

## Supporting Information

### Computational Determination of the Mechanism of Pd-Catalyzed Formation of Isatoic Anhydrides from *o*-Haloanilines, CO, and CO<sub>2</sub>

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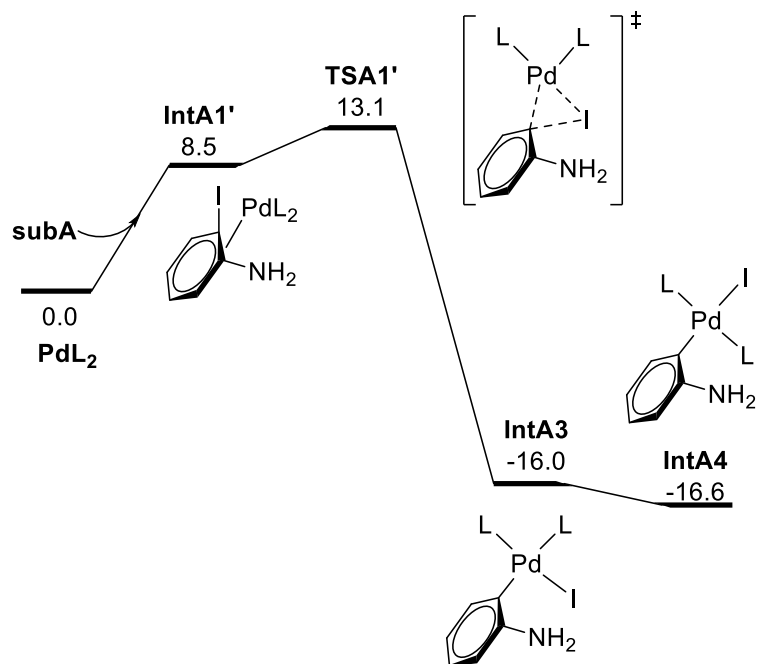
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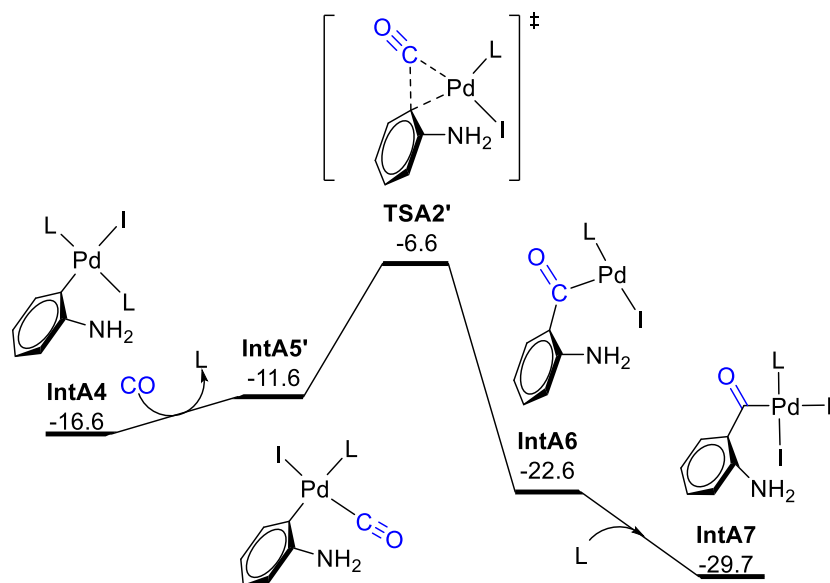
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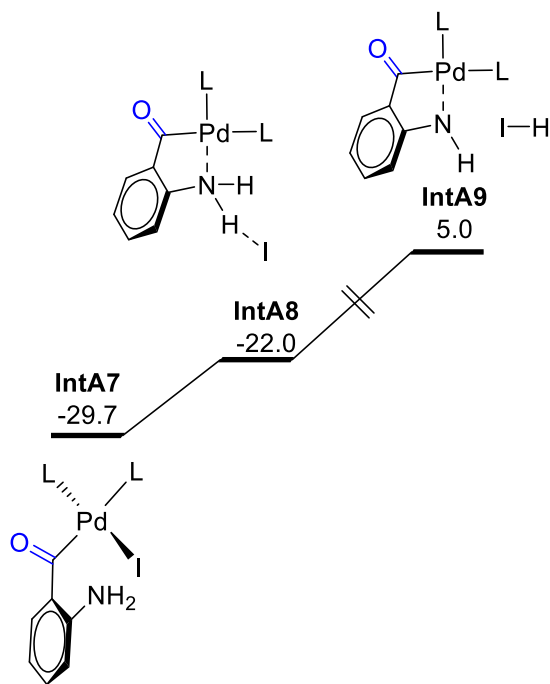
**Figure S1.** The Gibbs free energy (in kcal/mol) profiles of oxidative addition of *o*-iodoaniline with Pd(PPh<sub>3</sub>)<sub>2</sub>.

As shown in Figure S1, *o*-iodoaniline participates into reaction generates **IntA1'** without exchange with the ligand of active catalyst. Then oxidative addition via transition state **TSA1'** directly generates arylpalladium intermediate **IntA3**. This oxidative addition step has a 13.1 kcal/mol energy barrier.



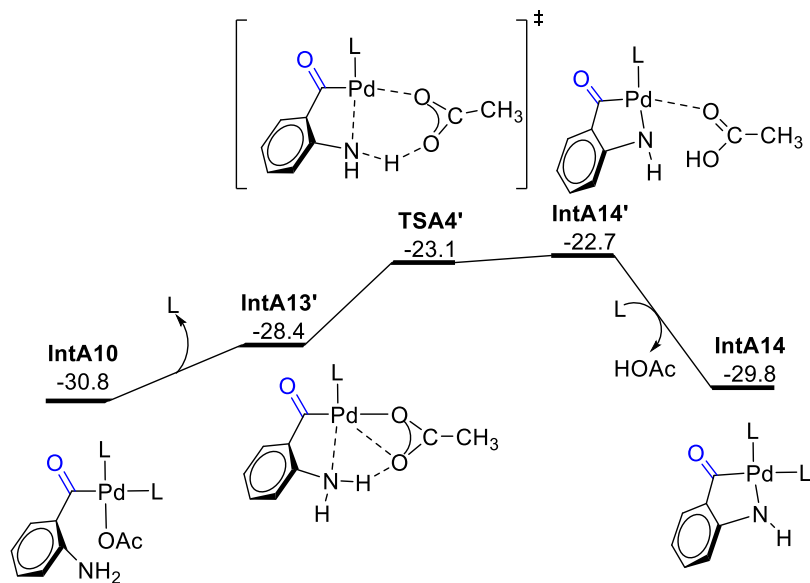
**Figure S2.** The Gibbs free energy (in kcal/mol) profiles of carbonylation of isomer **IntA5'**.

As shown in Figure S2, the ligand exchange of CO with one phosphine ligand of **IntA4** generates **IntA5'**, which is the isomer of **IntA5**. Then carbonylation via transition state **TSA2'** generates **IntA6** with an energy barrier of 10.0 kcal/mol.



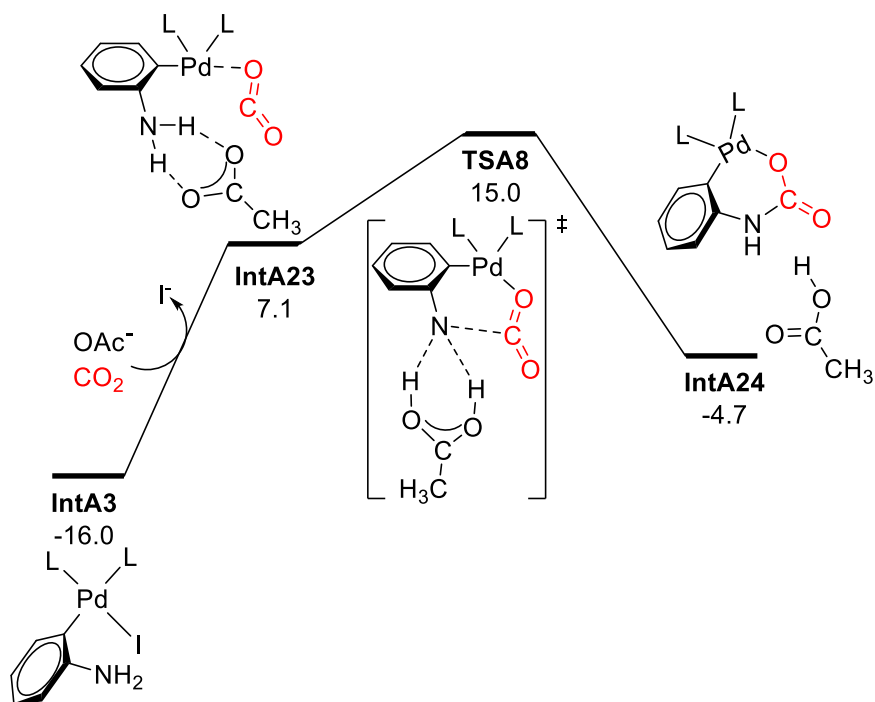
**Figure S3.** The Gibbs free energy (in kcal/mol) profiles of direct deprotonation of the amine by I.

In view of Figure S3, intermediate **IntA7** rearranges into **IntA8**, in which the amine group is coordinated with the Pd center and the I is coordinated with the amine through hydrogen-bonding interaction. However, calculated results indicate that the deprotonation energy of I to activate N-H bond is up to 34.7 kcal/mol. This hypothesis suggests that weakly basic I cannot activate N-H bond.



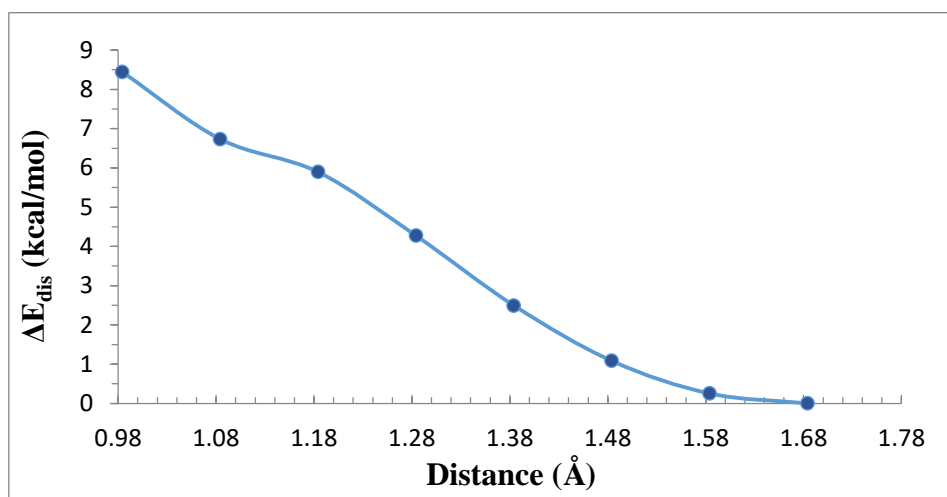
**Figure S4.** The Gibbs free energy (in kcal/mol) profiles of inner-CMD mechanism for the N-H activation of **IntA10**.

As indicated in Figure S4, **IntA10** converts to **IntA13'** through ligand exchange of  $\text{OAc}^-$  with phosphine ligand and coordination of amine group to the Pd center. **IntA13'** then goes through N-H bond activation via **TSA4'** and generates five-membered palladacycle **IntA14**. The energy barrier of this step is 8.1 kcal/mol.



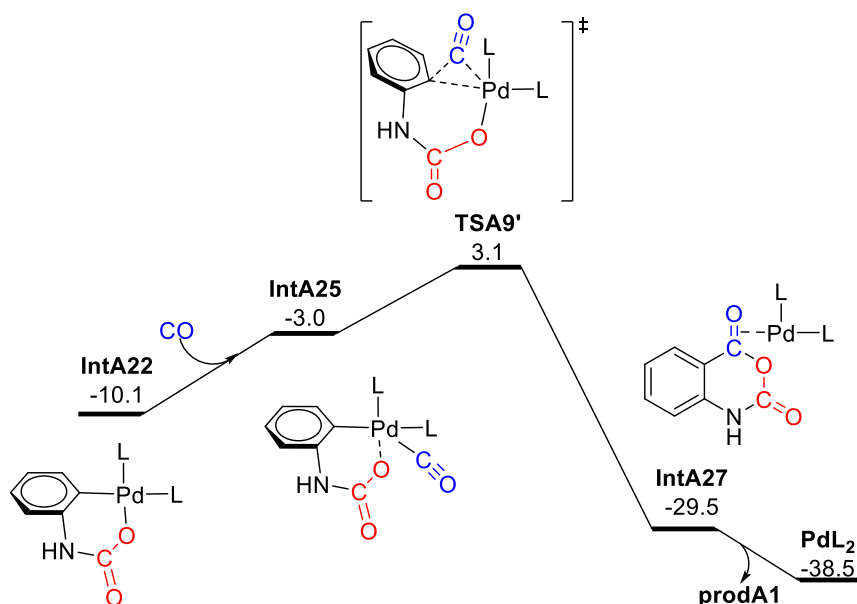
**Figure S5.** The Gibbs free energy (in kcal/mol) profiles of concerted N-H activation/carboxylation pathway of **IntA3**.

As shown in Figure S5, the dissociative  $\text{OAc}^-$  of **IntA23** is stabilized by the dual hydrogen-bonding interactions with amine group, and  $\text{CO}_2$  is coordinated to the Pd center. This process through transition state **TSA8** generates **IntA24** with an energy barrier of 31.0 kcal/mol.



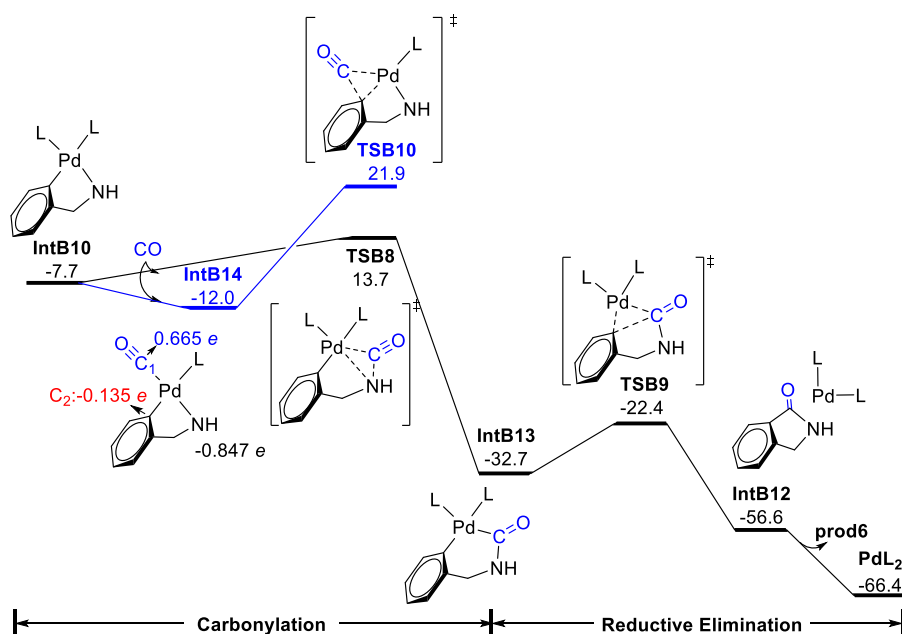
**Figure S6.** Energy profiles of the scanning result of N-H activation of **IntA19**.

In order to locate the N-H activation transition state of **IntA19**, a scan of the distance from amine-H to O (1.68 Å→0.98 Å), in interval of 0.1 Å, was performed. As shown in Figure S6, there is no obvious turning point in the scanning curve, which indicates that the N-H activation of **IntA19** is barrierless and endergonic.



**Figure S7.** The Gibbs free energy (in kcal/mol) profiles of regioselectivity of carbonylation in **IntA25**.

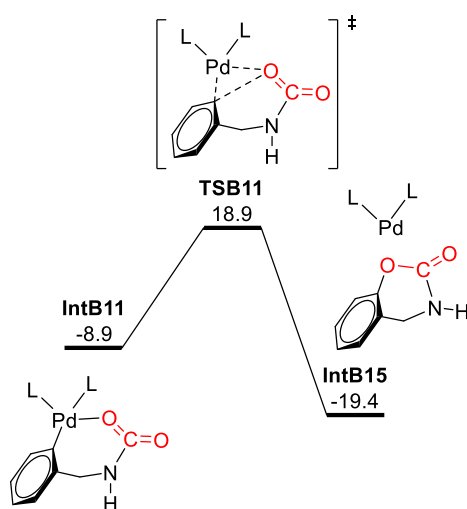
As shown in Figure S7, the regioselectivity of CO inserted into Ar-Pd bond via **TSA9'** with an energy barrier of 19.1 kcal/mol (**IntA3**  $\rightarrow$  **TSA9'**).



**Figure S8.** The Gibbs free energy (in kcal/mol) profiles for the formation of mono-carbonylation from **IntB10**.



In Figure S8, CO is inserted into the Pd-N bond through the transition state **TSB7** to complete the carbonylation step, and the energy barrier in this process is as high as 33.2 kcal/mol. However, when carbonylation occurs inserted into Pd-C bond, the energy barrier of **TSB10** is as high as 41.2 kcal/mol. In this regard, NBO analysis was performed on **IntB20**. It is found that C1 is an electron-poor atom, while C2 and N are electron-rich atoms with charges of  $-0.135e$  and  $-0.847e$ , respectively. NBO analysis results show that electron-poor C1 tends to combine with more electron-rich N, which results in the lower energy of carbonylation transition state **TSB8** than **TSB10**.



**Figure S9.** The Gibbs free energy (in kcal/mol) profiles of reductive elimination step of **IntB11** for the mono-carboxylation pathway.

As shown in Figure S9, the **IntB11** through **TSB11** to generate mono-carboxylation product with an energy barrier of 38.4 kcal/mol (**IntB9**→**TSB11**).

**Table S1. Thermal correction of Gibbs free energy (TCG, hartree) and total electronic energies (E, hartree) in Tetrahydrofuran solvent for all species involved in this study <sup>a</sup>**

Compounds	TCG	E	Compounds	TCG	E
CO	-0.014016	-113.281513931	IntA14'	0.383803	-1792.50618739
CO <sub>2</sub>	-0.008881	-188.560487267	IntA19	0.638647	-2715.12357479
OAc <sup>•</sup>	0.021462	-228.550979465	IntA20	0.577815	-2486.05121139
HOAc	0.035672	-229.039781581	TSA7	0.587481	-2674.61492785
<i>o</i> -Iodoaniline	0.075419	-298.257586322	IntA21	0.592568	-2674.62879735
PPh <sub>3</sub>	0.231568	-1035.91986079	IntA22	0.592111	-2674.65243620
I <sup>•</sup>	-0.016848	-11.5629944664	IntA25	0.598433	-2787.94299868
IntA0	0.480541	-2199.82771393	TSA9	0.600367	-2787.93865870
IntA1	0.324124	-1462.14754592	IntA26	0.601728	-2787.95307169
TSA1	0.322918	-1462.14534067	TSA10	0.601360	-2787.94587605
IntA2	0.327813	-1462.17133839	IntA27	0.598954	-2787.98569285
IntA3	0.588724	-2498.14355352	IntA23	0.644872	-2903.68187481
IntA4	0.587451	-2498.14327187	TSA8	0.647952	-2903.67242434
IntA5	0.332501	-1575.49310303	IntA24	0.651198	-2903.70714217
TSA2	0.331849	-1575.48094022	TSA11	0.581406	-2599.35241128
IntA6	0.334921	-1575.50748044	IntA28	0.585605	-2599.36989417
IntA7	0.596496	-2611.46868713	TSA12	0.590561	-2674.59305479
IntA10	0.646629	-2828.47023112	IntA29	0.591240	-2674.65712975
IntA13	0.645235	-2828.45673922	IntA30	0.329566	-1676.75375615
TSA4	0.642399	-2828.45367275	TSA13	0.329834	-1676.71351624
IntA14	0.585611	-2599.40350728	IntA31	0.333299	-1676.76205715
TSA5	0.595978	-2787.96069743	IntA32	0.596221	-2712.71785313
IntA15	0.598750	-2787.96443497	TSA14	0.593112	-2712.69698149
IntA16	0.599459	-2787.96833112	IntA33	0.594969	-2712.73294389
TSA6	0.601886	-2787.96039420	prodA4	0.084225	-512.887758751
IntA17	0.596125	-2787.98569285	TSA9'	0.600582	-2787.93552280
prodA1	0.088957	-588.142890826	subB	0.102649	-337.53656766
IntA1'	0.586782	-2498.10254656	IntB1	0.354034	-1501.42883238
TSA1'	0.587529	-2498.09606881	TSB1	0.356117	-1501.42769915
IntA5'	0.331000	-1575.48611168	IntB2	0.615215	-2537.42433793
TSA2'	0.332088	-1575.47918340	TSB2	0.361962	-1614.75945082
IntA8	0.595927	-2611.45584162	IntB3	0.623893	-2650.74520859
IntA9	0.587531	-2611.40437640	IntB4	0.675634	-2867.74263087
IntA11	0.651577	-3017.00756802	IntB5	0.612478	-2638.67020030
TSA3	0.654647	-3016.98851787	TSB3	0.625708	-2827.23042270
IntA12	0.657760	-3017.02061268	IntB6	0.629860	-2827.24643708
IntA13'	0.386342	-1792.51778257	TSB4	0.629162	-2827.23108779
TSA4'	0.381943	-1792.50504932	IntB7	0.624321	-2827.26249051

<sup>a</sup> The intermediates and transition states are calculated at the S10

M06/6-311+G(d,p)(SDD)// $\omega$ B97XD/6-31G(d)(LANL2DZ) level of theory.

**Table S1. Thermal correction of Gibbs free energy (TCG, hartree) and total electronic energies (E, hartree) in Tetrahydrofuran solvent for all species involved in this study <sup>a</sup>**

Compounds	TCG	E	Compounds	TCG	E
<b>prodB1</b>	0.116807	-627.41462726	<b>TSB9</b>	0.617496	-2638.67534194
<b>IntB8</b>	0.618616	-2537.42168164	<b>IntB14</b>	0.350418	-1602.70345325
<b>IntB9</b>	0.669193	-2754.43108652	<b>TSB10</b>	0.353894	-1602.65276140
<b>IntB10</b>	0.608186	-2525.34710172	<b>TSB11</b>	0.618592	-2713.88455408
<b>TSB5</b>	0.616845	-2713.91143432	<b>IntB15</b>	0.619720	-2713.94671244
<b>IntB11</b>	0.620888	-2713.93107278	<b>prodB4</b>	0.108676	-514.10078945
<b>TSB6</b>	0.627832	-2827.22071426			
<b>TSB7</b>	0.613449	-2638.66566413			
<b>IntB12</b>	0.615671	-2638.72811274			
<b>prodB2</b>	0.104620	-438.88547655			
<b>TSB8</b>	0.616683	-2638.61708221			
<b>IntB13</b>	0.617122	-2638.69148582			

<sup>a</sup> The intermediates and transition states are calculated at the M06/6-311+G(d,p)(SDD)// $\omega$ B97XD/6-31G(d)(LANL2DZ) level of theory.

**Cartesian coordinates for all optimized geometries**

**CO**

C 0.00000000 0.00000000 -0.64872700  
 O 0.00000000 0.00000000 0.48654500

**CO<sub>2</sub>**

C 0.00000000 0.00000000 0.00000000  
 O 0.00000000 0.00000000 1.16469000  
 O 0.00000000 0.00000000 -1.16469000

**OAc<sup>-</sup>**

O 0.80486600 -1.10406300 -0.00003400  
 C 0.21884500 0.00156800 -0.00007200  
 C -1.35042500 -0.05364300 -0.00000200  
 H -1.72550300 -1.08387300 -0.00164900  
 H -1.74158100 0.47170300 0.88196700  
 H -1.74190700 0.47482400 -0.87994300  
 O 0.69494300 1.16028700 0.00004200

**HOAc**

C -0.09757900 0.09997200 -0.08353700  
 O -0.66945500 1.11015800 -0.41246000  
 O -0.75822600 -1.02064200 0.27534000  
 H -1.70343200 -0.81078700 0.20438800

C 1.39308800 -0.09173900 -0.01200400  
 H 1.89237400 0.82556800 -0.32250700  
 H 1.68494800 -0.34866800 1.01066100  
 H 1.69452400 -0.92077300 -0.65894200

***o*-Iodoaniline**

C 2.52116800 -1.55153700 0.00722000  
 C 1.13521300 -1.45190700 0.00702700  
 C 0.52224400 -0.20332500 -0.00039700  
 C 1.26926000 0.98418800 -0.00755400  
 C 2.66977500 0.85594600 -0.00554100  
 C 3.28358200 -0.38577700 0.00007500  
 H 2.99495200 -2.52733200 0.01267000  
 H 0.52555300 -2.34879100 0.01356700  
 H 3.27302600 1.76040600 -0.01714000  
 H 4.36796600 -0.44233200 0.00042900  
 N 0.69442500 2.24292200 -0.06902900  
 H -0.25391900 2.32105900 0.27074000  
 H 1.28435700 2.99762200 0.24948100  
 I -1.61246000 -0.13106800 -0.00097200

**PPh<sub>3</sub>**

P 0.04663300 -0.04843700 -1.26144300  
 C -0.61156900 -3.22087400 1.34489300  
 H -1.21794700 -3.43917900 2.21934100

C	-2.66741300	0.50945500	-1.12231700	C	2.93038400	-0.31699100	4.35337400
H	-2.71180300	-0.11791700	-2.00946000	H	4.66412700	-1.51028600	3.90074400
C	-1.39224300	1.58031700	0.61731800	H	1.14166200	0.88143900	4.48681700
H	-0.44336700	1.78795300	1.10292500	H	3.06535600	-0.38599400	5.42899900
C	-1.43163600	0.75581200	-0.51168000	C	3.29117200	-1.33986200	-0.93827600
C	-2.56252300	2.13880000	1.12580300	C	2.67957100	-2.58814500	-1.10064800
H	-2.51608200	2.77925300	2.00197300	C	4.63233400	-1.18829800	-1.30197200
C	2.03661900	0.41419400	0.75758800	C	3.40030600	-3.66925600	-1.59687200
H	1.71163400	-0.50788900	1.23035600	H	1.62918000	-2.70187700	-0.84157000
C	1.42175200	0.84540600	-0.42216700	C	5.35053700	-2.26911100	-1.80810100
C	-0.69928500	-1.96914000	0.74019300	H	5.11832100	-0.22287000	-1.19459100
H	-1.37146100	-1.22103200	1.14976400	C	4.73800300	-3.51095300	-1.95217700
C	3.48564600	2.34625100	0.73996400	H	2.91440500	-4.63324100	-1.71574100
H	4.28619900	2.92586300	1.19032500	H	6.39096300	-2.13864700	-2.09154700
C	1.86308500	2.03437800	-1.01567600	H	5.29974900	-4.35218600	-2.34781500
H	1.40415800	2.37482500	-1.94092900	C	3.20631900	1.52254400	-0.67394100
C	0.07088100	-1.67062900	-0.38830100	C	4.25573900	2.03516600	0.09462500
C	-3.78711300	1.87642400	0.51772600	C	2.84757300	2.17698100	-1.85722900
H	-4.69848300	2.31230300	0.91658100	C	4.94114900	3.17395100	-0.32092900
C	3.06388400	1.15899000	1.33216400	H	4.53595600	1.54713300	1.02381400
H	3.53381500	0.81031300	2.24737500	C	3.53831500	3.30949300	-2.27626800
C	1.02156400	-3.90164300	-0.28929900	H	2.01405500	1.79643400	-2.44310000
H	1.69237800	-4.65255800	-0.69647900	C	4.58674200	3.80996200	-1.50781200
C	-3.83803600	1.05764700	-0.60787000	H	5.75229300	3.56581900	0.28594300
H	-4.78889200	0.85284200	-1.09117500	H	3.25103500	3.80729700	-3.19775800
C	0.92481200	-2.65543000	-0.90002000	H	5.12156200	4.69895200	-1.82937500
H	1.51920700	-2.44281000	-1.78552500	C	-3.22720100	-1.49824400	-0.72215800
C	0.25044900	-4.18771700	0.83484200	C	-4.28310600	-2.02159400	0.03012900
H	0.31794000	-5.16277400	1.30852000	C	-2.87785800	-2.11829400	-1.92659000
C	2.88103700	2.78462800	-0.43578800	C	-4.98404200	-3.13678000	-0.42191600
H	3.20841600	3.70697400	-0.90669100	H	-4.55626900	-1.56054800	0.97506500
<b>I</b>				C	-3.58405600	-3.22702900	-2.38192600
I	0.00000000	0.00000000	0.00000000	H	-2.03962000	-1.72997700	-2.50050100
<b>IntA0</b>				C	-4.63880300	-3.73823100	-1.62934800
Pd	-0.00015900	-0.00472600	-0.65624800	H	-5.80013300	-3.53736100	0.17250700
P	-2.26570100	-0.01325900	-0.22762200	H	-3.30396600	-3.69818700	-3.31949600
P	2.26530100	0.00936900	-0.22763200	H	-5.18573700	-4.60889800	-1.97940800
C	2.57921300	-0.15266500	1.57941800	C	-2.57699800	0.09464500	1.58394100
C	3.65460000	-0.86661700	2.11587000	C	-1.68288400	-0.56766000	2.43352500
C	1.67862600	0.47264200	2.44993900	C	-3.64406800	0.80322400	2.14362700
C	3.82751200	-0.94799600	3.49602300	C	-1.85725900	-0.53176500	3.81272100
H	4.35646600	-1.36899000	1.45645100	H	-0.83355000	-1.09470500	2.00531500
C	1.85466700	0.39529500	3.82719800	C	-3.81526500	0.84304500	3.52580400
H	0.82322900	1.00366100	2.03906900	H	-4.34063700	1.33393300	1.50099800

C	-2.92468700	0.17547100	4.36203800
H	-1.14936800	-1.04627600	4.45612300
H	-4.64532900	1.40157700	3.94879900
H	-3.05825400	0.21207200	5.43942700
C	-3.27318900	1.37220600	-0.89348600
C	-4.61597900	1.25067700	-1.26239200
C	-2.64499600	2.61701000	-1.01411300
C	-5.31937800	2.35717800	-1.73258300
H	-5.11496900	0.28884800	-1.18725400
C	-3.35094600	3.72347200	-1.47436400
H	-1.59335700	2.70807100	-0.75110300
C	-4.69035700	3.59487800	-1.83517800
H	-6.36123300	2.25001100	-2.02051300
H	-2.85216800	4.68431500	-1.56095400
H	-5.24060300	4.45616700	-2.20284000

### IntA1

H	-3.14810500	-1.50498300	-2.94448600
H	-3.14557200	0.05627000	-2.34276100
C	-3.01847300	-1.40323800	-0.92850300
C	-2.83377400	-2.78038100	-0.74367600
C	-2.90020200	-0.56602300	0.21751500
C	-2.57944700	-3.32289300	0.51241500
H	-2.91925100	-3.43309800	-1.60878400
C	-2.62520800	-1.12418500	1.48604300
C	-2.46743900	-2.50563300	1.62960600
H	-2.62320000	-0.48287600	2.36044500
I	-3.62869600	1.47912700	0.13506900
H	-2.46541000	-4.39830900	0.61026900
H	-2.26980200	-2.92259100	2.61118000
Pd	-0.82047100	-0.00360300	0.12854000
P	1.45333400	0.10029100	-0.00386700
C	2.33117000	0.21342100	1.60691800
C	3.51925000	-0.46543500	1.89148200
C	4.13996400	-0.30950400	3.12893300
C	3.58269000	0.52755100	4.09134800
C	2.39602700	1.20418900	3.81724700
C	1.77066400	1.04136100	2.58587600
C	2.22646400	1.45594800	-0.97628100
C	3.47630300	2.00764200	-0.67760500
C	4.01134900	3.01435000	-1.47750100
C	3.30536800	3.47894000	-2.58390100
C	2.05672700	2.94021400	-2.88505500
C	1.51880500	1.94041600	-2.08123900
C	2.17315100	-1.41197000	-0.76615300

C	3.35605100	-1.41343400	-1.51171400
C	3.85360800	-2.60143500	-2.04171800
C	3.17594200	-3.79931000	-1.83102000
C	1.99367400	-3.80576200	-1.09443700
C	1.49097000	-2.61874200	-0.57154200
H	3.96060500	-1.12345800	1.14866800
H	5.06033200	-0.84614100	3.34049200
H	4.06747200	0.64696300	5.05590200
H	1.95168800	1.85211800	4.56706700
H	4.03230700	1.65528700	0.18640400
H	4.98103200	3.43821000	-1.23290000
H	3.72342500	4.26558400	-3.20526800
H	1.49636900	3.30683300	-3.74009900
H	3.88884300	-0.48295900	-1.68586000
H	4.77126900	-2.58926200	-2.62271300
H	3.56453700	-4.72468900	-2.24643000
H	1.45558300	-4.73553300	-0.93408300
H	0.53401100	1.53354700	-2.29956800
H	0.55566500	-2.61846800	-0.01534800
H	0.83295700	1.55130100	2.37732200
N	-3.39486100	-0.90752400	-2.16787800

### TSA1

H	-3.33688200	-1.23171200	-2.99013300
H	-2.64591000	0.14437800	-2.31755400
C	-3.38695000	-1.18394200	-0.96068700
C	-3.96922400	-2.44954600	-0.80144200
C	-2.92516400	-0.53623400	0.21130500
C	-4.12756800	-3.02458100	0.45350500
H	-4.31699700	-2.97656000	-1.68696000
C	-3.11936300	-1.10344000	1.47865700
C	-3.70819100	-2.35928300	1.60145900
H	-2.82533500	-0.54524100	2.36130700
I	-2.79581500	1.85585000	0.14440200
H	-4.59338100	-4.00249000	0.53132600
H	-3.84661600	-2.80022900	2.58306200
Pd	-0.90485800	-0.15734900	0.14784000
P	1.41800800	-0.07873000	0.01946700
C	2.31216200	-0.82524200	1.43782100
C	3.49651300	-1.55518400	1.30204200
C	4.13505400	-2.07336800	2.42611400
C	3.59864100	-1.86514600	3.69379300
C	2.41626700	-1.14243600	3.83674100
C	1.77320500	-0.63152800	2.71430500
C	2.18739900	1.58007200	-0.13062700

C	3.47656500	1.86786700	0.32982700
C	4.01612200	3.13931700	0.15762500
C	3.27433700	4.13401100	-0.47527400
C	1.98773300	3.85709700	-0.92973200
C	1.44456700	2.58817800	-0.75263000
C	2.08878600	-0.99853500	-1.42210200
C	3.17923000	-0.56305500	-2.17967900
C	3.64259500	-1.32692300	-3.24880000
C	3.02554900	-2.53293000	-3.56787900
C	1.93605300	-2.97320400	-2.81899400
C	1.46638900	-2.20689200	-1.75801400
H	3.91969500	-1.72487500	0.31607100
H	5.05262800	-2.64262500	2.30948400
H	4.09730200	-2.27133200	4.56892700
H	1.98926200	-0.98406400	4.82252800
H	4.05905800	1.09969500	0.83039400
H	5.01629800	3.35407500	0.52245200
H	3.69589600	5.12644300	-0.60557600
H	1.39995100	4.63220800	-1.41221100
H	3.66716000	0.37687600	-1.93980300
H	4.48797200	-0.97611600	-3.83347900
H	3.38865700	-3.12644800	-4.40178300
H	1.44668000	-3.91067700	-3.06612300
H	0.43058200	2.37810700	-1.08379300
H	0.60593600	-2.54313000	-1.18307900
H	0.84055100	-0.08256500	2.82225800
N	-3.33217400	-0.58931300	-2.21103900

**IntA2**

H	1.90631700	-2.48100800	2.89962800
H	0.57854300	-1.75566500	2.19070300
C	2.07349200	-2.22259300	0.88513600
C	3.32425000	-2.84067200	0.75985200
C	1.38930600	-1.86060500	-0.28691400
C	3.88954400	-3.05967200	-0.49080300
H	3.86278100	-3.13350400	1.65883300
C	1.97381200	-2.05764300	-1.53461300
C	3.22215000	-2.66745100	-1.64705400
H	1.45525300	-1.72809300	-2.43168200
I	-3.19373700	-1.57236700	-0.15218500
H	4.86459400	-3.53355900	-0.55816300
H	3.66662500	-2.82499300	-2.62458900
Pd	-0.52472900	-1.31492200	-0.23205700
P	0.24675700	0.78335100	0.01957200
C	0.03836200	1.36249700	1.73897500

C	0.90065700	2.30769700	2.30451800
C	0.67640400	2.77119000	3.59742600
C	-0.40832500	2.29934200	4.33109100
C	-1.27424700	1.36513600	3.76814200
C	-1.05487400	0.89586100	2.47750600
C	-0.76215900	1.91625600	-0.99743600
C	-0.82495700	3.27594300	-0.67298300
C	-1.54446200	4.15068100	-1.47843300
C	-2.20259200	3.67596300	-2.61140300
C	-2.14271700	2.32462900	-2.93697900
C	-1.42617600	1.44417800	-2.13150800
C	1.96688000	1.17532400	-0.44475100
C	2.24691300	1.78179500	-1.67050200
C	3.56827100	1.97864100	-2.06525600
C	4.61153500	1.57124000	-1.24153700
C	4.33469900	0.96853100	-0.01535200
C	3.02030900	0.76897900	0.38394600
H	1.75121400	2.67919300	1.74186100
H	1.35321400	3.50136800	4.03055000
H	-0.57960200	2.66056100	5.34072500
H	-2.12552300	0.99746700	4.33242200
H	-0.32095800	3.65166600	0.21253900
H	-1.59621000	5.20328200	-1.21770900
H	-2.76925400	4.36025100	-3.23569900
H	-2.66501600	1.94745000	-3.81030800
H	1.43976500	2.09898900	-2.32313900
H	3.77774800	2.44981100	-3.02068800
H	5.64089100	1.71983100	-1.55382500
H	5.14500500	0.64136700	0.62847200
H	-1.40449400	0.38567600	-2.37294000
H	2.80971500	0.28322200	1.33276100
H	-1.74022000	0.17311800	2.04101400
N	1.58248400	-1.88233500	2.15138000

**IntA3**

Pd	-0.29116900	-0.97634800	-0.10947400
P	-1.54942200	0.97086500	-0.01005500
P	1.93061500	0.11088500	0.02442100
C	-0.57400200	4.23954900	-2.36796300
H	-0.48536900	5.31720300	-2.27035500
C	2.30428600	-1.09904900	2.52048700
H	1.47047300	-1.72843900	2.22675700
C	3.87048700	0.66295600	2.02262800
H	4.24005700	1.44055200	1.36073400
C	-0.60371000	1.23593800	2.59340800

H	-0.12364200	0.28148600	2.40302900	H	0.16715200	1.38500500	4.59089900
C	2.50468100	-0.90219900	-2.48695000	C	-0.74836600	1.47854500	-2.58968100
H	1.42798600	-0.85384300	-2.62267300	H	-0.80868800	0.39591300	-2.67420000
C	-2.05334700	3.02322400	1.87394800	C	2.63549800	3.84035400	-1.61280200
H	-2.72380400	3.45478400	1.13607100	H	2.94304500	4.23486600	-2.57658200
C	-1.37936600	1.82825400	1.59464700	C	1.84208100	2.80978200	0.83955400
C	4.44097100	-0.66765300	-1.07045800	H	1.54879300	2.42312200	1.80922500
H	4.88884600	-0.42243900	-0.11298100	C	-0.33483200	3.62770600	-3.59432800
C	-1.89067400	3.64776000	3.10538600	H	-0.07252700	4.22786600	-4.46053800
H	-2.40927900	4.57956800	3.30991500	C	-5.50518800	0.25723100	0.68124100
C	-4.00181600	1.38734700	-1.37205500	H	-6.08482600	-0.19830400	1.47796900
H	-3.42547500	1.82515700	-2.18043100	C	1.96633700	4.18430200	0.67090200
C	2.50895900	2.46416200	-1.44661600	H	1.75268000	4.84568700	1.50546300
H	2.72653000	1.80641900	-2.28151000	C	2.36887200	4.70459400	-0.55598400
C	-3.36626600	0.92749800	-0.21802500	H	2.47315200	5.77773300	-0.68772700
C	5.24935600	-1.12215100	-2.10823000	C	-2.07712700	-1.94845800	-0.22619700
H	6.31926800	-1.22193700	-1.95153400	C	-2.66697200	-2.48588200	0.92688700
C	2.11778500	1.93126400	-0.21548500	C	-2.74867000	-2.04283900	-1.43959900
C	4.68954900	-1.45381400	-3.33876400	C	-3.92839800	-3.08196300	0.83655200
H	5.32247200	-1.81094000	-4.14575200	C	-4.01157800	-2.63010600	-1.52634800
C	-0.91174600	3.47698200	-1.25373500	H	-2.29458100	-1.63643600	-2.34050100
H	-1.06787600	3.96987200	-0.30118000	C	-4.60274200	-3.14324900	-0.37845000
C	-6.13722600	0.71516800	-0.47296600	H	-4.38664600	-3.49698300	1.73291000
H	-7.21474500	0.62542900	-0.57494100	H	-4.52486500	-2.67869200	-2.48217000
C	-4.12744700	0.36500700	0.81244200	H	-5.58677500	-3.60131200	-0.42448300
H	-3.63800500	-0.00821400	1.70776400	N	-2.02295700	-2.35817100	2.17635900
C	2.90903800	-1.28472300	3.76081800	H	-2.40984200	-2.99163200	2.86735800
H	2.52996100	-2.04886300	4.43253300	H	-1.02799800	-2.54442700	2.08411900
C	-1.01131400	2.08977500	-1.35721800	I	0.84044100	-3.44530800	-0.19868500
C	-1.07830800	3.07056700	4.08082500				
H	-0.95582200	3.55936000	5.04286700	<b>IntA4</b>			
C	2.77684000	-0.12413100	1.63755600	Pd	0.02283000	-0.07703100	-0.43190800
C	-5.38527100	1.28291600	-1.49524500	P	-2.29665100	-0.06597200	-0.03943400
H	-5.87200800	1.64318100	-2.39672400	P	2.34787100	0.03431500	-0.01805600
C	3.06247800	-0.54951400	-1.25429500	C	-3.83802400	-2.81014100	2.63269700
C	-0.41719800	2.24209600	-3.70335500	H	-4.69286800	-3.47616700	2.70176000
H	-0.22004500	1.75362800	-4.65282200	C	3.30541300	-1.65697800	-2.00556800
C	4.47735700	0.47333900	3.25931100	H	2.42835900	-1.33652900	-2.55948500
H	5.32465000	1.09053600	3.54295600	C	4.60349000	-1.66641700	0.02888600
C	3.99581300	-0.49977900	4.13241800	H	4.75833200	-1.33680500	1.05231400
H	4.46786100	-0.64429000	5.09981500	C	-2.92949500	-1.22107800	-2.51383300
C	3.31462300	-1.34274100	-3.52752200	H	-1.86573700	-1.41635900	-2.59794400
H	2.86831500	-1.62034800	-4.47747900	C	3.03395900	2.35638800	-1.39499200
C	-0.44765500	1.85593700	3.82997500	H	2.20173200	2.09852200	-2.04026200
				C	-4.80592500	-0.35136700	-1.26691500

H	-5.20204000	0.16135800	-0.39489200
C	-3.42978000	-0.59382900	-1.37149100
C	4.41024400	1.89521800	0.52849100
H	4.66049300	1.27751400	1.38598000
C	-5.66734600	-0.75121100	-2.28187300
H	-6.73268300	-0.56168100	-2.19075500
C	-3.37372700	1.79032100	1.81413100
H	-3.25571700	1.02421500	2.57343700
C	2.27400900	0.83935800	2.68656400
H	2.38270400	1.85574700	2.32174100
C	-3.03971700	1.52369400	0.48637100
C	5.17645900	3.02135000	0.24973200
H	6.01509000	3.27436900	0.89150300
C	2.32371000	-0.23634000	1.79277300
C	4.87027100	3.81980900	-0.84995900
H	5.46604300	4.70224900	-1.06380900
C	-3.67698900	-2.01277600	1.50217900
H	-4.40353400	-2.06903200	0.69801800
C	-4.00795400	4.04049700	1.21577200
H	-4.37695600	5.02159200	1.50034900
C	-3.20416400	2.52473900	-0.47822900
H	-2.93562100	2.33031700	-1.51308100
C	4.21682500	-2.52962600	-2.59049300
H	4.05619500	-2.87297700	-3.60768900
C	-2.57445400	-1.16562200	1.39546100
C	-5.16173200	-1.38477700	-3.41553200
H	-5.83478600	-1.69362400	-4.21010300
C	3.49446700	-1.21857800	-0.69381100
C	-3.85845300	3.04624500	2.17523300
H	-4.11612200	3.24355700	3.21171600
C	3.32040000	1.56304300	-0.28331000
C	-1.80097100	-1.91835200	3.56135700
H	-1.05765900	-1.88284700	4.35192800
C	5.50780300	-2.54785400	-0.55405200
H	6.36224500	-2.89901100	0.01677300
C	5.31670000	-2.97799500	-1.86482000
H	6.02222400	-3.66814900	-2.31794200
C	3.80286900	3.48148100	-1.67535300
H	3.55907400	4.09820900	-2.53491000
C	-3.79471700	-1.61545100	-3.53088400
H	-3.39529900	-2.10620500	-4.41305300
C	-1.63101500	-1.13105900	2.42975500
H	-0.74882200	-0.50015400	2.34548400
C	2.07468800	0.61458200	4.04620700

