Your request submitted on 2024:11:05 at 12:13:33

Project:	**Forbexanthone**
Peaklist:	**Forbexanthone**
Requested by:	**gaetan.herbette@univ-amu.fr**
Requested from:	**78.113.48.9**
Requested via:	13C search

Result from Server - 01:	**Reference spectra:**	**74,435,185**	**Recall details**
Result from Server - 02:	**Reference spectra:**	**107,426,223**	**Recall details**
Result from Server - 03:	**Reference spectra:**	**177,099,966**	**Recall details**
Result from Server - 04:	**Reference spectra:**	**144,833,798**	**Recall details**
Result from Server - 05:	**Reference spectra:**	**111,570,000**	**Recall details**
All Server:	**Reference spectra:**	**615,365,172**	

Original data as given by the user	
Lines:	**164.5** **98.2** **167.2** **93.4** **158.7** **134.3** **148.0** **119.6** **113.3** **115.7** **181.5** **104.3** **147.5** **122.5** **132.2** **78.6** **28.6** **28.6** **56.4**
Selected range for molecular weight	**12.0 to 9999.0 amu**
Number of signals in reference compounds	**1 to 99**
Element: N	**May be present / May be absent**
Element: O	**May be present / May be absent**
Element: P	**May be present / May be absent**
Element: S	**May be present / May be absent**
Element: F	**May be present / May be absent**
Element: Cl	**May be present / May be absent**
Element: Br	**May be present / May be absent**
Element: I	**May be present / May be absent**
Element: other	**Must be absent**
No other significant lines present in reference compounds	
Constraints already used during search	

Remarks on the given input data	
Information:	**The given peaklist holds 19 lines**
Information:	**No signal multiplicities given**
Information:	**Deviation - default setting used**
Information:	**No restriction using number of signals given - default setting used**
Information:	**No restriction using elemental composition given - default setting used**
Information:	**No restriction using molecular weight given - default setting used**
Request accepted - result might be poor More sophisticated usage of restrictions recommended	

Recommendation:	Restrict resulting hitlist by number of signals
Recommendation:	Restrict resulting hitlist by elemental composition
Recommendation:	Restrict resulting hitlist by molecular weight

In order to verify your final structure proposal
[Checking the compatibility of your structure proposal and the experimental ^{13}C-NMR spectral data]
use the CSEARCH-Robot-Referee

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Your request holds too few constraints - Rating of result disabled
A well-defined request follows the rules below

Elemental composition	• P and F must be either absent or present • Unknown presence or absence of up to 5 elements	Recommendation: Select presence / absence of elements in reference compounds F and P are easily seen from NMR, you might know presence / absence of N, Cl and Br from MS N O P S F Cl Br I other Element must be absent: Element may be absent or present: Element must be present:
Molecular weight	Specified range lower/equal 250.0 amu	Recommendation: Limit your result by molecular weight and number of signals in reference compounds Molecular weight from 12 to 9999 Number of signals from 1 to 99 Use constraint for display only Use constraint already during search
Number of signals	Specified range lower/equal 15	

Use more restrictive constraints - Possibility for rating will be activated again

A general overview on selection of constraints is given here

Structures used for linking	
Database	Structures available
PUBCHEM	154,217,198
COCONUT	695,003
LOTUS	276,518
NPASS 2.0	96,235
npatlas 2.0	33,372
NP-MRD	280,096
SuperNatural 3.0	449,008

Summary of result	
Total number of entries shown:	75
Total number of spectra searched:	615,365,172
Total number of links to PUBCHEM:	116
Total number of links to NP-databases:	21
Total CPU-Usage (seconds):	2,305
Total I/O-Usage (MBytes):	10,298

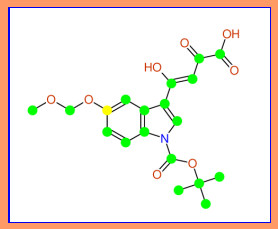
Structure Proposals sorted by Similarity

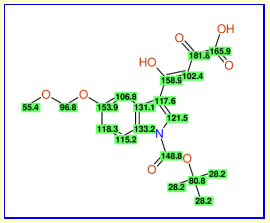
No constraints supplied - Recommendation: restrict by
1) Elemental composition and/or
2) Molecular weight and/or
3) Number of signals in reference

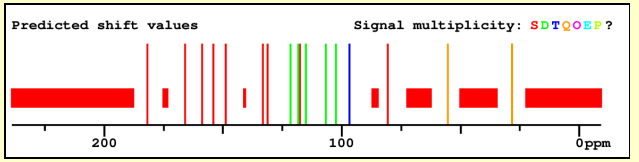
Structure proposal #1 Hide/Show Proposal — Molweight = 391.22 amu — Molecular formula: $C_{19}H_{21}NO_8$

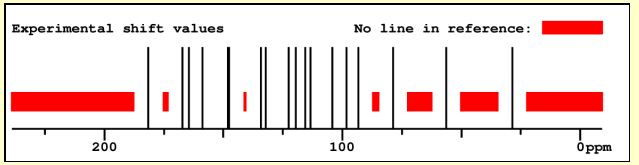
1.55 - 1.56ppm	4x found	ZIP-file	UTHVOLHTYQBNHY

PubChem PubChem PubChem





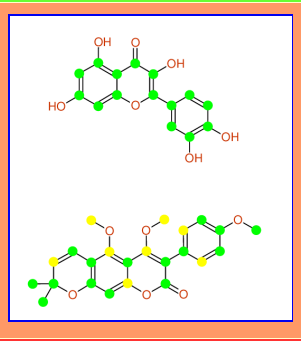


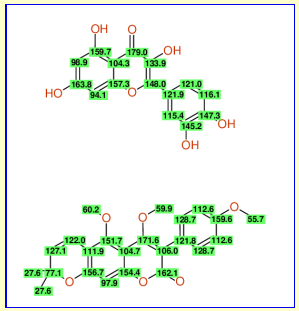


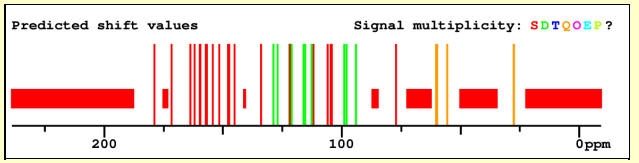
Structure proposal #2 Hide/Show Proposal — Molweight = 696.42 amu — Molecular formula: $C_{23}H_{22}O_6.C_{15}H_{10}O_7$

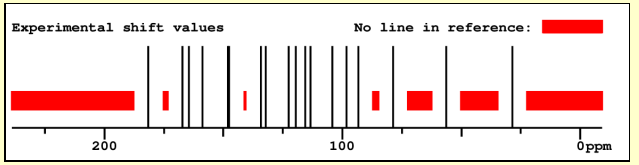
1.69 - 1.69ppm	1x found	ZIP-file	BFRWLXZOFXQFJV

PubChem





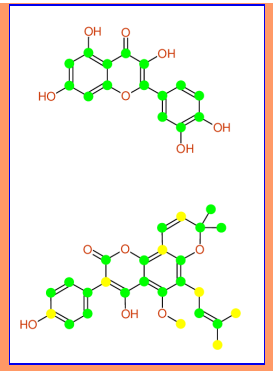


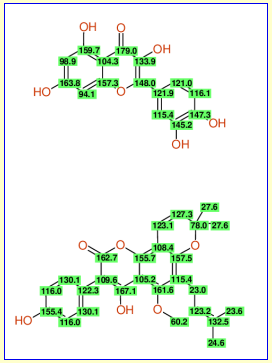


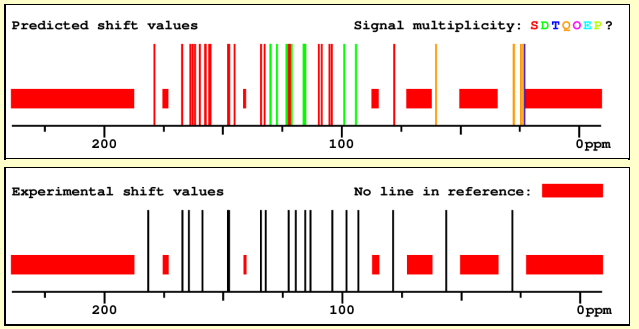
Structure proposal #3 Hide/Show Proposal — Molweight = 736.45 amu — Molecular formula: $C_{26}H_{26}O_6.C_{15}H_{10}O_7$

1.78 - 1.78ppm	1x found	ZIP-file	WIJRQEGGMARRGA

PubChem





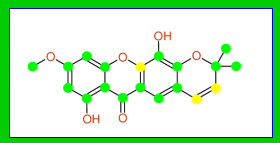


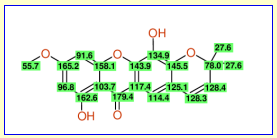
Structure proposal #4 Hide/Show Proposal **Molweight = 340.21 amu** **Molecular formula: $C_{19}H_{16}O_6$**

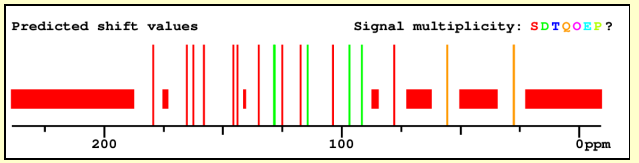
1.82 - 1.82ppm	2x found	ZIP-file	FDTSMQAHJQWMRR

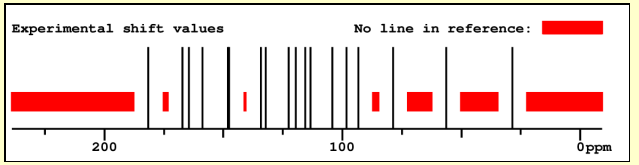
Known Natural Product

PubChem









Structure proposal #5 Hide/Show Proposal **Molweight = 624.31 amu** **Molecular formula: $C_{28}H_{32}O_{16}$**

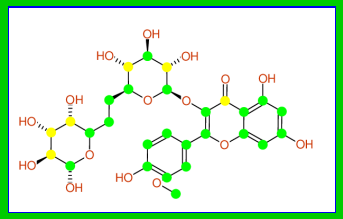
1.82 - 2.28ppm	5x found	ZIP-file	LOVOTONXXBWEEL

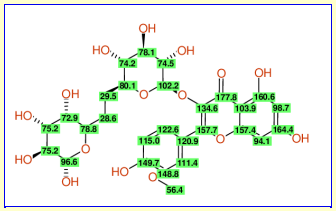
Known Natural Product

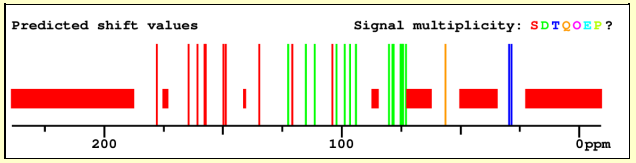
PubChem

PubChem

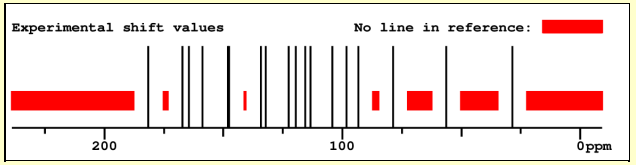
PubChem





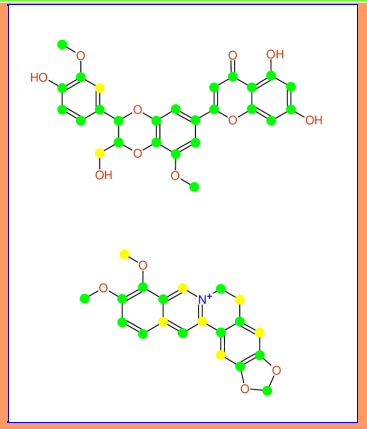


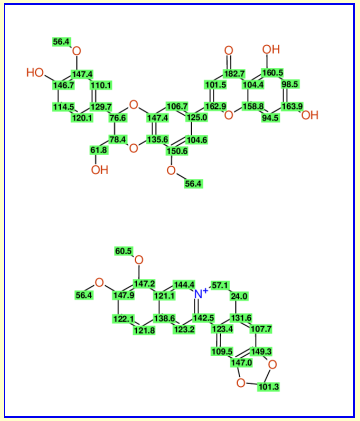
Different spectral pattern

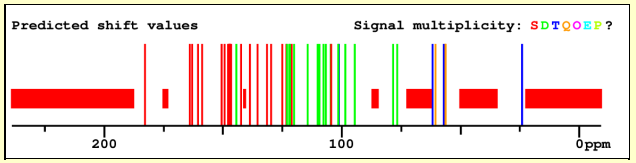


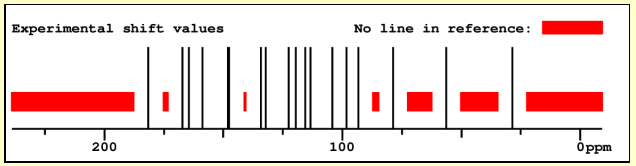
Structure proposal #6 Hide/Show Proposal **Molweight = 830.51 amu** **Molecular formula: $C_{46}H_{40}NO_{14}^{+}$**

1.85 - 1.86ppm **3x found** ZIP-file **BKAQIJPGVWTHRS**







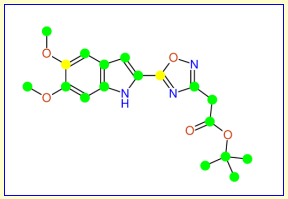


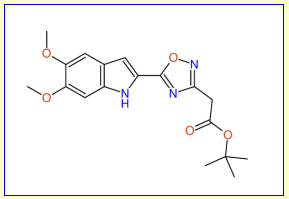
PubChem

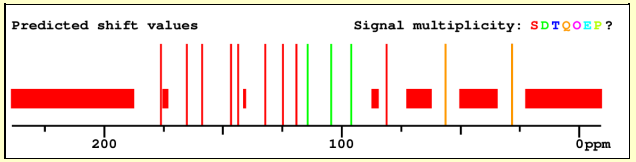
PubChem

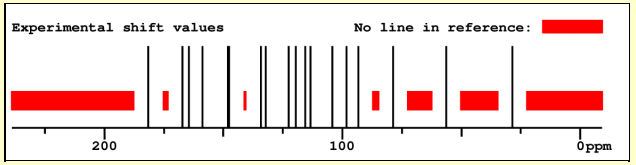
Structure proposal #7 Hide/Show Proposal **Molweight = 359.22 amu** **Molecular formula: $C_{18}H_{21}N_3O_5$**

1.89 - 1.89ppm **1x found** ZIP-file **YNWUVDJAFPSWDM**





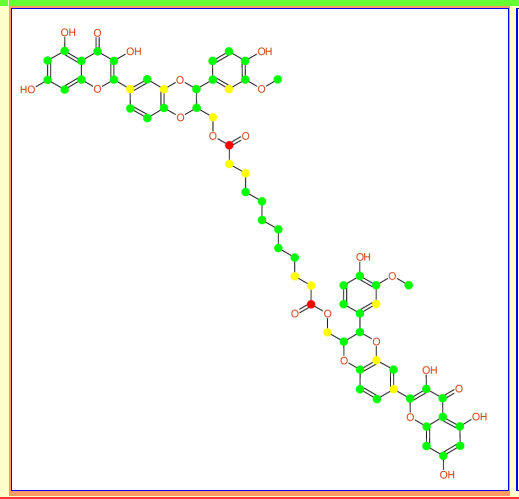


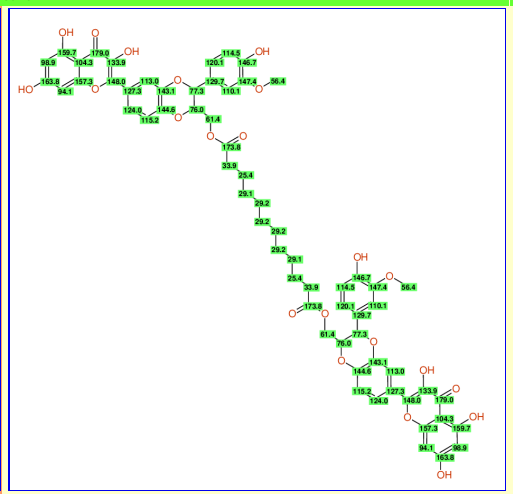


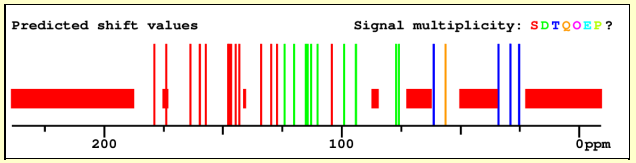
Structure proposal #8 Hide/Show Proposal **Molweight = 1154.68 amu** **Molecular formula: $C_{62}H_{58}O_{22}$**

