LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120221\
Data File : BP008186.D
Acq On : 02 Dec 2021 11:06
Operator : CG/JU
Sample : PB141105BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PB141105BL

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP008186.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.393	402	409	423	rBV	2068329	2977621	52.16%	10.903%
2	6.987	670	680	693	rBV	1789551	2924414	51.23%	10.708%
3	7.799	809	818	825	rBV	387252	599965	10.51%	2.197%
4	8.963	1007	1016	1031	rBV	1093030	1883769	33.00%	6.898%
5	10.599	1286	1294	1305	rBV	437647	765088	13.40%	2.801%
6	13.069	1707	1714	1730	rBV	2477536	3865334	67.71%	14.153%
7	14.446	1941	1948	1973	rBV	620304	988263	17.31%	3.619%
8	15.945	2195	2203	2231	rBV	1887484	3082639	54.00%	11.287%
9	17.210	2411	2418	2429	rBV	774845	1179072	20.65%	4.317%
10	19.486	2801	2805	2809	rBV	167746	177990	3.12%	0.652%
11	19.781	2849	2855	2868	rBV	4774394	5708704	100.00%	20.903%
12	20.504	2975	2978	2982	rBV	121096	135473	2.37%	0.496%
13	21.092	3074	3078	3086	rBV	137967	204097	3.58%	0.747%
14	21.310	3110	3115	3125	rBV	987554	1287100	22.55%	4.713%
