Interactions of Vinca Alkaloid Subunits with Chiral Amido[4]resorcinarenes: A Dynamic, Kinetic, and Spectroscopic Study.

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SUPPORTING INFORMATION

Kinetic plots (**Figures S1-S11**) of the gas-phase reaction between B and $[MHA]^+$ (A=catharanthine (**C**) or vindoline (**V**); **Figure S12**: $[\mathbf{4_R}•H•\mathbf{C}]^+$ and $[\mathbf{4_S}•H•\mathbf{C}]^+$ low-energy structures. **Tables 1S-3S**: NMR assignments. Docking and Molecular Dynamics Simulations: geometries and partial atomic charges.

Figure S1. Kinetic plots of the gas-phase reactions between B and $[\mathbf{1_R}\bullet H\bullet\mathbf{C}]^+$(open circles; [B]=7.0x10^9 molecule cm^{-3}) or $[\mathbf{1_S}\bullet H\bullet\mathbf{C}]^+$ (full circles; [B]=5.9x10^9 molecule cm^{-3})

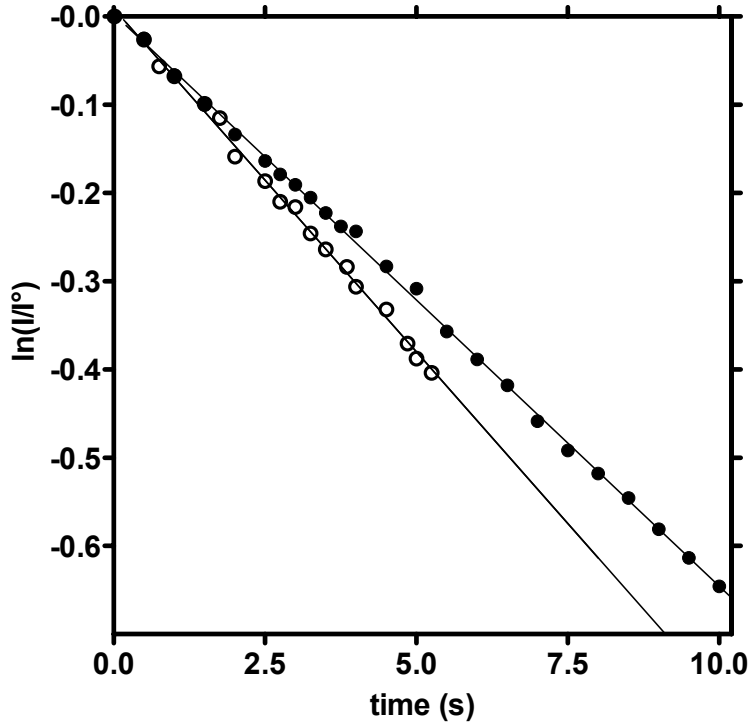


Figure S2. Kinetic plots of the gas-phase reactions between B and $[\mathbf{2_R}\bullet H\bullet\mathbf{C}]^+$(open circles; [B]=1.4x10^9 molecule cm^{-3}) or $[\mathbf{2_S}\bullet H\bullet\mathbf{C}]^+$ (full circles; [B]=1.5x10^9 molecule cm^{-3})

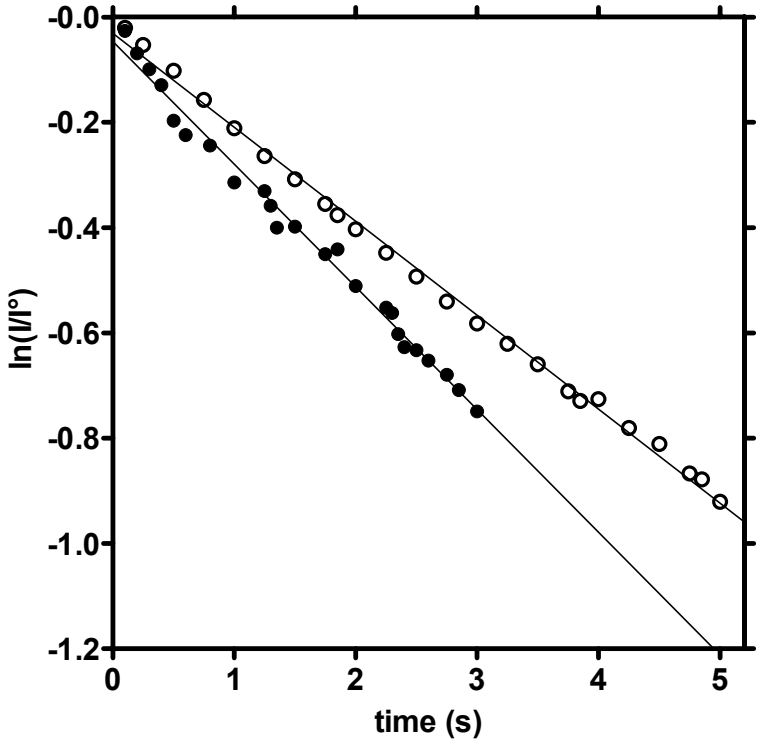


Figure S3. Kinetic plots of the gas-phase reactions between B and $[\mathbf{3_R}\bullet H\bullet\mathbf{C}]^+$(open circles; [B]=6.4x10^9 molecule cm^{-3}) or $[\mathbf{3_S}\bullet H\bullet\mathbf{C}]^+$ (full circles; [B]=7.0x10^9 molecule cm^{-3})

