LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121821\
Data File : BP008503.D
Acq On : 18 Dec 2021 23:11
Operator : CG/JU
Sample : M5115-10
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
EB-2021-12-15

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-BP121421.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP008503.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.852	312	317	334	rVB	107224	167154	4.07%	0.991%
2	5.322	391	397	421	rBV	412074	779988	18.98%	4.622%
3	5.922	494	499	510	rVB	32160	51031	1.24%	0.302%
4	6.928	664	670	695	rBV	192203	479288	11.66%	2.840%
5	7.716	795	804	814	rBV	159268	286523	6.97%	1.698%
6	8.887	996	1003	1030	rBV	505027	1066338	25.95%	6.319%
7	10.516	1272	1280	1298	rBV	176961	372957	9.08%	2.210%
8	12.993	1693	1701	1722	rBV	1413899	2311383	56.25%	13.698%
9	14.381	1928	1937	1950	rBV	294953	506989	12.34%	3.005%
10	15.881	2185	2192	2217	rBV	1043330	1982912	48.26%	11.751%
11	17.145	2401	2407	2422	rBV	352819	626991	15.26%	3.716%
12	18.063	2558	2563	2576	rBV5	22035	63763	1.55%	0.378%
13	19.716	2838	2844	2855	rBV	3360271	4109194	100.00%	24.352%
14	20.957	3051	3055	3063	rBV	133463	199353	4.85%	1.181%
15	21.257	3101	3106	3117	rBV	564996	828778	20.17%	4.911%
16	21.363	3119	3124	3144	rBV	1390865	2139864	52.08%	12.681%
17	23.616	3502	3507	3522	rVB2	392717	901814	21.95%	5.344%

