LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121721\
Data File : BP008478.D
Acq On : 17 Dec 2021 19:01
Operator : CG/JU
Sample : M5084-06
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C7

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: BP008478.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.857	311	318	328	rBV	73892	112373	2.12%	0.595%
2	5.328	392	398	419	rBV	395980	719675	13.59%	3.812%
3	6.934	664	671	692	rBV	201265	460153	8.69%	2.437%
4	7.728	799	806	816	rBV	161956	280710	5.30%	1.487%
5	8.892	997	1004	1028	rVB	503481	968292	18.29%	5.129%
6	9.922	1172	1179	1188	rBV3	28640	57200	1.08%	0.303%
7	10.522	1274	1281	1296	rBV	192119	390500	7.38%	2.068%
8	12.998	1692	1702	1719	rBV	1421765	2158666	40.77%	11.433%
9	14.380	1929	1937	1944	rBV	317750	514310	9.71%	2.724%
10	15.886	2187	2193	2212	rBV	1133867	1802946	34.05%	9.549%
11	17.145	2401	2407	2418	rBV	400432	628953	11.88%	3.331%
12	17.821	2518	2522	2528	rBV	62791	82446	1.56%	0.437%
13	18.051	2557	2561	2568	rBV2	69956	100853	1.90%	0.534%
14	19.292	2768	2772	2778	rBV	43225	63216	1.19%	0.335%
15	19.721	2840	2845	2856	rBV	3002553	3437813	64.93%	18.208%
16	20.968	3053	3057	3064	rBV2	124015	180057	3.40%	0.954%
17	21.256	3102	3106	3114	rBV	609277	787207	14.87%	4.169%
18	21.374	3121	3126	3152	rBV	3653851	5294307	100.00%	28.041%
19	23.621	3502	3508	3518	rVB2	395206	840725	15.88%	4.453%