H	2.03755000	1.45816400	4.72899200
C	2.16582500	-1.53920300	2.28175500
H	2.16588200	-2.38054600	1.59535000
C	-2.90557300	-2.76120800	3.66401200
H	-3.03320400	-3.38698600	4.54247400
C	-3.68146900	3.77569300	-0.11333300
H	-3.78658000	4.54990500	-0.86695400
C	1.97253700	-1.75837000	3.64123800
H	1.84811200	-2.77378000	4.00482000
C	1.92370000	-0.68337200	4.52640100
H	1.76873200	-0.85685900	5.58740600
C	-0.05002400	1.95260900	-0.33966200
C	-0.18954100	2.68311100	-1.53097800
C	0.00168100	2.64372400	0.86662100
C	-0.20864500	4.08120100	-1.48710700
C	-0.03070900	4.03761400	0.91387600
H	0.05315500	2.08625500	1.79851100
C	-0.12374800	4.75407900	-0.27357400
H	-0.31024700	4.64171600	-2.41478900
H	0.00900700	4.55224900	1.86926700
H	-0.14526600	5.84014200	-0.26008900
N	-0.37387700	2.02372100	-2.75678400
H	-0.05313200	2.53214300	-3.57023100
H	-0.05589000	1.06146000	-2.75829100
I	0.04039000	-2.83431400	-0.74298900

### IntA5

Pd	0.24537000	-1.42633200	-0.16433100
P	-0.04467000	0.91603300	0.01523900
C	0.99196300	0.82379700	2.60638800
H	1.48676300	-0.08583300	2.27891400
C	-0.44084500	2.71377000	2.14818100
H	-1.08859500	3.26594100	1.47397200
C	1.54135000	1.29741500	-2.23724900
H	1.23225600	0.29076000	-2.50445700
C	1.56457100	3.13148000	-0.66711600
H	1.26376100	3.56891300	0.27971100
C	-1.86883800	2.09788000	-1.77082600
H	-1.02346900	2.24739700	-2.43491900
C	2.40286700	3.84405800	-1.51880800
H	2.74734000	4.83254400	-1.23062400
C	-1.68095900	1.54498000	-0.50286100
C	2.80259300	3.29005100	-2.73185400
H	3.45960800	3.84715400	-3.39301100
C	1.19628400	1.29705000	3.89883600



H	1.83811800	0.74249900	4.57631400
C	0.17198200	1.52947800	1.72138400
C	1.12737700	1.85403000	-1.02378200
C	-0.23455800	3.18212900	3.44144500
H	-0.71605500	4.10033100	3.76389800
C	0.58310800	2.47380300	4.31862400
H	0.74143700	2.83971700	5.32875400
C	2.37003900	2.01639000	-3.09139500
H	2.69192500	1.57286000	-4.02827700
C	-3.14535700	2.46166200	-2.19272000
H	-3.28117200	2.89160300	-3.18053600
C	-2.78329100	1.36562300	0.34080300
H	-2.64913200	0.92795600	1.32571500
C	-4.05405100	1.72810000	-0.08577900
H	-4.90356300	1.57013600	0.57108300
C	-4.23860800	2.27399600	-1.35433200
H	-5.23430200	2.55136200	-1.68753000
C	-1.79111300	-1.60322400	-0.24638900
C	-2.54401200	-1.74007700	0.92860400
C	-2.42987800	-1.60948400	-1.48215600
C	-3.93292100	-1.89701600	0.82781300
C	-3.81411100	-1.74655600	-1.57622300
H	-1.84477300	-1.49242400	-2.39109900
C	-4.55999800	-1.89870000	-0.41175300
H	-4.52285700	-1.99762600	1.73667000
H	-4.29855400	-1.73797800	-2.54753000
H	-5.63872100	-2.01530600	-0.46428600
N	-1.94937400	-1.61081400	2.19032500
H	-2.42636500	-2.10091000	2.93529600
H	-0.95300500	-1.78996900	2.20389800
I	2.98947200	-1.41606900	-0.03180600
C	0.29698300	-3.38289900	-0.30433000
O	0.31531700	-4.51467900	-0.39186100

**TSA2**

Pd	-0.15132200	-1.38058500	-0.15897000
P	0.38147600	0.97252500	0.01869100
C	1.63464100	0.68160000	2.48048300
H	1.91005900	-0.30038500	2.10455400
C	0.52079100	2.80477600	2.18054500
H	-0.08592600	3.47629000	1.58004000
C	2.03283300	0.84309200	-2.21551300
H	1.57909900	-0.13136600	-2.37056600
C	2.30493300	2.83623400	-0.87898500
H	2.05268700	3.42695200	-0.00316900

C	-1.18205200	2.68278100	-1.60555200
H	-0.34162900	2.70362500	-2.29260100
C	3.25334300	3.30844200	-1.77880700
H	3.73428300	4.26593600	-1.60274100
C	-1.08412500	1.98650800	-0.39920100
C	3.58951900	2.55198300	-2.90030800
H	4.33406300	2.92069000	-3.59972200
C	2.05841900	1.08701400	3.74269600
H	2.65859000	0.41404000	4.34736600
C	0.86448900	1.54028600	1.68905500
C	1.68570400	1.60047700	-1.09413800
C	0.94317300	3.20344300	3.44494900
H	0.66952100	4.18556100	3.81904100
C	1.71252800	2.34550700	4.22715800
H	2.04071400	2.65794500	5.21418600
C	2.97975900	1.32051000	-3.11780000
H	3.24916500	0.72082700	-3.98156300
C	-2.35695500	3.35617600	-1.93307900
H	-2.42158000	3.89542500	-2.87351300
C	-2.17967400	1.96970100	0.47193300
H	-2.11966400	1.42079300	1.40816900
C	-3.34642800	2.64911500	0.14571400
H	-4.18938200	2.62594100	0.82951500
C	-3.43910100	3.34232000	-1.05943900
H	-4.35353900	3.86905600	-1.31596600
C	-2.28409400	-1.37605700	-0.25854900
C	-3.01696300	-1.24015800	0.94131900
C	-2.86441000	-1.00143500	-1.48167800
C	-4.34231700	-0.77764900	0.86581300
C	-4.15504500	-0.50753300	-1.53641700
H	-2.28907500	-1.12276400	-2.39497600
C	-4.89269000	-0.41695800	-0.35142700
H	-4.92218300	-0.67813600	1.77993100
H	-4.59184900	-0.21057200	-2.48339700
H	-5.91539000	-0.05203000	-0.38034500
N	-2.44592800	-1.49995900	2.16717100
H	-3.05824600	-1.78059800	2.91824100
H	-1.53367800	-1.93598900	2.18039700
I	2.31128500	-2.46216800	-0.05226500
C	-1.27840400	-2.89789900	-0.34276800
O	-1.68640100	-3.97640900	-0.45834800

**IntA6**

Pd	1.14423200	-0.73905800	-0.13115400
P	-1.18348900	-0.50514300	0.06499400

C	-3.52109000	0.10916400	3.39298500
H	-4.54525200	-0.08197500	3.69879800
C	-1.39374700	-3.27306400	0.07994000
H	-0.41145200	-3.24174000	0.54678700
C	-3.28431400	-2.14644700	-0.91330100
H	-3.78199500	-1.23330000	-1.22645700
C	-2.02879700	-2.08589100	-0.30053000
C	-3.89500200	-3.37735000	-1.13595700
H	-4.86815000	-3.41583300	-1.61608800
C	-2.63241100	1.83873500	-0.58587600
H	-2.73750300	2.00754900	0.48091800
C	-1.97076100	0.70331300	-1.05554600
C	-3.09118600	-0.28730800	2.13223400
H	-3.78192200	-0.78864000	1.46026500
C	-3.00204500	2.57343300	-2.85512300
H	-3.40160400	3.30160600	-3.55470400
C	-1.81935600	0.51405100	-2.43522700
H	-1.28272700	-0.35353600	-2.80932400
C	-1.77063100	-0.04886300	1.73314100
C	-3.25938500	-4.55416600	-0.74910900
H	-3.73607800	-5.51320400	-0.92791000
C	-3.14565600	2.77004500	-1.48575300
H	-3.65316100	3.65364300	-1.11102000
C	-1.32275900	0.97926300	3.87248800
H	-0.62948100	1.46688200	4.55107600
C	-2.00803000	-4.50116700	-0.14015800
H	-1.50405200	-5.41582400	0.15572500
C	-0.88507400	0.58110000	2.61119100
H	0.14691700	0.75492100	2.31370800
C	-2.63705000	0.74535200	4.26365500
H	-2.97425200	1.05179300	5.24948900
C	-2.33839300	1.44224900	-3.32948600
H	-2.21570200	1.28712800	-4.39684700
I	3.72984600	-1.38485300	-0.01416200
C	1.27775000	0.89480900	-1.22277000
O	1.35676200	0.69778600	-2.39694100
C	1.12282500	2.21869900	-0.57378300
C	1.54121600	2.56301500	0.73226800
C	0.44423300	3.16458800	-1.36327200
C	1.21933200	3.85083400	1.20142000
C	0.13424100	4.42069400	-0.88024000
C	0.52725100	4.75530500	0.41768100
H	1.52910700	4.12913800	2.20551000
H	-0.40992800	5.12624300	-1.49840100

H	0.29513900	5.73654200	0.82171100
H	0.13735000	2.86729500	-2.36035700
N	2.20389600	1.69810200	1.57423000
H	2.72777100	0.93083600	1.16608700
H	2.68450100	2.13016100	2.35048500

### IntA7

Pd	0.22039900	-0.75277800	-0.51755300
P	1.27191900	1.29367300	-0.11906700
P	-2.08346300	-0.08235700	0.12635700
C	0.32697600	3.54399400	3.22746600
H	0.05302800	4.56658800	3.46812500
C	-2.85664600	-0.58613200	-2.51020900
H	-1.87535100	-1.04121400	-2.60897000
C	-4.53141500	0.51722100	-1.16813000
H	-4.84752400	0.95455800	-0.22519800
C	-0.18255200	2.22394200	-2.30452300
H	-0.55965800	1.20634200	-2.35443600
C	-1.88294200	-1.69268400	2.36181500
H	-0.86276600	-1.31755900	2.38822400
C	1.25123400	3.87347700	-1.28544000
H	2.01253700	4.14153000	-0.55820600
C	0.73253000	2.57249400	-1.30833800
C	-4.03839900	-1.80308500	1.28729800
H	-4.71026300	-1.51888700	0.48393600
C	0.81421900	4.81956700	-2.20541000
H	1.21586100	5.82788100	-2.17392900
C	3.91068500	1.26797300	0.90449300
H	3.46724300	1.12983600	1.88498500
C	-2.65251400	1.65560500	2.30547000
H	-2.62257300	0.77624500	2.94000800
C	3.09932800	1.42315300	-0.22186900
C	-4.46706700	-2.70927300	2.25410000
H	-5.47173100	-3.11759000	2.19869400
C	-2.44729500	1.53703200	0.92900500
C	-3.61241400	-3.09609000	3.28137700
H	-3.94954900	-3.80427500	4.03246500
C	0.55718900	3.19160600	1.90093400
H	0.44186800	3.94087600	1.12621800
C	5.88361400	1.45824900	-0.47118400
H	6.96523300	1.46954900	-0.56753800
C	3.69537600	1.58102900	-1.47782900
H	3.07879600	1.67581400	-2.36624400
C	-3.71785200	-0.55515000	-3.60462300
H	-3.39458100	-0.97659600	-4.55143800

C	0.89150900	1.87728100	1.57365600	N	1.76365100	-2.30649400	1.65991600
C	-0.12529900	4.47039800	-3.17496700	H	0.99295300	-2.63690800	1.08341700
H	-0.46147500	5.21014900	-3.89546800	H	1.81635800	-2.85408600	2.51051800
C	-3.25618900	-0.05277800	-1.28142900	<b>IntA10</b>			
C	5.29603600	1.28465700	0.77775000	Pd	0.19606600	-0.83102900	-0.66838300
H	5.91536900	1.15544300	1.65992700	P	1.33584500	1.07176600	-0.05309600
C	-2.74511900	-1.28396600	1.33781400	P	-2.09198900	-0.09014600	0.04971300
C	0.74246200	1.27434500	3.91358000	C	0.56205000	2.88742900	3.59093000
H	0.80885800	0.52089400	4.69314700	H	0.34619200	3.87979100	3.97478900
C	-5.39111800	0.54247800	-2.26024000	C	-2.86892100	-0.35931600	-2.60691700
H	-6.37777100	0.98497900	-2.15965000	H	-2.02873800	-1.04634600	-2.66225600
C	-4.98432500	0.00680100	-3.48121200	C	-4.30230600	1.08914900	-1.30973300
H	-5.65550200	0.02994400	-4.33483900	H	-4.56139500	1.56805600	-0.37042300
C	-2.31809300	-2.58385700	3.33525400	C	-0.18325000	2.32059100	-2.03512000
H	-1.64159500	-2.89254000	4.12694100	H	-0.58468300	1.32787900	-2.21470100
C	-0.61339300	3.16895500	-3.23235700	C	-2.08592500	-2.31119000	1.70908300
H	-1.32835000	2.88147500	-3.99709900	H	-1.01803200	-2.12157500	1.77342700
C	0.96876500	0.91461400	2.58888800	C	1.33598000	3.78415100	-0.86835300
H	1.21150800	-0.11802100	2.33710700	H	2.13832300	3.93412800	-0.15133600
C	-2.90656100	2.89987900	2.87657800	C	0.78331000	2.50891100	-1.04374300
H	-3.06586200	2.97178200	3.94836400	C	-4.25639800	-1.76623200	0.80393200
C	-2.49026300	2.69376300	0.14041100	H	-4.88886800	-1.14305400	0.17891400
H	-2.34753600	2.62723400	-0.93279400	C	0.88013700	4.85774900	-1.62481000
C	0.42594600	2.59113700	4.23628600	H	1.30932300	5.84378200	-1.47437000
H	0.24363300	2.87130500	5.26968800	C	4.01076400	0.94256600	0.86155300
C	5.08017200	1.60411900	-1.59872000	H	3.60423600	0.71808400	1.84230500
H	5.53040200	1.72925600	-2.57887700	C	-2.60798700	1.15494200	2.53238900
C	-2.73860000	3.93568600	0.71289700	H	-2.64496800	0.15221600	2.94626900
H	-2.77049400	4.81859300	0.08116500	C	3.15729400	1.18546200	-0.21583800
C	-2.95240600	4.04236300	2.08489400	C	-4.80574200	-2.85387600	1.47484400
H	-3.15328900	5.01094100	2.53364100	H	-5.86562900	-3.06884100	1.37539400
I	-0.55899900	-3.35887200	-0.99549700	C	-2.39140500	1.33958700	1.16444400
C	2.00261900	-1.37331200	-1.23992700	C	-3.99712000	-3.67116800	2.26271500
O	2.15245200	-1.20730300	-2.42667400	H	-4.42597900	-4.52736500	2.77506800
C	3.11196700	-1.86376200	-0.36278300	C	0.76021600	2.71000700	2.22511900
C	2.98790900	-2.23939900	0.99294300	H	0.68033900	3.56535400	1.56438000
C	4.38733700	-1.83483600	-0.94632500	C	5.92713200	1.26562200	-0.56927000
C	4.15857700	-2.52139200	1.71557600	H	7.00412200	1.29620300	-0.70537500
C	5.53170500	-2.12356300	-0.22521700	C	3.70154700	1.45004200	-1.47752300
C	5.40822900	-2.45814900	1.12267900	H	3.04806300	1.61729600	-2.32888000
H	4.07053200	-2.80493400	2.76207700	C	-3.65481500	-0.11970400	-3.73085300
H	6.50683900	-2.07460200	-0.69865100	H	-3.40044900	-0.59853000	-4.67173300
H	6.29093100	-2.68202100	1.71539900	C	1.01751300	1.43727800	1.71340000
H	4.44696900	-1.54614200	-1.98988400	C	-0.11451100	4.66641400	-2.58341000

H	-0.46702900	5.50668700	-3.17426600
C	-3.18226700	0.25300200	-1.38647000
C	5.39019900	0.98185200	0.68210900
H	6.04487000	0.78404000	1.52520300
C	-2.89116500	-1.48756600	0.91728300
C	0.86123700	0.52643100	3.95034600
H	0.89359500	-0.33031200	4.61728900
C	-5.08479900	1.32396200	-2.43649700
H	-5.94956600	1.97712200	-2.36408200
C	-4.75863600	0.72502500	-3.65066100
H	-5.36704200	0.91300100	-4.53067700
C	-2.63778800	-3.39847200	2.37967800
H	-1.99749700	-4.04617300	2.96969300
C	-0.63557600	3.39455000	-2.79806200
H	-1.39378000	3.22821000	-3.55713100
C	1.05023100	0.34052800	2.58441800
H	1.22270200	-0.65961800	2.18618300
C	-2.78705800	2.24995100	3.37315100
H	-2.95475700	2.08729000	4.43360800
C	-2.33573000	2.64608600	0.66128100
H	-2.16261600	2.81711700	-0.39619000
C	0.62093300	1.80021400	4.45712400
H	0.46494900	1.94416900	5.52236400
C	5.07994900	1.49575400	-1.65008200
H	5.49138100	1.70587900	-2.63276600
C	-2.52271200	3.73758300	1.50169700
H	-2.48664600	4.74174100	1.08926500
C	-2.75330500	3.54275600	2.86095500
H	-2.90094500	4.39478200	3.51826300
C	1.87885000	-1.54818700	-1.50461400
O	1.92593500	-1.45175500	-2.70800400
C	3.02787200	-2.06771700	-0.70376500
C	2.94622400	-2.51863400	0.63206900
C	4.28345200	-1.97592300	-1.32220800
C	4.14561500	-2.79313900	1.31256500
C	5.45431500	-2.26406100	-0.64384400
C	5.37564500	-2.66217300	0.69107100
H	4.09346000	-3.13451200	2.34420800
H	6.41535300	-2.16155200	-1.13721600
H	6.28110800	-2.88356900	1.24982100
H	4.30844200	-1.63544100	-2.35185500
N	1.73214700	-2.67750000	1.28687200
H	0.98764000	-3.10905900	0.71337200
H	1.83237300	-3.19756800	2.15114600

O	-0.89087300	-2.47447200	-1.47651300
C	-0.96116300	-3.64488500	-0.95796500
O	-0.21869400	-4.09910600	-0.07620500
C	-2.12182700	-4.48505100	-1.46288900
H	-2.30836600	-4.30145300	-2.52360100
H	-1.93550500	-5.54546200	-1.28339100
H	-3.01718900	-4.18599600	-0.90381500

### IntA13

Pd	0.64081700	0.63552700	0.05875800
P	1.06266700	-1.63461100	0.17326700
P	-1.84327400	0.55485200	-0.06854500
C	-1.41880900	-4.36620000	-1.72263000
H	-1.98026000	-5.25900900	-1.46413500
C	-1.58951700	2.05120100	2.29526500
H	-0.54382600	2.13954700	2.01556500
C	-3.79972800	1.18177800	1.90284500
H	-4.48980200	0.58182400	1.31672900
C	0.19612500	-1.55467300	2.80688600
H	0.04462000	-0.49778600	2.60366600
C	-1.65766600	1.84543100	-2.50392400
H	-0.66507000	1.39383500	-2.54321500
C	0.92436600	-3.73502800	2.08245300
H	1.34182900	-4.38824000	1.32156800
C	0.71726700	-2.37730100	1.80389400
C	-3.75567700	2.23301100	-1.36190400
H	-4.40865200	2.08350600	-0.50777000
C	0.59938700	-4.25704300	3.32997800
H	0.76365600	-5.31122700	3.53176600
C	3.25593900	-1.62411700	-1.51125300
H	2.62615100	-1.00389500	-2.14530900
C	-3.52893000	-1.33517300	-1.32584900
H	-3.46480700	-0.70894000	-2.21027700
C	2.78425100	-2.07713200	-0.27306800
C	-4.17753500	3.04005200	-2.41139800
H	-5.15689000	3.50800800	-2.37199000
C	-2.86100900	-0.96548100	-0.15780200
C	-3.34204700	3.25449300	-3.50807900
H	-3.67159400	3.89288400	-4.32288400
C	-0.68526100	-3.71145000	-0.73784700
H	-0.70583800	-4.09991300	0.27332600
C	5.40147000	-2.64213800	-1.07347100
H	6.41812700	-2.86397200	-1.38505100
C	3.64260700	-2.77974900	0.57296600
H	3.31716500	-3.08354300	1.56133600

C	-2.03537000	2.65723300	3.46744400	H	4.26202300	2.37476300	2.44885300
H	-1.33689200	3.22273200	4.07695600	N	0.61962200	2.78235900	-0.22919000
C	0.03539900	-2.55474600	-1.04477200	H	-0.27311700	3.27146700	-0.20793600
C	0.06650800	-3.42976600	4.31659100	O	1.83772600	2.87350600	-2.59121300
H	-0.18754500	-3.83950100	5.28973000	H	0.99428800	2.83267200	-1.23551500
C	-2.46676300	1.31481800	1.49137800	C	2.02350600	1.69059900	-2.97416900
C	4.55609000	-1.91437800	-1.90788600	C	3.22448900	1.41635100	-3.87410700
H	4.91125900	-1.55738400	-2.87032700	H	4.04471200	1.04597100	-3.24654400
C	-2.49223500	1.62976400	-1.40162300	H	2.98773600	0.63997500	-4.60715300
C	-0.75843900	-2.70192900	-3.32603200	H	3.55876500	2.32715100	-4.37526300
H	-0.79137300	-2.29215100	-4.33131000	O	1.31483500	0.69847100	-2.64223900
C	-4.24541300	1.78741200	3.07256800	<b>TSA4</b>			
H	-5.28198700	1.67354900	3.37575100	Pd	0.45271800	0.78131500	0.02625000
C	-3.36483300	2.53036300	3.85615100	P	1.40190900	-1.32100300	0.22236500
H	-3.71350800	3.00019200	4.77107200	P	-1.94824600	0.14531800	-0.08257300
C	-2.08655100	2.65864800	-3.55210700	C	-0.35928100	-4.69165300	-1.43207000
H	-1.42271100	2.83166800	-4.39339600	H	-0.63346400	-5.69472000	-1.11911500
C	-0.13165600	-2.07764400	4.05485600	C	-2.12730200	1.95006500	2.05880300
H	-0.53880800	-1.42441000	4.82061300	H	-1.15028200	2.28989100	1.73155800
C	-0.02548300	-2.03903600	-2.34674000	C	-4.01147600	0.46400900	1.85258200
H	0.48529600	-1.11312600	-2.60052700	H	-4.50892800	-0.37151500	1.36869900
C	-4.28363700	-2.50515600	-1.36064300	C	0.64119000	-1.34415700	2.88947300
H	-4.79840900	-2.78207700	-2.27570100	H	0.18838300	-0.38487300	2.65056900
C	-2.93890500	-1.79793000	0.96603500	C	-2.06314600	1.17596000	-2.64719400
H	-2.41523800	-1.53173300	1.87990000	H	-0.98379800	1.02371400	-2.64495500
C	-1.44841000	-3.87116600	-3.02169800	C	1.94661200	-3.25849900	2.22215900
H	-2.02206800	-4.38461600	-3.78814700	H	2.51807100	-3.79609900	1.47059100
C	4.94461900	-3.06503800	0.17003100	C	1.33854600	-2.03901700	1.89756000
H	5.60477800	-3.60942000	0.83891300	C	-4.21108000	1.08297900	-1.53933900
C	-3.69750000	-2.96128600	0.92961000	H	-4.81474300	0.85141700	-0.66716700
H	-3.75456800	-3.59226600	1.81173100	C	1.83362100	-3.78210200	3.50558000
C	-4.37738900	-3.31487400	-0.23376500	H	2.30782900	-4.72911800	3.74504600
H	-4.97201400	-4.22328700	-0.26331200	C	3.47393100	-1.13662200	-1.63134400
C	2.38605500	1.05130400	0.99624700	H	2.68933400	-0.92464100	-2.35042900
O	3.17553000	0.28859900	1.49816200	C	-3.14464600	-2.23067200	-1.06284600
C	2.52167100	2.53874500	1.21679200	H	-3.27363600	-1.70817200	-2.00548800
C	1.58236400	3.38894800	0.63788700	C	3.16289900	-1.37813000	-0.28809100
C	3.54013400	3.05997500	2.01635500	C	-4.81851000	1.61377600	-2.67075700
C	1.63131300	4.75849200	0.88303800	H	-5.89038900	1.78875100	-2.67610100
C	3.59366100	4.42570100	2.26224300	C	-2.55505000	-1.58101900	0.02196800
C	2.63391500	5.26996600	1.70104800	C	-4.05222200	1.92510000	-3.79414400
H	0.90242900	5.41863200	0.42139000	H	-4.52900900	2.34315500	-4.67613100
H	4.37397200	4.83590100	2.89579700	C	0.23174200	-3.82703400	-0.51558400
H	2.67337200	6.33817200	1.89327900	H	0.39373800	-4.16880000	0.50021700

C	5.82882000	-1.32921400	-1.13538000
H	6.86370700	-1.31313900	-1.46476300
C	4.19926200	-1.56105600	0.62922200
H	3.98125700	-1.69404400	1.68257000
C	-2.72884100	2.55996600	3.15690900
H	-2.21617300	3.37203700	3.66366300
C	0.58101000	-2.52885500	-0.89418400
C	1.11885200	-3.09015300	4.48156100
H	1.03266400	-3.49984900	5.48366000
C	-2.76427800	0.90132800	1.38658800
C	4.79953300	-1.11901400	-2.05001100
H	5.02589700	-0.93182900	-3.09571800
C	-2.82901200	0.85819000	-1.52053500
C	-0.29393900	-2.96943200	-3.10862400
H	-0.50556400	-2.62058000	-4.11508600
C	-4.61179600	1.07358500	2.94887200
H	-5.57861600	0.72201900	3.29693000
C	-3.97301100	2.12564100	3.60209500
H	-4.44179400	2.59868800	4.45997700
C	-2.67909500	1.70625600	-3.78019000
H	-2.07413700	1.95271900	-4.64750800
C	0.52724300	-1.86875000	4.17408700
H	-0.01845400	-1.31765400	4.93387800
C	0.28888400	-2.09728100	-2.19488700
H	0.51348000	-1.07913200	-2.50084100
C	-3.57078200	-3.55133300	-0.94215700
H	-4.02649000	-4.04555100	-1.79494000
C	-2.37901000	-2.28238000	1.22165300
H	-1.91558700	-1.79545300	2.07473900
C	-0.61167000	-4.27099600	-2.73361800
H	-1.07139100	-4.94975900	-3.44634200
C	5.52494100	-1.54308100	0.20464800
H	6.32064600	-1.68492200	0.92992900
C	-2.80756800	-3.59827400	1.34026200
H	-2.66759900	-4.12534800	2.27944000
C	-3.41074200	-4.23528500	0.25792600
H	-3.74758700	-5.26385900	0.34847300
C	2.04296900	1.64664400	0.95053700
O	2.96615600	1.09789500	1.50308400
C	1.79219900	3.11606000	1.11471600
C	0.69802000	3.66417600	0.43537100
C	2.58350100	3.90630800	1.94943800
C	0.36584300	5.00569500	0.64645100
C	2.25591600	5.24034800	2.15055500

C	1.14006500	5.77888000	1.50396400
H	-0.48260800	5.44041400	0.12475500
H	2.85113000	5.85750300	2.81618600
H	0.87584100	6.82070000	1.66374200
H	3.42952300	3.44679600	2.45091500
N	0.03861200	2.81390600	-0.46926400
H	-0.91509700	3.11315500	-0.66000700
O	1.54073900	2.96706400	-2.44580400
H	0.72271600	2.85607800	-1.55250400
C	1.80497700	1.85297900	-3.02672800
C	3.08918900	1.83671400	-3.83340200
H	3.28532500	2.81474000	-4.27819300
H	3.91475700	1.60314900	-3.15076500
H	3.04675600	1.06358000	-4.60388000
O	1.11562900	0.82430100	-2.93934700

### IntA14

Pd	0.24710000	1.16144300	0.03027300
P	1.81645800	-0.56960900	-0.05166900
P	-1.79969400	-0.31470700	0.05347200
C	0.98842400	-3.86290300	-2.44233600
H	1.02121100	-4.94597700	-2.37493000
C	-2.44338300	1.10661700	2.35643600
H	-1.78274200	1.86110200	1.93325800
C	-3.53138100	-1.04372800	2.20297000
H	-3.70733900	-1.97907900	1.68017300
C	1.03927500	-1.19730700	2.54730400
H	0.37189600	-0.34589100	2.43683300
C	-2.53184700	0.90265100	-2.33936400
H	-1.46601800	1.08468200	-2.44194900
C	2.77164500	-2.62153700	1.66215400
H	3.47574200	-2.87068500	0.87296800
C	1.88271200	-1.55302300	1.49118300
C	-4.39273300	0.08232600	-1.04104300
H	-4.78174800	-0.39531000	-0.14652300
C	2.77535300	-3.35124400	2.84569000
H	3.46397600	-4.18237900	2.96497500
C	4.12084000	-0.45300300	-1.69077900
H	3.48560900	-0.77502200	-2.50961300
C	-2.28008300	-2.71004200	-1.37816800
H	-2.65136300	-2.08095300	-2.18060700
C	3.59419900	-0.29730100	-0.40619200
C	-5.27033200	0.51026800	-2.03093600
H	-6.33884800	0.36305200	-1.90496600
C	-1.83473300	-2.13596700	-0.18506400

C	-4.78048100	1.13017700	-3.17943300
H	-5.46790300	1.46649300	-3.95006800
C	1.36088100	-3.09645300	-1.34183000
H	1.66763600	-3.59374100	-0.42847500
C	6.30371800	0.19576600	-0.89399500
H	7.35603400	0.38701800	-1.08296800
C	4.43751300	0.11282000	0.63195100
H	4.04028700	0.25339200	1.63094400
C	-3.08187100	1.33748900	3.57202700
H	-2.90307800	2.26874400	4.10111300
C	1.30725700	-1.70367900	-1.40342200
C	1.90811700	-3.00709600	3.88178600
H	1.91674400	-3.57476800	4.80764900
C	-2.66203100	-0.08937200	1.66068900
C	5.46981600	-0.20665200	-1.93217300
H	5.86722800	-0.33463600	-2.93471200
C	-3.01470700	0.27208600	-1.18854200
C	0.48986400	-1.86075700	-3.68277900
H	0.14527400	-1.37206900	-4.58925200
C	-4.16493900	-0.80913200	3.41947600
H	-4.83501000	-1.55882100	3.83017800
C	-3.93965900	0.38085600	4.10730200
H	-4.43239200	0.56103500	5.05836000
C	-3.41153900	1.32667400	-3.33265200
H	-3.02554400	1.82056700	-4.21924100
C	1.04869000	-1.92244100	3.73664200
H	0.38593600	-1.63397400	4.54683500
C	0.85493000	-1.09448400	-2.58093200
H	0.79463800	-0.00929600	-2.63074000
C	-2.25366400	-4.09173500	-1.54934300
H	-2.60392800	-4.52046700	-2.48362600
C	-1.34664300	-2.97490300	0.82528100
H	-0.99442500	-2.55399300	1.76103400
C	0.56065800	-3.24936100	-3.61561600
H	0.27020400	-3.85226500	-4.47098500
C	5.78399800	0.35386200	0.38842700
H	6.42666300	0.67466300	1.20260100
C	-1.32325200	-4.35372000	0.65321400
H	-0.94601500	-4.98539800	1.45208200
C	-1.78067200	-4.91770600	-0.53536000
H	-1.76542200	-5.99529100	-0.67070800
C	1.61939400	2.64605400	0.37784700
O	2.73247900	2.45597600	0.80688500
C	1.02946200	3.97632700	0.15030700

C	-0.35404600	3.99352400	-0.14239900
C	1.77800100	5.15434600	0.23332100
C	-0.95490000	5.25509200	-0.38094500
C	1.17506500	6.37886300	-0.00118600
C	-0.19529900	6.40829500	-0.31118400
H	-2.01569900	5.30612900	-0.61510600
H	1.74697700	7.29970500	0.04880800
H	-0.67686600	7.36523300	-0.50030500
H	2.83494300	5.08060700	0.47316300
N	-0.98730100	2.80260700	-0.14848900
H	-1.95316900	2.81664300	-0.45145000

### TSA5

C	-0.89268000	2.71890400	0.61863900
O	-1.80804700	2.77727900	1.39614200
C	-0.21093400	3.89977400	0.03307200
C	1.07127200	3.65687800	-0.47155000
C	-0.78938100	5.16739800	-0.01956400
C	1.76264700	4.70924300	-1.08833000
C	-0.10483500	6.20173700	-0.64334100
C	1.16503900	5.95975100	-1.17979400
H	2.76463900	4.54338300	-1.47530500
H	-0.55105100	7.18806000	-0.72172300
H	1.70221400	6.76842000	-1.66842700
H	-1.77733100	5.31453600	0.40620800
N	1.60095600	2.39350000	-0.22287700
H	2.35560700	2.15608100	-0.86028300
C	2.61424900	2.45917700	1.48737000
O	3.70267900	2.07809100	1.18161100
O	1.83055400	2.82909400	2.30729700
Pd	0.02998200	0.99666400	0.03939200
P	-2.00724000	-0.18212800	0.02553200
C	-2.37971200	-1.02262600	-1.56099400
C	-3.57308700	0.71715500	0.31796500
C	-2.00535400	-1.50864200	1.29018400
C	-1.37826900	-1.16334600	-2.52205900
C	-3.65867500	-1.52490000	-1.83630700
C	-4.40761100	0.44841000	1.40064800
C	-3.93517700	1.70667400	-0.60218800
C	-2.65555600	-2.73653700	1.13511700
C	-1.25174700	-1.27843500	2.44550900
H	-0.39640400	-0.74325600	-2.33518400
C	-1.62949000	-1.83252800	-3.71631100
H	-4.46307200	-1.37970600	-1.12039900
C	-3.91122400	-2.19118100	-3.02981200

H	-4.13477200	-0.31037100	2.12722300
C	-5.59595000	1.15985400	1.55977600
H	-3.27920900	1.93403000	-1.43920900
C	-5.12061100	2.41032500	-0.44487100
C	-2.53450000	-3.72144600	2.11053000
H	-3.22749900	-2.94369500	0.23695800
C	-1.12232200	-2.26705700	3.41622200
H	-0.74454800	-0.32641500	2.57349700
C	-2.89373100	-2.35353800	-3.96854800
H	-0.83339800	-1.94503400	-4.44551200
H	-4.90595500	-2.57739500	-3.23114900
C	-5.95441800	2.13766700	0.63940200
H	-6.23853600	0.94791000	2.40908000
H	-5.39186600	3.17832600	-1.16288900
H	-3.03515500	-4.67586400	1.97577000
C	-1.75971300	-3.49293600	3.24644000
H	-0.50570800	-2.08235400	4.29018000
H	-3.09227600	-2.87501400	-4.90026200
H	-6.87950600	2.69208600	0.76656400
H	-1.65101100	-4.27120400	3.99590300
H	1.92829000	0.43677700	-2.64345700
C	2.93989100	0.23825600	-2.29420400
C	4.02560800	0.66429000	-3.05205500
C	3.13725200	-0.42258200	-1.07445000
H	3.85900800	1.17451900	-3.99602000
C	5.32133600	0.45136700	-2.58648300
P	1.64634400	-0.93954800	-0.14902700
C	4.43792100	-0.62518400	-0.61342400
C	5.52335100	-0.18762700	-1.36714500
H	6.17125500	0.79496600	-3.16842500
C	1.19524000	-2.53711900	-0.93789900
C	2.23858400	-1.45584400	1.50271100
H	4.60679100	-1.10421400	0.34519400
H	6.53103100	-0.33816000	-0.99234900
C	0.32792000	-3.39590400	-0.25255100
C	1.58667800	-2.87024700	-2.23735000
C	2.07454900	-0.57994900	2.57931000
C	2.84845200	-2.69714900	1.72045400
H	0.04023700	-3.17455900	0.76999600
C	-0.16214100	-4.54282600	-0.86496100
H	2.27420300	-2.23124900	-2.78245800
C	1.09844200	-4.02347600	-2.84684400
H	1.59949100	0.38570800	2.43522000
C	2.51246000	-0.93584000	3.85157500

H	2.97790400	-3.39033000	0.89437300
C	3.27875900	-3.05471400	2.99366200
H	-0.84214700	-5.18882300	-0.31762100
C	0.21420900	-4.85628200	-2.16853000
H	1.41296600	-4.26918400	-3.85706800
C	3.11056900	-2.17472200	4.06116400
H	2.38497600	-0.23867900	4.67381400
H	3.74713400	-4.02161400	3.15190500
H	-0.17302700	-5.74945900	-2.64956400
H	3.44896500	-2.45515100	5.05440800

### IntA15

C	-1.08607700	2.67925000	0.58061000
O	-2.06229600	2.72527300	1.27626000
C	-0.40818400	3.90132400	0.05268100
C	0.92275900	3.76289200	-0.32647700
C	-1.05900200	5.12834400	-0.05878700
C	1.61443000	4.85187300	-0.85169500
C	-0.37936500	6.21013700	-0.60634600
C	0.95112200	6.06590200	-1.00498200
H	2.66200400	4.75027000	-1.12065800
H	-0.88132800	7.16518900	-0.72610200
H	1.48226300	6.91398700	-1.42737500
H	-2.09139600	5.21059200	0.26578500
N	1.53005700	2.50220200	-0.06781500
H	2.29086300	2.31805200	-0.71807300
C	2.20497700	2.42017500	1.37990800
O	3.39195200	2.13575500	1.29937200
O	1.38078400	2.58682100	2.27828200
Pd	-0.04119200	1.00904500	0.07880700
P	-1.99029700	-0.28273400	0.02926700
C	-2.30235600	-1.11765500	-1.57140000
C	-3.61435300	0.49148400	0.35193700
C	-1.87365000	-1.61294500	1.28333500
C	-1.30824700	-1.13083000	-2.54993600
C	-3.53045300	-1.73549000	-1.84409100
C	-4.32848900	0.26060700	1.52590700
C	-4.13742400	1.35695100	-0.61448800
C	-2.48517100	-2.86321600	1.14741800
C	-1.08154900	-1.35949600	2.40752800
H	-0.36964000	-0.62088800	-2.36297800
C	-1.51214100	-1.78765700	-3.75986000
H	-4.33599500	-1.68605900	-1.11678200
C	-3.73523000	-2.39070400	-3.05253700
H	-3.92877000	-0.40077300	2.28797900



C	-5.55697600	0.88571500	1.72992100
H	-3.58048800	1.55104000	-1.52790900
C	-5.36279300	1.97574900	-0.41083000
C	-2.28648700	-3.84761600	2.10956000
H	-3.08618200	-3.08799800	0.27308800
C	-0.87537800	-2.34841000	3.36540100
H	-0.60243500	-0.39083100	2.52277100
C	-2.72221300	-2.42526500	-4.00929100
H	-0.72117700	-1.80028800	-4.50293500
H	-4.69028500	-2.86753900	-3.25156900
C	-6.07546400	1.74102100	0.76457600
H	-6.10539000	0.70370900	2.64919900
H	-5.76106200	2.64654000	-1.16612500
H	-2.75614300	-4.81951900	1.98947000
C	-1.47329000	-3.59568400	3.21383400
H	-0.22730400	-2.14543200	4.21191700
H	-2.88345300	-2.93811500	-4.95287000
H	-7.03221600	2.22856400	0.92654200
H	-1.30370600	-4.37349300	3.95234300
H	1.84876500	0.60947700	-2.61008700
C	2.87457000	0.49104300	-2.26498700
C	3.91678500	1.03094800	-3.01138700
C	3.13209700	-0.18375800	-1.06404300
H	3.70408400	1.54975100	-3.94141600
C	5.22754400	0.91752500	-2.55228200
P	1.69888100	-0.83727500	-0.13389700
C	4.44571800	-0.28257900	-0.60740300
C	5.48690200	0.26603700	-1.35065600
H	6.04305200	1.34895000	-3.12494400
C	1.31043500	-2.40750000	-1.00825700
C	2.36019100	-1.41757300	1.46971800
H	4.65539200	-0.76309800	0.34198300
H	6.50432200	0.19568700	-0.97883600
C	0.47672200	-3.33335500	-0.36985000
C	1.72753300	-2.66725700	-2.31623500
C	2.23014400	-0.60199500	2.59826200
C	3.00132900	-2.65718100	1.58908900
H	0.17847800	-3.17419100	0.66075900
C	0.03773000	-4.46969600	-1.03769600
H	2.39407900	-1.97837000	-2.82500700
C	1.29301100	-3.81164400	-2.98093500
H	1.74760500	0.36971100	2.53920100
C	2.72805600	-1.02728300	3.82707500
H	3.11154300	-3.29874700	0.71989800

C	3.49051800	-3.08008200	2.81989600
H	-0.61834500	-5.16741300	-0.52574600
C	0.43657200	-4.70834800	-2.35050300
H	1.62755800	-3.99966500	-3.99712900
C	3.35192000	-2.26560000	3.94205500
H	2.62891300	-0.37779000	4.69114200
H	3.98184700	-4.04516900	2.90138200
H	0.09008400	-5.59382900	-2.87490200
H	3.73598100	-2.59543800	4.90314900

### IntA16

C	1.96602600	1.19284300	-1.55624300
O	2.02583400	0.71487500	-2.66359100
C	3.03609700	2.01293700	-0.95133100
C	2.86302100	2.94003800	0.09780000
C	4.33072100	1.72086300	-1.41077300
C	4.02096700	3.48140000	0.68888800
C	5.45490300	2.27357000	-0.82829100
C	5.28840800	3.15027300	0.24486300
H	3.90608500	4.19514800	1.50113700
H	6.44514200	2.01658500	-1.18944100
H	6.15340700	3.59323400	0.73051400
H	4.42325700	1.00767600	-2.22293800
N	1.64475900	3.36440400	0.60984200
H	1.72128100	4.00682900	1.38640500
C	0.38746800	3.55821200	-0.04061800
O	-0.38871400	4.32244900	0.52041800
O	0.19074500	2.89904700	-1.12958600
Pd	0.25877900	0.80653800	-0.59653900
P	1.17197900	-1.18175100	0.14855500
C	0.76304500	-1.59301600	1.88302900
C	3.00382300	-1.24823700	0.19988000
C	0.69557400	-2.59029300	-0.91544400
C	-0.04743700	-0.72655000	2.61697100
C	1.30645900	-2.71690900	2.51903700
C	3.76403200	-1.95669500	-0.72992700
C	3.65148300	-0.48813100	1.18181600
C	0.34600400	-3.85569600	-0.44378000
C	0.72120000	-2.35266000	-2.29737800
H	-0.42915800	0.17584900	2.15333200
C	-0.36565600	-1.00137600	3.94452300
H	1.99633200	-3.36400400	1.98441300
C	0.98580900	-2.99603600	3.84248100
H	3.27696200	-2.54218400	-1.50318800
C	5.15635600	-1.91590300	-0.66905100

H	3.06804300	0.08692200	1.89610300
C	5.03748800	-0.45457700	1.24267000
C	0.05564400	-4.87978200	-1.34105600
H	0.26972500	-4.04550800	0.62077600
C	0.43408700	-3.38119100	-3.18811700
H	0.97786000	-1.36440500	-2.67305800
C	0.14043200	-2.14451700	4.55407000
H	-1.00695500	-0.31614000	4.49093300
H	1.40567300	-3.87376300	4.32454000
C	5.79381200	-1.17079800	0.31644300
H	5.74016100	-2.47253300	-1.39615700
H	5.52774900	0.14692100	2.00150900
H	-0.22330500	-5.85876600	-0.96277400
C	0.10701300	-4.64866400	-2.71155300
H	0.46413700	-3.18825500	-4.25621400
H	-0.10598800	-2.36577100	5.58834200
H	6.87845700	-1.13913100	0.35943200
H	-0.11775800	-5.45144300	-3.40784700
H	-1.37730900	2.57578000	1.63388300
C	-2.25874100	2.11889500	2.07584900
C	-2.78298000	2.65300300	3.25088200
C	-2.89170600	1.04167400	1.44850100
H	-2.28615400	3.49693500	3.71923300
C	-3.93901600	2.11648100	3.80866500
P	-2.16595800	0.42469700	-0.11945900
C	-4.07109400	0.52663400	1.99891400
C	-4.58651900	1.05604000	3.17657600
H	-4.34465300	2.53051100	4.72730000
C	-2.59412000	-1.35868700	-0.17634000
C	-3.25511400	1.17452700	-1.38770200
H	-4.58686300	-0.29605400	1.51261100
H	-5.49872500	0.64421500	3.59839400
C	-2.73253800	-1.97989700	-1.42427000
C	-2.67516500	-2.14457100	0.97739800
C	-2.78737800	2.29312600	-2.08324400
C	-4.55340900	0.70391700	-1.62110400
H	-2.64554400	-1.39365000	-2.33449400
C	-2.99563400	-3.34122700	-1.51182900
H	-2.54531500	-1.69479200	1.95587200
C	-2.93599500	-3.50966200	0.88726700
H	-1.78848700	2.67942500	-1.88960400
C	-3.61443000	2.92534400	-3.01084600
H	-4.92457000	-0.16493200	-1.08471700
C	-5.36927800	1.33643000	-2.55049500