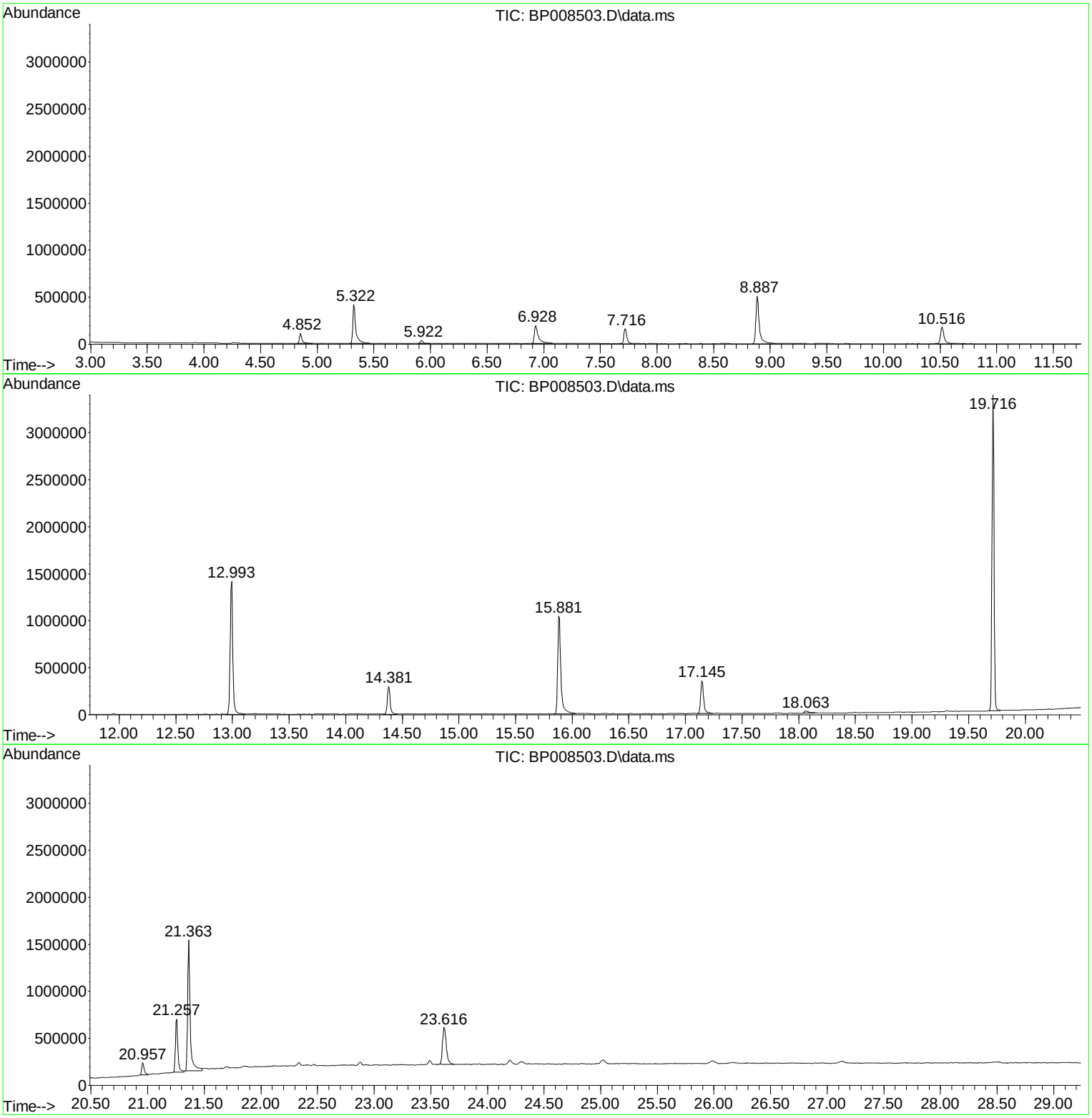
Sum of corrected areas: 16874320

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121821\
Data File : BP008503.D
Acq On : 18 Dec 2021 23:11
Operator : CG/JU
Sample : M5115-10
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
EB-2021-12-15

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP121421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121821\
Data File : BP008503.D
Acq On : 18 Dec 2021 23:11
Operator : CG/JU
Sample : M5115-10
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
EB-2021-12-15

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP121421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

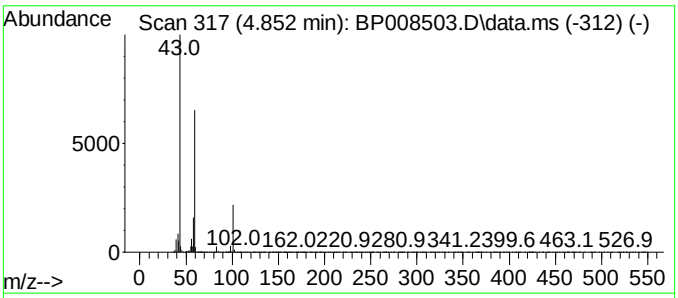
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

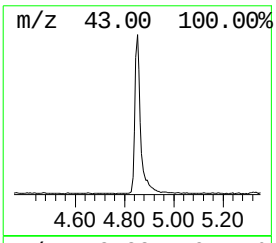
****

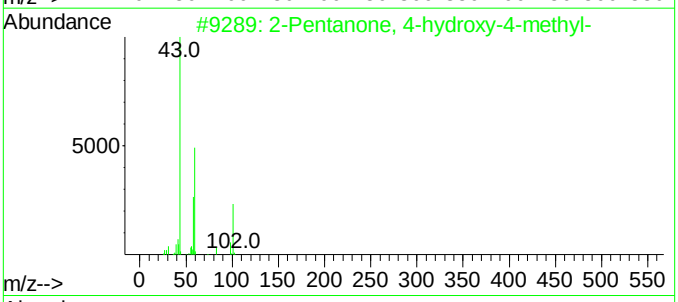
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

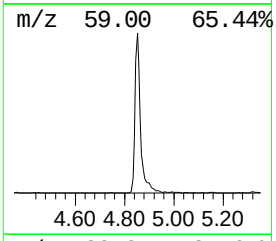
R.T.	EstConc	Area	Relative to ISTD	R.T.
4.852	11.67 ng	167154	1,4-Dichlorobenzene-d4	7.716