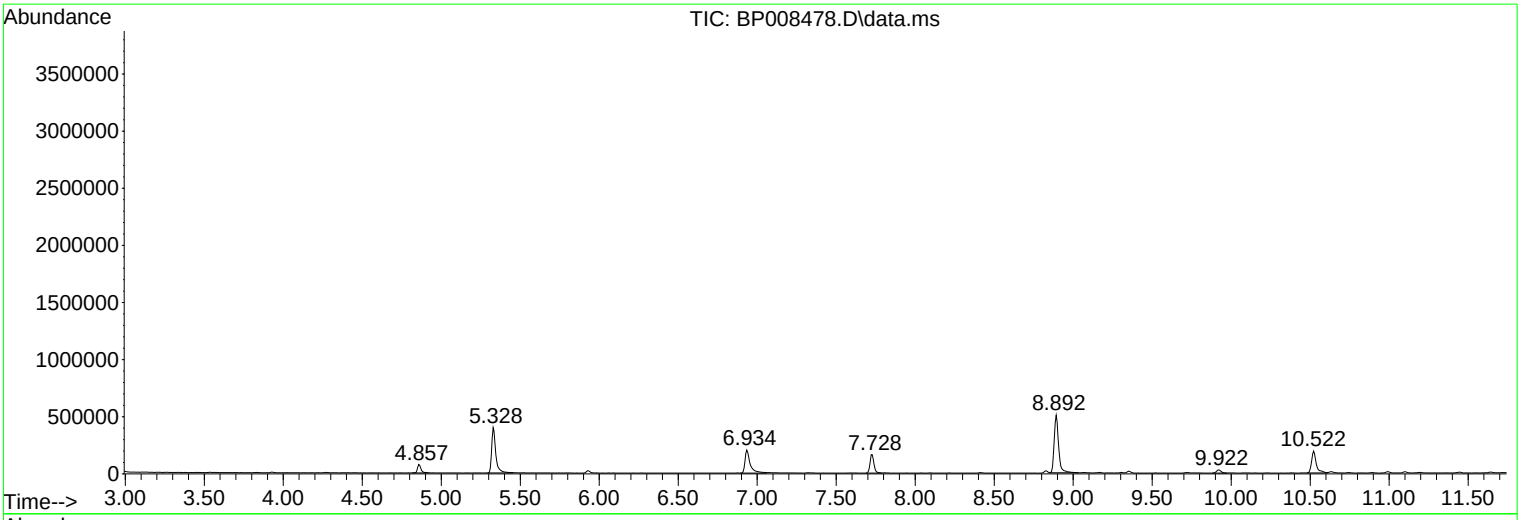
Sum of corrected areas: 18880402

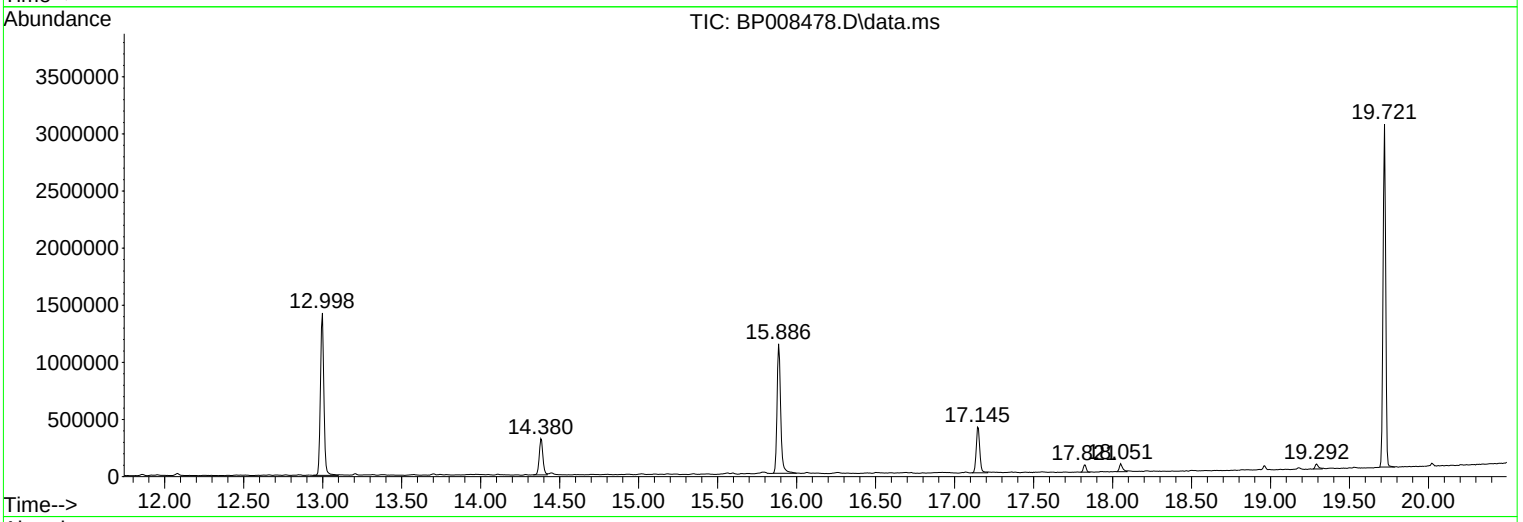
Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121721\
Data File : BP008478.D
Acq On : 17 Dec 2021 19:01
Operator : CG/JU
Sample : M5084-06
Misc :
ALS Vial : 13 Sample Multiplier: 1