15	21.428	3131	3135	3139	rBV	258221	354090	6.20%	1.297%
16	23.710	3517	3523	3534	rVB2	559538	1176597	20.61%	4.308%

Sum of corrected areas: 27310216

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BNA_P
ClientSampleId :
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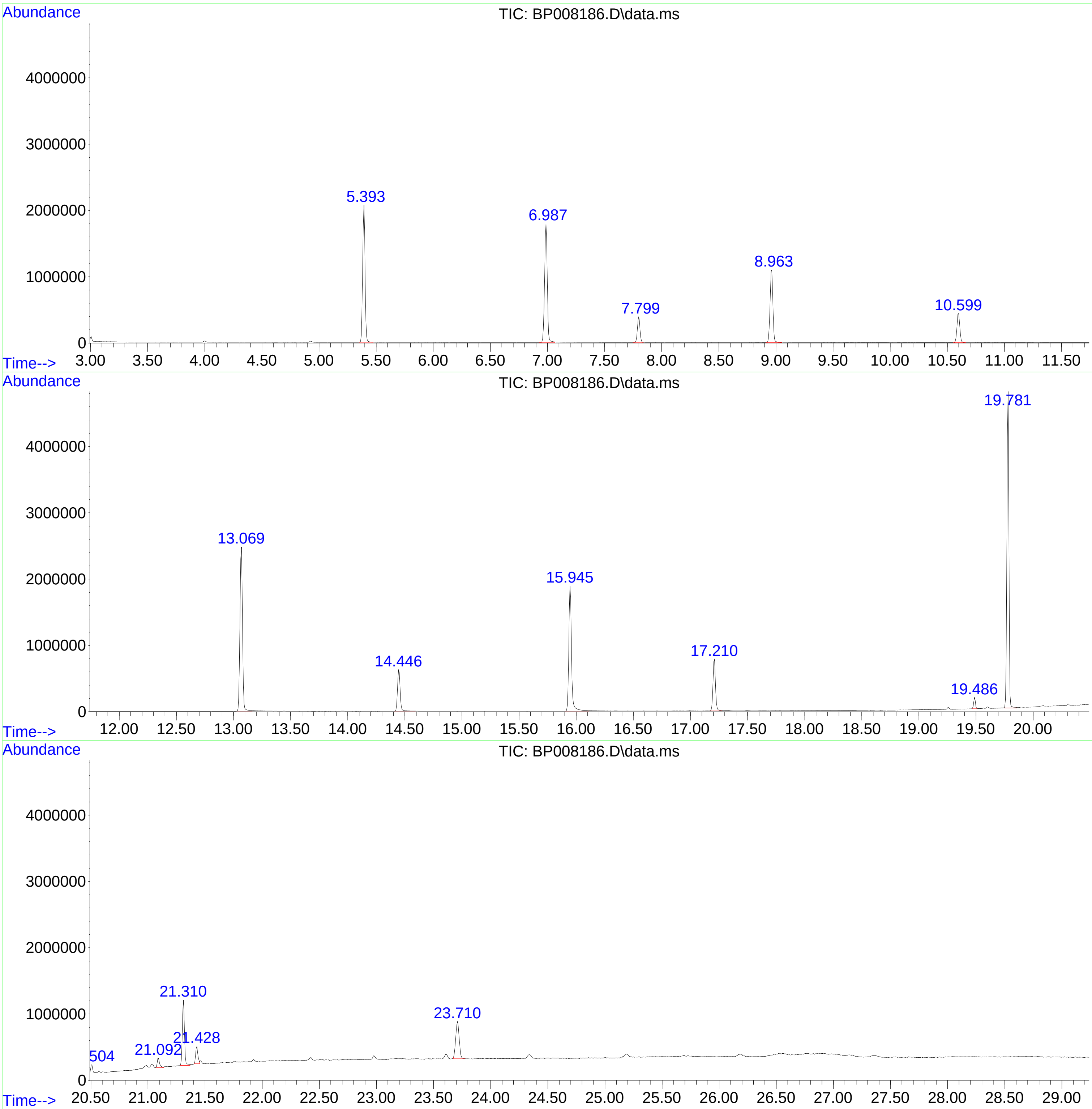
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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Data File : BP008186.D
Acq On    : 02 Dec 2021  11:06
Operator  : CG/JU
Sample    : PB141105BL
Misc      :
ALS Vial  : 3   Sample Multiplier: 1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title  : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

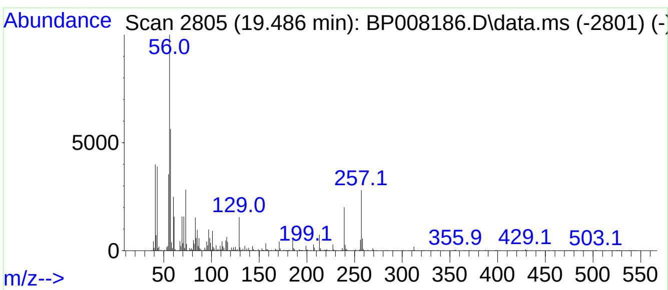
TIC Library    : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P
```

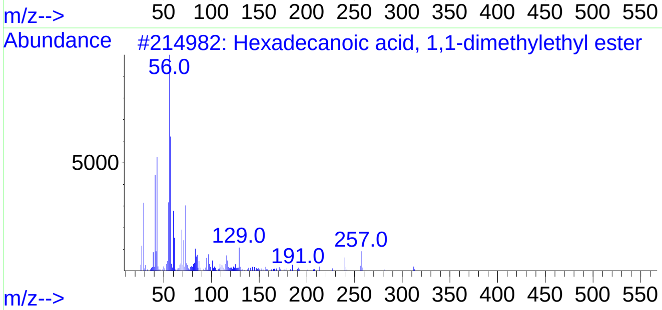
Instrument :
BNA_P
ClientSampleId :
PB141105BL

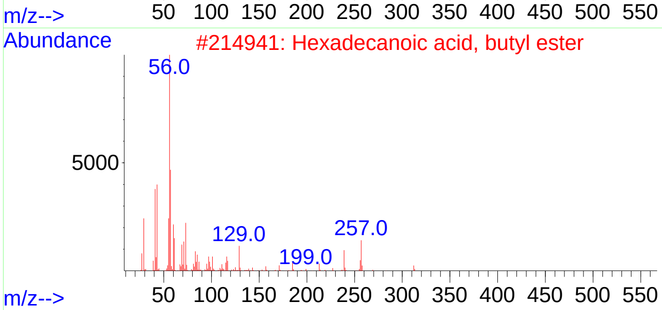
```
*********************************************************************
Peak Number  1  Hexadecanoic acid, 1,1-dime...  Concentration Rank  3
```

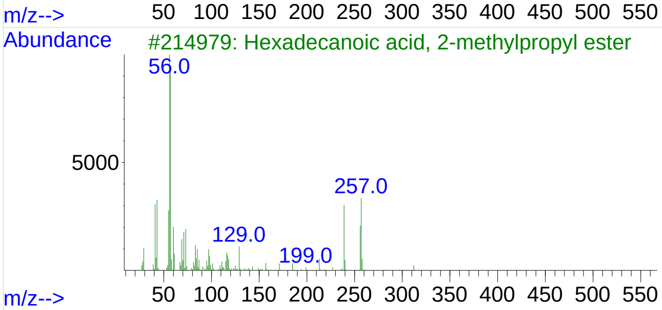
R.T.	EstConc	Area	Relative to ISTD	R.T.
