A theoretical survey of the ability of nanocarbon layers to deliver anti-cancer drug temozolomide to the target cancer cells

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1. General

SI 1 The calculated Gibbs free energy profiles for connected R-NH2 compound to SR_3-FG carbon at neutral and acidic conditions (in kcal mol-1)

Hydrolysis at acidic pH			Hydrolysis at neutral pH			ΔG(N) - ΔG(+H)	
Structure	**Gas**	**SM8**	**Structure**	**Gas**	**SM8**	**Gas**	**SM8**
H+R-D	-07.664	+6.565	N-R-D	+01.448	+08.224	+09.111	+01.660
H+TS-I	+02.058	+7.858	N-TS-I	+07.742	+07.753	+05.684	-00.105
H+P-I	-10.009	+4.214	N-P-I	+03.261	+06.223	+13.270	+02.009
H+TS-II	+39.226	+49.034	N-TS-II	+52.663	+56.951	+13.436	+07.918
H+P-II	-18.406	-12.541	N-P-II	+22.237	+30.416	+40.643	+42.956
H+P-III	-18.416	-12.467	N-P-III	-02.138	+5.021	+16.278	+17.488

SI 2 The calculated Gibbs free energy profiles for connected temozolomide to Sp2-FG carbon layers in two possible pathways at acidic condition (in kcal mol-1)

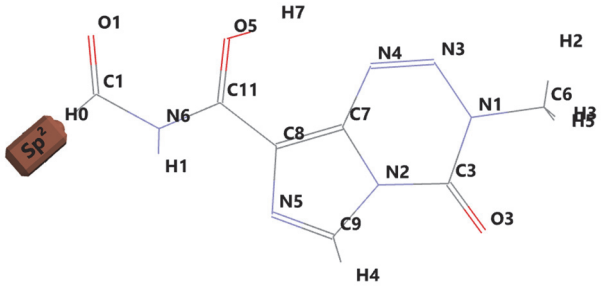
	(Path-O1)			(Path-O5)		$\Delta G_I - \Delta G_{II}$	
Structure	**Gas**	**SM8**	**Structure**	**Gas**	**SM8**	**Gas**	**SM8**
O1Sp^2-R-D	-3.60	-2.48	O5Sp2-R-D	-7.17	-3.73	-3.57	-1.25
O1Sp^2-R-TS-I	9.08	3.28	O5Sp2-R-TS-I	-1.04	-1.79	-10.13	-5.07
O1Sp^2-R-P-I	3.18	3.35	O5Sp2-R-P-I	-1.20	-1.17	-4.38	-4.52
O1Sp^2-R-TS-II	18.59	11.79	O5Sp2-R-TS-II	51.92	44.67	33.33	32.88
O1Sp^2-R-P-II	-15.85	-11.72	O5Sp2-R-P-II	-19.30	-18.47	-3.46	-6.75

SI 3 The calculated relative free energies for both temozolomide degradation paths (in kcal mol-1)

	(Path-B)		**(Path-II)**	
Structure	**Gas**	**SM8**	**Gas**	**SM8**
TMZ + water	-4.15/	-7.89	-4.15	- 7.89
TS-I (MTIC-acid)	+57.56	+59.35/	+72.10	+70.17
TS-II (MTIC-acid)	+62.17	+64.30/	+43.16	+48.14
Product (MTIC + CO_2)	+1.74	+3.94	- 20.93	- 10.18

1.1 O5 protonated

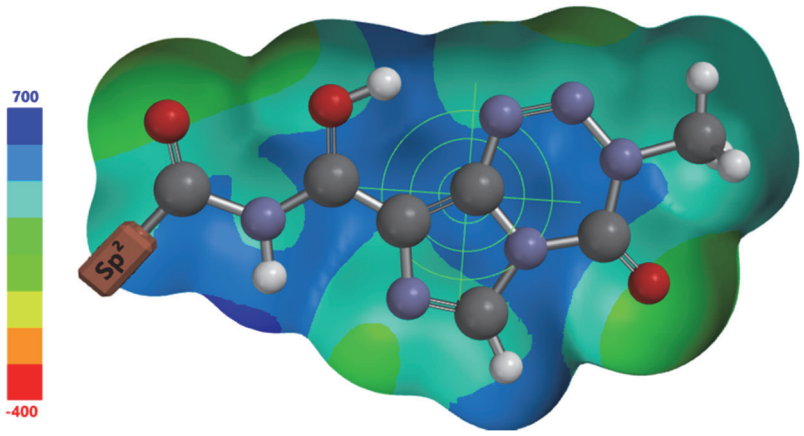
SI 4 Atomic electrostatic potential of O5 protonated of drug



Note: Average and variance below are in kcal/mol and (kcal/mol)^2 respectively

Atom#	All/Positive/Negative average			All/Positive/Negative variance		
1	**106.47283**	**106.47283**	**NaN**	**NaN**	**162.55554**	**NaN**
2	36.53225	36.53225	NaN	NaN	429.42097	NaN
3	141.49986	141.49986	NaN	NaN	230.35535	NaN
4	65.53084	65.53084	NaN	NaN	589.02772	NaN
5	113.79641	113.79641	NaN	NaN	345.53658	NaN
6	144.40344	144.40344	NaN	NaN	81.55148	NaN
8	81.11356	81.11356	NaN	NaN	489.46377	NaN
9	101.99493	101.99493	NaN	NaN	688.05943	NaN
10	141.77392	141.77392	NaN	NaN	205.92019	NaN
11	90.17211	90.17211	NaN	NaN	155.00593	NaN
12	111.71006	111.71006	NaN	NaN	302.07791	NaN
13	64.44903	64.44903	NaN	NaN	112.99678	NaN
14	**111.12776**	**111.12776**	**NaN**	**NaN**	**84.39273**	**NaN**
15	107.56618	107.56618	NaN	NaN	31.55635	NaN
16	54.67826	54.67826	NaN	NaN	679.55258	NaN
17	108.15455	108.15455	NaN	NaN	287.07256	NaN
18	74.34181	74.34181	NaN	NaN	19.12151	NaN
19	79.00774	79.00774	NaN	NaN	78.76455	NaN
20	78.85937	78.85937	NaN	NaN	80.62518	NaN
21	107.56924	107.56924	NaN	NaN	199.97019	NaN
22	110.47377	110.47377	NaN	NaN	531.91747	NaN
23	95.16594	95.16594	NaN	NaN	465.76611	NaN

SI 5 Surface electrostatic potential of O5 protonated of drug



SI 6 Atom contribution to orbitals range of atom number=1

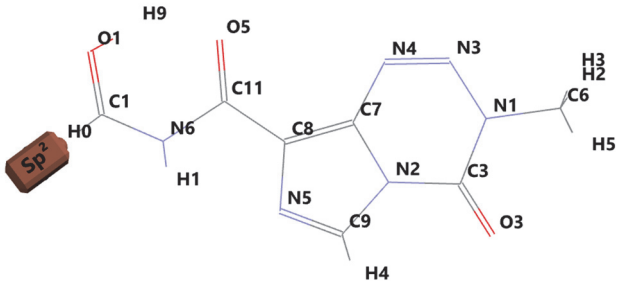
Orb#	Type	Ene(a.u.)	Occ	Composition	Population
55	Alpha&Beta	-0.4391	2.000	0.000%	0.000000
56	Alpha&Beta	-0.4276	2.000	8.120%	0.162402
57	**Alpha&Beta**	**-0.3288**	**2.000**	**0.016%**	**0.000320**
58	**Alpha&Beta**	**-0.2543**	**0.000**	**0.000%**	**0.000000**

SI 7 Atom contribution to orbitals range of atom number=14

Orb#	Type	Ene(a.u.)	Occ	Composition	Population
55	Alpha&Beta	-0.4391	2.000	0.000%	0.000002
56	Alpha&Beta	-0.4276	2.000	0.253%	0.005052
57	**Alpha&Beta**	**-0.3288**	**2.000**	**7.439%**	**0.148790**
58	**Alpha&Beta**	**-0.2543**	**0.000**	**0.279%**	**0.000000**

1.2 O1 protonated

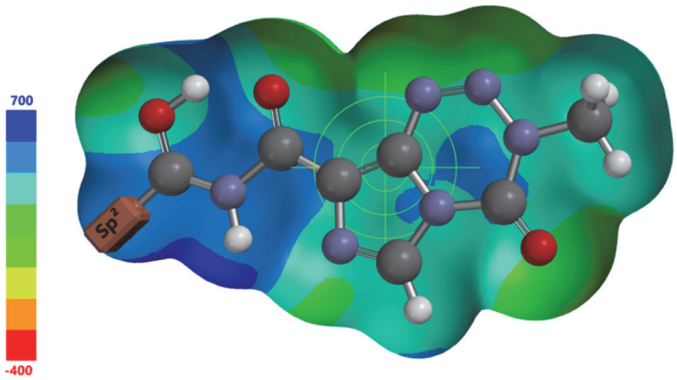
SI 8 Atomic electrostatic potential of O1 protonated of drug