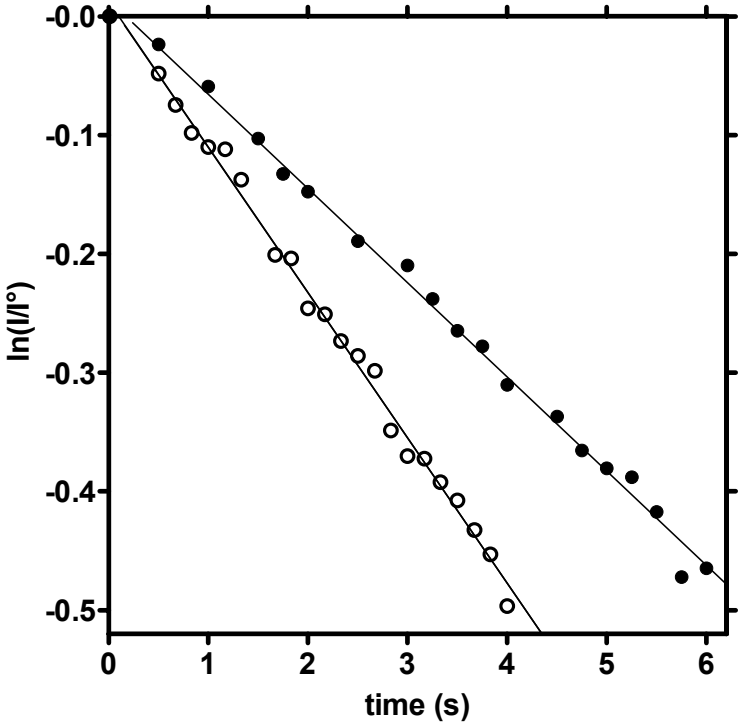


Figure S4. Kinetic plots of the gas-phase reactions between B and $[\mathbf{4_R}\bullet H\bullet\mathbf{C}]^+$(open circles; [B]=3.1x10^9 molecule cm^{-3}) or $[\mathbf{4_S}\bullet H\bullet\mathbf{C}]^+$ (full circles; [B]=3.1x10^9 molecule cm^{-3})

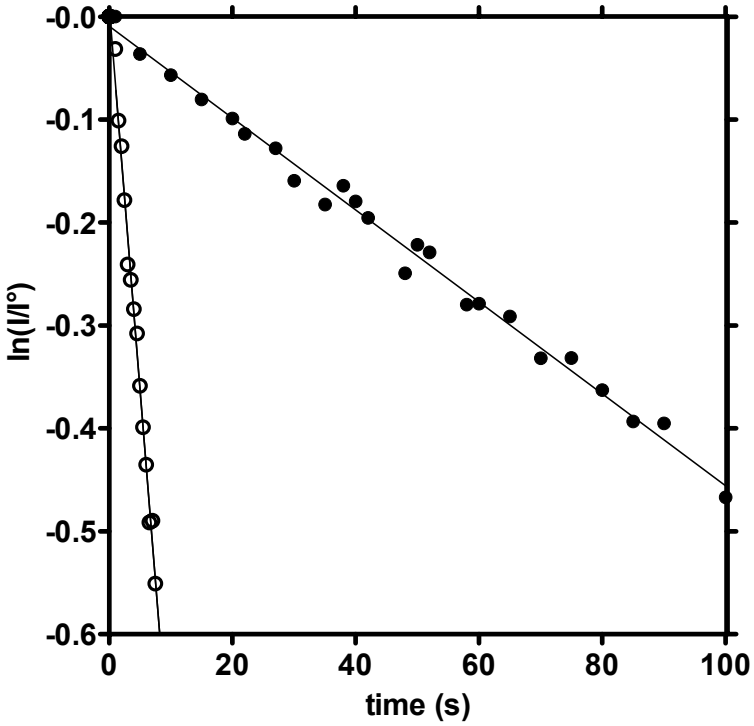


Figure S5. Kinetic plots of the gas-phase reactions between B and $[\mathbf{5_R}\bullet H\bullet\mathbf{C}]^+$(open circles; [B]=1.2x10^9 molecule cm^{-3}) or $[\mathbf{5_S}\bullet H\bullet\mathbf{C}]^+$ (full circles; [B]=2.0x10^9 molecule cm^{-3})

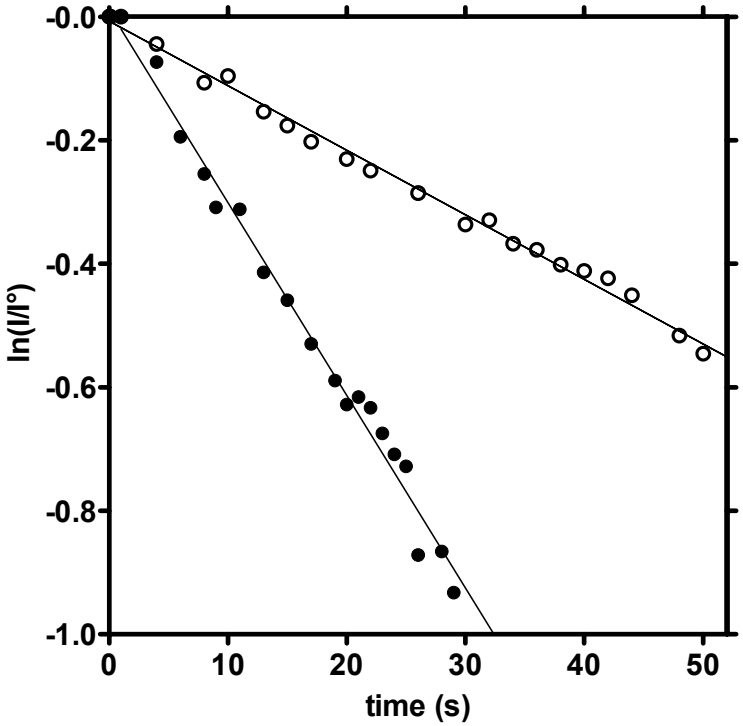


Figure S6. Kinetic plots of the gas-phase reactions between B and $[\mathbf{1_R}\bullet H\bullet\mathbf{V}]^+$(open circles; [B]=7.8x10^9 molecule cm^{-3}) or $[\mathbf{1_S}\bullet H\bullet\mathbf{V}]^+$ (full circles; [B]=7.4x10^9 molecule cm^{-3})

