6374	A97	A(3,18,51)	111.7637
A12	A(26,2,27)	106.1052	A98	A(3,18,52)	111.973
A13	A(2,3,4)	109.4595	A99	A(3,18,53)	109.4093
A14	A(2,3,18)	109.169	A100	A(51,18,52)	107.9762
A15	A(2,3,19)	108.8069	A101	A(51,18,53)	108.4552
A16	A(4,3,18)	115.4342	A102	A(52,18,53)	107.0944
A17	A(4,3,19)	107.3453	A103	A(3,19,20)	124.4174
A18	A(18,3,19)	106.4098	A104	A(3,19,21)	117.0604
A19	A(3,4,5)	116.6613	A105	A(20,19,21)	118.5219
A20	A(3,4,7)	112.9488	A106	A(19,21,54)	110.7456
A21	A(3,4,28)	104.0746	A107	A(16,22,23)	107.1886
A22	A(5,4,7)	112.4041	A108	A(16,22,55)	110.6657
A23	A(5,4,28)	103.1064	A109	A(16,22,56)	110.6912
A24	A(7,4,28)	106.1585	A110	A(23,22,55)	110.3475
A25	A(4,5,6)	109.9956	A111	A(23,22,56)	110.3062
A26	A(4,5,10)	112.3782	A112	A(55,22,56)	107.6642
A27	A(4,5,11)	106.6584	A113	A(22,23,57)	108.6301
A28	A(6,5,10)	109.7227			

Table S2. Natural Atomic Charge (NAC) and Mulliken Atomic Charges (MAC)

Trans-communic Acid

Atom	B3LYP/cc-pVTZ		BPW91/cc-pVTZ	
	NAC	MAC	NAC	MAC
C1	-0.37264	-0.210172	-0.39158	-0.184570
C2	-0.37394	-0.181480	-0.39305	-0.146777
C3	-0.10502	0.017765	-0.10737	-0.053453
C4	-0.20214	-0.088470	-0.21415	-0.082670
C5	0.03947	0.195040	0.03883	0.132844
C6	-0.39125	-0.211201	-0.41209	-0.182555
C7	-0.38089	-0.213059	-0.39943	-0.181108
C8	-0.41484	-0.192296	-0.43364	-0.148717
C9	0.03238	0.083649	0.02832	0.036022
C10	-0.24739	-0.077014	-0.25907	-0.080616
C11	-0.40952	-0.121554	-0.43064	-0.093336
C12	-0.13918	-0.249783	-0.14535	-0.244721
C13	-0.02360	0.130343	-0.02521	0.114838
C14	-0.59399	-0.356387	-0.62079	-0.319217
C15	-0.38901	-0.312633	-0.39932	-0.269140
C16	-0.59195	-0.318037	-0.62009	-0.294730
C17	-0.19547	-0.057696	-0.20559	-0.059038
C18	-0.37810	-0.307603	-0.38477	-0.273986
C19	-0.61323	-0.310576	-0.63674	-0.272944
C20	0.81086	0.281359	0.76094	0.267342
O21	-0.56784	-0.279214	-0.53643	-0.258425
O22	-0.67938	-0.240078	-0.65258	-0.210226
H23	0.20398	0.103803	0.21443	0.084517
H24	0.19011	0.092273	0.19972	0.090146
H25	0.20741	0.103692	0.21654	0.088403
H26	0.17211	0.075082	0.18160	0.073968
H27	0.17851	0.074093	0.19044	0.076420
H28	0.18552	0.077894	0.19596	0.071996
H29	0.19969	0.096248	0.20944	0.089227
H30	0.20185	0.099120	0.21092	0.082923
H31	0.20851	0.111870	0.21819	0.107481
H32	0.20697	0.090505	0.21629	0.071359
H33	0.19221	0.090056	0.20358	0.087680
H34	0.20195	0.090718	0.21473	0.093815
H35	0.20165	0.105682	0.21319	0.102123
H36	0.19693	0.093548	0.20714	0.089941
H37	0.17899	0.098120	0.18590	0.086242
H38	0.19605	0.084981	0.20533	0.078036
H39	0.19921	0.098709	0.20827	0.096089
H40	0.20328	0.098494	0.21223	0.094997
H41	0.19157	0.109604	0.19691	0.104274
H42	0.18811	0.103970	0.19305	0.091485
H43	0.19579	0.091133	0.20531	0.092404
H44	0.21896	0.111314	0.22801	0.110848
H45	0.21220	0.105883	0.22089	0.097683
H46	0.18790	0.098934	0.19363	0.083291
H47	0.19119	0.111207	0.19548	0.101167
H48	0.18224	0.106465	0.18652	0.096713