Note: Average and variance below are in kcal/mol and (kcal/mol)^2 respectively

Atom#	All/Positive/Negative average			All/Positive/Negative variance		
1	**116.21537**	**116.21537**	**NaN**	**NaN**	**10.00241**	**NaN**
2	78.91692	78.91692	NaN	NaN	156.70630	NaN
3	95.35919	95.35919	NaN	NaN	42.81479	NaN
4	51.40486	51.40486	NaN	NaN	180.13677	NaN
5	92.48953	92.48953	NaN	NaN	39.82413	NaN
6	97.76756	97.76756	NaN	NaN	17.57570	NaN
8	59.88754	59.88754	NaN	NaN	272.82927	NaN
9	58.26808	58.26808	NaN	NaN	302.80737	NaN
10	94.12508	94.12508	NaN	NaN	37.48450	NaN
11	92.41629	92.41629	NaN	NaN	11.57841	NaN
12	88.53052	88.53052	NaN	NaN	28.23650	NaN
13	76.75605	76.75605	NaN	NaN	60.57858	NaN
14	**103.21447**	**103.21447**	**NaN**	**NaN**	**48.60241**	**NaN**
15	108.57426	108.57426	NaN	NaN	13.13817	NaN
16	64.48590	64.48590	NaN	NaN	249.01889	NaN
17	119.01710	119.01710	NaN	NaN	57.02219	NaN
18	74.94049	74.94049	NaN	NaN	31.67130	NaN
19	70.83133	70.83133	NaN	NaN	41.65938	NaN
20	74.97649	74.97649	NaN	NaN	31.45839	NaN
21	87.11877	87.11877	NaN	NaN	42.40569	NaN
22	113.40525	113.40525	NaN	NaN	327.92764	NaN
23	99.92938	99.92938	NaN	NaN	138.64404	NaN

SI 9 Surface electrostatic potential of O1 protonated of drug



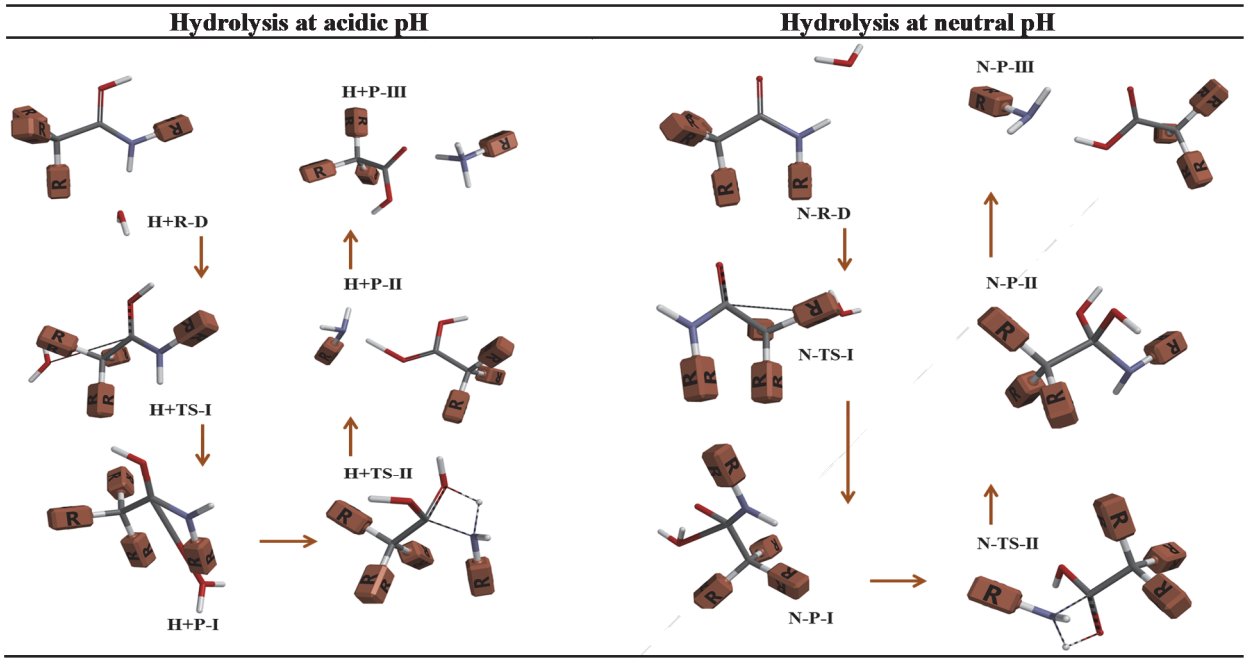
SI 10 Atom contribution to orbitals range of atom number=1

Orb#	Type	Ene(a.u.)	Occ	Composition	Population
55	Alpha&Beta	-0.4386	2.000	0.029%	0.000590
56	Alpha&Beta	-0.4190	2.000	0.001%	0.000012
57	**Alpha&Beta**	**-0.3091**	**2.000**	**0.198%**	**0.003956**
58	**Alpha&Beta**	**-0.2577**	**0.000**	**51.056%**	**0.000000**

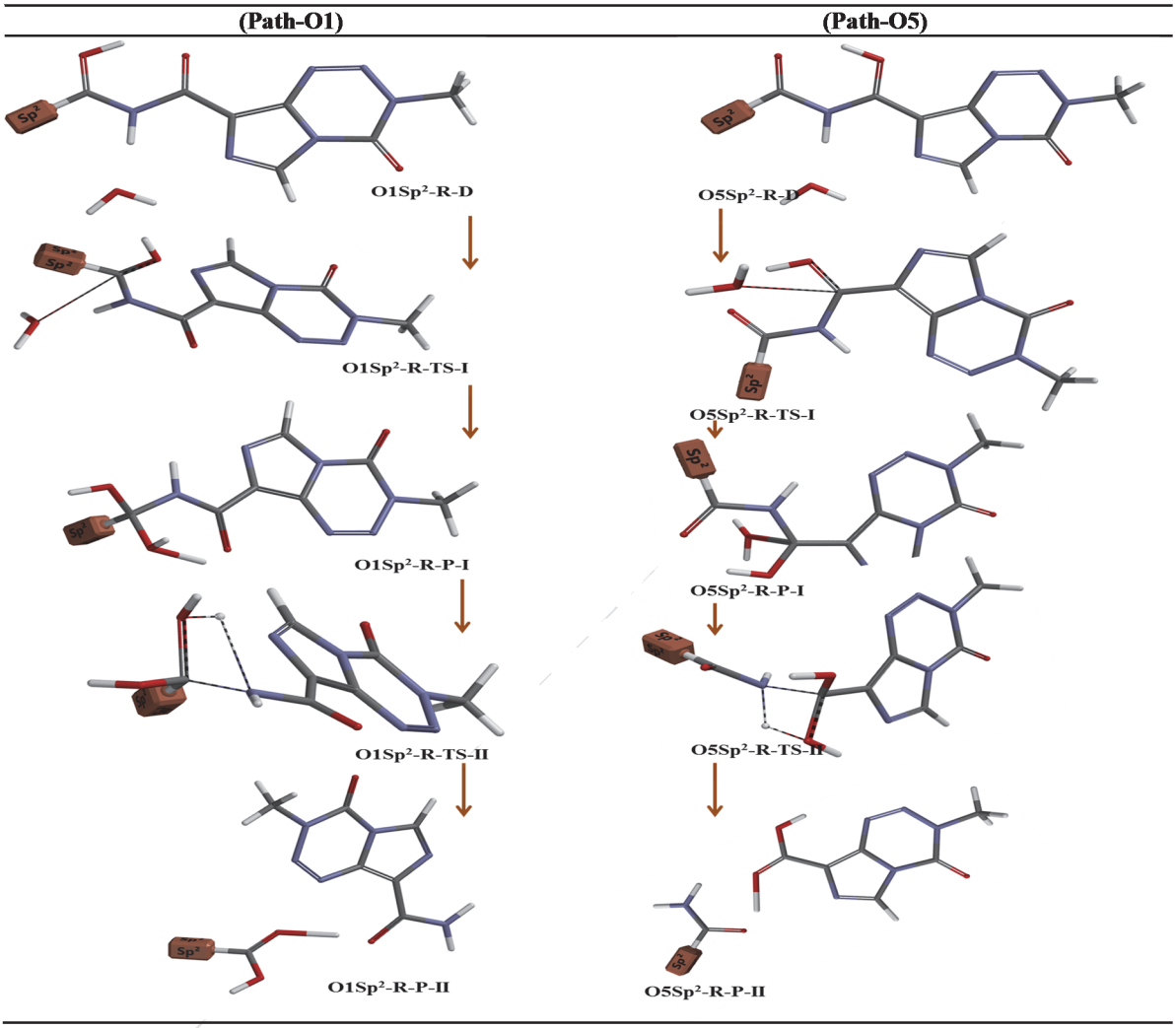
SI 11 Atom contribution to orbitals range of atom number=14