1.90 - 1.90ppm	1x found	ZIP-file	VAFHCRSYJGMPPG

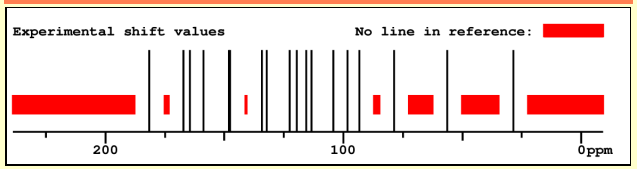
PubChem







Different spectral pattern

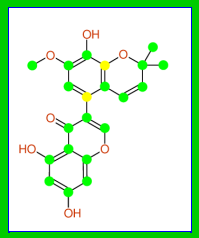


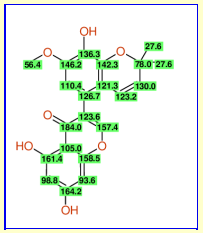
Structure proposal #9 Hide/Show Proposal **Molweight = 382.23 amu** **Molecular formula: $C_{21}H_{18}O_7$**

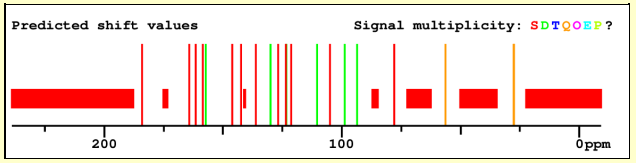
2.00 - 2.00ppm	2x found	ZIP-file	WHEMTMQWUKJLIV

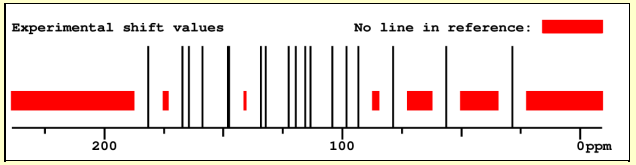
Known Natural Product

PubChem







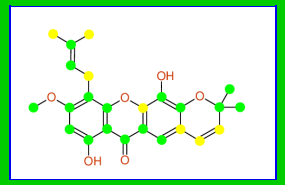


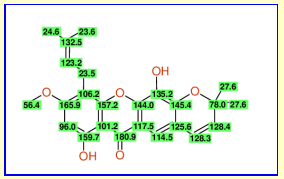
Structure proposal #10 Hide/Show Proposal Molweight = 408.26 amu Molecular formula: $C_{24}H_{24}O_6$

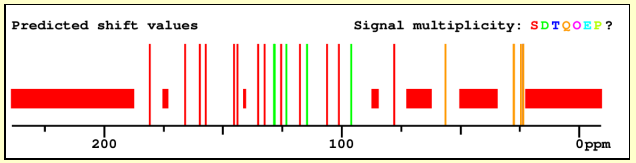
2.02 - 2.02ppm | 2x found | ZIP-file | OCYZJBDJUYIHMM

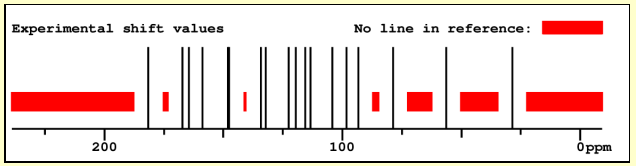
Known Natural Product

PubChem









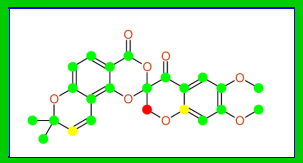
Structure proposal #11 Hide/Show Proposal Molweight = 424.25 amu Molecular formula: $C_{23}H_{20}O_8$

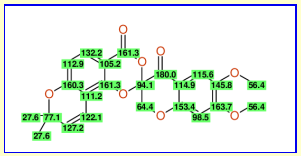
2.03 - 2.03ppm | 1x found | ZIP-file | NZIANEPQOIXOGI

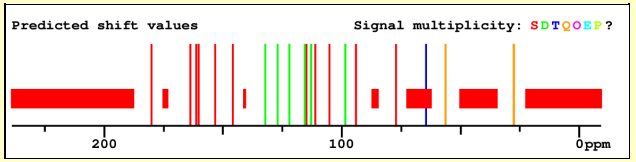
Known Natural Product

PubChem

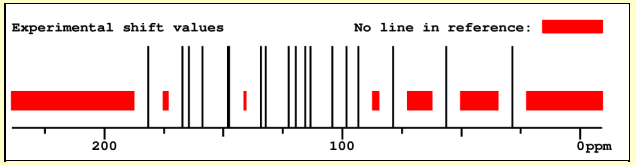
PubChem







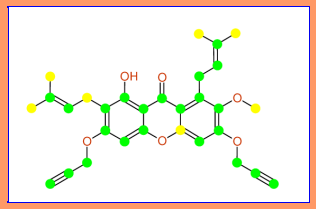
Different spectral pattern

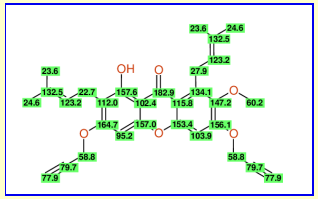


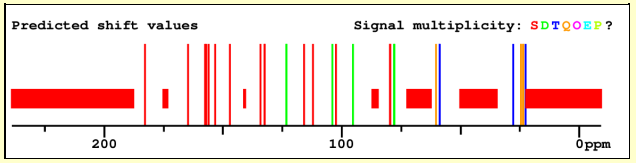
Structure proposal #12 Hide/Show Proposal Molweight = 486.33 amu Molecular formula: $C_{30}H_{30}O_6$

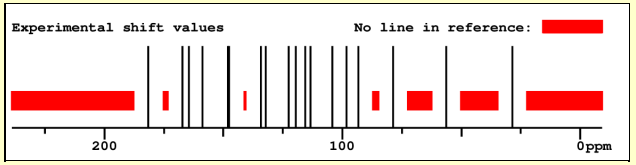
2.06 - 2.06ppm | 1x found | ZIP-file | JDNRLEDQUOYSPS

PubChem





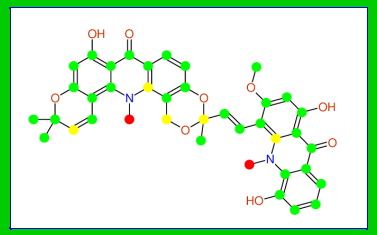


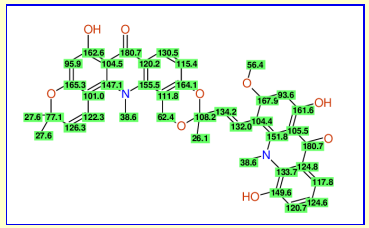


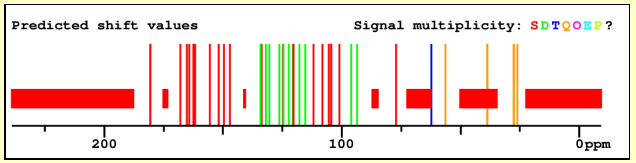
Structure proposal #13 Hide/Show Proposal **Molweight = 674.44 amu** **Molecular formula: $C_{39}H_{34}N_2O_9$**

2.06 - 2.10ppm	2x found	ZIP-file	QHXYPLIKIOHDHQ

Known Natural Product



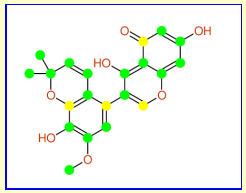


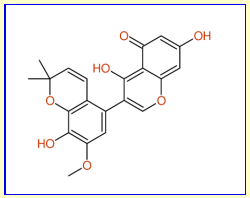


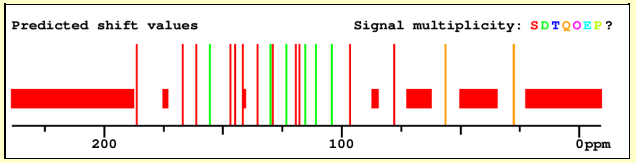
Different spectral pattern

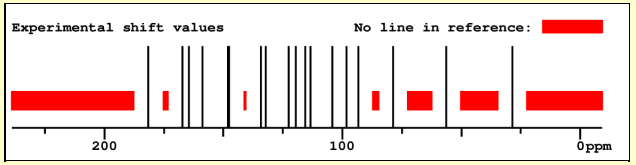
Structure proposal #14 Hide/Show Proposal **Molweight = 382.23 amu** **Molecular formula: $C_{21}H_{18}O_7$**

2.10 - 2.10ppm	1x found	ZIP-file	BMRPPBOVZCXJLM





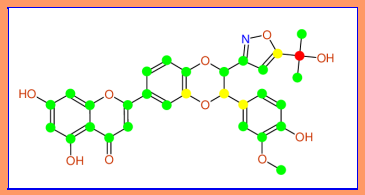


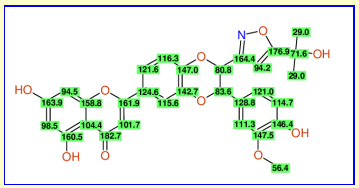


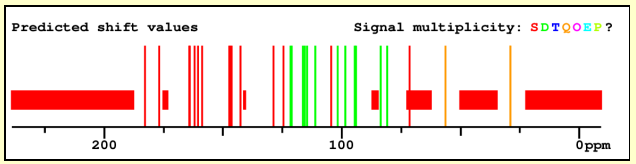
Structure proposal #15 Hide/Show Proposal **Molweight = 559.34 amu** **Molecular formula: $C_{30}H_{25}NO_{10}$**

2.12 - 2.12ppm | 1x found | ZIP-file | PBPYHFWRSVYWAZ

PubChem





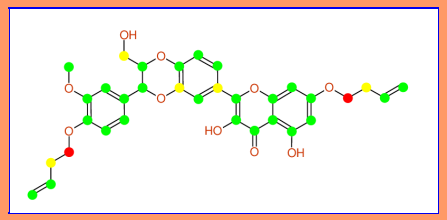


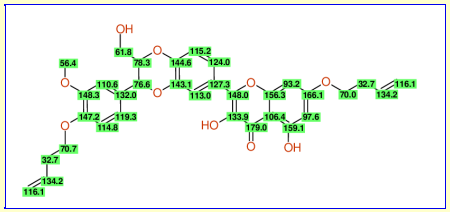
Different spectral pattern

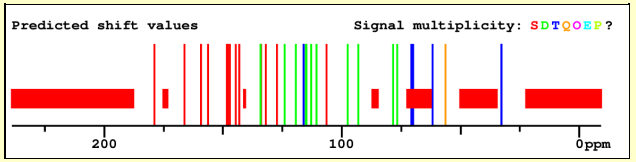
Structure proposal #16 Hide/Show Proposal **Molweight = 588.36 amu** **Molecular formula: $C_{33}H_{32}O_{10}$**

2.16 - 2.16ppm | 3x found | ZIP-file | JGWZSZSEHHNPCR

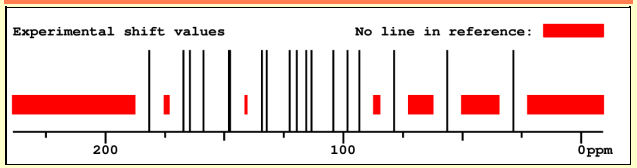
PubChem





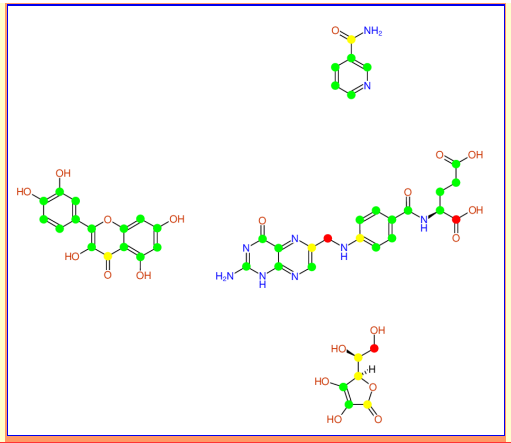


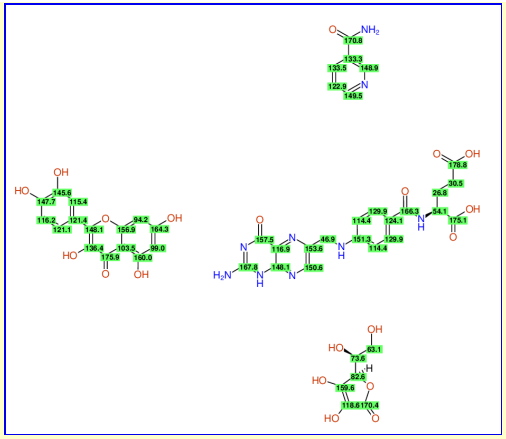
Different spectral pattern

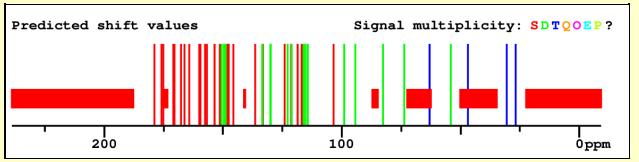


Structure proposal #17 Hide/Show Proposal **Molweight = 1041.58 amu** **Molecular formula: $C_{19}H_{19}N_7O_6.C_{15}H_{10}O_7.C_6H_6N_2O.C_6H_8O_6$**

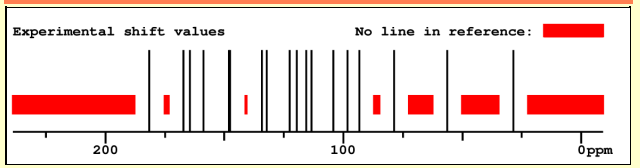
2.19 - 2.19ppm | 1x found | ZIP-file | IWMYFFJXCSPGGP







Different spectral pattern

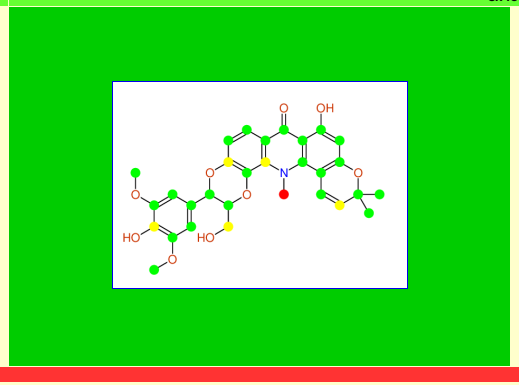


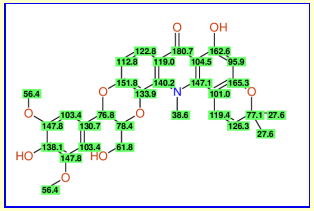
PubChem
PubChem

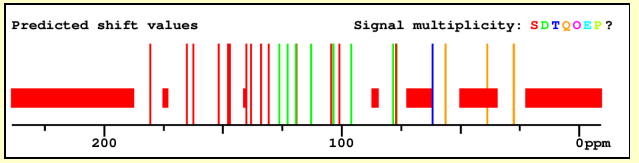
Structure proposal #18 Hide/Show Proposal **Molweight = 547.34 amu** **Molecular formula: $C_{30}H_{29}NO_9$**

2.19 - 2.19ppm **3x found** **ZIP-file** YCYRMTDEEUGSQO

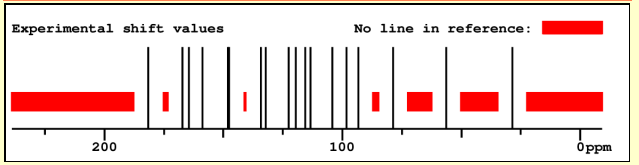
Known Natural Product







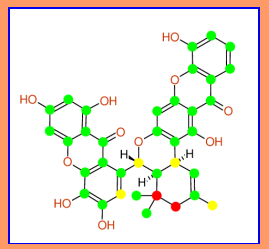
Different spectral pattern

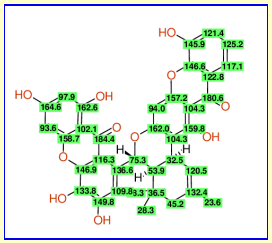


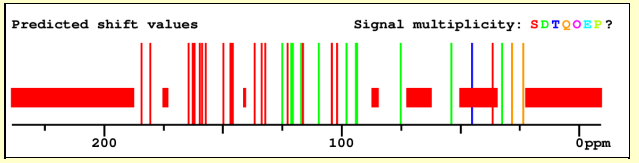
PubChem
PubChem
PubChem

Structure proposal #19 Hide/Show Proposal **Molweight = 636.40 amu** **Molecular formula: $C_{36}H_{28}O_{11}$**