19.486	2.77 ng	177990	Chrysene-d12	21.310

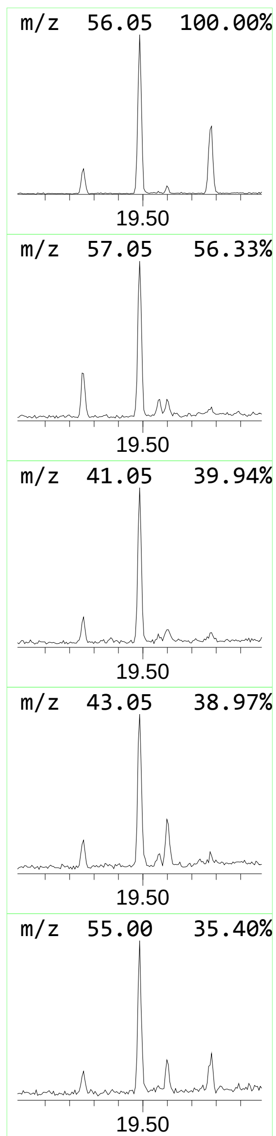
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	97
2	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	95
3	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	90
4	Methanimidamide, N'-(2,3-dihydro...	258	C14H18N4O	105949-64-2	35
5	1,3-Hexanediol, 2-ethyl- (isomer 1)	146	C8H18O2	1000484-18-2	32











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Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PB141105BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

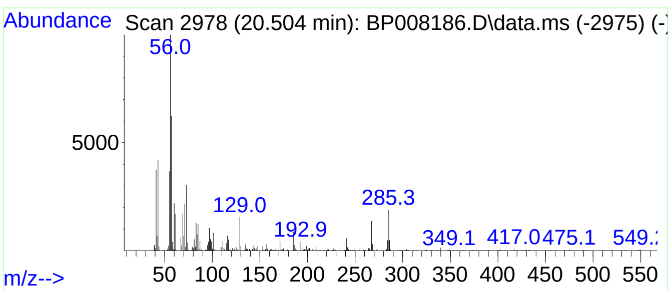
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

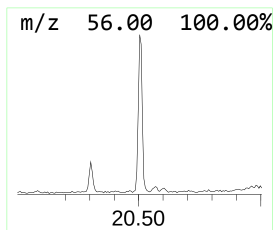
****

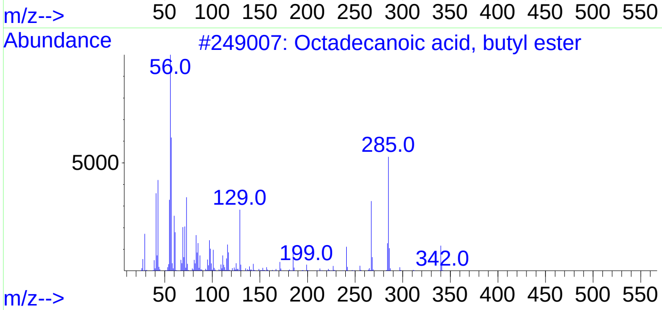
Peak Number 2 Octadecanoic acid, butyl ester Concentration Rank 4

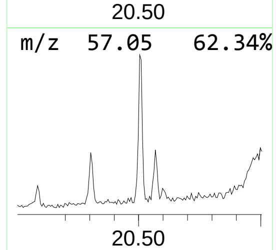
R.T.	EstConc	Area	Relative to ISTD	R.T.