H49	0.20375	0.093456	0.21150	0.084038
H50	0.21127	0.101310	0.22046	0.094722
H51	0.20827	0.102677	0.21720	0.095491
H52	0.47051	0.198258	0.46696	0.187705

Imbricatolic Acid

Atom	B3LYP/cc-pVTZ		BPW91/cc-pVTZ	
	NAC	MAC	NAC	MAC
C1	-0.37244	-0.209742	-0.39536	-0.179278
C2	-0.37376	-0.181773	-0.39458	-0.142928
C3	-0.10494	0.019101	-0.11193	-0.048833
C4	-0.20330	-0.089262	-0.21832	-0.079967
C5	0.04256	0.189471	0.03473	0.126935
C6	-0.39142	-0.209468	-0.41498	-0.177048
C7	-0.38024	-0.212942	-0.40404	-0.177532
C8	-0.41639	-0.192638	-0.43814	-0.145069
C9	0.04504	0.080079	0.03416	0.030997
C10	-0.25700	-0.077339	-0.27151	-0.074955
C11	-0.59366	-0.356783	-0.62390	-0.313347
C12	-0.40377	-0.318904	-0.41598	-0.272440
C13	-0.38277	-0.189169	-0.40722	-0.169829
C14	-0.36872	-0.148228	-0.39419	-0.131643
C15	-0.16925	-0.048005	-0.18520	-0.049758
C16	-0.39872	-0.159388	-0.42206	-0.140259
C17	-0.57913	-0.319951	-0.60557	-0.276417
C18	-0.59201	-0.317677	-0.62396	-0.287565
C19	0.81102	0.282149	0.76376	0.270559
O20	-0.56868	-0.280183	-0.54250	-0.265040
O21	-0.67936	-0.240319	-0.65260	-0.218249
C22	-0.02536	0.014451	-0.05739	0.024109
O23	-0.72474	-0.340617	-0.70559	-0.318704
H24	0.20360	0.103221	0.21656	0.082263
H25	0.19005	0.092056	0.20226	0.087941
H26	0.20698	0.103056	0.21953	0.086336
H27	0.17165	0.074199	0.17701	0.070421
H28	0.17912	0.074208	0.19783	0.073182
H29	0.18512	0.077645	0.19800	0.069961
H30	0.20053	0.095861	0.21294	0.086756
H31	0.20247	0.099523	0.21435	0.082004
H32	0.20825	0.111366	0.22352	0.105674
H33	0.20577	0.089357	0.21777	0.068921
H34	0.19453	0.092123	0.20604	0.086971
H35	0.20016	0.086627	0.21534	0.083685
H36	0.19499	0.083115	0.20686	0.075014
H37	0.19937	0.099866	0.21054	0.095737
H38	0.20460	0.101399	0.21570	0.095918
H39	0.18694	0.106980	0.19574	0.098560
H40	0.18895	0.104009	0.19707	0.090776
H41	0.19387	0.093318	0.20729	0.091928
H42	0.18434	0.082084	0.19638	0.068808
H43	0.18519	0.087491	0.19776	0.083622
H44	0.19094	0.096821	0.20459	0.095779