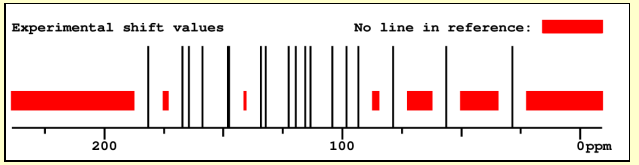
2.20 - 2.20ppm **2x found** **ZIP-file** QELMHHRFQHXGAO







Different spectral pattern

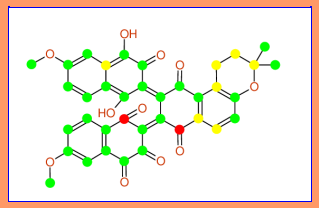


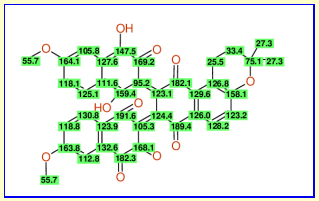
PubChem
PubChem

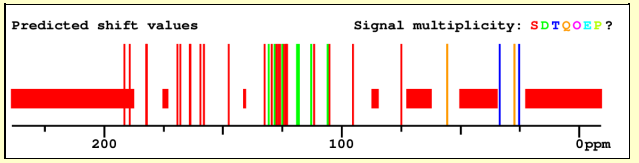
Structure proposal #20 Hide/Show Proposal **Molweight = 646.41 amu** **Molecular formula: $C_{37}H_{26}O_{11}$**

2.22 - 2.23ppm **4x found** **ZIP-file** CSURFSYIPWJGRK

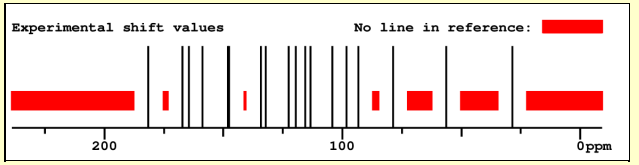
Pub Chem
Pub Chem







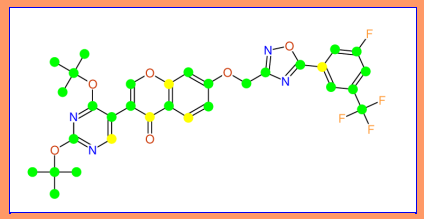
Different spectral pattern

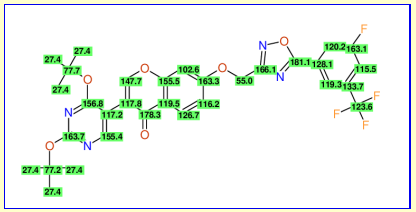


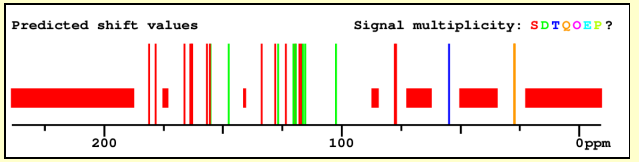
Structure proposal #21 Hide/Show Proposal **Molweight = 628.37 amu** **Molecular formula: $C_{31}H_{28}F_4N_4O_6$**

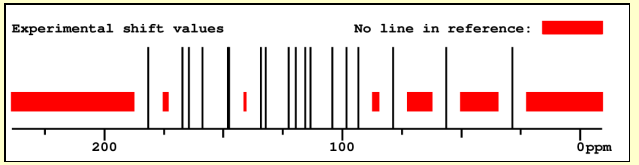
2.22 - 2.22ppm | 1x found | ZIP-file | KAHNJRAGQDDUMW

Pub Chem





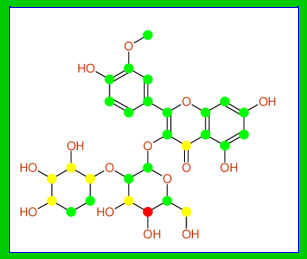


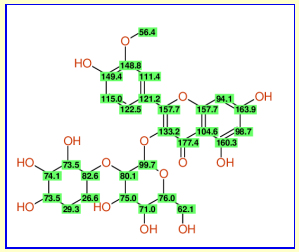


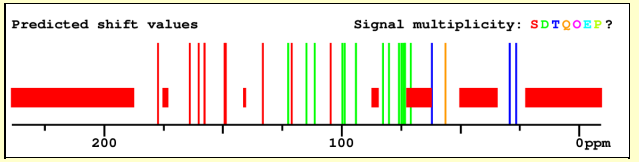
Structure proposal #22 Hide/Show Proposal **Molweight = 608.31 amu** **Molecular formula: $C_{28}H_{32}O_{15}$**

2.23 - 2.23ppm | 1x found | ZIP-file | VKSJLDQAVRCSPL

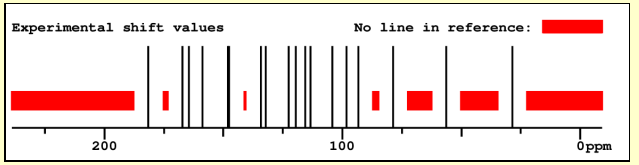
Known Natural Product
Pub Chem
Pub Chem
Pub Chem







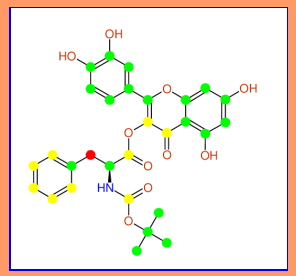
Different spectral pattern

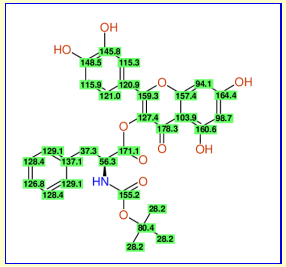


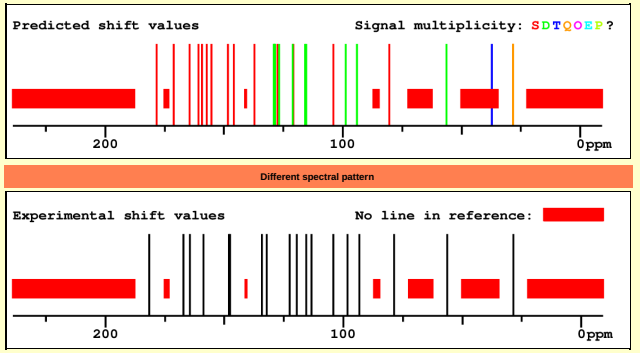
Structure proposal #23 Hide/Show Proposal **Molweight = 549.33 amu** **Molecular formula: $C_{29}H_{27}NO_{10}$**

2.24 - 2.24ppm | 1x found | ZIP-file | FPTSGAAACQGSOW

Pub Chem
Pub Chem



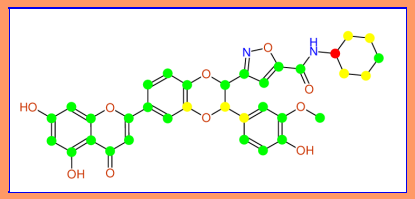


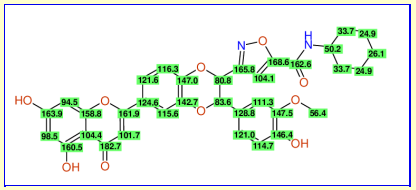


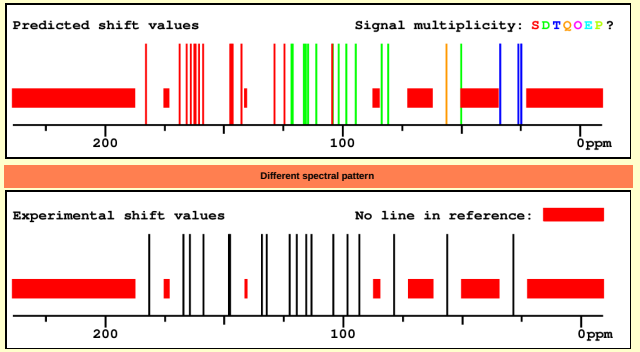
Structure proposal #24 Hide/Show Proposal **Molweight = 626.39 amu** **Molecular formula: $C_{34}H_{30}N_2O_{10}$**

2.24 - 2.24ppm | 1x found | ZIP-file | HWZOGELYLBCAHM

Pub Chem



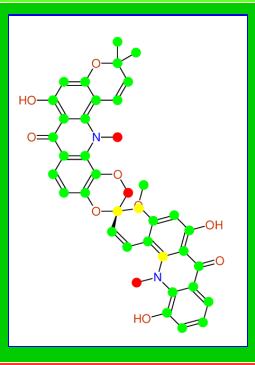


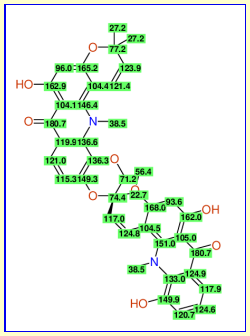


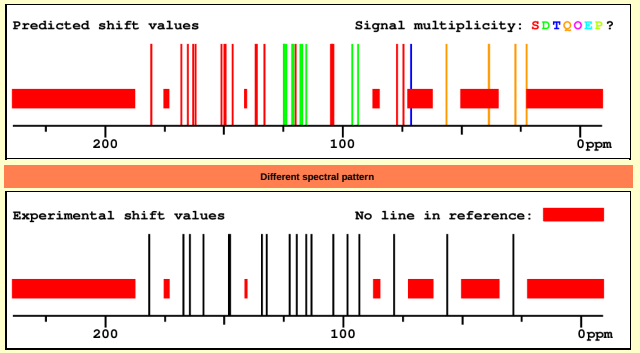
Structure proposal #25 Hide/Show Proposal **Molweight = 674.44 amu** **Molecular formula: $C_{39}H_{34}N_2O_9$**

2.24 - 2.28ppm | 7x found | ZIP-file | VULQLTOYHNVASU

Known Natural Product
Pub Chem
Pub Chem
Pub Chem
Pub Chem
Pub Chem
Pub Chem



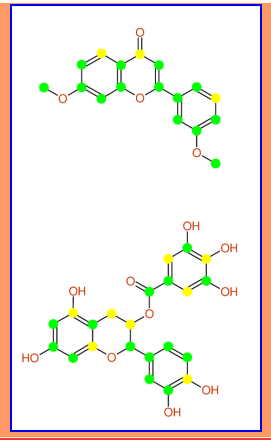


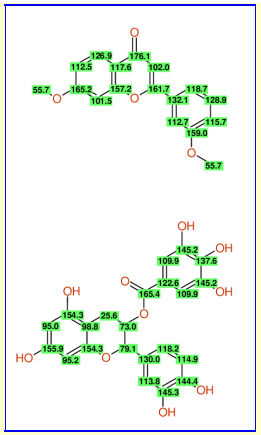


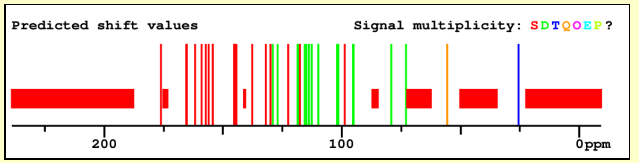
Structure proposal #26 Hide/Show Proposal **Molweight = 724.43 amu** **Molecular formula: $C_{22}H_{18}O_{10}.C_{17}H_{14}O_4$**

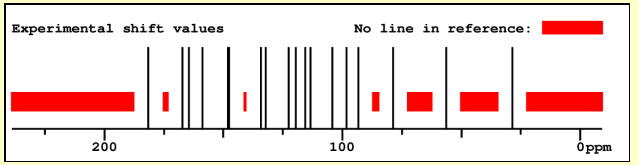
2.24 - 2.24ppm | 1x found | ZIP-file | VYUJFEJSRCUIKB

PubChem





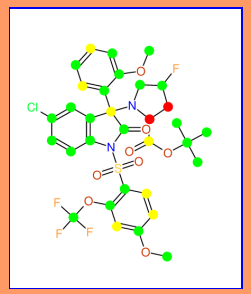


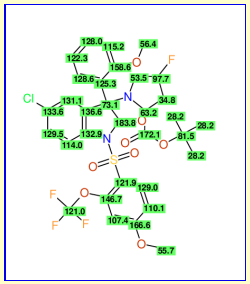


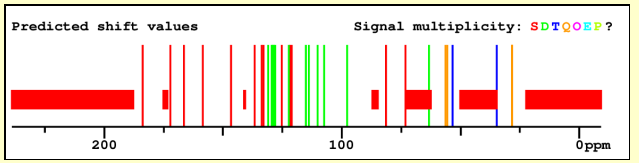
Structure proposal #27 Hide/Show Proposal **Molweight = 714.89 amu** **Molecular formula: $C_{32}H_{31}ClF_4N_2O_8S$**

2.25 - 2.46ppm	3x found	ZIP-file	PRJDIFHSZWLSGN

PubChem
PubChem
PubChem





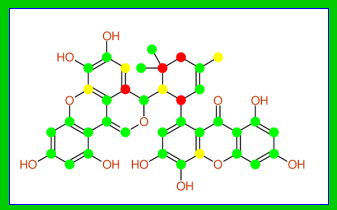


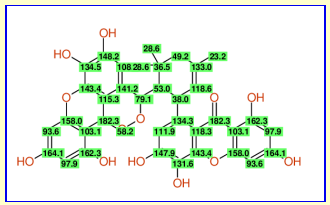
Different spectral pattern

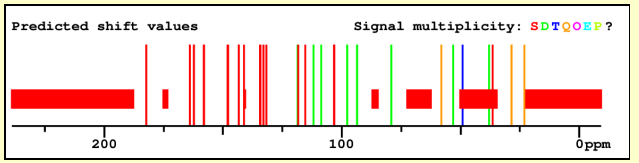
Structure proposal #28 Hide/Show Proposal **Molweight = 684.41 amu** **Molecular formula: $C_{37}H_{32}O_{13}$**

2.26 - 2.34ppm	4x found	ZIP-file	NBAWIKFNFWOFRT

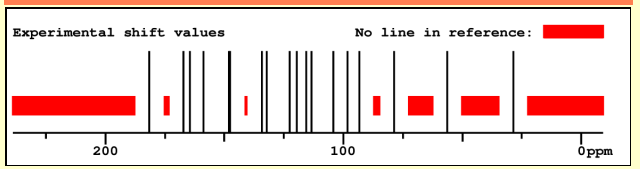
Known Natural Product
PubChem
PubChem







Different spectral pattern

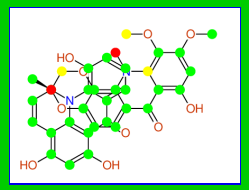


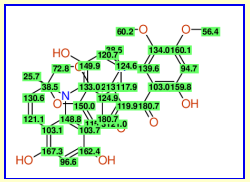
Structure proposal #29 Hide/Show Proposal **Molweight = 638.40 amu** **Molecular formula: $C_{35}H_{30}N_2O_{10}$**

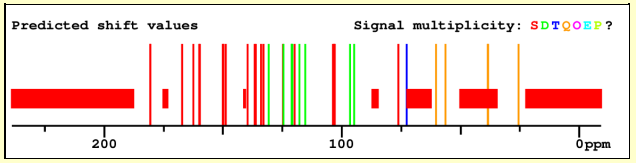
2.27 - 2.27ppm	1x found	ZIP-file	PQPGLMPQNHBXON

Known Natural Product

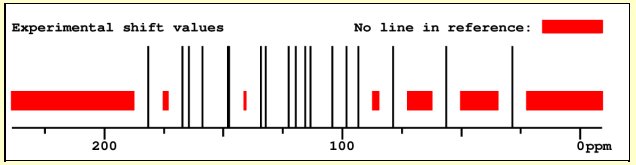
PubChem







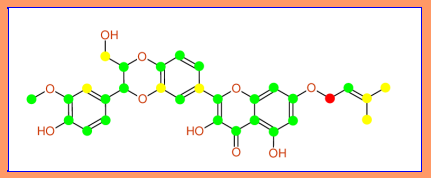
Different spectral pattern

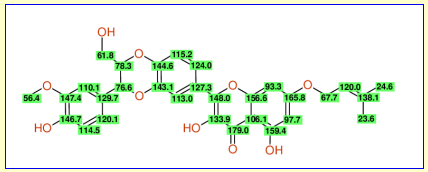


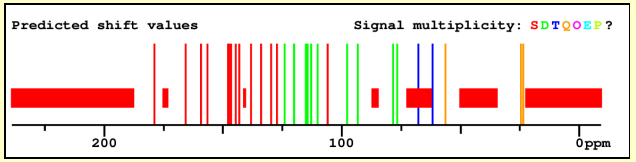
Structure proposal #30 Hide/Show Proposal **Molweight = 548.33 amu** **Molecular formula: $C_{30}H_{26}O_{10}$**