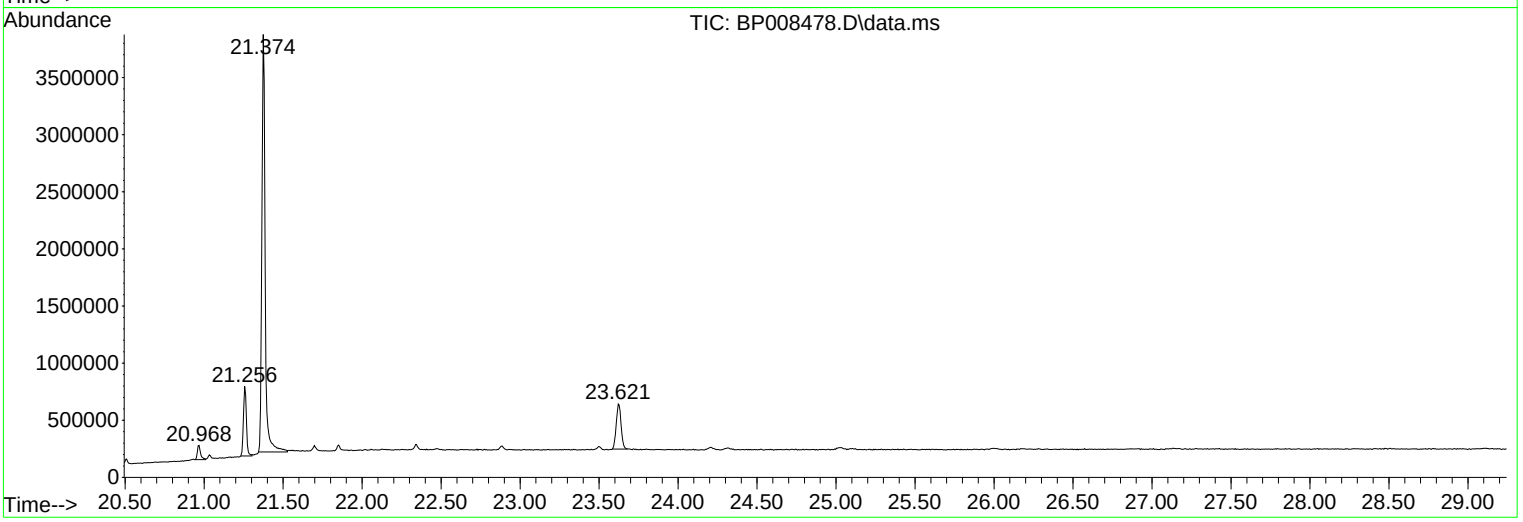
Instrument :
BNA_P
ClientSampleId :
C7

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\BP121721\
Data File : BP008478.D
Acq On : 17 Dec 2021 19:01
Operator : CG/JU
Sample : M5084-06
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C7

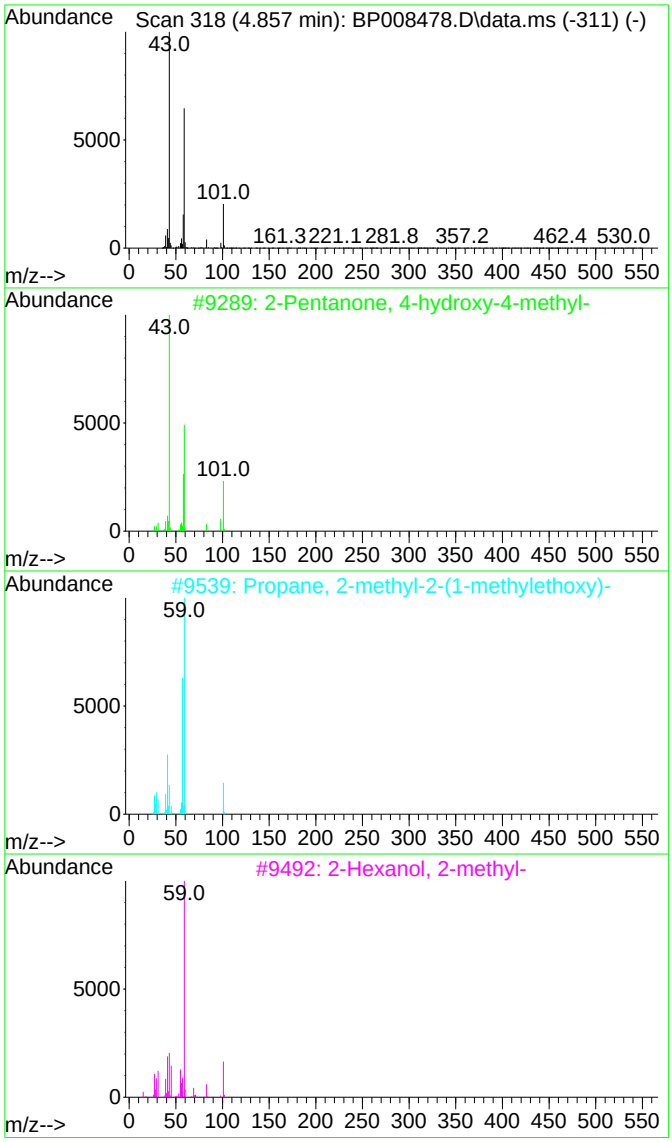
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP121421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