H	-3.10100000	-3.80475600	-2.48765000
C	-3.10891300	-4.10881700	-0.35530000
H	-3.00576700	-4.10089600	1.79567800
C	-4.89878100	2.44866200	-3.24823900
H	-3.24570400	3.79484200	-3.54636000
H	-6.37350300	0.96351100	-2.72994100
H	-3.31580100	-5.17270200	-0.42549800
H	-5.53791700	2.94272000	-3.97452800

### TSA6

Pd	-0.18567400	-0.82390500	-0.37255000
P	-1.29052500	1.16801000	0.07722300
P	2.24620100	-0.47190100	-0.05650900
C	-0.16216600	2.75863100	3.71745800
H	-0.49757100	2.69909300	4.74880200
C	2.95676800	-3.05092400	-0.79046300
H	2.10244000	-3.36121700	-0.19332400
C	4.36987900	-1.32964100	-1.73524300
H	4.62321300	-0.28126400	-1.86318600
C	-3.28536700	0.02540900	1.62372800
H	-2.49627600	-0.66267600	1.91954100
C	3.66535700	1.99929900	-0.25743100
H	4.20448400	1.71402800	0.64085300
C	-4.04544400	1.86513500	0.26214800
H	-3.85480200	2.63424900	-0.47980700
C	-3.01209300	1.02677700	0.68448600
C	2.03383100	1.52021400	-1.96585100
H	1.29281800	0.85361600	-2.39996300
C	-5.32717500	1.71523300	0.78595200
H	-6.12572200	2.36835100	0.44642100
C	-1.47514600	3.70528500	-1.18794700
H	-1.48128300	4.13943200	-0.19255300
C	4.31467900	-0.77752000	1.86849200
H	4.93126100	-1.16795100	1.06396100
C	-1.39101600	2.31706300	-1.34583100
C	2.24872300	2.77130900	-2.53274800
H	1.67414900	3.07120600	-3.40400900
C	2.99147200	-0.40208800	1.61379400
C	3.17243400	3.64321700	-1.95857800
H	3.33319800	4.62705400	-2.38953300
C	-0.88629300	2.10652300	2.72231000
H	-1.77650200	1.54923400	2.99454200
C	-1.51738400	3.99044900	-3.58313300
H	-1.56045400	4.64129900	-4.45166400
C	-1.38335100	1.77420600	-2.63501600

H	-1.31866800	0.69792100	-2.77219700
C	3.73083800	-4.02075000	-1.42020800
H	3.47013700	-5.06756500	-1.29855000
C	-0.47365500	2.16980900	1.38757600
C	-5.58363900	0.73734800	1.74173400
H	-6.58363100	0.62395300	2.14992900
C	3.27803000	-1.69688000	-0.94165000
C	-1.53347900	4.53688500	-2.30145000
H	-1.59047500	5.61304200	-2.16745800
C	2.72748400	1.12773500	-0.81507800
C	1.38843800	3.56534800	2.06530800
H	2.27685700	4.12746800	1.79462600
C	5.13519100	-2.30553600	-2.36752700
H	5.97913300	-2.01181000	-2.98512600
C	4.81741600	-3.65207900	-2.20918000
H	5.41334600	-4.41267200	-2.70567200
C	3.88667400	3.25078300	-0.82903900
H	4.61200400	3.92510700	-0.38247000
C	-4.55901500	-0.10709400	2.16240900
H	-4.75765500	-0.88987300	2.88734700
C	0.66736100	2.91622400	1.06967000
H	0.99785800	2.99601100	0.03977000
C	4.84156400	-0.65905300	3.15118500
H	5.86849900	-0.95721700	3.34109600
C	2.20319600	0.07759500	2.66353800
H	1.17001200	0.35538300	2.47903400
C	0.98109000	3.48334300	3.39376500
H	1.54960800	3.98367400	4.17191000
C	-1.44854100	2.60973900	-3.74739100
H	-1.43971300	2.17641300	-4.74298600
C	2.73436700	0.20419800	3.94306100
H	2.11100100	0.58729900	4.74540800
C	4.05421300	-0.16394400	4.18863400
H	4.46839300	-0.07305700	5.18869100
C	-1.69958700	-1.74249800	-1.41619200
O	-1.54600400	-1.50098700	-2.58865700
C	-2.94983900	-2.18137000	-0.76307600
C	-2.98383800	-3.07264800	0.31925800
C	-4.14170100	-1.63594900	-1.25170000
C	-4.22407400	-3.39855300	0.88618600
C	-5.36153200	-1.95223100	-0.67749000
C	-5.39467400	-2.84218500	0.39640100
H	-4.25866600	-4.10146500	1.71481500
H	-6.27655100	-1.51263600	-1.05945800

H	-6.34221200	-3.10714300	0.85632500
H	-4.08481600	-0.95049500	-2.09107300
N	-1.83396000	-3.63812800	0.84551900
H	-1.93250800	-4.26703300	1.62874300
C	-0.56896500	-3.69099600	0.25404000
O	0.30436800	-4.36201200	0.77709100
O	-0.43380200	-3.00322200	-0.85572400

### IntA17

Pd	0.06655500	-0.31511000	-0.87134900
P	2.32483400	-0.16156400	-0.37696400
P	-1.63009100	1.05610700	-0.15245900
C	1.96898100	2.04585500	3.08857900
H	1.76581800	3.08079200	3.34751200
C	-3.63004600	0.55491800	-1.99809600
H	-3.03323200	-0.32906500	-2.20696100
C	-3.93867400	2.61652400	-0.78611800
H	-3.59258400	3.33969400	-0.05231800
C	2.64577500	1.53144800	-2.55682400
H	1.84488600	0.92541700	-2.97464100
C	-1.24015600	0.26540300	2.47981200
H	-0.18824700	0.34973900	2.22539500
C	4.12501600	2.04460800	-0.73041900
H	4.49005600	1.85598500	0.27478500
C	3.11109700	1.24587800	-1.26944400
C	-3.56425700	0.43997600	1.86677100
H	-4.33701600	0.68438300	1.14423800
C	4.65132600	3.10808700	-1.45706600
H	5.43162700	3.72472200	-1.02034400
C	3.28985400	-2.67496200	-1.06337700
H	2.29844700	-2.82170600	-1.48096100
C	-1.03587800	3.45258800	1.30150100
H	-1.69604900	3.09219400	2.08500300
C	3.61073100	-1.47164300	-0.43349000
C	-3.92649500	-0.04435400	3.12469600
H	-4.97790200	-0.16328600	3.37215400
C	-0.86353800	2.70667700	0.13352400
C	-2.94771300	-0.36977800	4.06115400
H	-3.23232500	-0.74971300	5.03807300
C	2.11207800	1.69534300	1.74990200
H	2.00592000	2.46138000	0.98792000
C	5.49468400	-3.53136900	-0.58968100
H	6.22720200	-4.33153700	-0.64772200
C	4.88427600	-1.31127600	0.12676300
H	5.14143900	-0.38850900	0.63897800

C	-4.82341600	0.77485400	-2.68156000
H	-5.16049400	0.05662000	-3.42365000
C	2.36590900	0.36665700	1.38531200
C	4.17876000	3.38314500	-2.73848200
H	4.59029700	4.21420200	-3.30412300
C	-3.18373900	1.46541700	-1.03832000
C	4.23031600	-3.70119500	-1.14173600
H	3.96339800	-4.63433500	-1.62845600
C	-2.21745900	0.59015400	1.52853600
C	2.30198500	-0.25126000	3.72737300
H	2.36090600	-1.02191700	4.49006000
C	-5.12673800	2.84101900	-1.47377500
H	-5.70560700	3.73819200	-1.27441300
C	-5.57269400	1.91790500	-2.41945900
H	-6.50001100	2.09667100	-2.95621300
C	-1.60023600	-0.20298300	3.73764900
H	-0.82175200	-0.46404800	4.44682900
C	3.17681200	2.58916600	-3.29002100
H	2.80203700	2.79652100	-4.28815600
C	2.45290500	-0.60405400	2.38899500
H	2.60745500	-1.64626600	2.12861600
C	-0.33618000	4.64428500	1.48569900
H	-0.47088900	5.20965800	2.40358000
C	0.00960100	3.18444300	-0.85118800
H	0.17655200	2.59454800	-1.74769500
C	2.06395100	1.07425100	4.08242300
H	1.94458000	1.34756600	5.12701800
C	5.82099400	-2.33378800	0.04783300
H	6.80580000	-2.20050600	0.48642700
C	0.70954100	4.37097300	-0.66888300
H	1.40753200	4.70371600	-1.43163800
C	0.54170500	5.10161400	0.50689700
H	1.09866900	6.02115800	0.66173700
C	-1.87562500	-3.20034900	-0.97878100
C	-2.53683800	-2.78663800	0.17981100
C	-2.57147300	-3.30991000	-2.18569400
C	-3.89862700	-2.47745700	0.13283100
C	-3.92213300	-3.00867900	-2.23486600
C	-4.57660300	-2.58990200	-1.07078600
H	-4.40584700	-2.14449600	1.03193700
H	-4.46858600	-3.09315500	-3.16815400
H	-5.63256000	-2.34051500	-1.10626800
H	-2.02675000	-3.63585000	-3.06533400
N	-1.81425300	-2.70596900	1.35674600

H	-2.22633300	-2.27140100	2.17332800
C	-0.47437900	-2.97391100	1.46866800
O	0.15541200	-2.84665200	2.48409000
O	0.13311500	-3.45840400	0.34105000
C	-0.45061600	-3.54196300	-0.90684100
O	0.22821500	-3.91899900	-1.82505000

### prodA1

C	-0.70698200	1.39127000	0.00001000
O	-0.74316200	2.58900900	0.00013400
C	0.50653800	0.56407200	0.00000600
C	0.38859800	-0.82751800	0.00001600
C	1.76959400	1.16134600	-0.00002400
C	1.53413700	-1.62678200	-0.00002200
C	2.90834200	0.37335500	-0.00000800
C	2.78133800	-1.01960000	-0.00005900
H	1.44404900	-2.70901200	0.00008400
H	3.89129100	0.83139600	0.00003800
H	3.67095200	-1.64192600	-0.00000400
H	1.82557800	2.24475200	-0.00001500
N	-0.88446500	-1.37605700	0.00021900
H	-1.00893000	-2.37783700	-0.00041300
C	-2.05479900	-0.65404300	0.00000500
O	-3.14530200	-1.15404200	0.00003600
O	-1.91057200	0.70408700	-0.00026500

### IntA1'

Pd	-0.00702900	-0.56199200	-0.75599200
P	2.20998500	-0.07391500	-0.18097600
P	-1.48230800	1.16285200	-0.07523500
C	1.86798800	1.91357500	3.42908300
H	1.80005800	2.94351400	3.76619500
C	-2.91148500	1.14527400	-2.45829900
H	-2.23142900	0.33865900	-2.71871200
C	-3.67272100	2.79644000	-0.87437900
H	-3.58343600	3.28675200	0.09173100
C	2.66295000	1.73178800	-2.23831800
H	1.82234900	1.21485100	-2.69676500
C	-1.60107600	0.44853600	2.60057600
H	-0.52893300	0.61990500	2.57705000
C	4.16591200	2.00547200	-0.37733800
H	4.51722300	1.70448400	0.60572200
C	3.08500000	1.34135300	-0.96522500
C	-3.74188400	0.42711300	1.49530600
H	-4.34962000	0.58941600	0.61075000
C	4.78759800	3.06118600	-1.03540200

H	5.61849000	3.57737700	-0.56328400
C	4.57194200	-1.47501700	0.66358200
H	4.60047600	-0.82331900	1.53223300
C	-0.89249900	3.45187300	1.57561300
H	-1.59171000	3.06745000	2.31163800
C	3.53803300	-1.35033600	-0.26987700
C	-4.33092900	-0.06189600	2.66001400
H	-5.39818100	-0.26515600	2.67730500
C	-0.68709000	2.76365000	0.37840200
C	-3.56078300	-0.28460500	3.79776800
H	-4.02373200	-0.66425300	4.70411100
C	2.07710800	1.65417700	2.07595500
H	2.15928500	2.48742400	1.38509800
C	5.53450900	-3.28637200	-0.60983700
H	6.30632200	-4.03979100	-0.73731200
C	3.52069000	-2.20566500	-1.37553100
H	2.71893300	-2.11176800	-2.10389800
C	-3.88732400	1.56180000	-3.36139200
H	-3.96317400	1.08172000	-4.33309200
C	2.15397300	0.33842300	1.60950100
C	4.35041300	3.45196700	-2.30012700
H	4.83862700	4.27520100	-2.81378800
C	-2.80097200	1.75325600	-1.20720600
C	5.56016700	-2.44046700	0.49673700
H	6.35416700	-2.53121400	1.23249800
C	-2.37094800	0.69036500	1.45598900
C	1.79417700	-0.44997600	3.87659700
H	1.67603100	-1.27672400	4.57099200
C	-4.64954700	3.20973700	-1.77309600
H	-5.32290800	4.01929800	-1.50645300
C	-4.75845100	2.59103700	-3.01860300
H	-5.51940300	2.91818400	-3.72161100
C	-2.19234800	-0.02285300	3.76549500
H	-1.57582300	-0.20006100	4.64206300
C	3.29238800	2.77987400	-2.90568500
H	2.95139600	3.07433900	-3.89394800
C	1.99540900	-0.71058500	2.52620300
H	2.01770700	-1.73984100	2.17807800
C	-0.18115100	4.61947000	1.84797800
H	-0.34432200	5.13917500	2.78815200
C	0.22089800	3.28503800	-0.54865200
H	0.39121600	2.75582300	-1.48059800
C	1.73115200	0.86586900	4.33402600
H	1.56745900	1.07084900	5.38802900

C	4.51488000	-3.16426300	-1.54960800
H	4.48813100	-3.82053800	-2.41467000
C	0.93342100	4.44731700	-0.28047700
H	1.65524600	4.81314800	-1.00509900
C	0.73910600	5.11463700	0.92821600
H	1.30178500	6.01670100	1.15089200
C	-0.05850100	-2.72760200	-1.64220200
C	-1.26344600	-2.44807500	-0.95734300
C	-2.47918900	-2.21216100	-1.66946000
C	-2.42888300	-2.23124900	-3.05838000
C	-1.22491100	-2.46429600	-3.74300600
C	-0.05451800	-2.70830100	-3.05940700
H	0.77725200	-3.16932300	-1.11130200
H	-3.33838600	-2.02029700	-3.61563100
H	-1.23153200	-2.47234900	-4.82918100
H	0.86470200	-2.93687700	-3.58997400
N	-3.64310800	-1.86966400	-1.00931000
H	-4.49891800	-1.99811100	-1.52740100
H	-3.71299800	-2.12177600	-0.03340900
I	-1.36597700	-3.08359800	1.10827200

**TSA1'**

Pd	0.09422600	-0.82015900	-0.36200500
P	1.69124300	0.97641800	-0.18434400
P	-2.08017200	0.15819500	0.03471300
C	0.75688600	3.46216200	3.01341000
H	0.50599000	4.50473800	3.18379900
C	-3.17050700	-0.74008200	-2.36139100
H	-2.26770700	-1.34303200	-2.41096100
C	-4.52268200	0.90140400	-1.22112800
H	-4.67761000	1.57847100	-0.38561800
C	0.61077600	2.13616200	-2.46683600
H	0.06724500	1.19569400	-2.53506500
C	-2.09576000	-0.90116900	2.60592400
H	-1.09821100	-0.47304300	2.66105400
C	2.20606000	3.53637100	-1.32629300
H	2.92575700	3.68735200	-0.52622800
C	1.48423200	2.33795800	-1.39566400
C	-4.12106800	-1.32787300	1.37245600
H	-4.72159700	-1.22895300	0.47383700
C	2.01827300	4.52913400	-2.28123700
H	2.57659800	5.45809300	-2.21216400
C	4.26641900	0.50342400	0.94282600
H	3.78621700	0.49561000	1.91530400
C	-2.49404300	2.31920900	1.87725500

H	-2.72831200	1.58205500	2.63768200	C	-2.20800400	4.63910800	1.26146200
C	3.52700500	0.79695800	-0.20558500	H	-2.21623600	5.69182600	1.52936600
C	-4.62207600	-2.04712000	2.45662900	C	1.17641400	-2.53295900	0.30962800
H	-5.60622000	-2.50148300	2.38874100	C	2.58929300	-2.50974300	0.34379400
C	-2.18344600	1.91769100	0.57710800	C	0.42949400	-2.84181700	1.44979700
C	-3.86957600	-2.18339000	3.61820500	C	3.19814700	-2.65557100	1.59448200
H	-4.26326100	-2.74359300	4.46119900	C	1.06691200	-2.98998200	2.68445100
C	1.05478400	3.03425300	1.72153400	H	-0.64491900	-2.96540900	1.37270100
H	1.01185300	3.74809900	0.90673100	C	2.45063600	-2.88635500	2.74902500
C	6.26777000	0.20367200	-0.38031100	H	4.28121700	-2.58050300	1.65191500
H	7.32615900	-0.02981900	-0.44692900	H	0.47769300	-3.20712000	3.56999100
C	4.18594800	0.80224800	-1.44365300	H	2.96541700	-3.00450100	3.69819100
H	3.63115200	1.03025400	-2.35006300	N	3.33915300	-2.35572800	-0.80614300
C	-4.12574900	-0.82341100	-3.37224700	H	4.25849300	-1.95939800	-0.65779000
H	-3.96554600	-1.49544300	-4.21009200	H	2.85089600	-1.88745600	-1.55908700
C	1.35935700	1.69537900	1.47435200	I	0.12651800	-3.24761500	-1.72239700
C	1.12413000	4.32701000	-3.33236400	<b>IntA5'</b>			
H	0.98217000	5.10136500	-4.08066800	Pd	-1.03436300	0.40283300	-0.09353400
C	-3.36279600	0.11830900	-1.27633700	P	1.40078500	0.14359100	-0.00435000
C	5.62583800	0.20712100	0.85424300	C	1.34504000	-1.05804700	2.51118500
H	6.18288600	-0.02094400	1.75853800	H	0.36321200	-1.41189300	2.21151700
C	-2.85319600	-0.74703300	1.43629100	C	3.36508000	0.17675800	2.03015500
C	1.04921100	1.22020200	3.83458100	H	3.95391900	0.80252800	1.36589800
H	1.04124000	0.50174900	4.64946600	C	1.40351500	-1.33924200	-2.34879200
C	-5.47370200	0.81978900	-2.23210600	H	0.44244300	-0.86544700	-2.52780300
H	-6.36966100	1.43166700	-2.18136800	C	3.31053500	-1.72969100	-0.91894500
C	-5.27653100	-0.04401100	-3.30891600	H	3.84899900	-1.55118000	0.00683300
H	-6.01980500	-0.10520100	-4.09866400	C	3.01258500	1.83690900	-1.61732200
C	-2.60412800	-1.60298900	3.69196500	H	3.14525200	0.98857200	-2.28126700
H	-2.00564400	-1.70641900	4.59268500	C	3.82952100	-2.61419500	-1.85904800
C	0.42913000	3.12582000	-3.43116000	H	4.77043100	-3.11870800	-1.66140000
H	-0.25489000	2.95521600	-4.25719700	C	2.26336000	1.70155700	-0.44734000
C	1.33434900	0.78765600	2.54444400	C	3.14200000	-2.85584100	-3.04586400
H	1.52540400	-0.26853100	2.36628100	H	3.54731800	-3.54976400	-3.77621900
C	-2.50740400	3.67157600	2.21416000	C	1.86118900	-1.40987800	3.75494000
H	-2.74966400	3.96480200	3.23157700	H	1.27111000	-2.02849900	4.42398900
C	-1.89211800	2.90076100	-0.37671300	C	2.09494300	-0.26405200	1.63806200
H	-1.66328300	2.61237000	-1.39696200	C	2.09514600	-1.08399600	-1.16101400
C	0.75958900	2.56206900	4.07316100	C	3.87583900	-0.17609300	3.27495200
H	0.52453200	2.90023600	5.07817500	H	4.86106800	0.17169900	3.57067800
C	5.54216100	0.51169300	-1.53111400	C	3.12442300	-0.96950200	4.13882700
H	6.03324900	0.52114500	-2.49977300	H	3.52351600	-1.24190200	5.11137500
C	-1.89990200	4.24835700	-0.04048300	C	1.92918800	-2.21740000	-3.29060000
H	-1.66234700	4.98997900	-0.79770200	H	1.38181700	-2.41466400	-4.20690600

C	3.59601400	3.06157000	-1.93844500
H	4.17519500	3.15541700	-2.85209400
C	2.11049200	2.80877100	0.39749700
H	1.53831500	2.71497400	1.31785100
C	2.69899400	4.02600100	0.07875300
H	2.57536900	4.87489900	0.74417500
C	3.44167300	4.15554600	-1.09407100
H	3.89772500	5.10797800	-1.34661700
C	-3.06971300	0.67722500	-0.23521500
C	-3.84892600	0.75100600	0.92633500
C	-3.65001100	0.83349300	-1.48684600
C	-5.22020300	0.99894900	0.79392100
C	-5.01891100	1.07526400	-1.60925900
H	-3.03582100	0.76569000	-2.38101300
C	-5.79692200	1.16600600	-0.46043700
H	-5.83872600	1.05603300	1.68742400
H	-5.46536300	1.19417700	-2.59172200
H	-6.86341500	1.35776600	-0.53604100
N	-3.24958800	0.62207000	2.18990900
H	-3.92673200	0.49427600	2.93232600
H	-2.57433700	-0.13577000	2.21173200
I	-1.53351100	-2.23255700	0.00860100
C	-1.11169100	2.32489700	-0.08381600
O	-1.21226900	3.45807300	-0.06572700

**TSA2'**

Pd	-0.98815000	0.30490900	-0.09733400
P	1.39107200	0.18731000	-0.01957000
C	1.44121200	-1.13413300	2.43029500
H	0.54346000	-1.62701100	2.06708500
C	3.24397600	0.44273700	2.10509700
H	3.74806600	1.18898800	1.49850200
C	1.49276700	-1.37395600	-2.31569300
H	0.50029300	-0.97801100	-2.51025600
C	3.42168100	-1.57343800	-0.87448700
H	3.94466300	-1.31906400	0.04270700
C	3.05526100	1.90620400	-1.54885200
H	3.32347400	1.03567700	-2.13882600
C	4.00400200	-2.45351700	-1.78076300
H	4.97865400	-2.88113800	-1.56606000
C	2.17218900	1.78167900	-0.47476400
C	3.33543200	-2.78988100	-2.95558200
H	3.78939800	-3.48156600	-3.65897800
C	1.96108800	-1.46483400	3.67760000
H	1.45850100	-2.21028500	4.28619700

C	2.08127900	-0.17746600	1.63495500
C	2.16305900	-1.02604300	-1.14006500
C	3.75714200	0.11044500	3.35550300
H	4.65845300	0.59874600	3.71378300
C	3.11658300	-0.84244200	4.14301900
H	3.51750400	-1.09899900	5.11916300
C	2.08045500	-2.24969900	-3.22259300
H	1.54889200	-2.52199600	-4.12887100
C	3.59642300	3.15000400	-1.86979600
H	4.27923700	3.23636300	-2.70966700
C	1.84165600	2.91800000	0.27441600
H	1.15752800	2.83479700	1.11479400
C	2.38961000	4.15442300	-0.04197100
H	2.12607600	5.02680400	0.54797100
C	3.26701000	4.27316700	-1.11892800
H	3.69019700	5.24077100	-1.37137300
C	-3.01195600	0.93309000	-0.22011900
C	-3.84855200	0.75895100	0.89809700
C	-3.55460700	1.17054900	-1.48604200
C	-5.23384400	0.86656700	0.70911500
C	-4.92848400	1.25178900	-1.66234000
H	-2.88945600	1.30907700	-2.33397100
C	-5.76025700	1.11010800	-0.55079800
H	-5.89828900	0.73606700	1.55980900
H	-5.34627000	1.43372600	-2.64680800
H	-6.83754100	1.18291500	-0.66869200
N	-3.30467200	0.52651400	2.15394200
H	-3.98289200	0.25314200	2.85279200
H	-2.52075300	-0.11714800	2.14072800
I	-1.49694400	-2.37058100	-0.02525200
C	-1.47360400	2.12210700	0.05233500
O	-1.54834700	3.26142500	0.21447400

**IntA8**

Pd	-0.58598400	-0.07757300	0.61246900
P	0.24580200	2.00639000	0.04677300
P	1.43281400	-1.43871600	0.07053000
C	2.68507200	2.23387600	-3.30299300
H	3.65172200	2.64586100	-3.57658400
C	1.21040600	-2.04039900	2.79011800
H	0.20588200	-1.63452400	2.69477400
C	3.35930900	-2.56674700	1.83451600
H	4.04132600	-2.57401700	0.98936200
C	1.86139000	1.87242800	2.29459100
H	1.32673600	0.94577500	2.48538900

C	0.00998200	-2.81407300	-1.85100600
H	-0.49035200	-1.86229900	-2.01523000
C	2.21944800	3.83875800	0.94609200
H	1.95871700	4.46268900	0.09614300
C	1.53594800	2.63617300	1.16960500
C	1.59730100	-4.19195400	-0.65950100
H	2.35723700	-4.31320900	0.10647800
C	3.22742600	4.24734400	1.81299100
H	3.75276700	5.17902200	1.62642000
C	-2.10075400	3.06674100	-0.96264400
H	-2.19958100	2.11636800	-1.48130400
C	3.24700000	-1.13267800	-2.06808600
H	2.59073500	-1.78831500	-2.63161800
C	-1.01362000	3.32200300	-0.11855100
C	1.20706700	-5.28814000	-1.42130000
H	1.67050100	-6.25505200	-1.24849300
C	2.94801100	-0.81020800	-0.74335400
C	0.21982800	-5.15049600	-2.39721200
H	-0.08679600	-6.01252200	-2.98241600
C	2.22083500	2.39016300	-2.00028400
H	2.84620600	2.90240600	-1.27890700
C	-3.04040500	5.21971400	-0.41478300
H	-3.82864900	5.95808300	-0.52929200
C	-0.96493300	4.51884800	0.59724800
H	-0.15929700	4.71286200	1.29658000
C	1.63955500	-2.52110900	4.02430600
H	0.96616900	-2.49431200	4.87558600
C	0.98532800	1.85732400	-1.62643400
C	3.55776200	3.46661300	2.91908600
H	4.34534400	3.78786000	3.59419200
C	2.06296100	-2.05995900	1.68020600
C	-3.10469900	4.01514000	-1.11165300
H	-3.94438400	3.79792900	-1.76417300
C	0.99968900	-2.94412900	-0.87174600
C	0.70858300	0.98412100	-3.86989800
H	0.10741400	0.42731400	-4.58228100
C	3.78742200	-3.04759400	3.06763400
H	4.79561100	-3.43714500	3.17237200
C	2.92865400	-3.02625200	4.16443600
H	3.26620500	-3.39853900	5.12703200
C	-0.37995600	-3.91345000	-2.61105800
H	-1.16762700	-3.78942200	-3.34776000
C	2.86877700	2.28252800	3.16350700
H	3.11186500	1.67433700	4.02935400

C	0.24147900	1.13692700	-2.56939900
H	-0.71132500	0.68104900	-2.30538500
C	4.38898000	-0.61498100	-2.67355000
H	4.60964500	-0.87229400	-3.70498100
C	3.79870300	0.05246900	-0.04097500
H	3.57910600	0.31968200	0.98818300
C	1.92897800	1.53949800	-4.24236900
H	2.29726000	1.42051400	-5.25727900
C	-1.97390400	5.46596000	0.44334600
H	-1.92840800	6.39298800	1.00727500
C	4.93920400	0.56429200	-0.64778900
H	5.59147500	1.22791600	-0.08782200
C	5.23946100	0.22793200	-1.96583100
H	6.13120600	0.62632200	-2.44082200
C	-2.03916500	0.73131400	1.76267500
O	-2.05546700	1.83666000	2.24024100
C	-3.03204900	-0.31426200	2.19687000
C	-2.89222300	-1.61486000	1.72270600
C	-4.05906500	-0.00312100	3.08953900
C	-3.75227500	-2.61973300	2.15084300
C	-4.92235100	-1.00182500	3.51971700
C	-4.76294200	-2.30817400	3.05524400
H	-3.64713000	-3.62887600	1.76306400
H	-5.71839800	-0.76866400	4.21977600
H	-5.43972500	-3.08860600	3.38955900
H	-4.15190500	1.01923500	3.44058300
N	-1.85744500	-1.83443500	0.75016500
H	-1.44404200	-2.76248500	0.82012100
I	-3.25100800	-0.76950500	-2.27925100
H	-2.27754000	-1.74932700	-0.20296000

### IntA9

Pd	-0.59994000	-0.34448800	-0.59233600
P	-0.21410200	1.93969100	-0.21758700
P	1.73857900	-1.18436900	0.02625700
C	2.85759200	3.18799600	-2.69289300
H	3.93216200	3.33210900	-2.63385700
C	0.61363700	-2.42814900	2.22039700
H	-0.30326700	-2.34433000	1.64335600
C	2.99043000	-2.08346300	2.43799600
H	3.93499100	-1.72370900	2.04163800
C	0.55738600	1.31107800	2.36662000
H	-0.04569200	0.42198300	2.21154100
C	1.60091800	-2.53849000	-2.40724300
H	0.92082100	-1.74125700	-2.69259000



C	1.46264500	3.39752600	1.56959900
H	1.55982500	4.15169800	0.79438600
C	0.70067100	2.24785200	1.33901200
C	2.97728200	-3.62010400	-0.74568200
H	3.38965200	-3.66142500	0.25807600
C	2.10919400	3.57718700	2.78764400
H	2.70976200	4.46701200	2.95181100
C	-1.40215000	4.48897700	-0.40522800
H	-0.46630700	4.82145200	-0.84523100
C	3.99350100	-0.11515100	-1.27277500
H	3.71631100	-0.75125300	-2.10727400
C	-1.58460400	3.14369200	-0.07201500
C	3.28301000	-4.62593100	-1.65650500
H	3.93273400	-5.44338100	-1.35838700
C	3.25570800	-0.15228700	-0.08502300
C	2.75561400	-4.58596900	-2.94553100
H	2.99377600	-5.37338400	-3.65455600
C	2.16395300	2.78051600	-1.55501400
H	2.71380200	2.60673000	-0.63688300
C	-3.63377400	4.99072000	0.35963200
H	-4.43223000	5.70843300	0.52375300
C	-2.79958800	2.73209900	0.47612500
H	-2.95871000	1.68878300	0.72406700
C	0.57967500	-3.01299000	3.48207800
H	-0.36648800	-3.36588800	3.88046800
C	0.78297200	2.58622800	-1.60817400
C	1.98088200	2.62459600	3.79826400
H	2.48697800	2.76954500	4.74817500
C	1.81561700	-1.94819600	1.68986900
C	-2.42480800	5.40752700	-0.19177000
H	-2.27697700	6.44961100	-0.45942900
C	2.13447700	-2.56684800	-1.11418300
C	0.80523900	3.18830200	-3.95239300
H	0.27140300	3.33940500	-4.88579700
C	2.95498600	-2.66821100	3.70052900
H	3.87214700	-2.76264400	4.27447400
C	1.75002200	-3.12819400	4.22710800
H	1.72481700	-3.57671800	5.21584300
C	1.91635200	-3.54090400	-3.32057600
H	1.49338200	-3.50950700	-4.31989800
C	1.19256500	1.49634400	3.59156900
H	1.07728300	0.74997100	4.37136900
C	0.10724200	2.78175200	-2.82224300
H	-0.96310100	2.60267800	-2.87675000

C	5.08813400	0.73482300	-1.40037000
H	5.64764400	0.74916200	-2.33091500
C	3.63890900	0.68437500	0.97102800
H	3.08429100	0.68062900	1.90269800
C	2.18256400	3.39667400	-3.88990800
H	2.72612900	3.71462900	-4.77486000
C	-3.81893300	3.65234600	0.69422200
H	-4.76061500	3.31696700	1.11745100
C	4.73517500	1.53100500	0.84222300
H	5.01146700	2.17172600	1.67419700
C	5.46275900	1.56159700	-0.34517900
H	6.31801700	2.22338800	-0.44575400
C	-2.35318800	-0.01394200	-1.63114700
O	-2.65041300	1.06200100	-2.09324300
C	-3.07099700	-1.26997400	-1.85624900
C	-2.39214000	-2.44669600	-1.46093000
C	-4.33127800	-1.31557800	-2.46711800
C	-3.02789200	-3.68644700	-1.72274700
C	-4.94313400	-2.53302200	-2.69727100
C	-4.27243900	-3.71133100	-2.31995400
H	-2.53347500	-4.61092400	-1.43550400
H	-5.92068300	-2.58454900	-3.16499600
H	-4.74725400	-4.67278500	-2.50116000
H	-4.80509700	-0.38100100	-2.75277000
N	-1.19169700	-2.28790600	-0.87182200
H	-0.66129300	-3.13176100	-0.69921200
I	-3.06331100	-0.95637600	2.24151000
H	-2.01056900	-0.67548100	0.91387800

### IntA11

Pd	-0.10666700	-0.31163500	0.95441400
P	-1.25467600	0.90934600	-0.65994500
P	2.29249200	0.07331700	0.40727400
C	0.69383500	1.80828600	-4.20689000
H	0.90244800	2.68113200	-4.81825100
C	2.71800200	-0.10817900	3.15414700
H	1.89334100	-0.81495300	3.13066700
C	4.19181400	1.43943100	2.03665700
H	4.51910700	1.95028200	1.13577300
C	-0.93174900	3.08544100	1.06293300
H	-0.48927400	2.35914900	1.73989800
C	2.70650600	-2.39665400	-0.81094900
H	1.61896500	-2.48426500	-0.81060000
C	-2.01637400	3.61203600	-1.02323400
H	-2.44607300	3.29698900	-1.96969300

C	-1.40932000	2.66901200	-0.18225400
C	4.72997900	-1.19532300	-0.24953000
H	5.22344500	-0.33034700	0.18465400
C	-2.09745100	4.94697100	-0.64434900
H	-2.56540300	5.66748000	-1.30823700
C	-3.14148300	-0.69186400	-1.95062200
H	-2.30472100	-1.31104400	-2.25092100
C	3.32356800	1.41819000	-1.87783800
H	3.68214100	0.45535900	-2.22637100
C	-2.95309200	0.45097800	-1.16851000
C	5.49334500	-2.22746500	-0.78020900
H	6.57725100	-2.16209600	-0.76216000
C	2.65022100	1.51769200	-0.66081100
C	4.86711300	-3.34800700	-1.32635400
H	5.46511200	-4.15744200	-1.73509400
C	-0.01847600	1.95988900	-3.02104400
H	-0.33158600	2.95235200	-2.71962800
C	-5.52813600	-0.34522500	-1.90525600
H	-6.52912000	-0.65432400	-2.19232800
C	-4.06863100	1.17093600	-0.72747400
H	-3.94837800	2.03080300	-0.07738100
C	3.34578500	0.16850900	4.36481200
H	3.00597700	-0.32470700	5.27031100
C	-0.28572700	0.84974400	-2.21769700
C	-1.59095100	5.35570600	0.58830400
H	-1.65790600	6.39836000	0.88443400
C	3.13773500	0.52108600	1.97712100
C	-4.42345800	-1.08839100	-2.31289700
H	-4.54563500	-1.99203700	-2.90123200
C	3.33124700	-1.27129300	-0.26746200
C	0.91830500	-0.54950800	-3.78357900
H	1.29329600	-1.52936900	-4.06403000
C	4.81650300	1.71666600	3.24887300
H	5.63194300	2.43324300	3.28221800
C	4.39575100	1.08112700	4.41429300
H	4.88188900	1.30130600	5.36012700
C	3.47939000	-3.43175800	-1.33709100
H	2.98554400	-4.30672600	-1.74849100
C	-1.01835700	4.42192700	1.44573800
H	-0.64115700	4.72794800	2.41672300
C	0.20565400	-0.40554300	-2.59786600
H	0.03720400	-1.26946900	-1.95719700
C	3.52664300	2.55395600	-2.65947600
H	4.04839600	2.46244200	-3.60740300

C	2.17565300	2.76754100	-0.24545600
H	1.65622600	2.86058900	0.70293800
C	1.15557600	0.55492300	-4.59642500
H	1.71320500	0.44316500	-5.52180500
C	-5.34810400	0.78080000	-1.10761100
H	-6.20533800	1.34739500	-0.75702800
C	2.37072500	3.89698500	-1.02908800
H	1.98633200	4.85550100	-0.69305700
C	3.05273100	3.79206100	-2.24027900
H	3.20911200	4.67284600	-2.85625300
C	-1.61405200	-0.25211400	2.25034700
O	-0.97329700	0.10448500	3.21438100
C	-3.03744100	-0.50605700	2.16717400
C	-3.58698000	-1.52844600	1.34822000
C	-3.87537000	0.32375100	2.94372800
C	-5.00117400	-1.63409200	1.31694700
C	-5.24499500	0.20834300	2.87807800
C	-5.79730700	-0.78689300	2.05006300
H	-5.44213400	-2.40036100	0.68687100
H	-5.88486600	0.86413900	3.45852700
H	-6.87707500	-0.89319200	1.98760300
H	-3.41003200	1.07676500	3.57281600
N	-2.83071300	-2.42445100	0.68926500
H	-3.21987800	-2.96231600	-0.08051400
H	-1.83667100	-2.28281600	0.49975200
C	0.64381500	-3.69170200	1.55294600
O	0.87566900	-4.76097100	1.16443100
O	0.46571800	-2.65094100	2.06206500
C	-0.95647200	-3.63999700	-1.48869200
O	-0.41814700	-2.85532100	-0.62519500
O	-2.17210300	-3.75763300	-1.70797000
C	0.02886300	-4.47522900	-2.30777800
H	-0.49423900	-5.10990300	-3.02544300
H	0.72366100	-3.81484000	-2.84127800
H	0.62466700	-5.09703400	-1.63043800

### TSA3

Pd	0.17950100	-0.25596700	-0.91107900
P	0.92212700	1.33927700	0.60458500
P	-2.27412000	-0.38517600	-0.49877900
C	-1.48077000	2.54647700	3.74048300
H	-1.86676400	3.47831500	4.14275200
C	-2.50447600	-1.36924400	-3.08961100
H	-1.62291600	-1.94990600	-2.83273800
C	-4.19430400	0.25373700	-2.51037500

H	-4.63391000	0.94937700	-1.80186800	H	-2.39478900	-4.23507200	2.58756500
C	0.56451200	3.36349200	-1.29187100	C	0.61367100	4.67539900	-1.75823900
H	0.19525900	2.57417300	-1.93796800	H	0.25648500	4.90288800	-2.75786700
C	-2.35365600	-2.57171300	1.23363200	C	-0.52785300	0.16452900	2.66148100
H	-1.26703300	-2.49304200	1.27851300	H	-0.17027800	-0.77958000	2.25139400
C	1.56925400	4.07042900	0.78620000	C	-4.17981400	2.48706200	1.78899800
H	1.96401000	3.83406800	1.77050900	H	-4.78734800	2.52878600	2.68808500
C	1.02611100	3.05329300	-0.01145200	C	-2.60449800	2.36567800	-0.49044000
C	-4.50485900	-1.85723800	0.38376300	H	-1.99680900	2.32111900	-1.38929900
H	-5.09799400	-1.19912400	-0.24560300	C	-1.81754400	1.33424100	4.33429000
C	1.61465400	5.37867100	0.32036300	H	-2.45798400	1.31662700	5.21144100
H	2.03354500	6.15999200	0.94709900	C	5.00910000	1.22670800	0.99294100
C	2.81800700	-0.07575500	2.10837500	H	5.85974800	1.72978900	0.54369200
H	1.97885800	-0.62383900	2.51733800	C	-3.04040100	3.59664500	-0.01869300
C	-3.73645500	1.25183600	1.31986700	H	-2.75366600	4.50448900	-0.54110900
H	-3.99622900	0.34762200	1.85990600	C	-3.83526000	3.65881900	1.12475700
C	2.61249000	0.97976600	1.21502900	H	-4.17872500	4.61897900	1.49845300
C	-5.13257600	-2.84976300	1.12515600	C	1.81095600	0.12972500	-2.00706600
H	-6.21166300	-2.96153500	1.07469500	O	1.46708700	0.79210800	-2.95675400
C	-2.94875100	1.18109600	0.17168500	C	3.17716200	-0.40683700	-1.83854000
C	-4.37459400	-3.70443300	1.92635000	C	3.49700500	-1.51615300	-1.03308600
H	-4.86585600	-4.48230200	2.50402100	C	4.19294100	0.25378200	-2.54889200
C	-0.66577400	2.57604000	2.61294500	C	4.83313500	-1.93461600	-0.96881500
H	-0.44718300	3.52928000	2.14604000	C	5.50987000	-0.15635800	-2.45876100
C	5.20496000	0.16830900	1.87598500	C	5.82344600	-1.26144400	-1.66292100
H	6.21203700	-0.15756800	2.11859300	H	5.07732300	-2.79147600	-0.34846800
C	3.72084200	1.62478100	0.65348900	H	6.28656200	0.36901900	-3.00483700
H	3.58597000	2.42651000	-0.06557200	H	6.85269000	-1.59886600	-1.58274100
C	-3.07606500	-1.51192100	-4.35020700	H	3.91523700	1.10132600	-3.16706000
H	-2.63375800	-2.19961600	-5.06450100	N	2.52498200	-2.26099700	-0.36299400
C	-0.16738300	1.38554300	2.07762600	H	2.88805700	-2.92043700	0.34895400
C	1.12963800	5.68357400	-0.95105200	H	1.83329700	-1.73970500	0.18794700
H	1.16800600	6.70607700	-1.31491000	C	1.13054000	-3.26790300	-1.50518600
C	-3.06043000	-0.48547700	-2.15725800	O	1.40750500	-4.40247400	-1.40022600
C	4.10787200	-0.48478000	2.42920900	O	0.45997800	-2.36429400	-1.93520600
H	4.23884900	-1.34017600	3.08309300	C	1.40921100	-3.29418400	2.26756100
C	-3.11269800	-1.70611900	0.44319800	O	0.71591000	-2.44754100	1.61098900
C	-1.34622600	0.14510200	3.78609500	O	2.60472900	-3.57940000	2.05152800
H	-1.61925900	-0.81066000	4.22357800	C	0.67766900	-4.03149100	3.38961000
C	-4.76117400	0.11030900	-3.77349600	H	1.38380100	-4.45591200	4.10655600
H	-5.64049500	0.69083600	-4.03690800	H	-0.02618400	-3.36417700	3.89732400
C	-4.20360300	-0.77174800	-4.69515700	H	0.10110500	-4.85343500	2.94801300
H	-4.64569100	-0.87994200	-5.68119400				
C	-2.99221400	-3.56622600	1.97501900				
				<b>IntA12</b>			
				Pd	-0.19752500	-0.11111600	1.04549700

P	-0.75196400	1.67379000	-0.31324500	C	0.54547400	0.12466200	-3.85626400
P	2.16195100	-0.54540500	0.32828300	H	0.56194400	-0.86821500	-4.29590000
C	1.04845900	2.47418900	-3.96220600	C	5.45055400	-0.68027700	2.82521300
H	1.46616900	3.32671700	-4.48932200	H	6.48556900	-0.35084000	2.81339600
C	2.78770600	-1.51772100	2.85168600	C	4.95026000	-1.38015900	3.92094700
H	1.74891400	-1.84173000	2.86679000	H	5.59605300	-1.59767900	4.76689700
C	4.62515900	-0.40048300	1.74102200	C	1.45545400	-4.00396600	-1.73198800
H	5.02199700	0.15141700	0.89379200	H	0.58532600	-4.62506800	-1.92382500
C	0.34063700	3.32426300	1.63280200	C	0.71257400	4.53843100	2.20361800
H	0.53420400	2.39402200	2.15891100	H	1.21469400	4.54798300	3.16598700
C	1.31273100	-2.82796800	-1.00018100	C	0.03648700	0.29512700	-2.57396500
H	0.33351500	-2.53378000	-0.64432200	H	-0.33471300	-0.57063700	-2.03609200
C	-0.62846100	4.50239600	-0.23651700	C	3.96994500	1.85895100	-2.52001100
H	-1.19205600	4.49764900	-1.16534700	H	4.31444700	1.77686600	-3.54654600
C	-0.30813700	3.29372300	0.39595700	C	3.06283700	2.05664100	0.09335800
C	3.68892600	-2.44841100	-1.12359400	H	2.72019800	2.13913300	1.12037000
H	4.56580800	-1.86089300	-0.86498100	C	1.04453700	1.21745400	-4.55894300
C	-0.25247600	5.71405700	0.33171400	H	1.44648800	1.08758600	-5.55952500
H	-0.49965200	6.64483200	-0.16971900	C	-4.73183500	2.72990600	-0.12352600
C	-3.17031500	0.86023800	-1.46525900	H	-5.33601700	3.45749700	0.41034700
H	-2.57927300	0.10907000	-1.97839800	C	3.59592400	3.17282200	-0.53821800
C	3.42401600	0.74232600	-1.89066800	H	3.64674000	4.11755900	-0.00515300
H	3.33925800	-0.19089400	-2.43696000	C	4.05625300	3.07437800	-1.84973700
C	-2.55572400	1.80458800	-0.63579500	H	4.47548500	3.94377100	-2.34775300
C	3.83246000	-3.61265900	-1.86856900	C	-1.89632100	0.21221700	2.04583900
H	4.81923200	-3.92401600	-2.19820800	O	-1.88058800	1.11170000	2.84956100
C	2.96977700	0.82934500	-0.57459600	C	-3.09230700	-0.64158100	1.80640800
C	2.71551000	-4.39120400	-2.17437200	C	-3.09394900	-1.95455400	1.29670900
H	2.83476100	-5.30981700	-2.74134600	C	-4.31904900	-0.00270400	2.04512500
C	0.53669100	2.64847800	-2.67949000	C	-4.32761500	-2.54851100	0.98631300
H	0.58722500	3.62917500	-2.22191800	C	-5.52798600	-0.59953000	1.73723500
C	-5.33546400	1.79588500	-0.95806300	C	-5.52371300	-1.88074700	1.18923700
H	-6.41439100	1.78947700	-1.08024400	H	-4.33141700	-3.55341200	0.57253200
C	-3.34956500	2.73009700	0.04687600	H	-6.46001900	-0.07197900	1.91193300
H	-2.89750500	3.44493500	0.72619400	H	-6.45726400	-2.37122900	0.92927800
C	3.62256300	-1.79777000	3.93049300	H	-4.28739500	0.99995500	2.45673400
H	3.22667800	-2.34327500	4.78165800	N	-1.94911400	-2.72587800	1.00759000
C	0.00459200	1.56295600	-1.98116800	H	-2.19336100	-3.66547200	0.70361700
C	0.42834500	5.73221600	1.54803600	H	-1.86303800	-2.25882400	-0.75221500
H	0.71894700	6.67950100	1.99254900	C	-0.74265500	-2.83971800	1.81515400
C	3.28910000	-0.81719100	1.74850400	O	-0.21663900	-3.93726700	1.82520300
C	-4.55081800	0.85693100	-1.62279500	O	-0.34410400	-1.76604700	2.39476800
H	-5.01421800	0.11041300	-2.26040500	C	-2.12182900	-3.39901500	-2.25382600
C	2.42039400	-2.03681800	-0.69731100	O	-1.86835800	-2.18763100	-1.74314500