2.27 - 2.27ppm | 2x found | ZIP-file | UMHUIUBPLNPTMK

PubChem





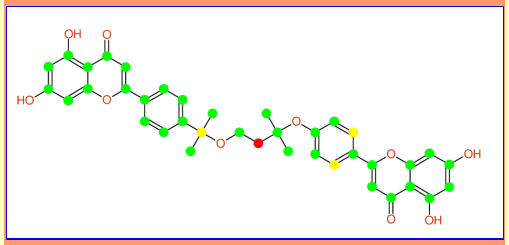


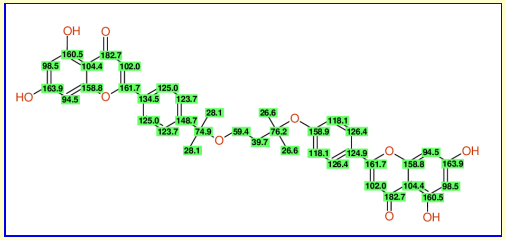
Different spectral pattern

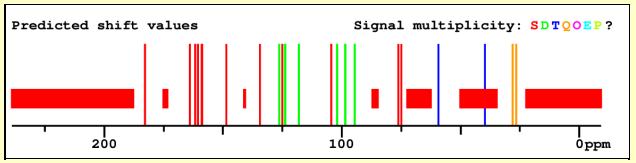
Structure proposal #31 Hide/Show Proposal **Molweight = 650.42 amu** **Molecular formula: $C_{38}H_{34}O_{10}$**

2.27 - 2.27ppm | 1x found | ZIP-file | WERCBVZGNWWFIL

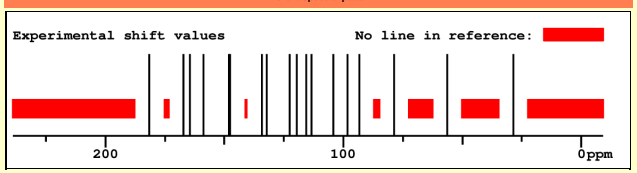
PubChem





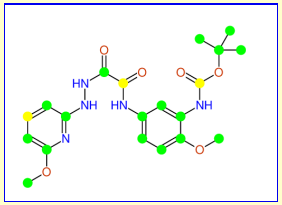


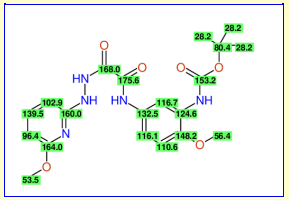
Different spectral pattern

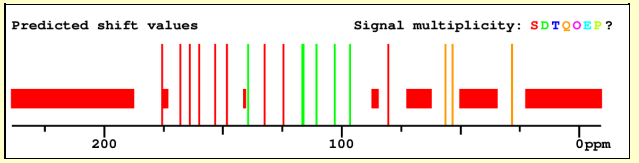


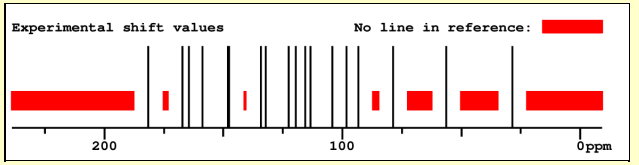
Structure proposal #32 Hide/Show Proposal **Molweight = 431.26 amu** **Molecular formula: $C_{20}H_{25}N_5O_6$**

2.28 - 2.28ppm | 1x found | ZIP-file | UCWUTNBKMOYHTJ





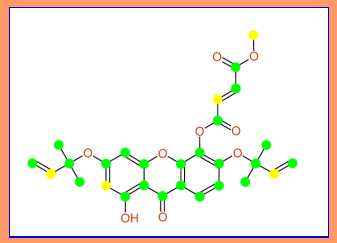


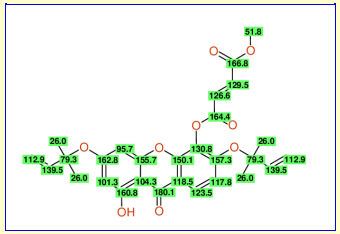


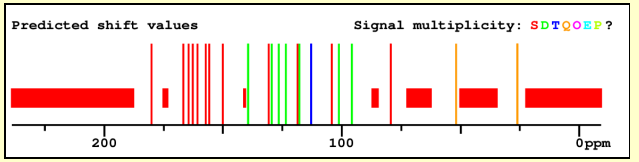
Structure proposal #33 Hide/Show Proposal **Molweight = 508.31 amu** **Molecular formula: $C_{28}H_{28}O_9$**

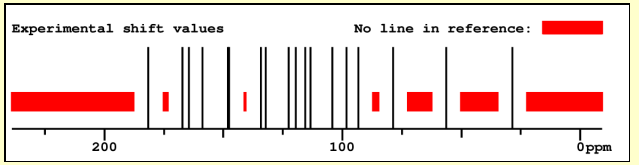
2.28 - 2.30ppm | **2x found** | ZIP-file | PGUSFGDXTAXCOY

PubChem
PubChem





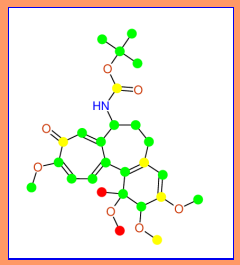


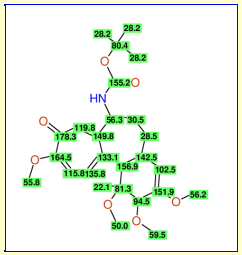


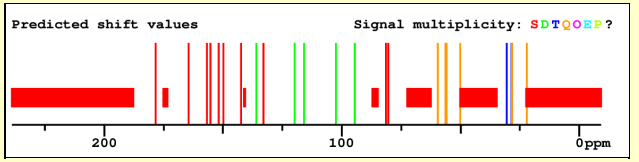
Structure proposal #34 Hide/Show Proposal **Molweight = 473.29 amu** **Molecular formula: $C_{26}H_{35}NO_7$**

2.29 - 2.29ppm | **1x found** | ZIP-file | FPECCRDHTWVNFW

PubChem



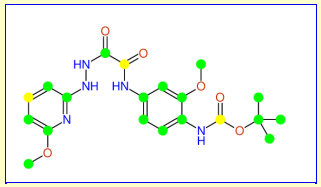


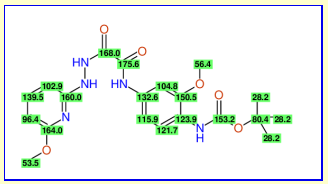


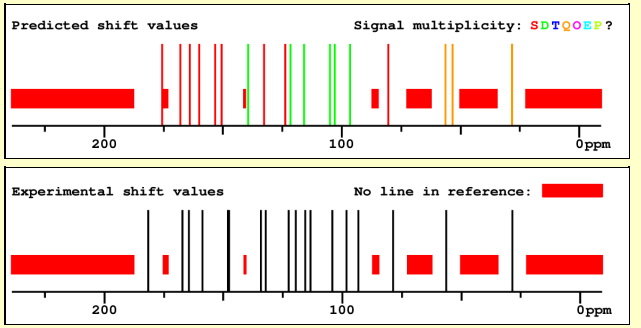
Different spectral pattern

Structure proposal #35 Hide/Show Proposal Molweight = 431.26 amu Molecular formula: $C_{20}H_{25}N_5O_6$

2.29 - 2.29ppm | 1x found | ZIP-file | KIYPWADWUVIQFL





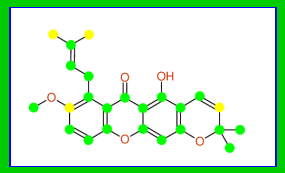


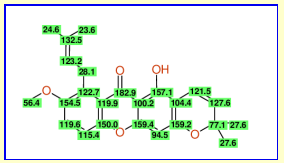
Structure proposal #36 Hide/Show Proposal Molweight = 392.26 amu Molecular formula: $C_{24}H_{24}O_5$

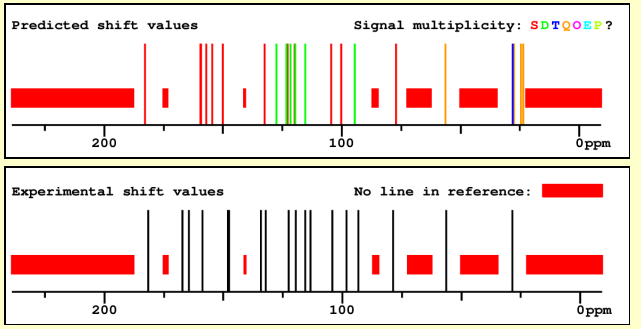
2.29 - 2.29ppm | 1x found | ZIP-file | PLKQPRRVFTZBAE

Known Natural Product

PubChem



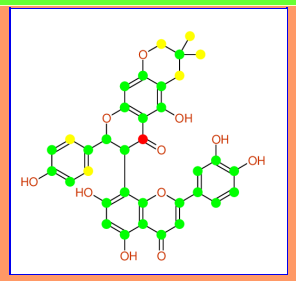


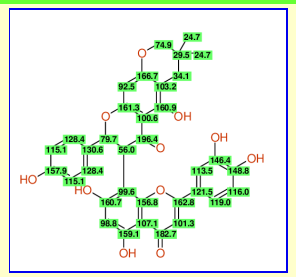


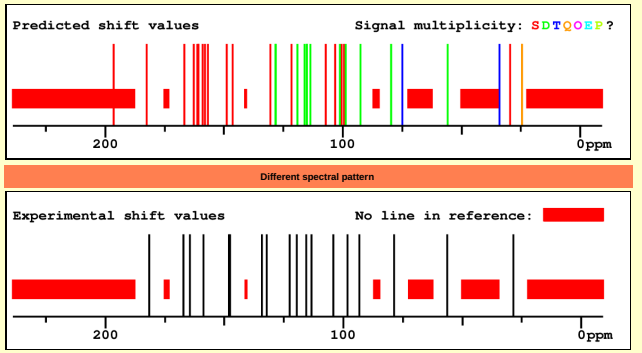
Structure proposal #37 Hide/Show Proposal Molweight = 624.38 amu Molecular formula: $C_{35}H_{28}O_{11}$

2.30 - 2.30ppm | 1x found | ZIP-file | FZFACVBRJAFBNP

PubChem



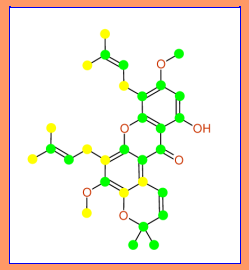


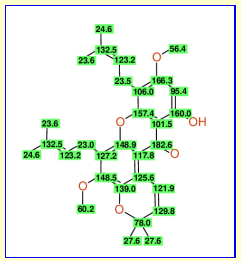


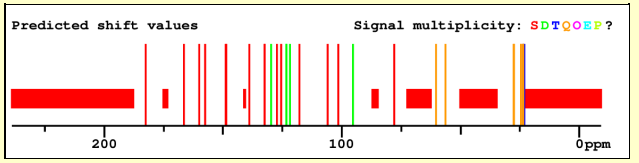
Structure proposal #38 Hide/Show Proposal Molweight = 490.33 amu Molecular formula: $C_{30}H_{34}O_6$

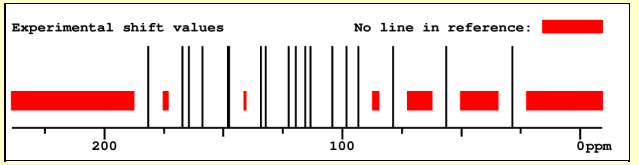
2.30 - 2.30ppm | 2x found | ZIP-file | NARALRJVEWSVHD

PubChem





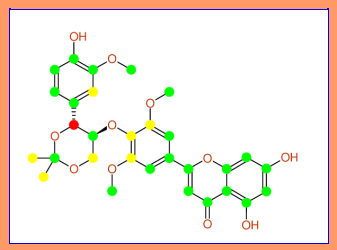


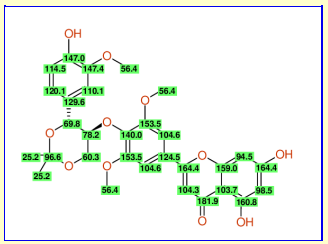


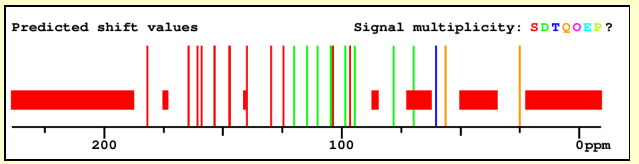
Structure proposal #39 Hide/Show Proposal **Molweight = 566.33 amu** **Molecular formula: $C_{30}H_{30}O_{11}$**

2.30 - 2.30ppm | 2x found | ZIP-file | ZZEOHFKNCQYMSG

PubChem
PubChem
PubChem





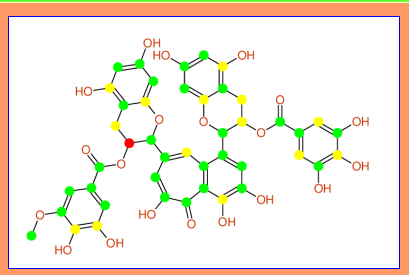


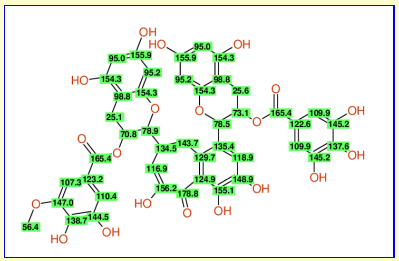
Different spectral pattern

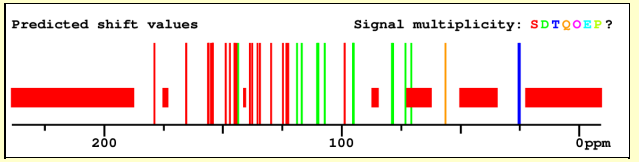
Structure proposal #40 Hide/Show Proposal **Molweight = 882.48 amu** **Molecular formula: $C_{44}H_{34}O_{20}$**

2.32 - 2.32ppm | 1x found | ZIP-file | FQXKSGFYFITSPQ

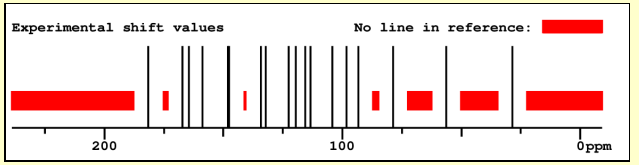
PubChem
PubChem





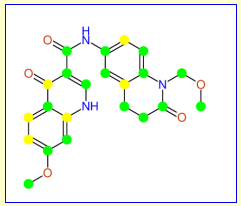


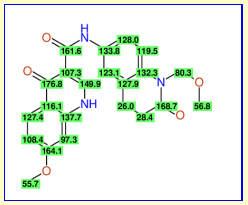
Different spectral pattern

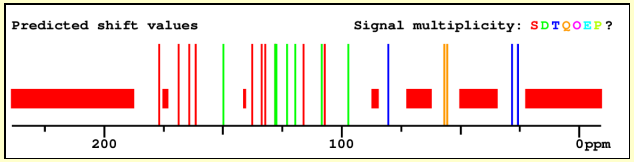


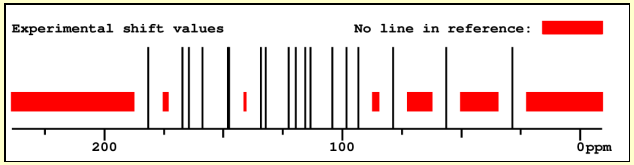
Structure proposal #41 Hide/Show Proposal **Molweight = 407.27 amu** **Molecular formula: $C_{22}H_{21}N_3O_5$**

2.32 - 2.32ppm	1x found	ZIP-file	GWBXZQDRCLYZIP





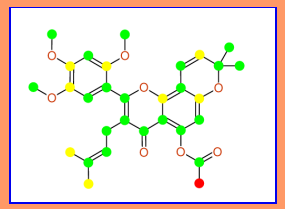


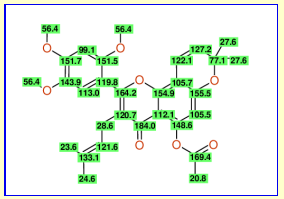


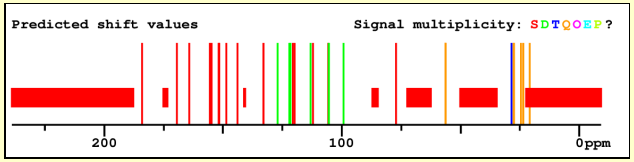
Structure proposal #42	Hide/Show Proposal	Molweight = 520.33 amu	Molecular formula: $C_{30}H_{32}O_8$