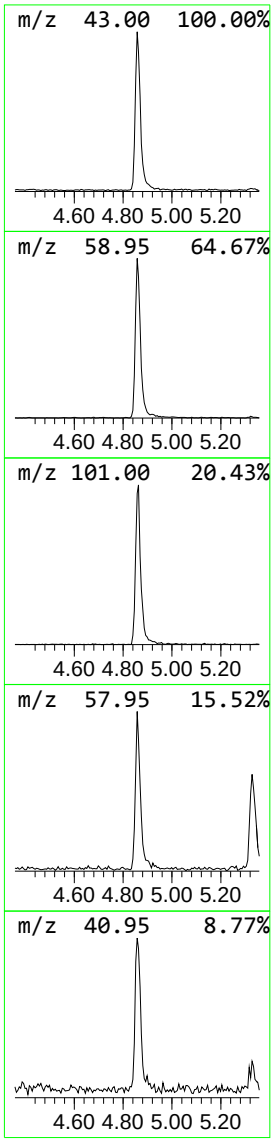
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.857	8.01 ng	112373	1,4-Dichlorobenzene-d4	7.728

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	40
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
5	1,2-Butanediol	90	C4H10O2	000584-03-2	23





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121721\
Data File : BP008478.D
Acq On : 17 Dec 2021 19:01
Operator : CG/JU
Sample : M5084-06
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C7

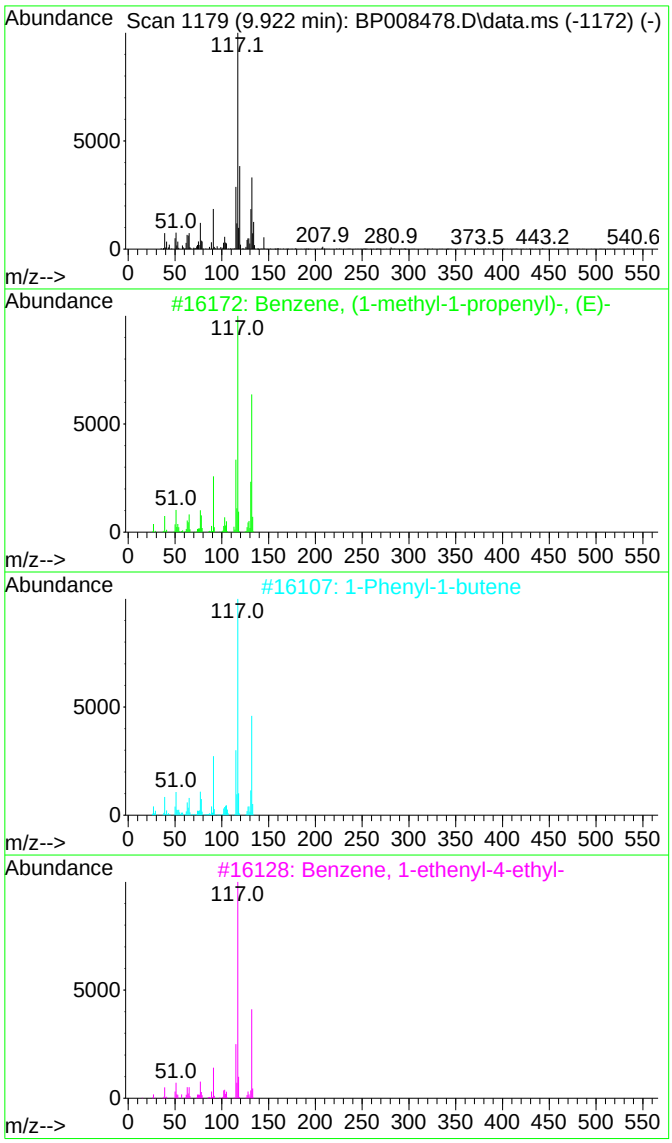
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP121421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

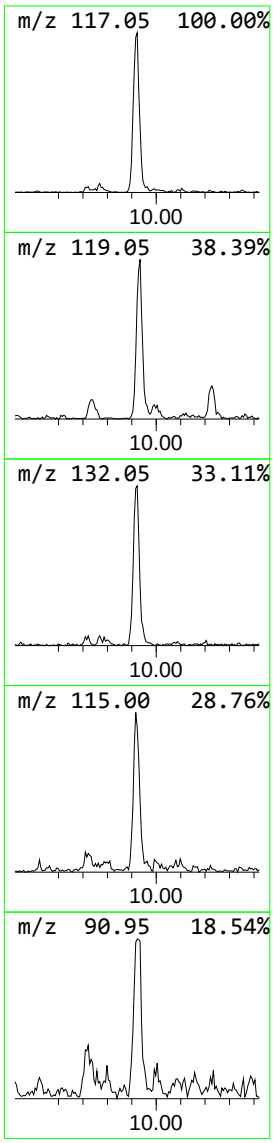
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Benzene, (1-methyl-1-propen... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.922	2.93 ng	57200	Naphthalene-d8	10.522