20.504	2.11 ng	135473	Chrysene-d12	21.310

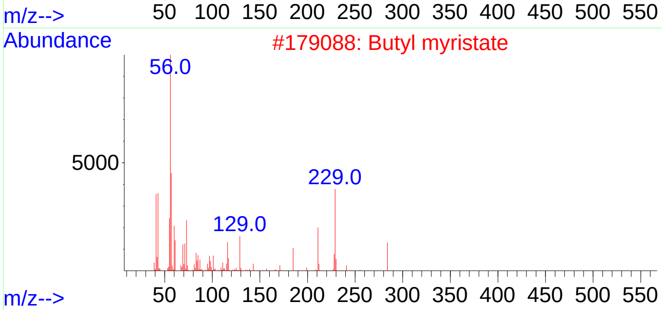
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	91
2	Butyl myristate	284	C18H36O2	000110-36-1	64
3	Octadecanoic acid, 2-methylpropy...	340	C22H44O2	000646-13-9	46
4	1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	35
5	1-Heptene, 2-methyl-	112	C8H16	015870-10-7	35

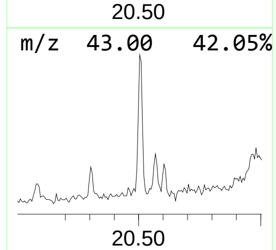


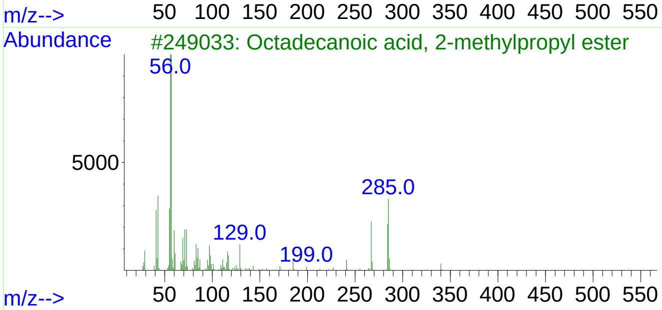


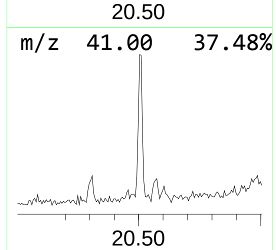


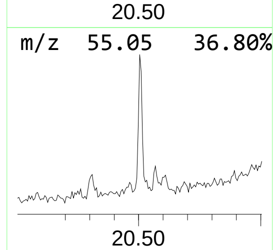












Library Search Compound Report

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BNA_P
ClientSampleId :
PB141105BL

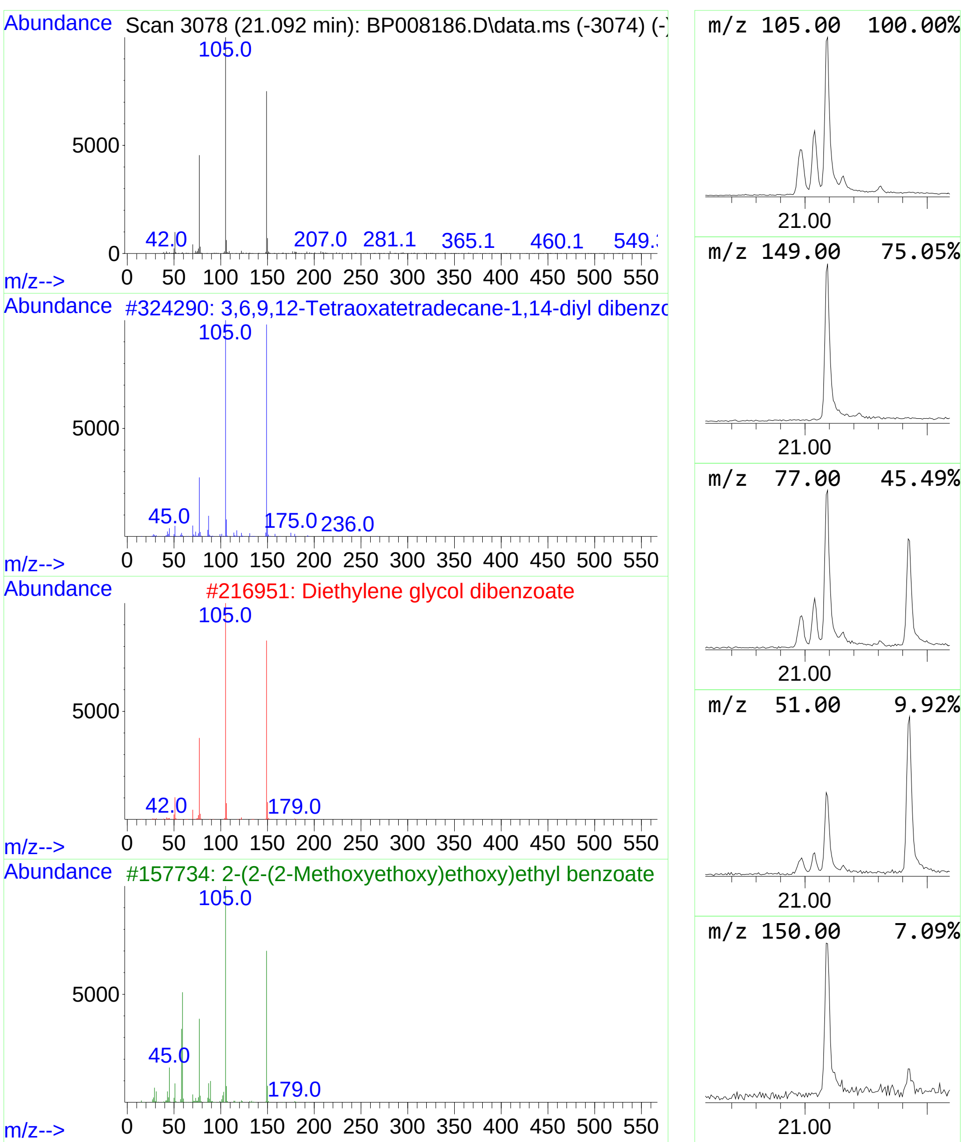
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 3,6,9,12-Tetraoxatetradecan... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.092	3.17 ng	204097	Chrysene-d12	21.310

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,6,9,12-Tetraoxatetradecane-1,1...	446	C24H30O8	1000366-97-0	74
2	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	72
3	2-(2-(2-Methoxyethoxy)ethoxy)eth...	268	C14H20O5	1000366-99-1	64
4	Phenyl(2-phenyl-1,3-dioxolan-2-y...	298	C18H18O4	006963-16-2	64
5	Benzoic acid, 2-(4-nitrophenoxy)...	287	C15H13NO5	1000368-92-7	56



Library Search Compound Report

```
Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120221\
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Sample    : PB141105BL
Misc      :
ALS Vial  : 3   Sample Multiplier: 1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title  : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library    : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P
```

Instrument :
BNA_P
ClientSampleId :
PB141105BL

```
*********************************************************************
Peak Number  4  Triphenylphosphine oxide        Concentration Rank  1

  R.T.     EstConc          Area       Relative to ISTD         R.T.