2.32 - 2.32ppm	1x found	ZIP-file	ROOBWRFBMSRDSD

PubChem





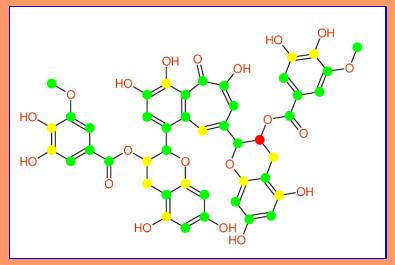


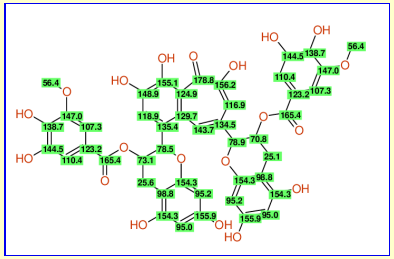
Different spectral pattern

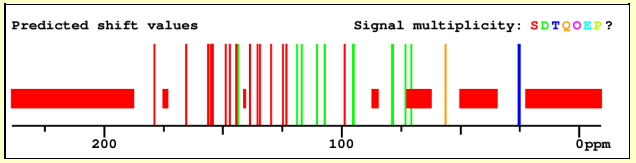
Structure proposal #43	Hide/Show Proposal	Molweight = 896.49 amu	Molecular formula: $C_{45}H_{36}O_{20}$

2.32 - 2.32ppm	1x found	ZIP-file	UBJBDUUSFQNEBA

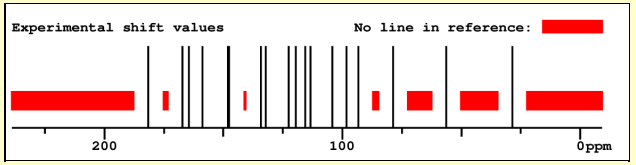
PubChem
PubChem







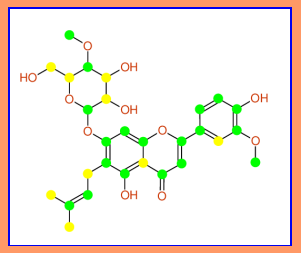
Different spectral pattern

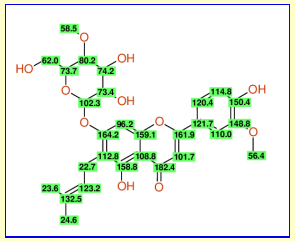


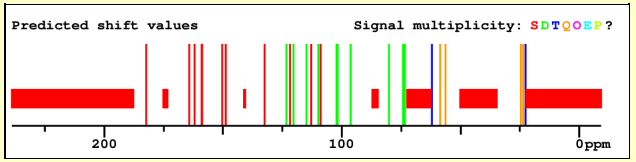
Structure proposal #44 Hide/Show Proposal **Molweight = 544.31 amu** **Molecular formula: $C_{28}H_{32}O_{11}$**

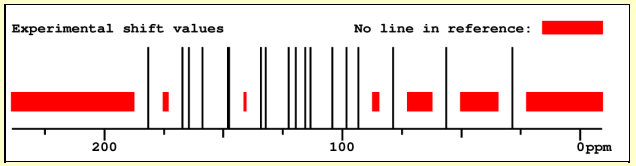
2.34 - 2.34ppm	1x found	ZIP-file	UOCDEBLBCGOGLG

PubChem
PubChem



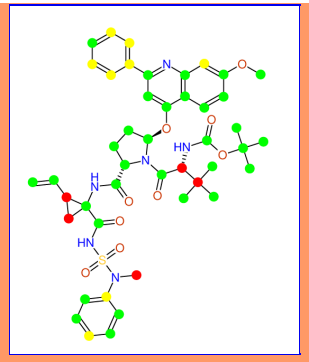


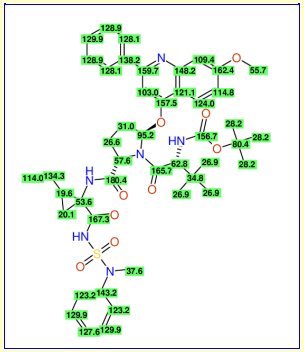


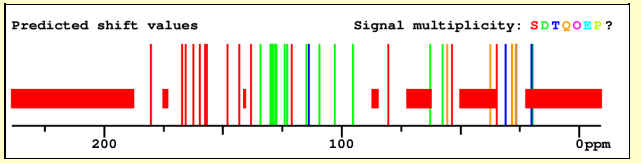


Structure proposal #45 Hide/Show Proposal **Molweight = 854.61 amu** **Molecular formula: $C_{45}H_{54}N_6O_9S$**

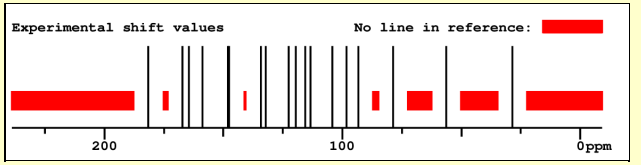
2.35 - 2.37ppm	4x found	ZIP-file	GGKVTMPLEOODRX





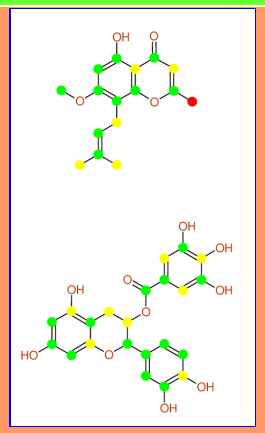


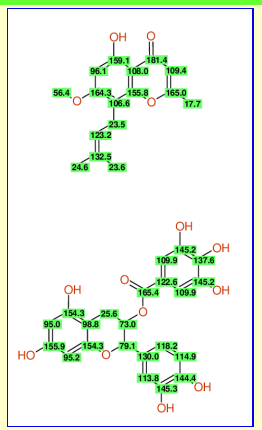
Different spectral pattern

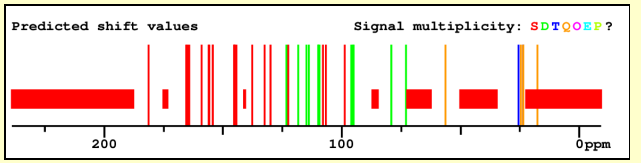


Structure proposal #46 Hide/Show Proposal **Molweight = 716.42 amu** **Molecular formula: $C_{22}H_{18}O_{10}.C_{16}H_{18}O_4$**

2.35 - 2.35ppm **1x found** ZIP-file **ONBQIVLYNCYRHK**



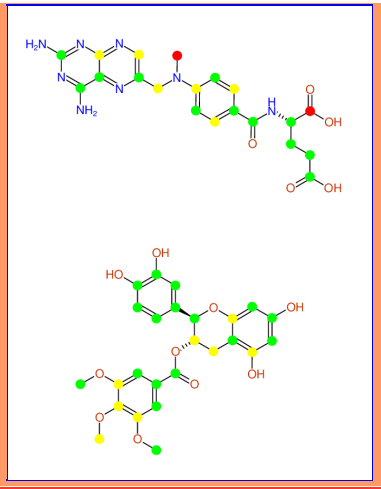


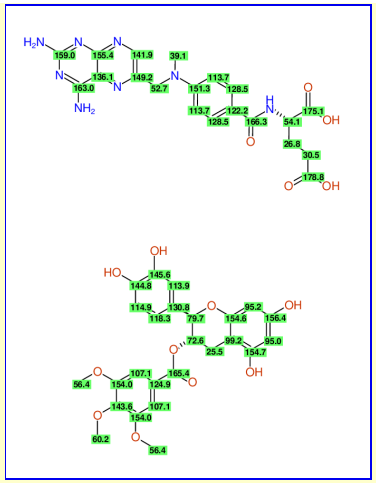


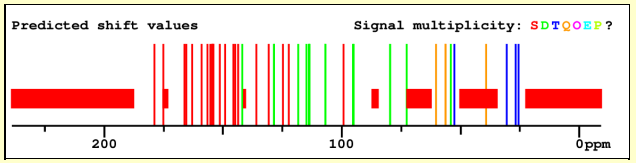
Different spectral pattern

Structure proposal #47 Hide/Show Proposal **Molweight = 938.56 amu** **Molecular formula: $C_{45}H_{46}N_8O_{15}$**

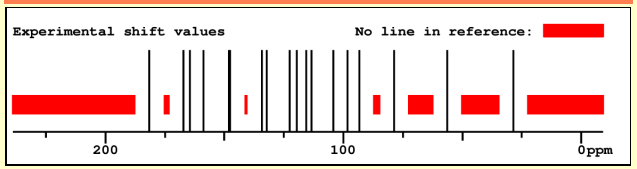
2.35 - 2.35ppm **2x found** ZIP-file **OPHPLXJLVOCOPC**







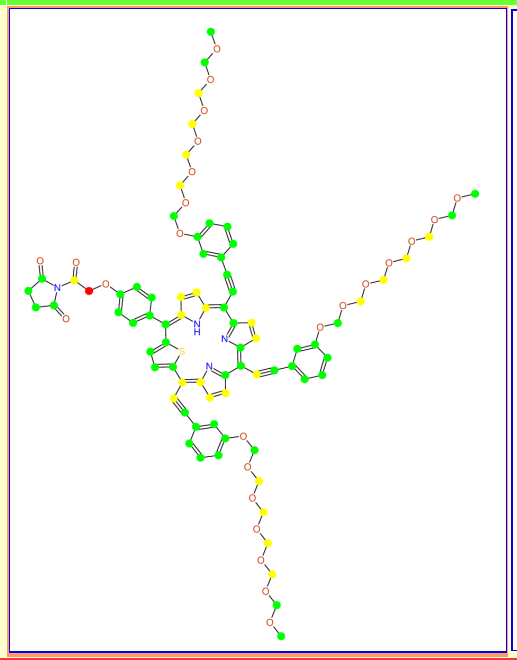
Different spectral pattern

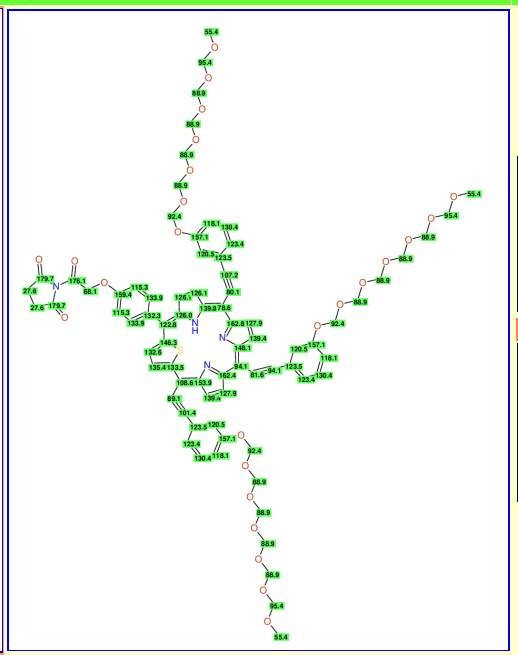


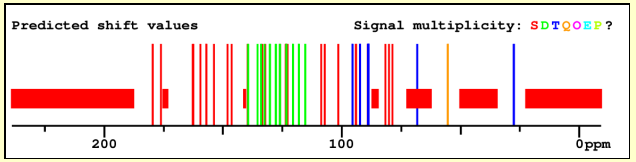
PubChem

Structure proposal #48 Hide/Show Proposal **Molweight = 1488.94 amu** **Molecular formula: $C_{77}H_{76}N_4O_{25}S$**

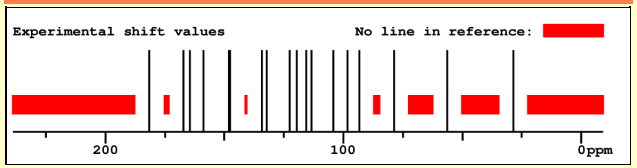
2.35 - 2.35ppm	1x found	ZIP-file	OYXBAMQTAYJYRS







Different spectral pattern



PubChem

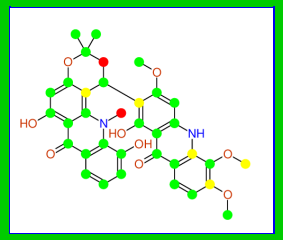
Structure proposal #49 Hide/Show Proposal **Molweight = 624.40 amu** **Molecular formula: $C_{35}H_{32}N_2O_9$**

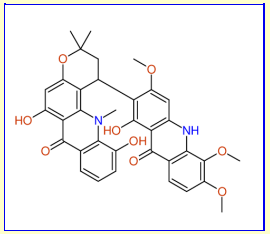
2.35 - 2.35ppm	2x found	ZIP-file	UIEVLPRKYIOBRT

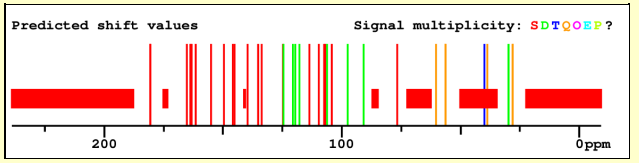
Known Natural Product

PubChem

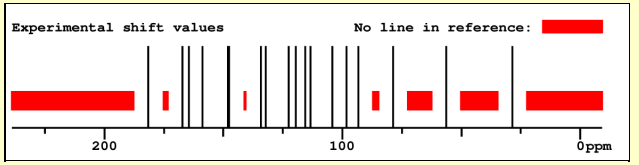
PubChem







Different spectral pattern

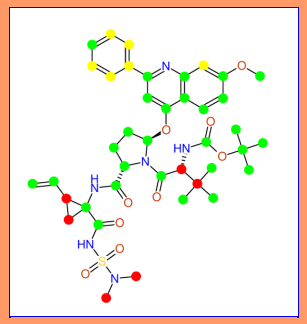


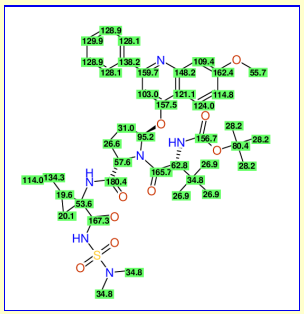
Structure proposal #50 Hide/Show Proposal **Molweight = 792.55 amu** **Molecular formula: $C_{40}H_{52}N_6O_9S$**

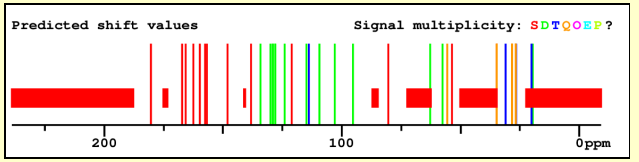
2.36 - 2.37ppm **2x found** ZIP-file ZJLHQUDFYRSQRM

PubChem

PubChem





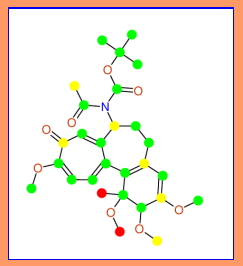


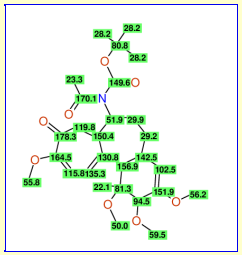
Different spectral pattern

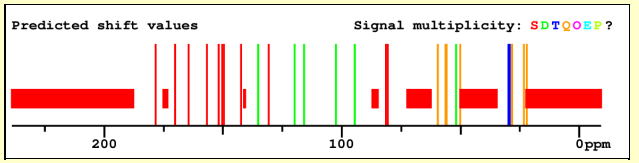
Structure proposal #51 Hide/Show Proposal **Molweight = 515.32 amu** **Molecular formula: $C_{28}H_{37}NO_8$**

