In [1]:

```
import pandas as pd
```

In [2]:

```
df = pd.read_csv('train_peptides.csv')
```

In [3]:

```
df.head()
```

Out[3]:

	visit_id	visit_month	patient_id	UniProt	Peptide	I
0	55_0	0	55	O00391	NEQEQPLGQWHLS	
1	55_0	0	55	O00533	GNPEPTFSWTK	
2	55_0	0	55	O00533	IEIPSSVQQVPTIIK	
3	55_0	0	55	O00533	KPQSAVYSTGSNGILLC(UniMod_4)EAEGEPQPTIK	
4	55_0	0	55	O00533	SMEQNGPGLEYR	

In [4]:

```
df.tail()
```

Out[4]:

	visit_id	visit_month	patient_id	UniProt	Peptide	F
981829	58648_108	108	58648	Q9UHG2	ILAGSADSEGVAAPR	
981830	58648_108	108	58648	Q9UKV8	SGNIPAGTTVDTK	
981831	58648_108	108	58648	Q9Y646	LALLVDTVGPR	
981832	58648_108	108	58648	Q9Y6R7	AGC(UniMod_4)VAESTAVC(UniMod_4)R	
981833	58648_108	108	58648	Q9Y6R7	GATTSPGVYELSSR	

In [5]:

```
df.shape
```

Out[5]:

```
(981834, 6)
```

In [6]:

```
df.columns
```

Out[6]:

```
Index(['visit_id', 'visit_month', 'patient_id', 'UniProt', 'Peptide',
       'PeptideAbundance'],
      dtype='object')
```

In [7]:

```
df.duplicated().sum()
```

Out[7]:

```
0
```

In [8]:

```
df.isnull().sum()
```

Out[8]:

```
visit_id            0
visit_month         0
patient_id          0
UniProt             0
Peptide             0
PeptideAbundance    0
dtype: int64
```

In [9]:

```
df.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 981834 entries, 0 to 981833
Data columns (total 6 columns):
 #   Column            Non-Null Count   Dtype  
---  ------            --------------   -----  
 0   visit_id          981834 non-null  object 
 1   visit_month       981834 non-null  int64  
 2   patient_id        981834 non-null  int64  
 3   UniProt           981834 non-null  object 
 4   Peptide           981834 non-null  object 
 5   PeptideAbundance  981834 non-null  float64
dtypes: float64(1), int64(2), object(3)
memory usage: 44.9+ MB
```

In [10]:

```
df.describe()
```

Out[10]:

	visit_month	patient_id	PeptideAbundance
count	981834.000000	981834.000000	9.818340e+05
mean	26.105061	32603.465361	6.428902e+05
std	22.913897	18605.934422	3.377989e+06
min	0.000000	55.000000	1.099850e+01
25%	6.000000	16566.000000	2.817425e+04
50%	24.000000	29313.000000	7.430830e+04
75%	48.000000	49995.000000	2.213388e+05
max	108.000000	65043.000000	1.787520e+08

In [11]:

```
df.nunique()
```

Out[11]:

```
visit_id              1113
visit_month             15
patient_id             248
UniProt                227
Peptide                968
PeptideAbundance    738931
dtype: int64
```

In [12]:

```
import matplotlib.pyplot as plt
import seaborn as sns
```

In [13]:

```
import warnings
warnings.filterwarnings('ignore')
```

In [14]:

```
df['visit_month'].unique()
```

Out[14]:

```
array([  0,   3,   6,  12,  18,  24,  30,  36,  48,  54,  60,  72,  84,
        96, 108], dtype=int64)
```

In [15]:

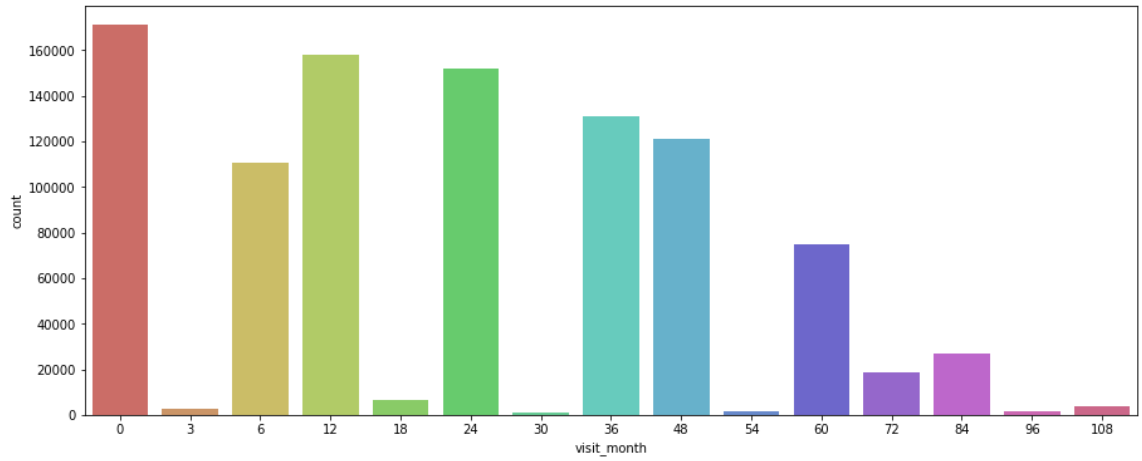
```
df['visit_month'].value_counts()
```

Out[15]:

```
0      171048
12     158114
24     152036
36     130903
48     121343
6      110733
60      74562
84      26729
72      18642
18       6822
108      3631
3        2742
96       1815
54       1801
30        913
Name: visit_month, dtype: int64
```

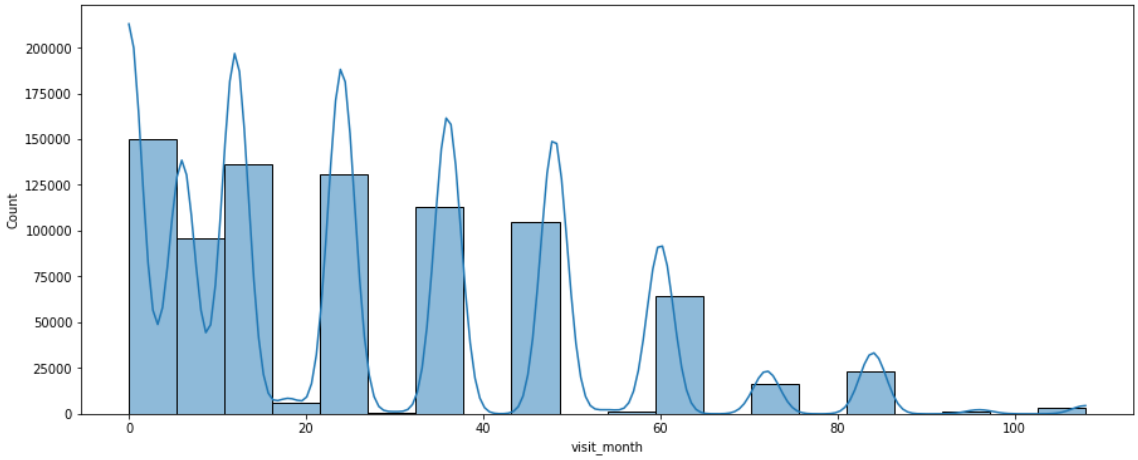
In [16]:

```
plt.figure(figsize=(15,6))
sns.countplot('visit_month', data = df, palette = 'hls')
plt.show()
```



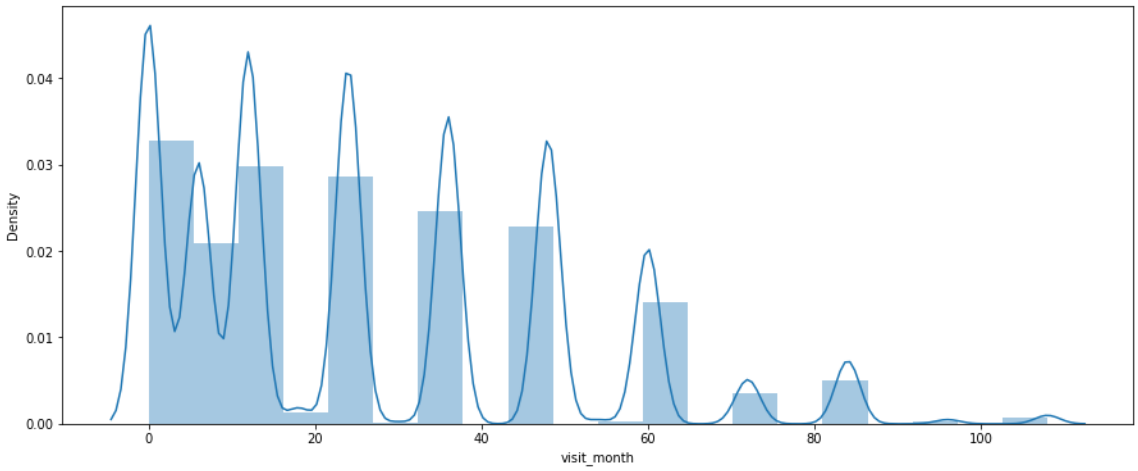
In [270]:

```
plt.figure(figsize=(15,6))
sns.histplot(df['visit_month'], kde = True, bins = 20, palette = 'hls')
plt.show()
```



In [272]:

```
plt.figure(figsize=(15,6))
sns.distplot(df['visit_month'], kde = True, bins = 20)
plt.show()
```



In [17]:

```
df['patient_id'].unique()
```

Out[17]:

```
array([   55,  1517,  1923,  2660,  3636,  3863,  4161,  4172,  5027,
        5178,  5645,  5742,  6054,  6211,  7051,  7117,  7568,  7832,
        8699, 10053, 10174, 10541, 10715, 10718, 11459, 11686, 11928,
       12516, 12636, 12703, 12755, 13368, 13618, 13968, 14035, 14124,
       14242, 14450, 14811, 15009, 15504, 15590, 16238, 16347, 16566,
       16574, 17154, 17414, 17727, 18183, 18204, 18553, 18560, 19088,
       20212, 20216, 20352, 20404, 20664, 20791, 21126, 21537, 21729,
       22126, 22623, 23192, 23244, 23391, 23636, 24278, 24690, 24820,
       24911, 25562, 25739, 25750, 25827, 25911, 26005, 26104, 26210,
       26809, 27079, 27300, 27464, 27468, 27715, 27971, 28327, 28342,
       28818, 29313, 29417, 30119, 30155, 30416, 30894, 30951, 31121,
       31154, 31693, 33548, 33558, 34182, 35231, 35465, 35477, 35675,
       35696, 36797, 37312, 37566, 38419, 39144, 40022, 40200, 40340,
       40751, 40874, 40967, 41444, 41617, 41628, 41871, 41883, 41930,
       42003, 42385, 42579, 44001, 44154, 44682, 45161, 45181, 46837,
       47103, 47513, 47881, 48780, 48928, 49239, 49672, 49683, 49995,
       50611, 50907, 51243, 51879, 51893, 51899, 52266, 53103, 54095,
       54406, 55240, 55256, 55302, 55662, 56073, 56075, 56119, 56317,
       56675, 56691, 56727, 57009, 57321, 57416, 57478, 57507, 57646,
       58189, 58270, 58648, 58653, 58823, 59550, 59574, 60170, 60326,
       60443, 60803, 61503, 61974, 62329, 62437, 62723, 62732, 62792,
       63875, 63889, 64669, 64674, 65043, 23175, 56538, 57468,   942,
        5036,  7151,  8344, 13360, 13852, 14270, 15245, 16778, 16931,
       20581, 20707, 24818, 31270, 33108, 37220, 40798, 44789, 47171,
       52119, 55096, 57108, 58674, 60788,  4923,  6420,  7265,  7886,
       10138, 13804, 14344, 17201, 20460, 20792, 27607, 27872, 27893,
       27987, 39719, 40650, 40876, 40980, 42086, 45662, 51708, 51846,
       52998, 54979, 58597,  7508, 12931], dtype=int64)
```

In [18]:

```
df['patient_id'].value_counts()
```

Out[18]:

```
20404    8272
23391    8147
62723    8111
26210    8076
18183    7965
         ...
55240    1810
52119    1804
25911    1782
42086    1781
41930     876
Name: patient_id, Length: 248, dtype: int64
```

In [19]:

```
df['UniProt'].unique()
```

Out[19]:

```
array(['O00391', 'O00533', 'O00584', 'O14498', 'O14773', 'O14791',
       'O15240', 'O15394', 'O43505', 'O60888', 'O75144', 'O75326',
       'O94919', 'P00441', 'P00450', 'P00734', 'P00736', 'P00738',
       'P00746', 'P00747', 'P00748', 'P00751', 'P01008', 'P01009',
       'P01011', 'P01019', 'P01023', 'P01024', 'P01031', 'P01033',
       'P01034', 'P01042', 'P01344', 'P01591', 'P01608', 'P01621',
       'P01717', 'P01780', 'P01833', 'P01834', 'P01857', 'P01859',
       'P01860', 'P01861', 'P01876', 'P01877', 'P02452', 'P02647',
       'P02649', 'P02652', 'P02655', 'P02656', 'P02671', 'P02675',
       'P02679', 'P02747', 'P02748', 'P02749', 'P02750', 'P02751',
       'P02753', 'P02760', 'P02763', 'P02765', 'P02766', 'P02768',
       'P02774', 'P02787', 'P02790', 'P04004', 'P04075', 'P04156',
       'P04180', 'P04196', 'P04207', 'P04211', 'P04216', 'P04217',
       'P04275', 'P04406', 'P04433', 'P05060', 'P05067', 'P05090',
       'P05155', 'P05156', 'P05408', 'P05452', 'P05546', 'P06310',
       'P06396', 'P06454', 'P06681', 'P06727', 'P07195', 'P07225',
       'P07333', 'P07339', 'P07602', 'P07711', 'P07858', 'P07998',
       'P08123', 'P08133', 'P08253', 'P08294', 'P08493', 'P08571',
       'P08603', 'P08637', 'P08697', 'P09104', 'P09486', 'P09871',
       'P10451', 'P10643', 'P10645', 'P10909', 'P11142', 'P11277',
       'P12109', 'P13473', 'P13521', 'P13591', 'P13611', 'P13671',
       'P13987', 'P14174', 'P14314', 'P14618', 'P16035', 'P16070',
       'P16152', 'P16870', 'P17174', 'P17936', 'P18065', 'P19021',
       'P19652', 'P19823', 'P19827', 'P20774', 'P20933', 'P23083',
       'P23142', 'P24592', 'P25311', 'P27169', 'P30086', 'P31997',
       'P35542', 'P36222', 'P36955', 'P36980', 'P39060', 'P40925',
       'P41222', 'P43121', 'P43251', 'P43652', 'P49588', 'P49908',
       'P51884', 'P54289', 'P55290', 'P61278', 'P61626', 'P61769',
       'P61916', 'P80748', 'P98160', 'Q02818', 'Q06481', 'Q08380',
       'Q12805', 'Q12841', 'Q12907', 'Q13283', 'Q13332', 'Q13451',
       'Q13740', 'Q14118', 'Q14508', 'Q14515', 'Q14624', 'Q15904',
       'Q16270', 'Q16610', 'Q562R1', 'Q6UX71', 'Q6UXB8', 'Q6UXD5',
       'Q7Z3B1', 'Q7Z5P9', 'Q8IWV7', 'Q8N2S1', 'Q8NBJ4', 'Q8NE71',
       'Q92520', 'Q92823', 'Q92876', 'Q96BZ4', 'Q96KN2', 'Q96PD5',
       'Q96S96', 'Q99435', 'Q99674', 'Q99832', 'Q99969', 'Q9BY67',
       'Q9HDC9', 'Q9NQ79', 'Q9NYU2', 'Q9UBR2', 'Q9UBX5', 'Q9UHG2',
       'Q9UNU6', 'Q9Y646', 'Q9Y6R7', 'P01594', 'P02792', 'P32754',
       'P60174', 'Q13449', 'Q99683', 'Q99829', 'Q9UKV8'], dtype=object)
```

In [20]:

```
df['UniProt'].value_counts()
```

Out[20]:

```
P02787    51916
P02768    40900
P01024    35253
P02751    27370
P02649    23082
          ...
Q6UX71      661
P01780      654
Q562R1      616
Q99832      606
Q99829      489
Name: UniProt, Length: 227, dtype: int64
```

In [21]:

```
df['Peptide'].unique()
```

Out[21]:

```
array(['NEQEQPLGQWHLS', 'GNPEPTFSWTK', 'IEIPSSVQQVPTIIK',
       'KPQSAVYSTGSNGILLC(UniMod_4)EAEGEPQPTIK', 'SMEQNGPGLEYR',
       'TLKIENVSYQDKGNYR', 'VIAVNEVGR', 'VMTPAVYAPYDVK',
       'VNGSPVDNHPFAGDVVFPR', 'ELDLNSVLLK', 'HGTC(UniMod_4)AAQVDALNSQK
K',
       'ALPGTPVASSQPR', 'LFGGNFAHQASVAR', 'LYQQHGAGLFDVTR',
       'VTEPISAESGEQVER', 'AYQGVAAPFPK', 'QQETAAAETETR', 'THLGEALAPLS
K',
       'ASGSPEPAISWFR', 'NIINSDGGPYVC(UniMod_4)R', 'TALASGGVLDASGDYR',
       'TQSSLVPALTDFVR', 'ALMSPAGMLR', 'GLYDVVSVLR',
       'SEGLLAC(UniMod_4)GTNAR', 'ILEVVNQIQDEER', 'QALNTDYLDSDYQR',
       'ADDLGKGGNEESTKTGNAGSR', 'TLVVHEKADDLGKGGNEESTK', 'ALYLQYTDETF
R',
       'EVGPTNADPVC(UniMod_4)LAK', 'FNKNNEGTYYSPNYNPQSR', 'GAYPLSIEPIGV
R',
       'KAEEEHLGILGPQLHADVGDKVK', 'MFTTAPDQVDKEDEDFQESNK',
       'MYYSAVDPTKDIFTGLIGPM(UniMod_35)K', 'NNEGTYYSPNYNPQSR',
       'QYTDSTFRVPVER', 'SVPPSASHVAPTETFTYFWTVPK',
```

In [22]:

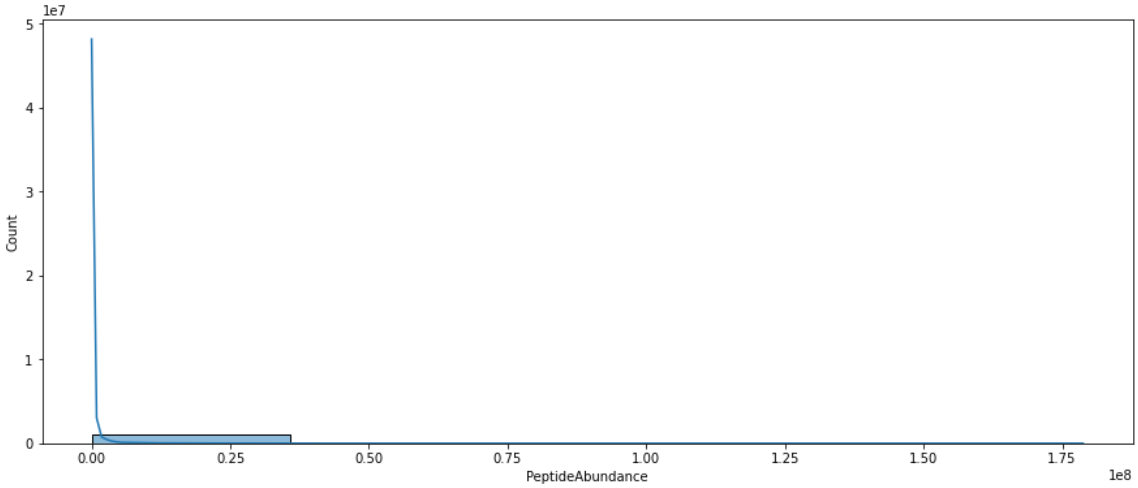
```
df['Peptide'].value_counts()
```

Out[22]:

```
TLLSNLEEAK                1113
IPTTFENGR                 1113
NILTSNNIDVK               1113
KYLYEIAR                  1113
AIGYLNTGYQR               1113
                          ...
HYEGSTVPEK                 605
SLEDQVEMLR                 599
TPSGLYLGTC(UniMod_4)ER     590
EPQVYTLPPSRDELTK           563
QALPQVR                    489
Name: Peptide, Length: 968, dtype: int64
```

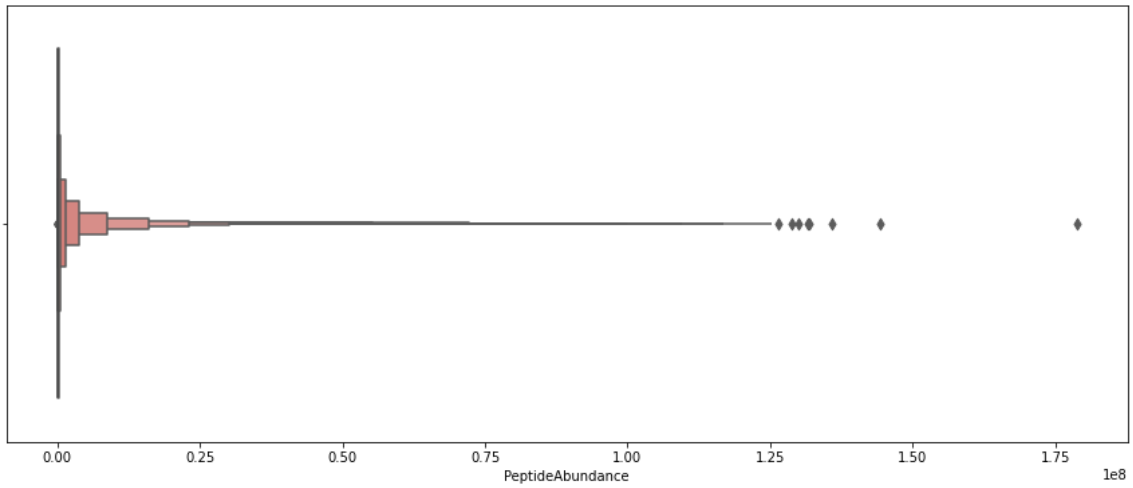
In [23]:

```
plt.figure(figsize=(15,6))
sns.histplot(df['PeptideAbundance'], bins = 5, kde = True, palette = 'hls')
plt.show()
```



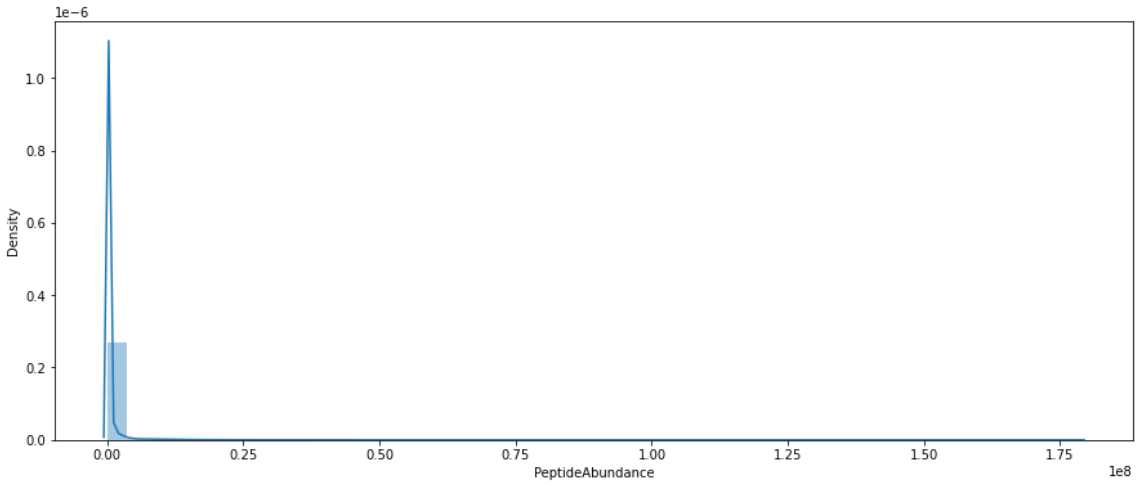
In [24]:

```
plt.figure(figsize=(15,6))
sns.boxenplot(df['PeptideAbundance'], palette = 'hls')
plt.show()
```



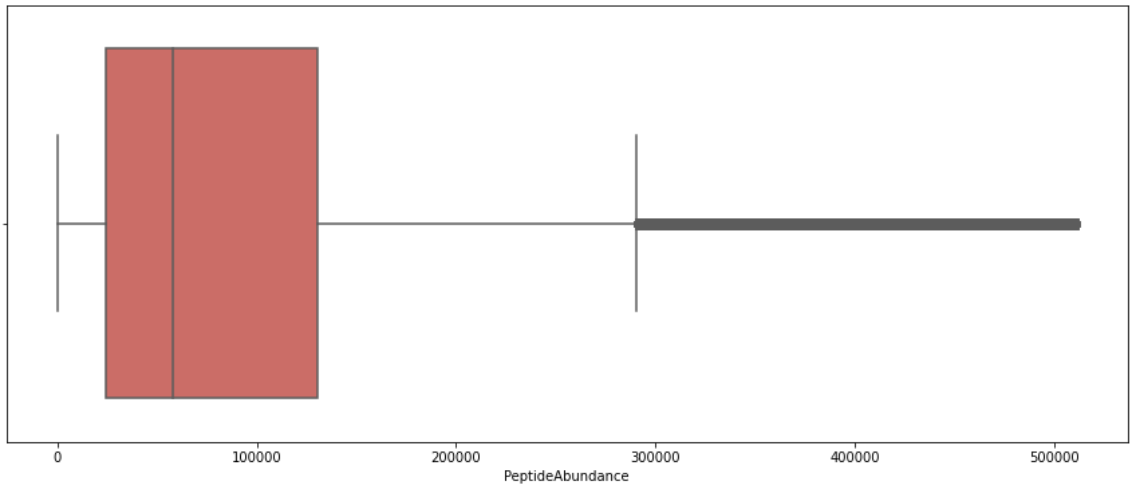
In [25]:

```
plt.figure(figsize=(15,6))
sns.distplot(df['PeptideAbundance'], kde = True)
plt.show()
```



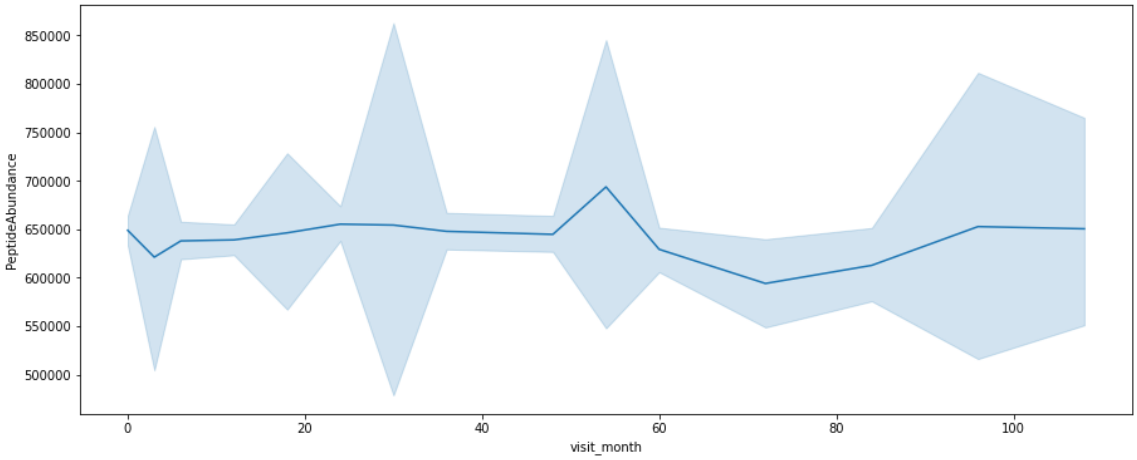
In [273]:

```
plt.figure(figsize=(15,6))
sns.boxplot(df['PeptideAbundance'], palette = 'hls')
plt.show()
```



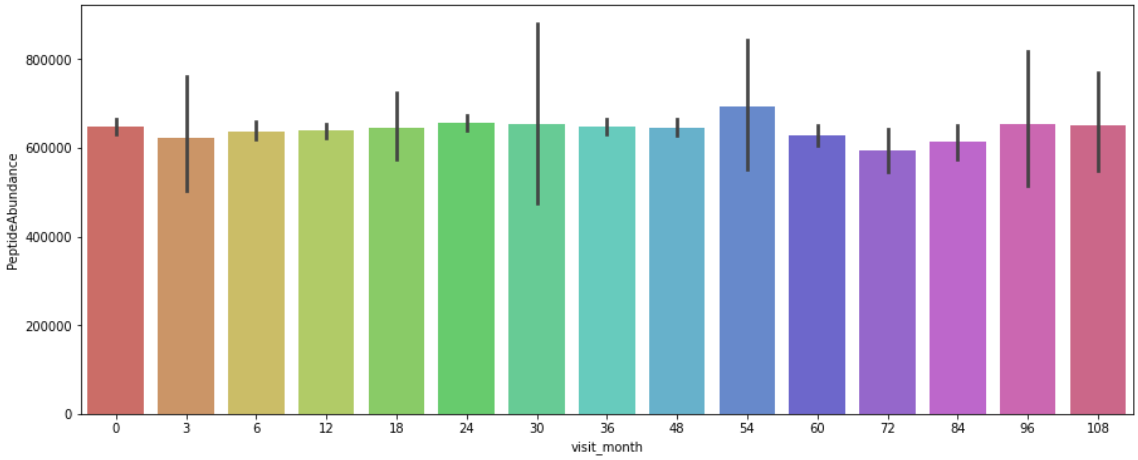
In [26]:

```
plt.figure(figsize=(15,6))
sns.lineplot(x = df['visit_month'], y = df['PeptideAbundance'], palette = 'hls')
plt.show()
```