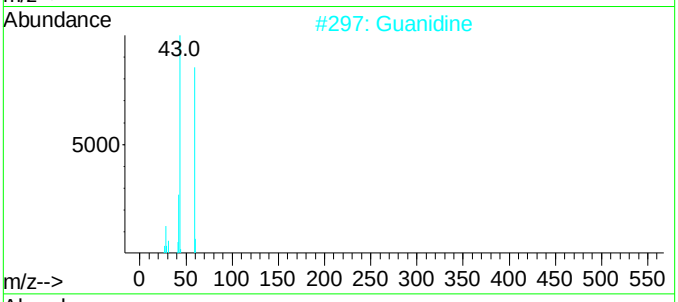
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Guanidine	59	CH5N3	000113-00-8	9
3	Acetone	58	C3H6O	000067-64-1	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	9

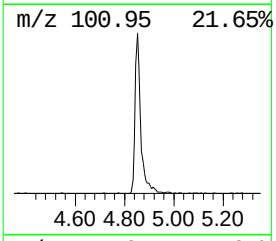


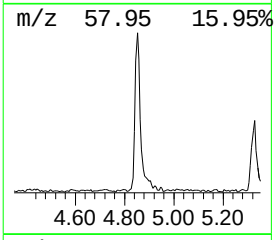


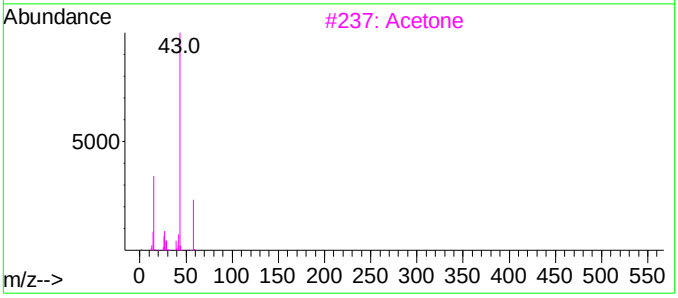


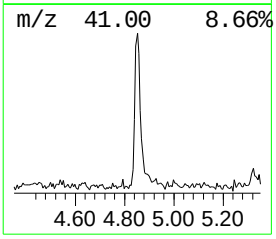












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Data File : BP008503.D
Acq On : 18 Dec 2021 23:11
Operator : CG/JU
Sample : M5115-10
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
EB-2021-12-15

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP121421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

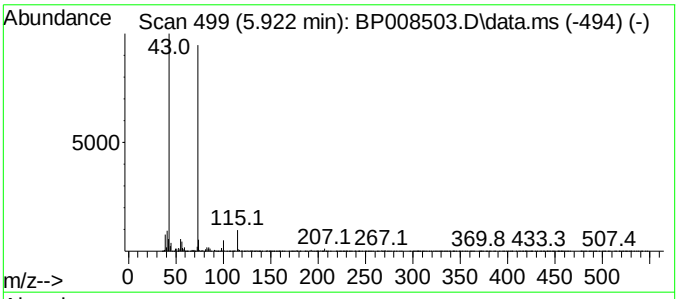
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

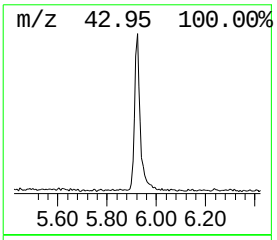
****

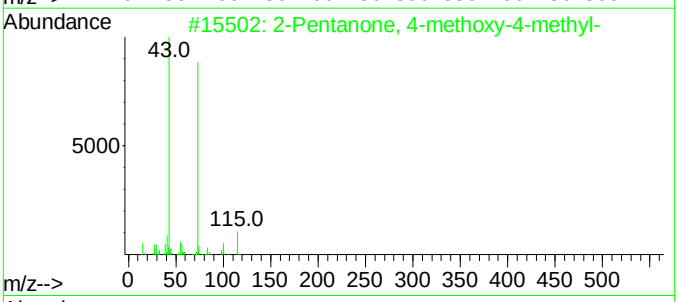
Peak Number 2 2-Pentanone, 4-methoxy-4-me... Concentration Rank 4

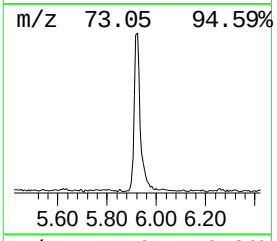
R.T.	EstConc	Area	Relative to ISTD	R.T.
5.922	3.56 ng	51031	1,4-Dichlorobenzene-d4	7.716

