LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121821\
Data File : BP008504.D
Acq On : 18 Dec 2021 23:45
Operator : CG/JU
Sample : M5115-08
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-6

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: BP008504.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	330	rVB	126557	185016	5.50%	1.135%
2	5.322	391	397	417	rBV	483263	852053	25.32%	5.226%
3	5.922	494	499	507	rBV	36871	57232	1.70%	0.351%
4	6.928	664	670	687	rBV	235074	524257	15.58%	3.216%
5	7.716	793	804	815	rBV	173317	301567	8.96%	1.850%
6	8.887	996	1003	1025	rBV	598627	1157099	34.39%	7.097%
7	10.516	1273	1280	1294	rBV	190717	398252	11.83%	2.443%
8	12.992	1694	1701	1717	rBV	1617730	2475227	73.56%	15.183%
9	14.375	1929	1936	1951	rBV	331614	546190	16.23%	3.350%
10	15.775	2170	2174	2180	rVB8	23065	39735	1.18%	0.244%
11	15.881	2186	2192	2208	rBV	1221071	1941281	57.69%	11.908%
12	17.139	2401	2406	2414	rBV	405973	586325	17.42%	3.596%
13	18.045	2556	2560	2567	rBV2	91254	128443	3.82%	0.788%
14	19.286	2768	2771	2778	rVB3	45086	64224	1.91%	0.394%
15	19.716	2838	2844	2853	rBV	2816317	3365074	100.00%	20.641%
16	20.492	2973	2976	2981	rVB	48950	51441	1.53%	0.316%
17	20.957	3052	3055	3061	rVB	68929	82190	2.44%	0.504%
18	21.251	3101	3105	3112	rBV	553234	734025	21.81%	4.502%
19	21.368	3120	3125	3136	rBV	1446748	1958014	58.19%	12.010%
20	23.615	3501	3507	3518	rVB2	409949	855337	25.42%	5.247%