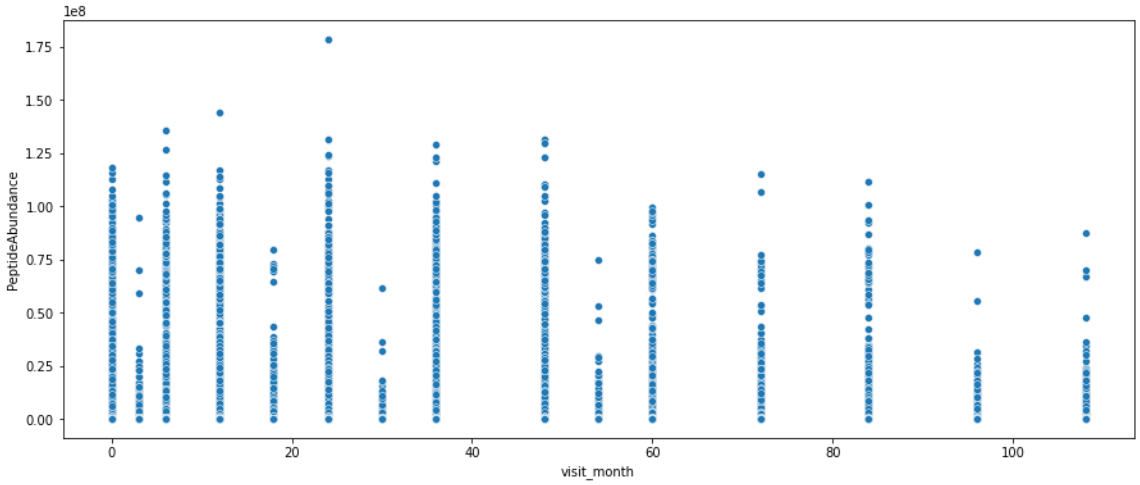
In [27]:

```
plt.figure(figsize=(15,6))
sns.barplot(x = df['visit_month'], y = df['PeptideAbundance'], palette = 'hls')
plt.show()
```



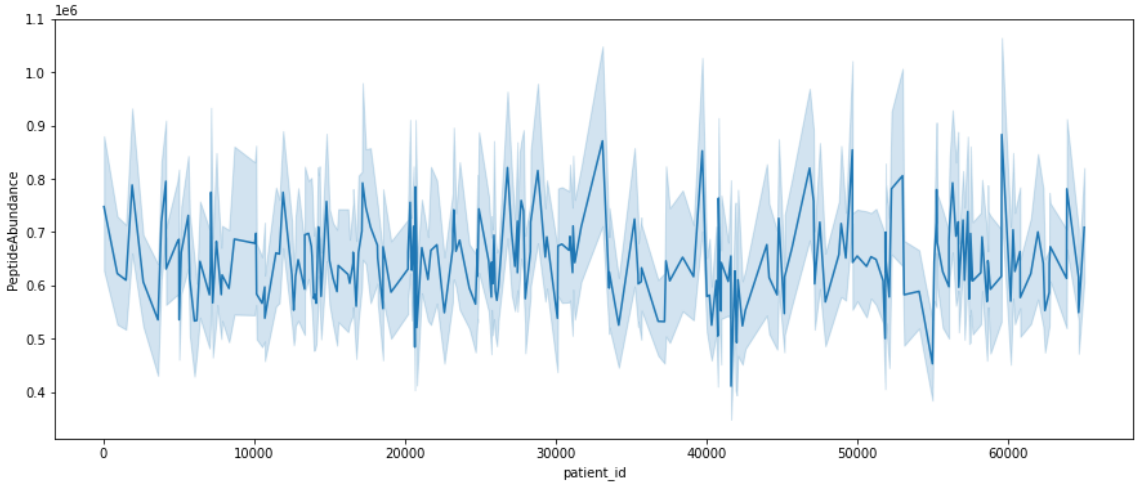
In [28]:

```
plt.figure(figsize=(15,6))
sns.scatterplot(x = df['visit_month'], y = df['PeptideAbundance'], palette = 'hls')
plt.show()
```



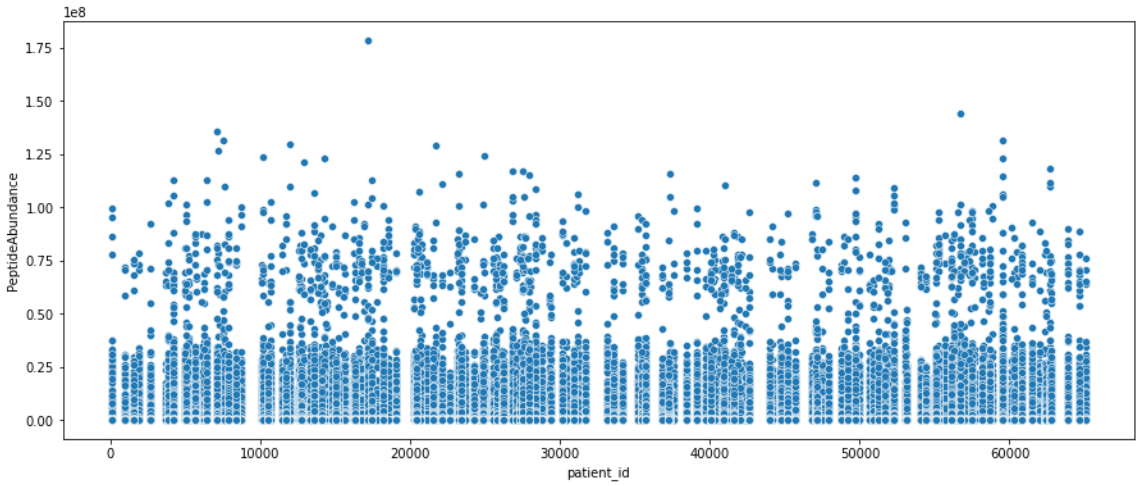
In [29]:

```
plt.figure(figsize=(15,6))
sns.lineplot(x = df['patient_id'], y = df['PeptideAbundance'], palette = 'hls')
plt.show()
```



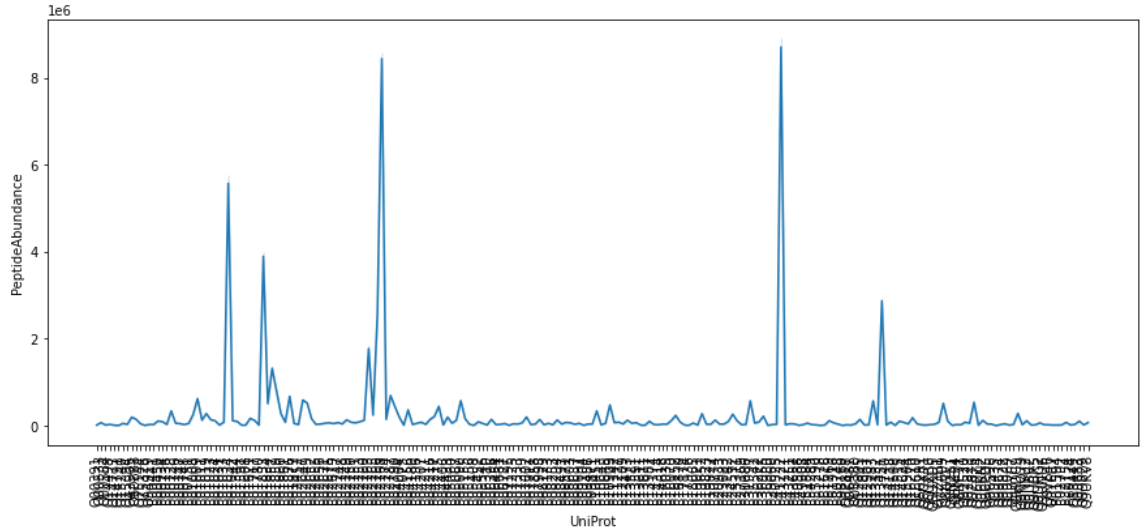
In [30]:

```
plt.figure(figsize=(15,6))
sns.scatterplot(x = df['patient_id'], y = df['PeptideAbundance'], palette = 'hls')
plt.show()
```



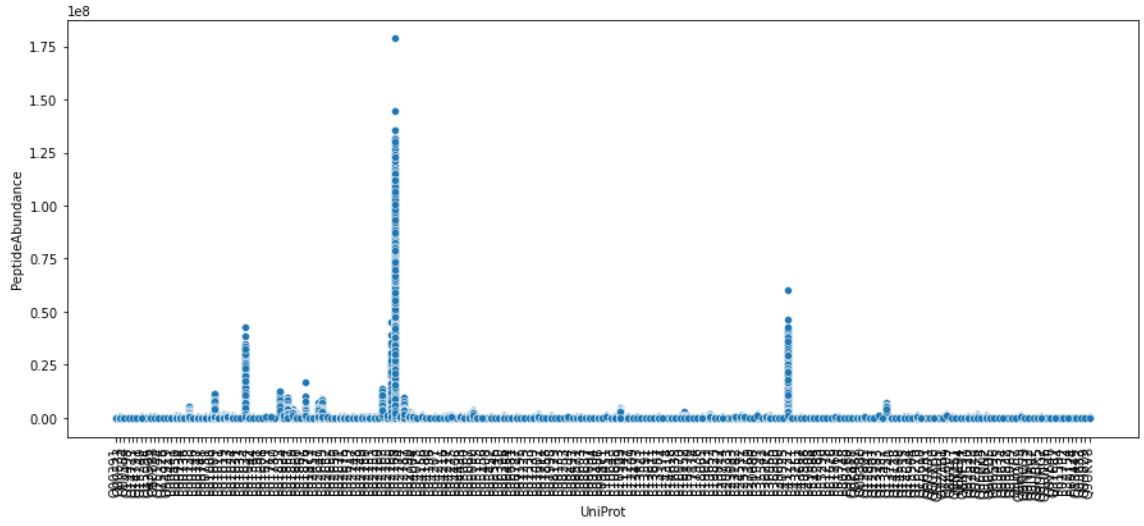
In [31]:

```
plt.figure(figsize=(15,6))
sns.lineplot(x = df['UniProt'], y = df['PeptideAbundance'], palette = 'hls')
plt.xticks(rotation = 90)
plt.show()
```



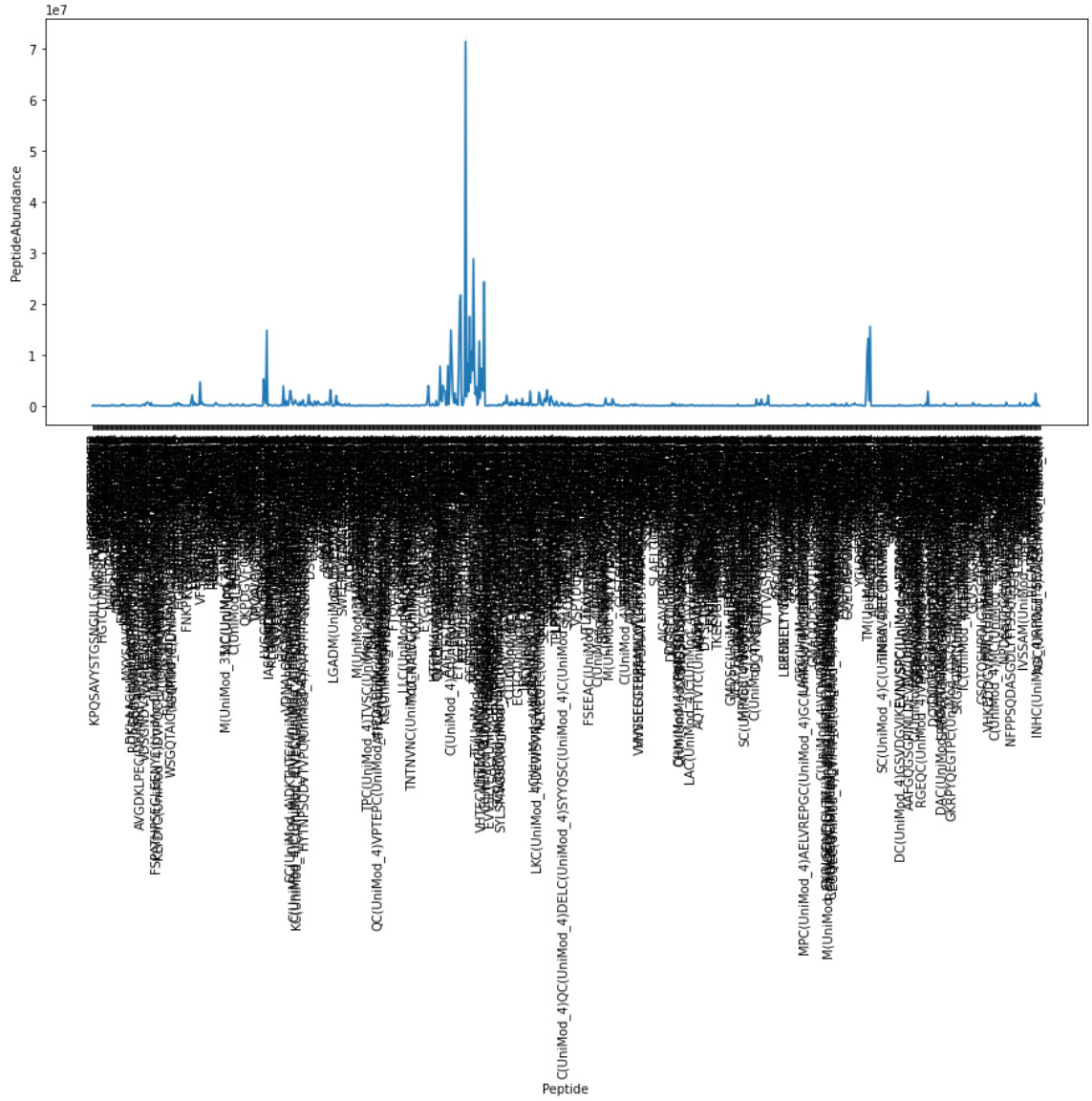
In [32]:

```
plt.figure(figsize=(15,6))
sns.scatterplot(x = df['UniProt'], y = df['PeptideAbundance'], palette = 'hls')
plt.xticks(rotation = 90)
plt.show()
```



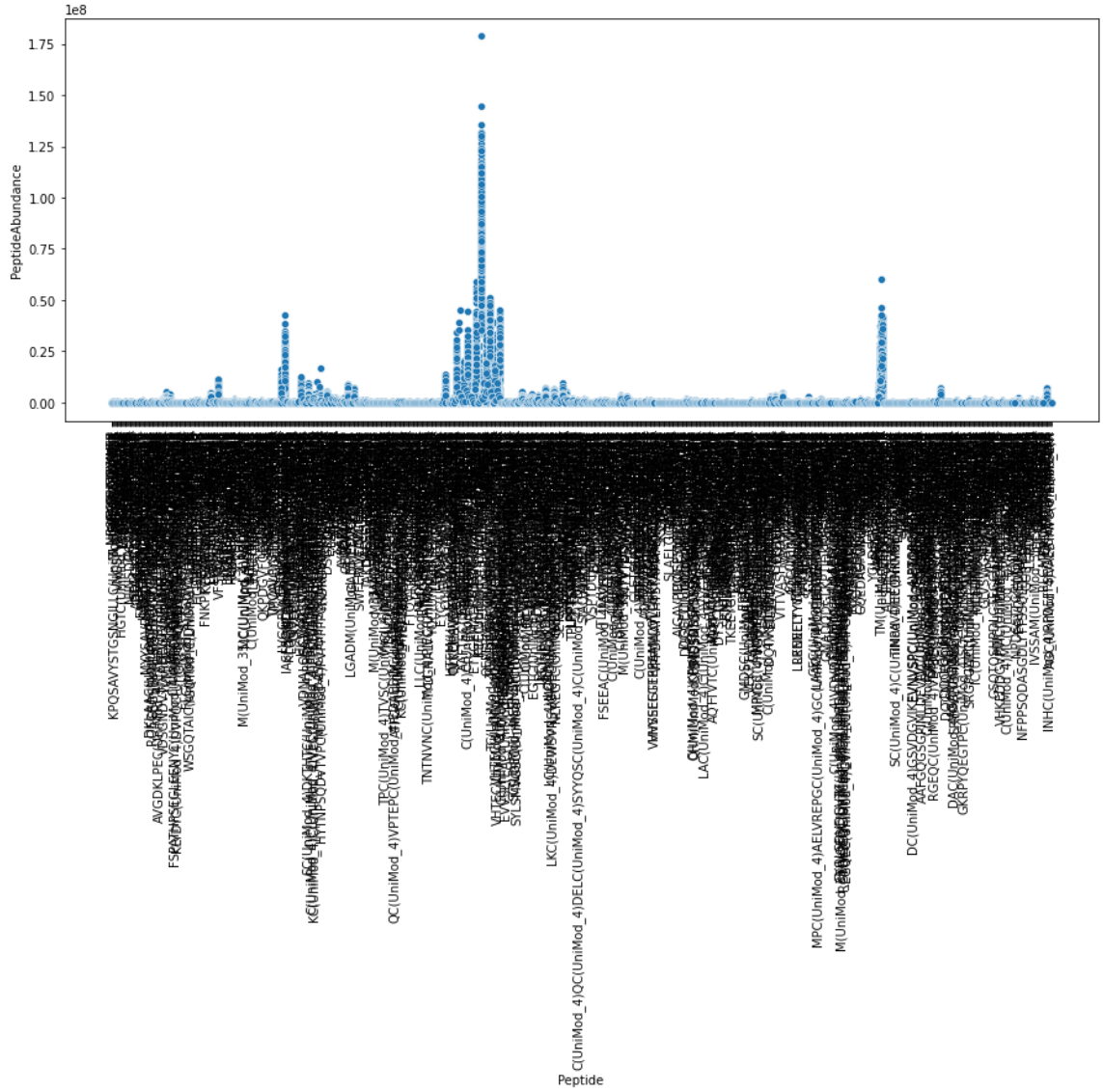
In [33]:

```
plt.figure(figsize=(15,6))
sns.lineplot(x = df['Peptide'], y = df['PeptideAbundance'], palette = 'hls')
plt.xticks(rotation = 90)
plt.show()
```



In [34]:

```
plt.figure(figsize=(15,6))
sns.scatterplot(x = df['Peptide'], y = df['PeptideAbundance'], palette = 'hls')
plt.xticks(rotation = 90)
plt.show()
```



In [36]:

```
Q1 = df.quantile(0.25)
Q3 = df.quantile(0.75)
IQR = Q3-Q1
```

In [37]:

```
print(IQR)
```

```
visit_month            42.0
patient_id          33429.0
PeptideAbundance    193164.5
dtype: float64
```

In [38]:

```
df = df[~((df < (Q1 - 1.5 * IQR)) |(df > (Q3 + 1.5 * IQR))).any(axis=1)]
```

In [39]:

```
df.shape
```

Out[39]:

```
(847363, 6)
```

In [40]:

```
df_corr = df.corr()
```

In [41]:

```
df_corr
```

Out[41]:

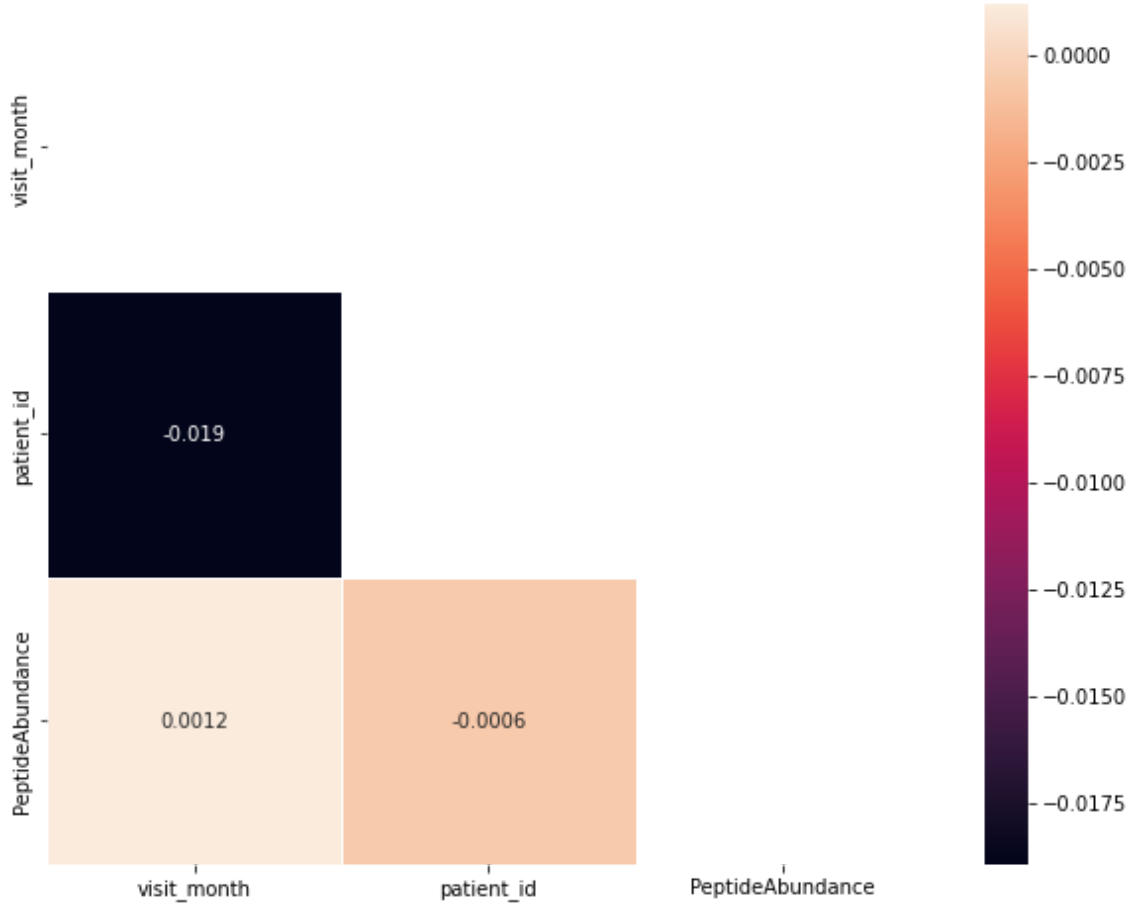
	visit_month	patient_id	PeptideAbundance
visit_month	1.000000	-0.018923	0.001200
patient_id	-0.018923	1.000000	-0.000602
PeptideAbundance	0.001200	-0.000602	1.000000

In [42]:

```
import numpy as np
```

In [43]:

```
plt.figure(figsize=(10, 8))
matrix = np.triu(df_corr)
sns.heatmap(df_corr, annot=True, linewidth=.8, mask=matrix, cmap="rocket");
plt.show()
```



In [45]:

```
df1 = pd.read_csv('train_proteins.csv')
```

In [46]:

```
df1.head()
```

Out[46]:

	visit_id	visit_month	patient_id	UniProt	NPX
0	55_0	0	55	O00391	11254.3
1	55_0	0	55	O00533	732430.0
2	55_0	0	55	O00584	39585.8
3	55_0	0	55	O14498	41526.9
4	55_0	0	55	O14773	31238.0

In [47]:

```
df1.tail()
```

Out[47]:

	visit_id	visit_month	patient_id	UniProt	NPX
232736	58648_108	108	58648	Q9UBX5	27387.8
232737	58648_108	108	58648	Q9UHG2	369437.0
232738	58648_108	108	58648	Q9UKV8	105830.0
232739	58648_108	108	58648	Q9Y646	21257.6
232740	58648_108	108	58648	Q9Y6R7	17953.1

In [48]:

```
df1.shape
```

Out[48]:

```
(232741, 5)
```

In [49]:

```
df1.columns
```

Out[49]:

```
Index(['visit_id', 'visit_month', 'patient_id', 'UniProt', 'NPX'], dtype
='object')
```

In [50]:

```
df1.duplicated().sum()
```

Out[50]:

```
0
```

In [51]:

```
df1.isnull().sum()
```

Out[51]:

```
visit_id       0
visit_month    0
patient_id     0
UniProt        0
NPX            0
dtype: int64
```

In [52]:

```
df1.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 232741 entries, 0 to 232740
Data columns (total 5 columns):
 #   Column       Non-Null Count   Dtype  
---  ------       --------------   -----  
 0   visit_id     232741 non-null  object 
 1   visit_month  232741 non-null  int64  
 2   patient_id   232741 non-null  int64  
 3   UniProt      232741 non-null  object 
 4   NPX          232741 non-null  float64
dtypes: float64(1), int64(2), object(2)
memory usage: 8.9+ MB
```

In [53]:

```
df1.describe()
```

Out[53]:

	visit_month	patient_id	NPX
count	232741.000000	232741.000000	2.327410e+05
mean	26.099205	32593.881873	2.712077e+06
std	22.874719	18608.479506	2.224155e+07
min	0.000000	55.000000	8.460820e+01
25%	6.000000	16566.000000	2.946440e+04
50%	24.000000	29313.000000	1.135560e+05
75%	48.000000	49995.000000	5.638940e+05
max	108.000000	65043.000000	6.138510e+08

In [54]:

```
df1.nunique()
```

Out[54]:

```
visit_id         1113
visit_month        15
patient_id        248
UniProt           227
NPX            218795
dtype: int64
```

In [55]:

```
df1['visit_month'].unique()
```

Out[55]:

```
array([  0,   3,   6,  12,  18,  24,  30,  36,  48,  54,  60,  72,  84,
        96, 108], dtype=int64)
```

In [56]:

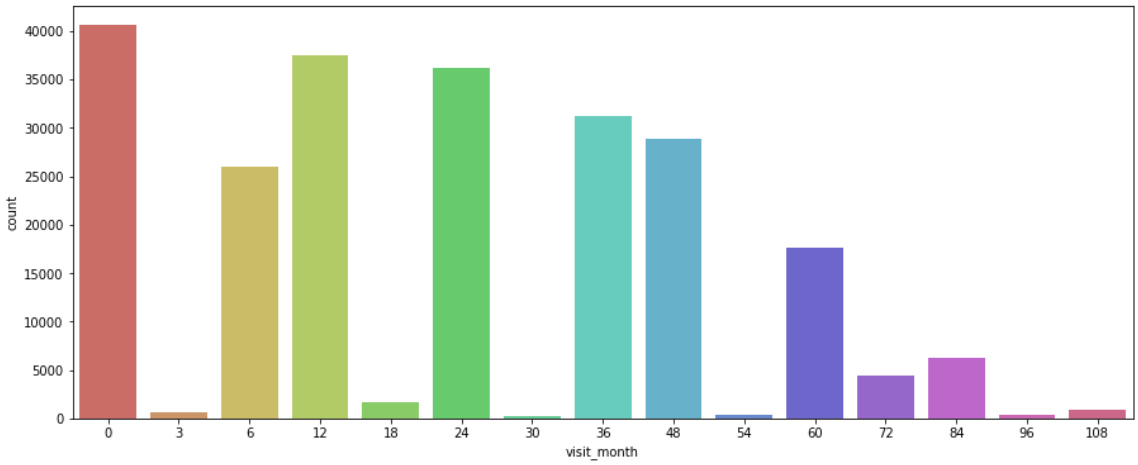
```
df1['visit_month'].value_counts()
```

Out[56]:

```
0      40587
12     37467
24     36225
36     31156
48     28838
6      25991
60     17572
84      6288
72      4407
18      1657
108      855
3        641
96       423
54       418
30       216
Name: visit_month, dtype: int64
```