O	-2.41813400	-4.35717000	-1.57382800
C	-1.95092100	-3.41958500	-3.74945600
H	-2.37616700	-4.33557600	-4.15945700
H	-2.41479300	-2.54083800	-4.20475100
H	-0.87898700	-3.38562600	-3.97498400

**IntA13'**

Pd	0.94047400	0.65102000	-0.51113500
P	-1.14079900	-0.27024500	0.00038900
C	-4.01752300	-0.98113500	-2.86984000
H	-5.04819900	-0.69721800	-3.06040100
C	-2.47561400	2.14893400	0.39204000
H	-1.81513200	2.52284700	-0.38407700
C	-3.14891000	0.37014700	1.88499400
H	-3.05226000	-0.64846300	2.24636800
C	-2.33494500	0.83132400	0.84483100
C	-4.08955000	1.21636500	2.46550700
H	-4.71339700	0.85004600	3.27535800
C	-1.84615100	-2.85087300	0.92549900
H	-2.51904600	-2.91066200	0.07551900
C	-1.04950600	-1.72018400	1.10795100
C	-3.37273700	-0.50688200	-1.72961100
H	-3.90602400	0.14144200	-1.04191800
C	-0.91196200	-3.83974000	2.91898300
H	-0.85591200	-4.66657900	3.62084700
C	-0.18156600	-1.65775800	2.20226600
H	0.45220300	-0.78441500	2.33859500
C	-2.04525600	-0.86121600	-1.47732300
C	-4.22973600	2.52416800	2.00998000
H	-4.96421700	3.18265100	2.46462800
C	-1.77396700	-3.90855600	1.82888300
H	-2.39166300	-4.78859000	1.67682400
C	-2.02270000	-2.17419000	-3.50694600
H	-1.49450000	-2.82678300	-4.19561000
C	-3.42236400	2.98667200	0.97377200
H	-3.52177200	4.00806600	0.61792300
C	-1.37091700	-1.69938700	-2.37472200
H	-0.34558300	-1.99158800	-2.16805100
C	-3.34517600	-1.81347100	-3.75879800
H	-3.85006200	-2.18167900	-4.64712900
C	-0.11606800	-2.71107400	3.10619600
H	0.56217400	-2.65488100	3.95220300
C	1.83493400	-1.12132100	-0.48664200
O	1.37780200	-2.22216100	-0.69868400
C	3.30719700	-0.95232700	-0.19357000

C	3.84938900	0.32465700	-0.32095800
C	4.11506300	-2.02318500	0.18754400
C	5.19627400	0.54963900	-0.06033200
C	5.45961200	-1.80150800	0.46216500
C	5.99578900	-0.51880800	0.33987800
H	5.61118400	1.54795000	-0.16333700
H	6.09404900	-2.62535200	0.77417400
H	7.04613600	-0.34867300	0.55647700
H	3.67233800	-3.01064200	0.26992000
N	2.93916200	1.35572100	-0.74446300
H	2.87804500	2.20778500	-0.14175300
H	3.12986600	1.66877000	-1.69465300
O	2.02381500	3.59966800	0.46767600
C	0.86908800	3.64906600	0.00758200
C	0.04826700	4.91749500	0.19305400
H	-0.76165700	4.71090500	0.90234600
H	0.66705800	5.72877000	0.57973600
H	-0.41217700	5.21062100	-0.75507100
O	0.25948400	2.71140000	-0.62094500

**TSA4'**

Pd	0.96732400	0.48460200	-0.60672000
P	-1.16803900	-0.30561400	-0.04209700
C	-4.08013200	-1.84503200	-2.52717900
H	-5.14643400	-1.71860800	-2.68957500
C	-2.55189200	2.04101600	-0.60237600
H	-2.08308200	1.95832800	-1.57745700
C	-2.89817200	1.20096300	1.63269800
H	-2.71812500	0.45584200	2.40109800
C	-2.30712900	1.06792700	0.37447700
C	-3.72122800	2.29080600	1.91044600
H	-4.17323400	2.38507600	2.89332300
C	-2.20324900	-2.35095500	1.61204900
H	-2.94005300	-2.52633800	0.83383900
C	-1.21818900	-1.37648700	1.43655800
C	-3.43805300	-1.09375200	-1.54647100
H	-4.00790300	-0.38573200	-0.95239300
C	-1.29441300	-2.89204400	3.78066800
H	-1.32194400	-3.48501300	4.69012400
C	-0.26825600	-1.17095300	2.44113300
H	0.51199300	-0.42710700	2.29937600
C	-2.06439200	-1.24489500	-1.33172900
C	-3.96646600	3.24947400	0.93296700
H	-4.61075400	4.09648300	1.14998900
C	-2.23860400	-3.10677200	2.78019000

H	-3.00333000	-3.86730900	2.90631200	H	-3.95711300	2.67136800	2.75063700
C	-1.99005600	-2.91039800	-3.08216000	C	-2.14703600	-2.24204700	1.78959100
H	-1.42276200	-3.61926800	-3.67766800	H	-2.90296000	-2.47676500	1.04615700
C	-3.38334900	3.11967500	-0.32699900	C	-1.16145600	-1.29231800	1.51035300
H	-3.56915500	3.86502400	-1.09457300	C	-3.42616000	-1.31589900	-1.42767200
C	-1.34251600	-2.16023000	-2.10612100	H	-4.00706700	-0.59425100	-0.86111600
H	-0.28074700	-2.29513800	-1.92596200	C	-1.18885400	-2.60854200	3.97352300
C	-3.35729200	-2.75240900	-3.29653600	H	-1.19763000	-3.12426400	4.92925900
H	-3.85904300	-3.33600500	-4.06288600	C	-0.18643100	-1.01174900	2.47195200
C	-0.30935900	-1.92219000	3.61069200	H	0.59401700	-0.28772400	2.25106800
H	0.43499200	-1.75743500	4.38371600	C	-2.04109800	-1.39680000	-1.24997700
C	1.86468800	-1.25069000	-0.28373400	C	-3.93360200	3.27489500	0.68431800
O	1.34407700	-2.34159900	-0.23994500	H	-4.57229900	4.13853500	0.84487000
C	3.33321400	-1.04796900	-0.09805900	C	-2.15791500	-2.89857300	3.01654100
C	3.84088300	0.21275000	-0.43895800	H	-2.92314600	-3.64082900	3.22303600
C	4.17479500	-2.08033400	0.32493800	C	-1.94912900	-3.16647900	-2.89388900
C	5.22580600	0.41448600	-0.38631500	H	-1.37057500	-3.88806700	-3.46261500
C	5.54275800	-1.86279500	0.39562100	C	-3.45593600	2.98639800	-0.59353200
C	6.06024700	-0.61596200	0.02841800	H	-3.71655500	3.62610200	-1.43133200
H	5.63575900	1.38396200	-0.65572200	C	-1.30459300	-2.32910900	-1.98916100
H	6.20905900	-2.65503700	0.72214500	H	-0.23273200	-2.40773400	-1.83684300
H	7.13251900	-0.44536100	0.07409800	C	-3.32777200	-3.07876700	-3.07150300
H	3.73905500	-3.04270800	0.57493400	H	-3.82737900	-3.73045400	-3.78235200
N	2.91646400	1.20484800	-0.80690100	C	-0.20334400	-1.66324300	3.70065800
H	2.56651800	2.39264200	-0.00901900	H	0.56051100	-1.44050800	4.43934700
H	3.15926000	1.61930500	-1.70513200	C	1.92616900	-1.21922700	-0.25360900
O	2.13562700	3.30878700	0.39887700	O	1.42811200	-2.31702400	-0.15863000
C	0.92948700	3.47411600	-0.04471500	C	3.38333500	-0.96199100	-0.08688500
C	0.26708600	4.77227600	0.33883000	C	3.84375000	0.30696500	-0.47336200
H	-0.79840600	4.59812900	0.50578000	C	4.26363700	-1.95512800	0.35343000
H	0.73524400	5.20407800	1.22464000	C	5.22724100	0.54414000	-0.45984200
H	0.37059300	5.47918800	-0.49145700	C	5.62524000	-1.69819800	0.38877000
O	0.32168500	2.66079400	-0.75876000	C	6.09730700	-0.44887400	-0.03211300
<b>IntA14'</b>				H	5.60601000	1.51510000	-0.76756400
Pd	0.96866100	0.46403800	-0.67291800	H	6.32128300	-2.46047800	0.72408100
P	-1.14299400	-0.34585300	-0.05253700	H	7.16523900	-0.24732400	-0.01781900
C	-4.06523600	-2.15409800	-2.33703300	H	3.86098700	-2.92182600	0.63990900
H	-5.14046400	-2.08225200	-2.47154600	N	2.88693000	1.25475000	-0.83422600
C	-2.63212000	1.88686600	-0.79762900	H	2.36554200	2.48237900	0.04986800
H	-2.24393600	1.68265200	-1.79071400	H	3.14575400	1.75032800	-1.68460900
C	-2.77377500	1.34069900	1.54724900	O	1.85896600	3.31220600	0.44045400
H	-2.51773400	0.70253000	2.38709300	C	0.68116000	3.41513200	-0.11062300
C	-2.29154300	1.04696600	0.27016400	C	-0.15105700	4.57560500	0.36144300
C	-3.58813300	2.45371100	1.75273500	H	-0.95576600	4.17781900	0.99018900

H 0.44157400 5.29175700 0.93146500  
H -0.62101600 5.05872600 -0.49804800  
O 0.22886400 2.62006500 -0.94231600

**IntA19**

C 1.63161400 -2.31062800 -0.91738600  
C 0.78428800 -3.29568300 -1.40674000  
C 3.00428400 -2.52198700 -0.93837200  
C 1.23997500 -4.49533200 -1.92881900  
C 3.48893300 -3.72810200 -1.45546000  
C 2.62119100 -4.70104100 -1.95010400  
H 0.54771100 -5.24658000 -2.30025400  
H 4.56047800 -3.90992300 -1.47152200  
H 3.02170200 -5.62850400 -2.34925400  
H 3.70466300 -1.77993700 -0.56506700  
N -0.58709000 -2.85257300 -1.24205900  
H -1.15229000 -2.88126000 -2.08563200  
O -1.85839800 -3.77467600 0.98840700  
H -1.08195900 -3.31420500 -0.43355100  
C -1.32322700 -3.14813000 1.94500800  
C -1.92977700 -3.35835300 3.33266300  
H -1.16908800 -3.24087500 4.10909300  
H -2.69703900 -2.59033400 3.49337700  
H -2.40712900 -4.33804100 3.40934900  
O -0.37150900 -2.32919500 1.85539700  
Pd 0.18141800 -0.98279400 -0.42435700  
P -1.85449900 0.30463500 -0.32120900  
C -2.61752800 0.67016800 1.29648300  
C -3.23167900 -0.50207700 -1.22812100  
C -1.65972800 1.90083500 -1.20171000  
C -1.97990200 0.23209800 2.46006200  
C -3.85167700 1.32636000 1.38880400  
C -3.92630400 0.11523800 -2.27171700  
C -3.59659000 -1.79320000 -0.82462700  
C -2.10605300 3.13421700 -0.72995700  
C -1.00664300 1.84493500 -2.44055000  
H -1.07672200 -0.37233400 2.39159500  
C -2.55097300 0.49467500 3.70455500  
H -4.38130900 1.61662800 0.48498900  
C -4.41168700 1.59337700 2.63228000  
H -3.65994900 1.11761700 -2.59189600  
C -4.96878000 -0.55312700 -2.91067600  
H -3.06647500 -2.30261000 -0.02034800  
C -4.63984400 -2.45256100 -1.46610000  
C -1.92040200 4.28630800 -1.49159600

H -2.57945900 3.20919900 0.24266500  
C -0.82320200 2.99340300 -3.20000500  
H -0.64659800 0.88788000 -2.81099200  
C -3.75534000 1.18514000 3.79315600  
H -2.05524200 0.14023700 4.60338600  
H -5.36641200 2.10691500 2.69646700  
C -5.32656400 -1.83685300 -2.51074900  
H -5.50165300 -0.06484500 -3.72157000  
H -4.90929800 -3.45412500 -1.14478200  
H -2.26468600 5.24144500 -1.10639300  
C -1.28572800 4.22001400 -2.72656400  
H -0.31711500 2.93161100 -4.15887300  
H -4.19736200 1.38706700 4.76465000  
H -6.13844100 -2.35652500 -3.01148400  
H -1.14249700 5.12097900 -3.31587400  
C 3.01349900 0.84969800 -1.02344000  
P 1.71166400 0.58761100 0.24157600  
C 2.66771800 0.67262500 -2.36635100  
C 4.31577000 1.24205500 -0.70272100  
C 2.56362100 0.12206300 1.79099800  
C 1.15022000 2.29326400 0.61286000  
H 1.66975000 0.32568300 -2.61620100  
C 3.59938200 0.90367000 -3.37269200  
H 4.61331800 1.36008700 0.33368600  
C 5.25130500 1.46052600 -1.70988000  
C 2.44671300 -1.18271800 2.27766300  
C 3.31666600 1.06361100 2.50880600  
C 1.40619400 3.36611000 -0.24243700  
C 0.43102700 2.51494300 1.79238700  
C 4.89394500 1.29767200 -3.04555400  
H 3.31813900 0.75775300 -4.41120700  
H 6.26339700 1.75402900 -1.44796200  
H 1.80526200 -1.89998200 1.77619000  
C 3.10773600 -1.54530000 3.45002400  
C 3.97763300 0.69257400 3.67263600  
H 3.36889900 2.09446700 2.16892600  
H 1.95265900 3.21081300 -1.16689500  
C 0.96166300 4.64373200 0.08723500  
H 0.23341100 1.69169300 2.47102100  
C -0.02022200 3.78925200 2.11383100  
H 5.62655500 1.46644300 -3.82922300  
H 3.00196300 -2.55835300 3.82515300  
C 3.87850900 -0.61742600 4.14095500  
H 4.56050700 1.42727300 4.22019400

H	1.16606100	5.47065200	-0.58597500
C	0.25120100	4.85891100	1.26373500
H	-0.58020400	3.94310400	3.03130500
H	4.39003700	-0.90608100	5.05473200
H	-0.09484500	5.85704900	1.51621000

**IntA20**

C	1.75014300	-2.58251100	-0.33676500
C	0.87228800	-3.67244400	-0.43552600
C	3.09720600	-2.77380200	-0.09922600
C	1.32895900	-4.98012700	-0.27473400
C	3.58498000	-4.09077200	-0.01798400
C	2.70436900	-5.16728800	-0.09058200
H	0.64482700	-5.82602900	-0.29503100
H	4.65007600	-4.26891700	0.10653800
H	3.09284100	-6.17931300	0.00052500
H	3.78308800	-1.93579800	0.01735100
N	-0.40618300	-3.15175700	-0.68823400
H	-1.14753700	-3.61954900	-0.17030800
Pd	0.21993000	-1.23341700	-0.20433700
P	-1.93660100	-0.22240300	-0.02183300
C	-2.35813200	0.57441100	1.57174900
C	-3.33804100	-1.38933900	-0.20800500
C	-2.21190600	1.00365000	-1.35043800
C	-1.38772100	0.61320900	2.57569100
C	-3.63704000	1.07609800	1.84268000
C	-4.33328200	-1.25431400	-1.17597100
C	-3.39464100	-2.46463500	0.68683800
C	-2.82185200	2.24666400	-1.18511600
C	-1.76121500	0.62517300	-2.62309500
H	-0.40509500	0.18798900	2.38938300
C	-1.67133200	1.18434100	3.81407400
H	-4.41842500	0.99934600	1.09112000
C	-3.91898600	1.65356100	3.07558600
H	-4.30345000	-0.42765700	-1.87897700
C	-5.37037100	-2.18327500	-1.24816200
H	-2.61720600	-2.58037500	1.43882600
C	-4.43197900	-3.38574500	0.61677800
C	-2.99966900	3.08996800	-2.27942400
H	-3.14116400	2.57400400	-0.20157300
C	-1.94741100	1.46578500	-3.71403800
H	-1.26527700	-0.33459200	-2.75273500
C	-2.93370900	1.71469000	4.06060000
H	-0.90441300	1.20792400	4.58255100
H	-4.91204800	2.04574800	3.27370800

C	-5.42262600	-3.24718800	-0.35447200
H	-6.13829800	-2.07150700	-2.00792700
H	-4.46463000	-4.21631300	1.31552800
H	-3.46711300	4.05985100	-2.13711400
C	-2.57158000	2.70010100	-3.54385800
H	-1.60034000	1.15858800	-4.69601800
H	-3.15796100	2.16125600	5.02488700
H	-6.23043400	-3.97042600	-0.41471000
H	-2.71444300	3.35998200	-4.39467400
C	2.98064800	0.64321000	-1.13644400
P	1.58309100	0.63345300	0.05131300
C	2.87359800	-0.12335700	-2.29994000
C	4.12006800	1.42891600	-0.93637400
C	2.35475500	0.74643500	1.71098700
C	0.84602600	2.29641600	-0.21837000
H	2.01044800	-0.76777000	-2.43728800
C	3.88675000	-0.09475400	-3.25473800
H	4.22586800	2.02048000	-0.03247300
C	5.13478100	1.44834000	-1.88650600
C	2.44381400	-0.42446200	2.47264300
C	2.86506500	1.94014600	2.23701000
C	0.84050500	2.84981700	-1.50308800
C	0.20369000	2.98656200	0.81483800
C	5.01746100	0.68911000	-3.04920000
H	3.79604800	-0.70069300	-4.15095100
H	6.01970600	2.05473200	-1.71759800
H	2.05641900	-1.35665200	2.07010200
C	3.03646800	-0.40120100	3.73243600
C	3.45386600	1.96053700	3.49693200
H	2.78697200	2.86312800	1.66989400
H	1.32229100	2.32585900	-2.32279300
C	0.22721700	4.07463700	-1.74160600
H	0.18696400	2.57698600	1.81872500
C	-0.40698100	4.21379000	0.57489600
H	5.81226600	0.70314200	-3.78931500
H	3.10166500	-1.31832600	4.30973700
C	3.54065100	0.78949000	4.24673600
H	3.84318000	2.89333600	3.89407300
H	0.22954200	4.48746500	-2.74560400
C	-0.39198100	4.76376500	-0.70272700
H	-0.89372500	4.73724300	1.39258400
H	3.99939600	0.80725600	5.23103300
H	-0.86802200	5.72166200	-0.89106400

**TSA7**



Pd	0.35737200	0.98502900	0.30736100	C	-3.06821500	0.97806800	-0.58676600
P	1.63735000	-0.86519700	-0.17484500	C	0.27858700	-0.72601600	-4.01182600
P	-1.82827000	-0.08470500	0.23473000	H	0.02357200	0.07406700	-4.70015700
C	0.46684900	-3.06962900	-3.49766100	C	-3.88610900	-1.27260800	3.62333700
H	0.34636400	-4.11038100	-3.78276800	H	-4.66957100	-1.97739100	3.88569500
C	-1.87881900	0.53127700	2.94185100	C	-3.31426800	-0.46528800	4.60417900
H	-1.09091800	1.23302800	2.67614900	H	-3.64981800	-0.54122400	5.63426500
C	-3.45524500	-1.18023100	2.30340200	C	-3.55749300	2.47113500	-2.42736600
H	-3.90057000	-1.81922800	1.54644100	H	-3.22501600	3.00691500	-3.31094600
C	0.82532500	-2.05378800	2.18911500	C	0.69959700	-3.07625700	3.12628600
H	0.36202600	-1.08930500	2.37608300	H	0.13766000	-2.90097200	4.03858200
C	-2.66235800	1.65928700	-1.73807400	C	0.71763300	-0.41074500	-2.73039200
H	-1.63633400	1.57318600	-2.08179900	H	0.78024200	0.63384500	-2.42943700
C	2.16305700	-3.49182600	0.79134800	C	-2.74398200	-3.08261800	-2.43849900
H	2.77830500	-3.64549500	-0.09050000	H	-3.11989000	-3.14423500	-3.45528500
C	1.53324200	-2.25843900	1.00159600	C	-1.77037100	-2.90185100	0.15598700
C	-4.37981800	1.12519400	-0.12833500	H	-1.39583300	-2.84910700	1.17223800
H	-4.70623100	0.61313300	0.77161600	C	0.15731100	-2.05734700	-4.40015300
C	2.03028400	-4.51635400	1.72206000	H	-0.19247000	-2.30522500	-5.39805900
H	2.51446500	-5.47189800	1.54448500	C	5.70425300	-0.72748100	0.45844800
C	3.90690100	0.08801000	-1.50234100	H	6.39936500	-1.04166200	1.23127700
H	3.21395700	0.42987000	-2.26418600	C	-1.91489200	-4.14653400	-0.44709800
C	-2.60073200	-1.83596400	-1.83700700	H	-1.64312000	-5.04150400	0.10492400
H	-2.87029100	-0.94325200	-2.39192800	C	-2.40463700	-4.24105300	-1.74673500
C	3.44096200	-0.62576500	-0.39378800	H	-2.51955800	-5.21257600	-2.21858900
C	-5.27113300	1.94358300	-0.81576700	C	1.83577700	2.30169300	0.74469300
H	-6.28637900	2.06050800	-0.44834500	C	0.95755500	3.37605300	0.91506800
C	-2.11689000	-1.73161400	-0.52999100	C	3.16216300	2.41103500	1.12002900
C	-4.86252500	2.61563600	-1.96524300	C	1.37381300	4.58401900	1.46576000
H	-5.55829800	3.26042600	-2.49379800	C	3.61040100	3.64114700	1.62837800
C	0.91473700	-2.75888800	-2.21681200	C	2.72541800	4.70222900	1.80636300
H	1.11299400	-3.56475000	-1.52023500	H	0.67626500	5.40405400	1.61866400
C	6.16139400	-0.02403200	-0.65095800	H	4.65834800	3.76435600	1.88983400
H	7.21644500	0.21289700	-0.74994200	H	3.09078200	5.63993500	2.21796200
C	4.34986800	-1.02491100	0.58977600	H	3.85989100	1.58399200	1.02699900
H	4.00606900	-1.55801900	1.47028900	N	-0.30521000	2.97639600	0.41114400
C	-2.31214700	0.43833300	4.26145100	H	-1.09109000	3.31499000	0.96324700
H	-1.86232900	1.07108300	5.02045700	C	-0.43946000	3.93932700	-1.55578000
C	1.05838500	-1.42741000	-1.82508100	O	-1.07253300	4.89475400	-1.27681500
C	1.28956300	-4.31319500	2.88598200	O	0.16968500	3.18965700	-2.24072300
H	1.18909600	-5.11499800	3.61150900				
C	-2.44408900	-0.27930700	1.95031100	<b>IntA21</b>			
C	5.25855300	0.38311600	-1.63059900	Pd	0.23192100	0.97103900	0.39303700
H	5.60515200	0.94210400	-2.49421600	P	1.64433200	-0.74618000	-0.15207600
				P	-1.93199800	-0.09134000	0.21860200

C	-0.27354800	-3.96549000	-1.89088300	C	-4.69912900	0.92616300	3.11779700
H	-0.72119400	-4.89941000	-1.56488400	H	-5.14610200	0.47407400	3.99846600
C	-3.55068100	2.07298300	0.84871400	C	-5.05677200	2.21446000	2.73397500
H	-3.10652900	2.53975800	-0.03137900	H	-5.78264300	2.77425000	3.31671400
C	-3.76859500	0.20564100	2.37153300	C	-2.52450100	0.33114300	-3.79082200
H	-3.50395900	-0.80159000	2.67781400	H	-1.95451500	0.72685600	-4.62532100
C	2.24358200	-1.14739500	2.52183300	C	2.71428600	-1.84782600	3.62815300
H	1.84006300	-0.14481000	2.64161200	H	2.68009800	-1.38738000	4.61076600
C	-1.96226500	0.33393000	-2.51637600	C	0.86282100	-1.56034700	-2.69514200
H	-0.97435800	0.76123100	-2.36606500	H	1.30248200	-0.62298700	-3.02171600
C	2.80584000	-3.01529400	1.10015300	C	-2.48785100	-4.13785800	0.94049700
H	2.83878800	-3.48012900	0.11918700	H	-3.02111900	-4.97702700	0.50331400
C	2.28071700	-1.72672500	1.24906500	C	-1.11766600	-1.98973700	2.03897500
C	-4.01193600	-0.58961900	-1.62356100	H	-0.56944100	-1.15292100	2.46371700
H	-4.61137700	-0.90007600	-0.77142900	C	-0.33189900	-3.58588900	-3.22701500
C	3.27025500	-3.71623300	2.20864900	H	-0.82133500	-4.22528000	-3.95551700
H	3.66913700	-4.71824000	2.08321600	C	5.41111700	-0.28687700	-1.75682900
C	2.96252900	1.05377100	-1.81765200	H	6.36572700	-0.80343300	-1.72129000
H	2.02590800	1.61234400	-1.81957100	C	-0.99145200	-3.25143700	2.60891100
C	-2.60501700	-2.87488300	0.36465700	H	-0.34310700	-3.38985800	3.46890900
H	-3.20264900	-2.75070000	-0.53176900	C	-1.67817900	-4.33123600	2.05668000
C	3.10649700	-0.11096500	-1.05294600	H	-1.57905100	-5.32082900	2.49289800
C	-4.56371800	-0.60134100	-2.89774300	C	1.74141800	2.22389800	0.86928200
H	-5.58338700	-0.94550700	-3.04299100	C	0.99434300	3.38959700	0.80466300
C	-1.91859200	-1.78835300	0.90806300	C	3.06529800	2.27497100	1.28326500
C	-3.81467300	-0.14814200	-3.98429800	C	1.51006700	4.63339500	1.13246300
H	-4.25186600	-0.14619400	-4.97860900	C	3.60927800	3.51936700	1.61750100
C	0.34151800	-3.14230900	-0.95152300	C	2.84293700	4.68302500	1.54491100
H	0.35080700	-3.44513200	0.09050000	H	0.90007300	5.53060900	1.06866100
C	5.26406000	0.86352500	-2.52746800	H	4.64714900	3.58190800	1.93399000
H	6.10614500	1.24614700	-3.09692200	H	3.28855200	5.63770000	1.80909500
C	4.33423800	-0.77741500	-1.02464300	H	3.68321900	1.38214500	1.33793400
H	4.46375600	-1.67025300	-0.42086900	N	-0.35159300	3.07847100	0.36316100
C	-4.48226600	2.78297100	1.59842800	H	-1.08860400	3.48750100	0.93079000
H	-4.75717800	3.78678300	1.28859700	C	-0.68924200	3.26366400	-1.12743800
C	0.92235600	-1.93480800	-1.34686600	O	-1.83146400	3.69011400	-1.29913100
C	3.22247600	-3.13510400	3.47362400	O	0.21197800	2.88644300	-1.88868900
H	3.58340600	-3.68497300	4.33774100				
C	-3.18826600	0.77552000	1.23609200	<b>IntA22</b>			
C	4.04114600	1.52804600	-2.55811600	Pd	0.38587400	0.96630000	0.44405800
H	3.92174000	2.43332000	-3.14491300	P	1.46641800	-0.97087500	-0.15589800
C	-2.69522000	-0.14997200	-1.43104400	P	-1.93966700	0.17720000	0.18578500
C	0.23581000	-2.37853100	-3.62627200	C	-0.04756500	-3.23942100	-3.29066000
H	0.18828400	-2.06836700	-4.66535700	H	-0.24961800	-4.28199700	-3.51638000
				C	-2.53004200	1.48259000	2.56144100

H	-1.78003400	2.19227000	2.22072800
C	-3.84841100	-0.51046500	2.19102400
H	-4.11092100	-1.37158600	1.58427800
C	0.79934600	-1.96817500	2.33143000
H	0.43497300	-0.95729900	2.50181200
C	-2.20442800	2.01766800	-1.89639000
H	-1.12134200	2.06754000	-1.87124500
C	1.85186000	-3.59390500	0.89451900
H	2.35016900	-3.85338600	-0.03463000
C	1.36643500	-2.29508100	1.09510100
C	-4.28536200	1.17982900	-1.00758700
H	-4.82564500	0.56050800	-0.29672100
C	1.72543000	-4.55475000	1.89179000
H	2.09824100	-5.56009300	1.72118200
C	3.62275200	0.12674800	-1.51393600
H	2.86440100	0.70891500	-2.02779900
C	-2.85374800	-1.83858200	-1.58464200
H	-3.09190900	-1.03798100	-2.27691300
C	3.25202900	-0.81928000	-0.55142700
C	-4.98750100	1.95559500	-1.92137900
H	-6.07330100	1.93693700	-1.92399400
C	-2.32125100	-1.54264200	-0.32811500
C	-4.29840400	2.76781100	-2.82163500
H	-4.84897000	3.38585700	-3.52482600
C	0.48039500	-2.90020400	-2.04821300
H	0.65200300	-3.68402300	-1.32106300
C	5.95145500	-0.32720700	-1.09273000
H	6.99945900	-0.12894900	-1.29622700
C	4.24735800	-1.50719300	0.14237000
H	3.98838600	-2.21648700	0.92073000
C	-3.20128800	1.69364500	3.76209100
H	-2.95081000	2.55976700	4.36714800
C	0.73209500	-1.56512200	-1.73127300
C	1.13324800	-4.22490800	3.10961500
H	1.03714300	-4.97647700	3.88743800
C	-2.84774500	0.37131800	1.76897900
C	4.96151300	0.36954400	-1.78364600
H	5.23311100	1.11815700	-2.52108000
C	-2.88592400	1.20071200	-0.99426300
C	-0.11579500	-0.91575000	-3.90993100
H	-0.36303900	-0.13327800	-4.62071000
C	-4.51252700	-0.29406900	3.39528400
H	-5.28649300	-0.98625400	3.71420500
C	-4.18767900	0.80583000	4.18417800

H	-4.70627600	0.97337100	5.12381200
C	-2.90872800	2.80119300	-2.80603200
H	-2.36674200	3.45570100	-3.48063700
C	0.68205200	-2.92771400	3.33339500
H	0.23477100	-2.65880500	4.28519200
C	0.41285300	-0.57550100	-2.67049500
H	0.56028900	0.47235100	-2.42185600
C	-3.07709400	-3.16065300	-1.96118300
H	-3.49048900	-3.37298100	-2.94263600
C	-2.00795900	-2.59852400	0.53697500
H	-1.60458600	-2.39144400	1.52244900
C	-0.33885100	-2.25283800	-4.22653000
H	-0.75572100	-2.52276200	-5.19222000
C	5.59186100	-1.26411700	-0.13225200
H	6.35652200	-1.80262100	0.41956700
C	-2.22584100	-3.91778100	0.15828700
H	-1.97455000	-4.72014000	0.84576200
C	-2.76507600	-4.20261900	-1.09430800
H	-2.94031900	-5.23230800	-1.39242300
C	2.14471400	1.88039200	0.79043800
C	2.32217000	3.12694500	0.17307900
C	3.15689100	1.38486000	1.60838000
C	3.55122600	3.78624400	0.29234700
C	4.37473600	2.05020400	1.74346600
C	4.57690000	3.24242700	1.05751000
H	3.69376500	4.74382900	-0.20458500
H	5.16025500	1.62770500	2.36304400
H	5.52504300	3.76721100	1.13414400
H	3.02044500	0.43529500	2.12129400
N	1.29137100	3.71535200	-0.58012400
H	1.53992100	4.57997600	-1.04153100
C	-0.05237500	3.79148600	-0.12351900
O	-0.74204800	4.71308100	-0.53355800
O	-0.44564200	2.85193100	0.67996900

### IntA25

Pd	-0.12214900	-0.97492700	-0.68833400
P	2.13294000	-0.21146600	-0.08170600
P	-1.43715400	0.93625900	0.00440900
C	1.82833200	2.36845400	3.09377400
H	1.62785200	3.42614200	3.23643600
C	-4.14785300	0.38779100	-0.39567900
H	-4.06363200	-0.22029900	0.49906400
C	-3.16845900	1.87977900	-2.01700800
H	-2.32804100	2.46088100	-2.38377600

C	2.70052300	0.87609200	-2.56372600
H	1.98260300	0.14089400	-2.91811000
C	-1.15466800	0.22483500	2.67568900
H	-0.36007300	-0.42143400	2.32257400
C	3.88284000	1.93741500	-0.75361100
H	4.11419500	2.02247900	0.30334900
C	2.96024900	0.98431200	-1.19345700
C	-2.92777200	1.80669600	2.24075100
H	-3.51499000	2.39850900	1.54408200
C	4.51105100	2.78232100	-1.66478100
H	5.21934700	3.52415000	-1.30841700
C	2.87992400	-2.87104700	0.37180500
H	1.85011900	-2.99933100	0.70314300
C	-0.65287600	3.61608500	0.57154700
H	-1.21020600	3.53230100	1.49823500
C	3.32237200	-1.61244200	-0.05649200
C	-3.22580900	1.84223400	3.59703700
H	-4.03681400	2.47035500	3.95390900
C	-0.60138000	2.53809800	-0.31748600
C	-2.49709500	1.05951800	4.49400000
H	-2.74622000	1.07523800	5.55120900
C	1.94128800	1.86283500	1.80338200
H	1.82988100	2.53486700	0.95906600
C	5.08892900	-3.77884600	-0.00001000
H	5.77490800	-4.62076600	0.01931200
C	4.65365400	-1.44997000	-0.45675600
H	5.01259000	-0.48519000	-0.79966500
C	-5.34694200	0.41494900	-1.09574700
H	-6.18775500	-0.17029900	-0.73700800
C	2.19060100	0.50134200	1.59806000
C	4.24091900	2.67098900	-3.02578800
H	4.73537200	3.32822400	-3.73492000
C	-3.04619000	1.11873900	-0.85318000
C	3.76716500	-3.94400500	0.40242400
H	3.41554400	-4.91347700	0.74218800
C	-1.88350500	0.99568200	1.77187100
C	2.20336900	0.16502200	3.99093800
H	2.29290200	-0.50555300	4.83985900
C	-4.37300800	1.90634000	-2.71536200
H	-4.45669400	2.50473300	-3.61785400
C	-5.46271900	1.17244800	-2.25867500
H	-6.39965700	1.18896600	-2.80760500
C	-1.46732100	0.24925400	4.03218700
H	-0.91166400	-0.39045400	4.70892900

C	3.33874100	1.70921500	-3.47580000
H	3.12767100	1.61082100	-4.53638400
C	2.31570400	-0.34765000	2.70248100
H	2.46622400	-1.41212400	2.56268200
C	0.04512600	4.78717400	0.29336200
H	0.00709000	5.61394300	0.99664100
C	0.14750700	2.66261600	-1.49013000
H	0.20558800	1.82245000	-2.17604300
C	1.95882900	1.52106700	4.19012900
H	1.86062200	1.91451700	5.19742400
C	5.53006700	-2.52989000	-0.42934100
H	6.55970700	-2.39314000	-0.74658800
C	0.84504500	3.83368200	-1.76996000
H	1.44469600	3.89842300	-2.67244200
C	0.80008000	4.89649900	-0.87302300
H	1.35540800	5.80672900	-1.07893800
C	-1.92749000	-1.83079400	-1.10011600
C	-2.61742000	-2.55894000	-0.11291200
C	-2.47073600	-1.70116600	-2.37774700
C	-3.85093900	-3.13553600	-0.47833700
C	-3.69501500	-2.26802100	-2.71651700
C	-4.38438800	-2.99197100	-1.74942500
H	-4.39623700	-3.70657300	0.27037200
H	-4.10203700	-2.13694300	-3.71410600
H	-5.34132800	-3.45092200	-1.98165800
H	-1.94116600	-1.11014800	-3.11999400
N	-2.24520400	-2.67877400	1.22292000
H	-2.93814100	-3.10778500	1.81903700
C	-0.97035000	-2.72764600	1.86064500
O	-0.97820700	-3.11032100	3.02841100
O	0.03775900	-2.33889300	1.18073600
C	0.56633900	-2.21634800	-2.07792000
O	0.92426100	-2.96919600	-2.85392100

**TSA9**

Pd	-0.16128600	-0.83918600	-0.80197800
P	2.10611300	-0.12943700	-0.18805800
P	-1.43102000	0.94315300	0.14362800
C	1.86238100	2.33494000	3.10465800
H	1.69221900	3.39007100	3.29797500
C	-4.16430000	0.39753600	-0.08813500
H	-4.00702100	-0.28796600	0.73764500
C	-3.32092500	2.02999600	-1.64903700
H	-2.51391700	2.64678300	-2.03195200
C	2.44464200	1.06701600	-2.65234900

H	1.73845300	0.30612900	-2.97760700
C	-1.07319000	-0.27248300	2.61115200
H	-0.37785500	-0.93130200	2.10670600
C	3.72000900	2.11770200	-0.89771000
H	4.03081300	2.17448800	0.14081700
C	2.80817000	1.13916200	-1.30313200
C	-2.68710100	1.52479200	2.60295900
H	-3.25619400	2.27939200	2.06650700
C	4.23550200	3.02399800	-1.82022200
H	4.93734500	3.78445400	-1.49141500
C	3.04852900	-2.73909600	0.18545800
H	2.01546600	-3.01423900	0.40012800
C	-0.69215800	3.59111400	0.90580500
H	-1.17347900	3.40927200	1.86027100
C	3.39586000	-1.43581300	-0.18570800
C	-2.91488000	1.32396100	3.95794700
H	-3.64135400	1.94013900	4.47940400
C	-0.66469100	2.59255400	-0.07157900
C	-2.22802700	0.31805800	4.64114600
H	-2.42157400	0.15392600	5.69737400
C	1.96106400	1.89003900	1.78975800
H	1.86644300	2.60607400	0.98076400
C	5.35547300	-3.42341600	-0.04403200
H	6.11688400	-4.19640200	0.00751700
C	4.72994500	-1.13668300	-0.48955600
H	5.01687000	-0.13427900	-0.78956200
C	-5.41775500	0.47866800	-0.68080000
H	-6.22678400	-0.14017400	-0.30591600
C	2.17236200	0.53547800	1.51685300
C	3.86027800	2.95093400	-3.15902600
H	4.26668500	3.65664100	-3.87748700
C	-3.10419500	1.17189200	-0.56920400
C	4.03200600	-3.72371000	0.25771100
H	3.74590200	-4.73076100	0.54434000
C	-1.74754200	0.73428300	1.92315300
C	2.18250600	0.08353200	3.89263400
H	2.25678900	-0.63020100	4.70710000
C	-4.57873300	2.10914800	-2.24072400
H	-4.73591900	2.78207000	-3.07846900
C	-5.62830200	1.33331300	-1.75964600
H	-6.60765100	1.39257200	-2.22510700
C	-1.31714700	-0.48442400	3.96580000
H	-0.79997000	-1.29795000	4.46323200
C	2.96860900	1.96486400	-3.57625700

H	2.67912100	1.89539000	-4.62042100
C	2.27794800	-0.36790100	2.58116800
H	2.39605800	-1.43083000	2.39405900
C	-0.05611500	4.80766500	0.68055500
H	-0.07348800	5.57263300	1.45126000
C	-0.00280800	2.84020300	-1.27690200
H	0.03758400	2.06453100	-2.03608600
C	1.97317700	1.43410300	4.15874000
H	1.88873000	1.78106700	5.18417500
C	5.70223200	-2.12755000	-0.42105600
H	6.73260500	-1.88597100	-0.66510000
C	0.63504000	4.05602000	-1.50276100
H	1.16796600	4.21692700	-2.43447700
C	0.61354800	5.04041600	-0.51942600
H	1.12087400	5.98617400	-0.68476400
C	-1.96689500	-1.70948700	-1.25447500
C	-2.52553000	-2.57937000	-0.30331000
C	-2.64186200	-1.44844200	-2.44311900
C	-3.79855800	-3.11035900	-0.54874300
C	-3.90488500	-1.98723900	-2.67879100
C	-4.48726500	-2.80853800	-1.71767100
H	-4.23510800	-3.77933600	0.18901500
H	-4.43141100	-1.75688500	-3.60010300
H	-5.47341500	-3.23253000	-1.88501500
H	-2.19922700	-0.78369000	-3.18047600
N	-1.88418100	-2.84796500	0.91375100
H	-2.44394700	-2.87307100	1.75209100
C	-0.54198000	-3.26227500	1.10697500
O	-0.12685700	-3.26168000	2.27322700
O	0.10991500	-3.59097100	0.05709300
C	0.40433500	-2.51399300	-1.72476400
O	0.75205600	-3.29288100	-2.48547700

### IntA26

Pd	-0.18958500	-0.99342100	-0.28751500
P	2.05867600	-0.07819800	-0.11950700
P	-1.52022600	0.97924000	0.14357600
C	1.94582600	3.60828600	1.69990500
H	1.55785600	4.59227400	1.45374900
C	-4.05861500	-0.04586800	0.60453800
H	-3.59200400	-0.52553100	1.46030400
C	-3.91101700	1.40030600	-1.31961200
H	-3.34100100	2.06183000	-1.96483600
C	2.10371900	-0.19493200	-2.88098100
H	1.53434300	-1.11047000	-2.73234500

C	-0.55280200	1.02076400	2.75148300
H	0.15534000	0.28189700	2.39095500
C	3.32509300	1.68325200	-1.97651700
H	3.69026900	2.25351800	-1.12830900
C	2.54512500	0.54188400	-1.77365800
C	-2.45681700	2.45386500	2.37219700
H	-3.24308700	2.82359600	1.71924300
C	3.63242500	2.10335100	-3.26816200
H	4.23349500	2.99605100	-3.41397000
C	3.10713700	-2.24852500	1.27048000
H	2.12022100	-2.34094200	1.71346800
C	-1.10002700	3.74711900	-0.45466800
H	-1.51305800	3.98883000	0.51916600
C	3.37939200	-1.26615400	0.31508600
C	-2.40260900	2.87437900	3.69599000
H	-3.13432400	3.58597400	4.06684800
C	-1.01343400	2.41600200	-0.87189700
C	-1.41785500	2.37473400	4.54750500
H	-1.37792900	2.70386600	5.58174900
C	1.87689800	2.59309400	0.75281500
H	1.44682100	2.80598800	-0.21894900
C	5.36826200	-3.06595600	1.08940700
H	6.14036800	-3.77153600	1.38218100
C	4.65553100	-1.18981500	-0.25093500
H	4.87654000	-0.43767600	-1.00217500
C	-5.39017600	-0.30402500	0.31285000
H	-5.95809200	-0.98051200	0.94377800
C	2.35814800	1.31161400	1.04356700
C	3.17359800	1.38084900	-4.36596500
H	3.41390600	1.70970600	-5.37298400
C	-3.30677700	0.80690200	-0.21187000
C	4.10053000	-3.14301700	1.65748600
H	3.86557900	-3.90867900	2.38988900
C	-1.51609100	1.53818600	1.88310800
C	2.99774500	2.09396400	3.24473700
H	3.44318400	1.89324000	4.21472000
C	-5.24957200	1.14092600	-1.60985300
H	-5.71098000	1.60700700	-2.47548900
C	-5.98856200	0.28772700	-0.79872700
H	-7.02854300	0.07930100	-1.03171900
C	-0.49883200	1.44292700	4.07689000
H	0.26224900	1.03863600	4.73651100
C	2.41761500	0.22662000	-4.16912900
H	2.07316100	-0.35324100	-5.02008900