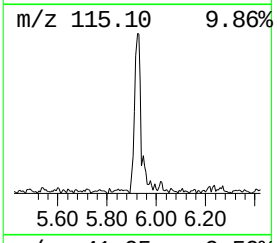
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	86
2	Butane, 2-methoxy-2,3,3-trimethyl-	130	C8H18O	027705-21-1	37
3	1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	27
4	1-Methoxyethanimine, N-acetyl-	115	C5H9NO2	099028-43-0	25
5	2,3-Dimethoxy-2,3-dimethylbutane	146	C8H18O2	006091-59-4	23

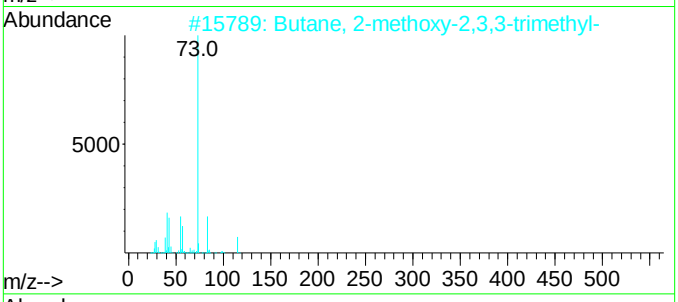


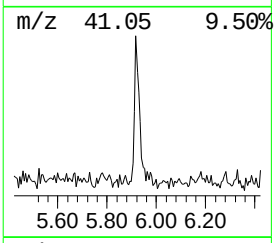


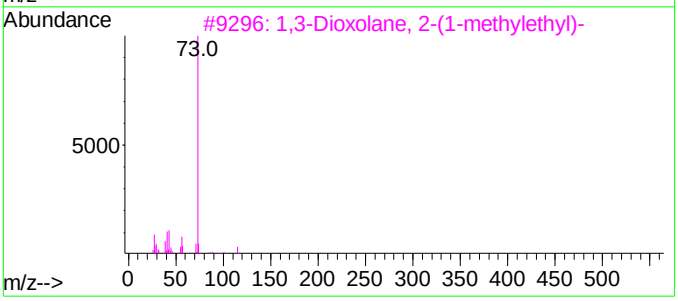


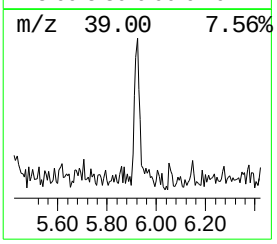












Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121821\
Data File : BP008503.D
Acq On : 18 Dec 2021 23:11
Operator : CG/JU
Sample : M5115-10
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
EB-2021-12-15

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP121421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

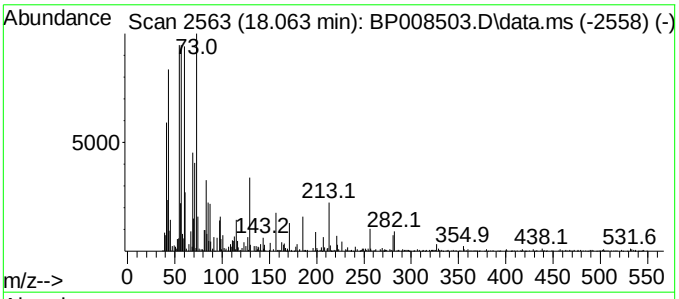
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

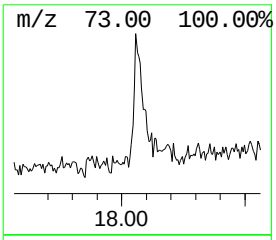
****

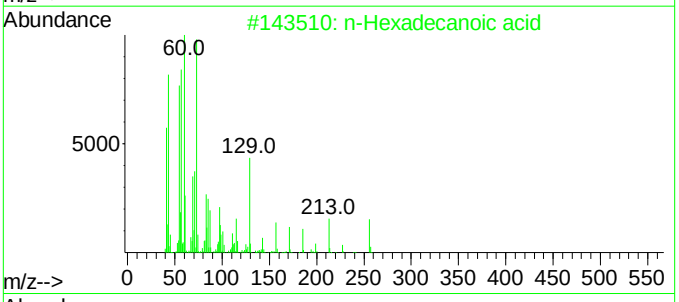
Peak Number 3 n-Hexadecanoic acid Concentration Rank 5