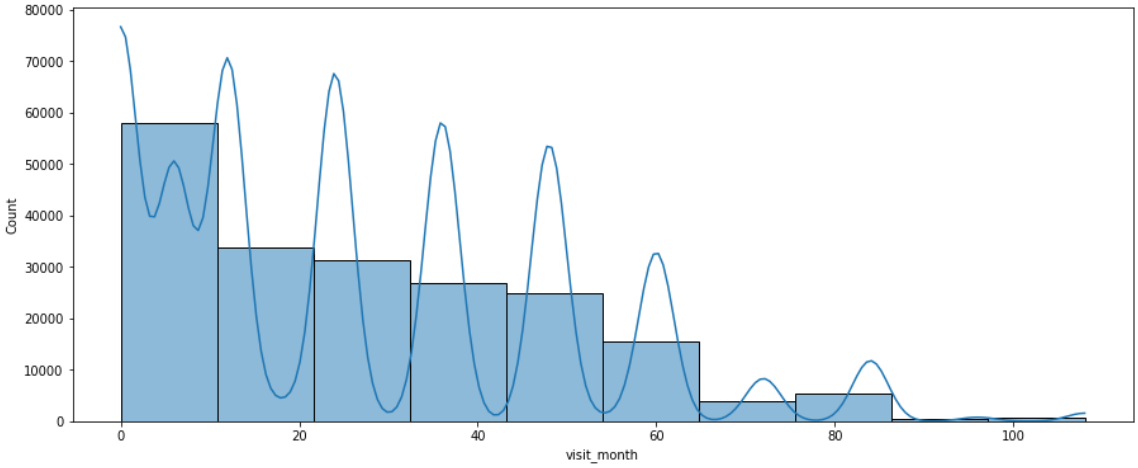
In [57]:

```
plt.figure(figsize=(15,6))
sns.countplot('visit_month', data = df1, palette = 'hls')
plt.show()
```



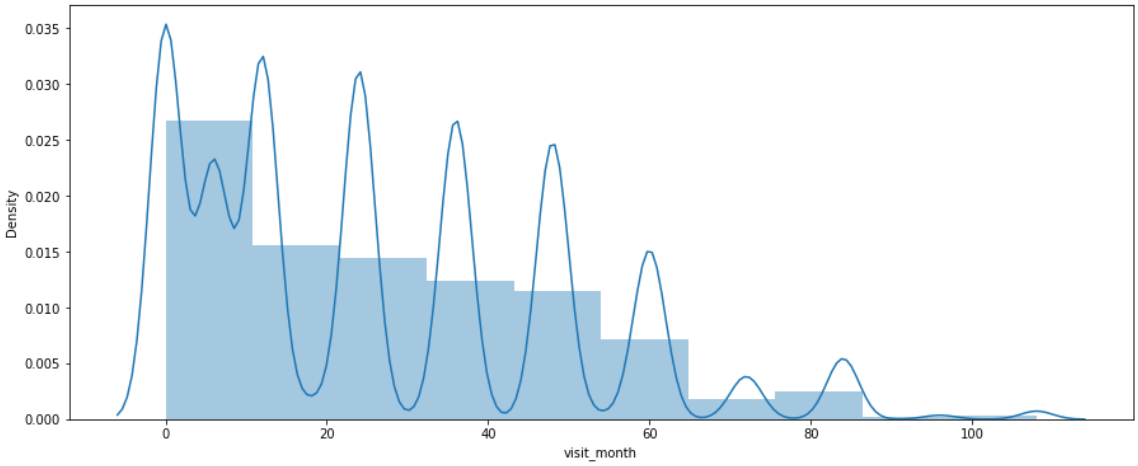
In [274]:

```
plt.figure(figsize=(15,6))
sns.histplot(df1['visit_month'], kde = True, bins = 10, palette = 'hls')
plt.show()
```



In [275]:

```
plt.figure(figsize=(15,6))
sns.distplot(df1['visit_month'], kde = True, bins = 10)
plt.show()
```



In [58]:

```
df1['patient_id'].unique()
```

Out[58]:

```
array([   55,  1517,  1923,  2660,  3636,  3863,  4161,  4172,  5027,
        5178,  5645,  5742,  6054,  6211,  7051,  7117,  7568,  7832,
        8699, 10053, 10174, 10541, 10715, 10718, 11459, 11686, 11928,
       12516, 12636, 12703, 12755, 13368, 13618, 13968, 14035, 14124,
       14242, 14450, 14811, 15009, 15504, 15590, 16238, 16347, 16566,
       16574, 17154, 17414, 17727, 18183, 18204, 18553, 18560, 19088,
       20212, 20216, 20352, 20404, 20664, 20791, 21126, 21537, 21729,
       22126, 22623, 23192, 23244, 23391, 23636, 24278, 24690, 24820,
       24911, 25562, 25739, 25750, 25827, 25911, 26005, 26104, 26210,
       26809, 27079, 27300, 27464, 27468, 27715, 27971, 28327, 28342,
       28818, 29313, 29417, 30119, 30155, 30416, 30894, 30951, 31121,
       31154, 31693, 33548, 33558, 34182, 35231, 35465, 35477, 35675,
       35696, 36797, 37312, 37566, 38419, 39144, 40022, 40200, 40340,
       40751, 40874, 40967, 41444, 41617, 41628, 41871, 41883, 41930,
       42003, 42385, 42579, 44001, 44154, 44682, 45161, 45181, 46837,
       47103, 47513, 47881, 48780, 48928, 49239, 49672, 49683, 49995,
       50611, 50907, 51243, 51879, 51893, 51899, 52266, 53103, 54095,
       54406, 55240, 55256, 55302, 55662, 56073, 56075, 56119, 56317,
       56675, 56691, 56727, 57009, 57321, 57416, 57478, 57507, 57646,
       58189, 58270, 58648, 58653, 58823, 59550, 59574, 60170, 60326,
       60443, 60803, 61503, 61974, 62329, 62437, 62723, 62732, 62792,
       63875, 63889, 64669, 64674, 65043, 23175, 56538, 57468,   942,
        5036,  7151,  8344, 13360, 13852, 14270, 15245, 16778, 16931,
       20581, 20707, 24818, 31270, 33108, 37220, 40798, 44789, 47171,
       52119, 55096, 57108, 58674, 60788,  4923,  6420,  7265,  7886,
       10138, 13804, 14344, 17201, 20460, 20792, 27607, 27872, 27893,
       27987, 39719, 40650, 40876, 40980, 42086, 45662, 51708, 51846,
       52998, 54979, 58597,  7508, 12931], dtype=int64)
```

In [59]:

```
df1['patient_id'].value_counts()
```

Out[59]:

```
62723    1929
20404    1924
23391    1919
26210    1912
18183    1899
         ...
55240     429
42086     427
25911     419
52119     417
41930     199
Name: patient_id, Length: 248, dtype: int64
```

In [60]:

```
df1['UniProt'].unique()
```

Out[60]:

```
array(['O00391', 'O00533', 'O00584', 'O14498', 'O14773', 'O14791',
       'O15240', 'O15394', 'O43505', 'O60888', 'O75144', 'O75326',
       'O94919', 'P00441', 'P00450', 'P00734', 'P00736', 'P00738',
       'P00746', 'P00747', 'P00748', 'P00751', 'P01008', 'P01009',
       'P01011', 'P01019', 'P01023', 'P01024', 'P01031', 'P01033',
       'P01034', 'P01042', 'P01344', 'P01591', 'P01608', 'P01621',
       'P01717', 'P01780', 'P01833', 'P01834', 'P01857', 'P01859',
       'P01860', 'P01861', 'P01876', 'P01877', 'P02452', 'P02647',
       'P02649', 'P02652', 'P02655', 'P02656', 'P02671', 'P02675',
       'P02679', 'P02747', 'P02748', 'P02749', 'P02750', 'P02751',
       'P02753', 'P02760', 'P02763', 'P02765', 'P02766', 'P02768',
       'P02774', 'P02787', 'P02790', 'P04004', 'P04075', 'P04156',
       'P04180', 'P04196', 'P04207', 'P04211', 'P04216', 'P04217',
       'P04275', 'P04406', 'P04433', 'P05060', 'P05067', 'P05090',
       'P05155', 'P05156', 'P05408', 'P05452', 'P05546', 'P06310',
       'P06396', 'P06454', 'P06681', 'P06727', 'P07195', 'P07225',
       'P07333', 'P07339', 'P07602', 'P07711', 'P07858', 'P07998',
       'P08123', 'P08133', 'P08253', 'P08294', 'P08493', 'P08571',
       'P08603', 'P08637', 'P08697', 'P09104', 'P09486', 'P09871',
       'P10451', 'P10643', 'P10645', 'P10909', 'P11142', 'P11277',
       'P12109', 'P13473', 'P13521', 'P13591', 'P13611', 'P13671',
       'P13987', 'P14174', 'P14314', 'P14618', 'P16035', 'P16070',
       'P16152', 'P16870', 'P17174', 'P17936', 'P18065', 'P19021',
       'P19652', 'P19823', 'P19827', 'P20774', 'P20933', 'P23083',
       'P23142', 'P24592', 'P25311', 'P27169', 'P30086', 'P31997',
       'P35542', 'P36222', 'P36955', 'P36980', 'P39060', 'P40925',
       'P41222', 'P43121', 'P43251', 'P43652', 'P49588', 'P49908',
       'P51884', 'P54289', 'P55290', 'P61278', 'P61626', 'P61769',
       'P61916', 'P80748', 'P98160', 'Q02818', 'Q06481', 'Q08380',
       'Q12805', 'Q12841', 'Q12907', 'Q13283', 'Q13332', 'Q13451',
       'Q13740', 'Q14118', 'Q14508', 'Q14515', 'Q14624', 'Q15904',
       'Q16270', 'Q16610', 'Q562R1', 'Q6UX71', 'Q6UXB8', 'Q6UXD5',
       'Q7Z3B1', 'Q7Z5P9', 'Q8IWV7', 'Q8N2S1', 'Q8NBJ4', 'Q8NE71',
       'Q92520', 'Q92823', 'Q92876', 'Q96BZ4', 'Q96KN2', 'Q96PD5',
       'Q96S96', 'Q99435', 'Q99674', 'Q99832', 'Q99969', 'Q9BY67',
       'Q9HDC9', 'Q9NQ79', 'Q9NYU2', 'Q9UBR2', 'Q9UBX5', 'Q9UHG2',
       'Q9UNU6', 'Q9Y646', 'Q9Y6R7', 'P01594', 'P02792', 'P32754',
       'P60174', 'Q13449', 'Q99683', 'Q99829', 'Q9UKV8'], dtype=object)
```

In [61]:

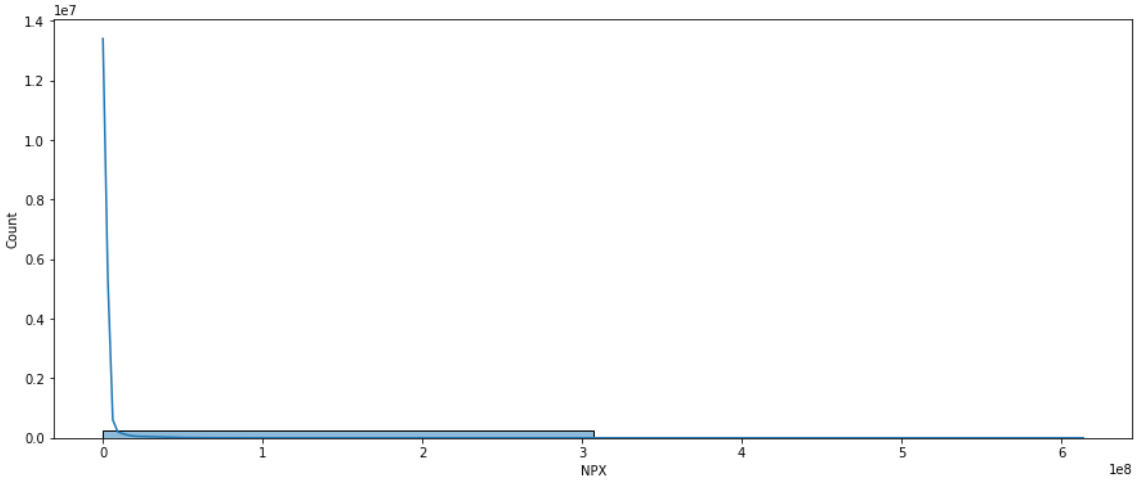
```
df1['UniProt'].value_counts()
```

Out[61]:

```
P01024    1113
P05090    1113
P01011    1113
P01023    1113
Q92520    1113
          ...
Q6UX71     661
P01780     654
Q562R1     616
Q99832     606
Q99829     489
Name: UniProt, Length: 227, dtype: int64
```

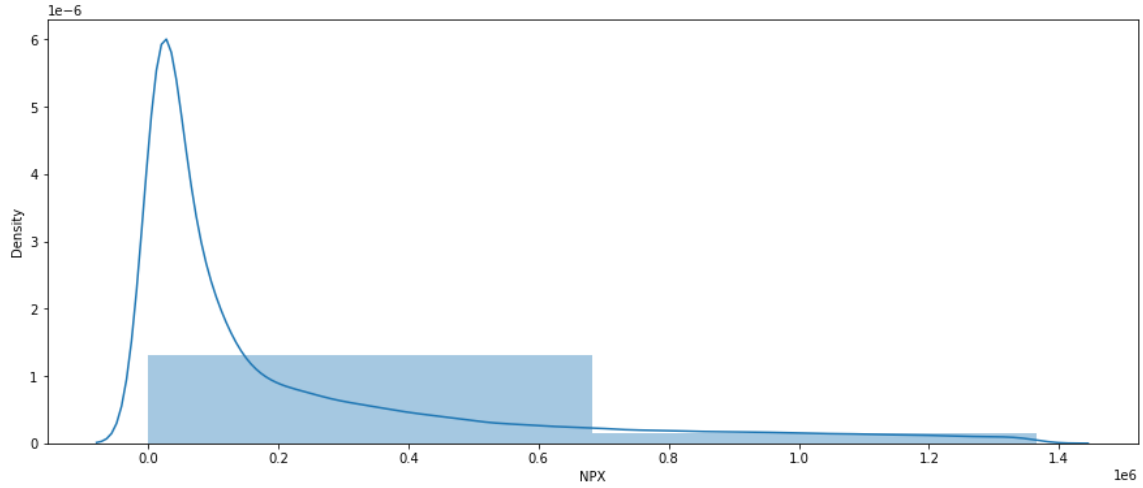
In [68]:

```
plt.figure(figsize=(15,6))
sns.histplot(df1['NPX'], kde = True, bins = 2, palette = 'hls')
plt.show()
```



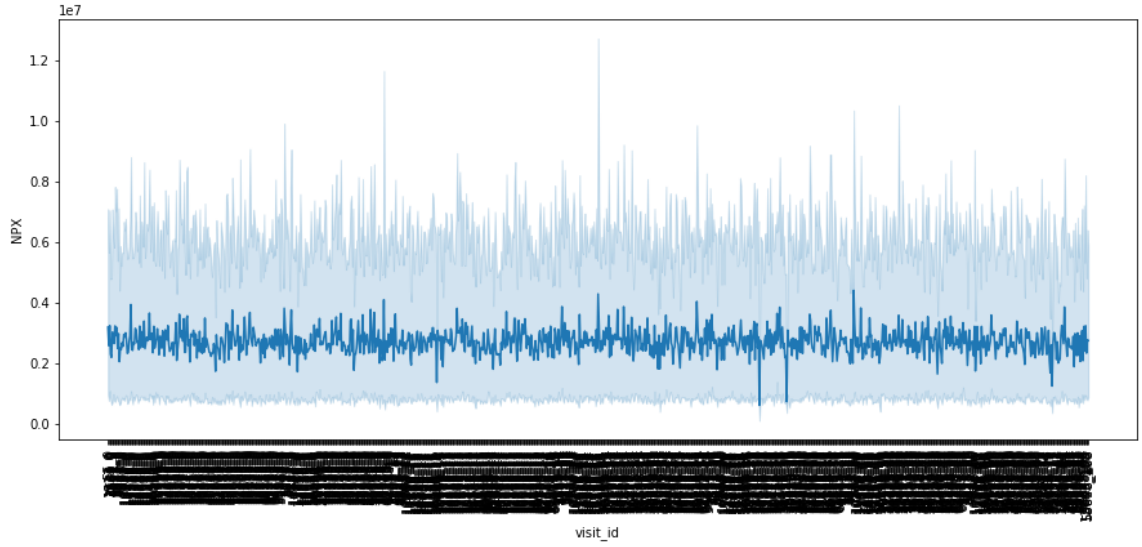
In [276]:

```
plt.figure(figsize=(15,6))
sns.distplot(df1['NPX'], kde = True, bins = 2)
plt.show()
```



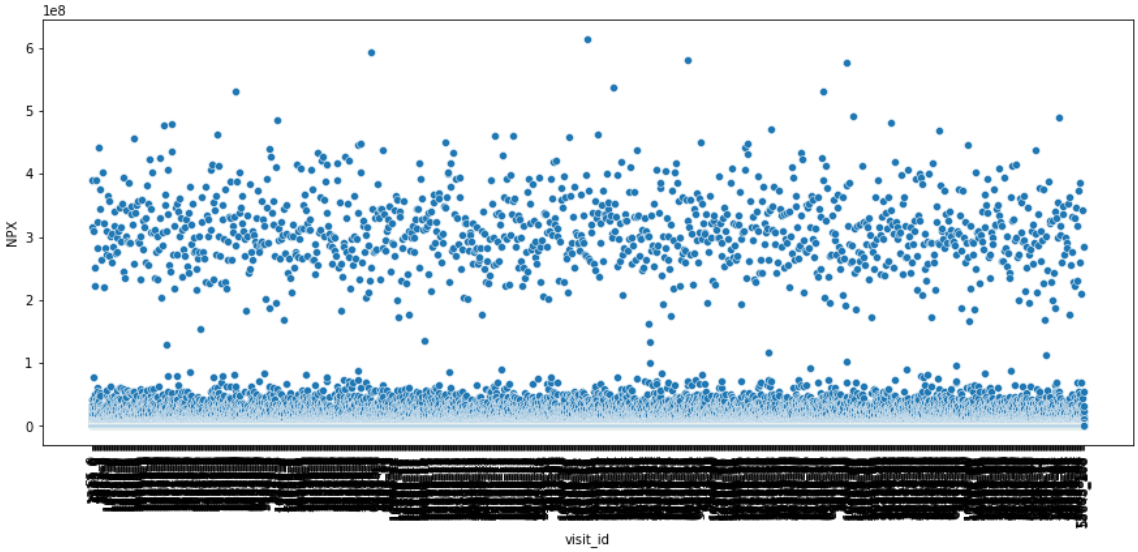
In [70]:

```
plt.figure(figsize=(15,6))
sns.lineplot(x = df1['visit_id'], y = df1['NPX'], palette = 'hls')
plt.xticks(rotation = 90)
plt.show()
```



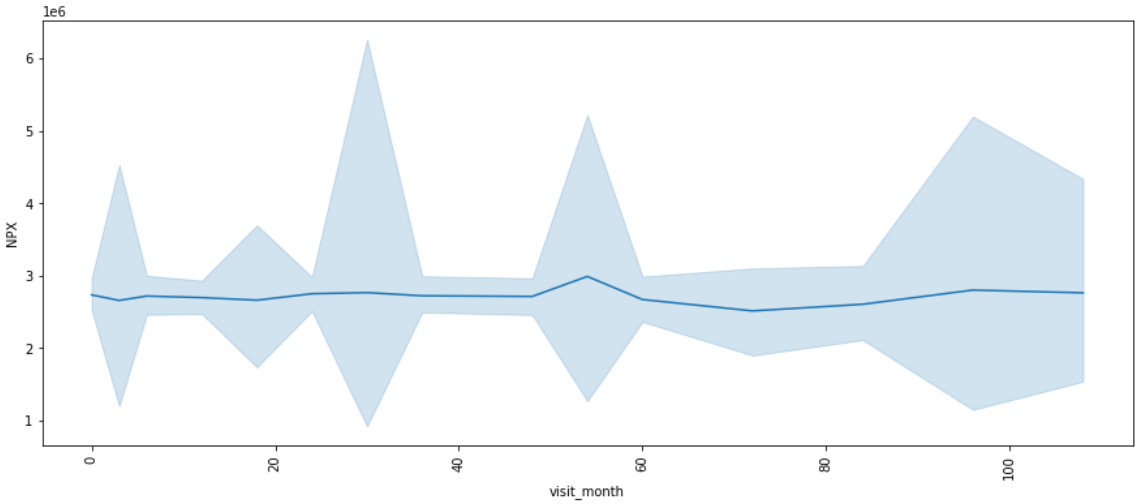
In [71]:

```
plt.figure(figsize=(15,6))
sns.scatterplot(x = df1['visit_id'], y = df1['NPX'], palette = 'hls')
plt.xticks(rotation = 90)
plt.show()
```



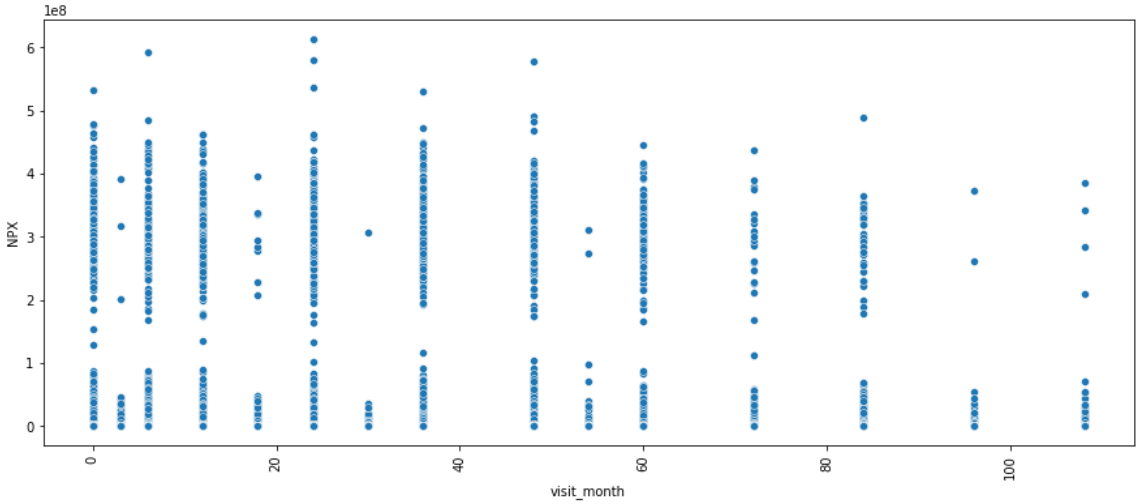
In [72]:

```
plt.figure(figsize=(15,6))
sns.lineplot(x = df1['visit_month'], y = df1['NPX'], palette = 'hls')
plt.xticks(rotation = 90)
plt.show()
```



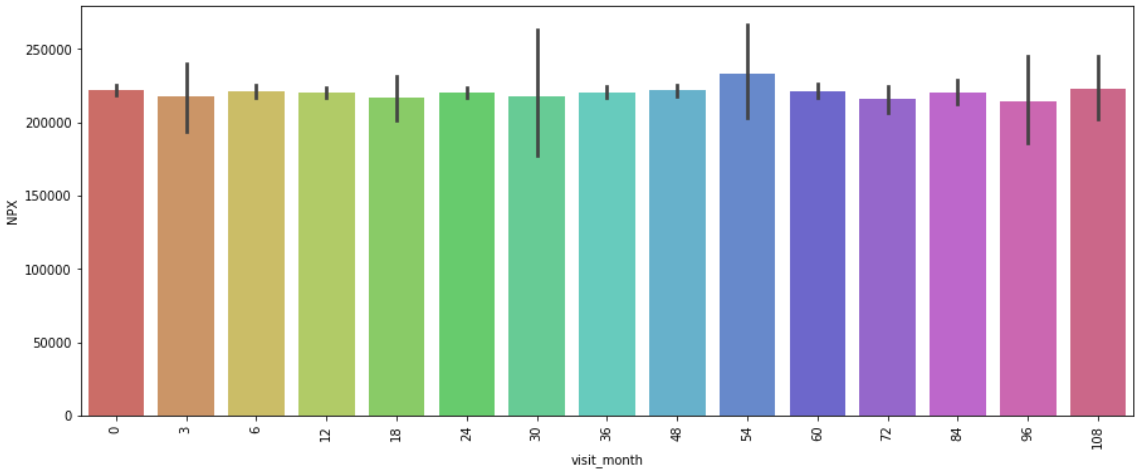
In [73]:

```
plt.figure(figsize=(15,6))
sns.scatterplot(x = df1['visit_month'], y = df1['NPX'], palette = 'hls')
plt.xticks(rotation = 90)
plt.show()
```



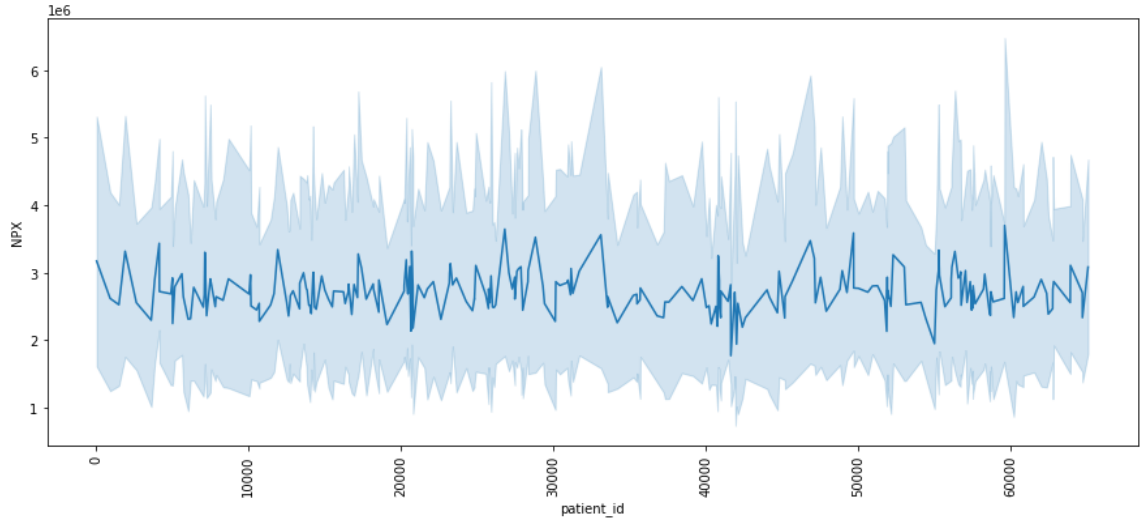
In [277]:

```
plt.figure(figsize=(15,6))
sns.barplot(x = df1['visit_month'], y = df1['NPX'], palette = 'hls')
plt.xticks(rotation = 90)
plt.show()
```



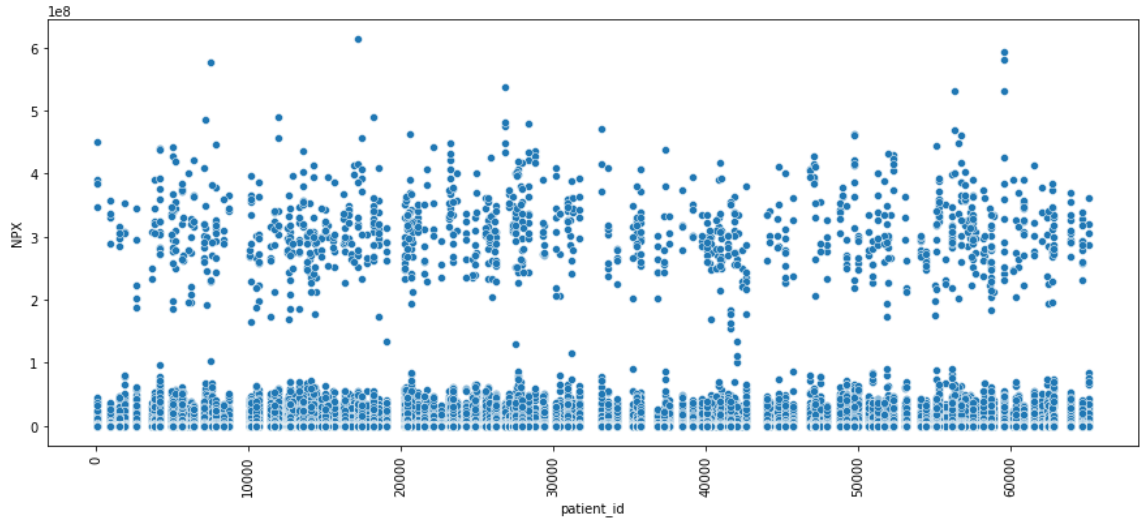
In [74]:

```
plt.figure(figsize=(15,6))
sns.lineplot(x = df1['patient_id'], y = df1['NPX'], palette = 'hls')
plt.xticks(rotation = 90)
plt.show()
```