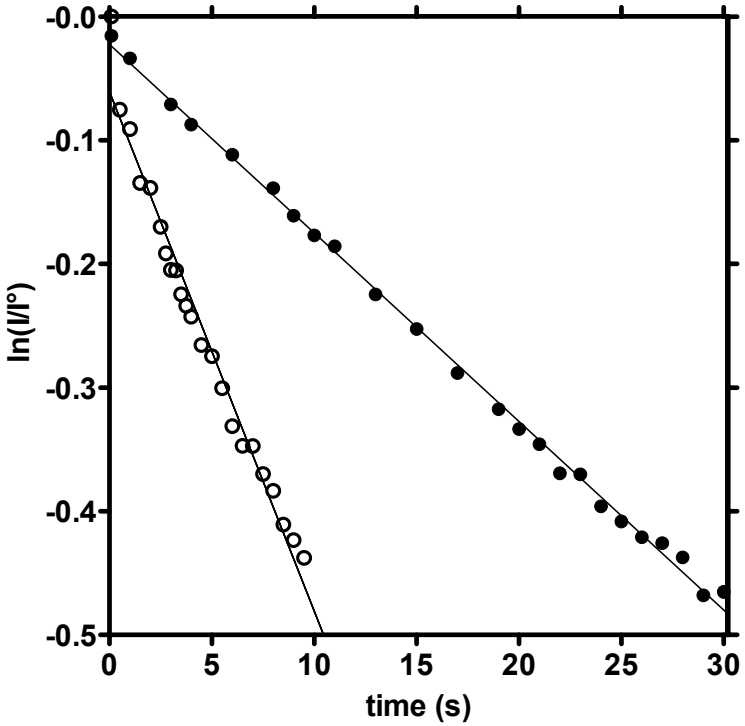


Figure S7. Kinetic plots of the gas-phase reactions between B and $[\mathbf{2_R}\bullet H\bullet\mathbf{V}]^+$(open circles; [B]=1.8x10^9 molecule cm^{-3}) or $[\mathbf{2_S}\bullet H\bullet\mathbf{V}]^+$ (full circles; [B]=1.6x10^9 molecule cm^{-3})

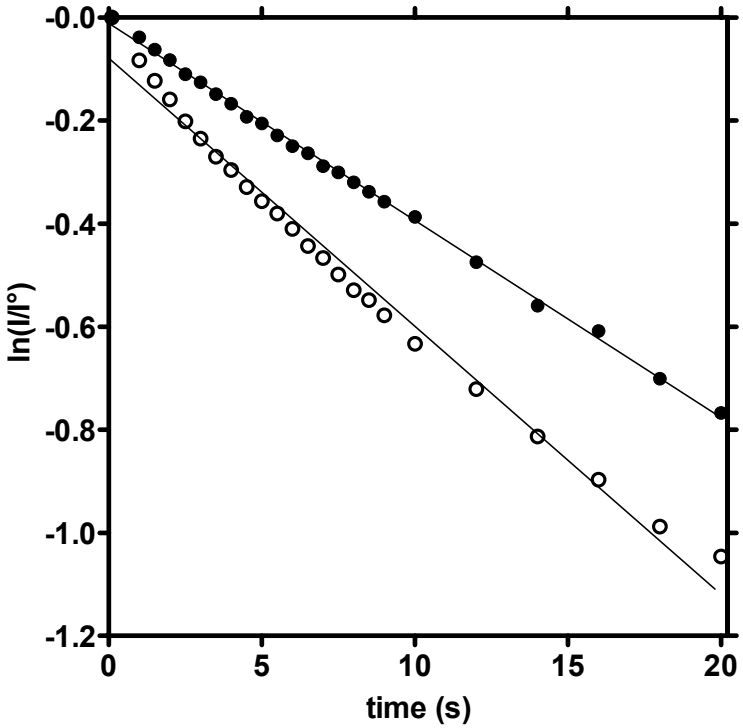


Figure S8. Kinetic plots of the gas-phase reactions between B and $[\mathbf{3_R}\bullet H\bullet\mathbf{V}]^+$(open circles; [B]=7.5x10^9 molecule cm^{-3}) or $[\mathbf{3_S}\bullet H\bullet\mathbf{V}]^+$ (full circles; [B]=7.4x10^9 molecule cm^{-3})

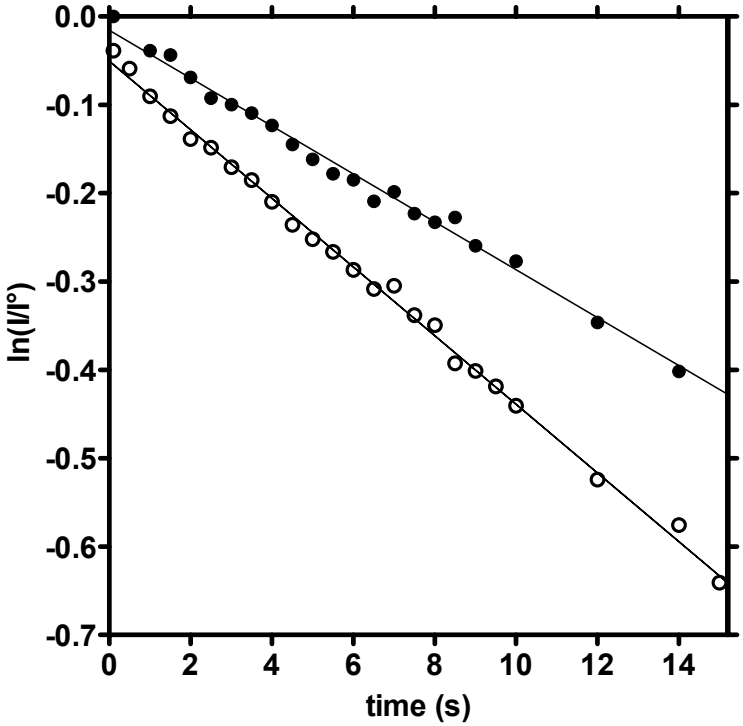


Figure S9. Kinetic plots of the gas-phase reactions between B and $[\mathbf{4_R}\bullet H\bullet\mathbf{V}]^+$(open circles; [B]=3.3x10^9 molecule cm^{-3}) or $[\mathbf{4_S}\bullet H\bullet\mathbf{V}]^+$ (full circles; [B]=3.0x10^9 molecule cm^{-3})