Orb#	Type	Ene(a.u.)	Occ	Composition	Population
55	Alpha&Beta	-0.4386	2.000	0.199%	0.003977
56	Alpha&Beta	-0.4190	2.000	0.010%	0.000202
57	**Alpha&Beta**	**-0.3091**	**2.000**	**9.894%**	**0.197885**
58	**Alpha&Beta**	**-0.2577**	**0.000**	**1.576%**	**0.000000**

SI 12 The input files of different pathways of Degradation mechanism of connected R-NH2 compounds to SR3-FG carbon layers at neutral and acidic conditions



SI 13 The input files of different pathways of Degradation mechanism of connected temozolomide to Sp^2-FG carbon layers at acidic conditions

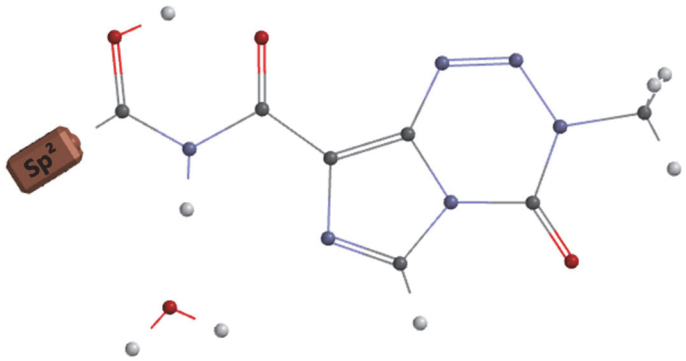


2. *Drug degradation mechanism*

2.1 The Cartesian Coordinates, Closed-Shell Molecular Orbital Coefficients Eigenvalues of the O1 protonated drug

SI 14 The Cartesian Coordinates, Closed-Shell Molecular Orbital Coefficients Eigenvalues of the O1 protonated drug

SI 15 O1Sp2-D-P(gas)



			Cartesian Coordinates (Angstroms)		
	Atom		X	Y	Z
1	C	C1	4.2165203	0.5912643	0.0000000
2	O	O1	4.3809990	1.8622948	0.0000000
3	C	C3	-2.8970316	-0.7332457	0.0000000
4	O	O3	-3.5896521	-1.7201144	0.0000000
5	N	N1	-3.3349034	0.5940164	0.0000000
6	N	N2	-1.4855086	-0.7746971	0.0000000
7	C	C6	-4.7818976	0.8842211	0.0000000
8	N	N3	-2.5466749	1.7067940	0.0000000
9	N	N4	-1.2747308	1.6148185	0.0000000

10	C	C7	-0.7155758	0.3711306	0.0000000
11	C	C8	0.6064504	-0.0887689	0.0000000
12	C	C9	-0.6359011	-1.8607257	0.0000000
13	N	N5	0.6154834	-1.4720571	0.0000000
14	C	C11	1.8080554	0.7124440	0.0000000
15	N	N6	3.0445712	-0.0186437	0.0000000
16	O	O5	1.8486558	1.9409247	0.0000000
17	H	H0	5.1196168	-0.0155337	0.0000000
18	H	H2	-5.0268613	1.4602164	0.8942488
19	H	H5	-5.3166710	-0.0639016	0.0000000
20	H	H3	-5.0268613	1.4602164	-0.8942488
21	H	H4	-1.0065019	-2.8763124	0.0000000
22	H	H1	3.0625763	-1.0610899	0.0000000
23	O	O2	3.3146189	-2.7578732	0.0000000
24	H	H6	3.9414637	-3.4983634	0.0000000
25	H	H8	2.4145836	-3.1229040	0.0000000
26	H	H9	3.4703025	2.3062830	0.0000000

Point Group = CS Order = 1 Nsymop = 2

Closed-Shell Molecular Orbital Coefficients

MO:	1	2	3	4	5
Eigenvalues:	-19.40574	-19.33497	-19.31953	-19.30211	-14.58968
(ev)	-528.05728	-526.13148	-525.71140	-525.23725	-397.00560

SI 16 O1Sp2-R-P (water)

Cartesian Coordinates (Angstroms)

	Atom		X	Y	Z
1	C	C1	4.1892374	0.6281420	0.0000000
2	O	O1	4.3548715	1.9076007	0.0000000
3	C	C3	-2.9086030	-0.7627866	0.0000000
4	O	O3	-3.5974041	-1.7680951	0.0000000
5	N	N1	-3.3718367	0.5465295	0.0000000
6	N	N2	-1.5059615	-0.7910713	0.0000000
7	C	C6	-4.8214030	0.8238436	0.0000000
8	N	N3	-2.5953082	1.6801863	0.0000000
9	N	N4	-1.3273366	1.6047562	0.0000000
10	C	C7	-0.7413183	0.3703165	0.0000000
11	C	C8	0.5794101	-0.0735922	0.0000000
12	C	C9	-0.6388634	-1.8636320	0.0000000
13	N	N5	0.6052218	-1.4504340	0.0000000
14	C	C11	1.7851059	0.7367652	0.0000000
15	N	N6	3.0083500	0.0197807	0.0000000
16	O	O5	1.7935913	1.9710688	0.0000000
17	H	H0	5.0936482	0.0187043	0.0000000
18	H	H2	-5.0761186	1.3974126	0.8933271
19	H	H5	-5.3520499	-0.1261311	0.0000000
20	H	H3	-5.0761186	1.3974126	-0.8933271
21	H	H4	-0.9831122	-2.8901955	0.0000000
22	H	H1	3.0392095	-1.0224555	0.0000000
23	O	O2	3.6086321	-2.7265780	0.0000000
24	H	H6	4.4126061	-3.2726292	0.0000000
25	H	H8	2.8607322	-3.3474065	0.0000000
26	H	H9	3.4503815	2.3507461	0.0000000

Point Group = CS Order = 1 Nsymop = 2

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Supplementary data – drug degradation mechanism

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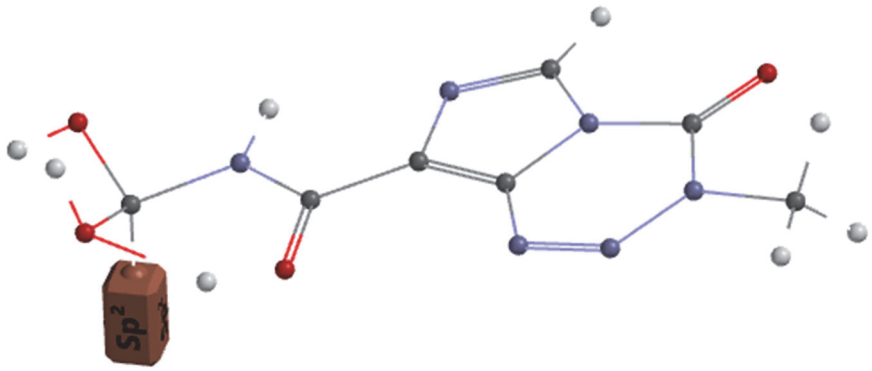
SI 17 O1Sp2-R-P-I (gas)



Cartesian Coordinates (Angstroms)

	Atom		X	Y	Z
1	C	C1	4.1954676	0.0014814	0.2943002
2	O	O1	4.9791080	0.9784480	-0.2777205
3	C	C3	-3.0973595	0.7046628	-0.0382191
4	O	O3	-3.8806864	1.6196286	-0.0705420
5	N	N1	-3.4322821	-0.6530402	-0.0354069
6	N	N2	-1.6960031	0.8616999	0.0025354
7	C	C6	-4.8609635	-1.0119772	-0.0747927
8	N	N3	-2.5667392	-1.7022816	-0.0012984
9	N	N4	-1.3053782	-1.5093942	0.0372113
10	C	C7	-0.8442646	-0.2270160	0.0397354
11	C	C8	0.4352824	0.3341667	0.0746955
12	C	C9	-0.9255927	2.0102157	0.0136481
13	N	N5	0.3466471	1.7111290	0.0575365
14	C	C11	1.7233566	-0.2978722	0.1137173
15	N	N6	2.8112107	0.4643786	0.0745083
16	O	O5	1.7753419	-1.6015838	0.1823714
17	H	H0	4.3748406	-0.1332713	1.3670159
18	H	H2	-4.9136815	-2.0992950	-0.0587182
19	H	H5	-5.3118161	-0.6150358	-0.9868891
20	H	H3	-5.3674134	-0.5866199	0.7944403
21	H	H4	-1.3632103	2.9984954	-0.0103478