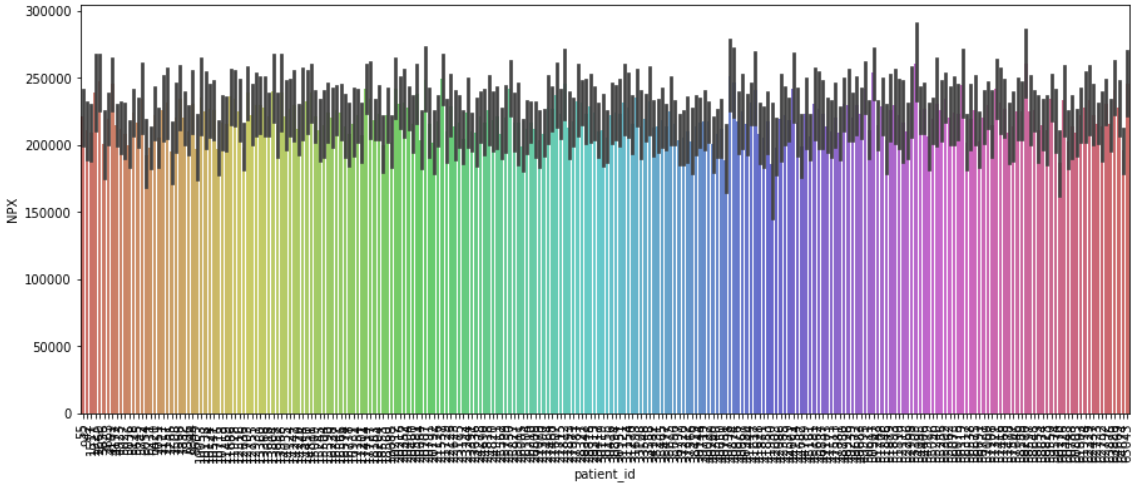
In [75]:

```
plt.figure(figsize=(15,6))
sns.scatterplot(x = df1['patient_id'], y = df1['NPX'], palette = 'hls')
plt.xticks(rotation = 90)
plt.show()
```



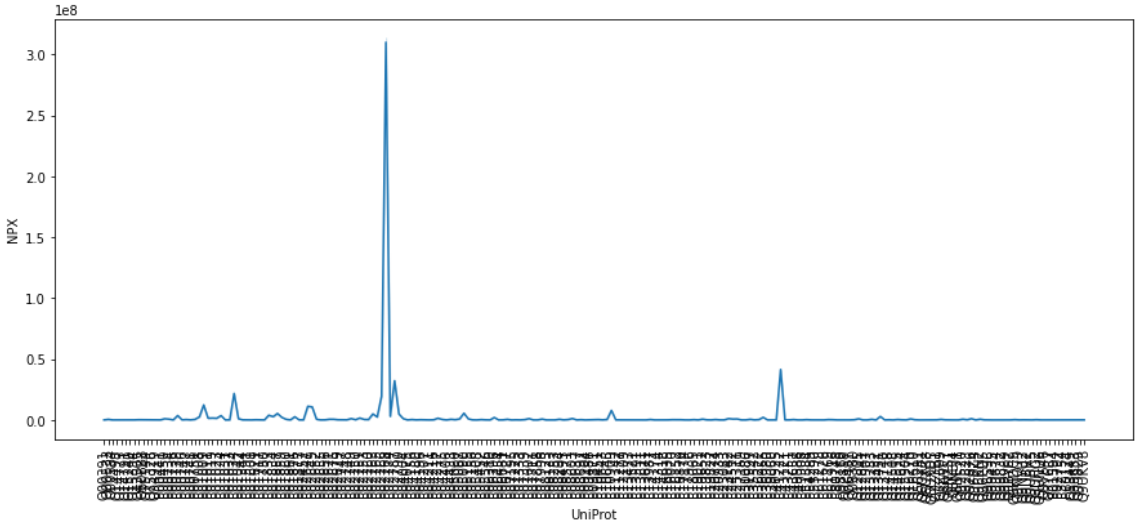
In [278]:

```
plt.figure(figsize=(15,6))
sns.barplot(x = df1['patient_id'], y = df1['NPX'], palette = 'hls')
plt.xticks(rotation = 90)
plt.show()
```



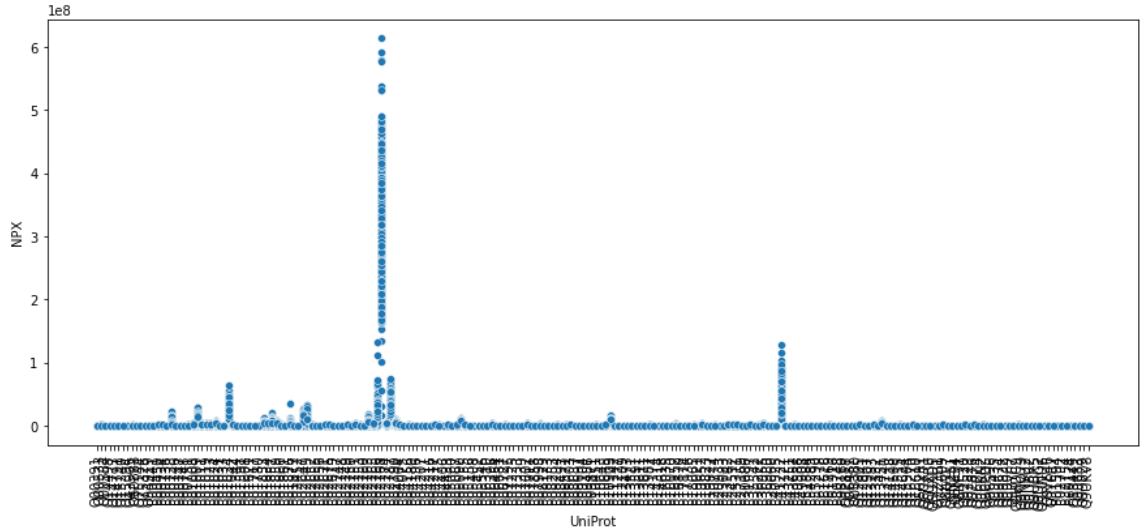
In [76]:

```
plt.figure(figsize=(15,6))
sns.lineplot(x = df1['UniProt'], y = df1['NPX'], palette = 'hls')
plt.xticks(rotation = 90)
plt.show()
```



In [77]:

```
plt.figure(figsize=(15,6))
sns.scatterplot(x = df1['UniProt'], y = df1['NPX'], palette = 'hls')
plt.xticks(rotation = 90)
plt.show()
```



In [160]:

```
Q1 = df1.quantile(0.25)
Q3 = df1.quantile(0.75)
IQR = Q3-Q1
```

In [161]:

```
print(IQR)
```

```
visit_month        42.0
patient_id      33429.0
NPX            534429.6
dtype: float64
```

In [162]:

```
df1 = df1[~((df1 < (Q1 - 1.5 * IQR)) |(df1 > (Q3 + 1.5 * IQR))).any(axis=1)]
```

In [163]:

```
df1.shape
```

Out[163]:

```
(200981, 5)
```

In [164]:

```
df1_corr = df1.corr()
```

In [165]:

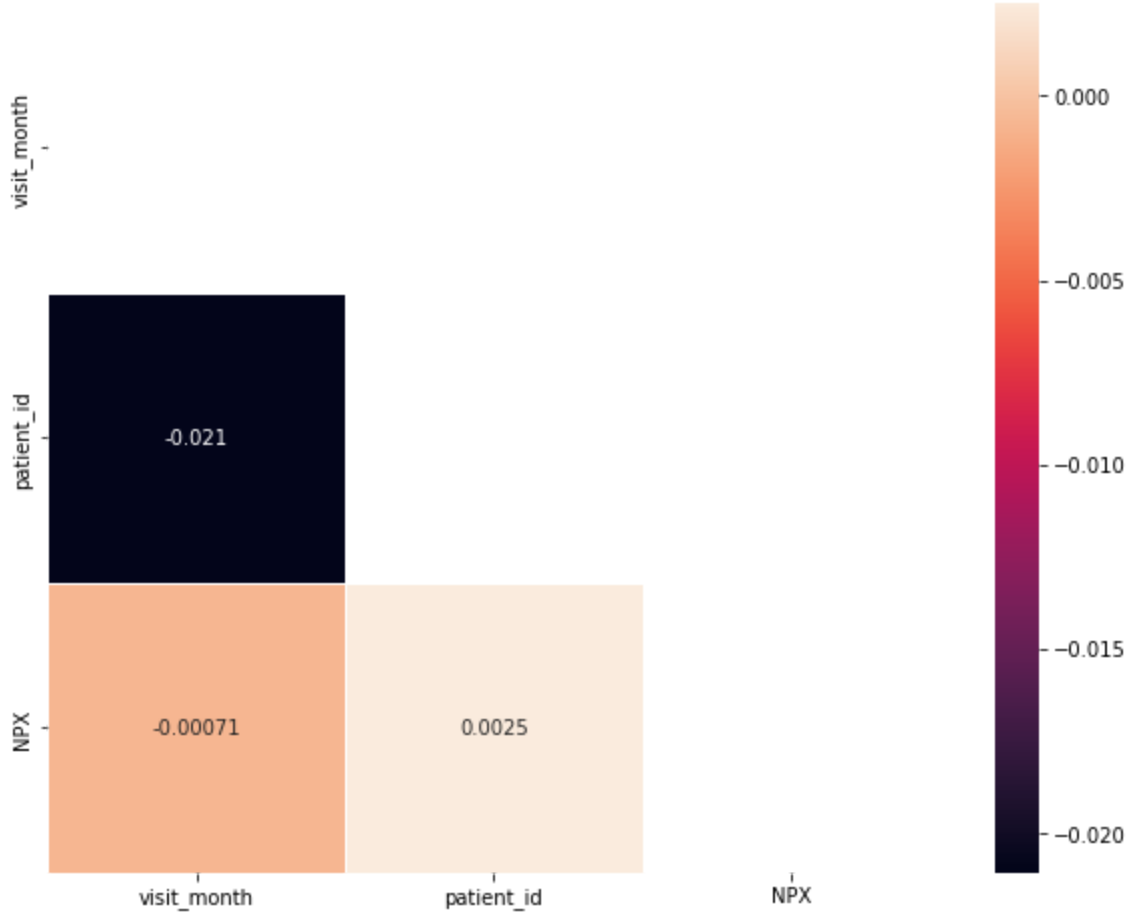
```
df1_corr
```

Out[165]:

	visit_month	patient_id	NPX
visit_month	1.000000	-0.021061	-0.000708
patient_id	-0.021061	1.000000	0.002519
NPX	-0.000708	0.002519	1.000000

In [166]:

```
plt.figure(figsize=(10, 8))
matrix = np.triu(df1_corr)
sns.heatmap(df1_corr, annot=True, linewidth=.8, mask=matrix, cmap="rocket");
plt.show()
```



In [78]:

```
df2 = pd.read_csv('train_clinical_data.csv')
```

In [79]:

```
df2.head()
```

Out[79]:

	visit_id	patient_id	visit_month	updrs_1	updrs_2	updrs_3	updrs_4	upd23b_clinical_stat
0	55_0	55	0	10.0	6.0	15.0	NaN	
1	55_3	55	3	10.0	7.0	25.0	NaN	
2	55_6	55	6	8.0	10.0	34.0	NaN	
3	55_9	55	9	8.0	9.0	30.0	0.0	
4	55_12	55	12	10.0	10.0	41.0	0.0	

In [80]:

```
df2.tail()
```

Out[80]:

	visit_id	patient_id	visit_month	updrs_1	updrs_2	updrs_3	updrs_4	upd23b_clinica
2610	65043_48	65043	48	7.0	6.0	13.0	0.0	
2611	65043_54	65043	54	4.0	8.0	11.0	1.0	
2612	65043_60	65043	60	6.0	6.0	16.0	1.0	
2613	65043_72	65043	72	3.0	9.0	14.0	1.0	
2614	65043_84	65043	84	7.0	9.0	20.0	3.0	

In [81]:

```
df2.shape
```

Out[81]:

```
(2615, 8)
```

In [82]:

```
df2.columns
```

Out[82]:

```
Index(['visit_id', 'patient_id', 'visit_month', 'updrs_1', 'updrs_2',
       'updrs_3', 'updrs_4', 'upd23b_clinical_state_on_medication'],
      dtype='object')
```

In [83]:

```
df2.duplicated().sum()
```

Out[83]:

```
0
```

In [84]:

```
df2.isnull().sum()
```

Out[84]:

```
visit_id                                0
patient_id                              0
visit_month                             0
updrs_1                                 1
updrs_2                                 2
updrs_3                                25
updrs_4                              1038
upd23b_clinical_state_on_medication  1327
dtype: int64
```

In [85]:

```
df2.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 2615 entries, 0 to 2614
Data columns (total 8 columns):
 #   Column                               Non-Null Count  Dtype  
---  ------                               --------------  -----  
 0   visit_id                             2615 non-null   object 
 1   patient_id                           2615 non-null   int64  
 2   visit_month                          2615 non-null   int64  
 3   updrs_1                              2614 non-null   float64
 4   updrs_2                              2613 non-null   float64
 5   updrs_3                              2590 non-null   float64
 6   updrs_4                              1577 non-null   float64
 7   upd23b_clinical_state_on_medication  1288 non-null   object 
dtypes: float64(4), int64(2), object(2)
memory usage: 163.6+ KB
```

In [86]:

```
df2.describe()
```

Out[86]:

	patient_id	visit_month	updrs_1	updrs_2	updrs_3	updrs_4
count	2615.000000	2615.000000	2614.000000	2613.00000	2590.000000	1577.000000
mean	32651.743786	31.190822	7.110559	6.74359	19.421236	1.861763
std	18535.758700	25.199053	5.525955	6.32323	15.000289	3.022112
min	55.000000	0.000000	0.000000	0.00000	0.000000	0.000000
25%	16574.000000	10.500000	3.000000	1.00000	6.000000	0.000000
50%	29417.000000	24.000000	6.000000	5.00000	19.000000	0.000000
75%	50611.000000	48.000000	10.000000	10.00000	29.000000	3.000000
max	65043.000000	108.000000	33.000000	40.00000	86.000000	20.000000

In [87]:

```
df2.nunique()
```

Out[87]:

```
visit_id                              2615
patient_id                             248
visit_month                             17
updrs_1                                 32
updrs_2                                 36
updrs_3                                 72
updrs_4                                 19
upd23b_clinical_state_on_medication      2
dtype: int64
```

In [89]:

```
mean_value = df2['updrs_1'].mean()
```

In [90]:

```
df2['updrs_1'] = df2['updrs_1'].replace({pd.np.nan: mean_value})
```

In [91]:

```
mean_value = df2['updrs_2'].mean()
```

In [92]:

```
df2['updrs_2'] = df2['updrs_2'].replace({pd.np.nan: mean_value})
```

In [93]:

```
mean_value = df2['updrs_3'].mean()
```

In [94]:

```
df2['updrs_3'] = df2['updrs_3'].replace({pd.np.nan: mean_value})
```

In [95]:

```
mean_value = df2['updrs_4'].mean()
```

In [96]:

```
df2['updrs_4'] = df2['updrs_4'].replace({pd.np.nan: mean_value})
```

In [97]:

```
df2['upd23b_clinical_state_on_medication'].fillna('Not Avaliable', inplace=True)
```

In [98]:

```
df2.isnull().sum()
```

Out[98]:

```
visit_id                              0
patient_id                            0
visit_month                           0
updrs_1                               0
updrs_2                               0
updrs_3                               0
updrs_4                               0
upd23b_clinical_state_on_medication    0
dtype: int64
```

In [279]:

```
df2['visit_id'].unique()
```

Out[279]:

```
array(['55_0', '55_3', '55_6', ..., '65043_60', '65043_72', '65043_84'],
      dtype=object)
```

In [100]:

```
df2['patient_id'].unique()
```

Out[100]:

```
array([   55,   942,  1517,  1923,  2660,  3636,  3863,  4161,  4172,
        4923,  5027,  5036,  5178,  5645,  5742,  6054,  6211,  6420,
        7051,  7117,  7151,  7265,  7508,  7568,  7832,  7886,  8344,
        8699, 10053, 10138, 10174, 10541, 10715, 10718, 11459, 11686,
       11928, 12516, 12636, 12703, 12755, 12931, 13360, 13368, 13618,
       13804, 13852, 13968, 14035, 14124, 14242, 14270, 14344, 14450,
       14811, 15009, 15245, 15504, 15590, 16238, 16347, 16566, 16574,
       16778, 16931, 17154, 17201, 17414, 17727, 18183, 18204, 18553,
       18560, 19088, 20212, 20216, 20352, 20404, 20460, 20581, 20664,
       20707, 20791, 20792, 21126, 21537, 21729, 22126, 22623, 23175,
       23192, 23244, 23391, 23636, 24278, 24690, 24818, 24820, 24911,
       25562, 25739, 25750, 25827, 25911, 26005, 26104, 26210, 26809,
       27079, 27300, 27464, 27468, 27607, 27715, 27872, 27893, 27971,
       27987, 28327, 28342, 28818, 29313, 29417, 30119, 30155, 30416,
       30894, 30951, 31121, 31154, 31270, 31693, 33108, 33548, 33558,
       34182, 35231, 35465, 35477, 35675, 35696, 36797, 37220, 37312,
       37566, 38419, 39144, 39719, 40022, 40200, 40340, 40650, 40751,
       40798, 40874, 40876, 40967, 40980, 41444, 41617, 41628, 41871,
       41883, 41930, 42003, 42086, 42385, 42579, 44001, 44154, 44682,
       44789, 45161, 45181, 45662, 46837, 47103, 47171, 47513, 47881,
       48780, 48928, 49239, 49672, 49683, 49995, 50611, 50907, 51243,
       51708, 51846, 51879, 51893, 51899, 52119, 52266, 52998, 53103,
       54095, 54406, 54979, 55096, 55240, 55256, 55302, 55662, 56073,
       56075, 56119, 56317, 56538, 56675, 56691, 56727, 57009, 57108,
       57321, 57416, 57468, 57478, 57507, 57646, 58189, 58270, 58597,
       58648, 58653, 58674, 58823, 59550, 59574, 60170, 60326, 60443,
       60788, 60803, 61503, 61974, 62329, 62437, 62723, 62732, 62792,
       63875, 63889, 64669, 64674, 65043], dtype=int64)
```

In [101]:

```
df2['patient_id'].value_counts()
```

Out[101]:

```
55096    17
57108    17
15009    17
16778    16
52266    16
         ..
13968     5
20792     5
62732     4
60443     3
14450     3
Name: patient_id, Length: 248, dtype: int64
```

In [102]:

```
df2['visit_month'].unique()
```

Out[102]:

```
array([  0,   3,   6,   9,  12,  18,  24,  30,  36,  42,  48,  54,  60,
        72,  84,  96, 108], dtype=int64)
```

In [103]:

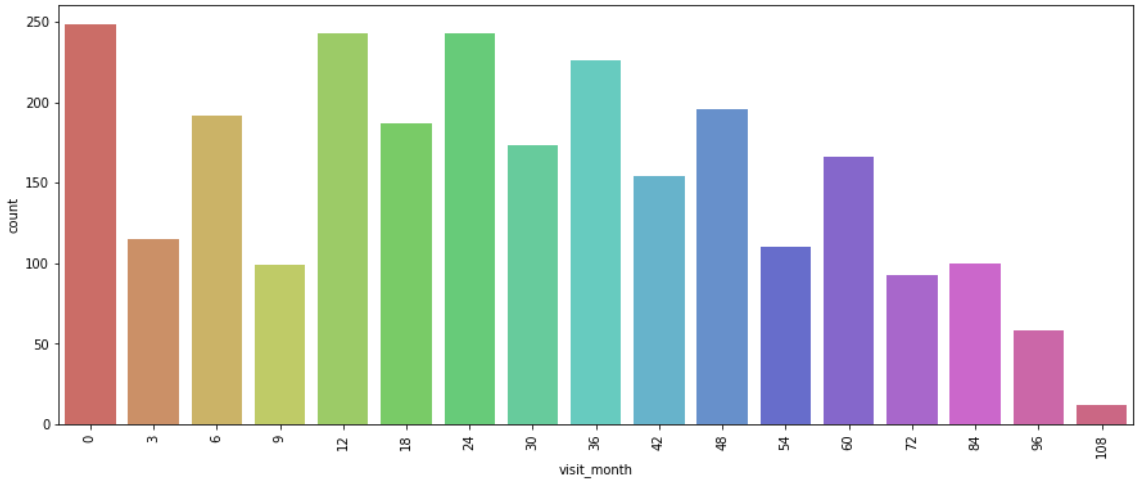
```
df2['visit_month'].value_counts()
```

Out[103]:

```
0      248
12     243
24     243
36     226
48     196
6      192
18     187
30     173
60     166
42     154
3      115
54     110
84     100
9       99
72      93
96      58
108     12
Name: visit_month, dtype: int64
```

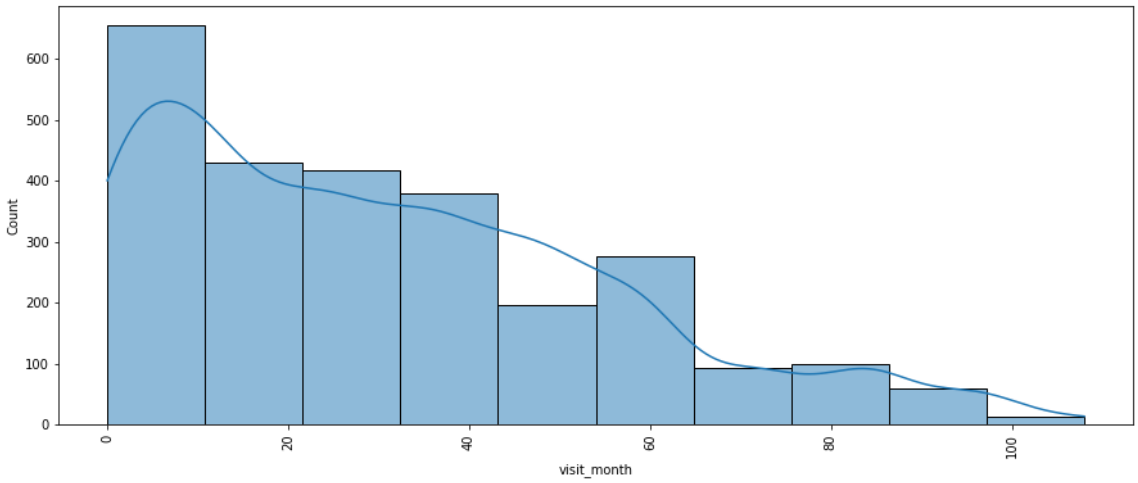
In [104]:

```
plt.figure(figsize=(15,6))
sns.countplot(x = df2['visit_month'], data = df2, palette = 'hls')
plt.xticks(rotation = 90)
plt.show()
```



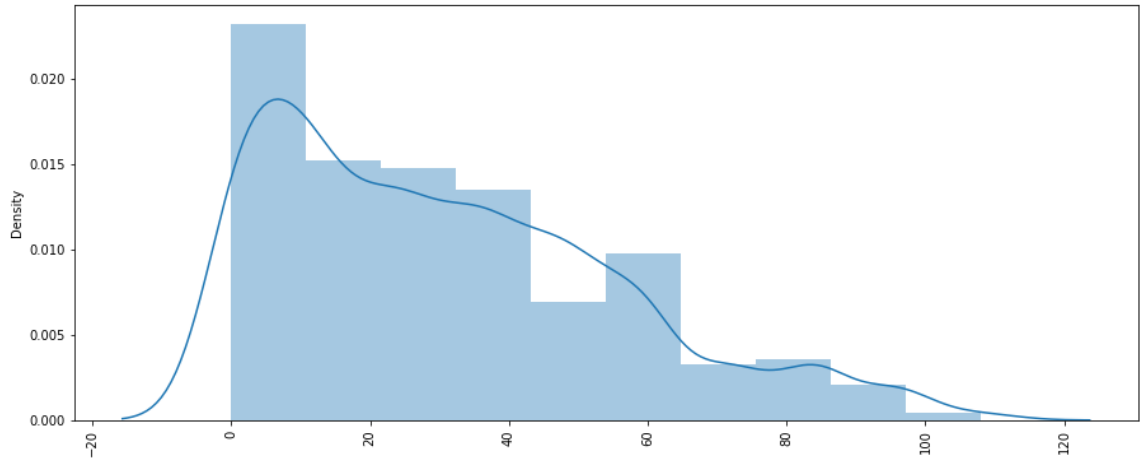
In [280]:

```
plt.figure(figsize=(15,6))
sns.histplot(x = df2['visit_month'], kde = True, bins = 10, palette = 'hls')
plt.xticks(rotation = 90)
plt.show()
```



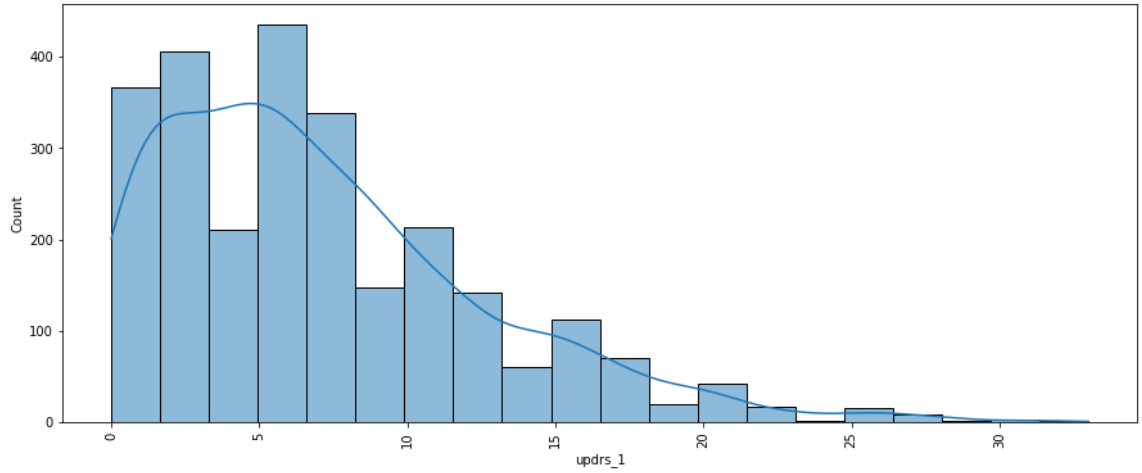
In [281]:

```
plt.figure(figsize=(15,6))
sns.distplot(x = df2['visit_month'], kde = True, bins = 10)
plt.xticks(rotation = 90)
plt.show()
```



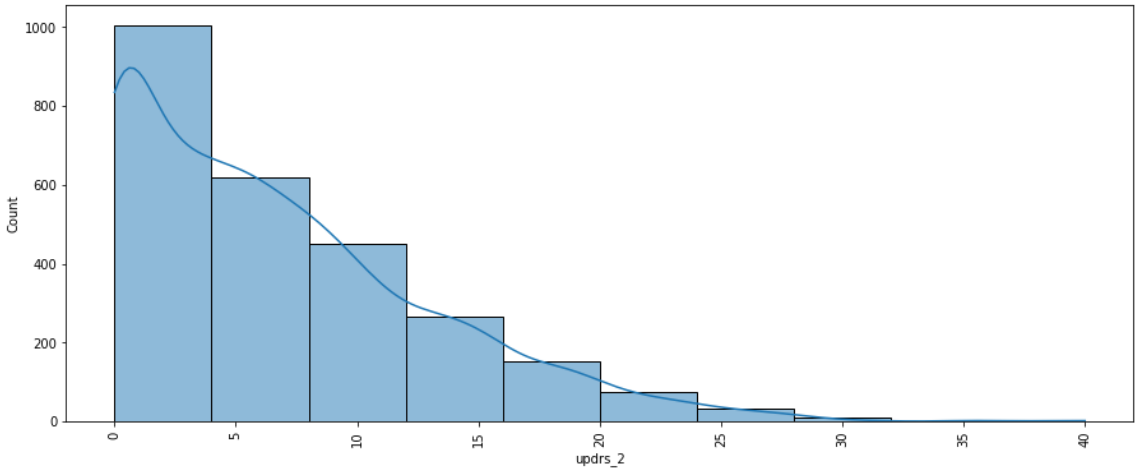
In [282]:

```
plt.figure(figsize=(15,6))
sns.histplot(x = df2['updrs_1'], kde = True, bins = 20, palette = 'hls')
plt.xticks(rotation = 90)
plt.show()
```



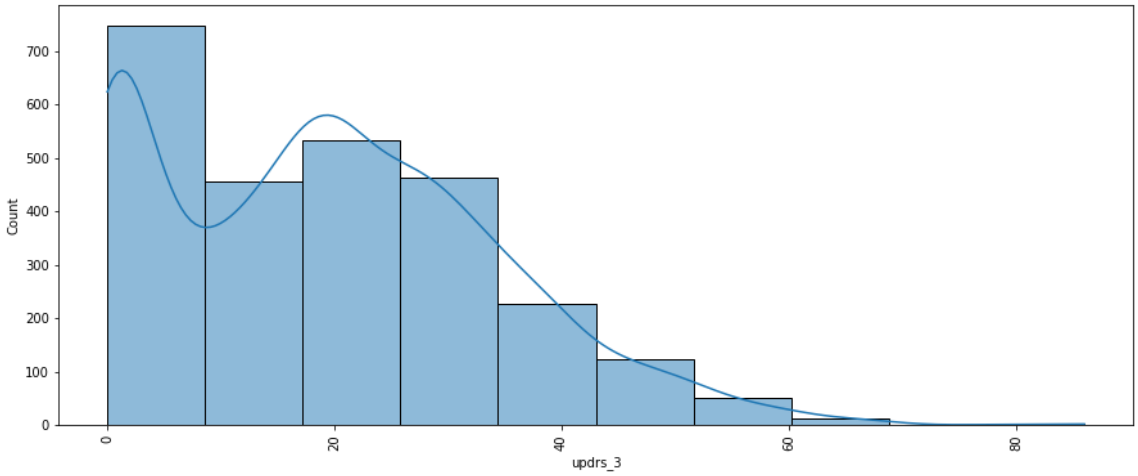
In [106]:

```
plt.figure(figsize=(15,6))
sns.histplot(x = df2['updrs_2'], kde = True, bins = 10, palette = 'hls')
plt.xticks(rotation = 90)
plt.show()
```