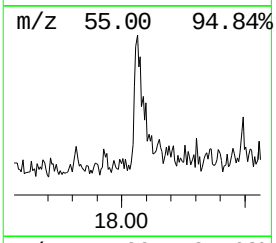
R.T.	EstConc	Area	Relative to ISTD	R.T.
18.063	2.03 ng	63763	Phenanthrene-d10	17.145

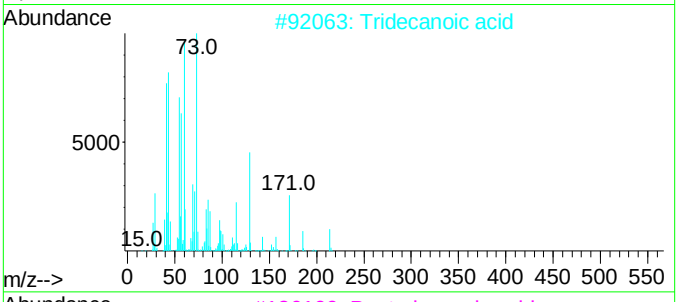
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2	Tridecanoic acid	214	C13H26O2	000638-53-9	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	72
4	Undecanoic acid	186	C11H22O2	000112-37-8	64
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	64

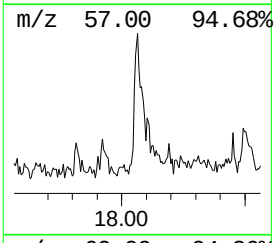


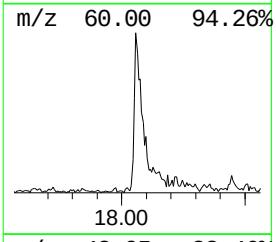


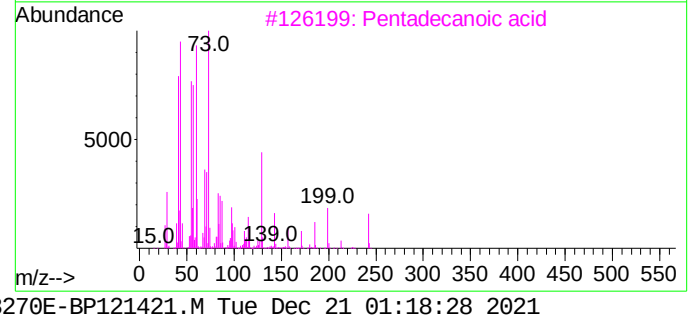


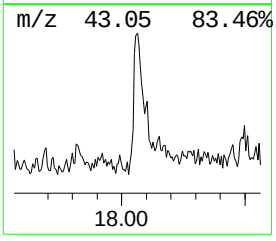












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Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
EB-2021-12-15

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP121421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

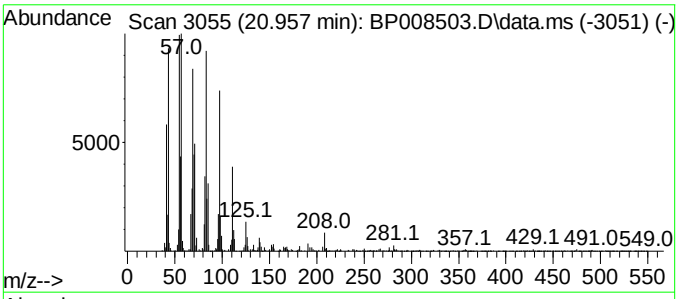
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

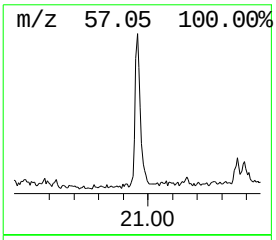
****

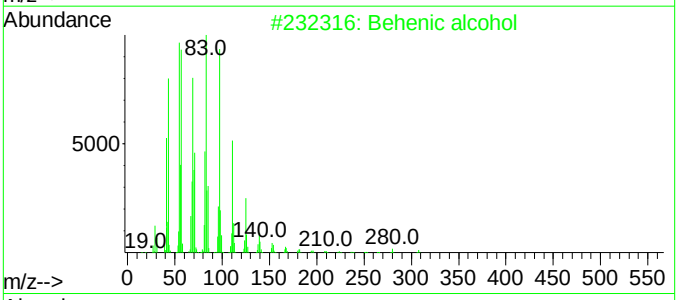
Peak Number 4 Behenic alcohol Concentration Rank 3