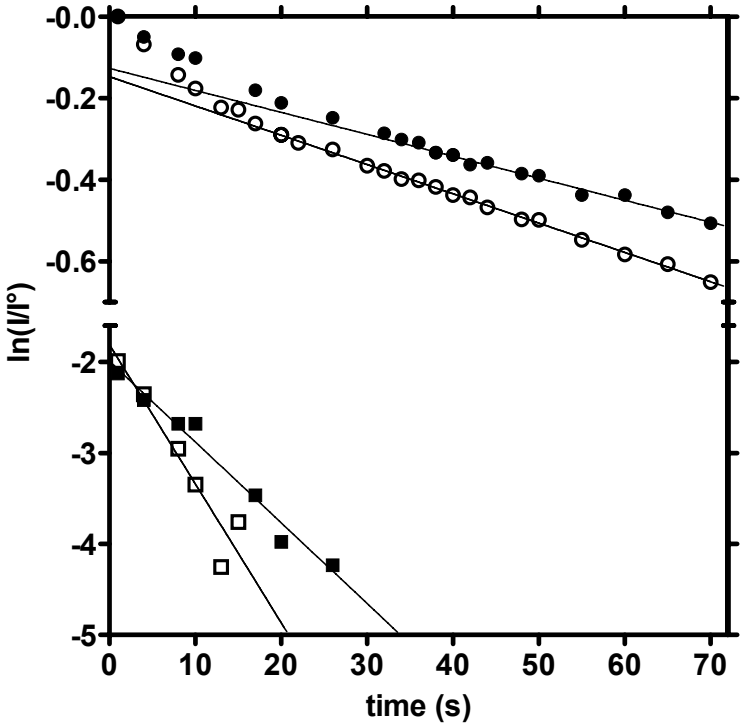


Figure S10. Time dependence of the relative abundance of the reactant and products of the gas-phase reaction between B and $[\mathbf{5_S}\bullet H\bullet \mathbf{V}]^+$([B]=2.0x10^9 molecule cm^{-3})

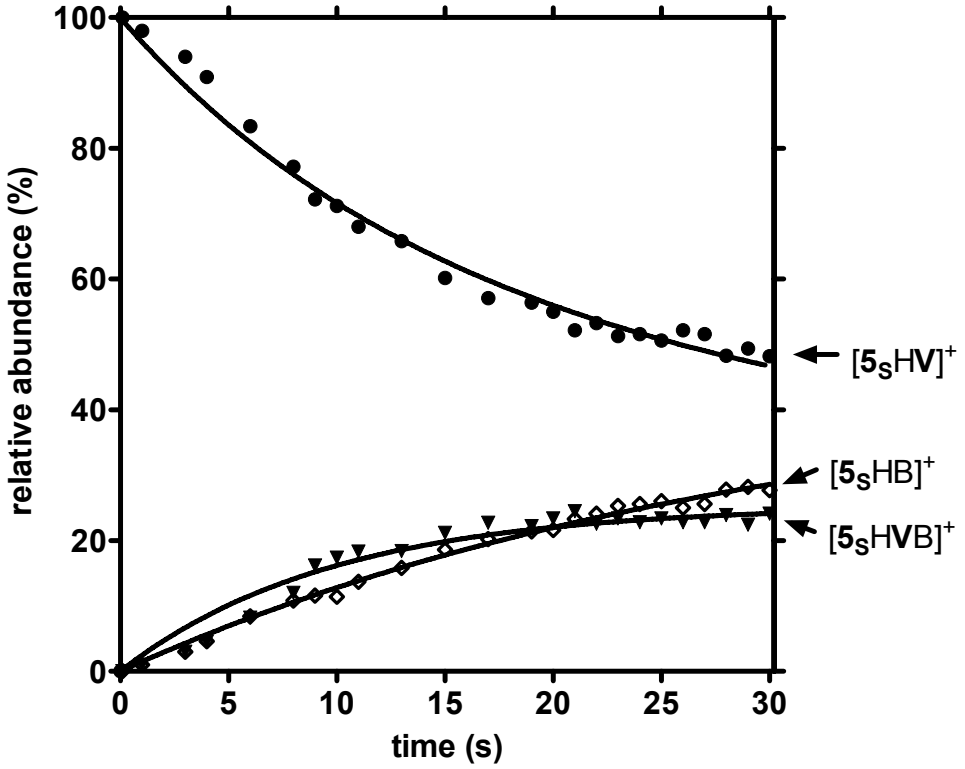
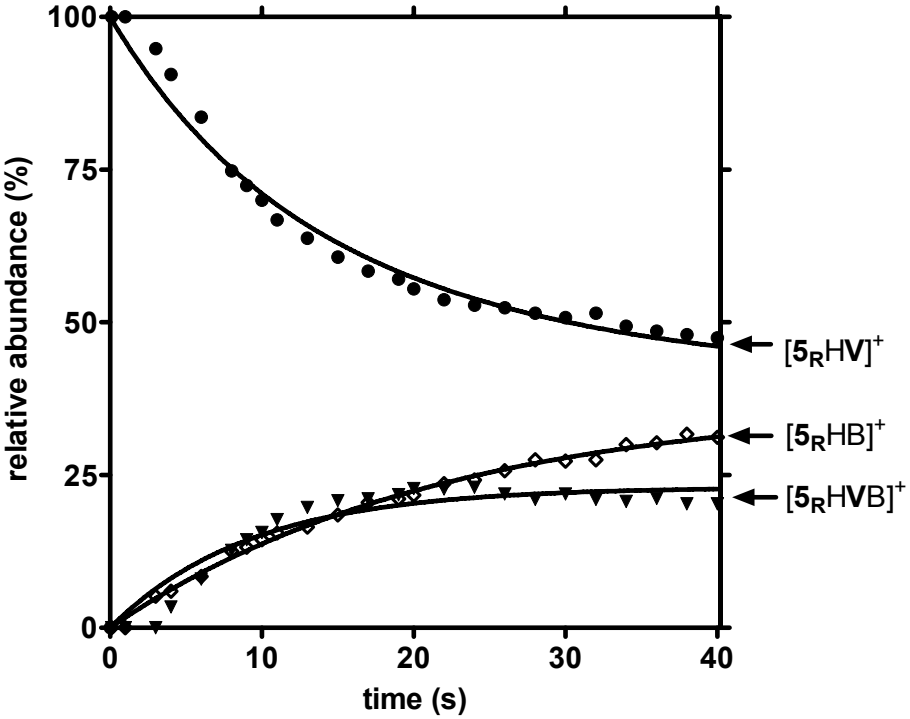
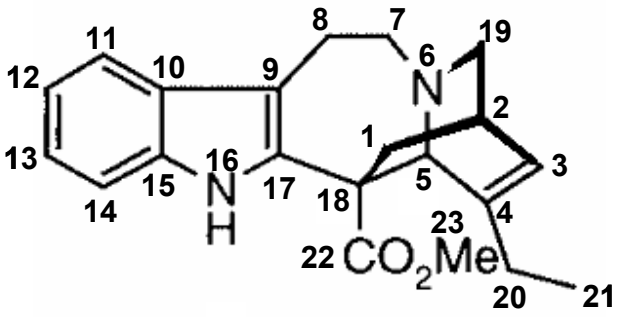


Figure S11. Time dependence of the relative abundance of the reactant and products of the gas-phase reaction between B and $[\mathbf{5_R}\bullet H\bullet\mathbf{V}]^+$([B]=1.9x10^9 molecule cm^{-3})




11
12
10
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N
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1
13
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17
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5
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NH
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23
22 CO2Me
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Table 1S. ^{1}H and ^{13}C assignments of **C** in CD_2Cl_2. ^{1}H and ^{13}C chemical shifts are reported with respect to the residual proton signal of CD_2Cl_2 (δ= 5.33 ppm) and to the carbon signal of CD_2Cl_2 l at (δ= 54. 2 ppm), respectively.