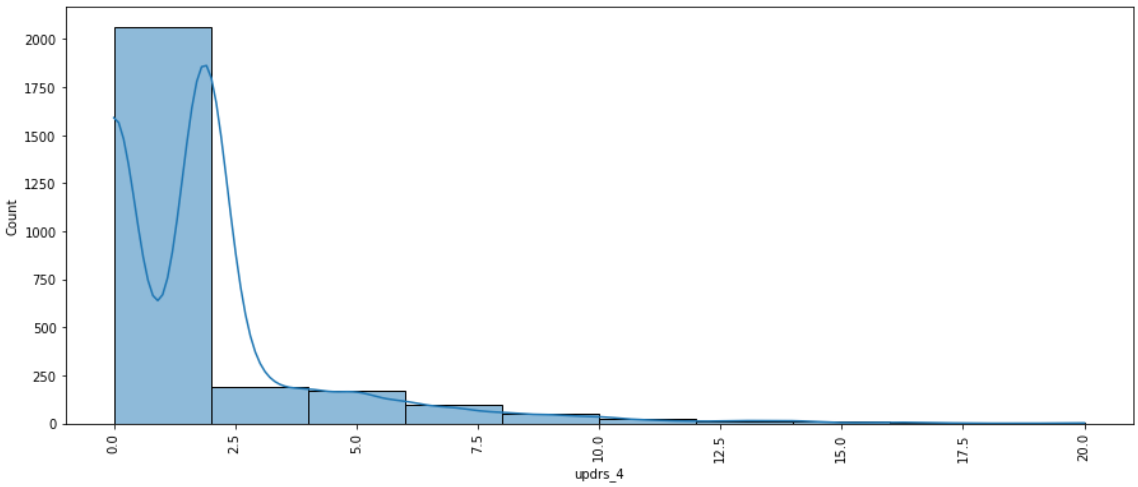
In [107]:

```
plt.figure(figsize=(15,6))
sns.histplot(x = df2['updrs_3'], kde = True, bins = 10, palette = 'hls')
plt.xticks(rotation = 90)
plt.show()
```



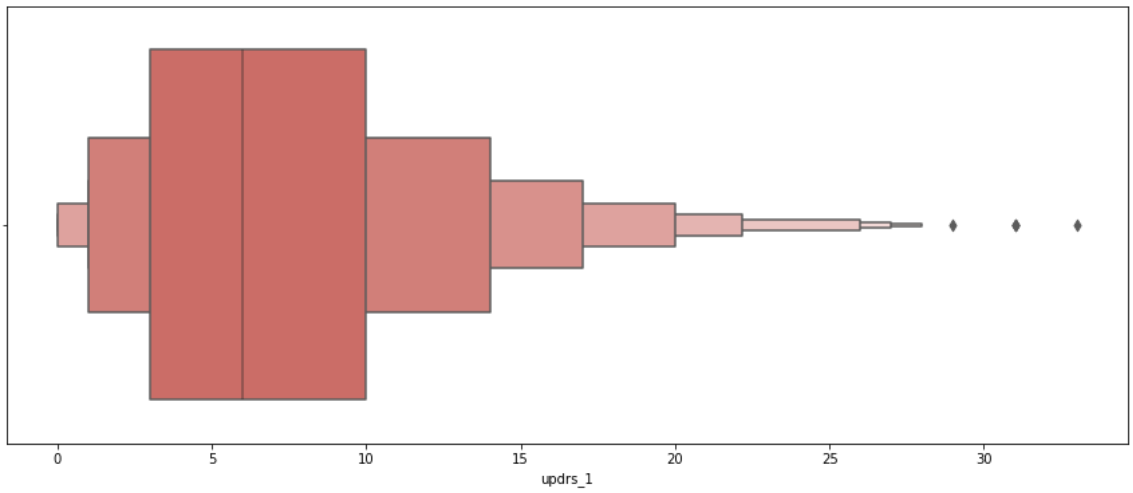
In [108]:

```
plt.figure(figsize=(15,6))
sns.histplot(x = df2['updrs_4'], kde = True, bins = 10, palette = 'hls')
plt.xticks(rotation = 90)
plt.show()
```



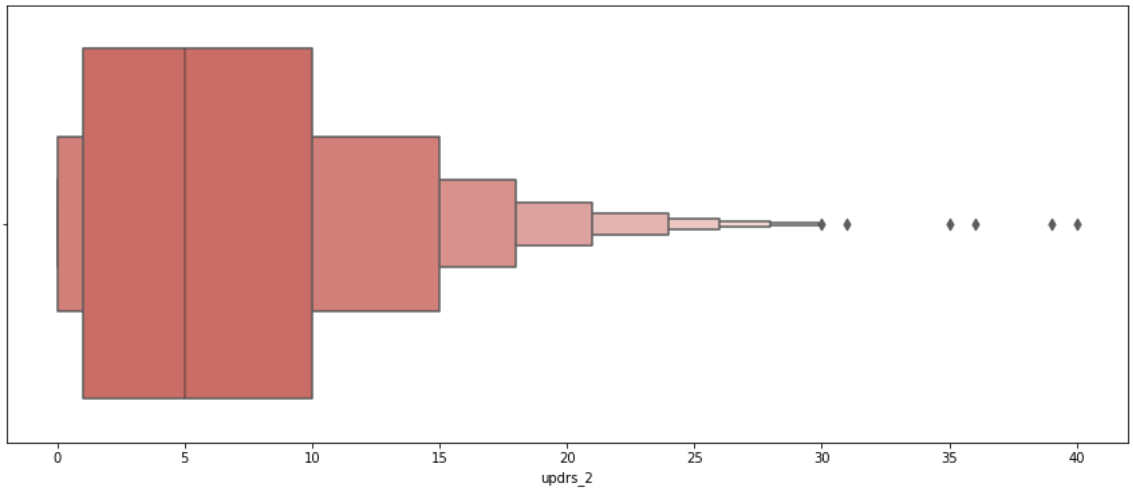
In [156]:

```
plt.figure(figsize=(15,6))
sns.boxenplot(x = df2['updrs_1'], data = df2, palette = 'hls')
plt.show()
```



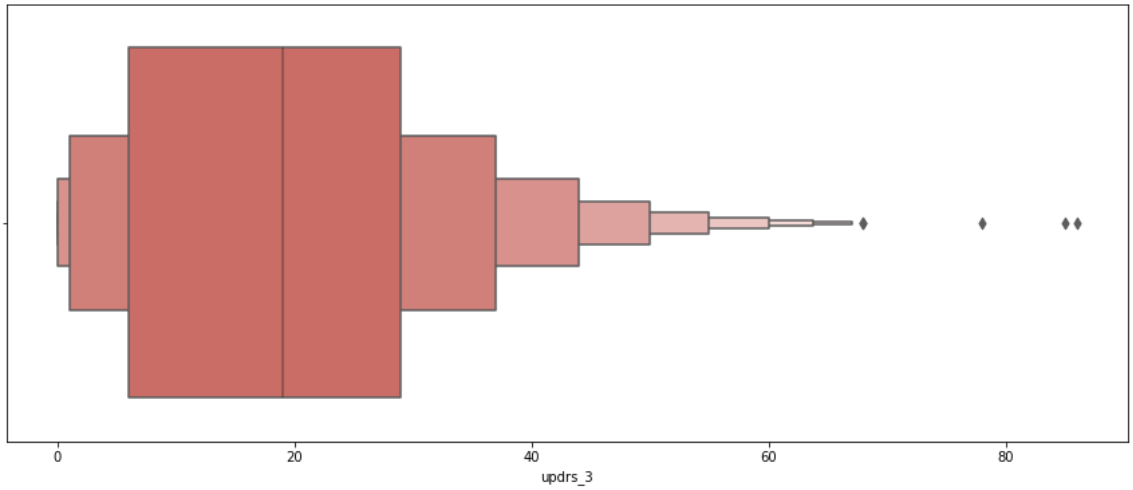
In [157]:

```
plt.figure(figsize=(15,6))
sns.boxenplot(x = df2['updrs_2'], data = df2, palette = 'hls')
plt.show()
```



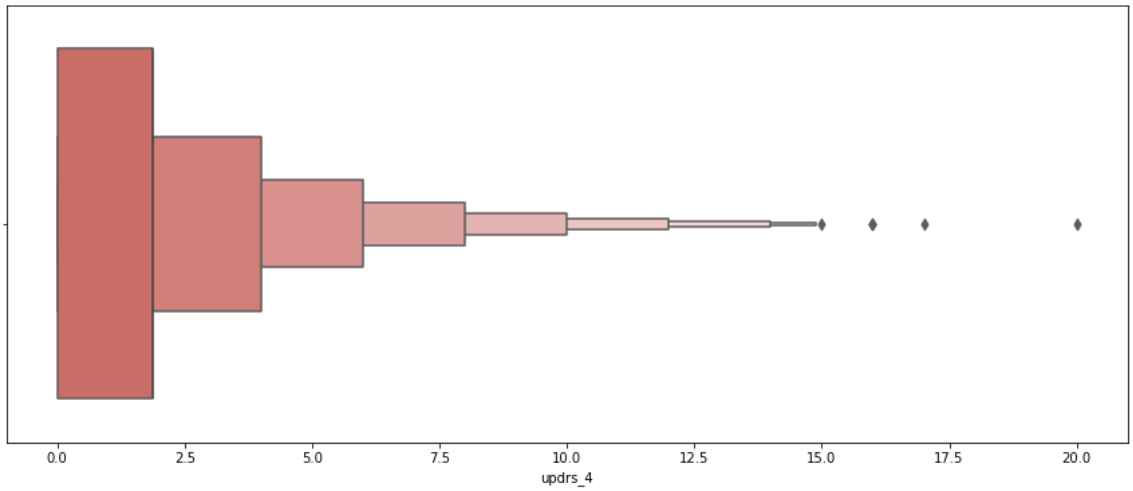
In [158]:

```
plt.figure(figsize=(15,6))
sns.boxenplot(x = df2['updrs_3'], data = df2, palette = 'hls')
plt.show()
```



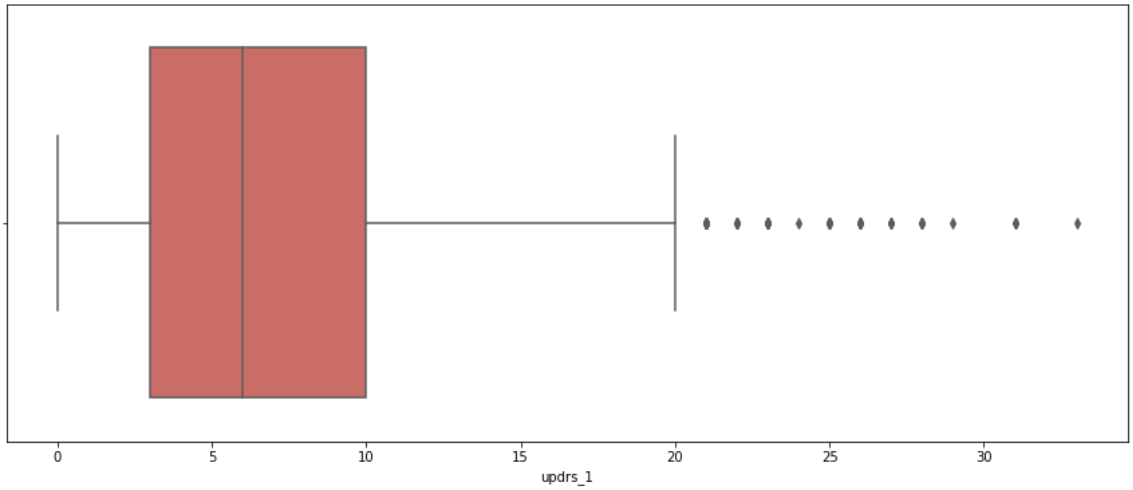
In [159]:

```
plt.figure(figsize=(15,6))
sns.boxenplot(x = df2['updrs_4'], data = df2, palette = 'hls')
plt.show()
```



In [283]:

```
plt.figure(figsize=(15,6))
sns.boxplot(x = df2['updrs_1'], data = df2, palette = 'hls')
plt.show()
```



In [109]:

```
df2['upd23b_clinical_state_on_medication'].unique()
```

Out[109]:

```
array(['Not Avaliable', 'On', 'Off'], dtype=object)
```

In [110]:

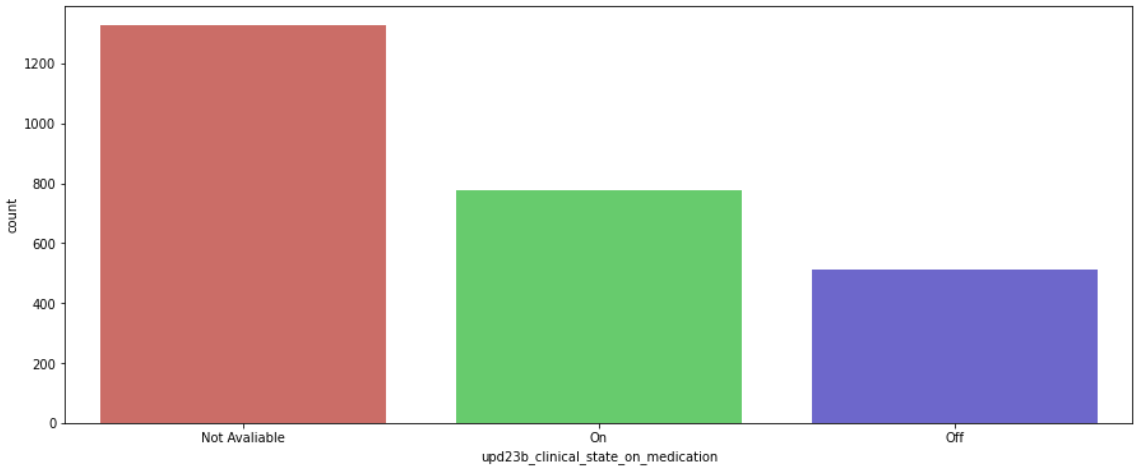
```
df2['upd23b_clinical_state_on_medication'].value_counts()
```

Out[110]:

```
Not Avaliable    1327
On                775
Off               513
Name: upd23b_clinical_state_on_medication, dtype: int64
```

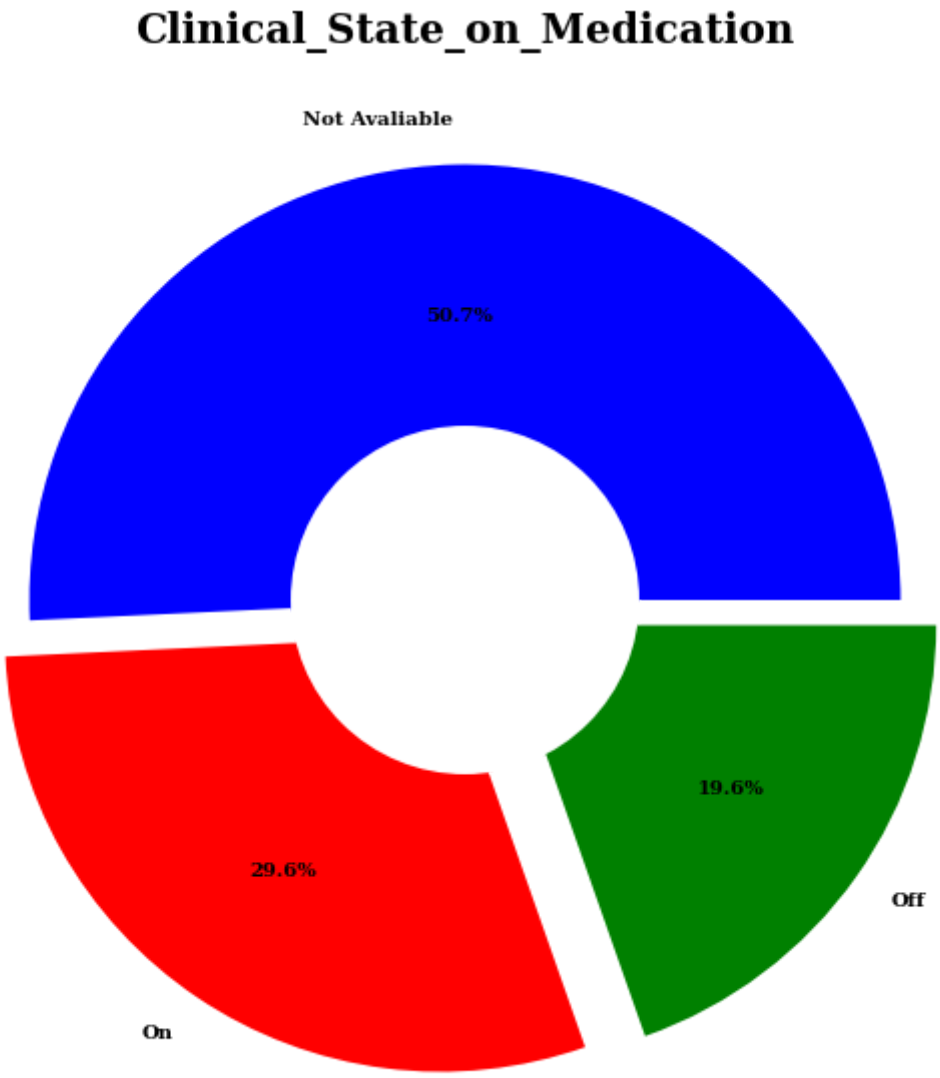
In [112]:

```
plt.figure(figsize=(15,6))
sns.countplot(x = df2['upd23b_clinical_state_on_medication'], data = df2, palette = 'hls
plt.show()
```



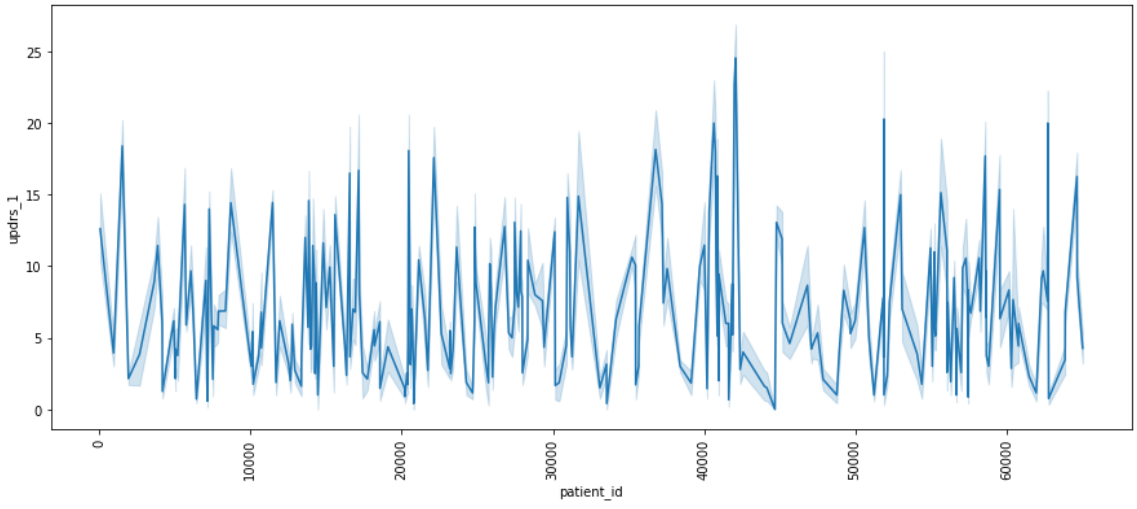
In [113]:

```
label_data = df2['upd23b_clinical_state_on_medication'].value_counts()

explode = (0.0, 0.1, 0.1)
plt.figure(figsize=(20, 10))
patches, texts, pcts = plt.pie(label_data,
                               labels = label_data.index,
                               colors = ['blue', 'red', 'green'],
                               pctdistance = 0.65,
                               shadow = True,
                               startangle = 0,
                               explode = explode,
                               autopct = '%1.1f%%',
                               textprops={ 'fontsize': 10,
                                           'color': 'black',
                                           'weight': 'bold',
                                           'family': 'serif' })
plt.setp(pcts, color='black')

hfont = {'fontname':'serif', 'weight': 'bold'}
plt.title('Clinical_State_on_Medication', size=20, **hfont)

centre_circle = plt.Circle((0,0),0.40,fc='white')
fig = plt.gcf()
fig.gca().add_artist(centre_circle)
plt.show()
```



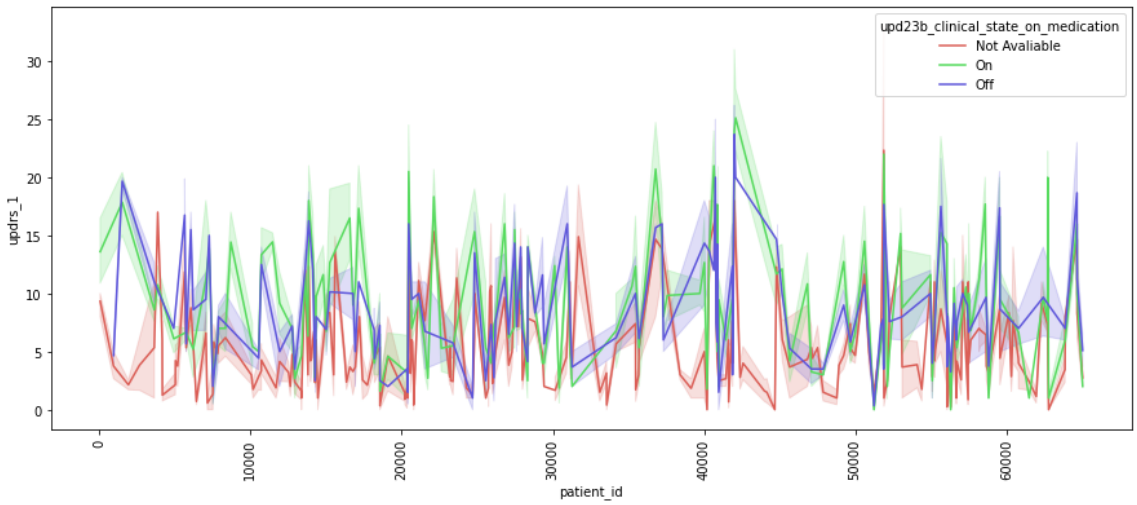
In [114]:

```
plt.figure(figsize=(15,6))
sns.lineplot(x = df2['patient_id'], y = df2['updrs_1'], palette = 'hls')
plt.xticks(rotation = 90)
plt.show()
```



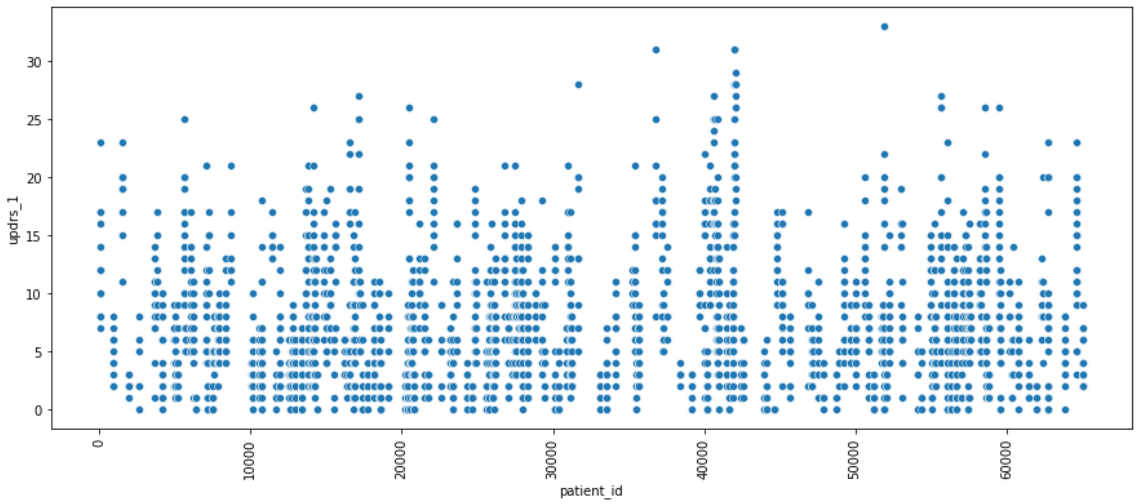
In [285]:

```
plt.figure(figsize=(15,6))
sns.lineplot(x = df2['patient_id'], y = df2['updrs_1'], hue = df2['upd23b_clinical_state_
plt.xticks(rotation = 90)
plt.show()
```



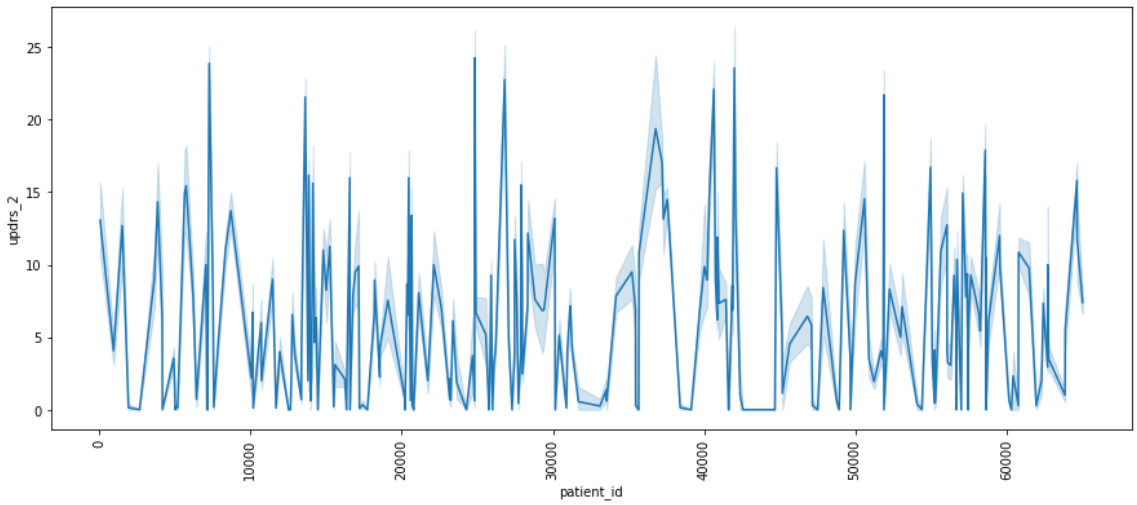
In [115]:

```
plt.figure(figsize=(15,6))
sns.scatterplot(x = df2['patient_id'], y = df2['updrs_1'], palette = 'hls')
plt.xticks(rotation = 90)
plt.show()
```



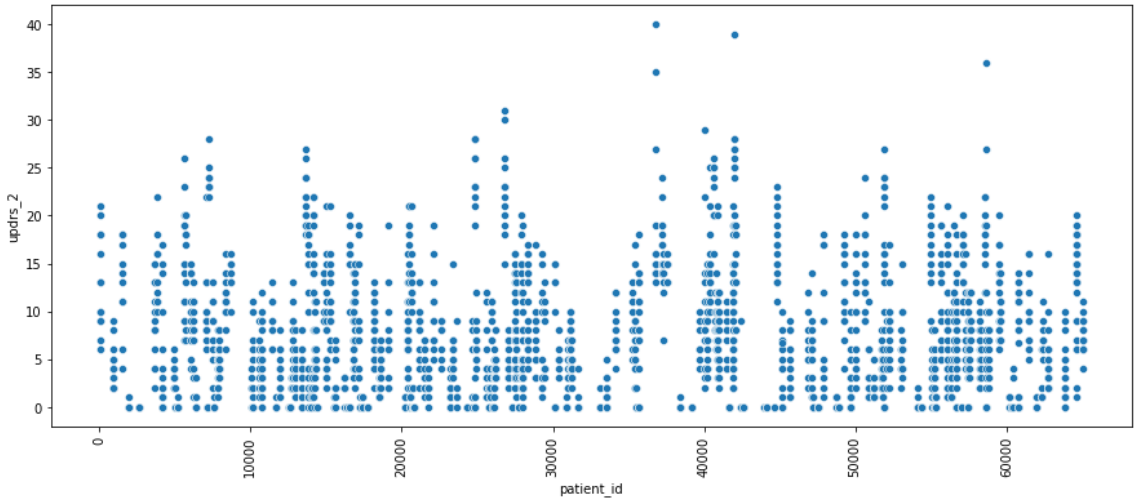
In [116]:

```
plt.figure(figsize=(15,6))
sns.lineplot(x = df2['patient_id'], y = df2['updrs_2'], palette = 'hls')
plt.xticks(rotation = 90)
plt.show()
```