2.41 - 2.41ppm **1x found** ZIP-file KQMXTGOLNWMWML

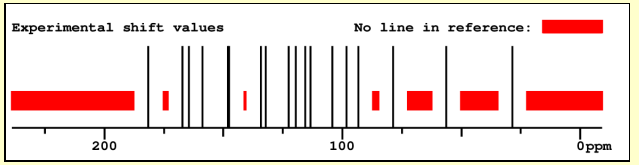
PubChem







Different spectral pattern



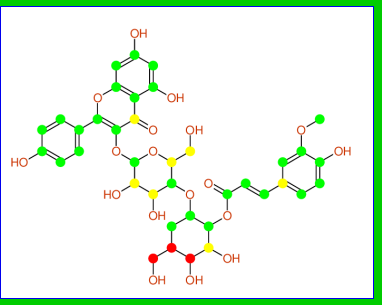
Structure proposal #52 Hide/Show Proposal **Molweight = 784.42 amu** **Molecular formula: $C_{38}H_{40}O_{18}$**

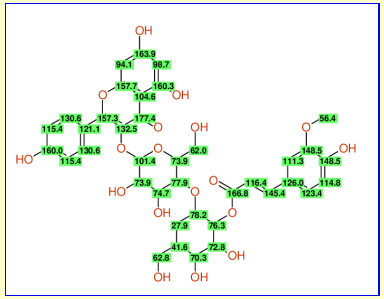
2.41 - 2.41ppm **1x found** ZIP-file LLECSJWFKSKWSI

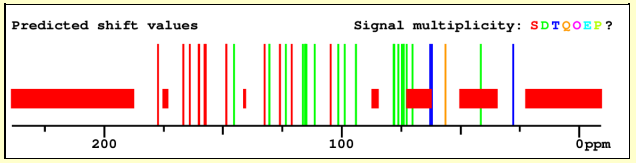
Known Natural Product

PubChem

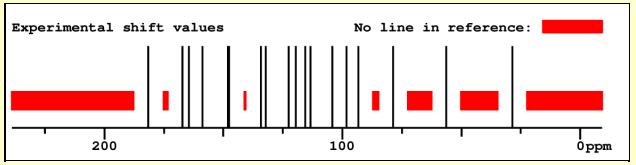
PubChem







Different spectral pattern



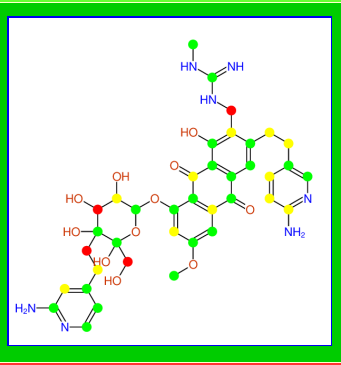
Structure proposal #53 Hide/Show Proposal **Molweight = 773.47 amu** **Molecular formula: $C_{38}H_{43}N_7O_{11}$**

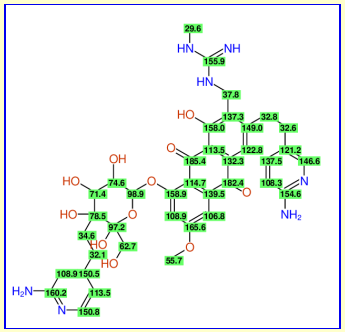
2.44 - 2.44ppm **1x found** ZIP-file HPBXXKPUKGNONL

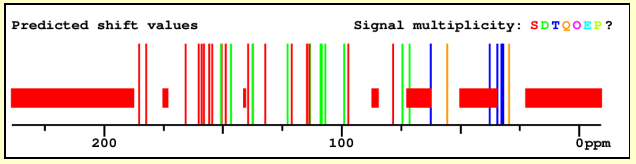
Known Natural Product

PubChem

PubChem



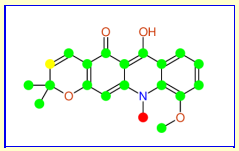


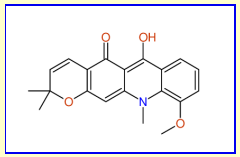


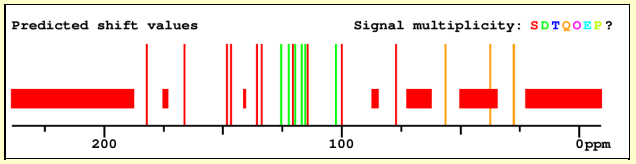
Different spectral pattern

Structure proposal #54 Hide/Show Proposal **Molweight = 337.23 amu** **Molecular formula: $C_{20}H_{19}NO_4$**

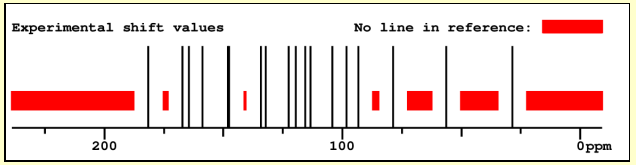
2.44 - 2.44ppm **1x found** ZIP-file RMLDGROOTDFTCL







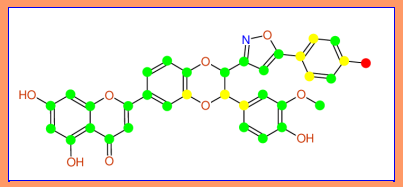
Different spectral pattern

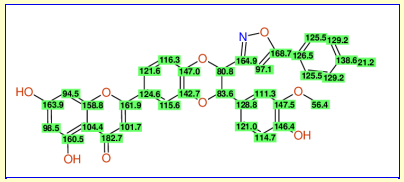


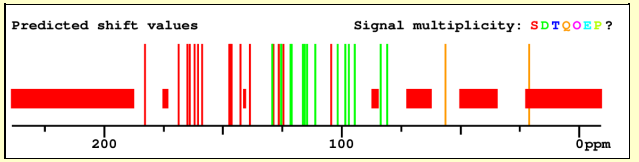
Structure proposal #55 Hide/Show Proposal **Molweight = 591.38 amu** **Molecular formula: $C_{34}H_{25}NO_9$**

2.45 - 2.45ppm **1x found** ZIP-file PYMDTGNTRMSSGF

PubChem





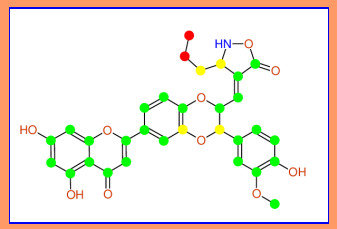


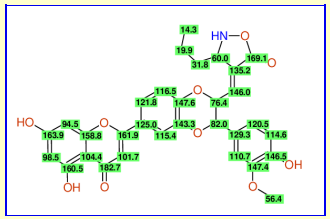
Different spectral pattern

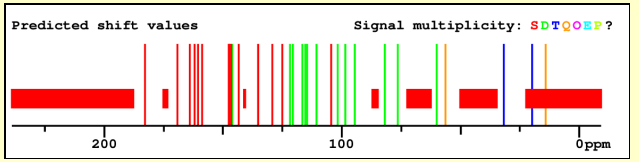
Structure proposal #56 Hide/Show Proposal Molweight = 573.35 amu Molecular formula: $C_{31}H_{27}NO_{10}$

2.46 - 2.46ppm | 1x found | ZIP-file | HXYDGAWCFNTNGI

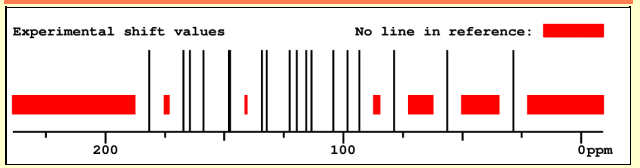
PubChem







Different spectral pattern



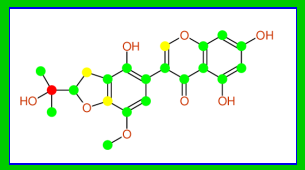
Structure proposal #57 Hide/Show Proposal Molweight = 400.23 amu Molecular formula: $C_{21}H_{20}O_8$

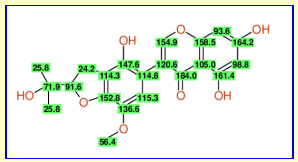
2.48 - 2.48ppm | 1x found | ZIP-file | FARFZQNVSOJULQ

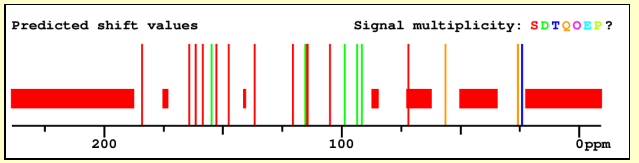
Known Natural Product

PubChem

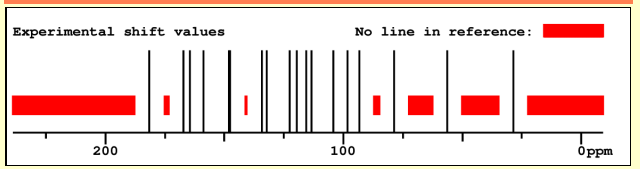
PubChem





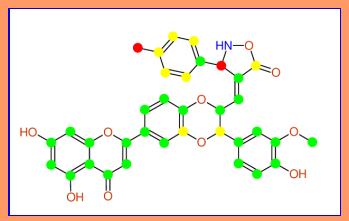


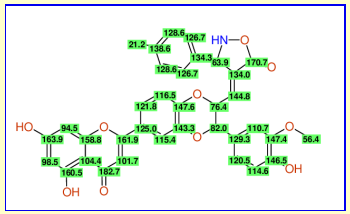
Different spectral pattern

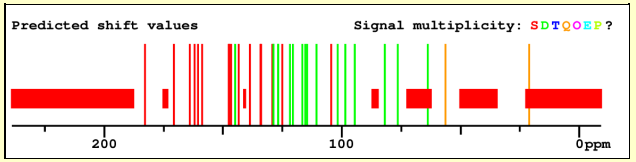


Structure proposal #58 Hide/Show Proposal Molweight = 621.39 amu Molecular formula: $C_{35}H_{27}NO_{10}$

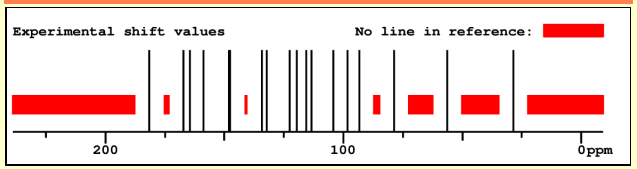
2.48 - 2.48ppm | 1x found | ZIP-file | HKLZTYORFMETHX







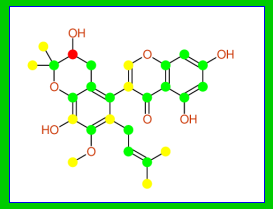
Different spectral pattern

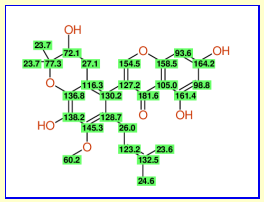


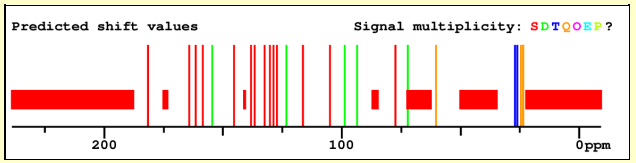
Structure proposal #59 Hide/Show Proposal **Molweight = 468.29 amu** **Molecular formula: $C_{26}H_{28}O_8$**

2.49 - 2.49ppm **1x found** ZIP-file ULBHYLFUEKDETJ

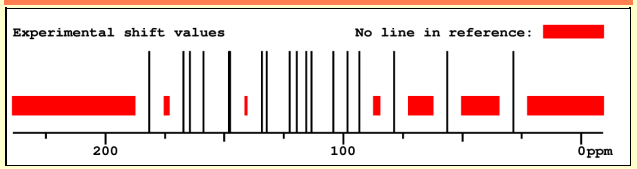
Known Natural Product







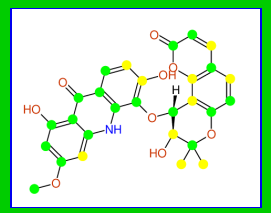
Different spectral pattern

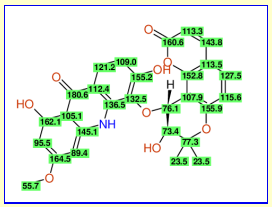


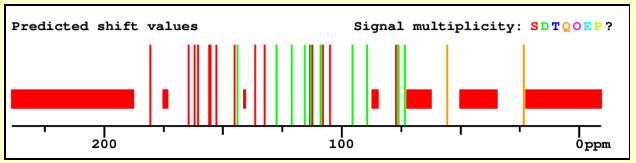
Structure proposal #60 Hide/Show Proposal **Molweight = 517.32 amu** **Molecular formula: $C_{28}H_{23}NO_9$**

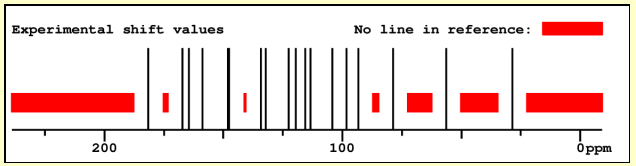
2.50 - 2.50ppm **1x found** ZIP-file LCGFAZIBUURPDA

Known Natural Product



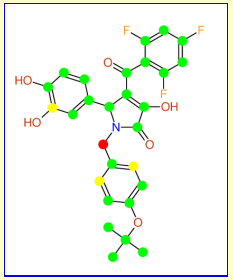


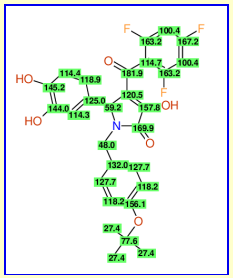


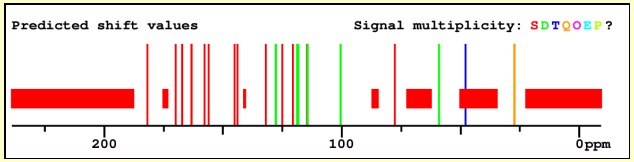


Structure proposal #61 Hide/Show Proposal **Molweight = 527.32 amu** **Molecular formula: $C_{28}H_{24}F_3NO_6$**

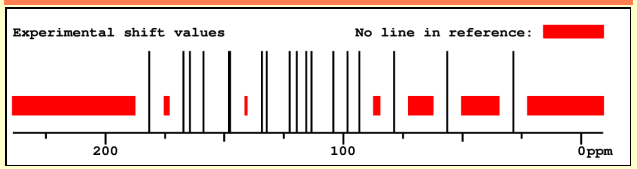
2.50 - 2.50ppm	1x found	ZIP-file	NGLNFRQYRKAJJV







Different spectral pattern



Structure proposal #62	Hide/Show Proposal	Molweight = 400.23 amu	Molecular formula: $C_{21}H_{20}O_8$

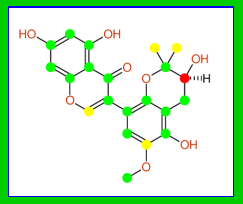
2.51 - 2.51ppm	1x found	ZIP-file	QVZMXQYIIGURQW

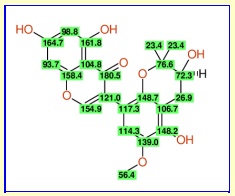
Known Natural Product

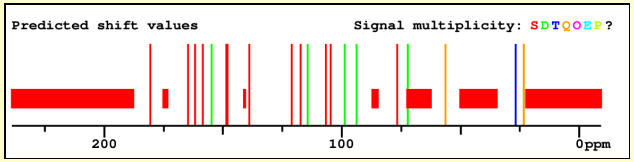
PubChem

PubChem

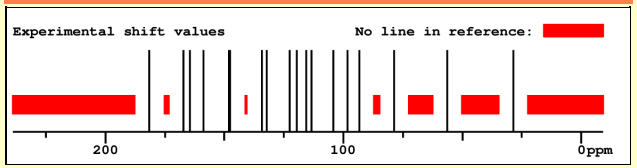
PubChem





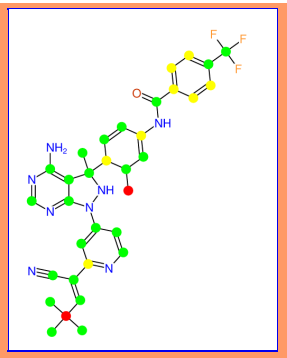


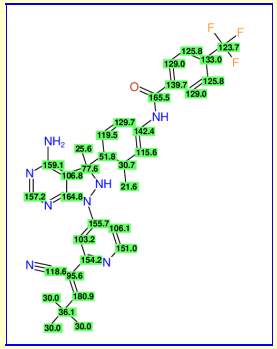
Different spectral pattern

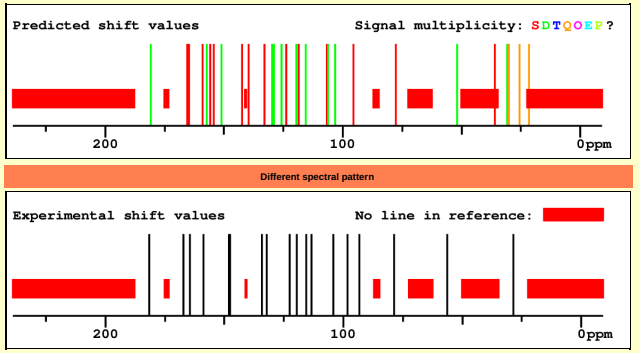


Structure proposal #63	Hide/Show Proposal	Molweight = 614.43 amu	Molecular formula: $C_{33}H_{33}F_3N_6O$