	Type	^{1}H (ppm)	m	J_{H-H} (Hz)	^{13}C (ppm)
1	CH_2	1' 1.967 1'' 2.891	dd m	13.5;2.2	37.27
2	CH	3.069	bs		29.83
3	CH	6.264	m		128.26
4	C				146.28
5	CH	4.769	s		60.33
7	CH_2	7' 3.470 7'' 4.075	m m		57.06
8	CH_2	8' 3.205 8'' 3.404	ddd ddd	17.5, 8.1, 3.2 17.5, 8.8, 3.2	20.00
10	C				128.40
11	CH	7.515	d	8.0	118.99
12	CH	7.149	ddd	8.0, 8.0, 1.0	120.99
13	CH	7.213	ddd	8.0,8.2, 1.1	123.81
14	CH	7.320	ddd	8.2, 0.8, 0.8	111.70
15	C				136.13
16	NH	8.000	s		
18	C				51.73
19	CH_2	19' 2.891 19'' 3.400	m m		53.21
20	CH_2	20' 2.210 20'' 2.751	ddq ddq	17.2, 2.2, 7.3 17.2, 2.2, 7.3	27.53
21	CH_3	1.137	t	7.3	10.5
22	CO				172.24
23	CH_3	3.775			54.09

Table 2S. Assignment of **C** in D_2O at pH = 10.8. ^{1}H and ^{13}C chemical shifts are reported with respect to methyl signal of ethanol at 1.131 ppm and 17.1 ppm, respectively.

	Type	^{1}H (ppm)	m	J_{H-H} (Hz)	^{13}C (ppm)
1	CH_2	1' 1.689 1'' 2.646	dd ddd	13.5, 2.2 13.5, 2.2, 2.8	36.7
2	CH	2.77	bs		30.2
3	CH	5.976	m		125.04
5	CH	4.062	s		62.20
7	CH_2	7' 3.179 7'' 3.361	ddd ddd	13.3, 8.2, 3.6 13.3, 10.1. 3.1	52.30
8	CH_2	8' 2.958 8'' 3.256	ddd ddd	16.9, 8.2, 3.9 16.9, 10.1, 4.3	
11	CH	7.559	d	8.0	118.15
12	CH	7.118	ddd	8.0, 8.0, 1.0	119.87
13	CH	7.175	ddd	8.8, 8,2, 1.1	122.28
14	CH	7.325	ddd	8.2, 0.8, 0.8	11.28
19	CH_2	19' 2.612 19'' 2.826	ddd bd	9.4, 2.8, 2.8 9.4	48.80
20	CH_2	20' 1.968 20'' 2.162	ddq ddq	17.1, 2.2, 7.3 17.1, 2.2, 7.3	32.2
21	CH_3	0.98	t	7.4	10.0
23	CH_3	3.719	s		53.30

Table 3S. ^{1}H Assignment of **C** in D_2O at pH = 5.4. ^{1}H Chemical shifts are reported with respect to methyl signal of ethanol at 1.131 ppm.

.

	Type	^{1}H (ppm)	m	J_{H-H} (Hz)
1	CH_2	1' 1.990 1'' 2.798	dd	13.7, 2.1
2	CH	3.13	bs	
3	CH	6.366	m	
5	CH	4.967	s	
7	CH_2	7' 3.600 7'' 3.929	m ddd	 13.3, 8.2, 3.6
8	CH_2	8' 3.28 8'' 3.42	ddd ddd	17.6, 8.6, 3.7 17.6, 8.6, 3.7
11	CH	7.588	ddd	8.0, 0.8, 0.8
12	CH	7.162	ddd	8.0, 8.0, 0.8
13	CH	7.233	ddd	8.0, 8.2, 0.8
14	CH	7.374	ddd	8.2, 0.8, 0.8
19	CH_2	3.207	m	
20	CH_2	20' 2.105 20'' 2.283	ddq ddq	17.5, 2.1, 7.4
21	CH_3	1.029	t	7.4
23	CH_3	3.720	s	