H45	0.18456	0.082366	0.19752	0.065373
H46	0.19922	0.089642	0.21025	0.074455
H47	0.19764	0.088484	0.20851	0.079373
H48	0.19714	0.095935	0.20676	0.083515
H49	0.19642	0.093632	0.20584	0.080442
H50	0.18839	0.086202	0.19819	0.079207
H51	0.19553	0.089963	0.20710	0.088827
H52	0.21871	0.111133	0.23231	0.109392
H53	0.21181	0.105600	0.22121	0.095730
H54	0.47065	0.198447	0.46698	0.192181
H55	0.14701	0.057735	0.15487	0.047745
H56	0.14885	0.063297	0.15757	0.056820
H57	0.45374	0.190377	0.45219	0.182946

Table S3.

Optimized molecular geometries of Trans-communic Acid (Fig1a) and Imbricatolic Acid (Fig 1b) at B3LYP/cc-pVTZ level of theory.

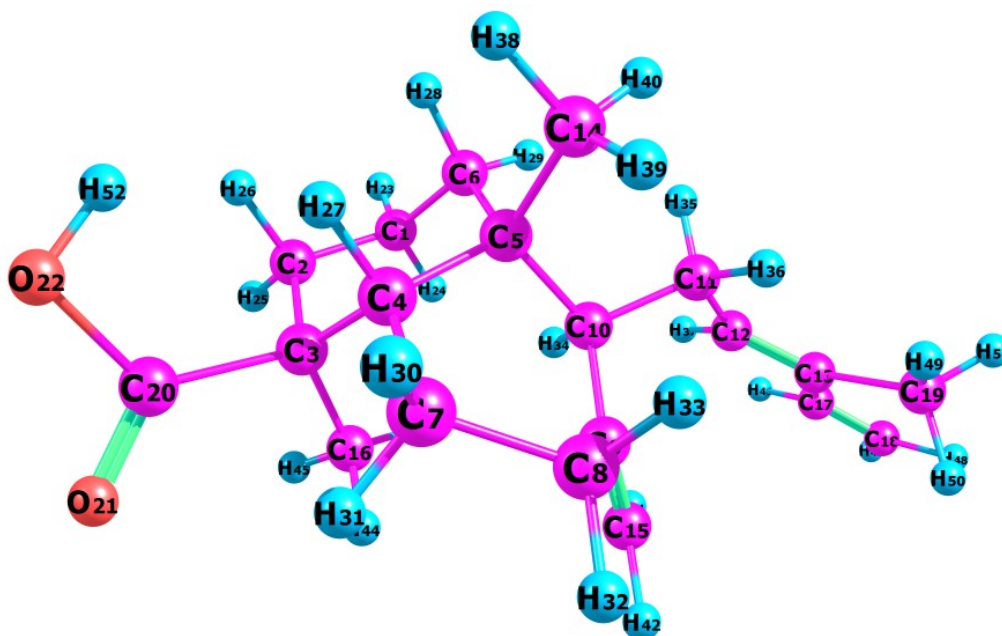


Fig1a

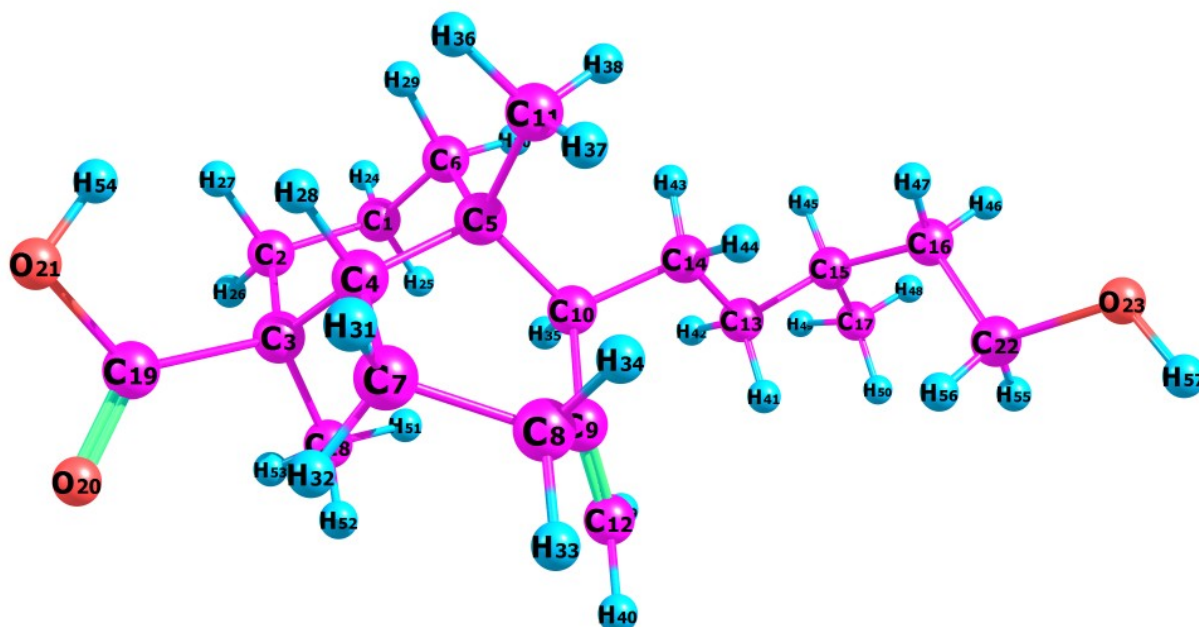


Fig1b

Molecular graphs showing C---H as well as H---H intramolecular interactions (dotted lines) in Trans-communic Acid (Fig 2a) and Imbricatolic Acid (Fig 2b). Red points correspond to ring critical points and green represent bond critical points (BCPs). Red spheres correspond to Oxygen atoms, dark grey spheres correspond to carbon atoms and light blue spheres correspond to hydrogen atoms.