Supplementary data – drug degradation mechanism

```
22 H   H1           2.6566841     1.4724397     0.0240254
23 O   O2           4.3678468    -1.2733803    -0.2801147
24 H   H6           2.7083268    -1.9195582     0.0768500
25 H   H8           4.5547694    -1.1682717    -1.2333270
26 H   H9           5.8708723     0.9768079     0.1108845

 Point Group = C1  Order =  1 Nsymop =  1

 Closed-Shell Molecular Orbital Coefficients
 MO:                    1          2          3          4          5
 Eigenvalues:     -19.38748  -19.35724  -19.34988  -19.30349  -14.59234
         (ev)    -527.56043 -526.73743 -526.53732 -525.27505 -397.07808
```

SI 18 O1Sp2-R-P-I water)

Cartesian Coordinates (Angstroms)

	Atom		X	Y	Z
1	C	C1	4.2024719	-0.0030002	0.2871368
2	O	O1	5.0123012	0.9404369	-0.3449280
3	C	C3	-3.1012071	0.6865336	-0.0371932
4	O	O3	-3.9047686	1.6015102	-0.0696261
5	N	N1	-3.4249140	-0.6634666	-0.0432480
6	N	N2	-1.7114458	0.8676056	0.0108967
7	C	C6	-4.8462074	-1.0505731	-0.0938903
8	N	N3	-2.5380409	-1.7102308	-0.0089915
9	N	N4	-1.2853390	-1.5003384	0.0364245
10	C	C7	-0.8308104	-0.2112468	0.0465970
11	C	C8	0.4325029	0.3708322	0.0843392
12	C	C9	-0.9599207	2.0236648	0.0261082
13	N	N5	0.3185676	1.7427962	0.0706101
14	C	C11	1.7342022	-0.2608772	0.1215423
15	N	N6	2.8202050	0.4877356	0.0756752
16	O	O5	1.7704084	-1.5710529	0.1960028
17	H	H0	4.3955087	-0.0873383	1.3610156
18	H	H2	-4.8782523	-2.1393213	-0.0881905
19	H	H5	-5.3039600	-0.6606127	-1.0053258
20	H	H3	-5.3701669	-0.6491079	0.7758123
21	H	H4	-1.4053484	3.0087187	0.0046115
22	H	H1	2.6916910	1.5017921	0.0288560
23	O	O2	4.3364816	-1.3073829	-0.2367329
24	H	H6	2.7172500	-1.8758914	0.0920683
25	H	H8	4.5057638	-1.2413250	-1.1992576
26	H	H9	5.8927162	0.9342834	0.0752741

Point Group = C1 Order = 1 Nsymop = 1

Incomplete wavefunction found in archive. 30339

DEBUG: 341 341 342 339

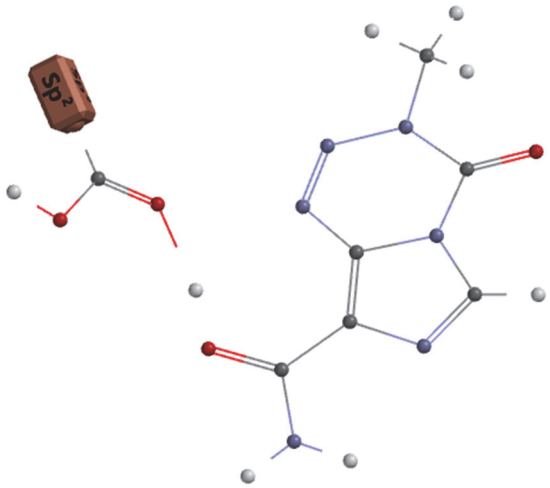
DEBUG: 1 -19.2445210310000 1.147838309600000E-005

1.147838309600000E-005

DEBUG: 2 0.000000000000000E+000 4.86120006530000

Supplementary data – drug degradation mechanism

SI 19 O1Sp2-R-P-II (gas)



Cartesian Coordinates (Angstroms)

	Atom		X	Y	Z
1	C	C1	-3.1910790	2.2784281	-0.6559046
2	O	O1	-2.5929068	1.2745673	-0.9936153
3	C	C3	2.7712854	0.1484588	-0.0990230
4	O	O3	3.9316839	-0.1161201	-0.2889190
5	N	N1	2.2668180	1.4230991	0.1767264
6	N	N2	1.7279833	-0.7988860	-0.1191376
7	C	C6	3.2227124	2.5413753	0.2473090
8	N	N3	0.9650709	1.7476216	0.4157373
9	N	N4	0.0564314	0.8541990	0.3785422
10	C	C7	0.4109740	-0.4320037	0.0974202
11	C	C8	-0.3083480	-1.6227648	0.0072381
12	C	C9	1.7605452	-2.1643559	-0.3159279
13	N	N5	0.5555628	-2.6702129	-0.2361746
14	C	C11	-1.7194419	-1.8939868	0.1962841
15	N	N6	-2.0908298	-3.1519297	0.3417307
16	O	O5	-2.6522177	-0.9984242	0.2629084
17	H	H0	-3.2838159	3.1509355	-1.3171489
18	H	H2	3.7479406	2.6325155	-0.7056769
19	H	H5	3.9474172	2.3540277	1.0428082
20	H	H3	2.6450214	3.4401278	0.4575558

Supplementary data – drug degradation mechanism

```
21 H   H4           2.6806352    -2.6985638    -0.5074223
22 H   H1          -1.3924073    -3.8884578     0.3139328
23 O   O2          -3.7674136     2.3741829     0.5381852
24 H   H6          -4.2098815     3.2333162     0.6632749
25 H   H9          -2.4626453    -0.0690075    -0.1039749
26 H   H8          -3.0725757    -3.3866850     0.4418322

 Point Group = C1  Order =  1 Nsymop =  1

 Closed-Shell Molecular Orbital Coefficients
 MO:                    1          2          3          4          5
 Eigenvalues:     -19.36219  -19.35999  -19.31228  -19.30140  -14.59201
         (ev)    -526.87224 -526.81238 -525.51408 -525.21791 -397.06899
```

SI 20 O1Sp2-R-P-II (water)

Cartesian Coordinates (Angstroms)

	Atom		X	Y	Z
1	C	C1	-2.9655052	2.3598248	-0.7973698
2	O	O1	-2.4117104	1.3005235	-1.0651437
3	C	C3	2.7271115	0.0738118	-0.1575881
4	O	O3	3.8722140	-0.2112151	-0.4606937
5	N	N1	2.3011386	1.3248461	0.2661229
6	N	N2	1.6612222	-0.8363685	-0.1889604
7	C	C6	3.2915919	2.4110111	0.3733349
8	N	N3	1.0237688	1.6648053	0.6387876
9	N	N4	0.0878971	0.8073799	0.5861741
10	C	C7	0.3678944	-0.4575624	0.1570081
11	C	C8	-0.3914619	-1.6140444	0.0164167
12	C	C9	1.6321088	-2.1771907	-0.5043879
13	N	N5	0.4176936	-2.6553269	-0.3808713
14	C	C11	-1.8042659	-1.8394818	0.2874191
15	N	N6	-2.2257300	-3.0609776	0.4877714
16	O	O5	-2.6911469	-0.8798611	0.3715855
17	H	H0	-2.9436314	3.2171916	-1.4855723
18	H	H2	3.7531934	2.5874602	-0.6002041
19	H	H5	4.0625548	2.1404161	1.0976993
20	H	H3	2.7538957	3.2986060	0.7061149
21	H	H4	2.5133533	-2.7229113	-0.8118249
22	H	H1	-1.5767227	-3.8465927	0.4670199
23	O	O2	-3.6305764	2.5277664	0.3480889
24	H	H6	-4.0127491	3.4310991	0.3973432
25	H	H9	-2.4503204	-0.0020469	-0.0707038
26	H	H8	-3.2165897	-3.2496495	0.6372639

Point Group = C1 Order = 1 Nsymop = 1

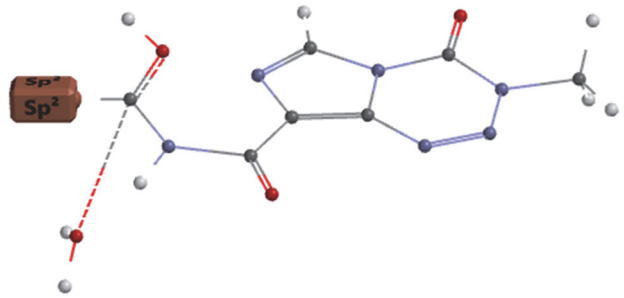
Incomplete wavefunction found in archive. 30339