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	70
2	1-Phenyl-1-butene	132	C10H12	000824-90-8	70
3	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	70
4	Indan, 1-methyl-	132	C10H12	000767-58-8	70
5	3-Phenylbut-1-ene	132	C10H12	000934-10-1	70





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121721\
Data File : BP008478.D
Acq On : 17 Dec 2021 19:01
Operator : CG/JU
Sample : M5084-06
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C7

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

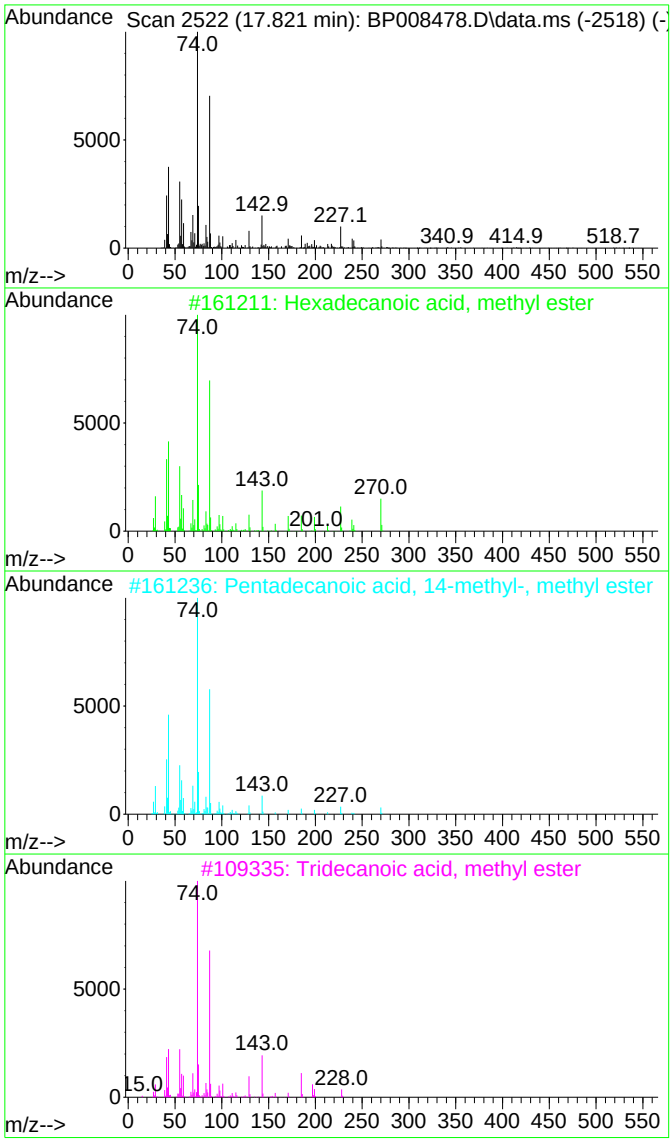
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

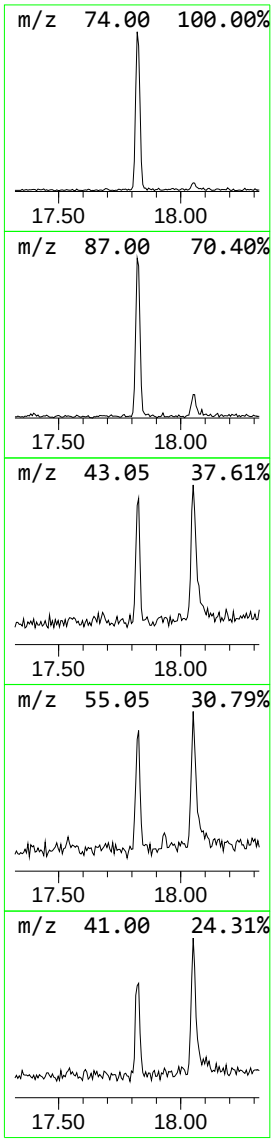
****

Peak Number 3 Hexadecanoic acid, methyl e... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.821	2.62 ng	82446	Phenanthrene-d10	17.145