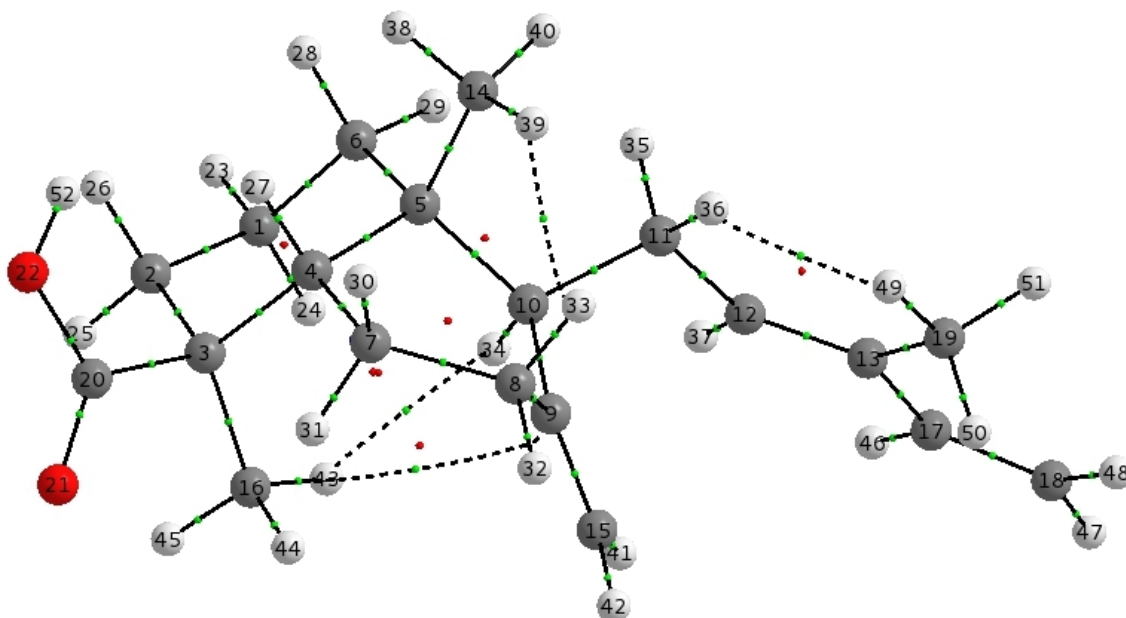


Fig2a

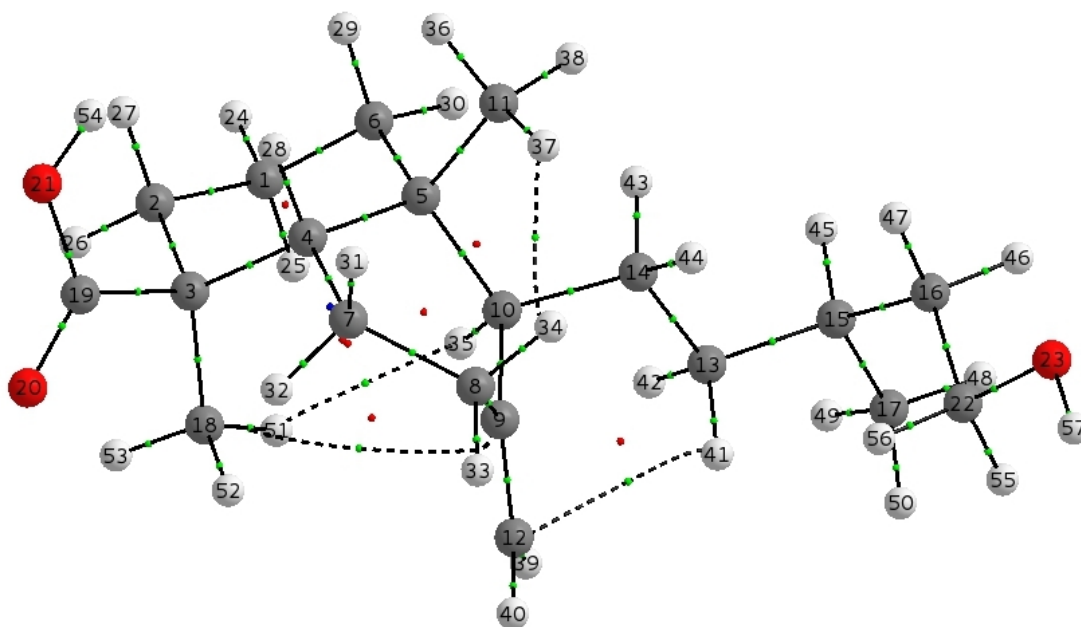