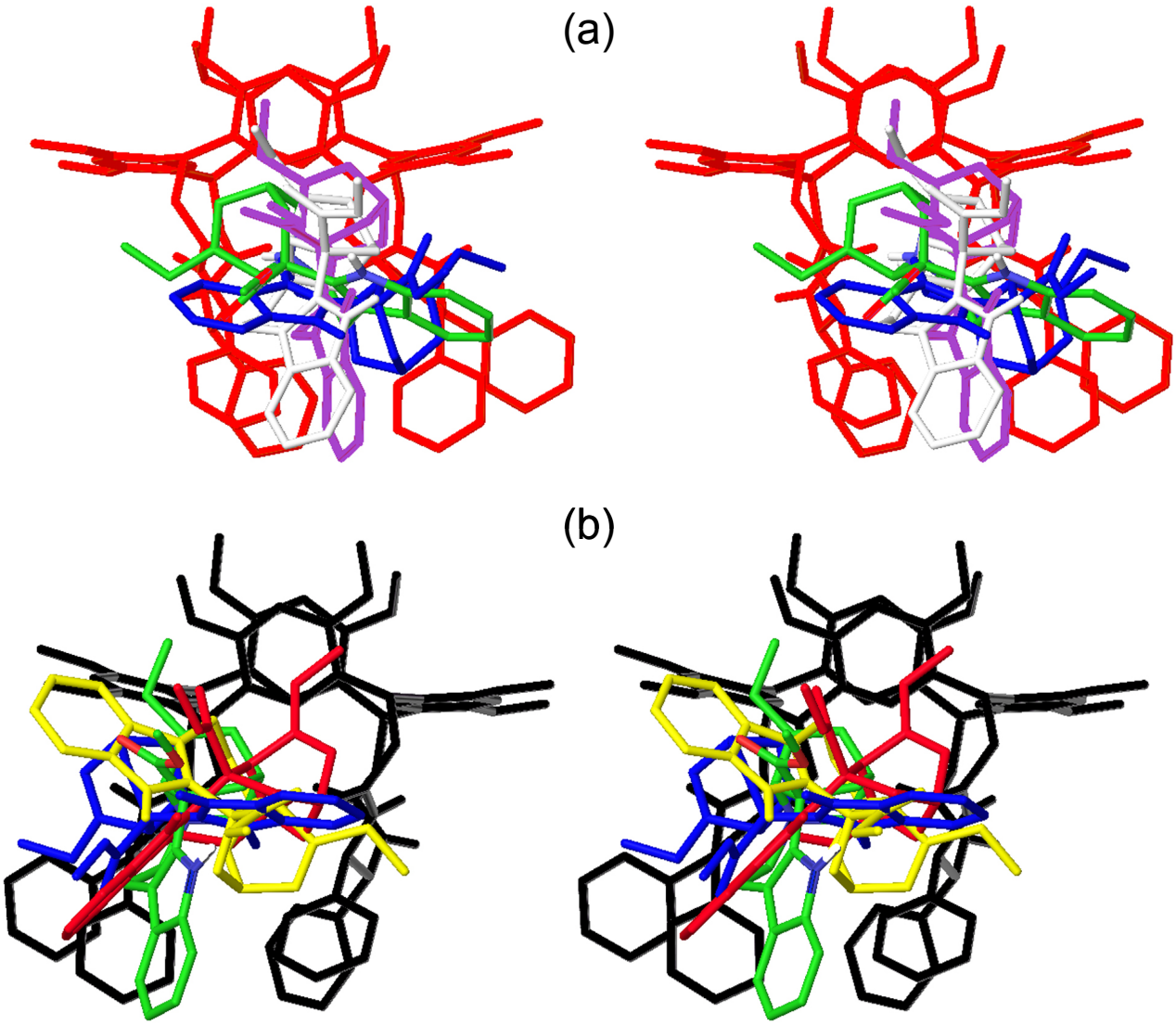

Figure S12. Tangles showing representative orientations of catharanthine In populated low-energy (a) [**4**$_S$•H•**C**]$^+$ (violet, white, and blue) and (b) [**4**$_R$•H•**C**]$^+$(yellow, red, and blue) complexes superimposed to the corresponding global minimumcomplex (green) shown in Figure 4 (crossed stereo view).

Cartesian coordinates and charges of **4$_S$** (mol2 format).

#Name: **4$_S$**

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@<TRIPOS>MOLECULE
amido[4]resorcinarene 4S
160   170    1
SMALL
NO_CHARGES