DEBUG: 341 341 342 339

DEBUG: 1 -19.2321884640000 4.267067416400000E-006 4.267067416400000E-006

DEBUG: 2 0.000000000000000E+000 4.84322859900000

SI 21 O1Sp2-R-TS-I (gas)



Cartesian Coordinates (Angstroms)

	Atom		X	Y	Z
1	C	C1	-3.7397796	0.1431716	-1.0592971
2	O	O1	-3.2668214	0.7555101	-2.1155330
3	C	C3	2.8566362	-0.8328800	-0.1768314
4	O	O3	3.5010328	-1.8147958	-0.4546601
5	N	N1	3.3818248	0.4056769	0.1919876
6	N	N2	1.4478880	-0.7842281	-0.1823378
7	C	C6	4.8459408	0.5474888	0.2522508
8	N	N3	2.6724460	1.5296076	0.5105732
9	N	N4	1.3980413	1.5221753	0.4896167
10	C	C7	0.7576791	0.3694863	0.1429911
11	C	C8	-0.5913627	0.0211252	0.0169603
12	C	C9	0.5215163	-1.7628162	-0.4845694
13	N	N5	-0.6985666	-1.2996718	-0.3707407
14	C	C11	-1.7489255	0.8566937	0.2393546
15	N	N6	-3.0551945	0.1095187	0.0300764
16	O	O5	-1.8165317	2.0041205	0.5822077
17	H	H0	-4.7138081	-0.3441568	-1.0956733
18	H	H2	5.2748137	0.3277883	-0.7280607
19	H	H5	5.2513779	-0.1505605	0.9884343
20	H	H3	5.0522120	1.5768343	0.5423420
21	H	H4	0.8163622	-2.7623047	-0.7715657
22	H	H1	-3.4756426	-0.3964203	0.8381852
23	O	O2	-4.4808932	-1.2492936	1.9716664

Supplementary data – drug degradation mechanism

```
24 H   H6          -4.3227713    -2.1662399     2.2499960
25 H   H8          -4.9359493    -0.8159391     2.7124521
26 H   H9          -3.8761873     0.7315014    -2.8749399

 Point Group = C1  Order =  1 Nsymop =  1

 Closed-Shell Molecular Orbital Coefficients
 MO:                    1          2          3          4          5
 Eigenvalues:      -19.41009  -19.33340  -19.31608  -19.29013  -14.57707
         (ev)     -528.17569 -526.08882 -525.61739 -524.91140 -396.66234
```

SI 22 O1Sp2-R-TS-I (water)

Cartesian Coordinates (Angstroms)

	Atom		X	Y	Z
1	C	C1	-3.7335709	0.2101107	-1.0720590
2	O	O1	-3.2408731	0.8622620	-2.0902181
3	C	C3	2.8339084	-0.8161574	-0.2076164
4	O	O3	3.4932259	-1.7906997	-0.5233674
5	N	N1	3.3543179	0.4067100	0.1938940
6	N	N2	1.4318921	-0.7875244	-0.2043415
7	C	C6	4.8186079	0.5695808	0.2453190
8	N	N3	2.6311854	1.5169424	0.5559794
9	N	N4	1.3596107	1.4955741	0.5422586
10	C	C7	0.7213113	0.3507601	0.1608186
11	C	C8	-0.6209484	-0.0056511	0.0238110
12	C	C9	0.5138798	-1.7622954	-0.5391671
13	N	N5	-0.7097911	-1.3113199	-0.4078644
14	C	C11	-1.7853757	0.8296165	0.2724654
15	N	N6	-3.0761724	0.1605375	0.0504677
16	O	O5	-1.7679153	1.9817083	0.6584502
17	H	H0	-4.6998607	-0.2997651	-1.1457158
18	H	H2	5.2444479	0.3927285	-0.7450465
19	H	H5	5.2461862	-0.1416449	0.9558913
20	H	H3	5.0130486	1.5924207	0.5668116
21	H	H4	0.8089591	-2.7525018	-0.8623258
22	H	H1	-3.5003507	-0.4076961	0.8283926
23	O	O2	-4.3722161	-1.3768739	1.9426014
24	H	H6	-3.9864672	-2.2452586	2.1565784
25	H	H8	-4.6092151	-0.9844908	2.8011148
26	H	H9	-3.8386931	0.8128104	-2.8696163

Point Group = C1 Order = 1 Nsymop = 1

Incomplete wavefunction found in archive. 30339

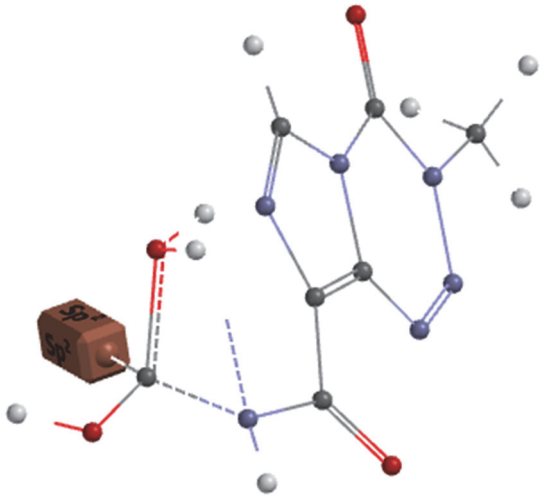
DEBUG: 341 341 342 339

DEBUG: 1 -19.2527984890000 -3.241690062800000E-005 -3.241690062800000E-005

Supplementary data – drug degradation mechanism

```
DEBUG: 2  0.000000000000000E+000   4.85983604150000
```

SI 23 O1Sp2-R-TS-II (gas)



Cartesian Coordinates (Angstroms)

	Atom		X	Y	Z
1	C	C1	3.5157289	-0.2244637	-0.5840006
2	O	O1	4.8351014	-0.1247245	-0.7731415
3	C	C3	-2.7400447	-0.9122763	-0.0101065
4	O	O3	-3.2843711	-1.9878430	0.0287257
5	N	N1	-3.3566724	0.3191594	-0.1755039
6	N	N2	-1.3362520	-0.7447086	0.1109191
7	C	C6	-4.8221937	0.3505056	-0.3233719
8	N	N3	-2.7372719	1.5446592	-0.2413645
9	N	N4	-1.4766261	1.6447337	-0.1282047
10	C	C7	-0.7393177	0.5089525	0.0580111
11	C	C8	0.6239501	0.2755573	0.2029214
12	C	C9	-0.3649389	-1.6828361	0.2844076
13	N	N5	0.8142833	-1.0900481	0.3397231
14	C	C11	1.6994188	1.2850482	0.3156079
15	N	N6	3.0397112	0.8509107	0.1336253
16	O	O5	1.4896081	2.4381724	0.6169386
17	H	H0	2.9066833	-0.5686666	-1.4198960
18	H	H2	-5.2862653	-0.1194366	0.5460887

```
19 H   H5          -5.1114946    -0.1907590    -1.2270632
20 H   H3          -5.1092338     1.3985657    -0.3943690
21 H   H4          -0.5676278    -2.7411987     0.3668645
22 H   H1           3.7321689     1.5444021     0.4126271
23 O   O2           3.2877932    -1.6548625     0.3216565
24 H   H6           3.7540966    -1.5816366     1.1793310
25 H   H8           2.2284900    -1.6130013     0.4721541
26 H   H9           5.1623070    -0.7700778    -1.4243460

 Point Group = C1  Order =  1 Nsymop =  1

 Closed-Shell Molecular Orbital Coefficients
 MO:                    1          2          3          4          5
 Eigenvalues:     -19.39024  -19.38533  -19.30636  -19.29858  -14.59758
         (ev)    -527.63542 -527.50186 -525.35309 -525.14138 -397.22049
```

SI 24 O1Sp2-R-TS-II (gas)

Cartesian Coordinates (Angstroms)

	Atom		X	Y	Z
1	C	C1	3.4481699	-0.1909381	-0.6542204
2	O	O1	4.7155788	-0.0059525	-1.0290450
3	C	C3	-2.7453998	-0.9028880	-0.0136058
4	O	O3	-3.3205526	-1.9767079	0.0303323
5	N	N1	-3.3506948	0.3235493	-0.2219298
6	N	N2	-1.3575075	-0.7574324	0.1467892
7	C	C6	-4.8100696	0.3696722	-0.4163770
8	N	N3	-2.7135641	1.5480304	-0.2976587
9	N	N4	-1.4577175	1.6295501	-0.1470259
10	C	C7	-0.7372174	0.4915751	0.0876611
11	C	C8	0.6151835	0.2388141	0.2741339
12	C	C9	-0.3852547	-1.6987332	0.3613069
13	N	N5	0.7945909	-1.1171573	0.4402627
14	C	C11	1.6927742	1.2429398	0.4129551
15	N	N6	3.0007095	0.8718805	0.1075206
16	O	O5	1.4619385	2.3751405	0.8362838
17	H	H0	2.7483049	-0.6322669	-1.3639246
18	H	H2	-5.3143417	-0.0407276	0.4613164
19	H	H5	-5.0871784	-0.2125889	-1.2985213
20	H	H3	-5.0795077	1.4166294	-0.5532377
21	H	H4	-0.5916792	-2.7582324	0.4563772
22	H	H1	3.7163049	1.5500584	0.3735779
23	O	O2	3.5250940	-1.6580260	0.3306327
24	H	H6	4.0990947	-1.5241155	1.1184218
25	H	H8	2.5858660	-1.7884940	0.6413414
26	H	H9	4.9868346	-0.6774902	-1.6878105