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	96
3	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	91
4	Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	90
5	Methyl tetradecanoate	242	C15H30O2	000124-10-7	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121721\
Data File : BP008478.D
Acq On : 17 Dec 2021 19:01
Operator : CG/JU
Sample : M5084-06
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C7

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

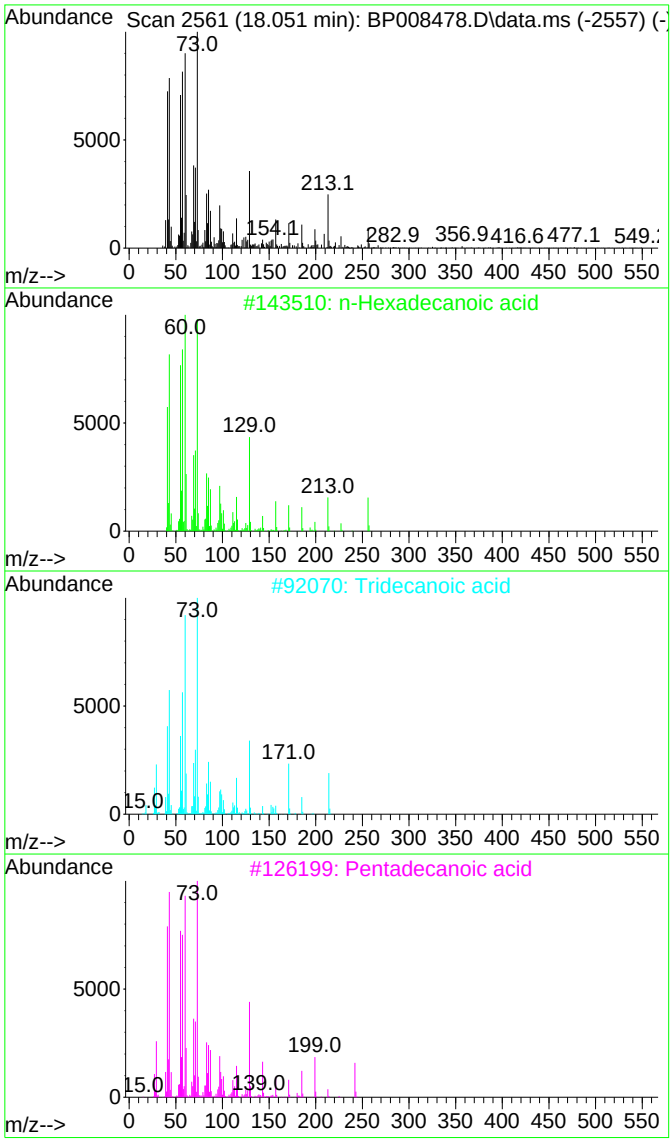
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

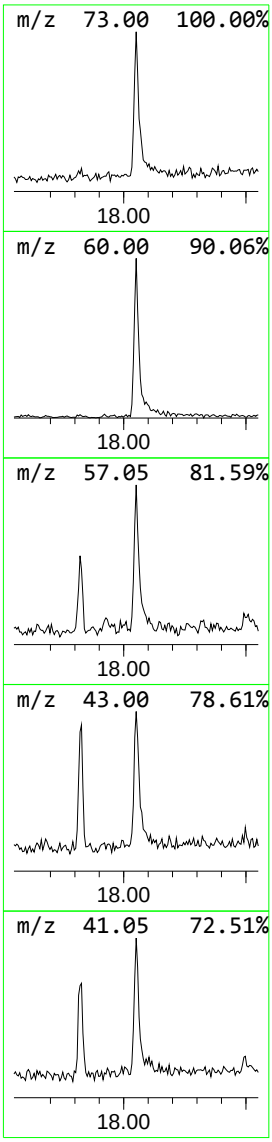
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.051	3.21 ng	100853	Phenanthrene-d10	17.145

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	81
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5	Octanoic acid	144	C8H16O2	000124-07-2	60





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121721\
Data File : BP008478.D
Acq On : 17 Dec 2021 19:01
Operator : CG/JU
Sample : M5084-06
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C7