C	2.92945900	1.07525800	2.29810000
H	3.31838900	0.09190900	2.54331000
C	-0.61069300	4.76676300	-1.26531800
H	-0.66946700	5.79737100	-0.92758900
C	-0.45089600	2.12787900	-2.11973400
H	-0.35987900	1.09454400	-2.44338500
C	2.49933300	3.36018600	2.95267200
H	2.54586500	4.15033100	3.69603000
C	5.64380300	-2.08911000	0.13467700
H	6.62987900	-2.03020400	-0.31657300
C	0.03846400	3.14723400	-2.93082300
H	0.50194100	2.89918000	-3.88051100
C	-0.03480300	4.46861800	-2.49957700
H	0.36058000	5.26661600	-3.12097700
C	-1.88176900	-2.08769900	-0.69912400
C	-2.34947900	-3.04528900	0.20302400
C	-2.63766200	-1.86850700	-1.85496100
C	-3.56304200	-3.70619900	0.00715700
C	-3.85044300	-2.51838400	-2.06308000
C	-4.32482600	-3.42865200	-1.12081700
H	-3.89387300	-4.44385900	0.73388500
H	-4.43180200	-2.30540200	-2.95566300
H	-5.27278600	-3.93582100	-1.27397200
H	-2.29617500	-1.14432100	-2.59063600
N	-1.59738400	-3.34045800	1.37743200
H	-2.03024800	-3.19785200	2.27877300
C	-0.25198200	-3.52971700	1.45273500
O	0.36105700	-3.53765200	2.50044500
O	0.36555000	-3.81967500	0.26637900
C	0.53805900	-2.83184400	-0.71409800
O	1.09899700	-3.17325300	-1.71847100

**TSA10**

Pd	-0.14556900	-0.95205000	-0.16393200
P	2.08846700	-0.06037300	-0.08232400
P	-1.56893200	0.99360800	0.14033500
C	1.91981600	3.73599000	1.48550800
H	1.52138100	4.69585200	1.17054100
C	-4.06715500	-0.14681400	0.54068500
H	-3.61554400	-0.54965500	1.44344300
C	-3.90472300	1.17690400	-1.46723400
H	-3.33763600	1.82307200	-2.13052600
C	2.13139300	-0.28729600	-2.84272200
H	1.52071200	-1.17016800	-2.66419500
C	-0.67314300	1.49627100	2.71933800

H	0.14926600	0.84424700	2.44315500
C	3.40571300	1.58620300	-2.00861100
H	3.78173100	2.18082500	-1.18187200
C	2.59369300	0.47557900	-1.76236700
C	-2.76544200	2.56952300	2.17762900
H	-3.58082900	2.74831800	1.48176800
C	3.72866500	1.94675400	-3.31426600
H	4.35434600	2.81639200	-3.49260400
C	3.11253100	-2.16643800	1.40700100
H	2.10929500	-2.24858200	1.81059800
C	-1.18098900	3.71877700	-0.63850200
H	-1.63319800	4.01519800	0.30271900
C	3.41434200	-1.20843000	0.43652200
C	-2.79374200	3.14858900	3.44159200
H	-3.62690100	3.78491100	3.72526800
C	-1.07201000	2.36554100	-0.96919000
C	-1.75760900	2.90885000	4.34342200
H	-1.78193100	3.36255800	5.32997800
C	1.87247600	2.65888000	0.60838000
H	1.44705700	2.79936800	-0.37925200
C	5.38132400	-2.97379700	1.33907700
H	6.14550100	-3.66590900	1.68091900
C	4.71202000	-1.13973800	-0.08070400
H	4.95770800	-0.40725900	-0.84391500
C	-5.37928300	-0.47126700	0.22367300
H	-5.94609400	-1.12341900	0.88117200
C	2.36753300	1.40585200	0.98927400
C	3.25363000	1.19443200	-4.38492200
H	3.50637400	1.47627700	-5.40309000
C	-3.31996100	0.68680000	-0.29876000
C	4.09279400	-3.04482000	1.85875700
H	3.82990900	-3.79294500	2.59958900
C	-1.69611500	1.74666600	1.80188900
C	2.96899900	2.34104600	3.14152300
H	3.40477700	2.21127700	4.12798500
C	-5.21901900	0.84270700	-1.78811900
H	-5.66414900	1.23066100	-2.69975000
C	-5.95860400	0.02139500	-0.94414800
H	-6.98275600	-0.23819000	-1.19556100
C	-0.69956100	2.08088500	3.98242800
H	0.10959600	1.88531300	4.67902900
C	2.46208300	0.07273200	-4.14554500
H	2.10058400	-0.52830400	-4.97455900
C	2.92478000	1.26038900	2.26364400

H	3.32238200	0.29965800	2.57671500
C	-0.66881200	4.69127900	-1.49306800
H	-0.74611300	5.74015200	-1.22149700
C	-0.46324800	2.00730500	-2.17711600
H	-0.35162000	0.95662000	-2.43139200
C	2.46168700	3.57927000	2.75845800
H	2.49049600	4.41822900	3.44730400
C	5.68920300	-2.02092500	0.36917300
H	6.69255200	-1.96766200	-0.04322400
C	0.04973400	2.97809900	-3.03128000
H	0.55035000	2.67586800	-3.94598900
C	-0.04619200	4.32336200	-2.68457300
H	0.36847600	5.08486500	-3.33846700
C	-1.62494400	-2.39619000	-0.62987200
C	-2.21469700	-3.16627900	0.37485500
C	-2.32901600	-2.22145200	-1.82792500
C	-3.50642200	-3.67757300	0.23240700
C	-3.61978000	-2.70896600	-1.97478600
C	-4.21359100	-3.42708900	-0.93511100
H	-3.94000200	-4.28142100	1.02564000
H	-4.16795000	-2.52847300	-2.89414200
H	-5.22203600	-3.81395900	-1.04650600
H	-1.85724400	-1.68243200	-2.64471600
N	-1.46363100	-3.44703400	1.53058100
H	-1.92250500	-3.54288000	2.42382500
C	-0.11237300	-3.66342600	1.57032200
O	0.49268200	-3.85044100	2.60322800
O	0.51217300	-3.74697800	0.36893700
C	0.27923400	-2.85875500	-0.70826200
O	0.73905300	-3.18112400	-1.77373900

### IntA27

Pd	0.06655500	-0.31511000	-0.87134900
P	2.32483400	-0.16156400	-0.37696400
P	-1.63009100	1.05610700	-0.15245900
C	1.96898100	2.04585500	3.08857900
H	1.76581800	3.08079200	3.34751200
C	-3.63004600	0.55491800	-1.99809600
H	-3.03323200	-0.32906500	-2.20696100
C	-3.93867400	2.61652400	-0.78611800
H	-3.59258400	3.33969400	-0.05231800
C	2.64577500	1.53144800	-2.55682400
H	1.84488600	0.92541700	-2.97464100
C	-1.24015600	0.26540300	2.47981200
H	-0.18824700	0.34973900	2.22539500

C	4.12501600	2.04460800	-0.73041900
H	4.49005600	1.85598500	0.27478500
C	3.11109700	1.24587800	-1.26944400
C	-3.56425700	0.43997600	1.86677100
H	-4.33701600	0.68438300	1.14423800
C	4.65132600	3.10808700	-1.45706600
H	5.43162700	3.72472200	-1.02034400
C	3.28985400	-2.67496200	-1.06337700
H	2.29844700	-2.82170600	-1.48096100
C	-1.03587800	3.45258800	1.30150100
H	-1.69604900	3.09219400	2.08500300
C	3.61073100	-1.47164300	-0.43349000
C	-3.92649500	-0.04435400	3.12469600
H	-4.97790200	-0.16328600	3.37215400
C	-0.86353800	2.70667700	0.13352400
C	-2.94771300	-0.36977800	4.06115400
H	-3.23232500	-0.74971300	5.03807300
C	2.11207800	1.69534300	1.74990200
H	2.00592000	2.46138000	0.98792000
C	5.49468400	-3.53136900	-0.58968100
H	6.22720200	-4.33153700	-0.64772200
C	4.88427600	-1.31127600	0.12676300
H	5.14143900	-0.38850900	0.63897800
C	-4.82341600	0.77485400	-2.68156000
H	-5.16049400	0.05662000	-3.42365000
C	2.36590900	0.36665700	1.38531200
C	4.17876000	3.38314500	-2.73848200
H	4.59029700	4.21420200	-3.30412300
C	-3.18373900	1.46541700	-1.03832000
C	4.23031600	-3.70119500	-1.14173600
H	3.96339800	-4.63433500	-1.62845600
C	-2.21745900	0.59015400	1.52853600
C	2.30198500	-0.25126000	3.72737300
H	2.36090600	-1.02191700	4.49006000
C	-5.12673800	2.84101900	-1.47377500
H	-5.70560700	3.73819200	-1.27441300
C	-5.57269400	1.91790500	-2.41945900
H	-6.50001100	2.09667100	-2.95621300
C	-1.60023600	-0.20298300	3.73764900
H	-0.82175200	-0.46404800	4.44682900
C	3.17681200	2.58916600	-3.29002100
H	2.80203700	2.79652100	-4.28815600
C	2.45290500	-0.60405400	2.38899500
H	2.60745500	-1.64626600	2.12861600

C	-0.33618000	4.64428500	1.48569900
H	-0.47088900	5.20965800	2.40358000
C	0.00960100	3.18444300	-0.85118800
H	0.17655200	2.59454800	-1.74769500
C	2.06395100	1.07425100	4.08242300
H	1.94458000	1.34756600	5.12701800
C	5.82099400	-2.33378800	0.04783300
H	6.80580000	-2.20050600	0.48642700
C	0.70954100	4.37097300	-0.66888300
H	1.40753200	4.70371600	-1.43163800
C	0.54170500	5.10161400	0.50689700
H	1.09866900	6.02115800	0.66173700
C	-1.87562500	-3.20034900	-0.97878100
C	-2.53683800	-2.78663800	0.17981100
C	-2.57147300	-3.30991000	-2.18569400
C	-3.89862700	-2.47745700	0.13283100
C	-3.92213300	-3.00867900	-2.23486600
C	-4.57660300	-2.58990200	-1.07078600
H	-4.40584700	-2.14449600	1.03193700
H	-4.46858600	-3.09315500	-3.16815400
H	-5.63256000	-2.34051500	-1.10626800
H	-2.02675000	-3.63585000	-3.06533400
N	-1.81425300	-2.70596900	1.35674600
H	-2.22633300	-2.27140100	2.17332800
C	-0.47437900	-2.97391100	1.46866800
O	0.15541200	-2.84665200	2.48409000
O	0.13311500	-3.45840400	0.34105000
C	-0.45061600	-3.54196300	-0.90684100
O	0.22821500	-3.91899900	-1.82505000

### IntA23

Pd	-0.28707300	-0.51831200	0.79527900
P	-1.41322100	0.86921100	-0.59366600
P	2.08660100	0.08790500	0.36726200
C	0.10898500	1.81063500	-4.31486700
H	0.26127900	2.69403500	-4.92773500
C	1.89521100	0.72431700	3.07330300
H	1.07473200	0.01078500	3.07541700
C	3.64107600	1.91862200	1.92093200
H	4.18527600	2.15465100	1.01138100
C	-0.59444900	3.03152100	0.96708200
H	0.01571000	2.30054000	1.49118200
C	2.86714300	-2.50354500	-0.24512400
H	1.80979400	-2.65789000	-0.46650900
C	-2.21486100	3.56733800	-0.73662900



H	-2.87865600	3.25811700	-1.53896600
C	-1.42423100	2.61756400	-0.07781600
C	4.66922600	-1.07962700	0.51539100
H	5.02622400	-0.12229400	0.88257600
C	-2.16143000	4.90603400	-0.36266400
H	-2.77815200	5.63403500	-0.88068600
C	-3.40929200	-0.72846300	-1.69292900
H	-2.60898000	-1.32221600	-2.12769200
C	3.10800100	0.74385600	-2.16702800
H	3.30463200	-0.31856600	-2.27286900
C	-3.15165000	0.40693200	-0.91791900
C	5.56636100	-2.12864200	0.35610100
H	6.61561200	-1.98193200	0.59495500
C	2.55170900	1.23803800	-0.98464400
C	5.11936600	-3.36680800	-0.10515300
H	5.82247100	-4.18604300	-0.22537200
C	-0.42404400	1.94812400	-3.03728200
H	-0.67530600	2.93704000	-2.66970800
C	-5.77168300	-0.49570400	-1.24134100
H	-6.79156900	-0.84824200	-1.36593900
C	-4.20821600	1.07029000	-0.28444300
H	-4.01599600	1.91172400	0.37256700
C	2.23621900	1.36721400	4.26001500
H	1.68222600	1.14751900	5.16750700
C	-0.60990000	0.81883200	-2.23655300
C	-1.32345800	5.30979900	0.67485600
H	-1.28642300	6.35503400	0.96692300
C	2.59208900	0.99183200	1.88850100
C	-4.71965800	-1.16976400	-1.85304900
H	-4.90486300	-2.05787500	-2.44941900
C	3.31409600	-1.26183500	0.21499300
C	0.28828400	-0.57040600	-3.99868000
H	0.55323600	-1.55834400	-4.36208100
C	3.98113600	2.56186800	3.10689900
H	4.79557800	3.28020100	3.11415400
C	3.27907600	2.28862700	4.27838200
H	3.54367700	2.79411600	5.20235400
C	3.77388700	-3.55126200	-0.40403900
H	3.41641200	-4.51479700	-0.75578100
C	-0.54163700	4.37092100	1.34134800
H	0.10854200	4.67468700	2.15615700
C	-0.22528400	-0.43761600	-2.71356400
H	-0.32696300	-1.31101100	-2.07769000
C	3.41707500	1.60711900	-3.21369800

H	3.84582800	1.20658300	-4.12719100
C	2.29056700	2.60918000	-0.88163800
H	1.85059900	3.01650000	0.02223200
C	0.45147600	0.55247800	-4.80333800
H	0.85641900	0.45192800	-5.80630400
C	-5.51238000	0.62239400	-0.45216300
H	-6.32424900	1.13839700	0.05119000
C	2.60739200	3.47063100	-1.92575600
H	2.40523200	4.53278100	-1.82326800
C	3.17627400	2.97200600	-3.09402400
H	3.42355300	3.64322300	-3.91118900
C	-2.08653200	-0.55091900	1.72105900
C	-2.98304900	-1.62894600	1.57134600
C	-2.38433200	0.48629600	2.60254500
C	-4.17984100	-1.59837700	2.30852500
C	-3.56925500	0.49631800	3.33830000
C	-4.47133100	-0.55031200	3.16885200
H	-4.88295300	-2.42020300	2.19331500
H	-3.78310000	1.31368200	4.02034200
H	-5.41081800	-0.55547000	3.71507700
H	-1.69584200	1.31995800	2.71002600
N	-2.68932300	-2.71140500	0.77183100
H	-3.48065400	-3.20884900	0.39041800
H	-1.92588400	-2.60840500	0.10255900
C	0.18306200	-3.54528800	1.83354600
O	0.07833700	-4.69220900	1.70287600
O	0.34642600	-2.41815100	2.12721000
C	-0.55076200	-3.63812400	-1.56046300
O	-0.17031200	-2.90607800	-0.57347500
O	-1.53839300	-3.41074900	-2.27060400
C	0.34083300	-4.84264600	-1.85986700
H	-0.12495300	-5.50222400	-2.59471200
H	1.29907700	-4.48701100	-2.25989900
H	0.55310600	-5.39424300	-0.93878000

**TSA8**

Pd	0.30990900	-0.31449200	-0.89728600
P	1.22486100	1.12164300	0.60900000
P	-2.10334500	-0.14821200	-0.43145800
C	-0.63108100	2.10803900	4.16124300
H	-0.88257800	3.01014100	4.71082000
C	-2.26953800	-0.17879700	-3.21186400
H	-1.37962000	-0.79924300	-3.15643900
C	-4.02644600	1.08245900	-2.14518700
H	-4.50116900	1.47293500	-1.25010200

C	0.47535600	3.24412600	-1.03589100	C	0.41634200	4.57765000	-1.42956000
H	-0.05357600	2.48354500	-1.60552300	H	-0.16437400	4.85636000	-2.30350600
C	-2.28140500	-2.68502900	0.69753400	C	-0.03301900	-0.19318400	2.71131500
H	-1.19929800	-2.62332300	0.83232500	H	0.18208400	-1.10299900	2.14940300
C	1.92215500	3.84503900	0.79777000	C	-3.72067500	1.85954800	2.78356800
H	2.52005400	3.56313300	1.65984200	H	-4.16965500	1.60101400	3.73768700
C	1.22019800	2.86609200	0.08367400	C	-2.54800000	2.50243100	0.35205400
C	-4.38397600	-1.76872100	-0.08334800	H	-2.10541000	2.76602400	-0.60262100
H	-4.94472500	-0.97242900	-0.56453300	C	-0.94413000	0.85780400	4.68546000
C	1.86282500	5.17785100	0.40462600	H	-1.42837500	0.77997000	5.65469600
H	2.41012100	5.92914000	0.96544200	C	5.32923800	0.93463300	0.62613300
C	3.19815300	-0.49079800	1.70488600	H	6.15656300	1.48654200	0.19022300
H	2.38337200	-1.09731500	2.07994200	C	-2.96406500	3.51423000	1.20825700
C	-3.30406100	0.84425900	1.92629000	H	-2.82472200	4.55201500	0.92021600
H	-3.43266900	-0.19262400	2.21904400	C	-3.55602300	3.19370800	2.42765700
C	2.95724000	0.69586300	1.00819900	H	-3.88276800	3.98184300	3.09962700
C	-5.04715300	-2.90818300	0.35312100	C	2.14328000	-0.23303500	-1.74178400
H	-6.12051100	-2.99587600	0.21295700	C	2.95811800	-1.37396500	-1.66267300
C	-2.71835100	1.15703100	0.69878100	C	2.54705100	0.84534000	-2.52378500
C	-4.33240000	-3.93818000	0.96520100	C	4.17172900	-1.39602200	-2.35688200
H	-4.85141800	-4.83047700	1.30353400	C	3.75515200	0.81410700	-3.22177000
C	-0.00512800	2.21450500	2.92316700	C	4.57009700	-0.30801700	-3.12464200
H	0.21058200	3.19933800	2.52488300	H	4.80611600	-2.27637800	-2.28579500
C	5.56392200	-0.25087500	1.31978100	H	4.05342500	1.66382500	-3.82885100
H	6.57813300	-0.62464500	1.42689400	H	5.52073800	-0.34209100	-3.64903700
C	4.03173700	1.40316400	0.45792700	H	1.92805300	1.73482400	-2.58983000
H	3.86220900	2.29548200	-0.13485000	N	2.50771000	-2.50133800	-0.96439300
C	-2.81741300	0.11300900	-4.45766900	H	3.21137600	-3.21657900	-0.81197200
H	-2.34139300	-0.26946000	-5.35536700	H	2.03957900	-2.32559200	-0.05671700
C	0.31678900	1.06266000	2.20040700	C	0.63787800	-3.33157400	-1.73962900
C	1.10755800	5.54582700	-0.70705700	O	0.81072900	-4.48425600	-1.64887900
H	1.06538400	6.58657300	-1.01386300	O	0.05400900	-2.32615700	-2.02166700
C	-2.86783000	0.30397300	-2.04144800	C	1.41207900	-3.60380500	1.81139500
C	4.49634000	-0.96670200	1.85113900	O	0.79005800	-2.68860500	1.15368300
H	4.64255600	-1.91959100	2.34792200	O	2.64084500	-3.72897600	1.86645400
C	-2.99879900	-1.65120500	0.08982000	C	0.51141100	-4.60627500	2.53518700
C	-0.65189400	-0.28876500	3.95357900	H	1.08670400	-5.22284500	3.22882700
H	-0.90696500	-1.26994600	4.34300400	H	-0.29083700	-4.08572700	3.07012800
C	-4.57155800	1.37365100	-3.39196500	H	0.04137100	-5.25718200	1.78801800
H	-5.47046900	1.97958400	-3.45703900				
C	-3.96752000	0.89147700	-4.55028800	<b>IntA24</b>			
H	-4.39290600	1.12173100	-5.52256300	Pd	-0.25241400	-0.46227600	0.91547200
C	-2.95724500	-3.82461700	1.13474500	P	-0.92267700	1.49058100	-0.10791400
H	-2.39429700	-4.62559400	1.60436800	P	2.09148700	-0.49620200	0.16170600
				C	0.62654600	2.53662300	-3.81725700

H	1.09967200	3.39343600	-4.28700800	H	6.35834700	0.31402000	2.62594000
C	2.83576500	-1.29860600	2.72178600	C	4.95370200	-0.83340700	3.78821400
H	1.86198100	-1.78038200	2.73467300	H	5.61519700	-0.92589300	4.64480200
C	4.52371400	-0.01640500	1.55935500	C	1.58173600	-3.78540400	-2.20671700
H	4.86085600	0.53056500	0.68446100	H	0.73929200	-4.27818200	-2.68154800
C	0.35514900	2.81523400	1.95401700	C	0.85657200	3.91177700	2.64974300
H	0.49164800	1.81166500	2.35133600	H	1.37617900	3.75929000	3.59049000
C	1.36319200	-2.64320900	-1.44328400	C	-0.52478100	0.33605400	-2.57795800
H	0.35458200	-2.26042400	-1.33432600	H	-0.95195000	-0.54292600	-2.10422200
C	-0.49646000	4.28691300	0.24375500	C	3.70849100	1.73050300	-2.91638400
H	-1.04479600	4.44896100	-0.67931300	H	4.00812700	1.56880900	-3.94753400
C	-0.31343900	2.98820100	0.73701200	C	2.92217500	2.13085500	-0.28383700
C	3.71928700	-2.52973700	-0.93200100	H	2.63053200	2.29535100	0.74881300
H	4.55240100	-2.05142900	-0.42449900	C	0.42013600	1.36762500	-4.54121800
C	0.01052700	5.38151400	0.93612300	H	0.71759000	1.31172800	-5.58414000
H	-0.13255800	6.38209900	0.53973400	C	-4.83104500	2.86092500	0.05819900
C	-3.45123300	0.59640000	-0.74613100	H	-5.36815300	3.74540000	0.38785600
H	-2.91897400	-0.31240900	-0.99788800	C	3.43692600	3.19002800	-1.02121100
C	3.19164200	0.66781600	-2.17868800	H	3.52704800	4.16970000	-0.56112800
H	3.09327600	-0.30906500	-2.64064600	C	3.83551700	2.99055900	-2.34166600
C	-2.73849700	1.70070600	-0.26838700	H	4.24162300	3.81565500	-2.91966300
C	3.93662600	-3.67037500	-1.69646800	C	-2.06328500	-0.67409100	1.77228100
H	4.93984100	-4.07631100	-1.78603900	C	-2.67007800	-1.92992500	1.66627900
C	2.79971700	0.85675700	-0.85270900	C	-2.72203500	0.32176200	2.49311600
C	2.86821400	-4.29878700	-2.33473900	C	-3.95840000	-2.13298300	2.16583600
H	3.03994200	-5.19653600	-2.92132300	C	-3.99637200	0.11705200	3.01667500
C	0.25464700	2.61279900	-2.47773400	C	-4.62573100	-1.10820700	2.82560500
H	0.47407700	3.51770900	-1.92501000	H	-4.43769200	-3.10004700	2.03538300
C	-5.52915800	1.75972100	-0.42400000	H	-4.49866200	0.91797900	3.55120400
H	-6.61386100	1.78100500	-0.47018500	H	-5.62977600	-1.27690400	3.20339600
C	-3.43947600	2.83312600	0.14310500	H	-2.25781900	1.29740300	2.61770200
H	-2.91932400	3.68760800	0.56168300	N	-2.00167100	-3.01243800	1.02343800
C	3.68939200	-1.41581400	3.81491100	H	-2.54614400	-3.86873900	1.05023700
H	3.36158700	-1.96999900	4.68923000	H	-2.02067600	-2.72574400	-0.68200500
C	-0.34097000	1.51858800	-1.85009900	C	-0.64065800	-3.35294600	1.39404500
C	0.69272300	5.19495100	2.13667900	O	-0.34413300	-4.53339000	1.38641600
H	1.08710600	6.05116500	2.67558900	O	0.13690500	-2.36241600	1.66308500
C	3.24753900	-0.59072000	1.58508500	C	-3.26639500	-2.50605200	-2.12666600
C	-4.83502100	0.61922000	-0.82523600	O	-2.00966400	-2.51505900	-1.66810400
H	-5.35995600	-0.26717000	-1.16707900	O	-4.22715500	-2.78238500	-1.44284600
C	2.42877100	-2.00596100	-0.80569400	C	-3.33271000	-2.05927600	-3.56552000
C	-0.14851300	0.26245000	-3.91390000	H	-4.32779700	-2.24982000	-3.96779200
H	-0.29305300	-0.66660700	-4.45725400	H	-3.12363900	-0.98387400	-3.61122500
C	5.37071800	-0.13689300	2.65733900	H	-2.57410600	-2.57117300	-4.16371300

**TSA11**

Pd	0.19250300	-0.60611600	-1.09873800
P	1.51314700	1.00101400	-0.08925900
P	-2.05422500	-0.21399800	-0.19708600
C	0.61061200	1.50427000	3.92574500
H	0.29531400	2.30191900	4.59138200
C	-3.00134400	0.10473800	-2.77921000
H	-2.04945000	-0.34811600	-3.04963500
C	-4.51382200	0.93088700	-1.09109500
H	-4.74875200	1.12496900	-0.04819200
C	0.18775700	3.10400700	-1.33440200
H	-0.38634500	2.30851600	-1.80478700
C	-1.76302500	-2.68412700	1.02438600
H	-0.70882900	-2.42355000	1.03496700
C	1.96850300	3.79109100	0.14044300
H	2.78419600	3.53952900	0.81339600
C	1.20469200	2.77044100	-0.43713600
C	-4.04041600	-2.17203100	0.41714700
H	-4.77228800	-1.50943600	-0.03515900
C	1.69266100	5.12302700	-0.14772400
H	2.28685000	5.90924200	0.30853100
C	4.19847300	0.77688100	0.85132000
H	3.79934500	0.78816300	1.86071900
C	-2.56975100	0.49230800	2.50685500
H	-2.62264100	-0.57111000	2.71686000
C	3.33816700	0.88338700	-0.24423200
C	-4.45345500	-3.38987500	0.95016300
H	-5.50315100	-3.66610800	0.91162700
C	-2.34598800	0.93885800	1.20298600
C	-3.52522700	-4.25073600	1.53094200
H	-3.85019400	-5.19998700	1.94708800
C	0.84659100	1.78714400	2.58165700
H	0.70369300	2.79871500	2.21684600
C	6.09460200	0.60752300	-0.63350200
H	7.16397800	0.49226600	-0.78458900
C	3.87167300	0.85472900	-1.53826100
H	3.21055800	0.90222600	-2.39816300
C	-3.90671000	0.47088300	-3.77142900
H	-3.66293300	0.29642000	-4.81508700
C	1.23354300	0.77155700	1.70836800
C	0.66173500	5.44764800	-1.02883300
H	0.45095500	6.48849200	-1.25667000
C	-3.29924100	0.32309700	-1.42989300
C	5.57082300	0.63815100	0.65561600

H	6.22972400	0.54960800	1.51455700
C	-2.69188000	-1.80689900	0.45185200
C	1.13912900	-0.81333100	3.53934300
H	1.25320300	-1.82974600	3.90438100
C	-5.41621600	1.30049200	-2.08354500
H	-6.35535000	1.77253700	-1.80996800
C	-5.11500500	1.06871400	-3.42422600
H	-5.81963700	1.36049800	-4.19750900
C	-2.17971500	-3.89444700	1.56979800
H	-1.44719400	-4.56207900	2.01412600
C	-0.08552500	4.43808600	-1.62797800
H	-0.87786300	4.68558500	-2.32820800
C	1.37141700	-0.53638200	2.19813500
H	1.66777000	-1.33926000	1.52531600
C	-2.72423500	1.40559400	3.54728000
H	-2.89622800	1.04173200	4.55602600
C	-2.26884400	2.31693100	0.96479200
H	-2.09423500	2.68531700	-0.04122900
C	0.75727800	0.20869300	4.40748600
H	0.56797600	-0.00834900	5.45478700
C	5.24185600	0.72017100	-1.73057400
H	5.64133800	0.68771200	-2.73955000
C	-2.42363900	3.22689700	2.00335200
H	-2.36136000	4.29143900	1.79689600
C	-2.65487000	2.77251000	3.30034300
H	-2.77735700	3.48185000	4.11384400
C	1.72073100	-1.59112800	-2.10060700
O	2.03464300	-1.23087200	-3.20479500
C	2.39676500	-2.49902800	-1.09122300
C	1.28904300	-3.32586800	-0.88401400
C	3.59484500	-2.65044300	-0.43921400
C	1.37191900	-4.41230500	-0.03061800
C	3.67573800	-3.73096900	0.46403900
C	2.59663200	-4.58887800	0.64452900
H	0.53939100	-5.09273200	0.12183900
H	4.59733700	-3.90457900	1.01111000
H	2.69727000	-5.42367300	1.33351900
H	4.43916700	-1.99005500	-0.61266400
N	0.27875000	-2.71835300	-1.64635600
H	-0.29931000	-3.27999800	-2.25961000

**IntA28**

Pd	-0.07940600	-0.33066500	-1.14271600
P	1.72440700	0.81007900	-0.25676800
P	-2.20908100	0.01043500	-0.34209100

C	0.38899900	1.69466500	3.55319700
H	-0.17572200	2.49092400	4.02888600
C	-3.68161900	-0.64559000	-2.60750200
H	-2.71208400	-0.96733700	-2.98185700
C	-5.00159500	0.35052100	-0.85530300
H	-5.07521100	0.79893000	0.13169300
C	1.21892400	3.08865200	-1.77567100
H	0.63790100	2.39645300	-2.38139100
C	-1.72973800	-1.15284600	2.15081900
H	-1.01513100	-0.34556200	2.27096600
C	2.62923100	3.49076500	0.13360600
H	3.15329800	3.12841400	1.01387500
C	1.87679400	2.60365000	-0.64352800
C	-3.42889500	-2.26697300	0.85818700
H	-4.05895600	-2.32901900	-0.02453100
C	2.70001400	4.83813500	-0.20208500
H	3.28071800	5.51884700	0.41375600
C	4.43225500	0.35455200	0.63242100
H	4.15455100	0.77211200	1.59592700
C	-3.01241300	1.80306100	1.76350400
H	-3.45313600	0.95352500	2.27681200
C	3.48530000	0.26693200	-0.39313900
C	-3.52628000	-3.25009800	1.84269900
H	-4.22975200	-4.06822500	1.71593900
C	-2.39655400	1.62963600	0.52124800
C	-2.73472100	-3.18102100	2.98632400
H	-2.81677000	-3.94536800	3.75377500
C	0.72939600	1.81201900	2.20739600
H	0.41953100	2.69538200	1.65828600
C	6.09916800	-0.67252400	-0.78234100
H	7.10949000	-1.04445600	-0.92751100
C	3.87311200	-0.28203700	-1.61865900
H	3.14558000	-0.36440100	-2.42106600
C	-4.82353500	-0.78096700	-3.39487400
H	-4.74922900	-1.21641400	-4.38717500
C	1.43969000	0.79435300	1.56203200
C	2.02959900	5.31426400	-1.32831500
H	2.08628800	6.36710800	-1.58965300
C	-3.75945200	-0.08557500	-1.33030400
C	5.72816100	-0.11668900	0.44037500
H	6.45028200	-0.05005800	1.24941500
C	-2.52850400	-1.20769200	1.00136100
C	1.45767400	-0.45975500	3.63918700
H	1.74121000	-1.35434400	4.18706000

C	-6.14147400	0.21986200	-1.64060000
H	-7.10032300	0.56347600	-1.26325000
C	-6.05425900	-0.34864500	-2.91109300
H	-6.94561700	-0.44793900	-3.52390000
C	-1.83895500	-2.12335900	3.13889800
H	-1.21095000	-2.05362300	4.02247000
C	1.29381200	4.43701500	-2.11920400
H	0.77577800	4.79989500	-3.00223700
C	1.78513900	-0.34963600	2.29232700
H	2.30669100	-1.16614700	1.80228000
C	-3.03802200	3.05744100	2.37028100
H	-3.50896400	3.17400200	3.34240100
C	-1.82697700	2.74233200	-0.10600300
H	-1.31997000	2.61051600	-1.05645500
C	0.75746100	0.56337600	4.27653200
H	0.49374700	0.47542800	5.32661000
C	5.16930300	-0.74841700	-1.81625300
H	5.44226700	-1.18355600	-2.77287200
C	-1.85707400	3.99664700	0.49240000
H	-1.38654100	4.83963800	-0.00559200
C	-2.45757900	4.15502400	1.74016800
H	-2.47003100	5.12908300	2.22085100
C	1.77427800	-2.77000700	-2.28059200
O	2.29221200	-2.64541700	-3.34966400
C	2.12708600	-3.14334700	-0.86126100
C	0.76005700	-3.19027700	-0.59746700
C	3.07939800	-3.41373200	0.09396900
C	0.22784500	-3.55550500	0.61408200
C	2.56895700	-3.78970500	1.35015600
C	1.19462700	-3.86097600	1.59059000
H	-0.83400400	-3.58756500	0.82879300
H	3.25789100	-4.02484000	2.15550700
H	0.84993000	-4.14558300	2.58066100
H	4.14500000	-3.33889100	-0.09453800
N	0.37229100	-2.68420700	-1.89441200
H	-0.34053200	-3.12990200	-2.46331300

**TSA12**

Pd	0.19306100	-1.00404600	-0.29353300
P	1.59878100	0.81721000	0.12997900
P	-2.13896600	-0.16805300	-0.20402400
C	0.25417400	4.03558100	2.35851600
H	0.30038600	5.12032900	2.32255000
C	-2.95190000	-2.46345000	-1.55775900
H	-1.92448900	-2.78722900	-1.41526000

C	-4.70096200	-0.83163300	-1.22409000
H	-5.03111000	0.13141600	-0.84344700
C	0.87856000	2.09434200	-2.23059500
H	-0.01611100	1.48385900	-2.15735400
C	-2.41803100	-1.10750300	2.37460800
H	-1.72875100	-1.88298600	2.04416900
C	3.03725700	2.75266400	-1.37931900
H	3.83086500	2.65822200	-0.64388400
C	1.88429600	1.96763700	-1.26799700
C	-3.73849300	0.86463900	1.93717500
H	-4.07586300	1.64748800	1.26437900
C	3.17385700	3.65353100	-2.43141700
H	4.07417400	4.25585700	-2.51082800
C	3.74167800	0.97317000	1.99792400
H	3.08355800	1.55560800	2.63526100
C	-2.05111600	2.63885700	-0.18648200
H	-1.76743400	2.55256400	0.85732500
C	3.29125800	0.51485300	0.75643800
C	-4.20229000	0.84278000	3.24961300
H	-4.89990800	1.60426200	3.58633700
C	-2.40642400	1.49792400	-0.91637000
C	-3.77710400	-0.15279300	4.12571500
H	-4.14062000	-0.16870600	5.14923000
C	0.91647900	3.28508600	1.39061300
H	1.45984300	3.78873900	0.59702500
C	5.89389800	-0.05082200	1.61170400
H	6.90409800	-0.27081200	1.94490100
C	4.15438500	-0.23557700	-0.04830200
H	3.81415600	-0.61218600	-1.00920600
C	-3.86508700	-3.30536800	-2.19136400
H	-3.53726800	-4.27351100	-2.55751000
C	0.85416900	1.88906700	1.41949600
C	2.16036400	3.78264900	-3.37862400
H	2.26907600	4.48770100	-4.19775500
C	-3.36359900	-1.21940300	-1.07490300
C	5.03717000	0.68908600	2.42251700
H	5.37716200	1.05097100	3.38855500
C	-2.83177900	-0.10100100	1.49342200
C	-0.53057600	2.00978200	3.40705400
H	-1.11344800	1.50221100	4.16974100
C	-5.60699100	-1.66919900	-1.86197600
H	-6.64176700	-1.35994900	-1.97685300
C	-5.18821400	-2.90822000	-2.34792400
H	-5.89841900	-3.56411300	-2.84313500

C	-2.89181900	-1.13340500	3.68262600
H	-2.56424400	-1.92265900	4.35233900
C	1.01203300	3.00249800	-3.27589400
H	0.21473100	3.09595600	-4.00684900
C	0.13684700	1.26113000	2.44297300
H	0.07020100	0.17681400	2.46385200
C	-2.04952300	3.89235100	-0.78825400
H	-1.76128600	4.76113000	-0.20401900
C	-2.76005200	1.64434400	-2.26311100
H	-3.03401400	0.77266400	-2.85031800
C	-0.47768300	3.40089600	3.36086200
H	-1.00935600	3.99054700	4.10195500
C	5.44925900	-0.51146800	0.37501700
H	6.10221000	-1.10218400	-0.26046300
C	-2.75969700	2.90129100	-2.86231900
H	-3.04062900	2.99678600	-3.90731000
C	-2.40079600	4.02873600	-2.12834000
H	-2.39298700	5.00736400	-2.59888800
C	1.58335500	-2.50597500	-0.80606000
C	2.45865100	-3.12821200	0.10410000
C	1.90762700	-2.46310500	-2.16247300
C	3.73404700	-3.50297400	-0.27899500
C	3.20467000	-2.82594000	-2.54083700
C	4.12022900	-3.31464500	-1.61070400
H	4.40323800	-3.97398400	0.43547900
H	3.49546100	-2.72034100	-3.58206200
H	5.11876700	-3.59969400	-1.92622500
H	1.19804800	-2.08982900	-2.89435700
N	1.77633400	-3.44181400	1.27350200
H	2.19599200	-3.90636700	2.06277200
C	0.40631500	-3.57536900	1.08068800
O	-0.36852800	-3.99677600	1.91539400
O	0.06136500	-3.19891200	-0.15953700

### IntA29

Pd	-0.02303200	-0.70532800	-0.67818200
P	1.66684100	0.80150100	-0.18289700
P	-2.21420600	-0.23914900	-0.10275400
C	0.90458300	3.39250600	2.96285300
H	0.95887400	4.45945200	3.16065000
C	-3.38372500	-1.63289000	-2.19353400
H	-2.36611200	-1.62729900	-2.57952400
C	-4.94561500	-1.04809500	-0.45529200
H	-5.16196500	-0.59508700	0.50777900
C	0.60727700	2.69016000	-1.91506500

H	-0.29471100	2.09188800	-1.81953200
C	-1.89385700	-1.56282700	2.31639100
H	-1.17554800	-2.15640300	1.75681500
C	2.93120500	3.06349900	-1.39001400
H	3.84479600	2.76704200	-0.88242500
C	1.77408500	2.28840400	-1.25587300
C	-3.45605200	0.26669300	2.42799200
H	-3.97352900	1.09833700	1.95787700
C	2.91938000	4.21737700	-2.16897100
H	3.82486900	4.80910200	-2.26910500
C	4.06352500	0.17055000	1.23085000
H	3.55080200	0.47234900	2.13844700
C	-1.97082300	2.47323400	0.55546500
H	-1.43711000	2.12156100	1.43332100
C	3.42898900	0.30008700	-0.00714000
C	-3.65558300	0.01151300	3.78173900
H	-4.33823100	0.63472600	4.35227000
C	-2.56084100	1.55378500	-0.32246100
C	-2.97861500	-1.03478600	4.40407500
H	-3.13222700	-1.22984500	5.46158800
C	1.35431400	2.89471900	1.74155800
H	1.73940300	3.58062500	0.99349000
C	6.01455000	-0.78021100	0.16531500
H	7.01437500	-1.19904100	0.23286300
C	4.10972100	-0.11438800	-1.16069100
H	3.62051500	-0.03485200	-2.12851300
C	-4.41032100	-2.23153600	-2.92060300
H	-4.19735800	-2.69257900	-3.88084000
C	1.27470000	1.52763600	1.46432500
C	1.74907900	4.61594900	-2.81134900
H	1.74094200	5.51965800	-3.41415800
C	-3.64056500	-1.03007300	-0.95830600
C	5.34528700	-0.37250400	1.31692500
H	5.81729700	-0.47851400	2.28898100
C	-2.57253400	-0.51842500	1.67954700
C	0.31268400	1.16324700	3.66213100
H	-0.10977600	0.48114800	4.39358100
C	-5.96971800	-1.65472800	-1.17488700
H	-6.97821200	-1.66775800	-0.77168500
C	-5.70463500	-2.24478300	-2.40984300
H	-6.50654700	-2.71757700	-2.96947400
C	-2.09812000	-1.82395100	3.66808000
H	-1.55522200	-2.63381600	4.14620700
C	0.59239800	3.85216700	-2.68006300

H	-0.32756600	4.15540400	-3.17078500
C	0.75893500	0.66782900	2.44207800
H	0.67402300	-0.39485000	2.23312900
C	-2.04675400	3.83794900	0.30711900
H	-1.57260900	4.53057700	0.99615800
C	-3.23108000	2.03462400	-1.45038800
H	-3.69575500	1.33924200	-2.14382900
C	0.37592800	2.53100400	3.92080800
H	0.01014700	2.92445900	4.86481300
C	5.39387200	-0.64056300	-1.07807800
H	5.91079600	-0.94951400	-1.98251800
C	-3.30137000	3.40432800	-1.70047000
H	-3.82513400	3.76185800	-2.58266700
C	-2.70786000	4.30935800	-0.82558700
H	-2.75867900	5.37583000	-1.02478600
C	1.09042700	-3.15485700	-0.33556500
C	2.41622900	-3.03971100	-0.76075200
C	0.02859400	-3.29175600	-1.21538000
C	2.74251700	-3.05031300	-2.10295000
C	0.36018500	-3.27173800	-2.58242600
C	1.68058500	-3.15177900	-3.01015400
H	3.77027300	-2.96317200	-2.43614400
H	-0.43518200	-3.36914300	-3.31413300
H	1.89467800	-3.14855200	-4.07415200
H	-0.98385100	-3.46566700	-0.87078400
N	3.16664800	-2.94951300	0.40441200
H	4.11214800	-2.59873900	0.47263200
C	2.33488100	-2.94135000	1.50183400
O	2.60124600	-2.77993200	2.66154500
O	1.05245700	-3.16963700	1.03786000

### IntA30

Pd	-0.98913100	-1.05133700	-0.12810200
P	1.05190500	0.14117300	-0.01808700
C	4.12702700	-1.78810200	1.96050100
H	4.61365000	-1.73606700	2.92983900
C	0.27693100	1.24331800	2.40470700
H	-0.39801400	0.39211900	2.45062200
C	1.92130500	2.54147400	1.20710500
H	2.53837100	2.70689000	0.32951800
C	1.08446800	1.42602200	1.27858200
C	1.95454200	3.45757300	2.25408500
H	2.60135200	4.32717900	2.18726900
C	2.98403600	1.18020200	-1.79252400
H	3.72333400	0.87441400	-1.05761700

C	1.62354600	0.94040200	-1.56126000	H	0.99155500	-0.92051900	-2.73066000
C	3.10258800	-0.89260200	1.65662100	C	3.65208600	-1.12053400	-0.61767000
H	2.80266700	-0.15110700	2.39033900	H	3.95304400	-0.84756900	0.38977500
C	2.46023000	2.17286700	-3.92635500	C	2.36574500	-0.81228300	-1.07368700
H	2.78461900	2.65016100	-4.84634700	C	4.55176800	-1.77042600	-1.45626800
C	0.68797100	1.31722000	-2.52889800	H	5.54997100	-2.00433100	-1.09846000
H	-0.36727800	1.14133300	-2.35568500	C	0.81344700	-2.64697400	0.94788200
C	2.46689400	-0.94695000	0.41516200	H	1.66448100	-2.92290400	0.33267700
C	1.15675200	3.26446000	3.37870900	C	0.37602200	-1.32189400	0.98978400
H	1.18234500	3.98266700	4.19286100	C	2.66318200	2.19694100	0.76117500
C	3.39876300	1.79637300	-2.96847800	H	2.44608100	2.55967300	-0.24150100
H	4.45595100	1.97715900	-3.13813700	C	-0.95840200	-3.28077800	2.46038200
C	3.89888200	-2.79771300	-0.21472500	H	-1.48574300	-4.04712600	3.02067100
H	4.20771100	-3.53585600	-0.94869600	C	-0.73245700	-0.98227900	1.77562100
C	0.31721700	2.15600400	3.45316600	H	-1.09248200	0.04395900	1.79160500
H	-0.31780000	2.00783600	4.32112800	C	2.15033900	0.96492900	1.18337900
C	2.87424500	-1.90987100	-0.51773600	C	4.17357800	-2.11546600	-2.75215900
H	2.39472100	-1.95588900	-1.49306200	H	4.87839900	-2.62054300	-3.40609700
C	4.52684900	-2.73974000	1.02882600	C	0.14566000	-3.62248800	1.68486500
H	5.32569600	-3.43520400	1.26792100	H	0.48492600	-4.65316100	1.64300600
C	1.10745300	1.93166900	-3.70518300	C	3.21862700	1.27918300	3.32836200
H	0.37227800	2.22043300	-4.44990300	H	3.43048100	0.92091400	4.33127000
C	-2.05378300	0.71886700	-0.18670500	C	2.89497400	-1.80899200	-3.20979500
O	-1.53766400	1.80897100	-0.29017400	H	2.59847600	-2.07395700	-4.22001000
C	-3.49488400	0.46876400	-0.11547500	C	2.43167200	0.51061100	2.47388200
C	-3.88031400	-0.89144200	-0.07657000	H	2.03251200	-0.44050700	2.81331300
C	-4.43802700	1.50389600	-0.09951400	C	3.72980500	2.50109000	2.90081300
C	-5.26826100	-1.17415500	-0.01320700	H	4.34067200	3.09906800	3.57036900
C	-5.78770000	1.20944000	-0.03564800	C	-1.39593100	-1.95879600	2.50775900
C	-6.18384900	-0.13972000	0.00718000	H	-2.27179700	-1.68865300	3.08877500
H	-5.60344600	-2.20788200	0.01871600	C	-1.70654300	-0.16752100	-1.43409500
H	-6.53017500	2.00029200	-0.01817500	O	-1.27947700	-0.79186400	-2.36471800
H	-7.24340700	-0.37993000	0.05730700	C	-2.83397900	-0.38528600	-0.58069700
H	-4.08298100	2.52979000	-0.13473200	C	-3.38175500	0.59809700	0.32234300
N	-2.89164300	-1.80623300	-0.10944600	C	-3.39059100	-1.69203300	-0.66114900
H	-3.17968300	-2.77421200	-0.07000900	C	-4.50269000	0.14944200	1.10772100
C	-0.17468300	-2.98024900	-0.05552300	C	-4.43949800	-2.07510000	0.12874600
O	0.10689700	-4.07830000	0.01716200	C	-4.99317300	-1.12385900	1.02166700
<b>TSA13</b>							
Pd	-0.52106400	1.39925800	-0.95556400	H	-4.94898000	0.86192900	1.79740100
P	1.13748800	0.00817000	-0.00169900	H	-4.84260300	-3.08019600	0.07153000
C	3.45272200	2.95925600	1.61430700	H	-5.83240000	-1.40974900	1.65151200
H	3.84579800	3.91362800	1.27770600	H	-2.93718100	-2.38989900	-1.35800800
C	1.99088300	-1.15603800	-2.37663400	N	-2.87675100	1.82014100	0.42932700
				H	-3.44216200	2.41888600	1.02858900