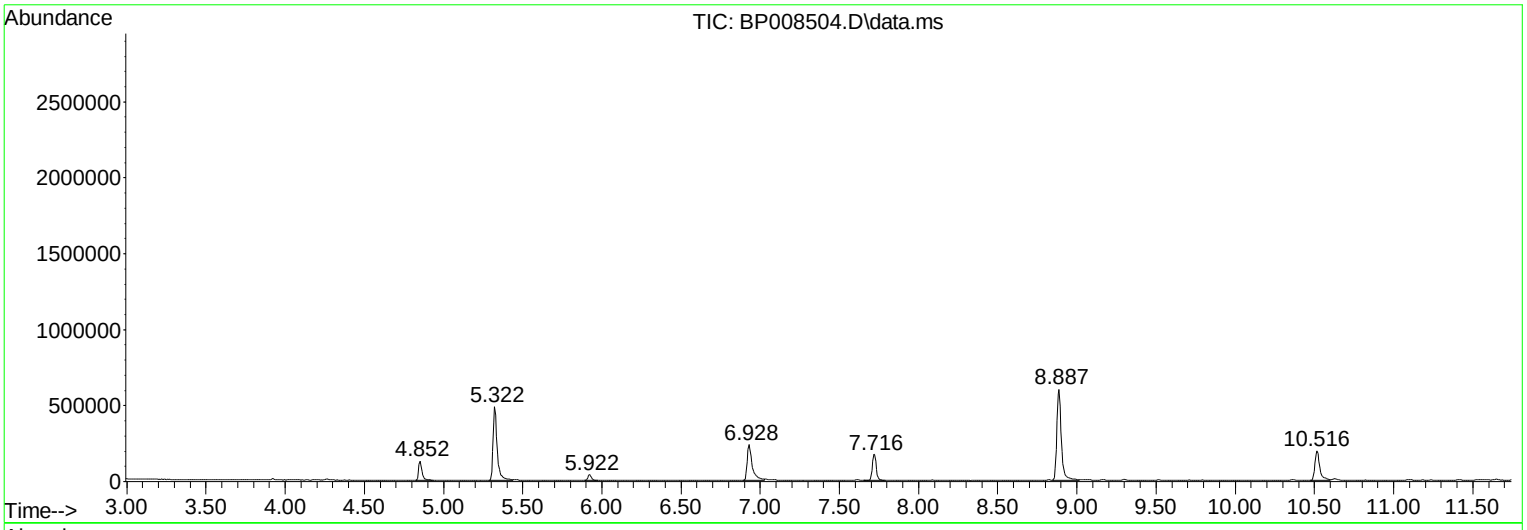
Sum of corrected areas: 16302982

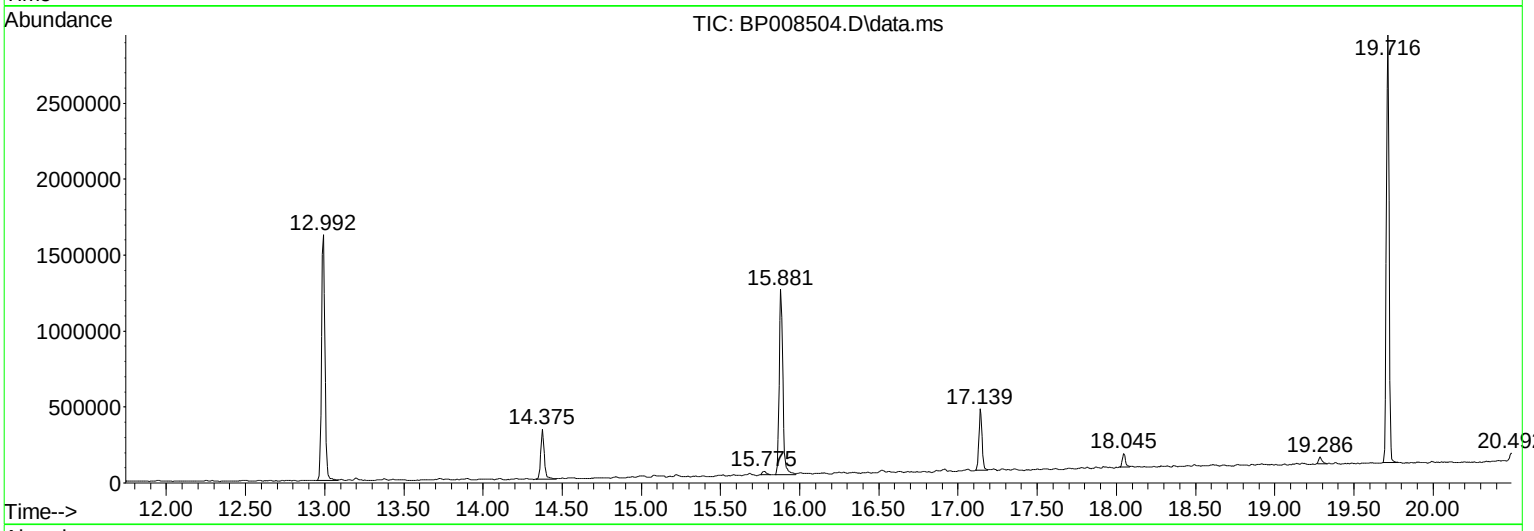
Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121821\
Data File : BP008504.D
Acq On : 18 Dec 2021 23:45
Operator : CG/JU
Sample : M5115-08
Misc :
ALS Vial : 18 Sample Multiplier: 1