2.53 - 2.53ppm	1x found	ZIP-file	HNGFDYDYOQVEPR



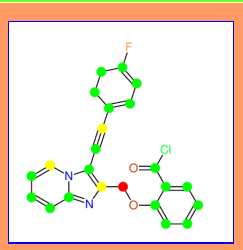


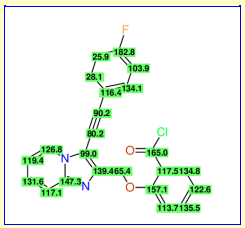


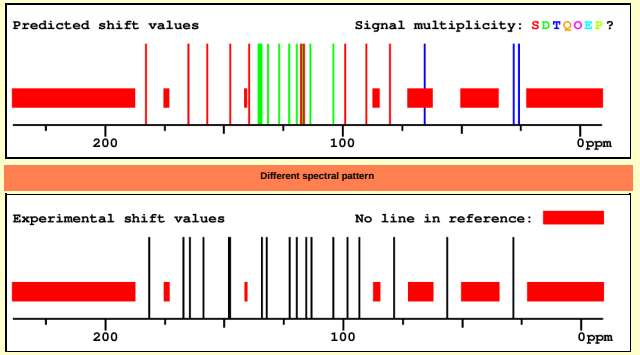
Pub Chem

Structure proposal #64 Hide/Show Proposal **Molweight = 406.73 amu** **Molecular formula: $C_{23}H_{16}ClFN_2O_2$**

2.54 - 2.54ppm **1x found** ZIP-file LOPPXGANJWGNHK







Pub Chem

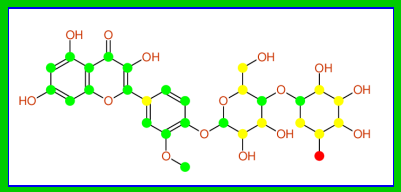
Structure proposal #65 Hide/Show Proposal **Molweight = 622.32 amu** **Molecular formula: $C_{29}H_{34}O_{15}$**

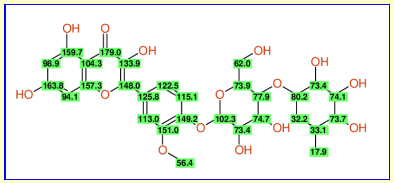
2.55 - 2.55ppm **1x found** ZIP-file OYIIRHRYYXKHHG

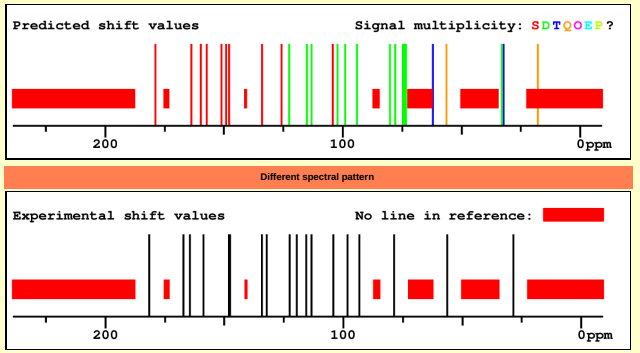
Known Natural Product

Pub Chem

Pub Chem

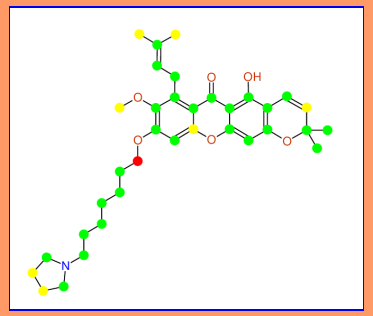


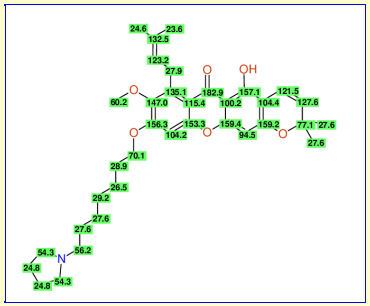


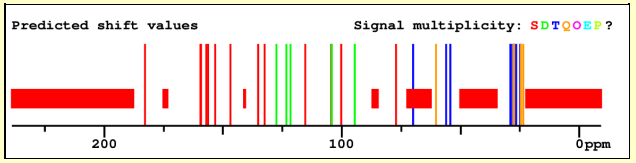


Structure proposal #66 Hide/Show Proposal **Molweight = 575.39 amu** **Molecular formula: $C_{35}H_{45}NO_6$**

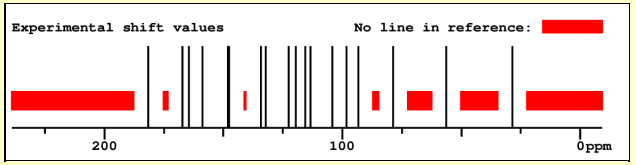
2.55 - 2.55ppm **1x found** ZIP-file RMVZUAIZGGPXDC







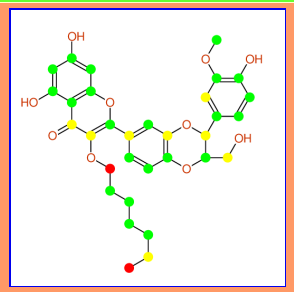
Different spectral pattern

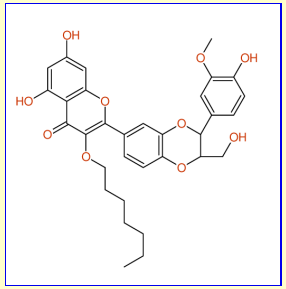


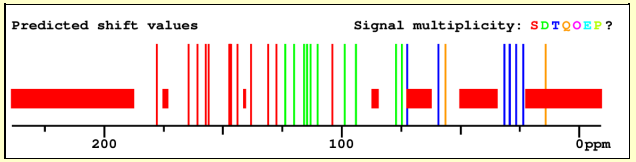
Pub Chem

Structure proposal #67 Hide/Show Proposal **Molweight = 578.35 amu** **Molecular formula: $C_{32}H_{34}O_{10}$**

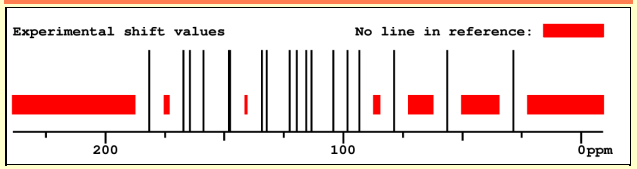
2.55 - 2.61ppm **4x found** ZIP-file JOJDSZIPMXOBLL







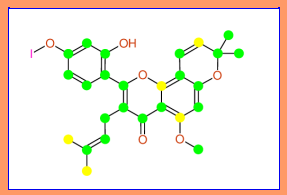
Different spectral pattern

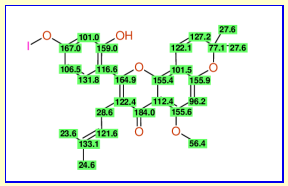


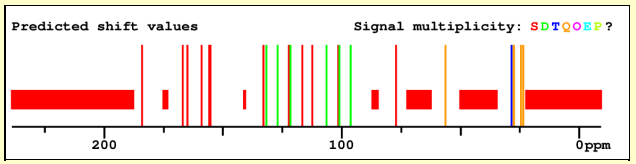
Pub Chem

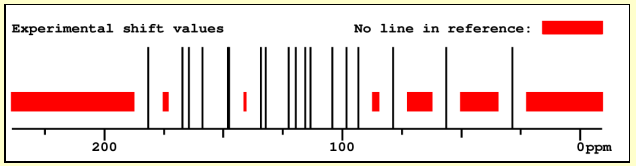
Structure proposal #68 Hide/Show Proposal **Molweight = 560.20 amu** **Molecular formula: $C_{26}H_{25}IO_6$**

2.56 - 2.56ppm **1x found** ZIP-file IPYSPVLEYMUDMN





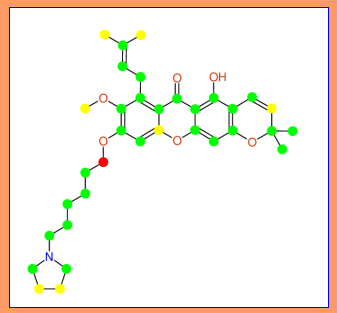


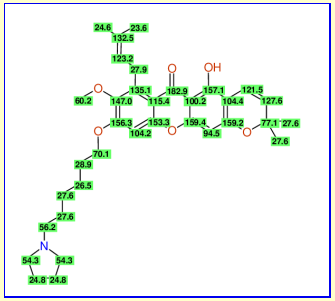


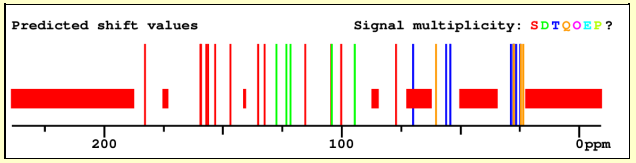
Pub Chem

Structure proposal #69 Hide/Show Proposal **Molweight = 561.38 amu** **Molecular formula: $C_{34}H_{43}NO_6$**

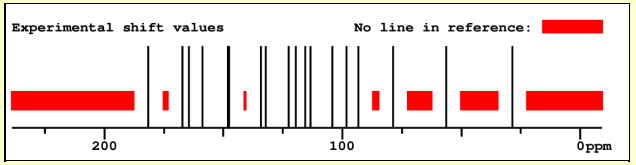
2.56 - 2.56ppm **1x found** ZIP-file KOINQBSLUHJYRH





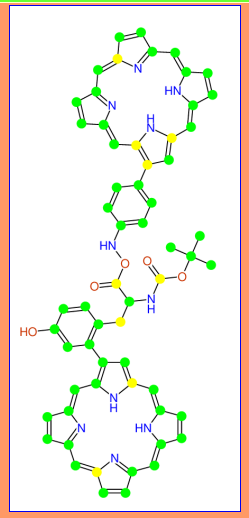


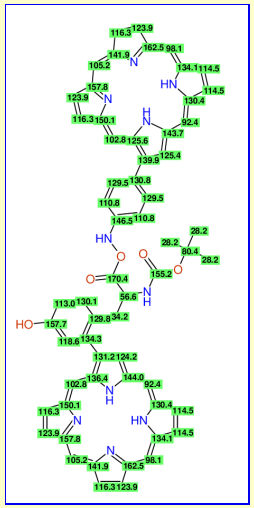
Different spectral pattern

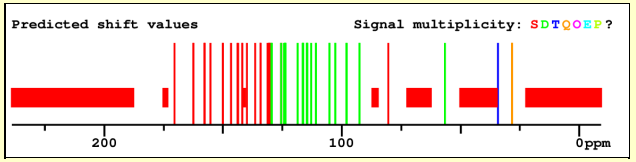


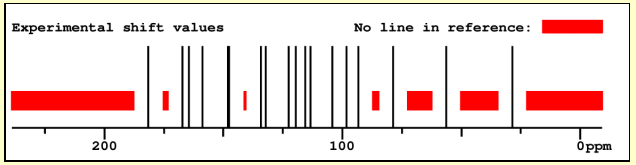
Structure proposal #70 Hide/Show Proposal **Molweight = 988.74 amu** **Molecular formula: $C_{60}H_{48}N_{10}O_5$**

2.56 - 2.56ppm **1x found** ZIP-file ONHAMRKWMJWYTR





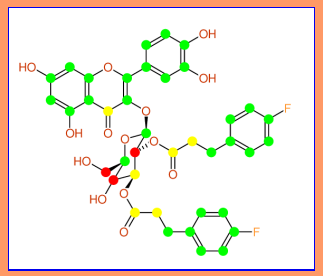


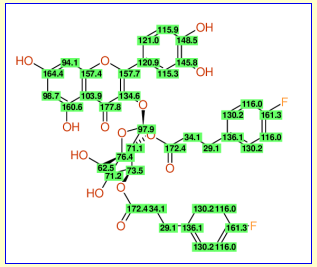


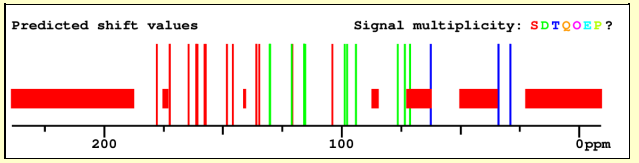
Structure proposal #71 Hide/Show Proposal **Molweight = 764.43 amu** **Molecular formula: $C_{39}H_{34}F_2O_{14}$**

2.57 - 2.57ppm **1x found** ZIP-file SOBUPDJFMNHVQS

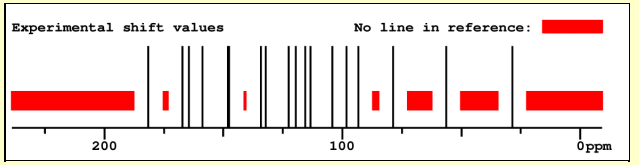
Pub Chem







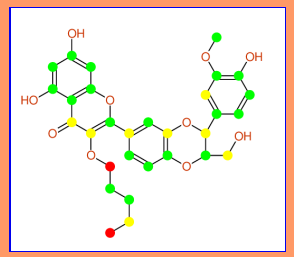
Different spectral pattern

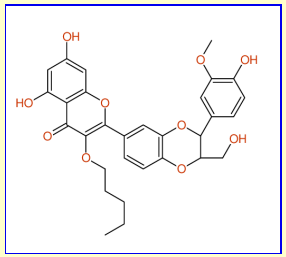


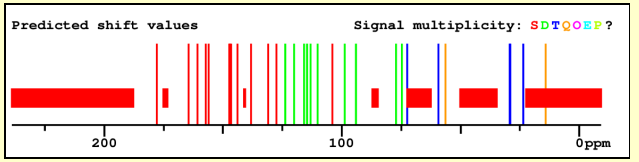
Structure proposal #72 Hide/Show Proposal **Molweight = 550.33 amu** **Molecular formula: $C_{30}H_{30}O_{10}$**

2.57 - 2.64ppm **4x found** ZIP-file AWIJZJKQVBMQJN

Pub Chem







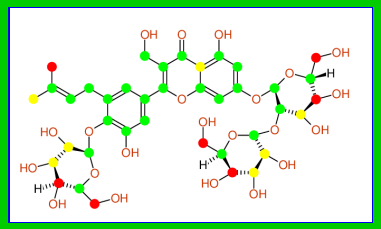
Different spectral pattern

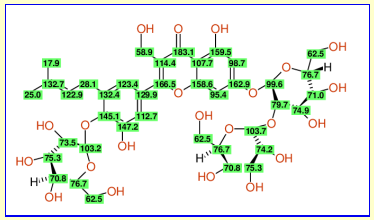
Structure proposal #73 Hide/Show Proposal **Molweight = 870.43 amu** **Molecular formula: $C_{39}H_{50}O_{22}$**

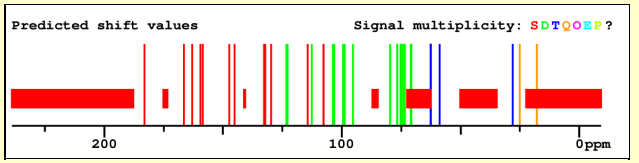
2.58 - 2.58ppm **1x found** ZIP-file XWEFVEFGSLLUFG

Known Natural Product

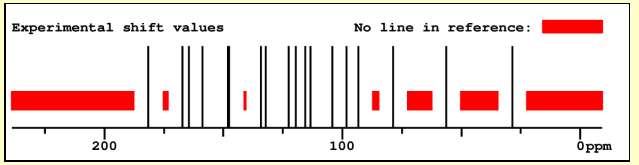
Pub Chem





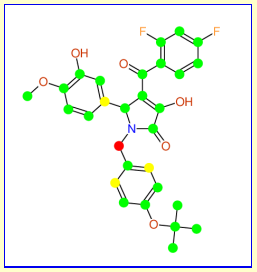


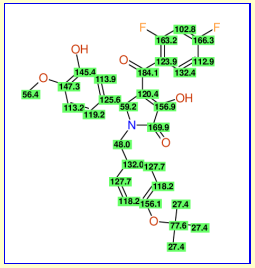
Different spectral pattern

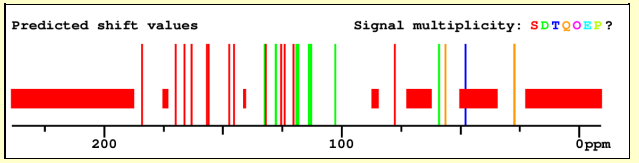


Structure proposal #74 Hide/Show Proposal **Molweight = 523.33 amu** **Molecular formula: $C_{29}H_{27}F_2NO_6$**