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

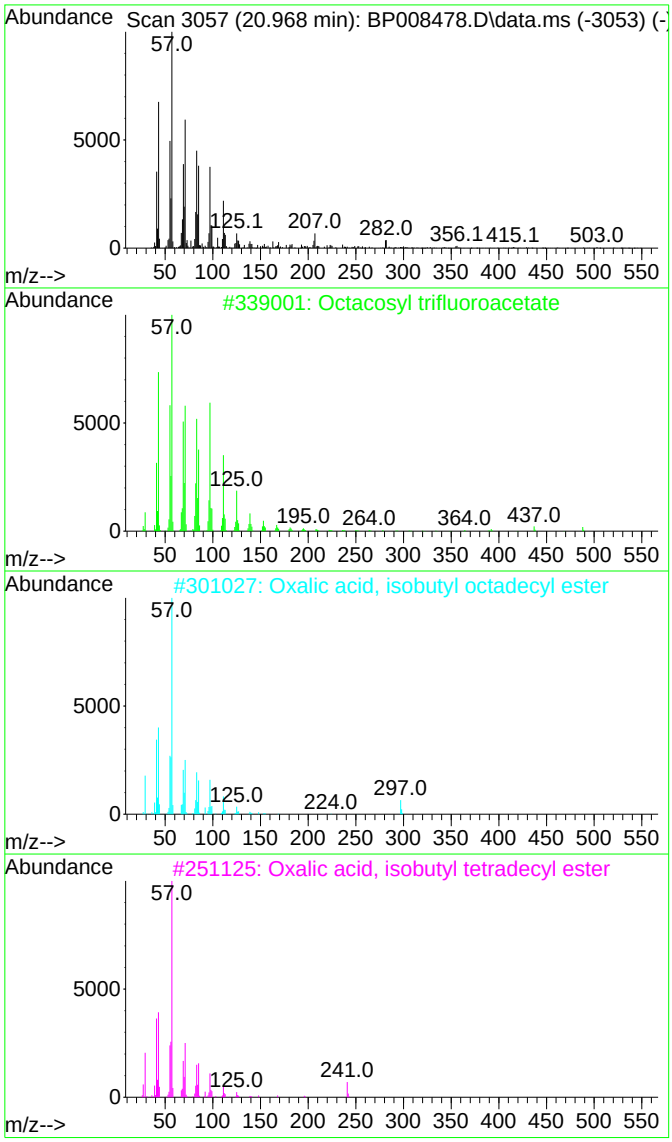
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

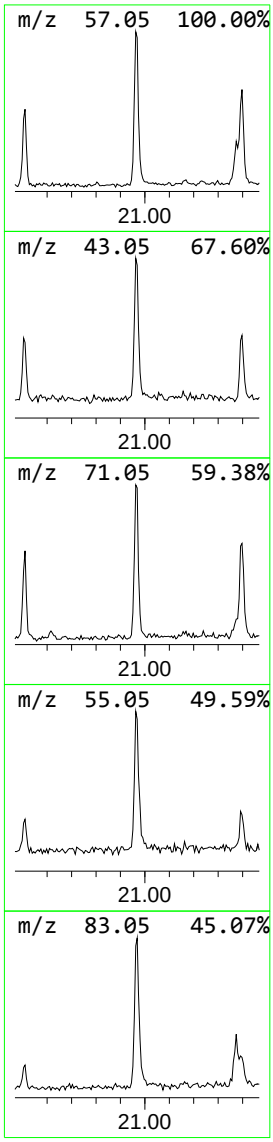
****

Peak Number 5 Octacosyl trifluoroacetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.968	4.57 ng	180057	Chrysene-d12	21.256

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	90
2	Oxalic acid, isobutyl octadecyl ...	398	C24H46O4	1000309-38-3	87
3	Oxalic acid, isobutyl tetradecyl...	342	C20H38O4	1000309-37-9	87
4	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	87
5	Oxalic acid, isobutyl heptadecyl...	384	C23H44O4	1000309-38-2	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121721\
Data File : BP008478.D
Acq On : 17 Dec 2021 19:01
Operator : CG/JU
Sample : M5084-06
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C7