C	-2.03955100	2.74018100	-1.28689600
O	-2.68737600	3.65408300	-1.55217400

### IntA31

Pd	0.91297000	-1.02316100	-0.19504000
P	-1.31308100	0.00249200	0.00312000
C	-3.31233800	-3.47369200	0.78712700
H	-3.18715200	-4.51796800	0.51818400
C	-1.27833400	1.40228300	-2.38801200
H	-0.25648000	1.63195400	-2.09874600
C	-3.38399000	0.31006800	-1.92104400
H	-4.00535300	-0.30996400	-1.28201600
C	-2.07013300	0.60709400	-1.54998500
C	-3.90180300	0.80571100	-3.11559200
H	-4.92284900	0.56737100	-3.39863000
C	-2.31069100	2.48197900	0.94734100
H	-2.97661500	2.47779000	0.08910800
C	-1.40269500	1.43574100	1.13170900
C	-2.39812100	-2.52883200	0.33181900
H	-1.56391300	-2.84825500	-0.29047000
C	-1.49896700	3.55204300	2.95191100
H	-1.53466400	4.37677500	3.65762800
C	-0.53558300	1.46415900	2.22781000
H	0.18965800	0.66500100	2.36020800
C	-2.54321200	-1.17892000	0.67076900
C	-3.11433900	1.60124300	-3.94228000
H	-3.51987900	1.98581600	-4.87355200
C	-2.35769900	3.53563700	1.85595900
H	-3.06356900	4.34681300	1.70407200
C	-4.52204400	-1.73872100	1.94508200
H	-5.34629000	-1.42883100	2.58061800
C	-1.80348900	1.89985100	-3.57541300
H	-1.18448300	2.51796500	-4.21874400
C	-3.61149200	-0.79159500	1.48553500
H	-3.72904100	0.25087900	1.76645000
C	-4.37548300	-3.07882600	1.59501800
H	-5.08564200	-3.81604600	1.95761600
C	-0.58753300	2.51519500	3.13703700
H	0.09131300	2.52972300	3.98429700
C	2.07747600	0.57137600	-0.34257000
O	1.51072100	1.61535400	-0.59112900
C	3.55071700	0.53004700	-0.14005400
C	4.31002600	-0.65420400	-0.05340100
C	4.20883500	1.76532300	-0.03379000
C	5.69705400	-0.55749400	0.13206600

C	5.57626200	1.85233000	0.15620200
C	6.32027200	0.67428300	0.23657900
H	6.28494200	-1.46968100	0.19588400
H	6.06080000	2.81962000	0.23850100
H	7.39560400	0.71453100	0.38329600
H	3.59834100	2.65903700	-0.10839300
N	3.76967600	-1.93133900	-0.15867900
H	4.41168900	-2.71526900	-0.12808300
C	2.44081000	-2.25087900	-0.21838600
O	2.06607900	-3.41498700	-0.26763100

### IntA32

Pd	-0.49127600	-0.96037300	-0.26162200
P	-1.11533500	1.36215400	0.07643000
P	1.97169500	-0.67145000	0.00668800
C	0.65325400	4.44805100	-2.05084300
H	1.18025300	5.37707500	-1.85458300
C	2.02071200	-1.96773600	2.47059300
H	1.03070800	-2.30698200	2.18579800
C	4.03956600	-0.75386900	1.96194800
H	4.61614300	-0.11279000	1.30152200
C	0.04462200	1.21112500	2.60293600
H	0.27560900	0.18918400	2.31826000
C	2.08596100	-1.87311900	-2.48938900
H	1.04975700	-1.55144300	-2.56408400
C	-0.95888800	3.34339500	2.10411600
H	-1.52975200	3.98533600	1.43850000
C	-0.62467400	2.04402500	1.70385400
C	4.11585300	-2.09215600	-1.20909800
H	4.67856300	-1.93864600	-0.29390500
C	-0.57761400	3.81288400	3.35605500
H	-0.83446600	4.82524800	3.65346300
C	-3.50087900	2.74586500	-0.64557800
H	-2.88773200	3.37999300	-1.27863700
C	3.02668500	1.42412900	-1.56381300
H	2.92292900	0.74190300	-2.40147800
C	-2.91597900	1.71077500	0.08461700
C	4.71055800	-2.76365800	-2.27280100
H	5.73217700	-3.12034700	-2.17967800
C	2.67245700	1.01120300	-0.27500500
C	3.99913900	-2.98096300	-3.44984200
H	4.46580400	-3.50490700	-4.27893900
C	0.20371700	3.67648900	-0.98186300
H	0.40161600	4.00545600	0.03220500
C	-5.67320700	2.14538300	0.22184800

H	-6.74543800	2.31164500	0.26939700
C	-3.72282300	0.89367900	0.88298400
H	-3.27866800	0.06797800	1.43398600
C	2.55826600	-2.34400400	3.69833200
H	1.97561200	-2.96543200	4.37173200
C	-0.46181500	2.47437600	-1.21859300
C	0.12059500	2.98281400	4.23285800
H	0.41496100	3.35227500	5.21082500
C	2.75437600	-1.16742700	1.58931800
C	-4.87597400	2.95955300	-0.57672600
H	-5.32392000	3.76299300	-1.15412100
C	2.79981300	-1.63868500	-1.31070700
C	-0.20711300	2.81706200	-3.60036400
H	-0.36755900	2.47665300	-4.61906000
C	4.57827600	-1.13522300	3.18644100
H	5.57628900	-0.80678300	3.46129200
C	3.83702800	-1.92918300	4.05840100
H	4.25592200	-2.22241100	5.01667100
C	2.68506900	-2.53436800	-3.55668400
H	2.11859400	-2.71191400	-4.46592300
C	0.42123000	1.67663600	3.86025400
H	0.94999800	1.01457200	4.53960900
C	-0.65693400	2.04134400	-2.53855400
H	-1.17739600	1.10339300	-2.72272900
C	3.53039900	2.70175500	-1.78485400
H	3.79987700	3.00255200	-2.79265100
C	2.80811200	1.92087800	0.78057000
H	2.53599100	1.63151200	1.78985400
C	0.44627400	4.02431300	-3.35873400
H	0.79920600	4.62877700	-4.18939900
C	-5.09342100	1.11120500	0.95431000
H	-5.70920600	0.46051400	1.56785000
C	3.31669000	3.19674100	0.55839600
H	3.42454600	3.88156600	1.39463700
C	3.68715800	3.58878400	-0.72425500
H	4.08809600	4.58318900	-0.89828600
C	-2.27878600	-1.31154600	-1.10749400
O	-2.56963000	-0.65936700	-2.09463700
C	-3.21714900	-2.30723400	-0.54394000
C	-2.74848500	-3.47194100	0.08577700
C	-4.59173000	-2.06537000	-0.62629300
C	-3.68141800	-4.36757500	0.62555000
C	-5.50931200	-2.94611200	-0.07313000
C	-5.04149700	-4.10300200	0.55126300

H	-3.32843000	-5.27617900	1.10711100
H	-6.57388400	-2.74357600	-0.13386200
H	-5.74307800	-4.80952500	0.98565600
H	-4.91470600	-1.15934300	-1.12963300
N	-1.39884100	-3.79715100	0.13960300
H	-1.16364700	-4.74471200	0.41368700
C	-0.28600700	-2.99718000	-0.09565700
O	0.80435400	-3.55099000	-0.00807600

### TSA14

Pd	-0.21324000	-0.86536500	-0.64048800
P	-1.33476500	1.13046200	-0.01096800
P	2.07522100	-0.45043500	0.04385300
C	0.23794900	4.68140400	-1.49747500
H	0.50587700	5.66951200	-1.13492100
C	1.69325700	-2.28378300	2.08437400
H	0.89603800	-2.64408700	1.43695000
C	3.48124800	-0.73137200	2.53045300
H	4.08015400	0.12939300	2.24812500
C	-0.54448000	0.73312300	2.61411100
H	-0.16758600	-0.20988500	2.22891600
C	3.05921300	-1.60419400	-2.29239800
H	2.01270700	-1.72298800	-2.55445900
C	-1.69075600	2.82129400	2.26115300
H	-2.24235900	3.49804600	1.61466100
C	-1.17188400	1.62733800	1.74349400
C	4.76756500	-0.94410100	-0.72055900
H	5.05857600	-0.51235100	0.23229800
C	-1.52863000	3.13515200	3.60611600
H	-1.92683800	4.06815400	3.99388000
C	-3.65355500	1.50488100	-1.56998100
H	-2.97837100	1.66609400	-2.40344700
C	3.02023600	2.01667800	-0.88961500
H	3.18733700	1.49167000	-1.82543300
C	-3.14734300	1.28889100	-0.28363300
C	5.74965300	-1.37888500	-1.60066300
H	6.79736300	-1.29047600	-1.32820500
C	2.53522200	1.32220700	0.22482400
C	5.38957900	-1.92581000	-2.83286500
H	6.15864900	-2.26581900	-3.52064100
C	-0.28992700	3.74699700	-0.61046600
H	-0.40320700	4.01652200	0.43315900
C	-5.91462500	1.30023900	-0.74495200
H	-6.98567100	1.30847600	-0.92448400
C	-4.04663700	1.05922800	0.76383100

H	-3.67840200	0.86314200	1.76585800
C	1.92639000	-2.90470900	3.30869500
H	1.31437500	-3.75037800	3.60820900
C	-0.62706000	2.46759300	-1.05300600
C	-0.86859700	2.24931700	4.45764600
H	-0.74506400	2.49710700	5.50791100
C	2.46854000	-1.19034500	1.68052200
C	-5.02623800	1.51231200	-1.79701900
H	-5.40079000	1.68291800	-2.80181200
C	3.41290700	-1.05531600	-1.05858600
C	0.12497100	3.06881200	-3.27987500
H	0.29296800	2.79285700	-4.31662300
C	3.71134300	-1.34967900	3.75533300
H	4.49789000	-0.97903000	4.40618800
C	2.93435600	-2.43757500	4.14724300
H	3.11329900	-2.91720400	5.10518400
C	4.04755600	-2.03767800	-3.17604700
H	3.75900800	-2.46962700	-4.12942900
C	-0.38836700	1.04077200	3.96360700
H	0.11235000	0.33432100	4.61907400
C	-0.39281400	2.12974900	-2.39461800
H	-0.61493500	1.12335300	-2.74488500
C	3.29892400	3.37621800	-0.81048200
H	3.67199300	3.89761200	-1.68672100
C	2.31080900	2.03054600	1.40966800
H	1.92156200	1.52315300	2.28515200
C	0.43721300	4.35031300	-2.83348700
H	0.84815100	5.08320100	-3.52183200
C	-5.41953300	1.07300400	0.53578500
H	-6.10150100	0.89743000	1.36270200
C	2.59208000	3.39171200	1.48797100
H	2.41556000	3.91964000	2.42074900
C	3.09313400	4.06750100	0.38050800
H	3.31355800	5.12943000	0.44056500
C	-1.81674600	-1.74295300	-1.66336800
O	-2.07235200	-1.27813200	-2.75744200
C	-2.78009800	-2.39102500	-0.73330800
C	-2.21230900	-3.45863500	-0.02607300
C	-4.09525400	-2.01594500	-0.50974400
C	-2.95434600	-4.15450600	0.91563200
C	-4.84474100	-2.69982100	0.44850500
C	-4.27454700	-3.75862800	1.14977100
H	-2.51943300	-4.99080100	1.45560100
H	-5.87266100	-2.40839800	0.63986900

H	-4.86221300	-4.29384900	1.89008300
H	-4.52351100	-1.20014800	-1.08313700
N	-0.88496900	-3.76623600	-0.39448800
H	-0.61507000	-4.74348500	-0.43279900
C	-0.34961800	-2.95132800	-1.39704400
O	0.45396600	-3.35905000	-2.20750900

### IntA33

Pd	-0.07120200	-0.94931000	0.49921600
P	-1.16551800	1.03565500	0.06719000
P	2.26842200	-0.50866300	0.17925800
C	0.44867600	3.39251900	-2.93983500
H	0.79204400	4.41386100	-3.07528600
C	2.93172100	-2.02854100	2.38808900
H	1.98325700	-2.51629300	2.17161700
C	4.57735200	-0.34130700	1.86651200
H	4.91650000	0.49127600	1.25669900
C	-0.08117300	2.07751600	2.41832300
H	0.37709100	1.09460800	2.50407300
C	1.97114300	-2.24341400	-1.98964400
H	0.90630400	-2.19616900	-1.77570100
C	-1.52354800	3.60033200	1.23278300
H	-2.19858500	3.80977000	0.40715000
C	-0.90078100	2.34936900	1.32099800
C	4.25858900	-1.67092000	-1.46465400
H	4.98097100	-1.14819000	-0.84335200
C	-1.29380100	4.57158400	2.20082600
H	-1.77702300	5.54071000	2.11877100
C	-3.55823400	1.61785000	-1.38173700
H	-2.93230300	1.85344500	-2.23657100
C	3.18892300	1.50498800	-1.59272300
H	3.20044800	0.74119100	-2.36315700
C	-2.97981700	1.19337600	-0.18503000
C	4.70081400	-2.45172800	-2.52530400
H	5.76456100	-2.53662200	-2.72784300
C	2.82698600	1.17501500	-0.28483800
C	3.77860600	-3.12795200	-3.32408600
H	4.12484700	-3.74057500	-4.15174300
C	-0.04910300	2.99530100	-1.70131200
H	-0.07484400	3.70874300	-0.88459400
C	-5.75634400	1.47057600	-0.39312500
H	-6.83412200	1.57847400	-0.47329400
C	-3.80874500	0.88689800	0.90039200
H	-3.36993300	0.53373600	1.83063400
C	3.71831900	-2.46636600	3.44881900

H	3.38085700	-3.29656800	4.06228900
C	-0.47998000	1.68287500	-1.50642700
C	-0.45482600	4.29762500	3.28014200
H	-0.28070100	5.05545700	4.03852800
C	3.35820100	-0.96474100	1.58386100
C	-4.94285200	1.75160700	-1.48395400
H	-5.38106200	2.08414400	-2.42062100
C	2.88982900	-1.55480600	-1.19267400
C	0.11186500	1.16748300	-3.79808100
H	0.17998100	0.44696200	-4.60760200
C	5.35695100	-0.77484200	2.93571500
H	6.30075900	-0.28116900	3.14890900
C	4.93020800	-1.83826600	3.72665600
H	5.54027300	-2.17552800	4.55964600
C	2.41856800	-3.02508900	-3.05355600
H	1.69493100	-3.55901600	-3.66190000
C	0.14407100	3.04678500	3.39318900
H	0.78352500	2.82081300	4.24157300
C	-0.38561400	0.76597000	-2.56324000
H	-0.70589000	-0.26444800	-2.42083400
C	3.52462100	2.81604100	-1.92100300
H	3.79961400	3.05562000	-2.94385700
C	2.79197500	2.18861100	0.68111300
H	2.51380900	1.95333700	1.70351000
C	0.52617900	2.48397300	-3.99006900
H	0.91860900	2.79678800	-4.95351100
C	-5.18491600	1.03395600	0.80114300
H	-5.81485300	0.79072800	1.65111800
C	3.12030000	3.49768700	0.35099400
H	3.08227200	4.26892500	1.11475400
C	3.49262300	3.81473800	-0.95381500
H	3.75089300	4.83703000	-1.21474300
C	-2.08088000	-2.51462000	-0.76583700
O	-1.59469800	-2.49594900	-1.88759500
C	-3.48183200	-2.35677600	-0.35450300
C	-3.56087400	-2.59100000	1.02960900
C	-4.62198000	-2.08381700	-1.10027700
C	-4.78681800	-2.54311000	1.68969600
C	-5.84998100	-2.04447200	-0.45170500
C	-5.92001400	-2.27358300	0.92796200
H	-4.85934200	-2.72579000	2.75764300
H	-6.75551900	-1.82611300	-1.00799400
H	-6.88706500	-2.23915600	1.42244900
H	-4.53454200	-1.90248000	-2.16687600

N	-2.31243000	-2.89551000	1.54190100
H	-2.07643900	-2.84653600	2.52020600
C	-1.32888700	-2.75542000	0.53810100
O	-0.13076600	-3.12660800	0.66022000

#### prodA4

C	1.18060100	0.89710800	0.00004000
O	1.74566600	1.96148100	0.00021700
C	-0.25614300	0.57642400	-0.00033500
C	-0.38129100	-0.82065800	-0.00009300
C	-1.37611700	1.39524100	-0.00024000
C	-1.62753700	-1.42676400	0.00000100
C	-2.63563800	0.79949000	0.00006900
C	-2.74832000	-0.59261000	0.00014100
H	-1.73417500	-2.50677500	0.00018100
H	-3.53019600	1.41298200	0.00025000
H	-3.73545000	-1.04530800	0.00027600
H	-1.25564100	2.47406300	-0.00029800
N	0.88213500	-1.42318900	0.00020800
H	1.04953800	-2.41760900	-0.00093000
C	1.90371300	-0.49238900	0.00007700
O	3.08875500	-0.70774000	-0.00007900

#### TSA9'

Pd	-0.12419800	-0.84910900	-0.67501700
P	2.14013000	-0.27055300	-0.16409200
P	-1.31393200	1.09408900	0.10790300
C	2.00624900	2.30411300	3.03922700
H	1.88490300	3.37258500	3.19099500
C	-4.00380300	0.51942200	-0.32867400
H	-3.89097300	-0.16171100	0.50932200
C	-3.08534100	2.17829200	-1.81875200
H	-2.26401100	2.81125400	-2.14044200
C	2.56210100	0.88029300	-2.64051500
H	1.77784300	0.19400300	-2.95260200
C	-1.15697700	0.01937300	2.65579900
H	-0.43551400	-0.66433400	2.22142900
C	3.95426200	1.80008700	-0.90059300
H	4.27819400	1.82651700	0.13528200
C	2.94706900	0.91541200	-1.29637800
C	-2.72505600	1.84624700	2.43795100
H	-3.23106400	2.58612100	1.82306100
C	4.54476500	2.65295800	-1.82891900
H	5.31990000	3.34242800	-1.50834900
C	2.83390000	-2.92684300	0.34284700
H	1.80813900	-3.03269800	0.69477000

C	-0.45483100	3.71754900	0.83134600	H	1.56010000	4.13991100	-2.45136600
H	-0.98261300	3.58933000	1.77023100	C	1.00519200	5.03848400	-0.56971700
C	3.29226100	-1.69831300	-0.14950600	H	1.58915400	5.93970000	-0.73133100
C	-3.05309400	1.72135400	3.78129700	C	-1.84124800	-1.90355600	-1.33774400
H	-3.79931600	2.37867900	4.21804500	C	-2.70646800	-2.56338400	-0.43109800
C	-0.47051000	2.70204300	-0.12826900	C	-2.28927000	-1.58261000	-2.62848100
C	-2.44266600	0.73679800	4.56143900	C	-4.00151500	-2.88142700	-0.90463000
H	-2.71920800	0.62802700	5.60623900	C	-3.57168100	-1.87640500	-3.05673100
C	2.10312600	1.80724800	1.74330900	C	-4.42471800	-2.54376900	-2.17520900
H	2.05627800	2.49778700	0.90815500	H	-4.68093800	-3.40292600	-0.23413100
C	5.00886300	-3.90124900	-0.05805000	H	-3.89893300	-1.60375100	-4.05427400
H	5.67539800	-4.75827100	-0.02587200	H	-5.43172800	-2.80841600	-2.48567600
C	4.61212600	-1.58382600	-0.59948700	H	-1.59850200	-1.09028600	-3.30804800
H	4.98113700	-0.64279800	-0.99401000	N	-2.44418000	-2.86148800	0.88595500
C	-5.21796700	0.58987500	-1.00061200	H	-3.23050500	-3.19884900	1.42209700
H	-6.04208400	-0.04076200	-0.68195700	C	-1.22602800	-2.97658400	1.64938100
C	2.24895900	0.43397200	1.52222500	O	-1.39432000	-3.26653700	2.83199000
C	4.14914400	2.61726200	-3.16358100	O	-0.14908300	-2.75424800	1.02064300
H	4.61347000	3.28150400	-3.88649900	C	0.02156700	-2.58358900	-1.50165300
C	-2.92708800	1.31476900	-0.73261000	O	0.32703500	-3.60402100	-1.93598600
C	3.69733400	-4.01811100	0.39188700	<b>subB</b>			
H	3.33223400	-4.96495100	0.77768800	C	-1.04488900	-1.68552700	0.22240300
C	-1.76075200	1.00019300	1.86997900	C	-0.49006600	-0.43347500	-0.02370300
C	2.20107500	0.07016300	3.91319300	C	-1.28973400	0.68609200	-0.27281300
H	2.22882800	-0.61531800	4.75445700	C	-2.67514500	0.49728100	-0.26422100
C	-4.30319000	2.24537900	-2.48996200	C	-3.24772800	-0.74536000	-0.01662000
H	-4.41623900	2.92451700	-3.32997000	C	-2.42836500	-1.84053100	0.22831200
C	-5.37094400	1.45114500	-2.08366700	H	-0.40310400	-2.53961600	0.40785200
H	-6.31987400	1.50301100	-2.60930800	H	-3.31555600	1.35430800	-0.45961400
C	-1.50438700	-0.11849700	3.99766300	H	-4.32770900	-0.85581100	-0.01777300
H	-1.05763300	-0.92139000	4.57322000	H	-2.85675800	-2.81924400	0.42138100
C	3.16098800	1.72330300	-3.57070100	C	-0.74389000	2.07717300	-0.50242100
H	2.85344700	1.68501900	-4.61136000	H	0.12947100	2.02907900	-1.16137400
C	2.29618400	-0.43249800	2.62004200	H	-1.51182900	2.66361100	-1.03482300
H	2.37659200	-1.50396200	2.47138300	N	-0.31511000	2.66211300	0.76437500
C	0.27930600	4.87889700	0.60906400	H	0.13094200	3.55973600	0.60260600
H	0.29385200	5.65734100	1.36635000	H	-1.12125200	2.82678500	1.36014300
C	0.24907200	2.87765000	-1.31369500	I	1.64151800	-0.30542600	-0.03197500
H	0.25902800	2.08447500	-2.05549400	<b>IntB1</b>			
C	2.05232600	1.43787800	4.12679000	C	2.76047800	1.35811300	-0.76379700
H	1.96581600	1.82552700	5.13733700	C	2.71176200	2.74622000	-0.63665400
C	5.46381900	-2.68286700	-0.55551500	C	2.80652000	0.58916700	0.43578200
H	6.48476200	-2.58507700	-0.91283600	C	2.69206600	3.38224800	0.60581700
C	0.98458000	4.03713400	-1.53665600	H	2.68424800	3.34478300	-1.54420800

C	2.76278700	1.22809000	1.69525200
C	2.69879800	2.62436000	1.76681100
H	2.86669800	0.64240400	2.60176900
I	3.45011600	-1.49477300	0.41037600
H	2.66100900	4.46596400	0.65823500
H	2.67489500	3.10297900	2.74099300
Pd	0.75719500	0.12397100	0.58262900
P	-1.49256500	-0.05173300	0.18002300
C	-2.75288300	0.29451000	1.46741400
C	-4.00769500	0.84768700	1.19360100
C	-4.92418000	1.05510700	2.22092200
C	-4.59774000	0.70928700	3.52994300
C	-3.34825100	0.16268300	3.81194200
C	-2.42842600	-0.03598000	2.78693000
C	-2.01464900	-1.67425600	-0.50705100
C	-3.25332900	-2.26795200	-0.25271900
C	-3.57677000	-3.49377300	-0.83151600
C	-2.66875700	-4.13184300	-1.67112500
C	-1.43041600	-3.54547500	-1.92682500
C	-1.09956800	-2.32736400	-1.34333500
C	-1.94688700	1.10521600	-1.18185000
C	-2.87856800	0.79211000	-2.17631500
C	-3.16414500	1.70462700	-3.18952000
C	-2.52149500	2.93917400	-3.22182800
C	-1.58836300	3.25910900	-2.23781100
C	-1.29962200	2.34671700	-1.22747800
H	-4.26954200	1.12307800	0.17594400
H	-5.89442000	1.48954800	1.99805300
H	-5.31376400	0.87272600	4.33014700
H	-3.08530900	-0.10017300	4.83230300
H	-3.96764300	-1.77764900	0.40230400
H	-4.54018500	-3.95007200	-0.62276900
H	-2.92203200	-5.08799700	-2.12011300
H	-0.71472800	-4.04431300	-2.57395500
H	-3.37686700	-0.17316000	-2.16620700
H	-3.88741000	1.44683600	-3.95780600
H	-2.74229700	3.64772700	-4.01489500
H	-1.07853000	4.21802500	-2.25991500
H	-0.12665500	-1.87414700	-1.53023200
H	-0.55348000	2.58556900	-0.47242500
H	-1.44354700	-0.44214400	3.00481700
C	2.77591200	0.74151600	-2.14354700
H	3.02441100	1.53724700	-2.86421300
H	3.57686600	-0.00394400	-2.20526200

N	1.51328000	0.06086800	-2.44000900
H	0.74935500	0.73276700	-2.42849300
H	1.54783500	-0.34159200	-3.37344000

**TSB1**

C	3.14630600	-1.28881300	0.70433400
C	3.60117000	-2.58288800	0.46707900
C	2.85196800	-0.47721800	-0.42272600
C	3.77074100	-3.08109500	-0.82603400
H	3.81833100	-3.22199400	1.32012500
C	3.02731100	-0.97007500	-1.72782300
C	3.47293700	-2.27918100	-1.91893400
H	2.86003300	-0.31866500	-2.57809600
I	2.93798400	1.82723000	-0.24479700
H	4.13051200	-4.09489300	-0.97171800
H	3.60076300	-2.65597900	-2.92943300
Pd	0.83634200	-0.10819100	-0.36164800
P	-1.47091200	-0.03351900	-0.14130500
C	-2.56893100	-0.26228900	-1.59208700
C	-3.81265500	-0.89814100	-1.52787500
C	-4.60376600	-1.01145600	-2.66805400
C	-4.16165900	-0.48868000	-3.88075900
C	-2.92177100	0.14159600	-3.95407600
C	-2.12663600	0.24723500	-2.81723500
C	-2.11568400	1.49400700	0.64783100
C	-3.38143200	2.02796500	0.39138000
C	-3.80518400	3.17864500	1.05236000
C	-2.97053200	3.80232100	1.97560400
C	-1.70568100	3.27768100	2.23271000
C	-1.27671900	2.13387300	1.56787200
C	-2.02715600	-1.34962800	1.01966100
C	-3.02658300	-1.16437300	1.97871500
C	-3.38546400	-2.20442900	2.83388900
C	-2.75160800	-3.43997100	2.73960000
C	-1.75244700	-3.63410900	1.78767300
C	-1.38971100	-2.59406600	0.93798700
H	-4.16287300	-1.31140600	-0.58614700
H	-5.56638200	-1.51105200	-2.60870600
H	-4.77969000	-0.57904500	-4.76933000
H	-2.56865800	0.54289900	-4.89936600
H	-4.03724800	1.54983100	-0.33052800
H	-4.78846600	3.58933100	0.84193400
H	-3.30176800	4.70105400	2.48782400
H	-1.04632700	3.76774900	2.94309800
H	-3.52271400	-0.20201400	2.06505300

H	-4.16132900	-2.04587000	3.57732700
H	-3.03153000	-4.24853700	3.40857000
H	-1.25125800	-4.59462200	1.71015700
H	-0.28241300	1.73122800	1.74997400
H	-0.59699100	-2.73917300	0.20667100
H	-1.14898800	0.72016800	-2.87407700
C	2.92469000	-0.80399400	2.11524800
H	3.38932300	-1.51964200	2.81149500
H	3.43190500	0.15764400	2.25373900
N	1.49666800	-0.58411900	2.36627300
H	0.99375000	-1.46771800	2.35903700
H	1.35508800	-0.16155600	3.28005100

**IntB2**

Pd	-0.01305000	-0.13556200	-0.19679300
P	-2.35789200	-0.06527700	0.09021500
P	2.36157700	-0.04417900	0.10284400
C	-4.86497800	-2.73895400	1.97551400
H	-5.88679900	-3.09098600	1.86974200
C	2.88758000	-1.19849500	-2.39505400
H	1.87995000	-1.59384600	-2.31333100
C	4.70872500	0.08953100	-1.47381400
H	5.12033100	0.71514400	-0.68758300
C	-2.69816200	-0.92445900	-2.53593500
H	-1.71287300	-1.36078300	-2.40053500
C	3.07379100	2.63472400	-0.23646000
H	2.77531200	2.48240000	-1.26908800
C	-4.56715800	0.32362900	-1.65561700
H	-5.03682000	0.87895700	-0.84915800
C	-3.28874900	-0.21964800	-1.48138700
C	3.40216600	1.79124900	1.99520100
H	3.38289900	0.97680100	2.71237800
C	-5.23840700	0.17080400	-2.86512200
H	-6.22816600	0.60017100	-2.98904300
C	-3.24148000	1.53820200	2.22698400
H	-3.13991400	0.64862200	2.84072100
C	2.08314400	-1.42522200	2.48808800
H	1.10256100	-0.95668600	2.50206200
C	-3.01742500	1.47052200	0.85000500
C	3.79338700	3.06267700	2.41178700
H	4.07622200	3.22319400	3.44807600
C	2.93041800	-1.20414800	1.39808200
C	3.82239700	4.11809500	1.50801100
H	4.12104500	5.10952000	1.83575900
C	-4.35882200	-1.81092800	1.07071900

H	-4.99109600	-1.44896600	0.26603700
C	-3.72936900	3.89567200	2.05697500
H	-3.99884100	4.83746900	2.52589700
C	-3.16288400	2.63229300	0.08388700
H	-2.98458700	2.60537900	-0.98587000
C	3.66847100	-1.49681200	-3.50866000
H	3.25868800	-2.12144700	-4.29676100
C	-3.04213800	-1.36074500	1.18871700
C	-4.64219000	-0.52873500	-3.91115400
H	-5.16657000	-0.64659100	-4.85496800
C	3.40085600	-0.40175900	-1.36661700
C	-3.59494500	2.74483500	2.82579000
H	-3.76567500	2.78088900	3.89775200
C	3.03423800	1.56692700	0.66823100
C	-2.75010700	-2.77328300	3.13064100
H	-2.11364500	-3.15716600	3.92198600
C	5.48591900	-0.21131900	-2.58769100
H	6.49804400	0.17605800	-2.65794600
C	4.96624100	-1.00416600	-3.60826900
H	5.57312400	-1.23740500	-4.47836700
C	3.46444900	3.89938100	0.17862300
H	3.47303000	4.71927400	-0.53276700
C	-3.37410900	-1.07836700	-3.74264000
H	-2.90807800	-1.63425300	-4.55088800
C	-2.23936300	-1.85499400	2.21980900
H	-1.20360600	-1.53775700	2.28825700
C	2.48105300	-2.24870300	3.53444700
H	1.81333500	-2.41595600	4.37424000
C	4.17522200	-1.83366000	1.36087200
H	4.83766100	-1.68557800	0.51386800
C	-4.06374300	-3.21745400	3.00870300
H	-4.45994900	-3.94415900	3.71188600
C	-3.51570100	3.83468900	0.68205000
H	-3.60867300	4.72835100	0.07281200
C	4.56699200	-2.66984300	2.40290500
H	5.53250600	-3.16499300	2.36027000
C	3.72441600	-2.87507600	3.49130800
H	4.03177900	-3.53022900	4.30109000
C	-0.05421300	1.88122200	-0.09382900
C	-0.18422100	2.62922900	-1.27400800
C	0.05844800	2.55314100	1.12523200
C	-0.16004200	4.02637600	-1.20322900
C	0.06171100	3.94266100	1.18669800
H	0.14839300	1.98423500	2.04660800

C	-0.03988800	4.68601800	0.01447100
H	-0.24689800	4.60486100	-2.12175000
H	0.15315800	4.44116000	2.14739100
H	-0.02479800	5.77177700	0.04729000
I	0.03186000	-2.91967100	-0.48470800
C	-0.44447500	1.97247300	-2.61535500
H	-1.51166200	1.72001100	-2.68300300
H	-0.24631400	2.70046900	-3.41886400
N	0.28518900	0.71930000	-2.77488000
H	-0.06156300	0.19683900	-3.57286000
H	1.27627200	0.88489300	-2.92455500

### TSB2

Pd	-0.30118400	-1.22146400	-0.51917100
P	0.55725500	0.98004800	0.00270500
C	0.80849400	0.08184900	2.60744200
H	1.34930900	-0.73922900	2.14098300
C	-0.36994600	2.18285800	2.42258400
H	-0.74775000	3.00497600	1.82270100
C	2.94930400	0.87993600	-1.40068100
H	2.41300600	0.21253200	-2.06831200
C	3.02512700	2.20052200	0.62191300
H	2.54186800	2.58510400	1.51562500
C	0.35415200	3.46574600	-1.35212200
H	1.43728700	3.45598600	-1.41700000
C	4.35092600	2.52746300	0.35673700
H	4.89818500	3.16329700	1.04623100
C	-0.31994100	2.42308500	-0.71016900
C	4.97424900	2.03708700	-0.78869300
H	6.01078500	2.28954200	-0.99209300
C	0.59487600	0.08316100	3.98117300
H	0.98216800	-0.73175900	4.58580700
C	0.31975300	1.13174300	1.81570700
C	2.31712300	1.37589700	-0.25755000
C	-0.58989000	2.17460300	3.79968900
H	-1.13363400	2.99357100	4.26127400
C	-0.11417900	1.12516100	4.57907700
H	-0.28896500	1.12009400	5.65086500
C	4.27307600	1.21532300	-1.66679600
H	4.76026500	0.81839300	-2.55179400
C	-0.35893900	4.52127600	-1.91598900
H	0.17700400	5.32316300	-2.41492600
C	-1.71802300	2.45743300	-0.64449100
H	-2.25877900	1.65792200	-0.14990500
C	-2.42643100	3.51616000	-1.19956300

H	-3.51060600	3.52282000	-1.13801800
C	-1.74799900	4.55033800	-1.84064600
H	-2.30056700	5.37455900	-2.28199200
C	-2.45137400	-0.97295000	-0.67442000
C	-3.17935000	-0.66289500	0.48673500
C	-2.92259500	-0.57291800	-1.93048000
C	-4.37116000	0.05191100	0.34910500
C	-4.09846500	0.15876500	-2.04642900
H	-2.36219500	-0.84161500	-2.82107600
C	-4.82565700	0.46711700	-0.89964800
H	-4.94767700	0.29604600	1.23870300
H	-4.44880900	0.47627900	-3.02342000
H	-5.75502400	1.02395000	-0.97668100
I	1.99887800	-2.63699000	-0.44168800
C	-1.56200000	-2.61329500	-0.73744400
O	-2.08917100	-3.63311100	-0.88117900
C	-2.67847300	-0.99425300	1.88320800
H	-2.07704800	-0.14483100	2.22820500
H	-3.54322300	-1.05631500	2.56118600
N	-1.83716500	-2.17473100	1.91258100
H	-1.10229700	-2.10664900	2.60516300
H	-2.36066000	-3.02948700	2.06111200

### IntB3

Pd	0.24636000	-0.57522000	-0.56104700
P	1.11343200	1.55041800	-0.09068000
P	-2.09132500	-0.21861100	0.15228000
C	-0.20284900	3.77631000	3.14801000
H	-0.61327800	4.76300500	3.33867200
C	-2.94782300	-0.65241400	-2.47753100
H	-1.90344500	-0.86159400	-2.68857500
C	-4.70135200	-0.10905200	-0.90951900
H	-5.01914200	0.14301600	0.09868800
C	-0.36078900	2.41022700	-2.29191000
H	-0.69120700	1.37625800	-2.34281200
C	-1.63974100	-1.63352100	2.49006700
H	-0.85031800	-0.90279700	2.64370800
C	0.99697300	4.12005000	-1.26515400
H	1.73451700	4.42134300	-0.52630800
C	0.53544300	2.79763400	-1.29308500
C	-3.46155900	-2.49429000	1.16903200
H	-4.09234800	-2.45322900	0.28738800
C	0.53005800	5.04551100	-2.19133400
H	0.88912600	6.06968600	-2.15863200
C	3.71785600	1.55200700	1.01415600



H	3.25123600	1.35433100	1.97330500	C	-3.22156500	3.68036200	0.70114600
C	-2.93905000	1.43981000	2.32892300	H	-3.33072000	4.54736700	0.05618400
H	-2.84337900	0.57476700	2.97625800	C	-3.50991700	3.77253300	2.06100400
C	2.93614900	1.76706500	-0.12388800	H	-3.84659600	4.71361300	2.48620600
C	-3.62460500	-3.53161800	2.08474100	I	-0.31506400	-3.16379800	-1.33151800
H	-4.39039800	-4.28160700	1.91210500	C	2.07689000	-1.00744900	-1.29560000
C	-2.65425200	1.33644300	0.96655400	O	2.23052800	-0.72567400	-2.45865400
C	-2.80547500	-3.61717000	3.20522400	C	3.22274800	-1.53551700	-0.46306600
H	-2.93322500	-4.43010100	3.91363700	C	3.15820500	-2.02885100	0.85261000
C	0.11833700	3.41080800	1.84377200	C	4.46875700	-1.45801400	-1.10579300
H	-0.05981300	4.11300200	1.03749100	C	4.34710700	-2.43948900	1.46585600
C	5.72819100	1.83739100	-0.28710000	C	5.63598000	-1.84922900	-0.47365800
H	6.81192300	1.85781700	-0.35132900	C	5.57385900	-2.34662700	0.82588600
C	3.56860100	2.01001700	-1.34815200	H	4.28571600	-2.85515000	2.46764200
H	2.97944000	2.14971800	-2.24873600	H	6.58783700	-1.76823400	-0.99020000
C	-3.88932200	-0.71306400	-3.50298100	H	6.47791300	-2.66556300	1.33700500
H	-3.56735900	-0.95275900	-4.51167100	H	4.49067800	-1.06953000	-2.11747900
C	0.62900600	2.14026900	1.57570200	C	1.90076400	-2.20949300	1.67914600
C	-0.38710800	4.65592600	-3.16678800	H	1.05595800	-1.67768200	1.21669700
H	-0.74729900	5.37960700	-3.89193900	H	2.06999700	-1.74555800	2.66188000
C	-3.34692100	-0.35274100	-1.17323100	N	1.63653400	-3.62737100	1.90232900
C	5.10588600	1.58562400	0.93127700	H	0.75034200	-3.71380400	2.39725700
H	5.69976500	1.40637600	1.82202700	H	1.47330700	-4.06062000	0.99412300
C	-2.47091600	-1.53323500	1.36730800				
C	0.47358300	1.60678800	3.93795700	<b>IntB4</b>			
H	0.60824000	0.89436000	4.74651700	Pd	0.32262900	0.63761200	0.45884600
C	-5.63950500	-0.17800800	-1.93200600	P	1.20170600	-1.47479300	0.06166100
H	-6.68757400	0.00798000	-1.71699600	P	-2.11503800	0.32765100	-0.04206700
C	-5.23299500	-0.47893600	-3.23167600	C	0.15940800	-4.06005000	-2.98147900
H	-5.96649800	-0.52993500	-4.03111200	H	0.12341000	-5.13273900	-3.14777000
C	-1.81215600	-2.66089300	3.40986400	C	-2.53511100	0.75688500	2.66778800
H	-1.16523500	-2.72090300	4.28072500	H	-1.73893300	1.48901700	2.54905000
C	-0.82444100	3.33644900	-3.22289000	C	-4.02240400	-0.88510200	1.70058700
H	-1.52205400	3.02068900	-3.99241400	H	-4.38645800	-1.44289000	0.84389700
C	0.78558500	1.23778400	2.63435000	C	-0.35513500	-2.31587100	2.21892500
H	1.15343700	0.23635100	2.43366800	H	-0.82601500	-1.34280900	2.13503400
C	-3.36540600	2.65108300	2.86997400	C	-2.14903000	2.53826700	-1.71109400
H	-3.58557700	2.71232700	3.93168700	H	-1.21488500	2.13458800	-2.09317500
C	-2.79876600	2.47290400	0.16000200	C	1.34628300	-3.88621000	1.54692000
H	-2.59725700	2.41294700	-0.90484800	H	2.20680400	-4.14298800	0.93540800
C	-0.01859100	2.88260300	4.19781200	C	0.70363400	-2.65394700	1.37183400
H	-0.27152200	3.17377300	5.21284200	C	-4.01327000	2.42654900	-0.17741600
C	4.95611300	2.05111700	-1.42544900	H	-4.54253500	1.92644900	0.62804900
H	5.43319500	2.23939400	-2.38246600	C	0.90514300	-4.77531500	2.52087700
				H	1.41060000	-5.72796600	2.64809600

C	3.68662800	-1.88926600	-1.22267200	H	5.72203200	-1.57880800	2.05297300
H	3.12221000	-1.97441600	-2.14606700	C	-3.00411900	-3.29922400	-1.72270100
C	-3.52131000	-0.62876200	-2.31332200	H	-2.78971300	-4.33775300	-1.49063600
H	-3.73096800	0.40875700	-2.55183500	C	-3.71529600	-2.96855300	-2.87452800
C	3.02190100	-1.69326700	-0.00947800	H	-4.06488100	-3.75084800	-3.54190200
C	-4.51254400	3.61515200	-0.70169700	C	2.08439200	1.17871000	1.24443600
H	-5.43121300	4.03569200	-0.30330500	O	2.22642100	0.89060800	2.41024100
C	-2.80328000	-0.95112900	-1.15995500	C	3.08035300	2.07314700	0.54837800
C	-3.83217600	4.26580300	-1.72883800	C	3.81686200	2.88839100	1.42001600
H	-4.21763100	5.19874400	-2.12971300	C	4.28260000	3.05067200	-1.29098900
C	0.59119900	-3.56629300	-1.75630900	C	4.75890700	3.78778400	0.94571200
H	0.87869900	-4.26171900	-0.97453400	C	4.99495800	3.86789200	-0.42360400
C	5.81229900	-1.85624900	-0.08194900	H	4.47746900	3.10664900	-2.36001200
H	6.89635400	-1.91346500	-0.11039000	H	5.30729600	4.41884700	1.63868000
C	3.76805500	-1.58709400	1.17082700	H	5.73482200	4.56068100	-0.81454100
H	3.26612400	-1.42282700	2.11884900	H	3.62492100	2.80057700	2.48381900
C	-3.10909000	0.53418700	3.91504300	N	1.38112900	2.00756600	-2.43934800
H	-2.74980500	1.09132000	4.77512400	H	0.94219300	2.55202400	-1.68768900
C	0.63158300	-2.18758000	-1.52552500	H	1.67874300	2.70400500	-3.11918900
C	-0.17510900	-4.44222800	3.33694000	O	-0.36036300	2.49214500	1.24227300
H	-0.51624600	-5.13959300	4.09639200	C	-0.26321900	3.61474000	0.61618600
C	-2.98578300	0.03975200	1.54931700	O	0.36049400	3.81267000	-0.42896400
C	5.07653400	-1.96745300	-1.25698400	C	-1.06621100	4.73995200	1.24794500
H	5.58191700	-2.11541800	-2.20665300	H	-1.03087200	4.68609500	2.33887400
C	-2.82712900	1.88339700	-0.67845800	H	-0.70371200	5.70898800	0.90028300
C	-0.18875800	-1.80890800	-3.76773800	H	-2.11103000	4.62203800	0.93579900
H	-0.49841400	-1.11723500	-4.54469100	C	3.31249800	2.15267600	-0.83747200
C	-4.58972100	-1.10568600	2.95387300	C	2.56725900	1.34862600	-1.88622100
H	-5.39213600	-1.83005900	3.05959300	H	3.25496600	1.11263700	-2.70647800
C	-4.13143700	-0.40141700	4.06336000	H	2.26751900	0.39064400	-1.46788900
H	-4.57221000	-0.57750400	5.04044100				
C	-2.65282300	3.72508000	-2.23360900	<b>IntB5</b>			
H	-2.10739200	4.23702600	-3.01978800	Pd	0.47778500	-0.91214900	-0.21968800
C	-0.80052000	-3.20835300	3.19004000	P	1.17704800	1.29318300	0.12014800
H	-1.62959000	-2.92475700	3.83117500	P	-1.99086800	-0.59495000	0.05487500
C	0.24502700	-1.30894300	-2.54304600	C	0.86739700	3.75388200	3.41731100
H	0.28049300	-0.23059000	-2.39258800	H	1.10359500	4.78119500	3.67817200
C	-3.97108100	-1.63387700	-3.16707200	C	-1.91571700	-1.23732200	-2.65428900
H	-4.52628900	-1.36766700	-4.06175100	H	-0.92148000	-0.79745800	-2.62321000
C	-2.54595800	-2.29845900	-0.87634800	C	-3.94848600	-1.89411700	-1.53314300
H	-1.98392300	-2.57015600	0.01363400	H	-4.54683700	-1.96368700	-0.62924500
C	-0.23710200	-3.18133900	-3.98727400	C	-0.36881200	3.51836400	-0.81089800
H	-0.58743400	-3.56825900	-4.93968000	H	-0.53320800	3.81236900	0.21990900
C	5.15449700	-1.66936400	1.13199000	C	-2.33830400	-2.81352300	1.65211200
				H	-1.50546400	-3.18040700	1.05012500