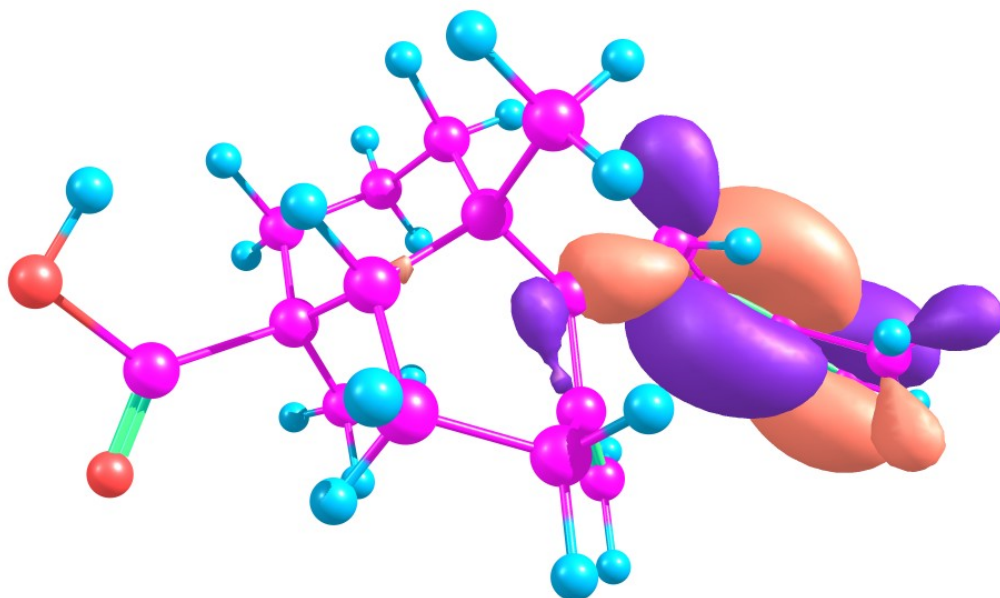
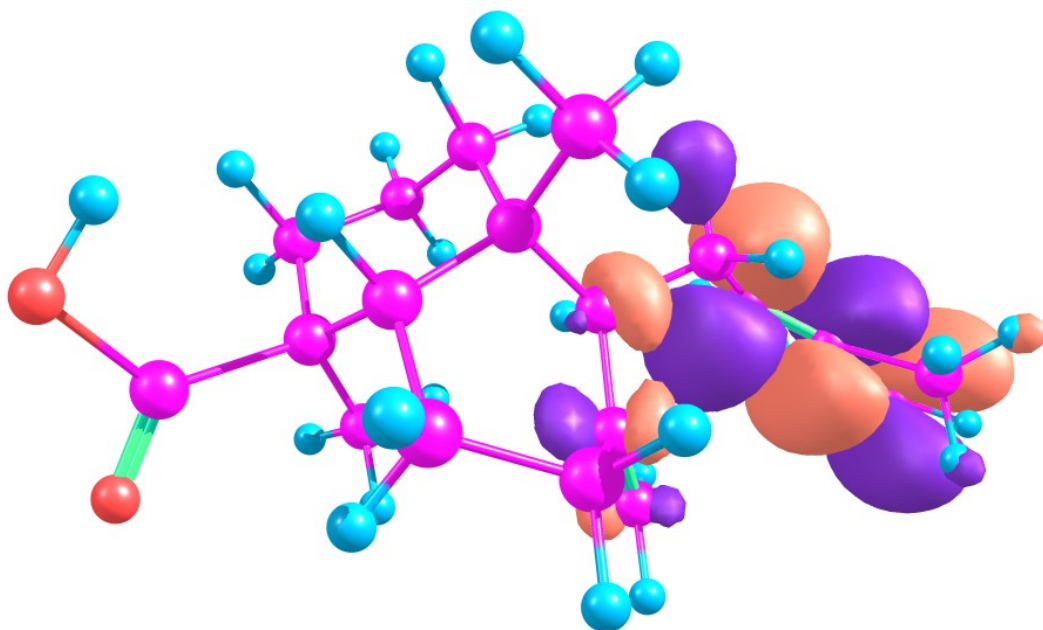