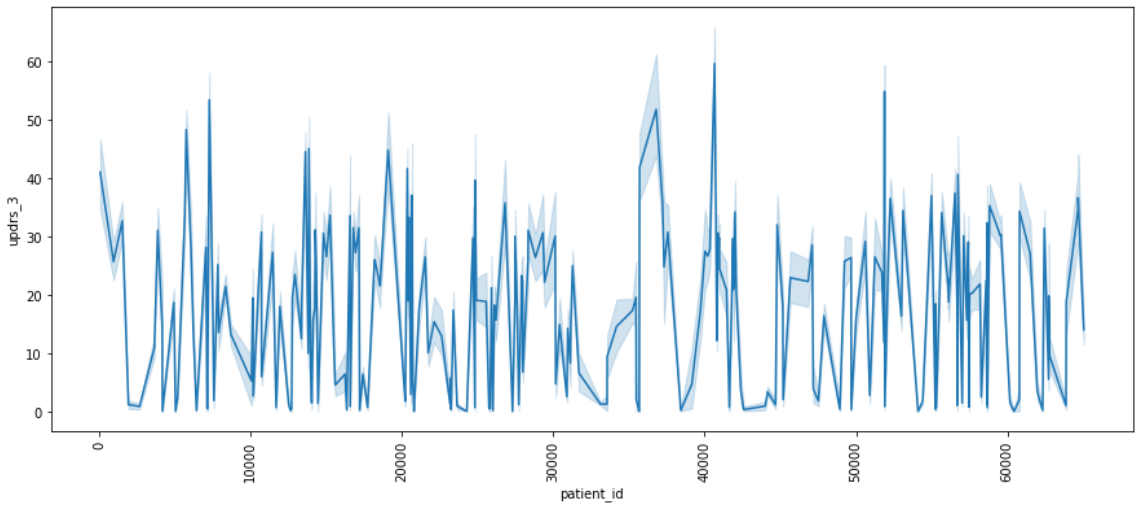
In [117]:

```
plt.figure(figsize=(15,6))
sns.scatterplot(x = df2['patient_id'], y = df2['updrs_2'], palette = 'hls')
plt.xticks(rotation = 90)
plt.show()
```



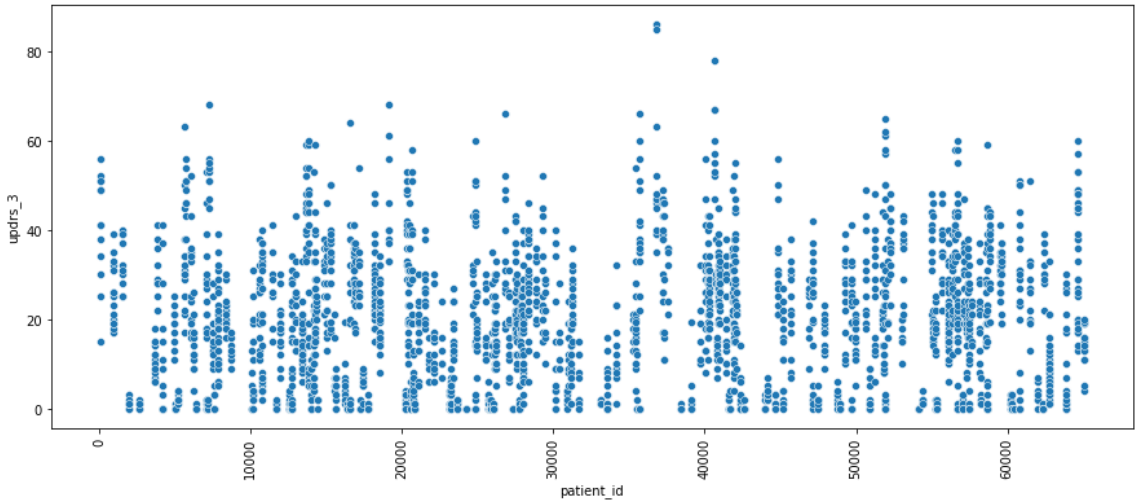
In [118]:

```
plt.figure(figsize=(15,6))
sns.lineplot(x = df2['patient_id'], y = df2['updrs_3'], palette = 'hls')
plt.xticks(rotation = 90)
plt.show()
```



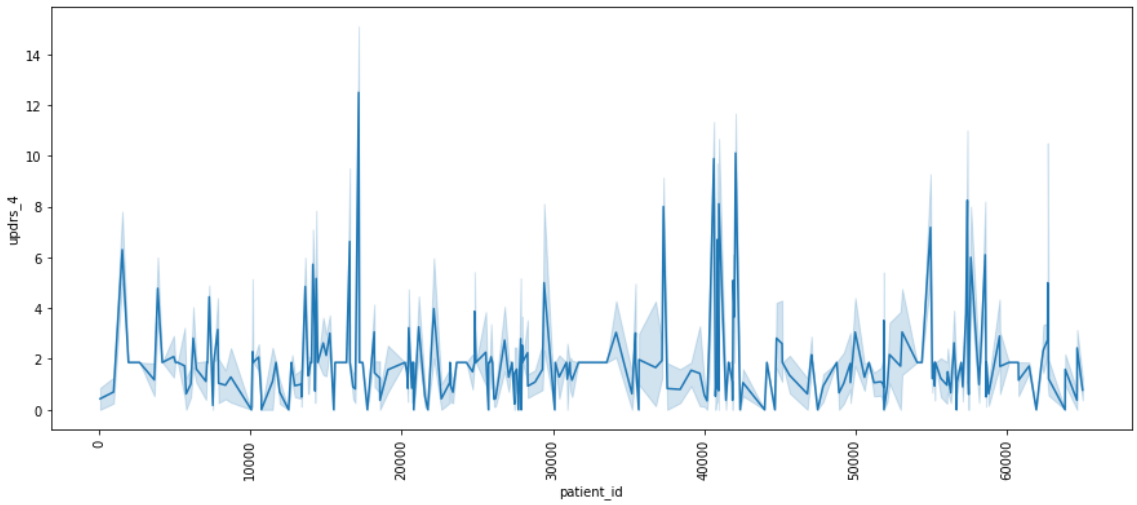
In [119]:

```
plt.figure(figsize=(15,6))
sns.scatterplot(x = df2['patient_id'], y = df2['updrs_3'], palette = 'hls')
plt.xticks(rotation = 90)
plt.show()
```



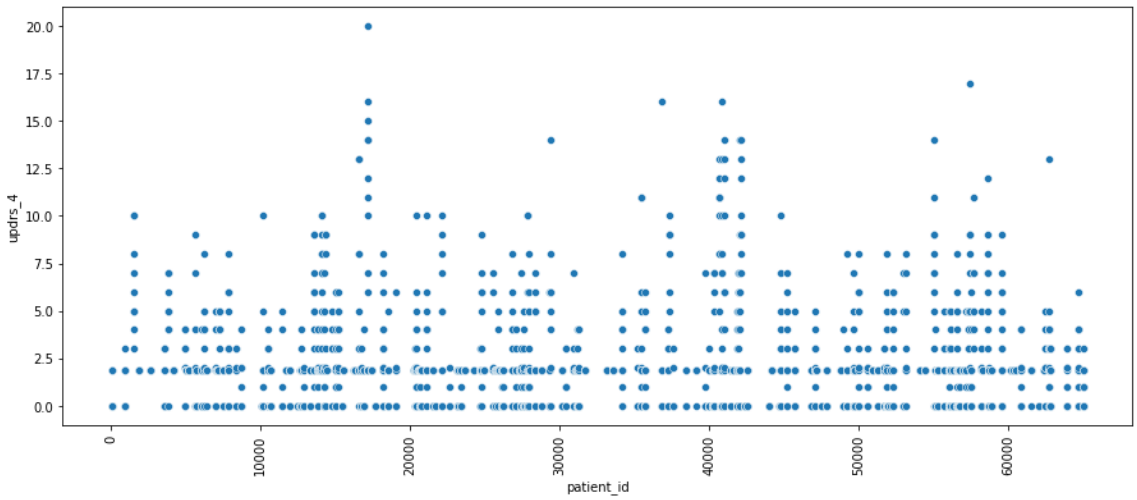
In [120]:

```
plt.figure(figsize=(15,6))
sns.lineplot(x = df2['patient_id'], y = df2['updrs_4'], palette = 'hls')
plt.xticks(rotation = 90)
plt.show()
```



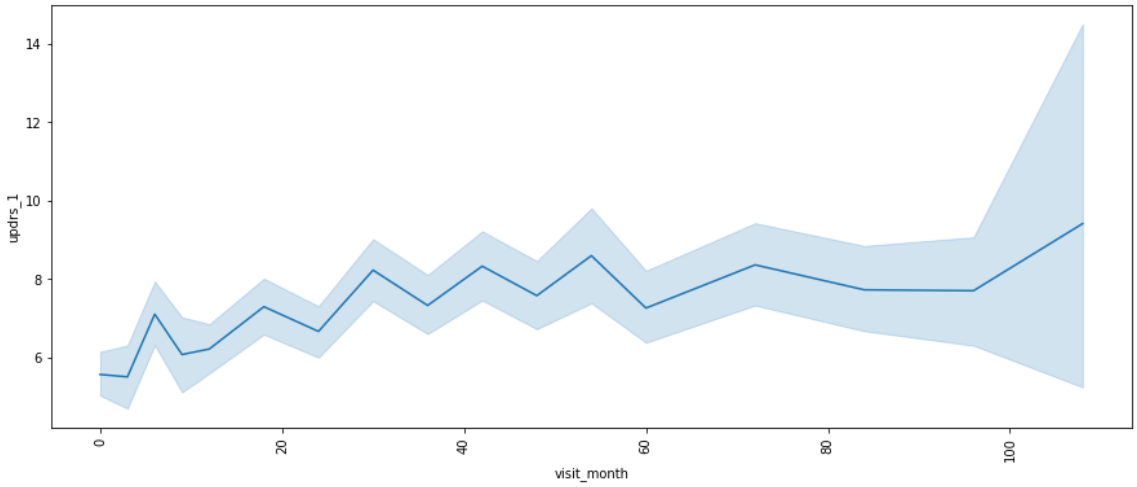
In [121]:

```
plt.figure(figsize=(15,6))
sns.scatterplot(x = df2['patient_id'], y = df2['updrs_4'], palette = 'hls')
plt.xticks(rotation = 90)
plt.show()
```



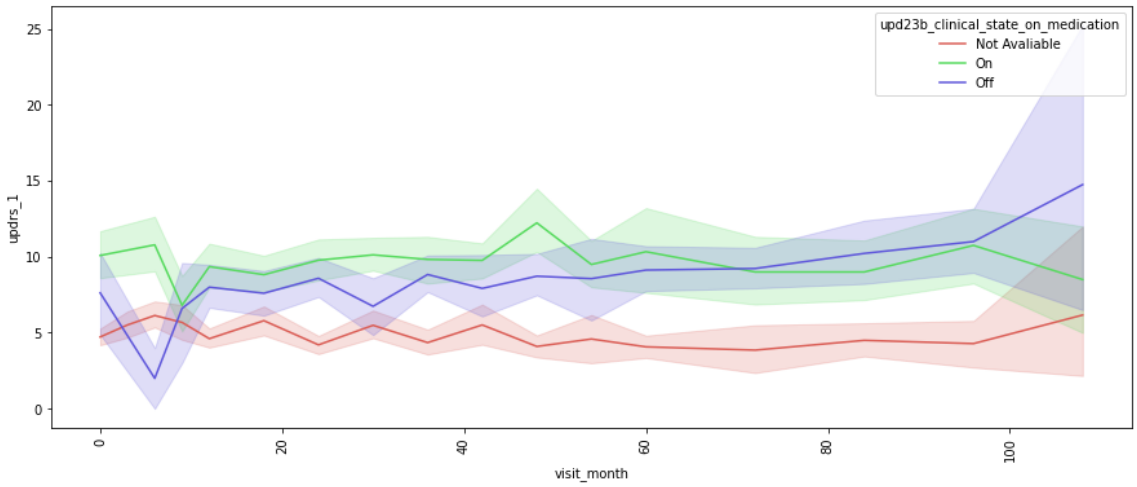
In [124]:

```
plt.figure(figsize=(15,6))
sns.lineplot(x = df2['visit_month'], y = df2['updrs_1'], palette = 'hls')
plt.xticks(rotation = 90)
plt.show()
```



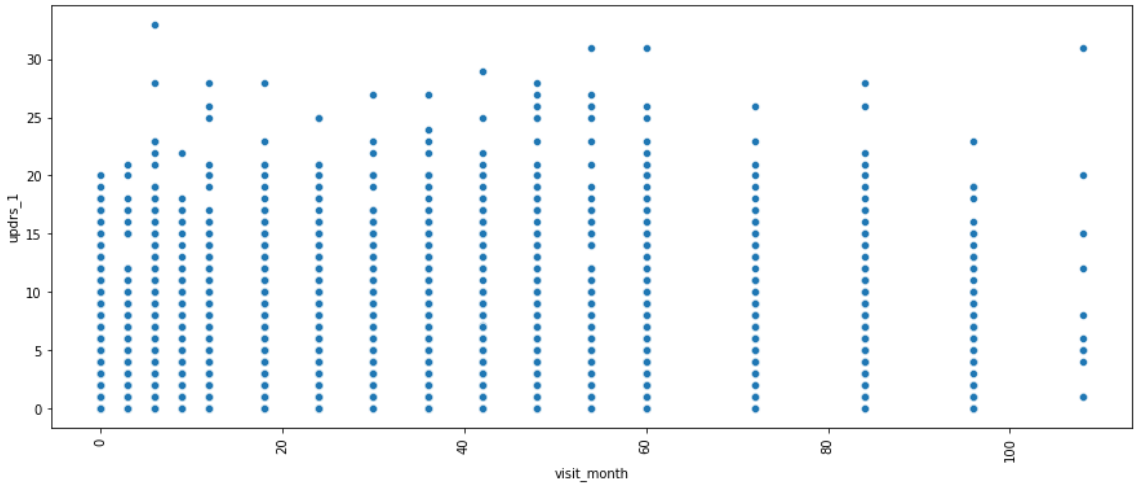
In [286]:

```
plt.figure(figsize=(15,6))
sns.lineplot(x = df2['visit_month'], y = df2['updrs_1'], hue = df2['upd23b_clinical_stat
plt.xticks(rotation = 90)
plt.show()
```



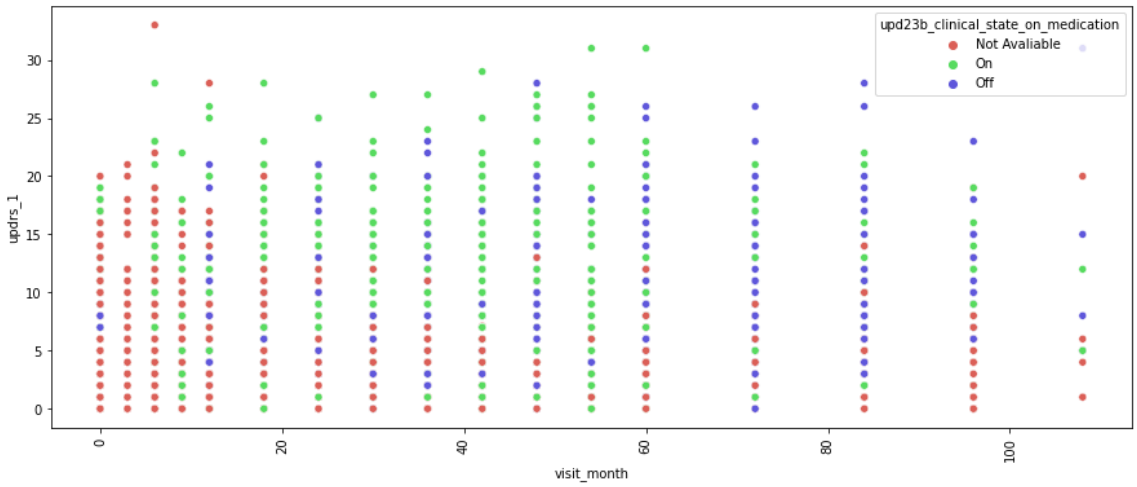
In [125]:

```
plt.figure(figsize=(15,6))
sns.scatterplot(x = df2['visit_month'], y = df2['updrs_1'], palette = 'hls')
plt.xticks(rotation = 90)
plt.show()
```



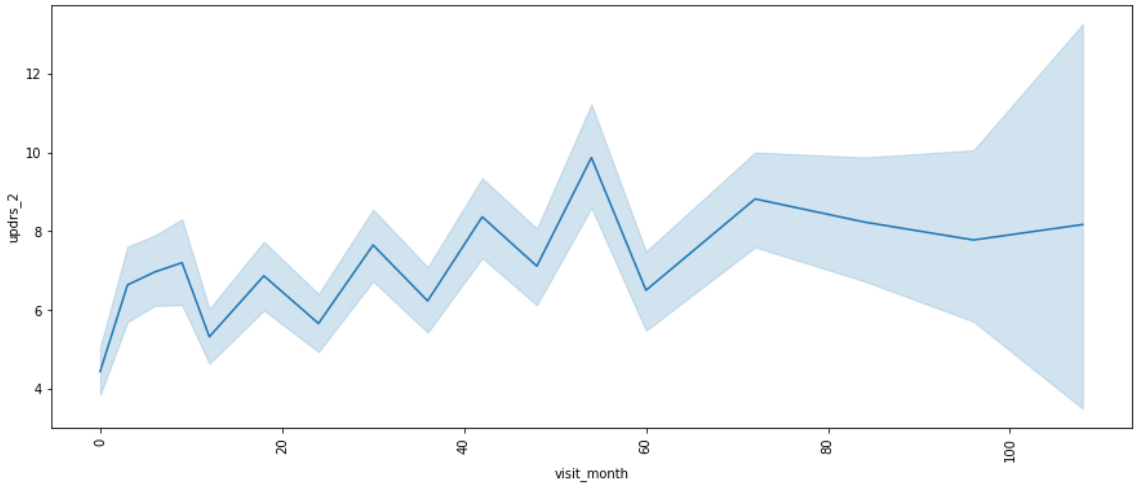
In [287]:

```
plt.figure(figsize=(15,6))
sns.scatterplot(x = df2['visit_month'], y = df2['updrs_1'],  hue = df2['upd23b_clinical_
plt.xticks(rotation = 90)
plt.show()
```



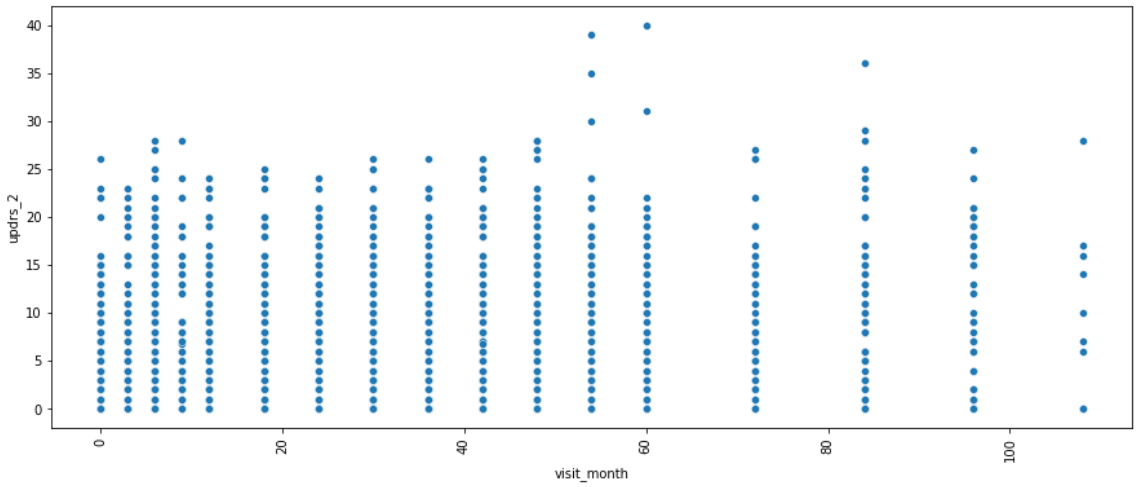
In [126]:

```
plt.figure(figsize=(15,6))
sns.lineplot(x = df2['visit_month'], y = df2['updrs_2'], palette = 'hls')
plt.xticks(rotation = 90)
plt.show()
```



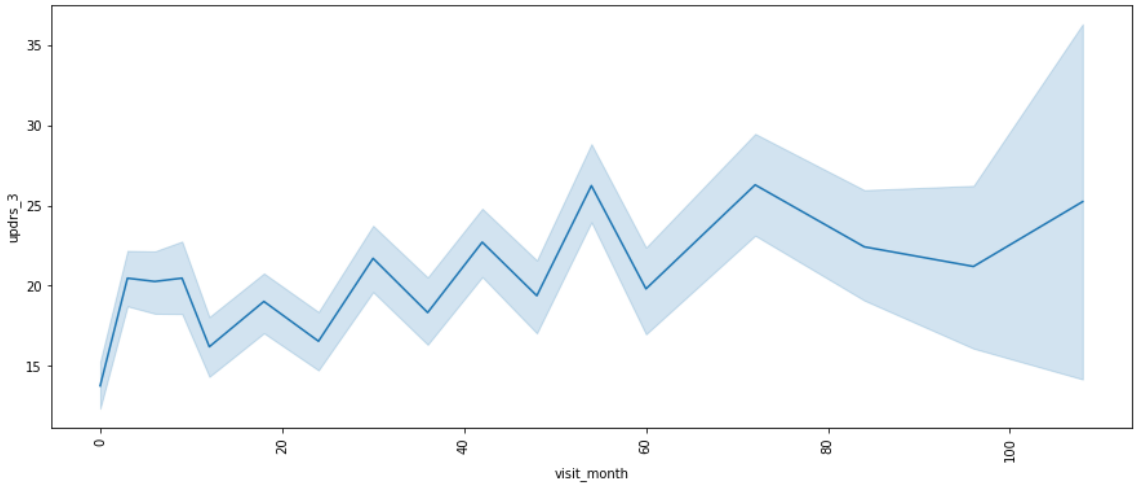
In [127]:

```
plt.figure(figsize=(15,6))
sns.scatterplot(x = df2['visit_month'], y = df2['updrs_2'], palette = 'hls')
plt.xticks(rotation = 90)
plt.show()
```



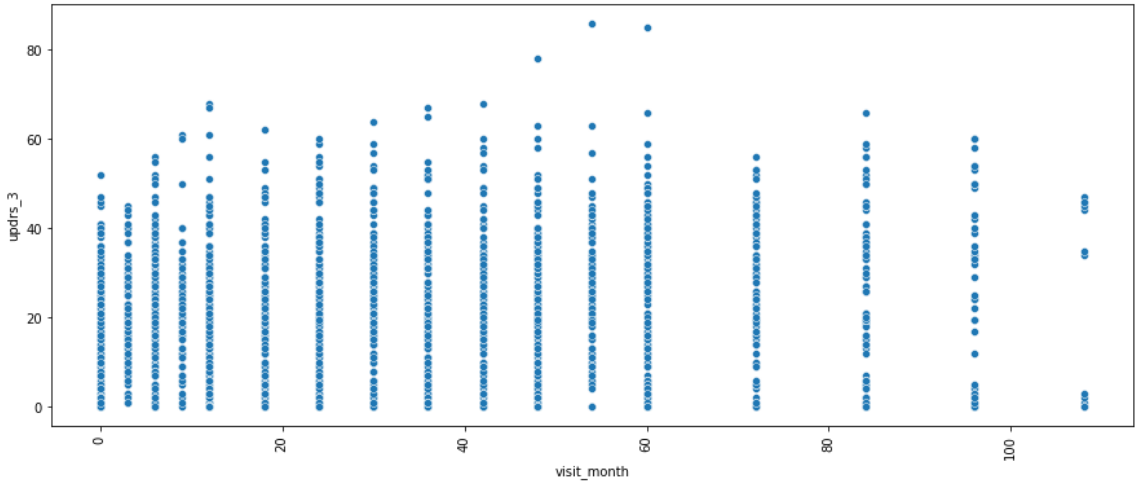
In [128]:

```
plt.figure(figsize=(15,6))
sns.lineplot(x = df2['visit_month'], y = df2['updrs_3'], palette = 'hls')
plt.xticks(rotation = 90)
plt.show()
```



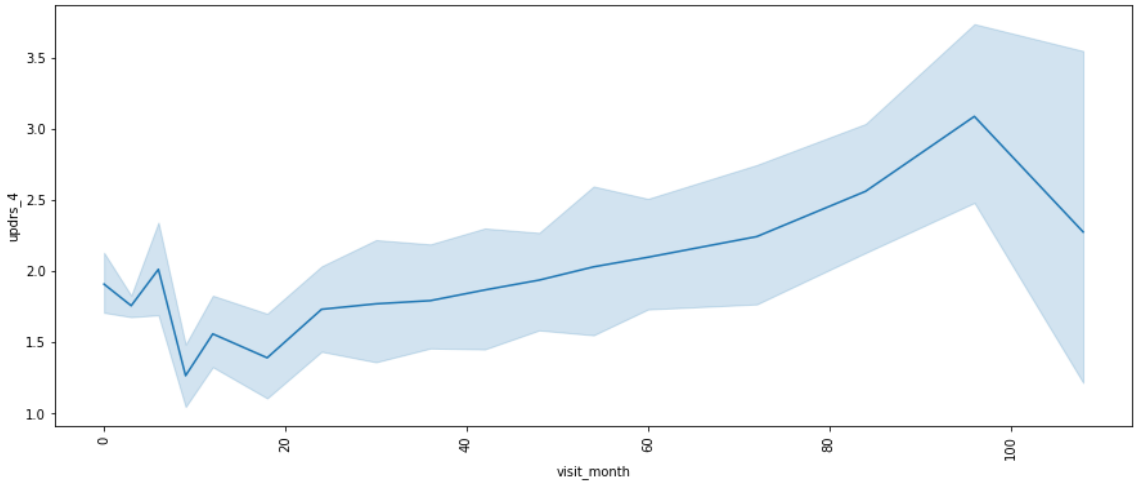
In [130]:

```
plt.figure(figsize=(15,6))
sns.scatterplot(x = df2['visit_month'], y = df2['updrs_3'], palette = 'hls')
plt.xticks(rotation = 90)
plt.show()
```



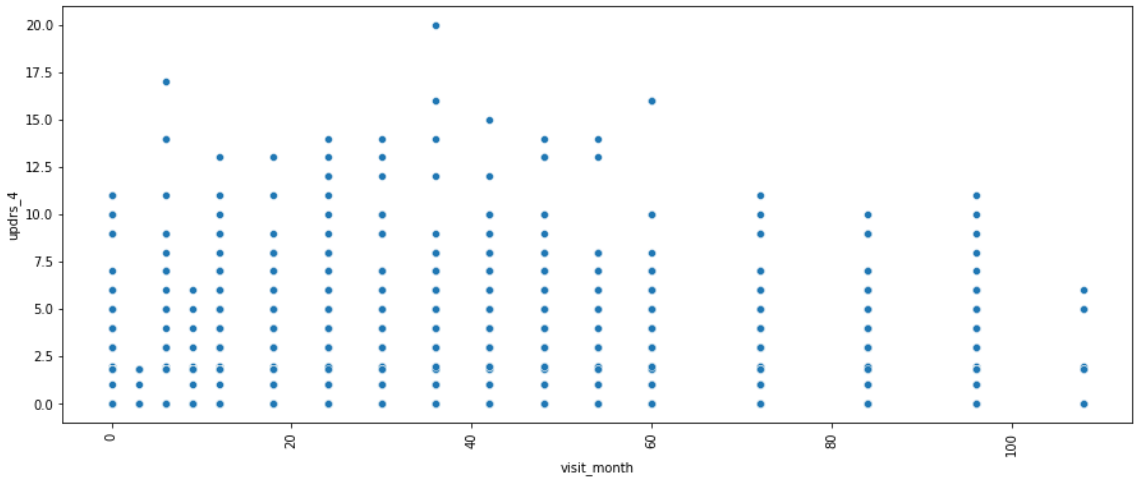
In [131]:

```
plt.figure(figsize=(15,6))
sns.lineplot(x = df2['visit_month'], y = df2['updrs_4'], palette = 'hls')
plt.xticks(rotation = 90)
plt.show()
```