---------------------------------------------------------------------
 21.427    5.50 ng         354090    Chrysene-d12                21.310

 Hit# of  5    Tentative ID             MW  MolForm       CAS#       Qual
---------------------------------------------------------------------
 1 Triphenylphosphine oxide            278 C18H15OP      000791-28-6 98
 2 (Carbethoxymethyl)-triphenylphos... 428 C22H22BrO2P   001530-45-6 64
 3 (E)-7-Benzylidene-1-azabicyclo[3... 293 C15H19NO3S    1000483-83-4 64
 4 Formaldehyde, (triphenylphosphor... 304 C19H17N2P     015990-54-2 42
 5 5-Methyl-8-phenylfuro[3',2':5,6]... 277 C16H11N3O2    1000460-07-9 38
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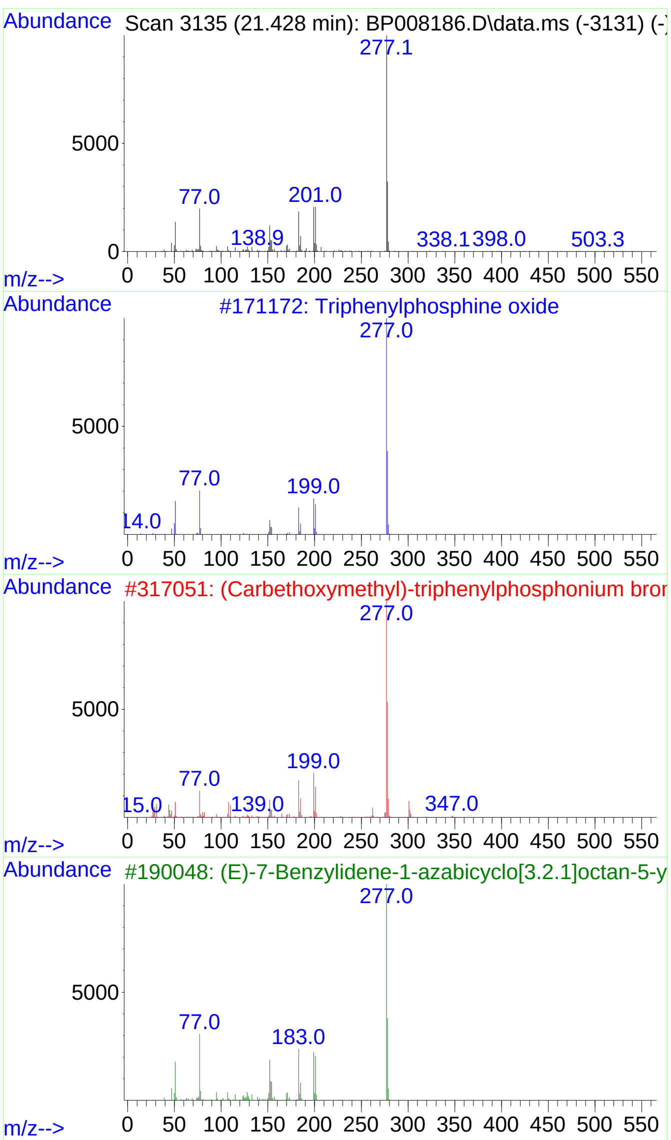

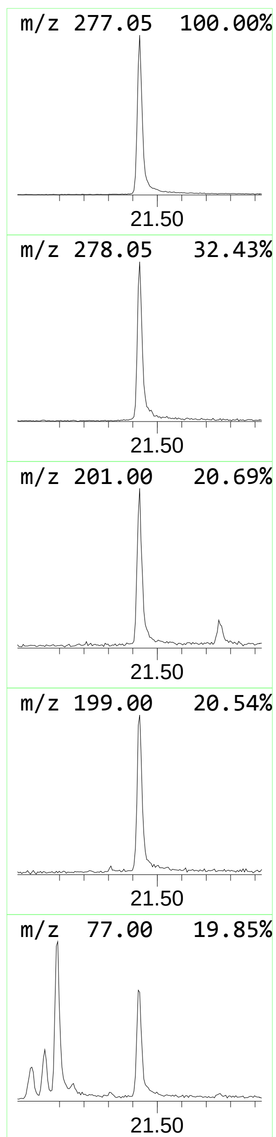

Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120221\
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Hexadecanoic ac...	19.486	2.8	ng	177990	5	21.310	1287100	20.0
Octadecanoic ac...	20.504	2.1	ng	135473	5	21.310	1287100	20.0
3,6,9,12-Tetrao...	21.092	3.2	ng	204097	5	21.310	1287100	20.0
Triphenylphosph...	21.427	5.5	ng	354090	5	21.310	1287100	20.0