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

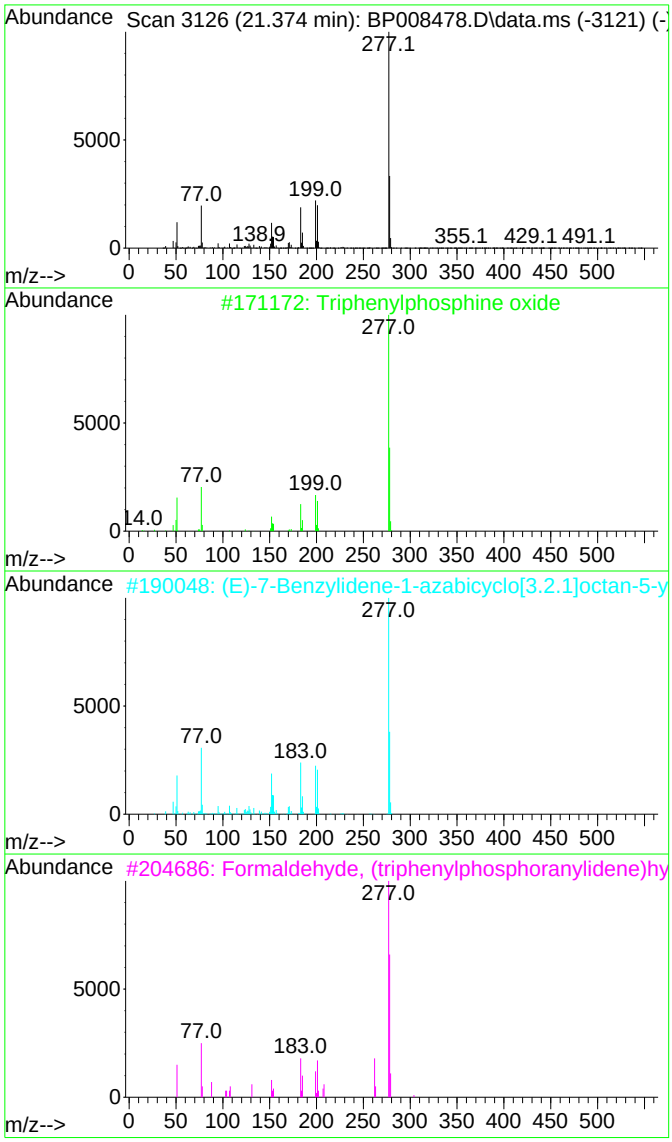
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

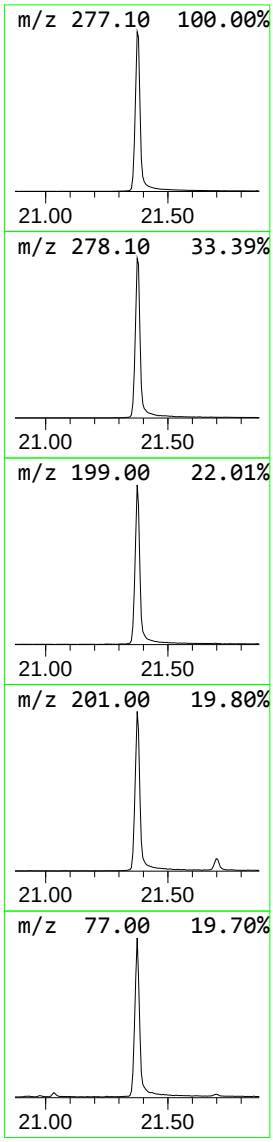
****

Peak Number 6 Triphenylphosphine oxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.374	134.51 ng	5294310	Chrysene-d12	21.256

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	96
2	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	91
3	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	37
4	1H-Indole-3-acetic acid, 5-[(tri...	277	C14H19NO3Si	072101-35-0	32
5	5-Methyl-8-phenylfuro[3',2':5,6]...	277	C16H11N3O2	1000460-07-9	28





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121721\
Data File : BP008478.D
Acq On : 17 Dec 2021 19:01
Operator : CG/JU
Sample : M5084-06
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C7

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-...	4.857	8.0	ng	112373	1	7.728	280710	20.0
Benzene, (1-met...	9.922	2.9	ng	57200	2	10.522	390500	20.0
Hexadecanoic ac...	17.821	2.6	ng	82446	4	17.145	628953	20.0
n-Hexadecanoic ...	18.051	3.2	ng	100853	4	17.145	628953	20.0
Octacosyl trifl...	20.968	4.6	ng	180057	5	21.256	787207	20.0
Triphenylphosph...	21.374	134.5	ng	5294310	5	21.256	787207	20.0