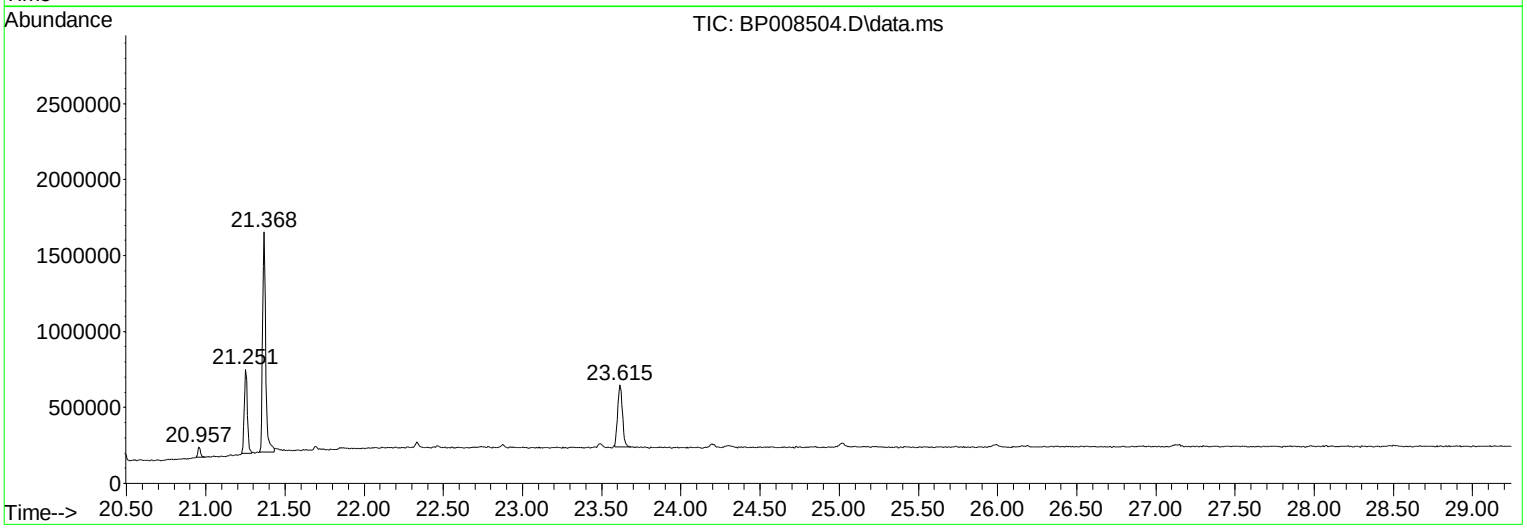
Instrument :
BNA_P
ClientSampleId :
MW-6

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 : BP008504.D
Acq On : 18 Dec 2021 23:45
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

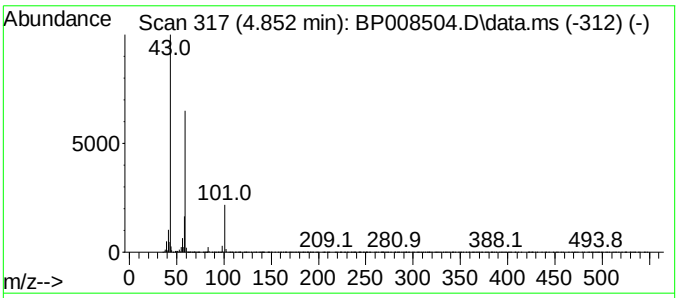
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

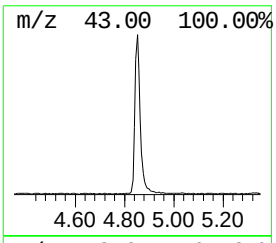
****

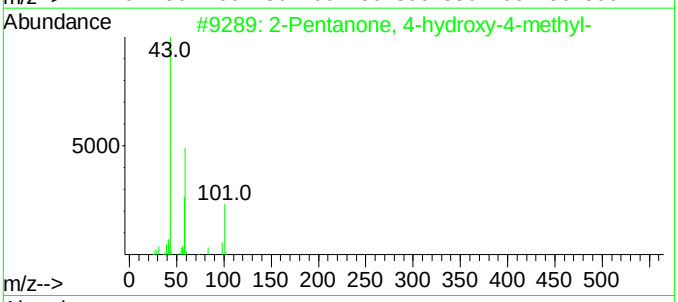
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

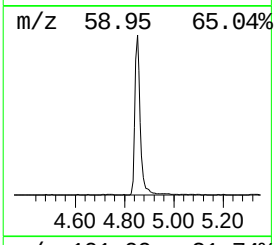
R.T.	EstConc	Area	Relative to ISTD	R.T.
4.852	12.27 ng	185016	1,4-Dichlorobenzene-d4	7.722

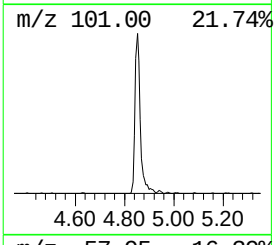
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	12
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9