@<TRIPOS>ATOM
      1 C           2.3711    6.4675    7.0410 C.ar      1 RES        -0.0520
      2 C           1.0822    6.1766    7.5341 C.ar      1 RES         0.0342
      3 C           0.1067    5.6965    6.6379 C.ar      1 RES        -0.1304
      4 C           0.4430    5.5123    5.2844 C.ar      1 RES        -0.0677
      5 C           1.7367    5.7678    4.7968 C.ar      1 RES        -0.1303
      6 C           2.7144    6.2642    5.6870 C.ar      1 RES         0.0342
      7 O           0.7430    6.3308    8.8581 O.3       1 RES        -0.1970
      8 C          -1.2949    5.3368    7.1225 C.3       1 RES         0.1928
      9 C           2.0995    5.4970    3.3376 C.3       1 RES         0.1928
     10 O           3.9756    6.5228    5.2022 O.3       1 RES        -0.1971
     11 C           1.6784    6.9018    9.7792 C.3       1 RES        -0.0488
     12 C           4.9828    7.0721    6.0583 C.3       1 RES        -0.0487
     13 C          -3.4317    7.7066    4.9883 C.ar      1 RES        -0.1489
     14 C          -2.4309    7.2381    5.8655 C.ar      1 RES         0.1003
     15 C          -2.3845    5.8632    6.1843 C.ar      1 RES        -0.0436
     16 C          -3.3614    5.0075    5.6376 C.ar      1 RES        -0.2435
     17 C          -4.3703    5.4744    4.7770 C.ar      1 RES         0.0024
     18 C          -4.3993    6.8427    4.4341 C.ar      1 RES         0.0311
     19 O          -1.4974    8.0779    6.4267 O.3       1 RES        -0.1893
     20 C          -5.4020    4.5139    4.1863 C.3       1 RES         0.1831
     21 O          -5.3694    7.2832    3.5640 O.3       1 RES        -0.1750
     22 C          -1.3596    9.4196    5.9489 C.3       1 RES        -0.0979
     23 C          -5.3369    8.6275    3.0747 C.3       1 RES        -0.1273
     24 C          -5.6254    3.6745    0.4508 C.ar      1 RES        -0.0489
     25 C          -6.0199    3.9800    1.7715 C.ar      1 RES         0.0283
     26 C          -5.0258    4.1623    2.7535 C.ar      1 RES        -0.1269
     27 C          -3.6740    3.9955    2.4019 C.ar      1 RES        -0.0520
     28 C          -3.2845    3.6608    1.0980 C.ar      1 RES        -0.1268
     29 C          -4.2683    3.5122    0.0983 C.ar      1 RES         0.0282
     30 O          -7.3382    4.0940    2.1462 O.3       1 RES        -0.1953
     31 C          -1.8105    3.3874    0.8228 C.3       1 RES         0.1832
     32 O          -3.8712    3.1952   -1.1788 O.3       1 RES        -0.1953
     33 C          -8.3755    3.9565    1.1692 C.3       1 RES        -0.0508
     34 C          -4.8363    2.8032   -2.1585 C.3       1 RES        -0.0508
     35 C          -0.3297    6.9385    0.7034 C.ar      1 RES        -0.1488
     36 C           0.7133    6.8715    1.6565 C.ar      1 RES         0.1003
     37 C           0.9329    5.6573    2.3458 C.ar      1 RES        -0.0435
     38 C           0.0608    4.5834    2.0897 C.ar      1 RES        -0.2436
     39 C          -0.9572    4.6272    1.1198 C.ar      1 RES         0.0025
     40 C          -1.1549    5.8292    0.4106 C.ar      1 RES         0.0311
     41 O           1.5216    7.9502    1.9341 O.3       1 RES        -0.1893
     42 O          -2.1446    5.8721   -0.5427 O.3       1 RES        -0.1750
     43 C           1.3426    9.1859    1.2340 C.3       1 RES        -0.0979
     44 C          -2.3844    7.0732   -1.2811 C.3       1 RES        -0.1273
     45 H          -6.3776    3.5508   -0.3085 H         1 RES         0.0771
     46 H          -2.8992    4.0926    3.1483 H         1 RES         0.1141
     47 H          -0.3206    5.1410    4.6188 H         1 RES         0.1227
     48 H           3.1182    6.8391    7.7202 H         1 RES         0.0742
     49 H          -0.4931    7.8580    0.1716 H         1 RES         0.1046
     50 H           0.1845    3.6870    2.6535 H         1 RES         0.1677
     51 H          -3.3358    3.9552    5.8552 H         1 RES         0.1677
     52 H          -3.4622    8.7527    4.7426 H         1 RES         0.1047
     53 H          -1.4951    5.8838    8.0441 H         1 RES         0.0003
     54 H           2.7887    6.2971    3.0742 H         1 RES         0.0003
     55 H           1.9711    7.9023    9.4580 H         1 RES         0.0740
     56 H           2.5557    6.2627    9.8843 H         1 RES         0.0740
     57 H           1.1933    6.9825   10.7520 H         1 RES         0.0740
     58 H           5.8851    7.2263    5.4665 H         1 RES         0.0740
     59 H           4.6649    8.0365    6.4566 H         1 RES         0.0740
     60 H           5.2180    6.3820    6.8693 H         1 RES         0.0740
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61	H	-6.3170	5.1053	4.1501	H	1 RES	0.0062
62	H	-0.4872	9.8621	6.4290	H	1 RES	0.0836
63	H	-2.2364	10.0128	6.2097	H	1 RES	0.0836
64	H	-1.1981	9.4259	4.8699	H	1 RES	0.0836
65	H	-5.5119	9.3358	3.8850	H	1 RES	0.0932
66	H	-6.1334	8.7405	2.3394	H	1 RES	0.0932
67	H	-4.3843	8.8322	2.5842	H	1 RES	0.0932
68	H	-1.6662	3.1893	-0.2388	H	1 RES	0.0062
69	H	-8.2716	4.7141	0.3912	H	1 RES	0.0740
70	H	-9.3346	4.1040	1.6654	H	1 RES	0.0740
71	H	-8.3643	2.9576	0.7315	H	1 RES	0.0740
72	H	-5.4272	1.9610	-1.7966	H	1 RES	0.0740
73	H	-4.2987	2.4854	-3.0517	H	1 RES	0.0740
74	H	-5.4806	3.6420	-2.4220	H	1 RES	0.0740
75	H	0.3523	9.5982	1.4300	H	1 RES	0.0835
76	H	1.4940	9.0449	0.1630	H	1 RES	0.0835
77	H	2.0883	9.8934	1.5960	H	1 RES	0.0835
78	H	-2.6784	7.8814	-0.6111	H	1 RES	0.0932
79	H	-3.2035	6.8832	-1.9742	H	1 RES	0.0932
80	H	-1.5014	7.3509	-1.8575	H	1 RES	0.0932
81	C	2.3550	2.8863	3.3145	C.2	1 RES	0.4622
82	O	2.2050	2.1837	2.3192	O.2	1 RES	-0.5509
83	C	3.0078	4.2587	3.1529	C.3	1 RES	-0.1508
84	C	-0.7337	2.9076	6.5085	C.2	1 RES	0.4816
85	O	-1.1692	2.8398	5.3618	O.2	1 RES	-0.5321
86	C	-1.3558	3.8575	7.5368	C.3	1 RES	-0.1583
87	N	1.9395	2.4985	4.5302	N.am	1 RES	-0.2594
88	N	0.3030	2.1754	6.9351	N.am	1 RES	-0.3848
89	C	0.9313	1.0384	6.2655	C.3	1 RES	-0.0372
90	C	-1.2413	-2.6229	7.1936	C.ar	1 RES	-0.1108
91	C	-1.9315	-1.5049	6.7004	C.ar	1 RES	-0.2107
92	C	-1.2348	-0.3241	6.3906	C.ar	1 RES	-0.0351
93	C	0.1601	-0.2358	6.5860	C.ar	1 RES	-0.0117
94	C	0.8409	-1.3665	7.0819	C.ar	1 RES	-0.1216
95	C	0.1482	-2.5524	7.3815	C.ar	1 RES	-0.1830
96	H	-1.7763	-3.5344	7.4210	H	1 RES	0.1372
97	H	-3.0000	-1.5485	6.5451	H	1 RES	0.1458
98	H	-1.7937	0.5102	5.9937	H	1 RES	0.1442
99	H	1.9113	-1.3373	7.2236	H	1 RES	0.1161
100	H	0.6874	-3.4127	7.7520	H	1 RES	0.1467
101	H	0.5881	2.3277	7.8900	H	1 RES	0.2917
102	H	3.8474	4.3134	3.8445	H	1 RES	0.0501
103	H	3.4164	4.3049	2.1424	H	1 RES	0.0501
104	H	-0.7943	3.7730	8.4673	H	1 RES	0.0581
105	H	1.9086	0.9389	6.7381	H	1 RES	0.1190
106	H	-2.3770	3.5531	7.7627	H	1 RES	0.0581
107	C	1.2162	1.2454	4.7648	C.3	1 RES	-0.0371
108	C	3.2515	-2.2410	3.1397	C.ar	1 RES	-0.1297
109	C	3.9396	-1.3567	3.9873	C.ar	1 RES	-0.1850
110	C	3.2859	-0.2231	4.5019	C.ar	1 RES	-0.0429
111	C	1.9393	0.0395	4.1798	C.ar	1 RES	0.0344
112	C	1.2624	-0.8508	3.3221	C.ar	1 RES	-0.0817
113	C	1.9113	-1.9852	2.8067	C.ar	1 RES	-0.1903
114	H	3.7519	-3.1101	2.7367	H	1 RES	0.1356
115	H	4.9734	-1.5439	4.2379	H	1 RES	0.1417
116	H	3.8251	0.4518	5.1486	H	1 RES	0.0989
117	H	0.2332	-0.6680	3.0511	H	1 RES	0.0747
118	H	1.3739	-2.6523	2.1471	H	1 RES	0.1434
119	H	2.0096	3.1510	5.2960	H	1 RES	0.2327
120	H	0.2715	1.3217	4.2273	H	1 RES	0.1560
121	C	-2.3831	0.9706	1.3519	C.2	1 RES	0.4622
122	O	-2.5500	0.4315	0.2591	O.2	1 RES	-0.5509
123	C	-1.3707	2.0930	1.5320	C.3	1 RES	-0.1508
124	C	-5.0574	2.0032	4.7888	C.2	1 RES	0.4816
125	O	-4.1525	1.6477	5.5399	O.2	1 RES	-0.5321
126	C	-5.8180	3.3058	5.0478	C.3	1 RES	-0.1583
127	N	-3.1011	0.6462	2.4322	N.am	1 RES	-0.2594
128	N	-5.4683	1.2458	3.7643	N.am	1 RES	-0.3848
129	C	-5.0997	-0.1578	3.5899	C.3	1 RES	-0.0372
130	C	-8.7569	-2.4725	3.2144	C.ar	1 RES	-0.1108
131	C	-7.8455	-2.7565	4.2447	C.ar	1 RES	-0.2107
132	C	-6.6630	-2.0059	4.3667	C.ar	1 RES	-0.0351
133	C	-6.3783	-0.9638	3.4627	C.ar	1 RES	-0.0117
134	C	-7.2985	-0.6879	2.4309	C.ar	1 RES	-0.1216
135	C	-8.4814	-1.4368	2.3066	C.ar	1 RES	-0.1830
136	H	-9.6654	-3.0511	3.1188	H	1 RES	0.1372
137	H	-8.0504	-3.5551	4.9435	H	1 RES	0.1458
138	H	-5.9671	-2.2387	5.1600	H	1 RES	0.1442