Point Group = C1 Order = 1 Nsymop = 1

Incomplete wavefunction found in archive. 30339

DEBUG: 341 341 342 339

DEBUG: 1 -19.2386550590000 2.291992267500000E-005

2.291992267500000E-005

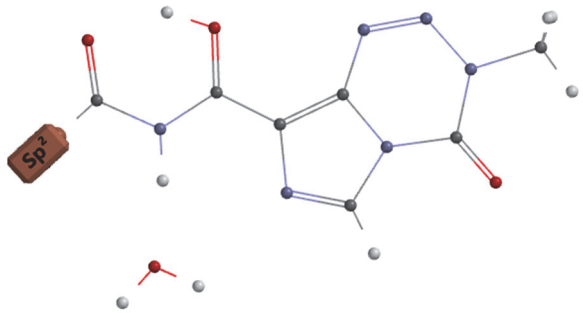
Supplementary data – drug degradation mechanism

```
DEBUG: 2  0.000000000000000E+000   4.83825449270000
```

2.2 *The Cartesian Coordinates, Closed-Shell Molecular Orbital Coefficients Eigenvalues of the O5 protonated drug*

SI 25 The Cartesian Coordinates, Closed-Shell Molecular Orbital Coefficients Eigenvalues of the O5 protonated drug

SI 26 O5Sp2-R-D (gas)



Cartesian Coordinates (Angstroms)

	Atom		X	Y	Z
1	C	C1	4.2433251	0.7125829	0.0000000
2	O	O1	4.3038257	1.9302367	0.0000000
3	C	C3	-2.8896776	-0.7425452	0.0000000
4	O	O3	-3.5915613	-1.7213526	0.0000000
5	N	N1	-3.3173611	0.5917669	0.0000000
6	N	N2	-1.4784776	-0.7947057	0.0000000
7	C	C6	-4.7639071	0.8910210	0.0000000
8	N	N3	-2.5224276	1.6925442	0.0000000
9	N	N4	-1.2488226	1.5909988	0.0000000
10	C	C7	-0.7020616	0.3435308	0.0000000
11	C	C8	0.6190507	-0.1297372	0.0000000
12	C	C9	-0.6336054	-1.8903347	0.0000000
13	N	N5	0.6178412	-1.5135541	0.0000000
14	C	C11	1.8280464	0.6336317	0.0000000
15	N	N6	3.0308787	0.0149958	0.0000000
16	O	O5	1.7407457	1.9271802	0.0000000
17	H	H0	5.1244411	0.0599682	0.0000000
18	H	H2	-5.0044270	1.4682530	0.8945652

19	H	H5	-5.3034077	-0.0543523	0.0000000
20	H	H3	-5.0044270	1.4682530	-0.8945652
21	H	H4	-1.0127761	-2.9029880	0.0000000
22	H	H1	3.0809092	-1.0242958	0.0000000
23	H	H7	2.6610042	2.3309038	0.0000000
24	O	O2	3.4188883	-2.7280696	0.0000000
25	H	H6	4.1307872	-3.3871988	0.0000000
26	H	H8	2.5742690	-3.2057166	0.0000000

Point Group = CS Order = 1 Nsymop = 2

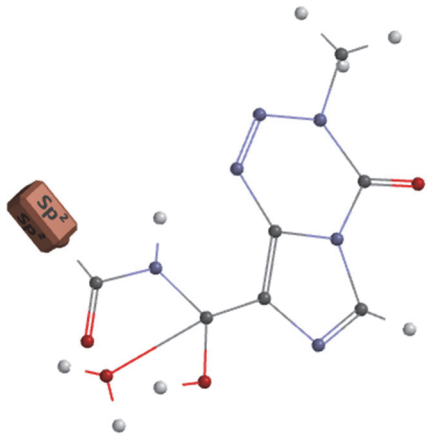
Closed-Shell Molecular Orbital Coefficients

MO:	1	2	3	4	5
Eigenvalues:	-19.39056	-19.33870	-19.31769	-19.31170	-14.60074
(ev)	-527.64418	-526.23309	-525.66139	-525.49838	-397.30639

SI 27 O5Sp2-R-D (water)

C	-0.90491	0.00000	-4.21239
O	-2.13394	0.00000	-4.26840
C	0.58577	0.00000	2.90303
O	1.57880	0.00000	3.60627
N	-0.73392	0.00000	3.34831
N	0.63173	0.00000	1.50036
C	-1.02872	0.00000	4.79539
N	-1.84967	0.00000	2.55941
N	-1.75950	0.00000	1.28988
C	-0.51654	0.00000	0.72466
C	-0.05171	0.00000	-0.59313
C	1.71995	0.00000	0.64485
N	1.32745	0.00000	-0.60229
C	-0.81965	0.00000	-1.80519
N	-0.20476	0.00000	-3.00455
O	-2.11888	0.00000	-1.71358
H	-0.26112	0.00000	-5.09947
H	-1.60506	0.89338	5.04154
H	-0.08513	0.00000	5.33647
H	-1.60506	-0.89338	5.04154
H	2.74084	0.00000	1.00577
H	0.83657	0.00000	-3.06858
H	-2.50940	0.00000	-2.64452
O	2.53397	0.00000	-3.58325
H	3.09195	0.00000	-4.37879
H	3.14093	0.00000	-2.82334

SI 28 O5Sp2-R-P-I (gas)



Cartesian Coordinates (Angstroms)

	Atom		X	Y	Z
1	C	C1	3.4894243	-1.5769800	0.4166819
2	O	O1	4.4852114	-0.8915841	0.5520781
3	C	C3	-2.9100607	0.4735212	0.0062726
4	O	O3	-3.8691358	1.1971885	-0.0366746
5	N	N1	-2.9609191	-0.9346956	-0.0839457
6	N	N2	-1.5798650	0.9075468	0.1527763
7	C	C6	-4.2885210	-1.5594621	-0.2394577
8	N	N3	-1.9162755	-1.7859340	-0.0443809
9	N	N4	-0.7237594	-1.3355952	0.0897520
10	C	C7	-0.5405122	0.0081033	0.1901938
11	C	C8	0.6115465	0.7850652	0.3410897
12	C	C9	-1.0287627	2.1797864	0.2791321
13	N	N5	0.2708645	2.1191513	0.3915752
14	C	C11	1.9567840	0.3080342	0.4259233
15	N	N6	2.2023182	-1.0287507	0.3796862
16	O	O5	2.9151575	1.1561818	0.5786657
17	H	H0	3.5072559	-2.6697770	0.3203844
18	H	H2	-4.1294121	-2.6352635	-0.2928975
19	H	H5	-4.7580738	-1.1894680	-1.1533702
20	H	H3	-4.9130064	-1.3014455	0.6186255
21	H	H4	-1.6413569	3.0709334	0.2806488
22	H	H1	1.3968319	-1.6489227	0.2509613

Supplementary data – drug degradation mechanism

```
23 H   H7           3.7955553     0.6747931     0.5945769
24 O   O2           2.7333344     0.4290401    -2.3042734
25 H   H6           3.0077999     1.3353516    -2.5197506
26 H   H8           2.8319309    -0.0632802    -3.1347992

 Point Group = C1  Order =  1 Nsymop =  1

 Closed-Shell Molecular Orbital Coefficients
 MO:                   1          2          3          4          5
 Eigenvalues:     -19.39191  -19.33967  -19.31877  -19.29858  -14.61356
         (ev)    -527.68099 -526.25932 -525.69059 -525.14127 -397.65536
```

SI 29 O5Sp2-R-P-I (water)

Cartesian Coordinates (Angstroms)