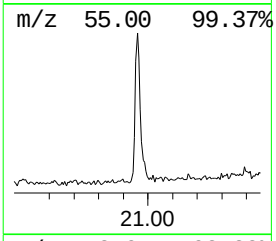
R.T.	EstConc	Area	Relative to ISTD	R.T.
20.957	4.81 ng	199353	Chrysene-d12	21.257

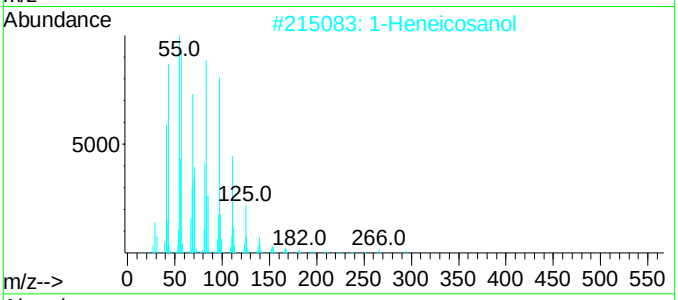
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	94
2	1-Heneicosanol	312	C21H44O	015594-90-8	91
3	2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	91
4	1-Tetracosene	336	C24H48	010192-32-2	91
5	Octacosanol	410	C28H58O	000557-61-9	91

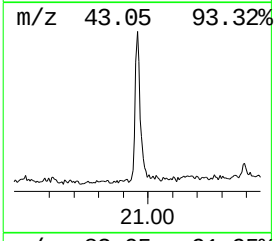


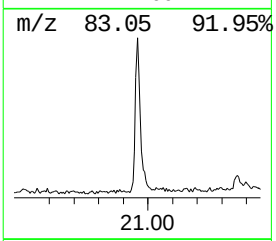


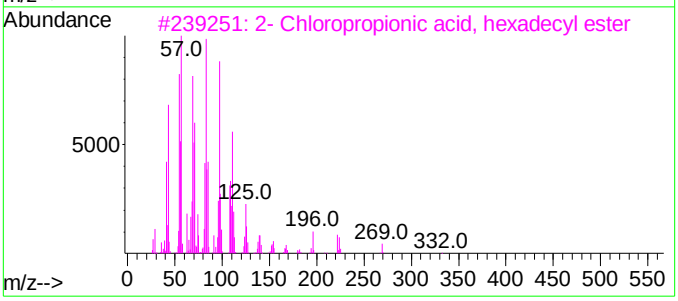


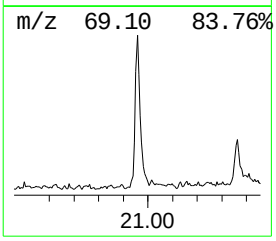












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Operator : CG/JU
Sample : M5115-10
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP121421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

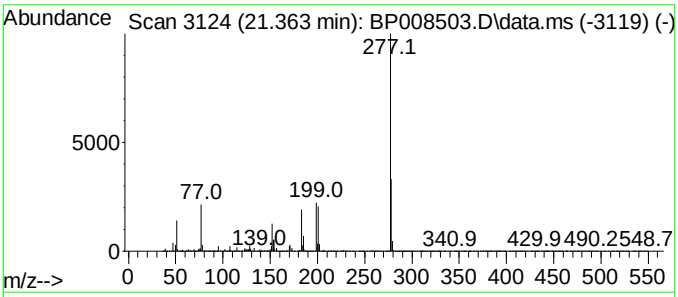
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