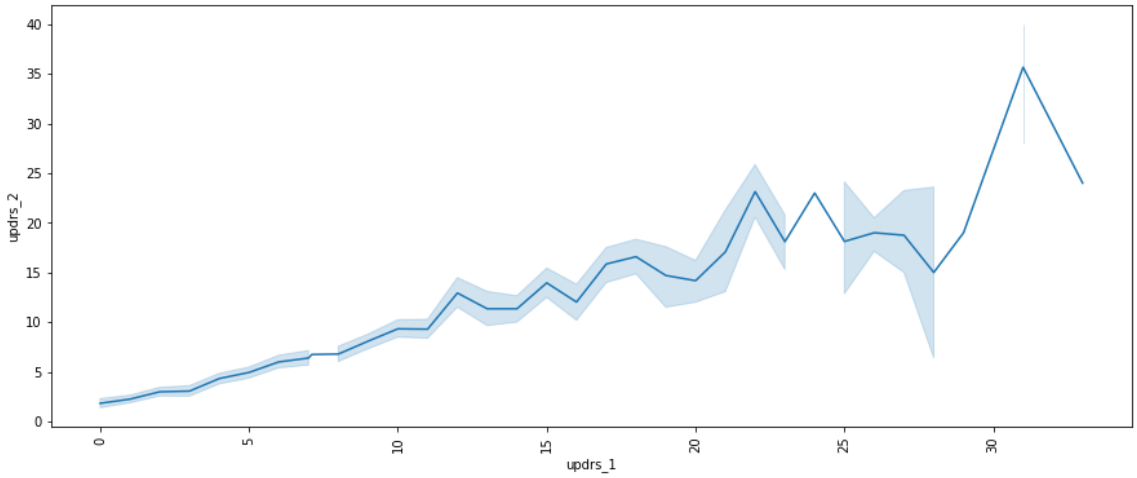
In [132]:

```
plt.figure(figsize=(15,6))
sns.scatterplot(x = df2['visit_month'], y = df2['updrs_4'], palette = 'hls')
plt.xticks(rotation = 90)
plt.show()
```



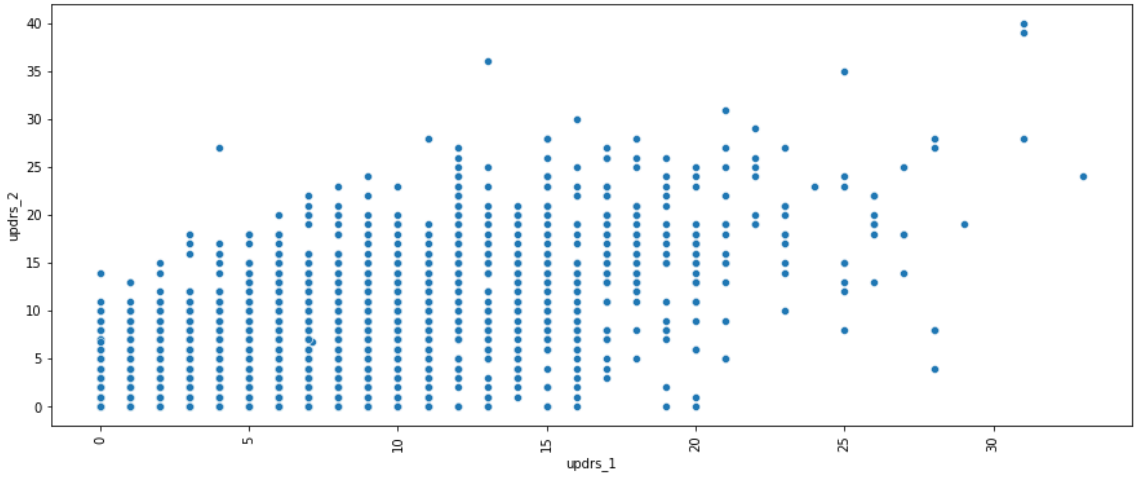
In [133]:

```
plt.figure(figsize=(15,6))
sns.lineplot(x = df2['updrs_1'], y = df2['updrs_2'], palette = 'hls')
plt.xticks(rotation = 90)
plt.show()
```



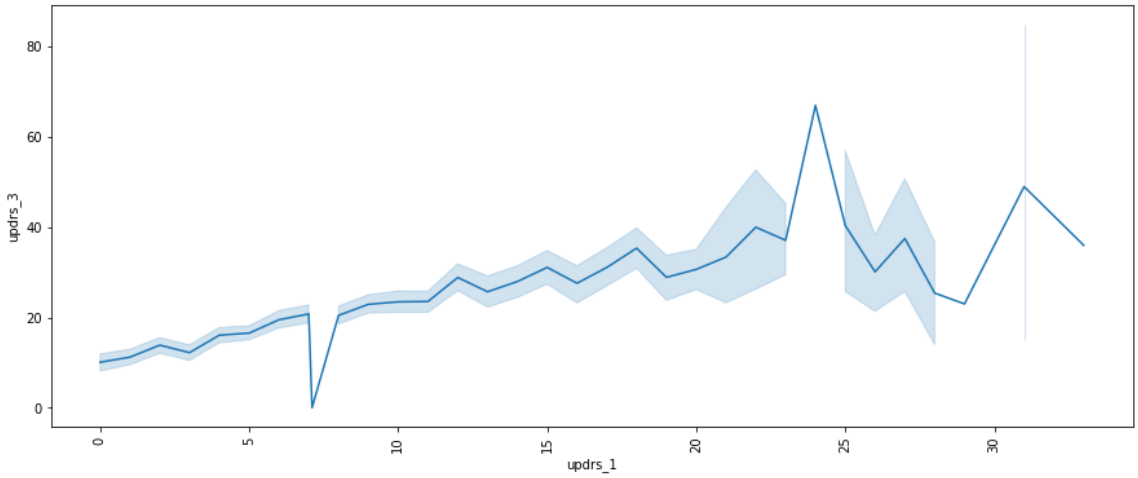
In [135]:

```
plt.figure(figsize=(15,6))
sns.scatterplot(x = df2['updrs_1'], y = df2['updrs_2'], palette = 'hls')
plt.xticks(rotation = 90)
plt.show()
```



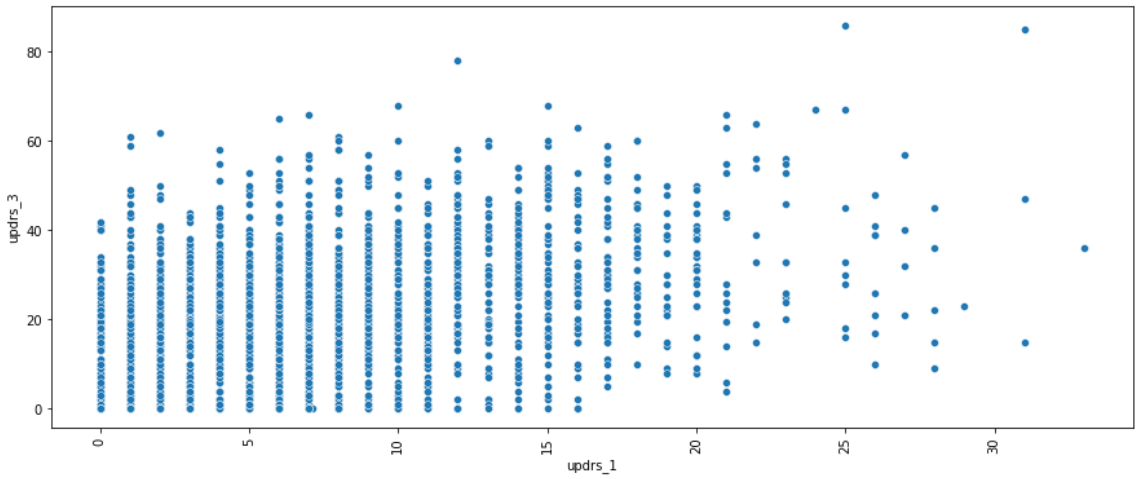
In [134]:

```
plt.figure(figsize=(15,6))
sns.lineplot(x = df2['updrs_1'], y = df2['updrs_3'], palette = 'hls')
plt.xticks(rotation = 90)
plt.show()
```



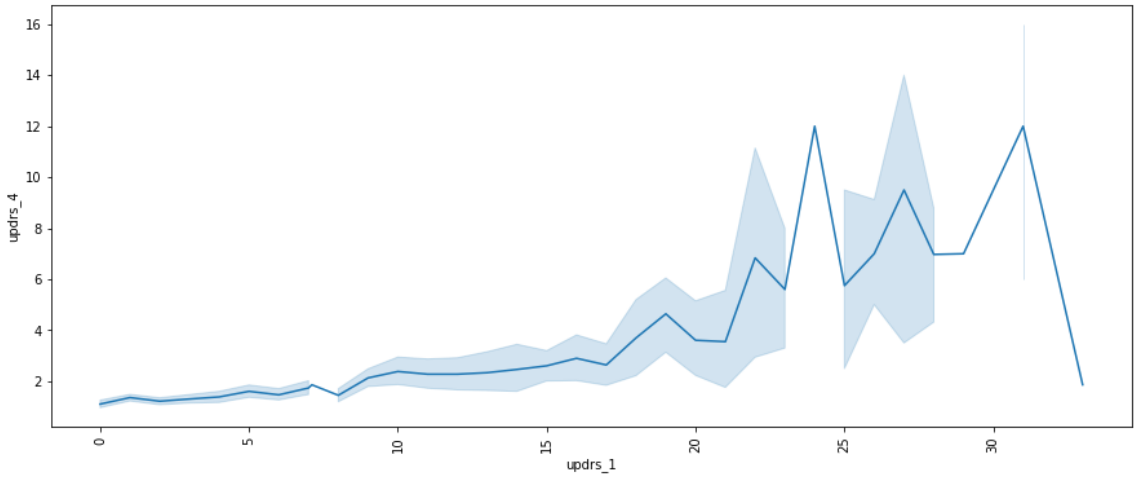
In [137]:

```
plt.figure(figsize=(15,6))
sns.scatterplot(x = df2['updrs_1'], y = df2['updrs_3'], palette = 'hls')
plt.xticks(rotation = 90)
plt.show()
```



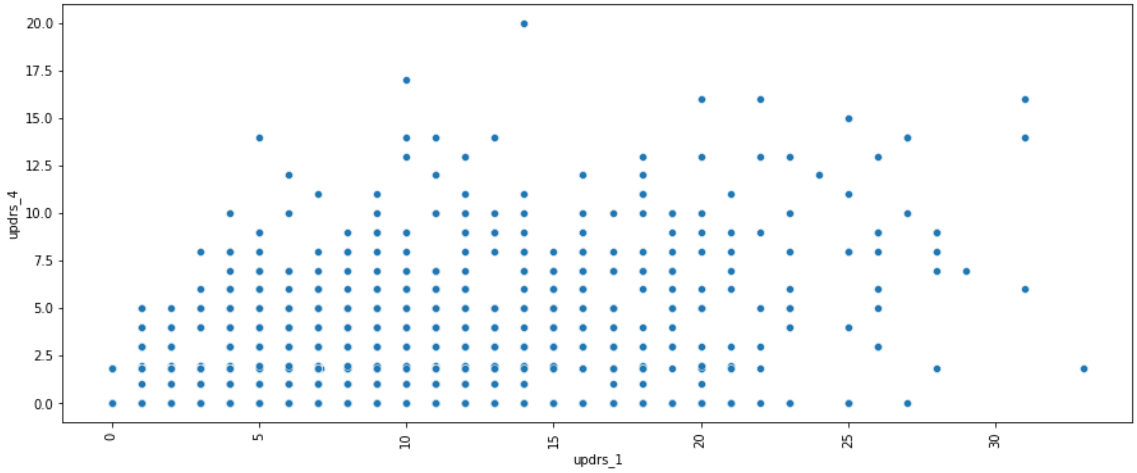
In [138]:

```
plt.figure(figsize=(15,6))
sns.lineplot(x = df2['updrs_1'], y = df2['updrs_4'], palette = 'hls')
plt.xticks(rotation = 90)
plt.show()
```



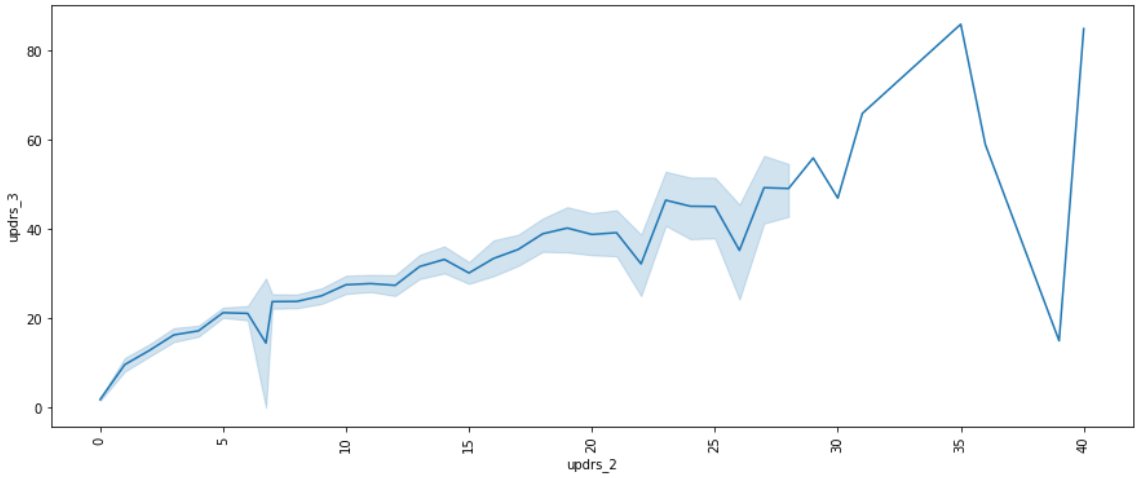
In [139]:

```
plt.figure(figsize=(15,6))
sns.scatterplot(x = df2['updrs_1'], y = df2['updrs_4'], palette = 'hls')
plt.xticks(rotation = 90)
plt.show()
```



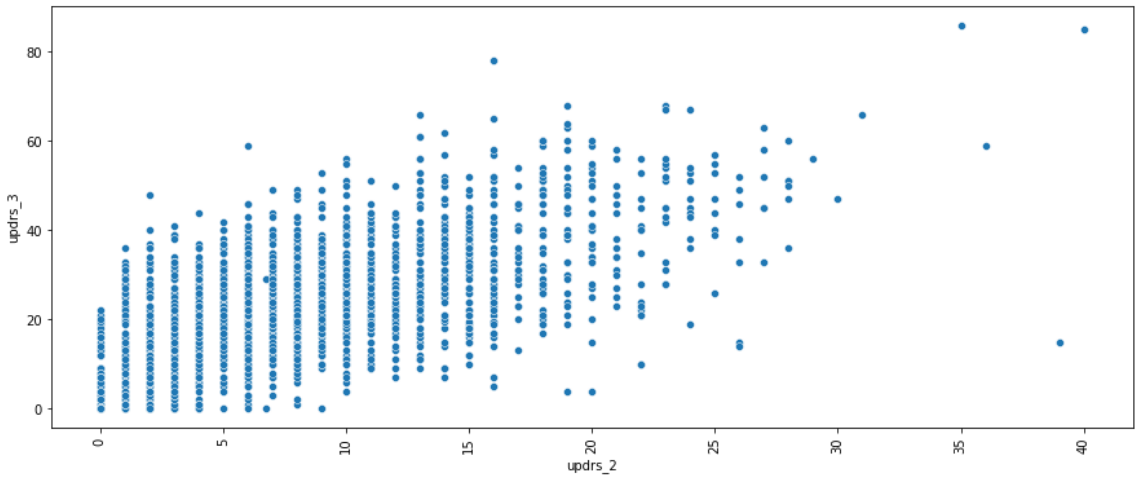
In [140]:

```
plt.figure(figsize=(15,6))
sns.lineplot(x = df2['updrs_2'], y = df2['updrs_3'], palette = 'hls')
plt.xticks(rotation = 90)
plt.show()
```



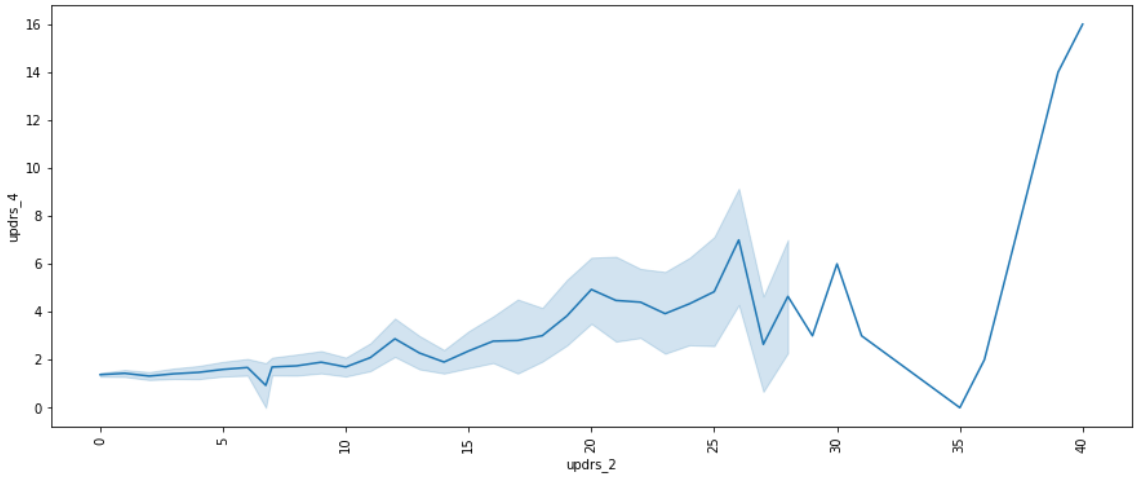
In [141]:

```
plt.figure(figsize=(15,6))
sns.scatterplot(x = df2['updrs_2'], y = df2['updrs_3'], palette = 'hls')
plt.xticks(rotation = 90)
plt.show()
```



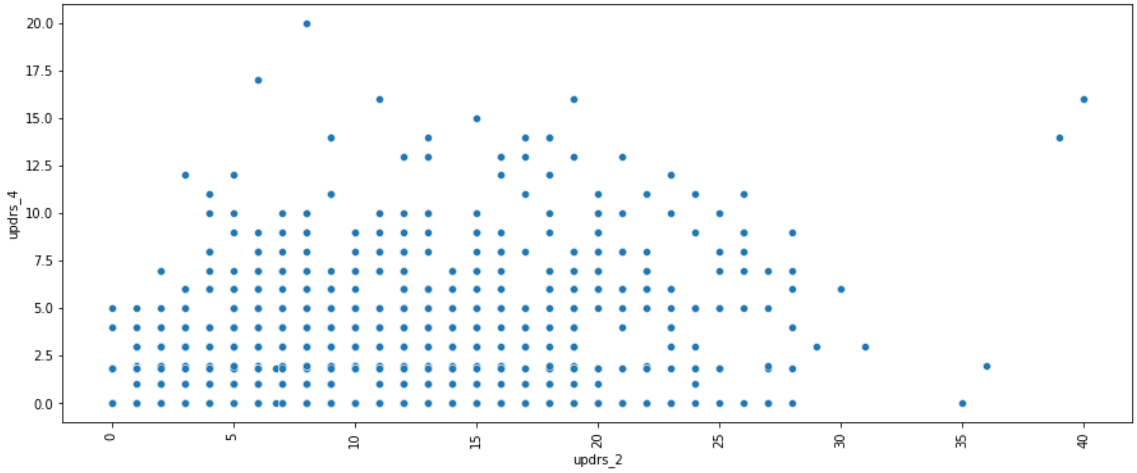
In [142]:

```
plt.figure(figsize=(15,6))
sns.lineplot(x = df2['updrs_2'], y = df2['updrs_4'], palette = 'hls')
plt.xticks(rotation = 90)
plt.show()
```



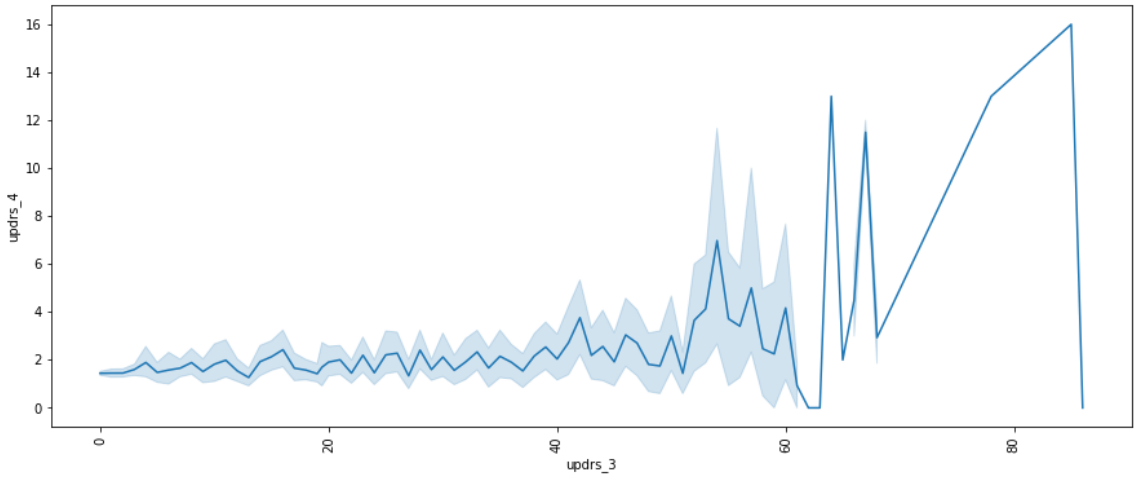
In [143]:

```
plt.figure(figsize=(15,6))
sns.scatterplot(x = df2['updrs_2'], y = df2['updrs_4'], palette = 'hls')
plt.xticks(rotation = 90)
plt.show()
```



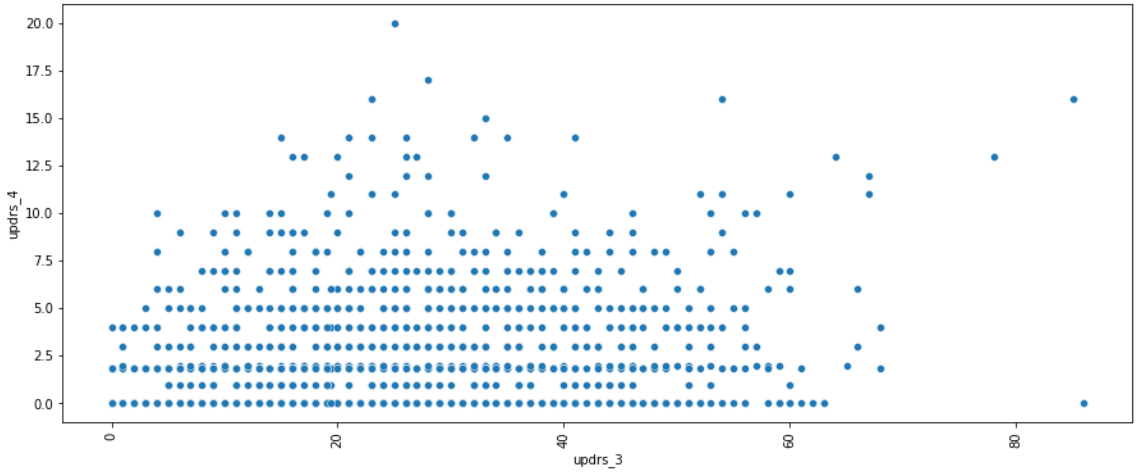
In [144]:

```
plt.figure(figsize=(15,6))
sns.lineplot(x = df2['updrs_3'], y = df2['updrs_4'], palette = 'hls')
plt.xticks(rotation = 90)
plt.show()
```



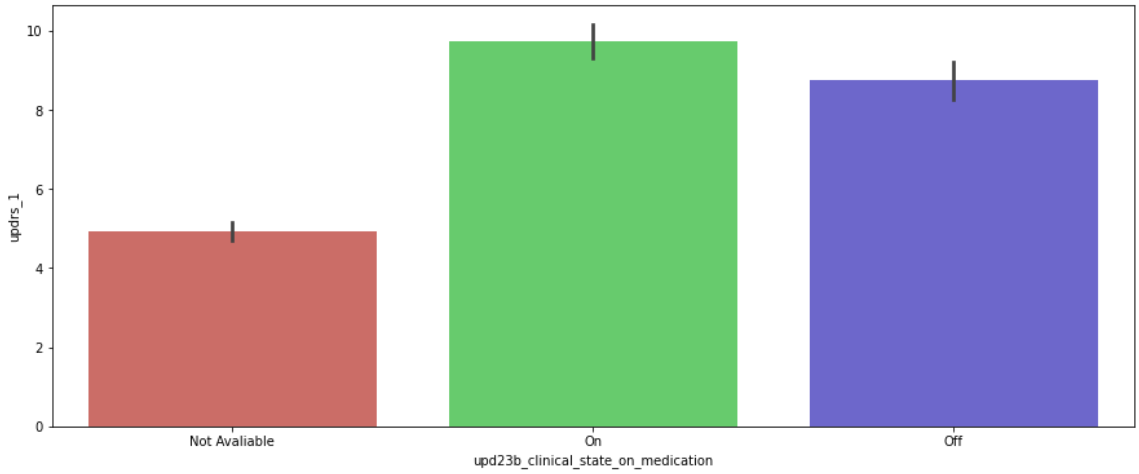
In [145]:

```
plt.figure(figsize=(15,6))
sns.scatterplot(x = df2['updrs_3'], y = df2['updrs_4'], palette = 'hls')
plt.xticks(rotation = 90)
plt.show()
```



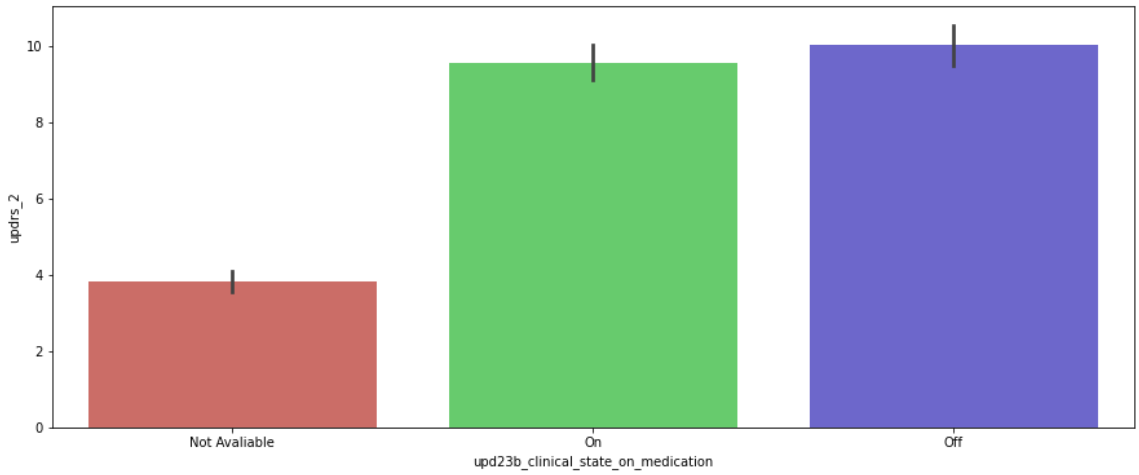
In [147]:

```
plt.figure(figsize=(15,6))
sns.barplot(y = df2['updrs_1'], x = df2['upd23b_clinical_state_on_medication'], palette
plt.show()
```



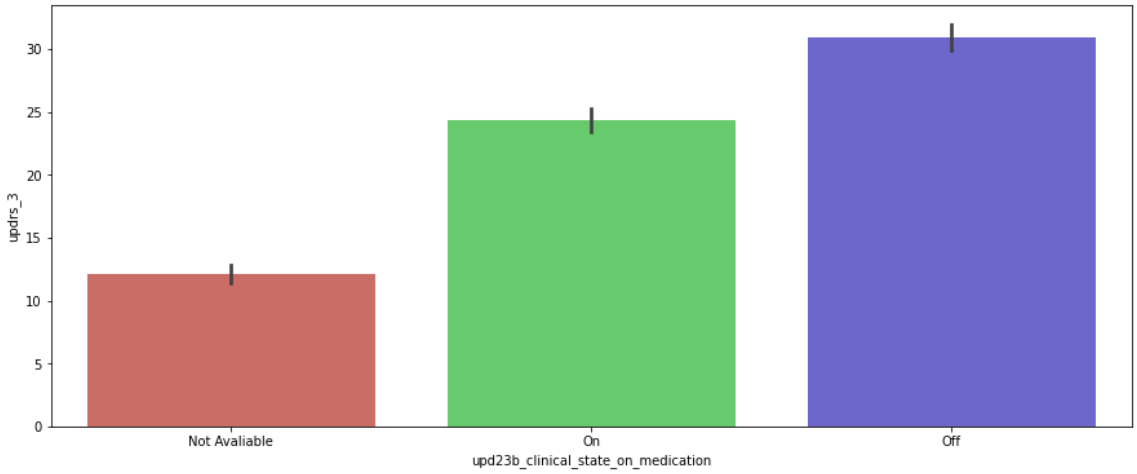
In [150]:

```
plt.figure(figsize=(15,6))
sns.barplot(y = df2['updrs_2'], x = df2['upd23b_clinical_state_on_medication'], palette
plt.show()
```