C	0.54817400	1.99773700	-2.45066900
H	1.13528600	1.11082500	-2.68496500
C	0.39499500	2.39203000	-1.11264200
C	-3.93902600	-1.05852400	2.10585100
H	-4.35018000	-0.07570400	1.89840600
C	-0.04474500	2.73696800	-3.46677200
H	0.08070200	2.42681100	-4.49993800
C	3.47326300	2.72840600	-0.76725700
H	2.79834700	3.38583400	-1.30715500
C	-2.67625900	1.82744500	1.28464100
H	-2.19397700	1.41170900	2.16302800
C	2.96772300	1.65256400	-0.03574500
C	-4.51575500	-1.84628000	3.09996400
H	-5.36727500	-1.46773000	3.65822900
C	-2.77091800	1.06854100	0.11050900
C	-4.00781700	-3.11304100	3.37228100
H	-4.45988500	-3.72498100	4.14776900
C	1.13369400	3.28721400	2.13506800
H	1.59403700	3.94778000	1.40510300
C	5.72219800	2.10945600	-0.14322700
H	6.79306600	2.28402900	-0.19170100
C	3.85222100	0.80771500	0.64193600
H	3.46835400	-0.04581300	1.19525200
C	-2.41692200	-1.73274100	-3.85448800
H	-1.81359600	-1.67238400	-4.75538200
C	0.82240500	1.96894600	1.78330900
C	-0.80095000	3.86784800	-3.16056100
H	-1.26858800	4.44149600	-3.95559800
C	-2.67967900	-1.31090600	-1.48498100
C	4.84704300	2.95325400	-0.82063700
H	5.23266500	3.78818400	-1.39832600
C	-2.84102900	-1.53308000	1.38249200
C	0.03447900	1.57728800	4.04004500
H	-0.38201200	0.90298800	4.78227900
C	-4.44549100	-2.39484800	-2.73250600
H	-5.43044700	-2.85174400	-2.75874200
C	-3.68164600	-2.31356600	-3.89455400
H	-4.07029100	-2.70740300	-4.82923300
C	-2.92355100	-3.59581300	2.64197800
H	-2.53043200	-4.58830200	2.84320900
C	-0.96290100	4.25328300	-1.83481300
H	-1.56750300	5.12038400	-1.58707500
C	0.28891200	1.11397500	2.75114300
H	0.06598500	0.08184500	2.48943800

C	-3.20823400	3.11018300	1.34940100
H	-3.12639200	3.67731200	2.27210900
C	-3.39718600	1.63437400	-1.00315400
H	-3.47392800	1.07338000	-1.92856700
C	0.31228000	2.90030300	4.36992500
H	0.11046300	3.26485900	5.37288400
C	5.22214100	1.03561400	0.59051400
H	5.89751800	0.36273400	1.11026000
C	-3.92570300	2.92117600	-0.93905600
H	-4.40626200	3.34490800	-1.81590900
C	-3.83721900	3.66152600	0.23525100
H	-4.25366900	4.66367200	0.28274000
C	2.17219400	-1.40979700	-1.15425800
O	2.43691400	-0.86746900	-2.20994700
C	3.07831700	-2.42878100	-0.54923900
C	2.58545300	-3.48448400	0.22024400
C	4.45768600	-2.26004400	-0.72848500
C	3.50257500	-4.35372400	0.81733800
C	5.35564800	-3.11982000	-0.11407700
C	4.87171200	-4.17193500	0.66538600
H	3.13037000	-5.18993100	1.40644900
H	6.42479500	-2.98058900	-0.24566700
H	5.56486500	-4.85704600	1.14594500
H	4.80151800	-1.43403300	-1.34369100
N	0.14647900	-2.96005200	-0.37877100
H	0.20366900	-3.25330000	-1.35327900
C	1.08863400	-3.73229000	0.39827900
H	0.86157800	-3.57906500	1.46534700
H	0.92636300	-4.80798700	0.21514400

### TSB3

Pd	0.59095400	-0.56098200	-0.38992600
P	0.73955500	1.75385400	0.07252000
P	-1.88798500	-0.85961200	-0.13292500
C	-1.77724900	3.78515300	2.67534000
H	-2.24033600	4.76364600	2.76447000
C	-1.61472200	-2.25784000	-2.52247900
H	-0.76458500	-1.59661900	-2.67473700
C	-3.42301100	-3.04844700	-1.13630200
H	-4.00041600	-3.00576100	-0.21828200
C	-0.91730400	3.24808300	-1.62439100
H	-1.73732200	2.91748700	-0.99752800
C	-1.64788700	-1.99428900	2.37362900
H	-0.59562600	-2.03829000	2.11271400
C	1.43490700	3.32152600	-2.15175300

H	2.45752300	3.02846200	-1.94549900
C	0.40054900	2.90057000	-1.30814600
C	-3.91045500	-1.37007700	1.81821000
H	-4.62865500	-0.93473800	1.12922400
C	1.15384500	4.09886400	-3.27078300
H	1.96662300	4.41902000	-3.91572000
C	2.77453600	3.59611400	0.78542500
H	2.15521500	4.36543800	0.33310600
C	-3.43063000	1.44667000	0.37237000
H	-3.15177200	1.31900400	1.41334600
C	2.36497700	2.25911700	0.75700800
C	-4.33972600	-1.83323500	3.05768400
H	-5.39065700	-1.76626700	3.32312000
C	-3.01058700	0.52189400	-0.59170900
C	-3.42466500	-2.37842900	3.95667400
H	-3.76244300	-2.73615800	4.92490100
C	-0.95318400	3.51050800	1.58744500
H	-0.78691200	4.27455800	0.83443000
C	4.78254500	2.96911000	1.96679000
H	5.72590300	3.24511400	2.42894100
C	3.16451000	1.28582600	1.36141900
H	2.84813700	0.24602600	1.36468200
C	-1.93926700	-3.20399500	-3.48959900
H	-1.35245700	-3.26418300	-4.40110800
C	-0.36349400	2.25147800	1.45332400
C	-0.15845000	4.45557000	-3.56913800
H	-0.37332700	5.06131900	-4.44473900
C	-2.36036100	-2.16433900	-1.33983700
C	3.98090700	3.94724700	1.38121100
H	4.29519800	4.98679900	1.38922900
C	-2.55746800	-1.44539200	1.46645100
C	-1.39852400	1.56496000	3.53583200
H	-1.57141000	0.79639800	4.28315700
C	-3.73895500	-4.00196700	-2.09996700
H	-4.56200600	-4.68878500	-1.92644400
C	-3.00176200	-4.07889200	-3.27852600
H	-3.24924400	-4.82543800	-4.02734300
C	-2.07850900	-2.46093200	3.61239600
H	-1.35778500	-2.88164700	4.30691800
C	-1.19353500	4.02449200	-2.74469700
H	-2.22395500	4.28374200	-2.96907200
C	-0.57526000	1.29147900	2.44839100
H	-0.09907900	0.31790500	2.36627800
C	-4.20686400	2.54283800	0.00889000

H	-4.51708700	3.25009500	0.77212700
C	-3.37817700	0.72470800	-1.92588100
H	-3.06308900	0.02257700	-2.69131800
C	-2.01052300	2.81153100	3.64475400
H	-2.66240300	3.02711800	4.48624600
C	4.36965500	1.64049700	1.96187000
H	4.98511700	0.87092100	2.41767500
C	-4.15257800	1.82324600	-2.28710700
H	-4.42861300	1.96416200	-3.32780000
C	-4.57020900	2.73568300	-1.32176200
H	-5.17548500	3.59196200	-1.60457900
C	2.40798100	-0.41854200	-1.25906100
O	2.63415700	0.49952200	-2.02133300
C	3.47048300	-1.42970000	-0.97218800
C	3.18562600	-2.79779100	-0.90700900
C	4.76949900	-0.96144900	-0.75926800
C	4.22333400	-3.67860600	-0.60532100
C	5.79022300	-1.85031900	-0.44366400
C	5.51385600	-3.21303800	-0.36715200
H	4.00970000	-4.74216200	-0.54085500
H	6.79619200	-1.48293000	-0.26248700
H	6.30334100	-3.91647900	-0.11819600
H	4.96123000	0.10479500	-0.83236900
N	0.82989700	-2.61956400	-0.29620400
H	-0.06714100	-3.07356100	-0.45871000
C	1.78480200	-3.29537100	-1.16600700
H	1.76591200	-4.37502700	-0.96078800
H	1.54487300	-3.17553700	-2.23809000
C	1.69895900	-3.18628700	1.80636900
O	1.78525400	-4.34723900	1.64491100
O	1.74972900	-2.12151500	2.31177200

### IntB6

Pd	0.20992500	0.71527400	-0.66275200
P	1.07649800	-1.29727800	0.08515400
P	-2.18264700	0.44654000	-0.15040300
C	-0.78874900	-3.08030700	3.30249600
H	-0.73292900	-3.02076200	4.38509300
C	-3.05538900	3.06650900	-0.27609500
H	-2.33058100	3.21782400	0.52008500
C	-4.13055300	1.59930600	-1.87119400
H	-4.26335700	0.61571800	-2.31133100
C	2.37225200	0.33831300	1.91664700
H	1.54306300	1.02155700	1.73858100
C	-3.75944200	-1.92374900	-0.53072800

H	-4.22116600	-1.74035100	0.43337100
C	3.54059600	-1.72235000	1.45297600
H	3.62696100	-2.66258300	0.91806300
C	2.44714900	-0.88225400	1.23291100
C	-2.17852500	-1.33737300	-2.25051100
H	-1.41066900	-0.67152600	-2.63968100
C	4.54699500	-1.34670600	2.33771300
H	5.39884900	-2.00245300	2.49231000
C	2.04482500	-3.82039700	-0.74896600
H	1.88191500	-4.14804300	0.27392900
C	-4.13951800	0.34281500	1.89100100
H	-4.88082900	0.41250300	1.09901600
C	1.72791800	-2.50681100	-1.12300700
C	-2.52962000	-2.47466500	-2.96980900
H	-2.04093900	-2.68578600	-3.91612100
C	-2.77557700	0.34785300	1.57185200
C	-3.49588900	-3.34424300	-2.46699600
H	-3.76659500	-4.23776100	-3.02182900
C	0.06357500	-2.30064500	2.52724300
H	0.77961300	-1.64749600	3.01553000
C	2.71963300	-4.31685000	-3.01031500
H	3.10707400	-5.01938500	-3.74228800
C	1.88581300	-2.12045900	-2.45690600
H	1.61281800	-1.11808800	-2.76956900
C	-3.81728200	4.12795600	-0.74848800
H	-3.68913800	5.11385000	-0.31168100
C	-0.00230900	-2.35260200	1.13200200
C	4.46643700	-0.13323300	3.01503400
H	5.25736500	0.16174700	3.69826600
C	-3.21415800	1.79269600	-0.83596100
C	2.54395300	-4.71665900	-1.68613900
H	2.78853800	-5.73091600	-1.38519900
C	-2.78817400	-1.05008900	-1.02137200
C	-1.77022500	-3.99543000	1.30476100
H	-2.48466100	-4.65136800	0.81733600
C	-4.88573600	2.67085000	-2.34383100
H	-5.59681400	2.51315800	-3.14967900
C	-4.73109400	3.93430300	-1.78315600
H	-5.32006200	4.76894400	-2.15275800
C	-4.11111400	-3.06325700	-1.25046200
H	-4.86253100	-3.73874900	-0.85147800
C	3.37548500	0.70580400	2.80635500
H	3.30985300	1.65973200	3.31983200
C	-0.92622300	-3.21099300	0.52659300

H	-0.99150300	-3.27265800	-0.55596000
C	-4.54877500	0.27865400	3.21733600
H	-5.60800500	0.27139600	3.45685700
C	-1.83404200	0.35053200	2.60016700
H	-0.78061500	0.43297900	2.35774300
C	-1.70826800	-3.92814100	2.69367500
H	-2.37376800	-4.53593000	3.29941800
C	2.38534900	-3.02284100	-3.39429400
H	2.50598200	-2.70899800	-4.42652900
C	-2.24429500	0.29214000	3.92921700
H	-1.50201800	0.29795400	4.72178800
C	-3.59905700	0.24408500	4.23816300
H	-3.91975300	0.20139300	5.27513100
C	1.87949500	1.23694400	-1.67482600
O	1.74746700	1.17569000	-2.87190600
C	3.14113700	1.72548000	-1.01709600
C	4.13989400	0.76056400	-0.86334000
C	4.57237600	3.33111800	0.04484000
C	5.33997300	1.07120200	-0.23897700
C	5.55260200	2.36329600	0.23028400
H	4.75504700	4.34939400	0.38193000
H	6.09953300	0.30566800	-0.11621900
H	6.48455100	2.62136500	0.72459100
H	3.96608100	-0.24787800	-1.22930500
N	1.35646100	4.22410400	0.31460500
H	1.71313800	4.42208100	1.23952200
C	0.32168700	3.29325800	0.33566800
O	-0.20906800	3.00084600	1.41762900
O	0.00605800	2.82666700	-0.83378400
C	3.35605900	3.04288900	-0.58146200
C	2.33927000	4.15962000	-0.75313200
H	2.87080000	5.11661600	-0.79298500
H	1.78883900	4.04416700	-1.68744100

**TSB4**

Pd	0.16816400	0.76317200	-0.29279200
P	1.08968000	-1.31025000	0.13768300
P	-2.27409400	0.56255200	-0.09132700
C	-0.53242500	-3.20167700	3.42654900
H	-0.31145500	-3.28427800	4.48683100
C	-2.69819600	3.27960300	-0.33054400
H	-1.91272500	3.34210000	0.41914900
C	-4.09644900	1.94882900	-1.78780600
H	-4.41090800	0.98135200	-2.16881600
C	2.91039900	-0.17164500	1.88076500

H	2.15038300	0.60303000	1.96306300
C	-3.89783900	-1.68972200	-0.78493900
H	-4.48302600	-1.49546600	0.10868100
C	3.68429800	-2.23456600	0.89866600
H	3.53725600	-3.07848800	0.23151400
C	2.69125200	-1.26249000	1.03166800
C	-2.09244200	-1.11994000	-2.27659800
H	-1.26054900	-0.47205800	-2.54375600
C	4.88052200	-2.11491900	1.60078700
H	5.65165900	-2.87080600	1.48326900
C	1.45930200	-3.77418000	-1.23405200
H	1.37072600	-4.26050600	-0.26651300
C	-4.50058000	0.67946600	1.66499100
H	-5.05040800	1.13297700	0.84461600
C	1.36003300	-2.38050700	-1.32612200
C	-2.36938100	-2.24085300	-3.05078600
H	-1.75641800	-2.45810200	-3.92034200
C	-3.15376400	0.33773700	1.49619000
C	-3.40960700	-3.09526500	-2.68889300
H	-3.61901800	-3.98055000	-3.28221300
C	0.33470500	-2.49383600	2.59735000
H	1.21862900	-2.02855400	3.02214800
C	1.73060900	-3.93125100	-3.62599500
H	1.87233900	-4.53420200	-4.51822400
C	1.43560300	-1.77433600	-2.58481700
H	1.33357600	-0.69553000	-2.67512700
C	-3.29731400	4.43536500	-0.81863000
H	-2.97986100	5.40351300	-0.44295500
C	0.06627000	-2.37560400	1.23043300
C	5.09009700	-1.02906700	2.44654200
H	6.02706200	-0.93433900	2.98756300
C	-3.10192200	2.02732800	-0.81017200
C	1.64495100	-4.54415200	-2.37729800
H	1.71695400	-5.62455700	-2.29395200
C	-2.84615400	-0.83813100	-1.12996400
C	-1.94075800	-3.69579200	1.53831100
H	-2.82854100	-4.15492000	1.11428000
C	-4.68603500	3.11138300	-2.27942400
H	-5.45617200	3.04364200	-3.04246700
C	-4.28917100	4.35402200	-1.79426200
H	-4.74862200	5.25969000	-2.17988300
C	-4.17676400	-2.81272500	-1.56171200
H	-4.99069700	-3.47387000	-1.27764300
C	4.10054800	-0.05967500	2.59012600

H	4.26312700	0.79650000	3.23740800
C	-1.07576400	-2.99358000	0.70736200
H	-1.29403400	-2.92813100	-0.35399400
C	-5.13455900	0.44925100	2.88141100
H	-6.17929500	0.71931100	3.00521900
C	-2.44952400	-0.21379800	2.56774900
H	-1.39859600	-0.45619700	2.45114000
C	-1.67533300	-3.79721100	2.90156900
H	-2.35617200	-4.33880000	3.55139100
C	1.62652300	-2.54719400	-3.72791300
H	1.68536100	-2.06303300	-4.69809100
C	-3.08618700	-0.44902300	3.78273500
H	-2.52651300	-0.88550200	4.60448300
C	-4.42887700	-0.12009300	3.94036900
H	-4.92559300	-0.29726600	4.89009400
C	1.71151600	1.71924300	-1.28194000
O	1.37160200	1.68933700	-2.44327700
C	3.13981100	1.79724400	-0.81746300
C	3.91043500	0.66954500	-1.10994400
C	5.09201500	2.82506600	0.14008300
C	5.25123600	0.60473600	-0.75988100
C	5.84371300	1.68418000	-0.11454800
H	5.56476900	3.68352600	0.61177300
H	5.82232600	-0.29166600	-0.97833000
H	6.88899900	1.64504800	0.17691400
H	3.44504900	-0.17377300	-1.60991400
N	1.97070400	4.12571600	1.03863100
H	2.22908200	4.25301600	2.00541600
C	0.88383200	3.31502800	0.83818000
O	0.12636000	3.00195100	1.74818000
O	0.72360200	2.95959800	-0.43606600
C	3.74348300	2.91209000	-0.21418800
C	3.00239000	4.21175700	0.02308300
H	3.71221200	4.98421500	0.33261800
H	2.53537500	4.55128800	-0.90553900

### IntB7

Pd	0.00253300	0.46745100	-0.51687000
P	1.98625300	-0.60827700	0.03434700
P	-2.17164900	-0.32452300	-0.18403800
C	2.21543400	-4.23558900	2.05705800
H	2.76736100	-4.66964000	2.88598700
C	-3.93004600	1.78214500	0.21546400
H	-3.21492900	2.08036200	0.97770800
C	-4.64151200	0.24586900	-1.50334900

H	-4.49202100	-0.65914900	-2.08448700	H	-3.37853700	-5.05231800	-1.32750200
C	2.12798800	0.14714900	2.72647500	C	2.58898800	0.89214100	3.80805900
H	1.24997200	-0.47930000	2.85221400	H	2.07933000	0.81896900	4.76386600
C	-2.91137700	-3.01338200	-0.83344600	C	0.80148800	-3.11260900	-0.05476300
H	-3.31162600	-3.09486100	0.17231500	H	0.22453100	-2.66675300	-0.86017500
C	3.85732200	1.08394600	1.33990200	C	-4.00943300	-1.66792300	3.28169400
H	4.35843100	1.16853400	0.38071200	H	-5.00835700	-1.68931800	3.70788300
C	2.76281400	0.22441200	1.47794400	C	-1.46000400	-1.59164100	2.18812000
C	-1.83314800	-1.73405400	-2.56414900	H	-0.46614300	-1.56253500	1.75670000
H	-1.37132100	-0.80717300	-2.89780200	C	1.26050500	-4.99178300	1.38180900
C	4.31201400	1.83979100	2.41933100	H	1.06183600	-6.01498400	1.68727800
H	5.16537700	2.49994400	2.29101400	C	4.11146700	-0.98531100	-3.44504300
C	4.66057500	-1.28194700	-0.73225400	H	3.88961500	-0.87825400	-4.50308000
H	4.87821500	-1.41508500	0.32416200	C	-1.66568000	-2.20237900	3.41951100
C	-3.80388900	-1.07045800	2.04000100	H	-0.82539400	-2.64806100	3.94454000
H	-4.64467200	-0.63573000	1.50832900	C	-2.94348100	-2.23729300	3.97266200
C	3.38460700	-0.87131700	-1.13545500	H	-3.10831100	-2.70490600	4.93923100
C	-1.87899800	-2.83365300	-3.41412400	C	-1.03087800	3.47741400	-0.53925300
H	-1.47197500	-2.75863000	-4.41838100	O	-1.95852700	3.81153700	-1.22444300
C	-2.52396200	-1.02535000	1.48088900	C	0.26839700	3.00748000	-1.11151800
C	-2.43027100	-4.03433200	-2.96990700	C	0.22887500	2.45078100	-2.39993200
H	-2.45477900	-4.89911300	-3.62657500	C	2.67778200	3.10013300	-1.25008000
C	2.46658700	-2.91995400	1.67511800	C	1.40907400	2.21722600	-3.09864000
H	3.21000500	-2.34034900	2.21518800	C	2.63345500	2.55467200	-2.52895800
C	5.38311700	-1.37003800	-3.03260400	H	3.63421400	3.35847400	-0.80375100
H	6.16043900	-1.56045700	-3.76692900	H	1.36839000	1.78642200	-4.09425900
C	3.11935600	-0.73562800	-2.49910100	H	3.55536400	2.37415000	-3.07254700
H	2.12526300	-0.43009600	-2.81257400	H	-0.73908400	2.27049100	-2.85552300
C	-5.06163000	2.55661300	-0.00863300	N	0.85356700	3.14532600	1.84611300
H	-5.21421400	3.46098800	0.57224000	H	1.38719000	2.49966900	2.41346400
C	1.75361000	-2.34187400	0.62101500	C	-0.46333200	2.85332600	1.75506200
C	3.68235800	1.74603200	3.65770000	O	-1.07588200	2.09213600	2.45921300
H	4.03644500	2.33399600	4.49892000	O	-1.14157600	3.63587900	0.81944600
C	-3.71081700	0.61691800	-0.52972200	C	1.50988700	3.32180000	-0.52470000
C	5.65584200	-1.52015600	-1.67331400	C	1.55700500	3.93642000	0.85411300
H	6.64396000	-1.83203800	-1.34762000	H	2.59150000	4.02589800	1.19126300
C	-2.35024700	-1.80891400	-1.26431100	H	1.12799900	4.94544300	0.83696900
C	0.55801400	-4.42949800	0.31908600				
H	-0.19736000	-5.00230600	-0.21035000	<b>prodB1</b>			
C	-5.77039400	1.03019500	-1.73168800	C	0.64313900	1.35809800	-0.39827400
H	-6.48610700	0.73272400	-2.49299900	O	0.62166900	2.52285400	-0.68494700
C	-5.98319500	2.18485200	-0.98510200	C	-0.59130700	0.56656000	-0.10737500
H	-6.86274900	2.79617700	-1.16578800	C	-1.68538400	1.26671900	0.40308200
C	-2.94601900	-4.12016700	-1.68009800	C	-1.92513700	-1.43713700	-0.19242800
				C	-2.88919200	0.61350100	0.63629000

C -3.00928300 -0.73993800 0.33444700  
H -2.02679100 -2.49183600 -0.43469800  
H -3.73298000 1.16066800 1.04399800  
H -3.94895600 -1.25569200 0.50715800  
H -1.57653100 2.32694900 0.60536400  
N 1.59613600 -1.54327300 -0.02639800  
H 1.68964300 -2.31648100 0.61620300  
C 2.13386100 -0.38332400 0.43543400  
O 2.85966000 -0.26990100 1.38430700  
O 1.85235800 0.71064100 -0.38308700  
C -0.70828200 -0.79845500 -0.41549600  
C 0.48324500 -1.54999600 -0.96401000  
H 0.22314300 -2.59177200 -1.16319400  
H 0.82005800 -1.11383400 -1.91024900

**IntB8**

Pd -0.27700400 -0.92579500 -0.01178800  
P -1.53542400 1.03296200 -0.10948300  
P 1.97248300 0.10646300 0.11142100  
C -0.29731500 4.40294400 -2.18148100  
H -0.25905000 5.47842800 -2.03697200  
C 2.68790000 -1.64734600 2.16775400  
H 1.98438500 -2.31913800 1.68876400  
C 3.84583000 0.46438100 2.23135200  
H 4.03353000 1.45388200 1.82669900  
C -1.02451200 1.39493300 2.60472800  
H -0.42367700 0.49392500 2.49402900  
C 2.55249200 -0.66650800 -2.50399800  
H 1.47905200 -0.79128500 -2.59636800  
C -2.51900600 3.02775100 1.64564200  
H -3.09665600 3.39660700 0.80268100  
C -1.69748200 1.90414400 1.49176900  
C 4.49037200 -0.21705300 -1.14257100  
H 4.93330300 0.04321200 -0.18592700  
C -2.62136900 3.65939200 2.88003900  
H -3.25586000 4.53395800 2.98766800  
C -3.66771900 1.15974600 -1.97150400  
H -2.93933200 1.49407300 -2.70283200  
C 2.61871200 2.67436400 -0.92628500  
H 2.94126400 2.16417800 -1.82741300  
C -3.28647800 0.92843300 -0.64883900  
C 5.31396500 -0.46022300 -2.23639700  
H 6.39196500 -0.39017600 -2.12516900  
C 2.12577200 1.94336700 0.15708700  
C 4.75784000 -0.79724500 -3.46849400

H 5.40238300 -0.99022400 -4.32113100  
C -0.78483900 3.59221300 -1.16042900  
H -1.10539600 4.04541600 -0.22909500  
C -5.93681000 0.52671000 -1.44739400  
H -6.96379300 0.36197400 -1.75963600  
C -4.24967500 0.50514500 0.27336100  
H -3.96923700 0.31229700 1.30388600  
C 3.38903500 -2.06332100 3.29557900  
H 3.21395000 -3.05695000 3.69761900  
C -0.82462100 2.20777100 -1.32411600  
C -1.92397600 3.16090800 3.97945000  
H -2.01026000 3.65151400 4.94453100  
C 2.90470000 -0.37692300 1.62467800  
C -4.98828300 0.96067800 -2.36655200  
H -5.27163000 1.14399800 -3.39878500  
C 3.10158800 -0.31318300 -1.26974400  
C 0.13491100 2.46004400 -3.53672700  
H 0.50255300 2.01007100 -4.45395700  
C 4.54296600 0.04790700 3.36184500  
H 5.26768200 0.71395600 3.82099100  
C 4.31383600 -1.21576300 3.89901500  
H 4.85837300 -1.54005400 4.78114400  
C 3.37658500 -0.90101900 -3.60059000  
H 2.93757200 -1.18584600 -4.55190000  
C -1.13586000 2.02219200 3.84355300  
H -0.60789400 1.61720700 4.70189700  
C -0.34909400 1.64904600 -2.51653500  
H -0.36253200 0.56891500 -2.63977600  
C 2.69882100 4.06310200 -0.86252400  
H 3.08337100 4.61385400 -1.71573900  
C 1.70994200 2.63726300 1.29916700  
H 1.34775900 2.09106000 2.16233100  
C 0.15558900 3.84248400 -3.37174300  
H 0.53666300 4.48031400 -4.16380000  
C -5.56394600 0.30192500 -0.12423400  
H -6.29466500 -0.04604900 0.59908800  
C 1.78191100 4.02372200 1.36014400  
H 1.45089500 4.53759400 2.25789900  
C 2.28195300 4.74245700 0.27724000  
H 2.34533900 5.82588700 0.32192100  
C -2.07271600 -1.87842700 -0.02471300  
C -2.67060200 -2.26843700 1.18015100  
C -2.72200000 -2.15334100 -1.22932200  
C -3.90936900 -2.91964000 1.14572000



C	-3.95900900	-2.78742700	-1.25026400
H	-2.25607900	-1.86658600	-2.16751400
C	-4.56041300	-3.17136800	-0.05462400
H	-4.36779400	-3.23393000	2.08200400
H	-4.44903500	-2.98475700	-2.19964900
H	-5.52332300	-3.67413100	-0.05805000
I	0.75871800	-3.39884200	-0.71561200
C	-2.05045500	-1.97541700	2.53012800
H	-2.45472900	-2.68624900	3.26778700
H	-2.35690300	-0.97312300	2.86471100
N	-0.59052900	-1.98241900	2.46894100
H	-0.18643400	-1.84439400	3.39132500
H	-0.26281200	-2.88098300	2.11879300

**IntB9**

C	2.13875400	-1.79331500	-0.70601000
C	2.07879800	-2.87725000	-1.60160300
C	3.35727600	-1.54898200	-0.06818700
C	3.20499200	-3.65484600	-1.86486400
C	4.48492600	-2.32591900	-0.33098300
C	4.41518300	-3.37649300	-1.23874800
H	3.12959700	-4.49645500	-2.55012200
H	5.41790500	-2.10676000	0.18155400
H	5.28964300	-3.98742600	-1.44351500
H	3.45615300	-0.74385100	0.65239200
N	-0.29284000	-2.73197100	-1.29444100
H	-1.21302900	-2.73339100	-1.72715900
Pd	0.32459500	-0.89480300	-0.39049800
P	-1.96599100	-0.16023000	-0.15968600
C	-2.54782800	0.44061900	1.46265900
C	-3.14646200	-1.52283300	-0.48414300
C	-2.38182800	1.08917500	-1.43377600
C	-1.66703100	0.38133000	2.54386200
C	-3.86374500	0.87071200	1.67158800
C	-4.16711700	-1.45572700	-1.43520500
C	-2.97885100	-2.68493100	0.28198000
C	-3.14903200	2.23565700	-1.23185900
C	-1.86041200	0.84086700	-2.71179300
H	-0.68391600	-0.05414000	2.40948400
C	-2.07174100	0.81919500	3.80232100
H	-4.58376800	0.83943300	0.85837100
C	-4.26368800	1.31473200	2.92670800
H	-4.30062800	-0.55992600	-2.03478800
C	-5.01833500	-2.54423000	-1.61769200
H	-2.15909200	-2.74701400	0.99747100

C	-3.82956400	-3.76727800	0.08916200
C	-3.41313600	3.10121200	-2.29136100
H	-3.51932700	2.48028400	-0.24317600
C	-2.12811800	1.70170600	-3.76859500
H	-1.23171000	-0.03272300	-2.87158700
C	-3.36223600	1.30348300	3.99073800
H	-1.37474800	0.76847700	4.63338800
H	-5.28349600	1.65552000	3.07920400
C	-4.85055700	-3.69839500	-0.85762400
H	-5.81156100	-2.48816400	-2.35765500
H	-3.67833700	-4.66989200	0.67274700
H	-4.00395500	3.99520400	-2.11509400
C	-2.91282500	2.83459200	-3.56044000
H	-1.72003800	1.49201400	-4.75292700
H	-3.67781900	1.64747800	4.97152900
H	-5.51128200	-4.54738100	-1.00799700
H	-3.12218400	3.51167900	-4.38337600
C	2.76659900	1.45362400	-0.96874300
P	1.33776500	1.11644600	0.13496300
C	2.65402000	1.05250700	-2.30446300
C	3.93654200	2.08555600	-0.54638300
C	1.94520400	1.23289600	1.85644200
C	0.33798400	2.65048600	-0.04909900
H	1.76591800	0.51431600	-2.62551900
C	3.68069000	1.30297200	-3.20665600
H	4.06178100	2.37425200	0.49146700
C	4.97174400	2.32140200	-1.44770200
C	1.90960100	0.08857300	2.65990500
C	2.40979200	2.44085700	2.39610800
C	0.29573000	3.33470000	-1.26787100
C	-0.42110400	3.13089300	1.02305400
C	4.84433700	1.93746000	-2.77853400
H	3.58093200	0.98242300	-4.23919800
H	5.88292100	2.80149600	-1.10350200
H	1.48587700	-0.84276500	2.28136300
C	2.35822900	0.15149700	3.97795500
C	2.86049900	2.49475900	3.70948900
H	2.39770700	3.34702500	1.79662700
H	0.87247300	2.97917000	-2.11526200
C	-0.47214300	4.48593300	-1.40285700
H	-0.40642400	2.61662900	1.97743800
C	-1.19168200	4.28113500	0.88406100
H	5.65461300	2.11955800	-3.47819100
H	2.31926500	-0.74248900	4.59280800

C	2.84016300	1.34662100	4.50093400	H	-4.44582700	-0.90159400	-1.02306800
H	3.21942100	3.43452900	4.11844700	C	-3.98200000	-1.62090800	-2.99242500
H	-0.49361600	5.00536000	-2.35586000	H	-4.19443200	0.63463100	1.98110200
C	-1.21332300	4.96575200	-0.32674400	C	-5.34673200	2.30557000	1.28136000
H	-1.77142000	4.63956900	1.72940800	H	-2.73662300	2.59129700	-1.56176300
H	3.18890400	1.39113200	5.52870200	C	-4.54443400	3.38978300	-0.71515400
H	-1.81043200	5.86663800	-0.43450600	C	-3.13314300	-2.79443300	2.46258400
C	0.74973300	-3.18107500	-2.23155400	H	-3.32854200	-2.36238200	0.37157600
H	0.63054100	-2.62642200	-3.17160900	C	-1.85998500	-1.21973300	3.76591500
H	0.64247800	-4.24980500	-2.45686200	H	-1.05744700	0.45785700	2.68329400
C	0.37218700	-3.41929800	1.77903300	C	-3.01650500	-1.71180800	-3.99443400
C	1.55770900	-3.80084700	2.66315000	H	-0.99920600	-1.21549100	-4.57169300
H	1.48299400	-3.32598600	3.64631800	H	-4.97971100	-2.01553700	-3.16021000
H	1.63989500	-4.88488200	2.76995800	C	-5.47958500	3.29617200	0.31363400
H	2.46890400	-3.43364900	2.17297100	H	-6.07102300	2.22851200	2.08703200
O	-0.02513800	-4.26504600	0.93924800	H	-4.63621900	4.16723300	-1.46751100
O	-0.09017900	-2.24820600	1.91726600	H	-3.69509600	-3.72078700	2.38903300
H	-0.32631200	-3.37848800	-0.46499400	C	-2.60768600	-2.39231800	3.68625400

### IntB10

C	1.99014800	2.45135700	0.04386000	H	-3.25986000	-2.18576600	-4.94088000
C	1.72524400	3.82577700	0.21452000	H	-6.30752000	3.99746900	0.36239900
C	3.32629500	2.08428800	-0.16336100	H	-2.76942900	-2.99708300	4.57383100
C	2.75083100	4.77113900	0.17778400	C	2.77097300	-0.83605300	1.22893700
C	4.35432800	3.02599800	-0.19335600	P	1.44502000	-0.76105200	-0.04012900
C	4.06933500	4.37639500	-0.02148800	C	2.61841700	-0.04279300	2.36943500
H	2.51297800	5.82590200	0.30346400	C	3.88171400	-1.67729500	1.12645900
H	5.37865100	2.69821200	-0.35336300	C	2.24895600	-1.08172900	-1.66202700
H	4.86534000	5.11603100	-0.04852700	C	0.57675500	-2.35626600	0.27628500
H	3.60459400	1.04522100	-0.30748100	H	1.77885200	0.64397300	2.42997600
N	-0.56429700	3.13401500	-0.03588200	C	3.55328600	-0.10169000	3.39851900
H	-1.42866800	3.14973700	0.50004600	H	4.02793700	-2.28695700	0.24090200
Pd	0.27304800	1.30095600	0.02144200	C	4.82237700	-1.72576100	2.15008500
P	-1.93222500	0.33500900	0.01417200	C	2.34513600	-0.02590400	-2.57505400
C	-2.39052400	-0.50433400	-1.54894400	C	2.73749500	-2.34220700	-2.03053300
C	-3.34795300	1.49030200	0.18931100	C	0.55026400	-2.90756200	1.56118800
C	-2.20169000	-0.83602500	1.39623600	C	-0.10225300	-3.01790500	-0.75254000
C	-1.44281600	-0.56738500	-2.57287300	C	4.65701100	-0.94229800	3.28983700
C	-3.67583200	-1.00834900	-1.78240500	H	3.42710500	0.52453500	4.27645700
C	-4.28521400	1.40496400	1.22185100	H	5.68772700	-2.37509200	2.05554200
C	-3.48271500	2.49501400	-0.77908400	H	1.96495300	0.95480900	-2.30135100
C	-2.93267700	-2.02154300	1.32176400	C	2.93119700	-0.22259600	-3.82285600
C	-1.65260500	-0.45095800	2.62646200	C	3.32471100	-2.53612400	-3.27602300
H	-0.45885200	-0.13384500	-2.41845400	H	2.63450400	-3.18515100	-1.35332300
C	-1.75066900	-1.17235600	-3.78896600	H	1.06302100	-2.40983400	2.37775100

C	-0.12443100	-4.09897900	1.80527800
H	-0.09326000	-2.61708700	-1.75969600
C	-0.77930500	-4.20799200	-0.50631400
H	5.39347400	-0.98045700	4.08716000
H	3.00043800	0.60833600	-4.51815000
C	3.42395500	-1.47539900	-4.17413000
H	3.69860600	-3.51879800	-3.54798700
H	-0.13511200	-4.51041100	2.80986900
C	-0.78749500	-4.75533500	0.77274800
H	-1.29592000	-4.70667800	-1.32112500
H	3.87964400	-1.62871300	-5.14804800
H	-1.31200500	-5.68670000	0.96581300
C	0.29932100	4.19980000	0.46096000
H	0.17385900	4.37787400	1.54489800
H	0.05481200	5.15606200	-0.03282100

**TSB5**

Pd	-0.22147100	1.02985400	-0.10735000
P	-1.58968200	-0.88026500	0.04381800
P	2.00134400	0.01503200	-0.14038500
C	-0.26086300	-4.59810800	1.31676100
H	-0.33626600	-5.63789700	1.01146900
C	2.58842700	2.00813600	-1.99911300
H	1.52783200	1.94366900	-2.23082300
C	4.47658200	1.32990200	-0.66067500
H	4.90545800	0.72955700	0.13551700
C	-1.23598400	-2.08692800	-2.41525200
H	-0.18181300	-2.00665100	-2.17133400
C	2.43115600	0.31188700	2.56384400
H	1.61150800	1.02200200	2.48916500
C	-3.55195800	-1.72960300	-1.84881800
H	-4.31576100	-1.37550700	-1.16359300
C	-2.20143700	-1.63703900	-1.50608500
C	3.90883800	-1.29656900	1.53477100
H	4.25628700	-1.83436700	0.65747000
C	-3.92914700	-2.27140300	-3.07615700
H	-4.98234700	-2.33145100	-3.33368600
C	-3.90357100	-1.73946600	1.40123100
H	-3.71293100	-2.70814100	0.94655800
C	2.04371100	-2.76555200	-0.63620600
H	1.91220000	-2.89144700	0.43314500
C	-3.06119400	-0.65518300	1.12057400
C	4.50005800	-1.54074700	2.77064400
H	5.30633500	-2.26414800	2.84840300
C	2.19842500	-1.48713900	-1.18323800

C	4.05919100	-0.85992900	3.90369400
H	4.52004600	-1.05496800	4.86768900
C	-0.89146200	-3.61127300	0.56164200
H	-1.43831500	-3.88633500	-0.33509900
C	-5.21347800	-0.35877000	2.87957300
H	-6.05138500	-0.24236800	3.56082300
C	-3.29377900	0.56905100	1.74890800
H	-2.63663700	1.40767100	1.54920900
C	3.39835400	2.89976800	-2.69453700
H	2.96944900	3.51408600	-3.48040400
C	-0.79660600	-2.27207900	0.94214100
C	-2.96467100	-2.73188000	-3.96634300
H	-3.26262700	-3.15555600	-4.92088500
C	3.12248700	1.20715800	-0.98100800
C	-4.97913000	-1.58961300	2.26744000
H	-5.62901400	-2.43504200	2.47292800
C	2.86250500	-0.37468200	1.42466800
C	0.55933900	-2.91947100	2.84208100
H	1.13630700	-2.63680000	3.71752000
C	5.28280400	2.23255100	-1.34955800
H	6.33217300	2.32472300	-1.08568900
C	4.74762000	3.01508700	-2.36861600
H	5.37848700	3.71965900	-2.90239400
C	3.02899000	0.07108900	3.79746800
H	2.67979700	0.60677700	4.67492200
C	-1.61485600	-2.64000400	-3.63158000
H	-0.85023600	-2.99016800	-4.31860700
C	-0.08280300	-1.93686100	2.09750700
H	-0.01865500	-0.89711500	2.40733300
C	2.05064600	-3.89110300	-1.45460100
H	1.91917100	-4.87168900	-1.00734500
C	2.36895900	-1.36423700	-2.56763700
H	2.49578300	-0.38520100	-3.01788300
C	0.47380200	-4.25448600	2.44898600
H	0.97678100	-5.02509500	3.02576400
C	-4.36743200	0.71453600	2.62476000
H	-4.53785000	1.67265400	3.10582900
C	2.37429900	-2.49133600	-3.38378900
H	2.50783700	-2.37531400	-4.45525800
C	2.21032800	-3.75907000	-2.83050200
H	2.21085000	-4.63810500	-3.46816500
C	-1.71852900	2.27767500	-0.74691200
C	-1.32376700	3.62939900	-0.81000900
C	-3.00357600	1.95493600	-1.19592000

C	-2.20756200	4.61048500	-1.26103300
C	-3.87923500	2.93321000	-1.66402000
C	-3.48634000	4.26792600	-1.68690400
H	-1.88825500	5.65050000	-1.28203500
H	-4.87044400	2.64828000	-2.00778700
H	-4.16994500	5.03624700	-2.03799700
H	-3.35202900	0.92724400	-1.19157600
N	0.58798000	2.83994800	0.38854000
H	1.60568300	2.86301400	0.37098300
C	0.09188400	3.93687000	-0.43035500
H	0.16197100	4.88981700	0.11685500
H	0.68169700	4.06505900	-1.35681400
C	-0.31043400	3.23864200	2.60141300
O	-0.45519600	4.39464400	2.48217800
O	-0.29078200	2.13951900	3.02372000

**IntB11**

Pd	0.26908400	-0.90038000	-0.38243200
P	1.54296100	0.91154000	0.22393400
P	-2.06892700	-0.06333400	-0.20389000
C	0.31087300	3.55162300	3.15477900
H	0.40454100	4.61044300	3.37748100
C	-2.54695200	-1.66286300	-2.45131300
H	-1.46909400	-1.77336600	-2.50189600
C	-4.52222000	-0.85528500	-1.31904000
H	-4.98043300	-0.30583000	-0.50106700
C	0.82883300	2.36809700	-2.02013000
H	0.05025600	1.61880400	-2.12327300
C	-2.81257800	-1.63345600	1.92654200
H	-2.30619000	-2.42694500	1.37956800
C	2.76167300	3.22886600	-0.85641100
H	3.49923600	3.14609000	-0.06284100
C	1.74913400	2.26852000	-0.97432200
C	-3.64947800	0.63043600	2.08057700
H	-3.77178300	1.62478200	1.66397600
C	2.83523300	4.28102100	-1.76265200
H	3.62438600	5.02068200	-1.66701500
C	3.48001500	0.09484200	2.08115800
H	2.69280400	0.16911000	2.82507900
C	-1.94738800	2.71843000	0.23971600
H	-1.63032800	2.47489600	1.24707700
C	3.24025700	0.48050300	0.76016900
C	-4.22299100	0.33209100	3.31485500
H	-4.78128800	1.09778800	3.84593800
C	-2.32653500	1.70112600	-0.64525200