	Atom		X	Y	Z
1	C	C1	3.9930683	-1.4390812	0.0472942
2	O	O1	4.9648924	-0.6977002	-0.0751224
3	C	C3	-2.5028392	0.5146127	0.4845417
4	O	O3	-3.4616766	1.2609081	0.5216062
5	N	N1	-2.5737516	-0.8774641	0.5842875
6	N	N2	-1.1772800	0.9405228	0.3509421
7	C	C6	-3.9014285	-1.5005456	0.7401026
8	N	N3	-1.5320176	-1.7411795	0.5310448
9	N	N4	-0.3392485	-1.3053134	0.3960527
10	C	C7	-0.1330152	0.0371309	0.3066375
11	C	C8	1.0177031	0.8181778	0.1701118
12	C	C9	-0.6281922	2.2100924	0.2376709
13	N	N5	0.6716873	2.1559290	0.1302535
14	C	C11	2.3768302	0.3707155	0.0812051
15	N	N6	2.6850798	-0.9474944	0.1276956
16	O	O5	3.3128056	1.2642955	-0.0437245
17	H	H0	4.0621665	-2.5324663	0.1038614
18	H	H2	-3.7402997	-2.5742041	0.8240951
19	H	H5	-4.5176584	-1.2730185	-0.1308330
20	H	H3	-4.3824086	-1.1140882	1.6400802
21	H	H4	-1.2392135	3.1006473	0.2447039
22	H	H1	1.9213084	-1.6305526	0.2281522
23	H	H7	4.2053476	0.7961563	-0.0930348
24	O	O2	-2.0418769	-0.3085760	-3.2084697
25	H	H6	-2.2602296	0.4326422	-3.8024074
26	H	H8	-1.7162139	-0.9981537	-3.8162507

Point Group = C1 Order = 1 Nsymop = 1

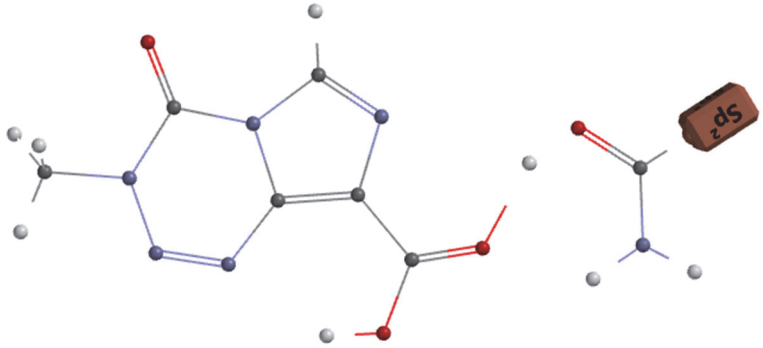
Incomplete wavefunction found in archive. 30338

DEBUG: 341 341 342 338

DEBUG: 1 -19.2559151410000 1.778720358600000E-005 1.778720358600000E-005

DEBUG: 2 0.000000000000000E+000 0.000000000000000E+000

SI 30 O5Sp2-R-P-II (gas)



Cartesian Coordinates (Angstroms)

	Atom		X	Y	Z
1	C	C1	5.2140308	0.8867682	0.0000000
2	O	O1	4.0531203	1.4285779	0.0000000
3	C	C3	-2.9527794	0.9675769	0.0000000
4	O	O3	-3.5565097	2.0100649	0.0000000
5	N	N1	-3.5485957	-0.3055854	0.0000000
6	N	N2	-1.5498069	0.8555414	0.0000000
7	C	C6	-5.0210645	-0.3697509	0.0000000
8	N	N3	-2.9145993	-1.5084771	0.0000000
9	N	N4	-1.6393656	-1.5524809	0.0000000
10	C	C7	-0.9413081	-0.3832273	0.0000000
11	C	C8	0.4219736	-0.1291638	0.0000000
12	C	C9	-0.5415410	1.8025551	0.0000000
13	N	N5	0.6395599	1.2285751	0.0000000
14	C	C11	1.5038500	-1.1089892	0.0000000
15	N	N6	5.4462084	-0.4015287	0.0000000
16	O	O5	2.6954262	-0.7738779	0.0000000
17	H	H0	6.0556490	1.5763664	0.0000000
18	H	H2	-5.2926715	-1.4241985	0.0000000
19	H	H5	-5.4081167	0.1300206	-0.8903165
20	H	H3	-5.4081167	0.1300206	0.8903165
21	H	H4	-0.7489310	2.8633581	0.0000000
22	H	H1	6.3990486	-0.7494414	0.0000000
23	H	H7	3.2961204	0.7450025	0.0000000

Supplementary data – drug degradation mechanism

```
24 O  O2          1.1933752    -2.3965256     0.0000000
25 H  H6          0.2208246    -2.5534521     0.0000000
26 H  H8          4.6701248    -1.0705165     0.0000000

 Point Group = CS  Order =  1 Nsymop =  2

 Closed-Shell Molecular Orbital Coefficients
 MO:                   1          2          3          4          5
 Eigenvalues:     -19.38152  -19.35189  -19.31288  -19.29808  -14.58965
         (ev)    -527.39824 -526.59197 -525.53056 -525.12763 -397.00482
```

SI 31 O5Sp2-R-P-II (water)

Cartesian Coordinates (Angstroms)

	Atom		X	Y	Z
1	C	C1	5.4554266	0.8686926	0.0000000
2	O	O1	4.2635106	1.3980104	0.0000000
3	C	C3	-3.0124586	0.9682939	0.0000000
4	O	O3	-3.6144432	2.0257002	0.0000000
5	N	N1	-3.6164210	-0.2895210	0.0000000
6	N	N2	-1.6165575	0.8571177	0.0000000
7	C	C6	-5.0904085	-0.3574636	0.0000000
8	N	N3	-2.9810846	-1.5005949	0.0000000
9	N	N4	-1.7088567	-1.5478486	0.0000000
10	C	C7	-0.9988758	-0.3852555	0.0000000
11	C	C8	0.3632448	-0.1262472	0.0000000
12	C	C9	-0.6118496	1.8044872	0.0000000
13	N	N5	0.5711401	1.2326599	0.0000000
14	C	C11	1.4628892	-1.0995751	0.0000000
15	N	N6	5.7210067	-0.4016338	0.0000000
16	O	O5	2.6452065	-0.7783428	0.0000000
17	H	H0	6.2734596	1.5843793	0.0000000
18	H	H2	-5.3600413	-1.4133567	0.0000000
19	H	H5	-5.4823816	0.1366563	-0.8916877
20	H	H3	-5.4823816	0.1366563	0.8916877
21	H	H4	-0.8161059	2.8672246	0.0000000
22	H	H1	6.6943620	-0.7041779	0.0000000
23	H	H7	3.5294331	0.7195188	0.0000000
24	O	O2	1.1416482	-2.4123705	0.0000000
25	H	H6	0.1678428	-2.5608530	0.0000000
26	H	H8	4.9960382	-1.1188752	0.0000000

Point Group = CS Order = 1 Nsymop = 2

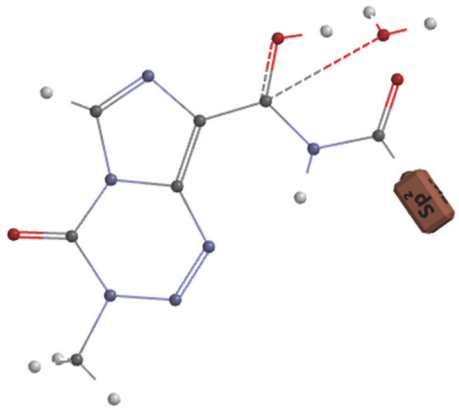
Incomplete wavefunction found in archive. 30339

DEBUG: 341 341 342 339

DEBUG: 1 -19.2285514210000 -2.122158338400000E-005 -2.122158338400000E-005

DEBUG: 2 0.000000000000000E+000 4.93567476630000

SI 32 O5Sp2-R-TS-I (gas)



Cartesian Coordinates (Angstroms)

	Atom		X	Y	Z
1	C	C1	3.3443514	-1.5962353	0.5012911
2	O	O1	4.3383551	-0.9377904	0.7238506
3	C	C3	-3.0319563	0.4885498	-0.0751752
4	O	O3	-3.9900593	1.2128258	-0.1247906
5	N	N1	-3.0830257	-0.9199449	-0.1632946
6	N	N2	-1.7018434	0.9218456	0.0781347
7	C	C6	-4.4102559	-1.5447786	-0.3258396
8	N	N3	-2.0399831	-1.7719660	-0.1135883
9	N	N4	-0.8479126	-1.3226733	0.0293064
10	C	C7	-0.6641942	0.0211628	0.1276422
11	C	C8	0.4887527	0.7976266	0.2826366
12	C	C9	-1.1500468	2.1942124	0.2017778
13	N	N5	0.1486577	2.1325553	0.3228897
14	C	C11	1.8351645	0.3190886	0.3882806
15	N	N6	2.0757597	-1.0171427	0.3317267
16	O	O5	2.7844724	1.1720819	0.5505797
17	H	H0	3.3340563	-2.6910868	0.4217251
18	H	H2	-4.2499437	-2.6200778	-0.3844910
19	H	H5	-4.8767962	-1.1704681	-1.2394318
20	H	H3	-5.0371077	-1.2914755	0.5319720
21	H	H4	-1.7616144	3.0860066	0.1929416
22	H	H1	1.2681523	-1.6296125	0.1808045