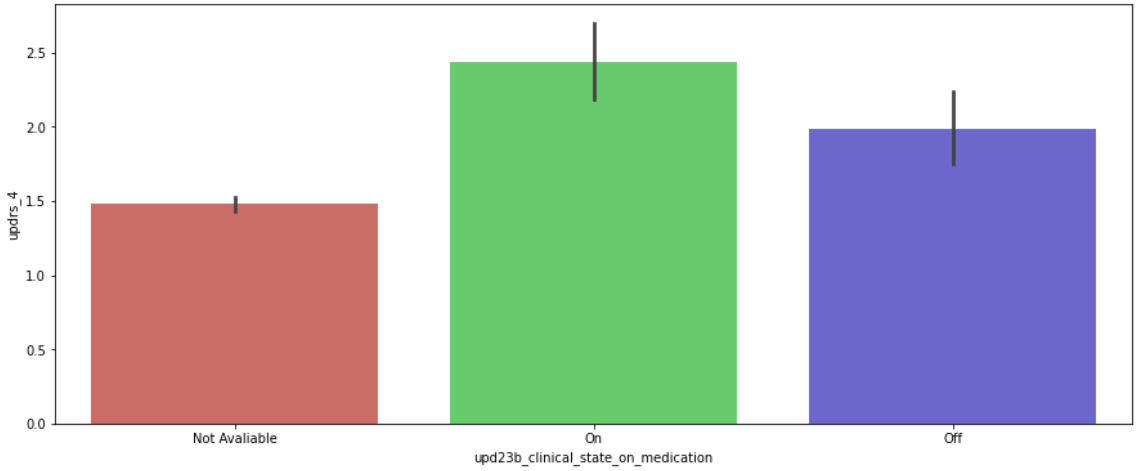
In [151]:

```
plt.figure(figsize=(15,6))
sns.barplot(y = df2['updrs_3'], x = df2['upd23b_clinical_state_on_medication'], palette
plt.show()
```



In [152]:

```
plt.figure(figsize=(15,6))
sns.barplot(y = df2['updrs_4'], x = df2['upd23b_clinical_state_on_medication'], palette
plt.show()
```



In [155]:

```
plt.figure(figsize=(15,6))
sns.pairplot(df2, palette = 'hls')
plt.show()
```

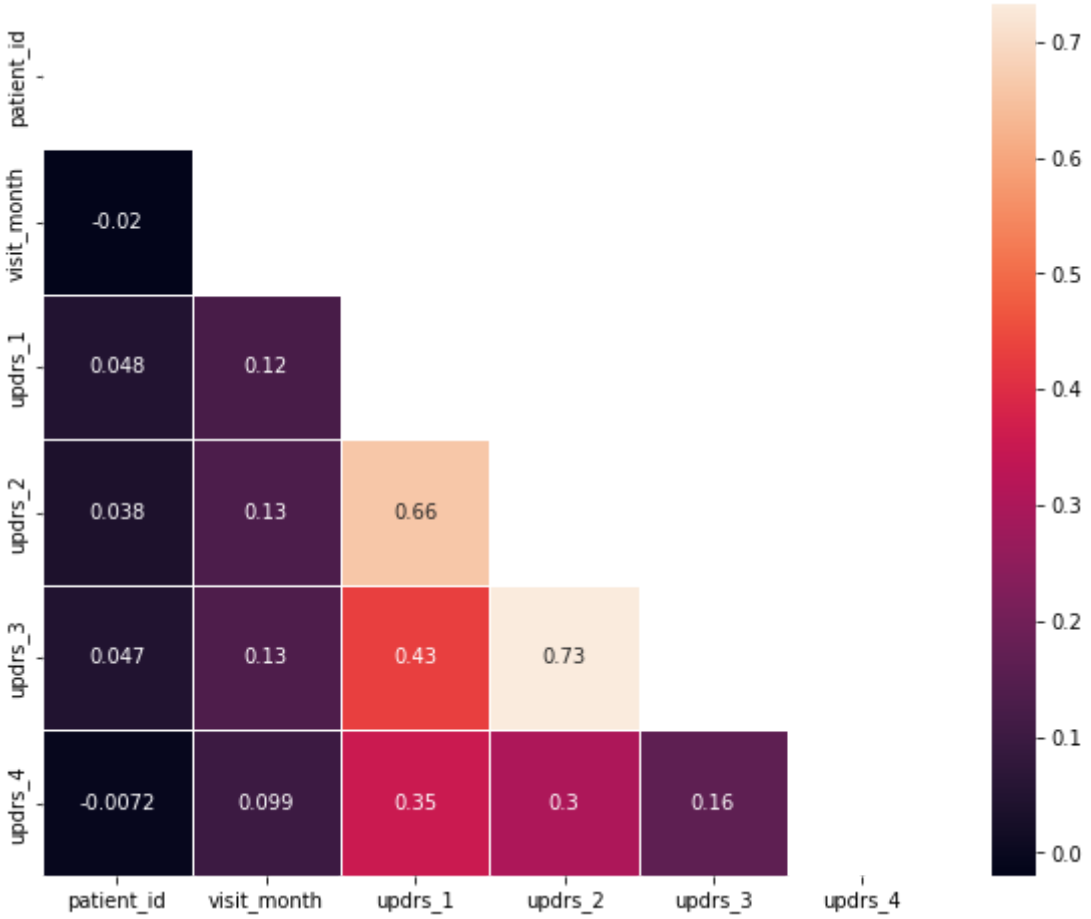
```
<Figure size 1080x432 with 0 Axes>
```

In [153]:

```
df2_corr = df2.corr()
```

In [154]:

```
plt.figure(figsize=(10, 8))
matrix = np.triu(df2_corr)
sns.heatmap(df2_corr, annot=True, linewidth=.8, mask=matrix, cmap="rocket");
plt.show()
```



In [168]:

```
df.shape
```

Out[168]:

```
(847363, 6)
```

In [169]:

```
df1.shape
```

Out[169]:

```
(200981, 5)
```

In [170]:

```
df2.shape
```

Out[170]:

```
(2615, 8)
```

In [171]:

```
df.columns
```

Out[171]:

```
Index(['visit_id', 'visit_month', 'patient_id', 'UniProt', 'Peptide',
       'PeptideAbundance'],
      dtype='object')
```

In [172]:

```
df1.columns
```

Out[172]:

```
Index(['visit_id', 'visit_month', 'patient_id', 'UniProt', 'NPX'], dtype
='object')
```

In [173]:

```
df2.columns
```

Out[173]:

```
Index(['visit_id', 'patient_id', 'visit_month', 'updrs_1', 'updrs_2',
       'updrs_3', 'updrs_4', 'upd23b_clinical_state_on_medication'],
      dtype='object')
```

In [174]:

```
df_new = df.merge(df1, on=['visit_id', 'visit_month', 'patient_id', 'UniProt'])
df_new = df_new.merge(df2, on=['visit_id', 'visit_month', 'patient_id'])
```

In [175]:

```
df_new.head()
```

Out[175]:

	visit_id	visit_month	patient_id	UniProt	Peptide	I
0	55_0	0	55	O00391	NEQEQPLGQWHLS	
1	55_0	0	55	O00533	GNPEPTFSWTK	
2	55_0	0	55	O00533	IEIPSSVQQVPTIIK	
3	55_0	0	55	O00533	KPQSAVYSTGSNGILLC(UniMod_4)EAEGEPQPTIK	
4	55_0	0	55	O00533	SMEQNGPGLEYR	

In [177]:

```
df_new.tail()
```

Out[177]:

	visit_id	visit_month	patient_id	UniProt	Peptide	F
539644	58648_108	108	58648	Q9UHG2	ILAGSADSEGVAAPR	
539645	58648_108	108	58648	Q9UKV8	SGNIPAGTTVDTK	
539646	58648_108	108	58648	Q9Y646	LALLVDTVGPR	
539647	58648_108	108	58648	Q9Y6R7	AGC(UniMod_4)VAESTAVC(UniMod_4)R	
539648	58648_108	108	58648	Q9Y6R7	GATTSPGVYELSSR	

In [176]:

```
df_new.shape
```

Out[176]:

```
(539649, 12)
```

In [178]:

```
df_new.columns
```

Out[178]:

```
Index(['visit_id', 'visit_month', 'patient_id', 'UniProt', 'Peptide',
       'PeptideAbundance', 'NPX', 'updrs_1', 'updrs_2', 'updrs_3', 'updrs_
4',
       'upd23b_clinical_state_on_medication'],
      dtype='object')
```

In [179]:

```
df_new.duplicated().sum()
```

Out[179]:

```
0
```

In [180]:

```
df_new.isnull().sum()
```

Out[180]:

```
visit_id                             0
visit_month                          0
patient_id                           0
UniProt                              0
Peptide                              0
PeptideAbundance                     0
NPX                                  0
updrs_1                              0
updrs_2                              0
updrs_3                              0
updrs_4                              0
upd23b_clinical_state_on_medication    0
dtype: int64
```

In [181]:

```
df_new.info()
```

```
<class 'pandas.core.frame.DataFrame'>
Int64Index: 539649 entries, 0 to 539648
Data columns (total 12 columns):
 #   Column                             Non-Null Count   Dtype  
---  ------                             --------------   -----  
 0   visit_id                           539649 non-null  object 
 1   visit_month                        539649 non-null  int64  
 2   patient_id                         539649 non-null  int64  
 3   UniProt                            539649 non-null  object 
 4   Peptide                            539649 non-null  object 
 5   PeptideAbundance                   539649 non-null  float64
 6   NPX                                539649 non-null  float64
 7   updrs_1                            539649 non-null  float64
 8   updrs_2                            539649 non-null  float64
 9   updrs_3                            539649 non-null  float64
 10  updrs_4                            539649 non-null  float64
 11  upd23b_clinical_state_on_medication  539649 non-null  object 
dtypes: float64(6), int64(2), object(4)
memory usage: 53.5+ MB
```

In [182]:

```
df_new.describe()
```

Out[182]:

	visit_month	patient_id	PeptideAbundance	NPX	updrs_1	
count	539649.000000	539649.000000	539649.000000	5.396490e+05	539649.000000	53964
mean	26.758738	32652.382856	71166.236653	4.322718e+05	6.538131	
std	22.912143	18626.760180	81205.642003	3.938369e+05	5.329968	
min	0.000000	55.000000	46.765000	8.460820e+01	0.000000	
25%	6.000000	16566.000000	19537.900000	8.643140e+04	2.000000	
50%	24.000000	29417.000000	42528.700000	3.096000e+05	5.000000	
75%	48.000000	50611.000000	90343.100000	7.138080e+05	9.000000	
max	108.000000	65043.000000	511044.000000	1.365430e+06	33.000000	2

In [183]:

```
df_new.nunique()
```

Out[183]:

```
visit_id                              1068
visit_month                             15
patient_id                             248
UniProt                                226
Peptide                                844
PeptideAbundance                    430488
NPX                                 178139
updrs_1                                 30
updrs_2                                 29
updrs_3                                 65
updrs_4                                 18
upd23b_clinical_state_on_medication      3
dtype: int64
```

In [184]:

```
df_new['visit_month'].unique()
```

Out[184]:

```
array([  0,   3,   6,  12,  18,  24,  30,  36,  48,  54,  60,  72,  84,
        96, 108], dtype=int64)
```

In [185]:

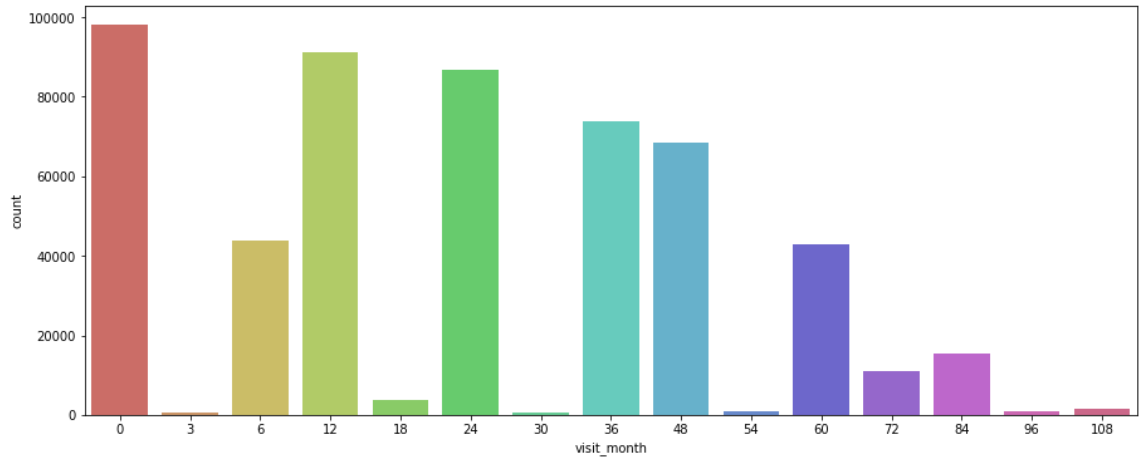
```
df_new['visit_month'].value_counts()
```

Out[185]:

```
0      98054
12     91046
24     86690
36     73811
48     68616
6      43886
60     42897
84     15400
72     10943
18      3815
108     1516
96      1012
54       969
3        514
30       480
Name: visit_month, dtype: int64
```

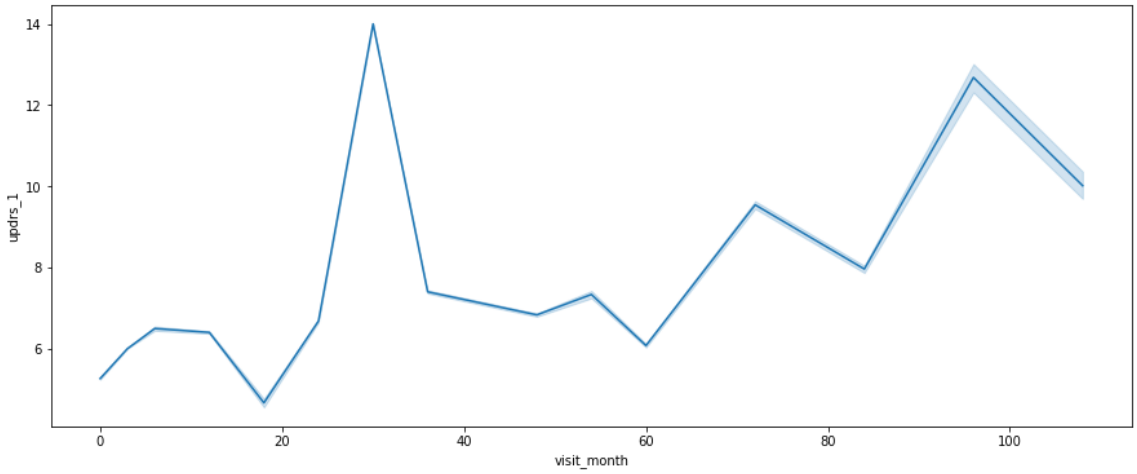
In [186]:

```
plt.figure(figsize=(15,6))
sns.countplot(df_new['visit_month'], data = df_new, palette = 'hls')
plt.show()
```



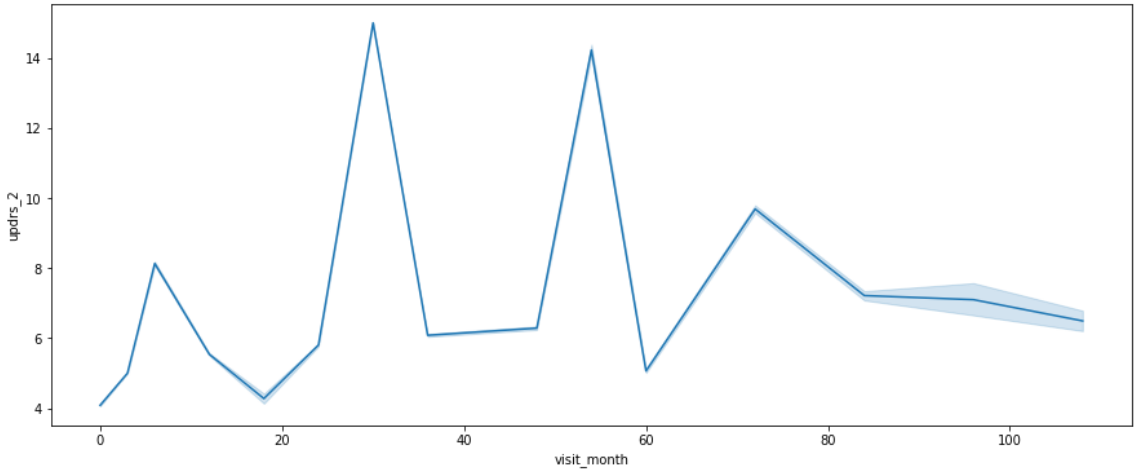
In [190]:

```
plt.figure(figsize=(15,6))
sns.lineplot(x = df_new['visit_month'], y = df_new['updrs_1'], data = df_new, palette =
plt.show()
```



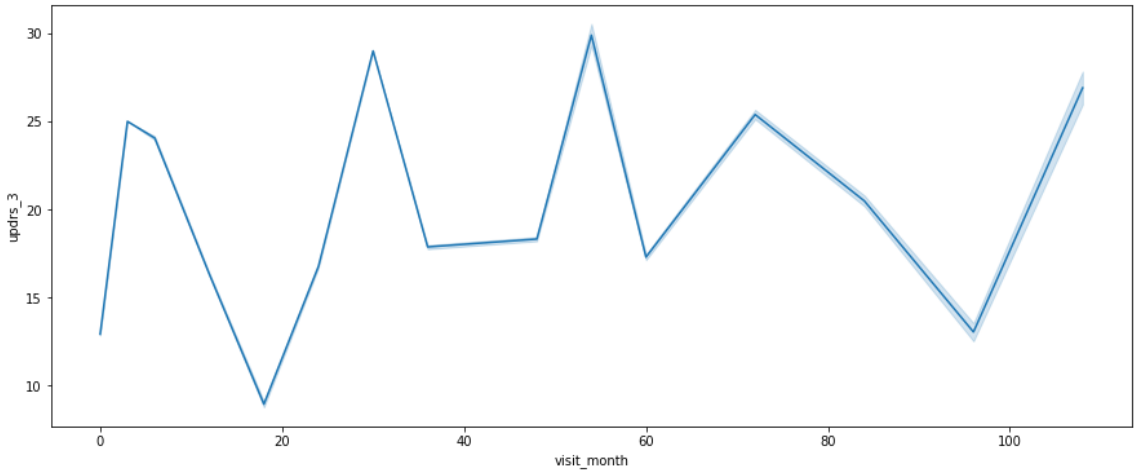
In [191]:

```
plt.figure(figsize=(15,6))
sns.lineplot(x = df_new['visit_month'], y = df_new['updrs_2'], data = df_new, palette =
plt.show()
```



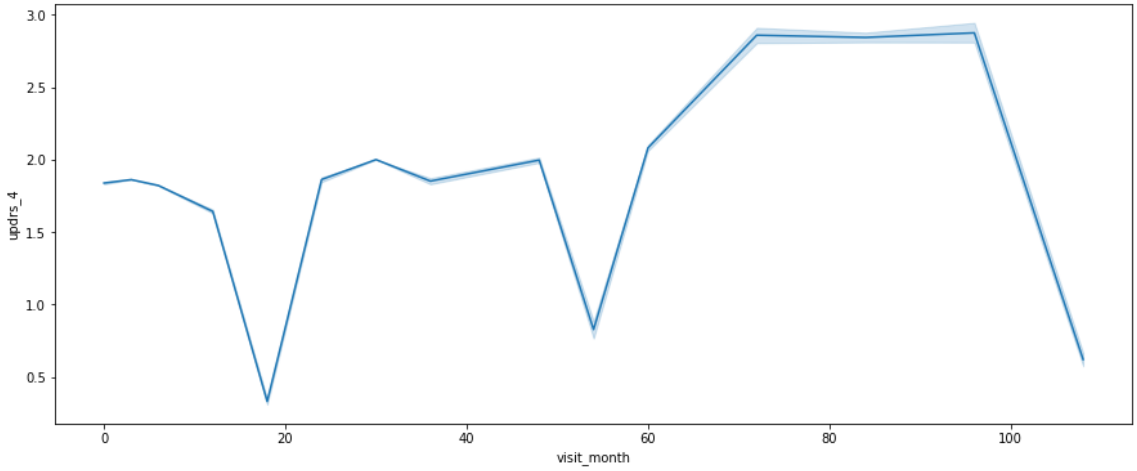
In [192]:

```
plt.figure(figsize=(15,6))
sns.lineplot(x = df_new['visit_month'], y = df_new['updrs_3'], data = df_new, palette =
plt.show()
```



In [193]:

```
plt.figure(figsize=(15,6))
sns.lineplot(x = df_new['visit_month'], y = df_new['updrs_4'], data = df_new, palette =
plt.show()
```



In [202]:

```
df_new.columns
```

Out[202]:

```
Index(['visit_id', 'visit_month', 'patient_id', 'UniProt', 'Peptide',
       'PeptideAbundance', 'NPX', 'updrs_1', 'updrs_2', 'updrs_3', 'updrs_
4',
       'upd23b_clinical_state_on_medication'],
      dtype='object')
```

In [206]:

```
df_new_1 = df_new[['PeptideAbundance', 'NPX', 'updrs_1']]
```

In [207]:

```
df_new_1
```

Out[207]:

	PeptideAbundance	NPX	updrs_1
0	11254.30	11254.3	10.0
1	102060.00	732430.0	10.0
2	174185.00	732430.0	10.0
3	27278.90	732430.0	10.0
4	30838.70	732430.0	10.0
...	...	...	...
539644	202820.00	369437.0	6.0
539645	105830.00	105830.0	6.0
539646	21257.60	21257.6	6.0
539647	5127.26	17953.1	6.0
539648	12825.90	17953.1	6.0

539649 rows × 3 columns

In [208]:

```
X = df_new_1.drop('updrs_1', axis =1)
y = df_new_1['updrs_1']
```

In [209]:

```
from sklearn import preprocessing
scaler = preprocessing.MinMaxScaler()
X= scaler.fit_transform(X)
```

In [210]:

```
from sklearn.model_selection import train_test_split
X_train, X_test, y_train, y_test = train_test_split(X, y,
                                                    test_size=0.30)
```

In [211]:

```
from sklearn.linear_model import LinearRegression
```

In [212]:

```
lr = LinearRegression()
```

In [213]:

```
lr.fit(X_train,y_train)
```

Out[213]:

```
LinearRegression()
```

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In [214]:

```
y_pred = lr.predict(X_test)
```

In [215]:

```
from sklearn.metrics import mean_squared_error
```

In [216]:

```
RMSE_lr = mean_squared_error(y_test, y_pred, squared = False)
RMSE_lr
```

Out[216]:

```
5.30827489979071
```

In [219]:

```
from sklearn.metrics import r2_score
```

In [220]:

```
r2 = r2_score(y_test, y_pred)
r2
```

Out[220]:

```
-2.6721576411148362e-05
```

In [217]:

```
from sklearn.model_selection import cross_val_score
```

In [218]:

```
cross_val_score(lr, X_train, y_train, cv=10)
```

Out[218]:

```
array([-5.27375550e-05,  3.37670713e-05, -1.58026404e-06, -1.99379959e-05,
       -7.52700358e-05,  1.86911454e-05, -1.63380315e-05, -6.99537494e-06,
        1.35883401e-05,  6.12006435e-05])
```

In [265]:

```
from sklearn.model_selection import GridSearchCV

# Define the grid of hyperparameters to search
param_grid = {'fit_intercept': [True, False],
              'normalize': [True, False]}

# Create a linear regression model
lin_reg = LinearRegression()

# Create a grid search object
grid_search = GridSearchCV(lin_reg, param_grid, )
cv=5
# Fit the grid search to the data
grid_search.fit(X_train, y_train)

# Get the best hyperparameters
best_fit_intercept = grid_search.best_params_['fit_intercept']
best_normalize = grid_search.best_params_['normalize']

# Train a linear regression model with the best hyperparameters
lin_reg_best = LinearRegression(fit_intercept=best_fit_intercept,
                                normalize=best_normalize)
lin_reg_best.fit(X_train, y_train)
```

Out[265]:

```
LinearRegression(normalize=True)
```

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In [266]:

```
y_pred = lin_reg_best.predict(X_test)
```

In [267]:

```
r2 = r2_score(y_test, y_pred)
r2
```

Out[267]:

```
-2.6721576411148362e-05
```

In [221]:

```
from sklearn.tree import DecisionTreeRegressor
```

In [222]:

```
dt = DecisionTreeRegressor(random_state=0)
```

In [223]:

```
dt.fit(X_train, y_train)
```

Out[223]:

```
DecisionTreeRegressor(random_state=0)
```

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In [224]:

```
y_pred = dt.predict(X_test)
```

In [225]:

```
RMSE_dt = mean_squared_error(y_test, y_pred, squared = False)
RMSE_dt
```

Out[225]:

```
5.770982107341489
```

In [226]:

```
cross_val_score(dt, X_train, y_train, cv=10)
```

Out[226]:

```
array([-0.26053411, -0.28087271, -0.23617434, -0.21194405, -0.20917041,
       -0.22644514, -0.43629063, -0.2066975 , -0.15947303, -0.24562276])
```

In [227]:

```
r2 = r2_score(y_test, y_pred)
r2
```

Out[227]:

```
-0.1819640005104295
```

In [268]:

```
# Define the grid of hyperparameters to search
param_grid = {'max_depth': [1, 2, 3, 4, 5],
              'min_samples_split': [2, 3, 4]}

# Create a decision tree regression model
dtr = DecisionTreeRegressor()

# Create a grid search object
grid_search = GridSearchCV(dtr, param_grid, cv=5)

# Fit the grid search to the data
grid_search.fit(X_train, y_train)

# Get the best hyperparameters
best_max_depth = grid_search.best_params_['max_depth']
best_min_samples_split = grid_search.best_params_['min_samples_split']

# Train a decision tree regression model with the best hyperparameters
dtr_best = DecisionTreeRegressor(max_depth=best_max_depth,
                                 min_samples_split=best_min_samples_split)
dtr_best.fit(X_train, y_train)
```

Out[268]:

```
DecisionTreeRegressor(max_depth=5, min_samples_split=4)
```

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In [228]:

```
from sklearn.ensemble import RandomForestRegressor
```

In [229]:

```
rf = RandomForestRegressor(max_depth=5, random_state=0)
```

In [230]:

```
rf.fit(X_train, y_train)
```

Out[230]:

```
RandomForestRegressor(max_depth=5, random_state=0)
```

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In [231]:

```
y_pred = rf.predict(X_test)
```

In [232]:

```
RMSE_rf = mean_squared_error(y_test, y_pred, squared = False)
RMSE_rf
```

Out[232]:

```
5.30474267933126
```

In [233]:

```
r2 = r2_score(y_test, y_pred)
r2
```

Out[233]:

```
0.0013037067378985912
```

In [269]:

```
# Define the grid of hyperparameters to search
param_grid = {'n_estimators': [10, 50, 100],
              'max_depth': [1, 2, 3, 4, 5]}

# Create a random forest regression model
rfr = RandomForestRegressor()

# Create a grid search object
grid_search = GridSearchCV(rfr, param_grid, cv=5)

# Fit the grid search to the data
grid_search.fit(X_train, y_train)

# Get the best hyperparameters
best_n_estimators = grid_search.best_params_['n_estimators']
best_max_depth = grid_search.best_params_['max_depth']

# Train a random forest regression model with the best hyperparameters
rfr_best = RandomForestRegressor(n_estimators=best_n_estimators,
                                 max_depth=best_max_depth)
rfr_best.fit(X_train, y_train)
```

Out[269]:

```
RandomForestRegressor(max_depth=5, n_estimators=10)
```

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In [234]:

```
from xgboost import XGBRegressor
```

In [235]:

```
model = XGBRegressor()
model.fit(X_train, y_train)
```

Out[235]:

```
XGBRegressor(base_score=0.5, booster='gbtree', callbacks=None,
             colsample_bylevel=1, colsample_bynode=1, colsample_bytree=1,
             early_stopping_rounds=None, enable_categorical=False,
             eval_metric=None, gamma=0, gpu_id=-1, grow_policy='depthwis
e',
             importance_type=None, interaction_constraints='',
             learning_rate=0.300000012, max_bin=256, max_cat_to_onehot=4,
             max_delta_step=0, max_depth=6, max_leaves=0, min_child_weight
=1,
             missing=nan, monotone_constraints='()', n_estimators=100, n_j
obs=0,
             num_parallel_tree=1, predictor='auto', random_state=0, reg_al
pha=0,
             reg_lambda=1, ...)
```

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In [236]:

```
y_pred = model.predict(X_test)
```

In [237]:

```
RMSE_xg = mean_squared_error(y_test, y_pred, squared = False)
RMSE_xg
```

Out[237]:

```
5.21380418046862
```

In [238]:

```
r2 = r2_score(y_test, y_pred)
r2
```

Out[238]:

```
0.03525124767452825
```

In [ ]:

```
from sklearn.model_selection import GridSearchCV
param_grid = {
    'max_depth': [3, 5, 7],
    'learning_rate': [0.01, 0.1, 0.5],
    'n_estimators': [50, 100, 200]
}

model = XGBRegressor()
grid_search = GridSearchCV(model, param_grid, cv=5, scoring='neg_mean_squared_error')
grid_search.fit(X_train, y_train)

y_pred = grid_search.predict(X_test)

mse = mean_squared_error(y_test, y_pred)
print("MSE:", mse)

# Print the best hyperparameters from GridSearchCV
print("Best hyperparameters:", grid_search.best_params_)
```