C	-4.08559100	-0.94095200	3.86059300
H	-4.53228100	-1.17133700	4.82368900
C	0.94029800	3.02634500	2.03056100
H	1.50047300	3.68447200	1.37428000
C	5.74559200	-0.50738300	1.51191200
H	6.71557500	-0.90049900	1.80133600
C	4.27233200	0.37936800	-0.17847700
H	4.09862500	0.65785000	-1.21217100
C	-3.35266200	-2.28262900	-3.40332800
H	-2.89324200	-2.85333300	-4.20442000
C	0.81225600	1.66871200	1.72513600
C	1.90078800	4.38325900	-2.79207800
H	1.95990200	5.20712300	-3.49717400
C	-3.12834900	-0.93942700	-1.40832200
C	4.72796400	-0.39691100	2.45378500
H	4.90088000	-0.69598700	3.48324500
C	-2.92604300	-0.34352300	1.38894700
C	-0.56646200	1.37119400	3.69748000
H	-1.17130700	0.72248000	4.32317300
C	-5.32330500	-1.47750900	-2.26869200
H	-6.40444800	-1.41222000	-2.19038700
C	-4.73767300	-2.18989100	-3.31412700
H	-5.36393100	-2.68164900	-4.05287700
C	-3.39064900	-1.92389100	3.15767000
H	-3.29837900	-2.92867700	3.55830900
C	0.89929800	3.42612700	-2.92102900
H	0.16853700	3.49819000	-3.72012200
C	0.06478100	0.84509100	2.57416400
H	-0.05896000	-0.20853800	2.33711900
C	-1.97138200	4.05112500	-0.15589900
H	-1.66652500	4.82015300	0.54766100
C	-2.74082100	2.05624300	-1.93444600
H	-3.04453500	1.28743900	-2.63796400
C	-0.44885300	2.72815500	3.98458400
H	-0.95227700	3.14642100	4.85104400
C	5.51579600	-0.11385600	0.19587600
H	6.30117500	-0.20427300	-0.54782300
C	-2.76231400	3.39161600	-2.32900000
H	-3.08805900	3.64734300	-3.33322900
C	-2.37258700	4.39281400	-1.44419200
H	-2.38410400	5.43300200	-1.75576900
C	1.98250100	-1.73753200	-0.99791900
C	2.49937000	-1.40834900	-2.24899300
C	3.72291100	-3.36932400	-0.70886300

C	3.64177600	-2.05420300	-2.72457800
C	4.26173000	-3.02710400	-1.94719400
H	4.19529800	-4.14503700	-0.10996900
H	4.04776800	-1.78974600	-3.69765000
H	5.15667900	-3.52681500	-2.30694600
H	2.03224500	-0.63102400	-2.85065100
N	0.83272100	-4.04496500	0.95353400
H	0.74621300	-4.71736900	1.70114000
C	-0.44088600	-3.75098000	0.44718100
O	-1.37488300	-4.45319300	0.83600100
O	-0.58260300	-2.79879200	-0.42638800
C	2.57641100	-2.73721400	-0.22887200
C	1.95277600	-3.12752700	1.08878300
H	2.69951000	-3.63552400	1.70796600
H	1.66423900	-2.20864100	1.62873000

**TSB6**

Pd	-0.14977700	-1.00060800	-0.38406700
P	2.07331900	-0.12471600	-0.21587400
P	-1.45339500	0.98685300	0.15217400
C	2.06350400	3.23584600	2.15660800
H	1.79546500	4.28313600	2.05182400
C	-4.04344300	0.00460000	0.37099200
H	-3.66204500	-0.49364400	1.25762600
C	-3.70445400	1.45644900	-1.52249100
H	-3.06947200	2.10717100	-2.11559000
C	2.01277900	0.26822600	-2.96265000
H	1.36030600	-0.60152100	-2.94936300
C	-0.71405200	0.80819300	2.82771300
H	0.01934300	0.06553500	2.51760000
C	3.34635900	1.89480600	-1.79323700
H	3.75335700	2.30157900	-0.87290700
C	2.50632100	0.77797800	-1.75647300
C	-2.58243300	2.28226100	2.38719600
H	-3.29773000	2.71515800	1.69243800
C	3.66378800	2.50103100	-3.00589000
H	4.31146800	3.37263300	-3.01585700
C	3.22652900	-2.59608900	0.44557900
H	2.23766200	-2.93658200	0.74549500
C	-0.86818900	3.77139100	-0.06798700
H	-1.21537400	3.88643400	0.95324800
C	3.45508600	-1.31503700	-0.05761300
C	-2.65583400	2.59542400	3.73847600
H	-3.41772500	3.28384500	4.09222800
C	-0.88741200	2.51526400	-0.67981700

C	-1.75959700	2.01660900	4.63877100
H	-1.82585200	2.25573700	5.69638000
C	1.98846100	2.39722900	1.04955300
H	1.66217500	2.80478600	0.09941000
C	5.58646900	-3.08994100	0.26492100
H	6.41490800	-3.78183600	0.38872300
C	4.75872100	-0.92493700	-0.39683900
H	4.95187500	0.06635700	-0.79481500
C	-5.36607600	-0.18414700	-0.00812800
H	-6.00675800	-0.83013700	0.58427900
C	2.32551000	1.04471700	1.16381300
C	3.15988500	1.99072200	-4.19850600
H	3.41003300	2.46392100	-5.14348700
C	-3.20154200	0.83133700	-0.37969100
C	4.29653600	-3.47601100	0.60615900
H	4.10138600	-4.46465300	1.00918900
C	-1.59934600	1.39594400	1.92206300
C	2.80596400	1.38304400	3.50498100
H	3.11204300	0.97729400	4.46431200
C	-5.02960700	1.26034500	-1.90409300
H	-5.41088500	1.75525600	-2.79244700
C	-5.86289100	0.44248800	-1.14819300
H	-6.89687700	0.29305900	-1.44463900
C	-0.80017200	1.12003900	4.18366600
H	-0.11129400	0.64121600	4.87208800
C	2.33747700	0.86630300	-4.17515900
H	1.94653700	0.45456600	-5.10088400
C	2.73063300	0.53706300	2.40298000
H	2.92391100	-0.52343400	2.52326700
C	-0.35779900	4.87267000	-0.74881500
H	-0.33395900	5.84188100	-0.25949400
C	-0.40210400	2.38693300	-1.98465100
H	-0.39325500	1.41032800	-2.46007600
C	2.47468700	2.73033400	3.38640700
H	2.52742900	3.38318600	4.25288500
C	5.81683700	-1.80941000	-0.23836100
H	6.82258900	-1.49987200	-0.50761100
C	0.10435800	3.48808300	-2.66715100
H	0.50371600	3.36097500	-3.66828600
C	0.13405100	4.73284900	-2.04504100
H	0.54543500	5.59243800	-2.56565800
C	-1.78681800	-2.24724200	-1.06269300
C	-2.32475700	-1.92101100	-2.31024600
C	-3.83569200	-3.33357300	-0.46533100

C	-3.63117100	-2.27619000	-2.62490900	H	-5.40280900	-1.56264400	3.70652100
C	-4.38172400	-2.99522100	-1.69933600	C	-2.73197700	1.17043800	0.29991400
H	-4.43597700	-3.88447200	0.25550800	C	-4.02164900	-3.17580900	3.35110100
H	-4.05730400	-1.99725600	-3.58340100	H	-4.46075300	-3.82261700	4.10532700
H	-5.40288200	-3.28162800	-1.93344000	C	1.61422500	3.16082000	2.06606900
H	-1.71962900	-1.38573200	-3.03702300	H	2.12744100	3.74418000	1.30632600
N	-1.08124200	-2.34663200	1.79334600	C	5.79329300	1.51409000	-0.75158500
H	-1.48112100	-1.70835700	2.46775500	H	6.86206700	1.55875400	-0.93924600
C	0.28315000	-2.72507300	2.12177000	C	3.94882600	1.06491400	0.73526200
O	0.91000800	-1.87079000	2.78605600	H	3.58987900	0.74367200	1.70902500
O	0.66979300	-3.80442300	1.62777200	C	-2.68482600	-1.69426000	-3.77144300
C	0.08888500	-2.71777600	-1.16665200	H	-2.07365200	-1.81580500	-4.66082800
O	0.48674200	-3.67567500	-1.66744500	C	1.09637300	1.90016300	1.74410400
C	-2.53813900	-2.95802900	-0.11590700	C	-0.93311200	3.88195900	-2.99280000
C	-1.97467500	-3.33631400	1.24116300	H	-1.45455600	4.48662800	-3.72921200
H	-2.80742400	-3.56116600	1.92114800	C	-2.86589500	-1.11830200	-1.42712200
H	-1.37520000	-4.24979200	1.13594400	C	4.89165300	1.83647300	-1.76193300
<b>TSB7</b>				H	5.25356500	2.13450100	-2.74149100
Pd	0.35486800	-0.93576100	-0.20694200	C	-2.88936000	-1.50766500	1.41663900
P	1.24408000	1.18294900	0.06797100	C	0.38096000	1.63485100	4.04325800
P	-2.05988800	-0.52562700	0.11125600	H	-0.08615800	1.02944300	4.81433100
C	1.48998000	3.66370300	3.35614700	C	-4.82420400	-1.81776400	-2.66602200
H	1.88824400	4.64556300	3.59398500	H	-5.88803800	-2.03468700	-2.69449300
C	-2.09337300	-1.27548600	-2.58164800	C	-4.04903000	-1.96444700	-3.81531000
H	-1.02302200	-1.08546500	-2.54931600	H	-4.50897300	-2.29574600	-4.74191600
C	-4.23579600	-1.39727100	-1.47861300	C	-2.93001600	-3.61434200	2.60376700
H	-4.84308700	-1.28957900	-0.58396000	H	-2.51757400	-4.60500000	2.77212000
C	-0.12020200	3.57163000	-0.73982700	C	-0.78369600	4.34421200	-1.68970900
H	-0.04666400	3.93251700	0.28019600	H	-1.19976200	5.30462700	-1.40048000
C	-2.35969300	-2.78523600	1.64360600	C	0.49700200	1.13567400	2.74764200
H	-1.51066900	-3.11863600	1.04585900	H	0.12348900	0.14233300	2.50845100
C	0.23272400	1.85559000	-2.40056400	C	-2.96176600	3.15851800	1.67259500
H	0.61817200	0.87495000	-2.67509900	H	-2.81583000	3.65611500	2.62693400
C	0.40450500	2.32764700	-1.09046000	C	-3.30972000	1.86318200	-0.76727000
C	-3.98942300	-1.07519800	2.16195300	H	-3.43795500	1.37507700	-1.72782500
H	-4.40848100	-0.08733600	1.99360900	C	0.86744700	2.90288200	4.34512400
C	-0.42571200	2.63342400	-3.34631300	H	0.77638800	3.29471700	5.35399500
H	-0.54968400	2.25795700	-4.35771200	C	5.31700800	1.12857200	0.49916800
C	3.52011800	1.78387200	-1.52431500	H	6.01078400	0.86180400	1.29070300
H	2.83136700	2.04345300	-2.32141400	C	-3.71653000	3.18577500	-0.61189600
C	-2.55726500	1.83773800	1.51921800	H	-4.15999500	3.70979200	-1.45337300
H	-2.10742500	1.32080400	2.36081100	C	-3.54666000	3.83683800	0.60544200
C	3.03615200	1.40385700	-0.27056000	H	-3.86346400	4.86925900	0.72216500
C	-4.54980400	-1.90717900	3.12883700	C	1.85764300	-1.68950700	-1.29829500

O	1.87499000	-1.35455900	-2.46709500	C	2.08653200	2.22683900	0.27907600
C	2.95424000	-2.38499500	-0.58181000	C	5.94287100	0.23713300	-2.93802200
C	2.61935700	-3.44120000	0.25961800	H	6.82650900	0.16043900	-3.56486600
C	4.27468800	-1.95006300	-0.70261500	C	-3.74431500	2.82512600	-0.20543400
C	3.61734100	-4.04820100	1.01802500	H	-4.56600300	2.13915700	-0.01923400
C	5.26479000	-2.55996300	0.05806500	C	-5.91644200	-1.48473800	-1.78543900
C	4.93473000	-3.60695300	0.92006700	H	-6.80194700	-1.97148900	-2.18368400
H	3.36650200	-4.87662300	1.67739100	C	-3.88451700	-0.23414400	-2.13130100
H	6.29304900	-2.21838400	-0.01861500	H	-3.17452900	0.23903600	-2.80603500
H	5.71001900	-4.08692600	1.51108600	C	1.88424200	-1.53517700	3.26321900
H	4.50866500	-1.12744700	-1.37209600	H	1.07815700	-1.75996500	3.95320700
N	0.29733100	-3.02565900	-0.52550900	C	-2.44731400	2.32898300	-0.37938900
H	0.13426800	-3.38535400	-1.45806800	C	-1.66394500	-0.14456600	4.35082400
C	1.16164200	-3.87530500	0.25794600	H	-1.52279500	-0.31613900	5.41413000
H	0.81341800	-3.90796400	1.30264700	C	2.62649600	-0.47718300	1.20502400
H	1.11327700	-4.91072000	-0.11081300	C	-5.66549400	-1.49968500	-0.41718300
<b>IntB12</b>				H	-6.35677900	-1.99616300	0.25780900
Pd	0.03268700	-0.11174900	-0.99369300	C	3.66537400	0.44056600	-1.32108500
P	-2.04714400	0.54230200	-0.22150500	C	-1.64543800	4.59513300	-0.67218400
P	2.13770000	0.47655700	-0.29965000	H	-0.81902400	5.27679600	-0.84895000
C	-3.98828600	4.19299900	-0.26987400	C	4.16870400	-1.78328000	2.54382100
H	-4.99927400	4.56757200	-0.13726500	H	5.16650500	-2.18645800	2.69275700
C	1.61774700	-0.77311000	2.13151700	C	3.16302800	-2.04705300	3.47148100
H	0.60363100	-0.42982300	1.95097500	H	3.37151200	-2.65915100	4.34408100
C	3.90599000	-0.99825600	1.42183500	C	4.78042600	-0.44394000	-3.28499300
H	4.70390900	-0.80829800	0.71146000	H	4.75173600	-1.05129500	-4.18489600
C	-1.94874800	1.38277400	2.49695800	C	-1.76896100	1.15409600	3.86031500
H	-2.02270100	2.40172600	2.13016400	H	-1.71255700	1.99893000	4.54111800
C	3.64699200	-0.33659800	-2.48172600	C	-1.40174700	3.22515800	-0.61831400
H	2.72745300	-0.84883300	-2.75669800	H	-0.39363300	2.84459600	-0.75687200
C	-1.88891500	-0.99194100	2.10765400	C	2.15761900	4.58959500	-0.26858400
H	-1.88425600	-1.83676500	1.42793400	H	2.38309800	5.37707300	-0.98227500
C	-2.01391800	0.30921100	1.60409200	C	1.58803700	2.55791700	1.54310500
C	4.83944300	1.12712600	-0.98520500	H	1.34691400	1.77874200	2.25874300
H	4.86370800	1.74618000	-0.09230200	C	-2.93829000	5.08049900	-0.50053000
C	-1.72865600	-1.22212000	3.46893800	H	-3.13083500	6.14865600	-0.54811800
H	-1.61892200	-2.24395400	3.81851400	C	-5.02495700	-0.83992600	-2.64324200
C	-4.53142500	-0.87165800	0.09774200	H	-5.21390800	-0.82163100	-3.71281500
H	-4.35279200	-0.88392900	1.16847800	C	1.37719100	3.88742900	1.89516900
C	2.36217900	3.25958300	-0.62505400	H	0.98436800	4.12310600	2.87993500
H	2.73548300	3.02535900	-1.61829000	C	1.66179000	4.90862200	0.99303100
C	-3.62575200	-0.23895300	-0.75479100	H	1.49435900	5.94546600	1.26931300
C	5.97005300	1.02637800	-1.78854700	C	0.21553800	-3.82249200	1.07581100
H	6.87432400	1.56421900	-1.51903700	O	-0.25098400	-3.99544300	2.18992700

C	-0.51671300	-3.57716600	-0.19787100
C	0.40105600	-3.24714000	-1.18744000
C	-1.88466400	-3.58757200	-0.43840500
C	-0.03752600	-2.86793900	-2.45195400
C	-2.32882700	-3.22228600	-1.70393400
C	-1.41267700	-2.84922800	-2.69285800
H	0.66428200	-2.59588000	-3.23556600
H	-3.39237100	-3.19613600	-1.91908500
H	-1.77958200	-2.53921900	-3.66679900
H	-2.57924400	-3.86137700	0.35026500
N	1.54534400	-3.78394000	0.74008800
H	2.24035000	-3.66679300	1.46355400
C	1.79743700	-3.38550200	-0.63305300
H	2.35524000	-2.44513000	-0.67964100
H	2.37081300	-4.15100800	-1.17203400

**prodB2**

C	-1.59059300	-0.56217900	0.00003600
O	-2.27984900	-1.56337000	0.00002100
C	-0.10316300	-0.45429700	0.00012400
C	0.25967000	0.88716000	0.00012300
C	0.84239500	-1.46978200	-0.00003700
C	1.59846800	1.25476500	0.00002500
C	2.18623900	-1.10694400	-0.00004100
C	2.55711400	0.24170200	-0.00003900
H	1.89881500	2.29893400	0.00006500
H	2.95527200	-1.87335900	-0.00009200
H	3.61089000	0.50465300	-0.00007800
H	0.52710800	-2.50845900	-0.00003300
N	-2.03392600	0.73914400	-0.00013300
H	-3.01787300	0.95372800	-0.00011700
C	-0.98666400	1.74117700	-0.00001200
H	-1.03923400	2.38391100	-0.88826500
H	-1.03949600	2.38393000	0.88820900

**TSB8**

Pd	0.24248600	-1.12813300	0.02314900
P	-2.02117300	-0.24188900	0.08236500
P	1.48105200	0.85149700	-0.12775000
C	-2.20816200	3.80114900	-0.63782700
H	-1.87559300	4.70001000	-0.12725600
C	3.99242100	-0.03549500	-0.88325800
H	3.45291100	-0.51660800	-1.69423200
C	3.99238600	1.32689400	1.10868100
H	3.46484400	1.92534200	1.84506000
C	-1.98167900	-0.95955800	2.76563200

H	-1.23256900	-1.67711300	2.43974700
C	0.30866000	1.40271100	-2.60018700
H	-0.34241100	0.56956700	-2.35882900
C	-3.52809500	0.82031900	2.25375600
H	-3.99430200	1.49057200	1.53806100
C	-2.56492700	-0.09971400	1.82763900
C	2.20779500	2.78701600	-2.06174700
H	3.03772600	3.03495000	-1.40530100
C	-3.88467100	0.89463200	3.59731300
H	-4.62798900	1.61891800	3.91714000
C	-2.91528000	-1.94218800	-1.91774500
H	-1.92824500	-1.76745000	-2.33926900
C	1.02773700	3.43085000	1.03010400
H	1.39493800	3.87161800	0.10934500
C	-3.25233900	-1.35378000	-0.69412200
C	2.04164000	3.47946600	-3.25545300
H	2.73022100	4.27754600	-3.51685800
C	0.98331900	2.04166700	1.17763700
C	1.00040200	3.14203000	-4.11895600
H	0.87121400	3.68427600	-5.05113000
C	-2.04097700	2.56731000	-0.01959800
H	-1.59905300	2.52712300	0.96968800
C	-5.07156800	-3.01525200	-2.01261300
H	-5.77689000	-3.66668800	-2.52000500
C	-4.50611100	-1.60768300	-0.13453600
H	-4.77760800	-1.16606500	0.81934300
C	5.36011000	-0.22754700	-0.75516000
H	5.88563300	-0.84870600	-1.47357400
C	-2.44716400	1.38899000	-0.65614100
C	-3.29139800	0.04379300	4.52633300
H	-3.56932400	0.10423600	5.57460100
C	3.29762000	0.73949600	0.05243300
C	-3.82408400	-2.76251500	-2.57770600
H	-3.55147700	-3.21683000	-3.52563200
C	1.32495600	1.75682800	-1.71215800
C	-3.22105300	2.71648400	-2.52977500
H	-3.69134700	2.76755700	-3.50750700
C	5.36762300	1.13530600	1.23283200
H	5.90107900	1.59273000	2.06099500
C	6.05068300	0.35586600	0.30670400
H	7.11984300	0.19688900	0.41217700
C	0.14037400	2.09855400	-3.79414100
H	-0.66315700	1.81942200	-4.46859500
C	-2.34512400	-0.88848000	4.10684700



H	-1.88444500	-1.56126600	4.82387500	C	0.51441300	1.39915800	-2.59886200
C	-3.05213700	1.47962600	-1.91381300	H	-0.17520000	0.59586700	-2.36199400
H	-3.39113500	0.58284500	-2.42255400	C	-3.33942600	1.23318400	2.12655400
C	0.55405200	4.25904100	2.04345700	H	-3.67509500	1.94530600	1.37947900
H	0.58161500	5.33706800	1.91332200	C	-2.56794000	0.12973500	1.75121500
C	0.47725200	1.50105900	2.36434000	C	2.41652200	2.75685200	-2.00956100
H	0.41864500	0.42189500	2.47355100	H	3.22362800	3.00251300	-1.32439300
C	-2.79042200	3.87984400	-1.89961800	C	-3.67243300	1.43635500	3.46337500
H	-2.91423500	4.84284500	-2.38588300	H	-4.26641900	2.30141400	3.74361100
C	-5.40864000	-2.44017800	-0.79051200	C	-3.00994300	-2.09712700	-1.74512100
H	-6.37728600	-2.64136400	-0.34274900	H	-1.97935100	-2.17273100	-2.07945600
C	-0.00426900	2.32767300	3.37480700	C	1.19009900	3.47399900	1.06423800
H	-0.42692800	1.88614800	4.27218500	H	1.61595400	3.89939300	0.16144100
C	0.02874800	3.71011700	3.21219300	C	-3.33352400	-1.25789800	-0.67624800
H	-0.35827700	4.36002300	3.99148100	C	2.31617100	3.42424100	-3.22486900
C	1.97436900	-2.15138200	0.44798400	H	3.03097100	4.20315900	-3.47354500
C	2.41137200	-3.08627600	-0.48858000	C	1.08681900	2.08711000	1.20797800
C	2.75079700	-1.90861200	1.58436500	C	1.30793500	3.08571300	-4.12629900
C	3.65371500	-3.70554800	-0.32042700	H	1.23079800	3.60816600	-5.07540500
C	3.98268900	-2.53316400	1.75246300	C	-1.81688000	2.59342800	-0.33538400
C	4.44616300	-3.42293000	0.78497800	H	-1.36363200	2.60931000	0.64900800
H	3.99194800	-4.43049600	-1.05952200	C	-5.30857200	-2.80710500	-1.90201100
H	4.58544000	-2.31451700	2.62987200	H	-6.07632200	-3.41317700	-2.37420100
H	5.41212700	-3.90639700	0.90187900	C	-4.65377700	-1.20358700	-0.22253700
H	2.41545600	-1.19622400	2.33422700	H	-4.91477700	-0.56237000	0.61421900
C	-0.43236700	-3.16268500	-0.03771400	C	5.42383000	-0.32864000	-0.64187600
O	-0.80951600	-4.29949200	-0.07175400	H	5.94713100	-0.93591200	-1.37371300
C	1.52119300	-3.48685800	-1.64751200	C	-2.32355000	1.39653500	-0.85504200
H	1.99009000	-3.19242700	-2.59853800	C	-3.24583800	0.53465400	4.43419100
H	1.45289700	-4.58773100	-1.65183400	H	-3.50409600	0.69518800	5.47717800
N	0.19674300	-2.87801900	-1.54167700	C	3.37316300	0.67976000	0.15063800
H	-0.43164100	-3.41092500	-2.14279000	C	-3.99509600	-2.86521100	-2.35864800
<b>IntB13</b>				H	-3.73096100	-3.51983200	-3.18376100
Pd	0.21672200	-1.16474700	0.07702600	C	1.49871900	1.75292500	-1.67470600
P	-2.02346200	-0.19008100	0.02812600	C	-3.00615500	2.60101700	-2.84415600
P	1.56609800	0.86639000	-0.07320500	H	-3.47959100	2.59778200	-3.82181300
C	-1.89294200	3.77414900	-1.06449100	C	5.42088300	0.93927200	1.40759900
H	-1.48330600	4.68691300	-0.64213400	H	5.94554600	1.33797400	2.27102000
C	4.06698500	-0.08377700	-0.79528800	C	6.10383300	0.18020800	0.46396900
H	3.53449500	-0.51449700	-1.63878400	H	7.16360300	-0.02078900	0.59067400
C	4.05834100	1.19129100	1.25205500	C	0.41314200	2.06726300	-3.81594600
H	3.53189900	1.78050400	1.99703300	H	-0.36796500	1.78959600	-4.51664600
C	-2.16044500	-0.78850200	2.72820800	C	-2.49887700	-0.58144600	4.06189600
H	-1.61000800	-1.67960300	2.43179800	H	-2.17998700	-1.30000800	4.81106100

C	-2.92950000	1.41677800	-2.11544200	H	-0.20467900	1.19268500	-2.32590000
H	-3.34123600	0.50483800	-2.53643500	C	-3.34532600	1.05317800	2.20886800
C	0.70132300	4.31942500	2.05559100	H	-3.71428100	1.80923200	1.52263200
H	0.77392600	5.39576400	1.92863700	C	-2.56818400	-0.00700400	1.73377400
C	0.50729000	1.56582300	2.37001500	C	2.72211800	2.83675400	-1.81532100
H	0.40082300	0.48975700	2.48128200	H	3.55668700	2.87682800	-1.12029000
C	-2.48107600	3.78098600	-2.32610900	C	-3.63497200	1.16231700	3.56656400
H	-2.53355900	4.70113800	-2.90031100	H	-4.23201300	1.99661000	3.92348700
C	-5.63557400	-1.97842000	-0.83102900	C	-3.15461300	-2.18390900	-1.68419700
H	-6.65755700	-1.93721400	-0.46602700	H	-2.11756800	-2.39050100	-1.93419200
C	0.01563800	2.41065500	3.36073100	C	1.23198600	3.42067000	1.20822200
H	-0.46312000	1.98539700	4.23722800	H	1.67448700	3.88869800	0.33458100
C	0.10647600	3.79017000	3.20022900	C	-3.45544600	-1.21093000	-0.72934800
H	-0.29062200	4.45432700	3.96224300	C	2.71766600	3.65162900	-2.94233600
C	1.88968100	-2.34960900	0.29553400	H	3.54419100	4.33381000	-3.11925700
C	2.10968000	-3.36742800	-0.63973600	C	1.11417400	2.02964100	1.27423200
C	2.83446400	-2.17220200	1.30785400	C	1.65605400	3.59032400	-3.84427800
C	3.28414700	-4.11661500	-0.62098100	H	1.65395500	4.22842800	-4.72347700
C	4.00241500	-2.93457200	1.34636500	C	-1.87392400	2.58678400	-0.18791000
C	4.24256100	-3.89180600	0.36630300	H	-1.41144400	2.53157400	0.79148900
H	3.44370900	-4.89502500	-1.36564300	C	-5.50263800	-2.68138000	-1.93615000
H	4.73132200	-2.76499700	2.13450300	H	-6.29945200	-3.25290200	-2.40360100
H	5.15691600	-4.47866500	0.38266600	C	-4.79081400	-0.98444000	-0.37694700
H	2.68639200	-1.40746200	2.06677900	H	-5.03508600	-0.23641700	0.37204700
C	-0.61326500	-3.02663700	0.18386200	C	5.36134400	-0.55578600	-0.55845500
O	-1.39855200	-3.37707200	1.05364900	H	5.87835000	-1.13650400	-1.31629900
C	0.96771800	-3.67864000	-1.58645500	C	-2.38910000	1.43055200	-0.78702200
H	0.82318800	-2.85922100	-2.30216400	C	-3.16003700	0.20752800	4.46118000
H	1.16285700	-4.58473100	-2.16809700	H	-3.38279200	0.29587200	5.52081800
N	-0.27419300	-3.88400300	-0.84242400	C	3.34662200	0.53297200	0.22279500
H	-0.51592100	-4.84852300	-0.64020800	C	-4.17729900	-2.91452200	-2.28691600
<b>TSB9</b>				H	-3.93274000	-3.67227900	-3.02556800
Pd	0.15572700	-1.08231100	-0.10552100	C	1.66040300	1.95541600	-1.57494800
P	-2.08411200	-0.21639800	-0.02749200	C	-3.05320100	2.76918600	-2.69633100
P	1.57689700	0.88869300	-0.08713000	H	-3.52075100	2.83440100	-3.67472700
C	-1.94630600	3.81484400	-0.83452800	C	5.34396700	0.53944500	1.58677700
H	-1.53149300	4.69483000	-0.35200900	H	5.85145200	0.82963100	2.50232600
C	4.03101500	-0.20839800	-0.74706500	C	6.02173000	-0.18393200	0.61138600
H	3.51250900	-0.53046500	-1.64634200	H	7.06050700	-0.46247100	0.76331400
C	4.01145700	0.90048000	1.39312000	C	0.60606200	2.70517800	-3.62159600
H	3.49205900	1.47017000	2.15810200	H	-0.22327200	2.64880000	-4.31993200
C	-2.10784200	-0.97579800	2.63599000	C	-2.40468600	-0.86519600	3.99114100
H	-1.52933300	-1.82445800	2.27357100	H	-2.04371900	-1.62221300	4.68118100
C	0.61238300	1.88662700	-2.49550500	C	-2.98424000	1.53780500	-2.04847100

H	-3.39552800	0.65623100	-2.53124300
C	0.74384400	4.21623000	2.24137700
H	0.83009900	5.29697800	2.17339400
C	0.51784300	1.45245300	2.40130500
H	0.39318600	0.37390800	2.44989400
C	-2.53163200	3.91053400	-2.09423100
H	-2.58155400	4.86864000	-2.60288700
C	-5.80844000	-1.71669500	-0.97645500
H	-6.84206600	-1.53649100	-0.69586500
C	0.02928000	2.24613600	3.43425300
H	-0.46122500	1.77826200	4.28232900
C	0.13572700	3.63213800	3.35097400
H	-0.25969800	4.25788100	4.14579700
C	1.61747500	-2.61520700	0.19143700
C	2.10918500	-3.32551000	-0.90486600
C	2.41724700	-2.49222300	1.33316300
C	3.40764000	-3.82285800	-0.91554700
C	3.71193100	-3.00234800	1.33532700
C	4.21447100	-3.65023200	0.20743900
H	3.77545300	-4.37983200	-1.77493100
H	4.33730500	-2.88351800	2.21535500
H	5.22513300	-4.04840100	0.21514600
H	2.03698300	-1.98377200	2.21494600
C	-0.24791500	-3.11058300	0.04462200
O	-0.90200800	-3.56071900	0.97170700
C	1.04463900	-3.63487300	-1.93760800
H	0.98693600	-2.85411800	-2.70590900
H	1.24478400	-4.58191600	-2.44794100
N	-0.22471500	-3.73758800	-1.21399000
H	-0.59946200	-4.67845400	-1.14995500

**IntB14**

Pd	-1.30765700	0.43391000	-0.09002900
P	1.08506900	-0.01147300	-0.00984000
C	0.78460800	-0.86986100	2.61419600
H	0.00451500	-0.11327200	2.65856100
C	2.46796400	-2.06559800	1.36239000
H	3.00742200	-2.24097900	0.43642700
C	0.95223300	-1.93411800	-2.00315800
H	-0.01289100	-2.14591100	-1.54115400
C	2.99017700	-0.62415700	-2.01979800
H	3.60834100	0.16700200	-1.60654900
C	2.09962000	2.45756200	-0.76938500
H	1.37639600	2.38109000	-1.57808500
C	3.44832900	-1.35518300	-3.11273800

H	4.41915600	-1.12768800	-3.54306900
C	2.21101000	1.42209800	0.16733800
C	2.66452900	-2.37236800	-3.65064300
H	3.02362300	-2.93995500	-4.50437100
C	1.07476200	-1.63545700	3.73900500
H	0.52581700	-1.46948200	4.66089100
C	1.48253500	-1.07691700	1.41918900
C	1.73948300	-0.90925900	-1.46281900
C	2.75345500	-2.83303700	2.48811800
H	3.51699900	-3.60322400	2.43464100
C	2.05956500	-2.61849200	3.67623100
H	2.28190800	-3.22128800	4.55170900
C	1.42077600	-2.66085200	-3.09306000
H	0.80843200	-3.45468900	-3.51057800
C	2.91755900	3.57763000	-0.68503500
H	2.82306200	4.37137100	-1.41972300
C	3.15178300	1.53160500	1.19348600
H	3.25263500	0.73703400	1.92620800
C	3.96428300	2.66034700	1.28224500
H	4.68963300	2.73705300	2.08670700
C	3.85020600	3.68242300	0.34553200
H	4.48479200	4.56059100	0.41743100
C	-3.34862300	0.37385000	-0.05154000
C	-3.86728100	-0.93085400	-0.16085900
C	-4.24159400	1.43966800	0.09194800
C	-5.24522200	-1.14374700	-0.13519000
C	-5.61886300	1.22026900	0.12256700
C	-6.12200500	-0.07188100	0.00807000
H	-5.63596300	-2.15594900	-0.21931100
H	-6.29705000	2.06196500	0.23637700
H	-7.19429600	-0.24565800	0.03636300
H	-3.87983700	2.46023900	0.18508000
N	-1.50288800	-1.57816600	0.01650000
H	-1.32606200	-1.81355900	0.99253000
C	-2.85520500	-2.02645900	-0.33313100
H	-2.85309000	-2.33780200	-1.38949300
H	-3.12813700	-2.92200000	0.24435300
C	-1.24723900	2.35943900	-0.22601700
O	-1.25250800	3.49932600	-0.27789400

**TSB10**

Pd	-1.19856600	0.03460100	0.15273900
P	1.08453400	0.04615500	0.04810600
C	1.26284300	-0.46281400	2.77094900
H	0.44508300	0.25033200	2.84592600

C	2.81989100	-1.72242200	1.42175600
H	3.22240800	-1.99267700	0.45018400
C	1.01271500	-2.09251300	-1.70909000
H	0.12327800	-2.38068500	-1.13720000
C	2.81817500	-0.52194200	-2.11558200
H	3.34468300	0.39503500	-1.86886800
C	1.40663700	2.70145300	-0.72705400
H	0.41875200	2.59550700	-1.16438900
C	3.26284000	-1.30916700	-3.17429200
H	4.13279700	-1.00050800	-3.74643000
C	1.98281300	1.63661600	-0.02775300
C	2.59194900	-2.48539100	-3.49832300
H	2.94012600	-3.09741000	-4.32559000
C	1.77965700	-1.05028700	3.91977800
H	1.36825800	-0.79134700	4.89064100
C	1.78408200	-0.79028600	1.51470200
C	1.69508800	-0.91281800	-1.38057100
C	3.33251700	-2.31293300	2.57442200
H	4.13487500	-3.04020700	2.49441100
C	2.81587200	-1.97695400	3.82223600
H	3.21534300	-2.44141600	4.71890500
C	1.47189200	-2.87327600	-2.76587600
H	0.94447200	-3.78769700	-3.02132400
C	2.08911700	3.90792100	-0.85002600
H	1.63244000	4.72931300	-1.39359600
C	3.24401400	1.79856300	0.55576000
H	3.69774200	0.98058700	1.10755300
C	3.92050100	3.00869400	0.43497800
H	4.89737000	3.12750300	0.89417200
C	3.34532200	4.06328200	-0.26978100
H	3.87387500	5.00758400	-0.36146200
C	-3.36397800	0.63174300	-0.12304800
C	-3.77081900	-0.69881800	-0.43052700
C	-4.24407200	1.49723600	0.54339100
C	-5.07892100	-1.06279300	-0.09436000
C	-5.53889700	1.10550700	0.85132000
C	-5.95815000	-0.17965800	0.52082700
H	-5.40421100	-2.07785100	-0.30659600
H	-6.21464700	1.80006900	1.34025300
H	-6.96880800	-0.50071300	0.75651400
H	-3.91924900	2.50565200	0.78276500
N	-1.68104000	-2.04290600	-0.01025200
H	-2.07439700	-2.40233900	0.86062100
C	-2.80107100	-1.78250200	-0.92319000

H	-2.38810300	-1.47431900	-1.89628200
H	-3.38704700	-2.69488300	-1.12184800
C	-2.01177400	1.56447800	-0.57873000
O	-2.07639800	2.52766400	-1.25571000

### TSB11

Pd	0.19564800	-0.94480600	-0.33196600
P	1.58509500	0.85894400	0.14864300
P	-2.14445800	-0.07321300	-0.22330400
C	0.32651700	3.99673600	2.53626100
H	0.40618700	5.07982400	2.55859600
C	-3.00454900	-2.36579700	-1.54960700
H	-1.99390600	-2.72720700	-1.38055000
C	-4.70307700	-0.66580700	-1.28321100
H	-5.00593500	0.31561600	-0.92720600
C	0.90361600	2.10910400	-2.24232800
H	0.04677000	1.44317900	-2.22162000
C	-2.57733100	-1.07329000	2.30792800
H	-1.98288600	-1.91003400	1.94501600
C	2.96885400	2.89086600	-1.27186200
H	3.72907000	2.83338900	-0.49796400
C	1.85940200	2.03813900	-1.22592100
C	-3.68586500	1.03578000	1.92910400
H	-3.93753000	1.87018000	1.28199900
C	3.10712900	3.80727600	-2.30926400
H	3.97253300	4.46287000	-2.33731800
C	3.72973700	0.85363900	2.01694400
H	3.06202900	1.35186700	2.71317300
C	-1.95246600	2.72836500	-0.20572500
H	-1.65853700	2.62838700	0.83378300
C	3.28819200	0.53006100	0.73020400
C	-4.17574200	1.00997400	3.23246900
H	-4.80393000	1.82238600	3.58636100
C	-2.35508500	1.60213900	-0.93459100
C	-3.86688500	-0.05358900	4.07582500
H	-4.25083300	-0.07300100	5.09175900
C	0.97366400	3.27861000	1.53463900
H	1.53758100	3.80718800	0.77236000
C	5.89821500	-0.08607400	1.52454900
H	6.91176200	-0.32501400	1.83342500
C	4.16320400	-0.11460100	-0.15045900
H	3.82782200	-0.39512700	-1.14574400
C	-3.93889400	-3.18939900	-2.17704400
H	-3.63995800	-4.17872000	-2.50931800
C	0.86609100	1.88565800	1.48726800

C	2.14066500	3.88097300	-3.31063700
H	2.25098900	4.59711000	-4.11982100
C	-3.38186100	-1.09660400	-1.10570900
C	5.02880700	0.54447100	2.41112500
H	5.36229600	0.80256900	3.41207800
C	-2.86849300	0.00438900	1.46227600
C	-0.53118100	1.94418200	3.46911600
H	-1.13832300	1.41574400	4.19785200
C	-5.62753100	-1.48596400	-1.91642700
H	-6.64932200	-1.14444000	-2.05437600
C	-5.24407500	-2.75034900	-2.36575700
H	-5.96940500	-3.39367500	-2.85569800
C	-3.07629600	-1.10097400	3.60611200
H	-2.84965500	-1.94676000	4.24830500
C	1.03982200	3.03057500	-3.27616100
H	0.28144500	3.07947800	-4.05132000
C	0.11943700	1.22745700	2.46966600
H	0.01267000	0.14680400	2.42695500
C	-1.91773400	3.98398800	-0.80155500
H	-1.59460500	4.84055000	-0.21748500
C	-2.71830200	1.76600200	-2.27656700
H	-3.02819600	0.90661600	-2.86379200
C	-0.43340000	3.33281900	3.49832000
H	-0.95304300	3.89879200	4.26585200
C	5.46263500	-0.41322100	0.24325800
H	6.12489100	-0.92166200	-0.45072300
C	-2.68363300	3.02511400	-2.87051700
H	-2.97295700	3.13390600	-3.91190600
C	-2.28091200	4.13746600	-2.13662500
H	-2.24727600	5.11730600	-2.60343700
C	1.61587100	-2.40308600	-0.84135600
C	1.85299500	-2.40810200	-2.22399600
C	3.80963000	-3.31332600	-0.45231800
C	3.10354300	-2.79854000	-2.69237400
C	4.09103900	-3.25279600	-1.81719900
H	4.55908600	-3.68491300	0.24320800
H	3.29867400	-2.76485600	-3.76105600
H	5.05433000	-3.58032600	-2.19447100
H	1.07132800	-2.10178300	-2.91318800
N	0.92419900	-3.62808000	1.64500100
H	0.67220300	-3.95590800	2.56442000
C	-0.14661200	-3.61975600	0.78816900
O	-1.22773100	-4.07877500	1.12195300
O	0.03955400	-3.13171400	-0.44839000

C	2.58742800	-2.88726700	0.04755600
C	2.20345100	-2.94473300	1.49247800
H	2.95421400	-3.49554900	2.06757200
H	2.14694900	-1.92224200	1.90477100

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Pd	-0.04406600	-0.58746800	-0.81070800
P	1.64348200	0.85193800	-0.11993400
P	-2.23514500	-0.17218100	-0.16589500
C	0.94935400	2.98379300	3.37091000
H	1.02353400	4.01083600	3.71764900
C	-3.42930600	-1.19893900	-2.44890500
H	-2.42142600	-1.10369200	-2.84852100
C	-4.95784600	-0.96536000	-0.60258800
H	-5.15757400	-0.69643400	0.43052300
C	0.53352400	2.91602700	-1.61161000
H	-0.34618200	2.27885100	-1.61045100
C	-1.92913400	-1.79965100	2.05366900
H	-1.23223800	-2.33478000	1.41543600
C	2.83401600	3.29967700	-1.00371700
H	3.75279300	2.97230100	-0.52528300
C	1.70440300	2.47320100	-0.98777900
C	-3.46651300	0.01932600	2.41389800
H	-3.97932300	0.90887700	2.05852600
C	2.78977100	4.54312900	-1.62782500
H	3.67434700	5.17371700	-1.63581000
C	4.12502300	0.22033900	1.15516700
H	3.62632100	0.40394300	2.10239600
C	-1.96756000	2.42621100	0.84091900
H	-1.42858400	1.95462500	1.65719400
C	3.42939900	0.40767200	-0.04225000
C	-3.65365600	-0.40395500	3.72646100
H	-4.32387200	0.14811100	4.37936900
C	-2.57097700	1.63691500	-0.14771600
C	-2.97712000	-1.52478500	4.20496000
H	-3.11769500	-1.84570400	5.23341500
C	1.37859200	2.65839700	2.08591500
H	1.76782300	3.43807600	1.43858400
C	6.11547900	-0.41242000	-0.06221800
H	7.15575400	-0.72445600	-0.06927000
C	4.09709100	0.17032200	-1.25077600
H	3.56345400	0.29955100	-2.18927800
C	-4.46212400	-1.68053300	-3.24984100
H	-4.26413300	-1.95991200	-4.28076000
C	1.27179200	1.34624800	1.61662400

C	1.61415500	4.97984000	-2.23498900
H	1.58045500	5.95257200	-2.71755200
C	-3.66629400	-0.82908400	-1.12139000
C	5.45700800	-0.19296100	1.14514000
H	5.98527300	-0.32770400	2.08511500
C	-2.59943100	-0.67556000	1.56302900
C	0.32252900	0.68809000	3.75192400
H	-0.10850800	-0.08649500	4.37880200
C	-5.98814100	-1.45748500	-1.39729400
H	-6.98579200	-1.56487500	-0.98129900
C	-5.74341500	-1.81257600	-2.72275800
H	-6.54999300	-2.19642500	-3.34071100
C	-2.11350800	-2.22399300	3.36603500
H	-1.55437600	-3.08190300	3.72468600
C	0.48577100	4.16491800	-2.22352600
H	-0.43813900	4.49562300	-2.68828600
C	0.74870700	0.36572700	2.46814300
H	0.63212900	-0.65362900	2.11367800
C	-2.04123100	3.81205700	0.78362900
H	-1.55667400	4.40243800	1.55569300
C	-3.25274700	2.26965200	-1.19028400
H	-3.72996900	1.67739700	-1.96606900
C	0.41416500	2.00308500	4.20284300
H	0.06330800	2.26443500	5.19707700
C	5.43084900	-0.22380200	-1.26289500
H	5.93657300	-0.38927700	-2.21024800
C	-3.32146000	3.66104600	-1.24857000
H	-3.85535900	4.13749400	-2.06620700
C	-2.71429800	4.43610700	-0.26515800
H	-2.76368300	5.51994400	-0.31528100
C	1.06845300	-3.13176200	-0.79735700
C	0.04927800	-2.94747800	-1.73581800
C	2.75093900	-2.63212200	-2.43029800
C	0.41400400	-2.57121000	-3.03407400
C	1.75492100	-2.41704300	-3.38010000
H	3.79751400	-2.50333500	-2.69061900
H	-0.36224400	-2.42318300	-3.77811600
H	2.02313600	-2.13337200	-4.39270900
H	-0.97738000	-3.17732200	-1.47376900
N	2.76052500	-2.89569900	1.24484000
H	3.32592400	-2.65549600	2.04386500
C	1.48118200	-3.23287800	1.54085500
O	1.00406700	-3.24950100	2.65239200
O	0.69788300	-3.55400300	0.46556400

C	2.41240300	-2.97513100	-1.12726800
C	3.41230700	-3.17085800	-0.02481400
H	3.81842300	-4.19391100	-0.04088900
H	4.24695300	-2.47498000	-0.13821900

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C	0.27991300	-0.58291300	0.09305100
C	1.32847000	-1.49263900	0.01361300
C	1.81663800	1.24941200	-0.02754600
C	2.63058400	-1.01679200	-0.07951800
C	2.87882400	0.35510200	-0.10164000
H	2.00226500	2.32041000	-0.04860200
H	3.45436000	-1.72098600	-0.14082300
H	3.89567000	0.72572600	-0.18031200
H	1.10579800	-2.55397400	0.02585900
N	-1.86715000	0.98867700	-0.24894300
H	-2.72491000	1.51166100	-0.34358300
C	-2.09397100	-0.34327600	-0.04263000
O	-3.17673900	-0.86800700	-0.09975900
O	-0.98776100	-1.10572000	0.20864000
C	0.50620300	0.78837700	0.07580600
C	-0.68100800	1.70104500	0.19579100
H	-0.79257900	2.05135900	1.23375700
H	-0.54846500	2.58498800	-0.43630600