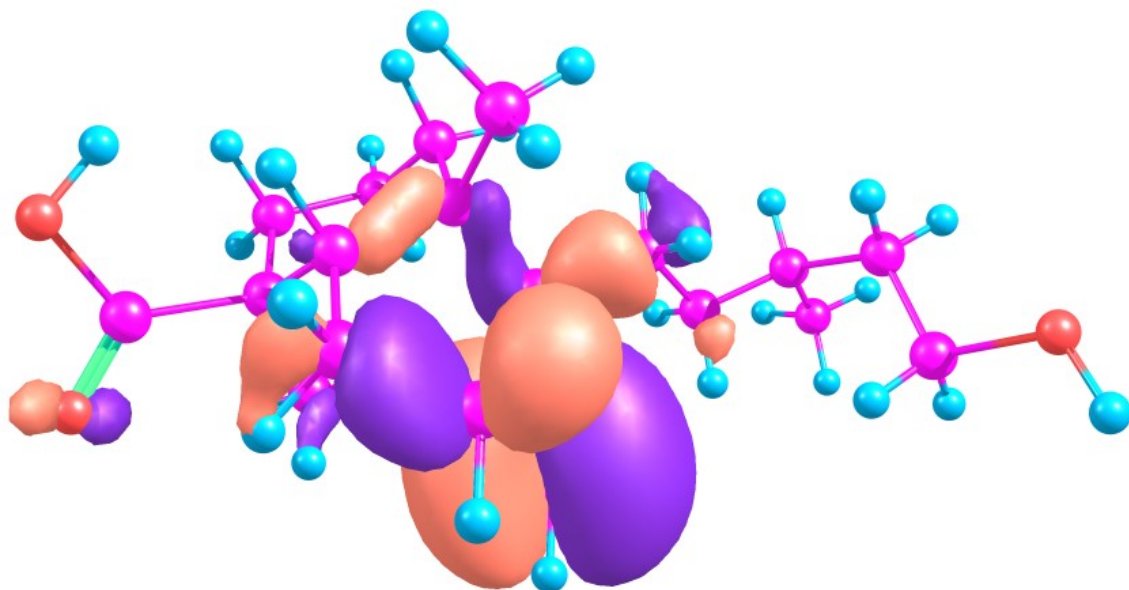
Fig2b



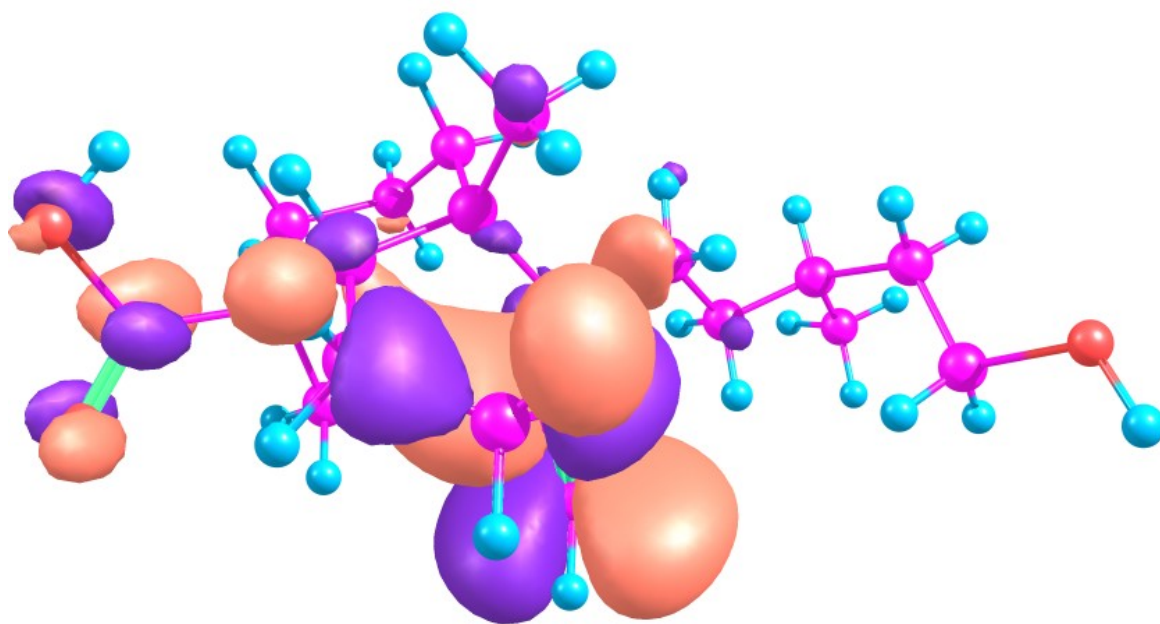
Trans-cinnamic Acid (HOMO)



Trans-cinnamic Acid (LUMO)



Imbricatolic Acid (HOMO)



Imbricatolic Acid (LUMO)