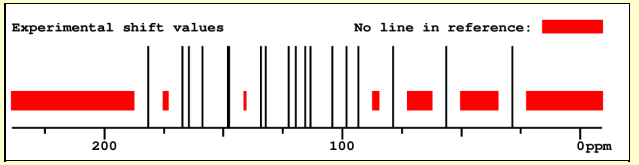
2.60 - 2.60ppm **1x found** ZIP-file ZBVLMEYGYPTOFY





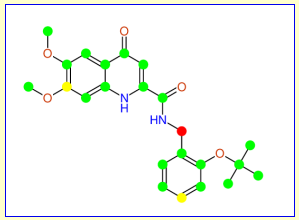


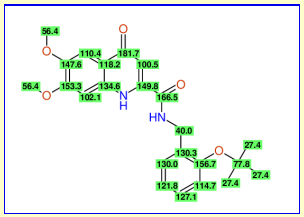
Different spectral pattern

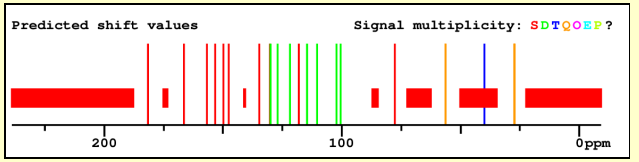


Structure proposal #75 Hide/Show Proposal **Molweight = 410.27 amu** **Molecular formula: $C_{23}H_{26}N_2O_5$**

2.61 - 2.61ppm **1x found** ZIP-file JNHKHVGMCKVKLN

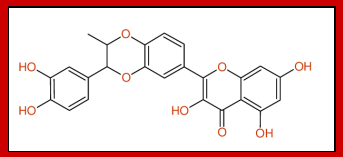


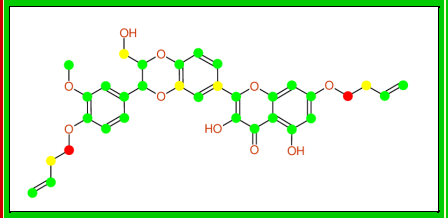


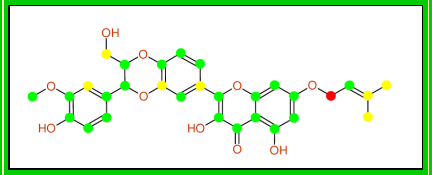


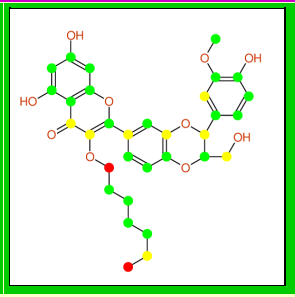
Different spectral pattern

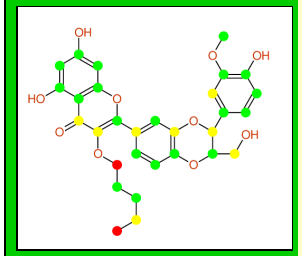
Summary of Ring Systems / Substitution Patterns found in Reference Compounds
Sorted by 1) Occurence and 2) Deviation

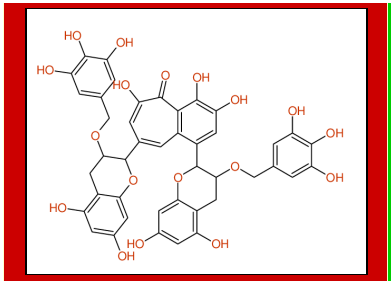


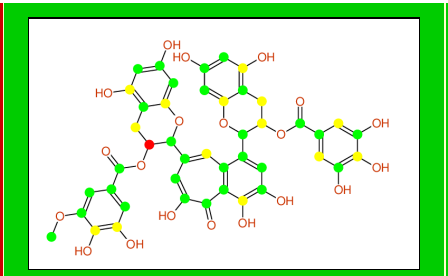


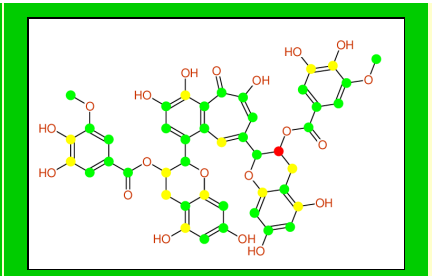


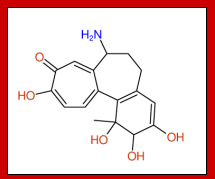


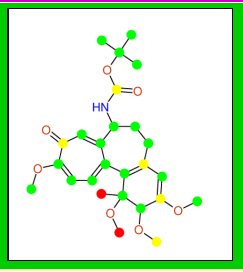


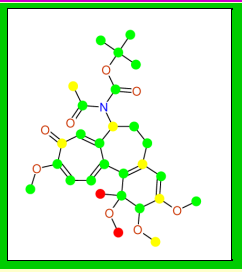


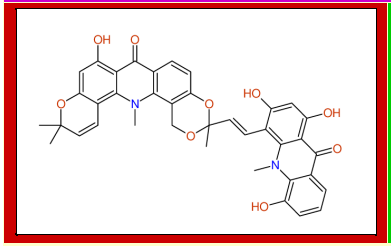


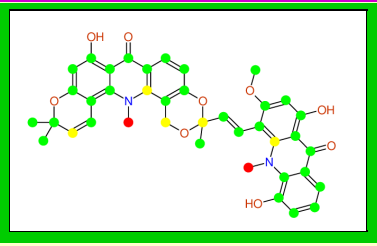


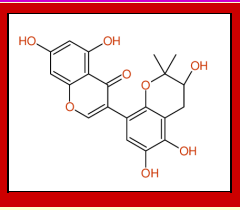


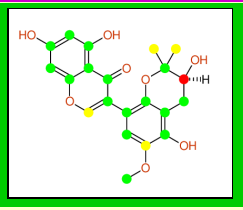


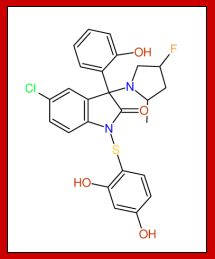
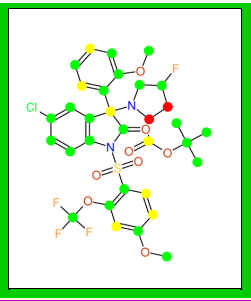
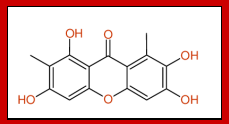
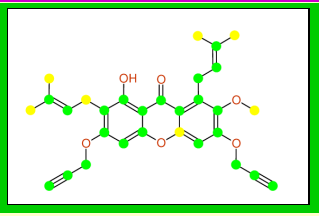
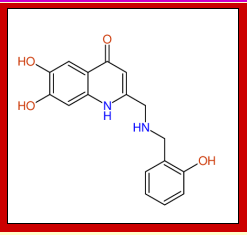
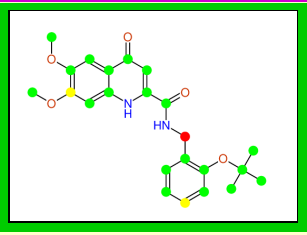
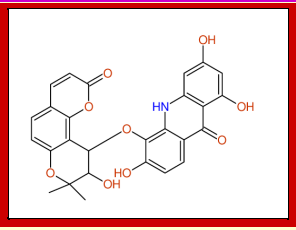
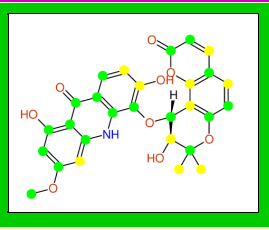
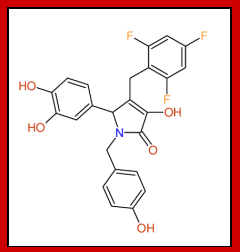
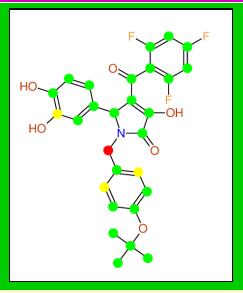


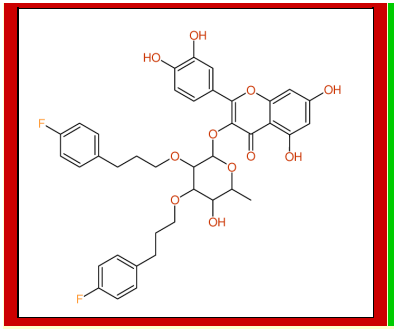
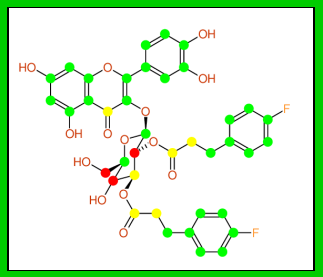
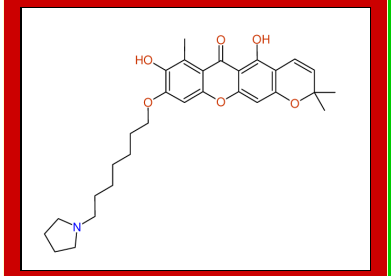
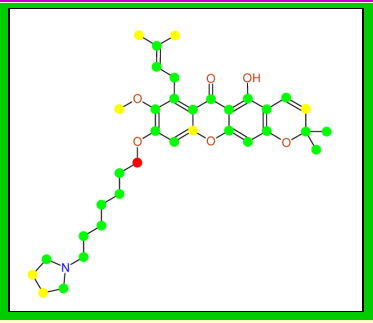
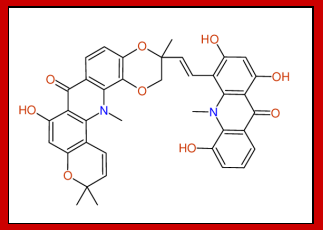
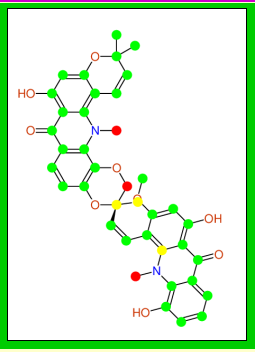
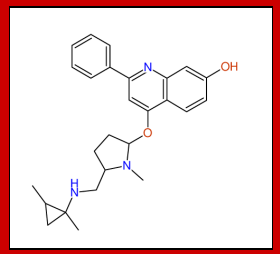
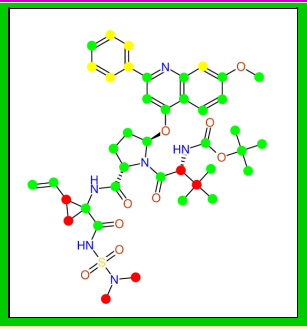


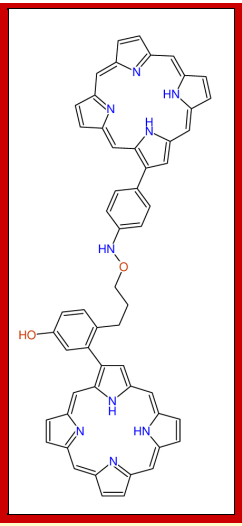




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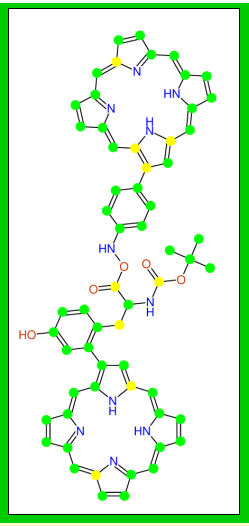
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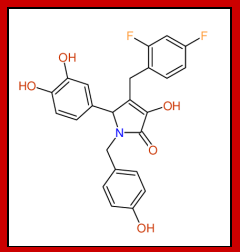
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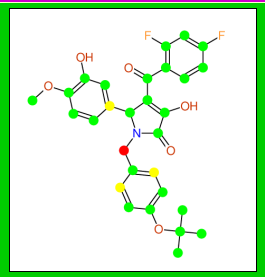
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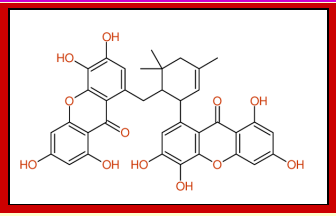
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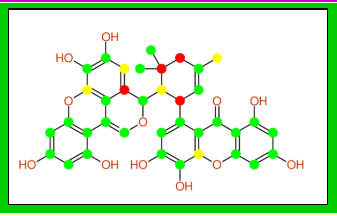
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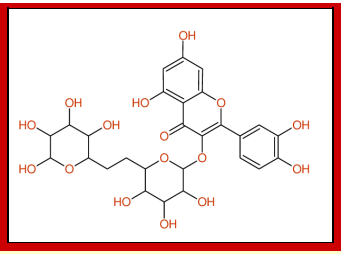

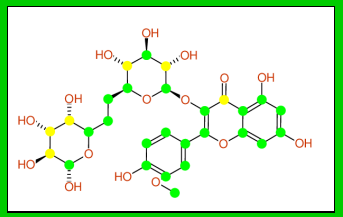

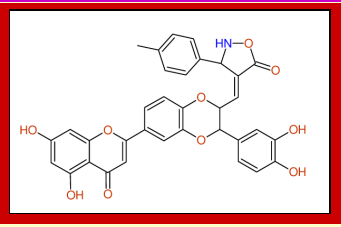

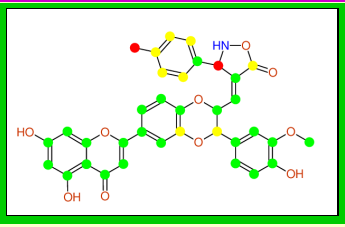

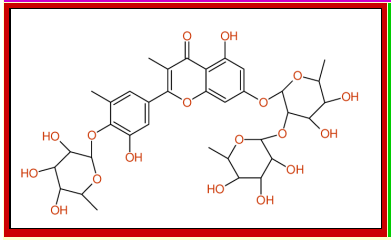

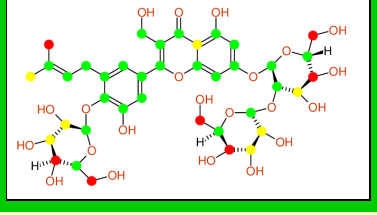

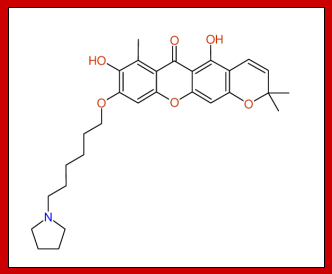

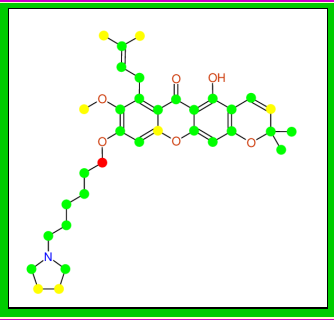

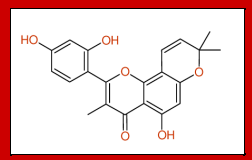

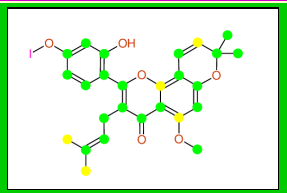

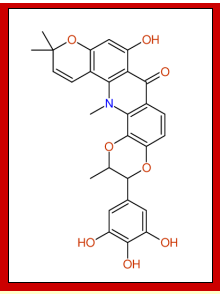

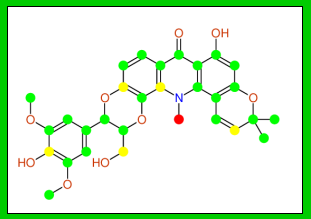

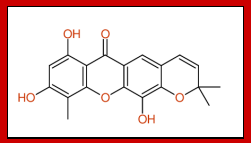

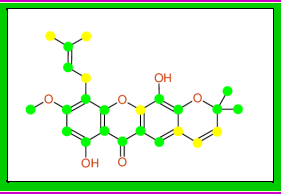

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