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    141 H          -6.1776    1.6281    3.1569 H         1 RES         0.2917
    142 H          -0.3992    1.7708    1.1546 H         1 RES         0.0501
    143 H          -1.3025    2.2573    2.6055 H         1 RES         0.0501
    144 H          -5.7441    3.5667    6.1037 H         1 RES         0.0581
    145 H          -4.5746   -0.4918    4.4876 H         1 RES         0.1190
    146 H          -6.8695    3.1022    4.8425 H         1 RES         0.0581
    147 C          -4.1402   -0.3651    2.4091 C.3       1 RES        -0.0371
    148 C          -2.3277   -4.3192    2.4524 C.ar      1 RES        -0.1297
    149 C          -3.3940   -4.0412    1.5803 C.ar      1 RES        -0.1850
    150 C          -3.9755   -2.7607    1.5612 C.ar      1 RES        -0.0429
    151 C          -3.5015   -1.7447    2.4135 C.ar      1 RES         0.0344
    152 C          -2.4315   -2.0365    3.2826 C.ar      1 RES        -0.0817
    153 C          -1.8456   -3.3126    3.3049 C.ar      1 RES        -0.1903
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    155 H          -3.7660   -4.8096    0.9182 H         1 RES         0.1417
    156 H          -4.7941   -2.5594    0.8860 H         1 RES         0.0989
    157 H          -2.0470   -1.2714    3.9370 H         1 RES         0.0747
    158 H          -1.0205   -3.5089    3.9762 H         1 RES         0.1434
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  88   44   80 1
  89   81   82 2
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  92   83  102 1
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Cartesian coordinates and charges of **C** (mol2 format).

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SMALL
NO_CHARGES


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      4 C4          -6.6010   -2.8512  -11.9315 C.ar      1 UNK          0.0574
      5 C5          -6.7333   -1.5331  -11.4402 C.ar      1 UNK         -0.2130
      6 C6          -6.0698   -0.4504  -12.0455 C.ar      1 UNK         -0.1736
      7 C7          -5.2511   -0.6586  -13.1667 C.ar      1 UNK         -0.1542
      8 C8          -5.0963   -1.9544  -13.6823 C.ar      1 UNK         -0.2437
      9 C9          -5.7604   -3.0305  -13.0716 C.ar      1 UNK          0.1141
     10 C10         -8.0720   -4.4260  -10.4145 C.3       1 UNK          0.0168
     11 H11         -7.3599   -1.3506  -10.5806 H         1 UNK          0.1583
     12 H12         -6.1918    0.5471  -11.6463 H         1 UNK          0.1360
     13 H13         -4.7434    0.1762  -13.6300 H         1 UNK          0.1440
     14 H14         -4.4684   -2.1209  -14.5449 H         1 UNK          0.1625
     15 C15         -6.8457   -6.5761  -12.4666 C.3       1 UNK         -0.0590
     16 H16         -5.3276   -4.8196  -14.1120 H         1 UNK          0.2925
     17 C17         -7.7348   -7.1094  -11.3049 C.3       1 UNK         -0.0331
     18 N18         -7.1639   -6.7241  -10.0065 N.3       1 UNK         -0.2636
     19 C19         -7.5606   -5.4388   -9.3877 C.3       1 UNK          0.1724
     20 H20         -8.2409   -3.4902   -9.8823 H         1 UNK          0.0233
     21 H21         -9.0369   -4.7373  -10.8129 H         1 UNK          0.0233
     22 C22         -7.6715   -8.6378  -11.3249 C.2       1 UNK         -0.0942
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     31 C31         -5.7291   -7.1019   -9.9047 C.3       1 UNK         -0.0407
     32 C32         -6.4408   -9.1277  -11.1748 C.2       1 UNK         -0.1847
     33 C33         -5.3568   -8.0648  -11.0494 C.3       1 UNK          0.0596
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     39 H39         -5.2892   -7.9573  -13.1793 H         1 UNK          0.0319
     40 H40         -8.7730   -6.7997  -11.4264 H         1 UNK          0.1186
     41 C41         -8.9097   -9.5198  -11.4792 C.3       1 UNK          0.0315
     42 C42         -9.8317   -9.3602  -10.2687 C.3       1 UNK         -0.0640
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     44 H44         -8.6141  -10.5666  -11.5586 H         1 UNK          0.0329
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     46 H46        -10.6946  -10.0167  -10.3825 H         1 UNK          0.0182
     47 H47         -9.2951   -9.6298   -9.3585 H         1 UNK          0.0182
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Cartesian coordinates and charges of protonated catharanthine **CH**$^+$ (mol2 format).

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SMALL
NO_CHARGES


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     26 C26        -9.8225    1.1197   -5.1787 C.3       2 ****       -0.0451
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     29 H29        -9.7901    1.3428   -4.1127 H         2 ****        0.1111
     30 H30       -10.2746    0.1358   -5.3202 H         2 ****        0.1111
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