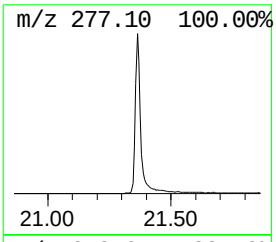
****

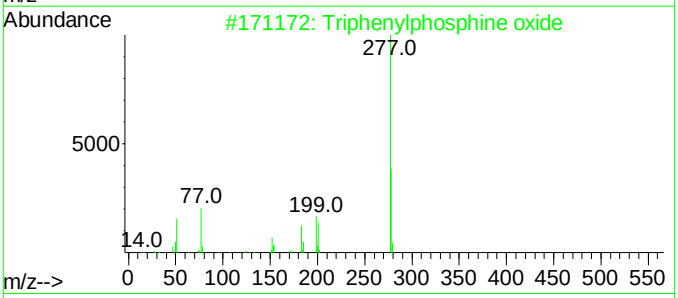
Peak Number 5 Triphenylphosphine oxide Concentration Rank 1

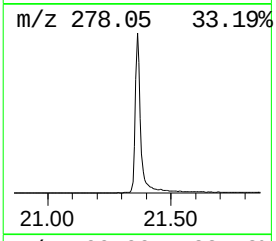
R.T.	EstConc	Area	Relative to ISTD	R.T.
21.363	51.64 ng	2139860	Chrysene-d12	21.257

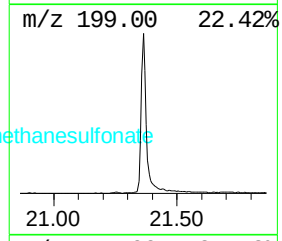
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	95
2	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	64
3	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	50
4	3-(3,4-Dichlorophenyl)-2-thioxo-...	277	C9H5Cl2NOS2	017046-34-3	25
5	2-Indolinone, 2TMS derivative	277	C14H23NOSi2	010416-65-6	9

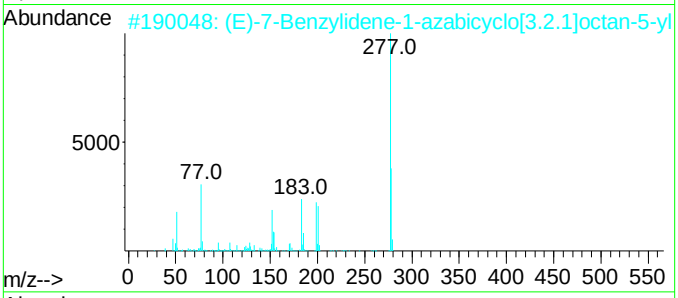


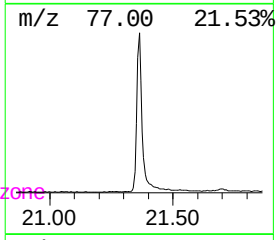


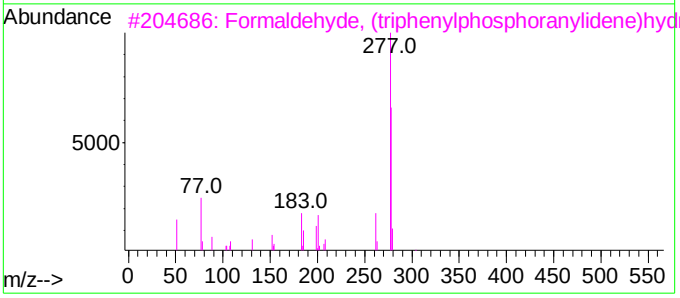


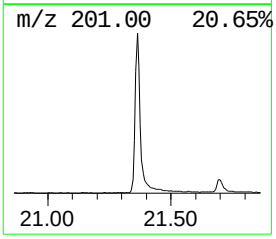












Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121821\
Data File : BP008503.D
Acq On : 18 Dec 2021 23:11
Operator : CG/JU
Sample : M5115-10
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
EB-2021-12-15

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP121421.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
2-Pentanone, 4-...	4.852	11.7	ng	167154	1	7.716	286523	20.0
2-Pentanone, 4-...	5.922	3.6	ng	51031	1	7.716	286523	20.0
n-Hexadecanoic ...	18.063	2.0	ng	63763	4	17.145	626991	20.0
Behenic alcohol	20.957	4.8	ng	199353	5	21.257	828778	20.0
Triphenylphosph...	21.363	51.6	ng	2139860	5	21.257	828778	20.0