Supplementary data – drug degradation mechanism

```
23 H   H7           3.6734701     0.7177505     0.5293065
24 O   O2           4.1458326     0.3491445    -1.8605739
25 H   H6           5.0442771    -0.0031692    -1.9674985
26 H   H8           4.0442378     0.9955625    -2.5777569

 Point Group = C1  Order =  1 Nsymop =  1

 Closed-Shell Molecular Orbital Coefficients
 MO:                   1          2          3          4          5
 Eigenvalues:     -19.39176  -19.33567  -19.31955  -19.29183  -14.61439
         (ev)    -527.67695 -526.15048 -525.71204 -524.95751 -397.67805
```

SI 33 O5Sp2-R-TS-I (water)

Cartesian Coordinates (Angstroms)

	Atom		X	Y	Z
1	C	C1	3.5140763	-0.8688678	1.0802912
2	O	O1	4.4286548	-0.0524516	1.0159223
3	C	C3	-3.0371467	0.3270744	-0.2523932
4	O	O3	-4.0346641	0.9376325	-0.5825323
5	N	N1	-3.0176043	-1.0157266	0.1392671
6	N	N2	-1.7503886	0.8781153	-0.2135040
7	C	C6	-4.2947246	-1.7550030	0.1627890
8	N	N3	-1.9277908	-1.7311914	0.5133553
9	N	N4	-0.7741692	-1.1836009	0.5314064
10	C	C7	-0.6585950	0.1238019	0.1718268
11	C	C8	0.4312826	0.9938114	0.0922461
12	C	C9	-1.2864377	2.1531708	-0.5060816
13	N	N5	0.0051750	2.2383578	-0.3292459
14	C	C11	1.8049653	0.7063475	0.3918438
15	N	N6	2.1881356	-0.5270176	0.7944152
16	O	O5	2.6754826	1.6635721	0.2706677
17	H	H0	3.6504752	-1.9171800	1.3692106
18	H	H2	-4.0685232	-2.7687725	0.4893110
19	H	H5	-4.7321845	-1.7628716	-0.8368651
20	H	H3	-4.9833688	-1.2724755	0.8581863
21	H	H4	-1.9471416	2.9423389	-0.8344640
22	H	H1	1.4747138	-1.2643254	0.8737588
23	H	H7	3.5873886	1.3035584	0.5108562
24	O	O2	4.0054973	-1.6688471	-2.3921356
25	H	H6	4.9192074	-1.3685605	-2.5435076
26	H	H8	3.5956436	-1.6255274	-3.2748546

Point Group = C1 Order = 1 Nsymop = 1

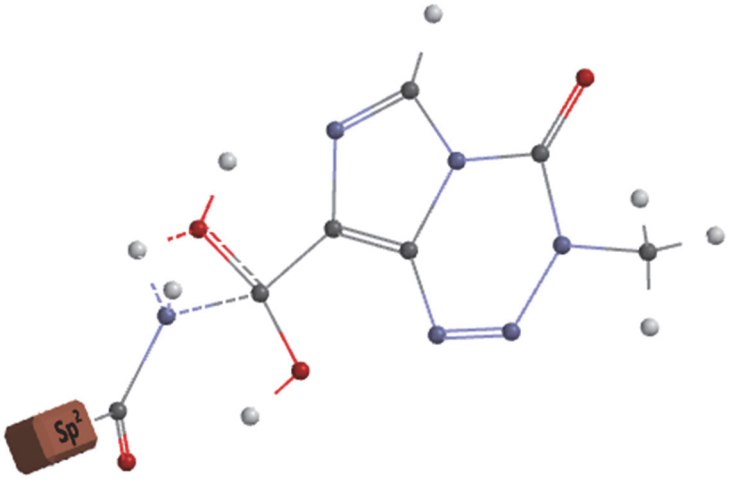
Incomplete wavefunction found in archive. 30338

DEBUG: 341 341 342 338

DEBUG: 1 -19.2559441900000 2.037866303600000E-005 2.037866303600000E-005

DEBUG: 2 0.000000000000000E+000 0.000000000000000E+000

SI 34 O5Sp2-R-TS-II (gas)



Cartesian Coordinates (Angstroms)

	Atom		X	Y	Z
1	C	C1	-3.7712293	-1.2303802	0.8981319
2	O	O1	-4.3648173	-1.4373225	-0.1275553
3	C	C3	2.9151391	0.4525702	0.1042059
4	O	O3	3.8412050	1.2162618	0.2152540
5	N	N1	3.0109453	-0.9347486	-0.0013515
6	N	N2	1.5602677	0.8579226	0.0669370
7	C	C6	4.3560878	-1.5371690	0.0046398
8	N	N3	1.9750471	-1.8237858	-0.1068489
9	N	N4	0.7719558	-1.4131394	-0.1485229
10	C	C7	0.5349442	-0.0687686	-0.0814355
11	C	C8	-0.6205692	0.6927507	-0.0964090
12	C	C9	1.0026995	2.1080395	0.1341448
13	N	N5	-0.3102473	2.0217711	0.0421820
14	C	C11	-2.0441794	0.3187635	-0.3189120
15	N	N6	-2.7632945	-0.1973542	0.9858829
16	O	O5	-2.2280123	-0.4197947	-1.4080274
17	H	H0	-3.9502289	-1.7561140	1.8472129
18	H	H2	4.9115075	-1.2011529	-0.8743391
19	H	H5	4.2193230	-2.6175965	-0.0188486
20	H	H3	4.8886466	-1.2325975	0.9082090

Supplementary data – drug degradation mechanism

```
21 H   H4           1.5891983     3.0092170     0.2437630
22 H   H1          -2.1277015    -0.3103711     1.7797999
23 H   H7          -3.1551631    -0.7420281    -1.4742069
24 O   O2          -2.8599656     1.5772697    -0.2722257
25 H   H6          -2.2286993     2.3472000    -0.2135306
26 H   H8          -3.2042369     1.0226333     0.8082298

 Point Group = C1  Order =  1 Nsymop =  1

 Closed-Shell Molecular Orbital Coefficients
 MO:                    1          2          3          4          5
 Eigenvalues:     -19.40167  -19.36767  -19.35788  -19.30419  -14.60143
         (ev)    -527.94657 -527.02142 -526.75497 -525.29399 -397.32534
```

SI 35 O5Sp2-R-TS-II (water)

Cartesian Coordinates (Angstroms)

	Atom		X	Y	Z
1	C	C1	-3.6990444	-1.2802149	0.8717300
2	O	O1	-4.2696326	-1.5404147	-0.1711490
3	C	C3	2.9022847	0.4328999	0.0884976
4	O	O3	3.8558344	1.1861213	0.1978066
5	N	N1	2.9823335	-0.9455330	-0.0132381
6	N	N2	1.5693859	0.8667708	0.0464640
7	C	C6	4.3101170	-1.5811443	0.0235856
8	N	N3	1.9220179	-1.8255039	-0.1154595
9	N	N4	0.7323123	-1.3888469	-0.1535363
10	C	C7	0.5118792	-0.0413351	-0.0819846
11	C	C8	-0.6256595	0.7444185	-0.0888962
12	C	C9	1.0322092	2.1245303	0.1214783
13	N	N5	-0.2817309	2.0630984	0.0374316
14	C	C11	-2.0649095	0.3730351	-0.2741160
15	N	N6	-2.7170496	-0.2381774	0.9697721
16	O	O5	-2.2503151	-0.3241546	-1.4374414
17	H	H0	-3.9041283	-1.7710224	1.8336322
18	H	H2	4.9126436	-1.2345306	-0.8177895
19	H	H5	4.1491727	-2.6561221	-0.0442366
20	H	H3	4.8164933	-1.3307490	0.9579239
21	H	H4	1.6293783	3.0181063	0.2308236
22	H	H1	-2.0854613	-0.3533956	1.7806120
23	H	H7	-3.1422495	-0.7389581	-1.4144392
24	O	O2	-2.8963753	1.5951863	-0.1797025
25	H	H6	-2.3122654	2.3918559	-0.0645427
26	H	H8	-3.2318189	0.9851154	0.9001018

Point Group = C1 Order = 1 Nsymop = 1

Incomplete wavefunction found in archive. 30339

DEBUG: 341 341 342 339

DEBUG: 1 -19.2510413760000 6.695441548500000E-007 6.695441548500000E-007

DEBUG: 2 0.000000000000000E+000 4.83671845200000

Supplementary data – drug degradation mechanism