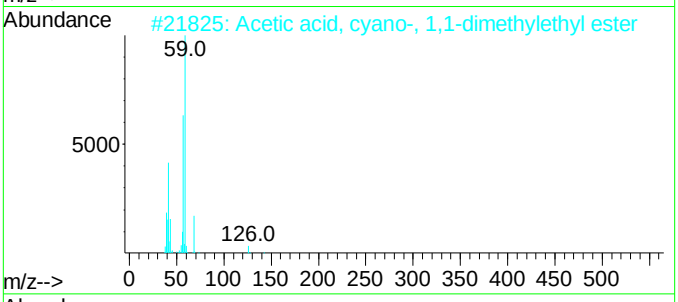


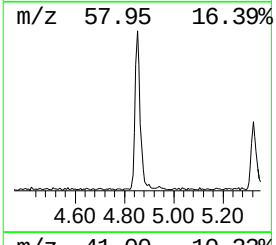


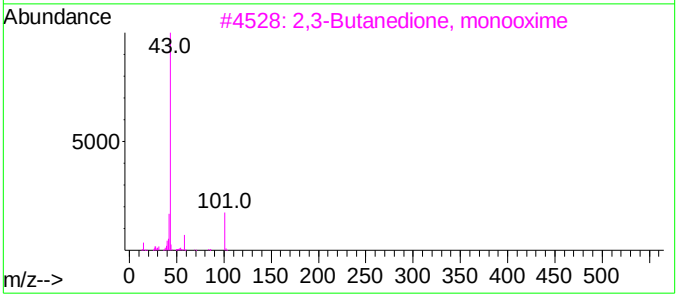


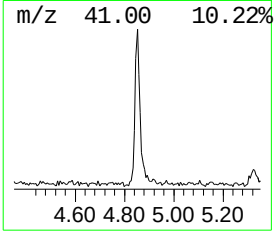












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Data File : BP008504.D
Acq On : 18 Dec 2021 23:45
Operator : CG/JU
Sample : M5115-08
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-6

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

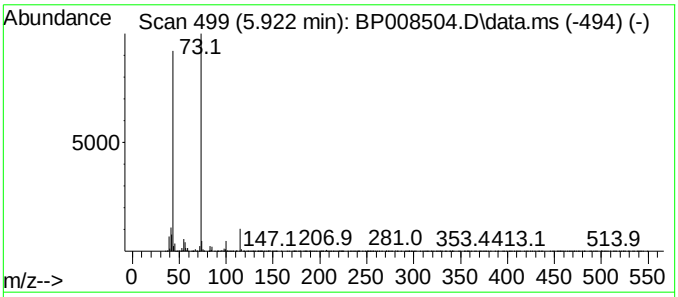
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

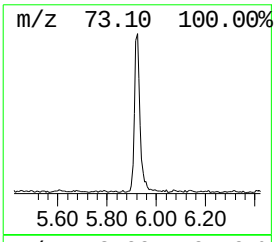
****

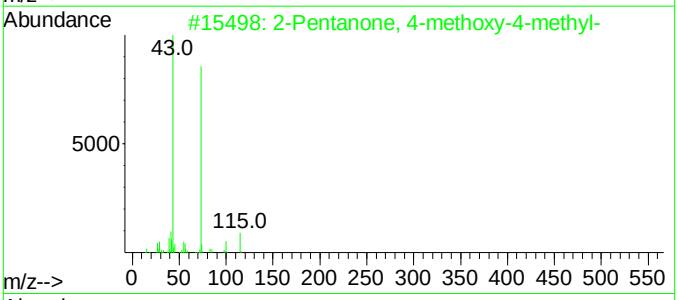
Peak Number 2 2-Pentanone, 4-methoxy-4-me... Concentration Rank 4

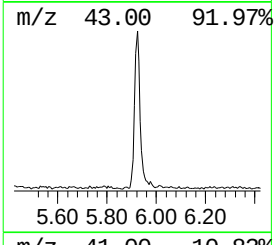
R.T.	EstConc	Area	Relative to ISTD	R.T.
5.922	3.80 ng	57232	1,4-Dichlorobenzene-d4	7.722

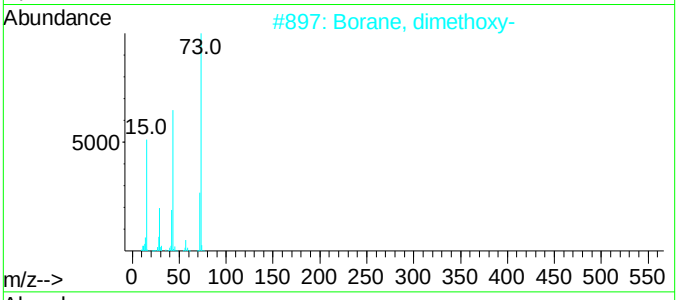
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2	Borane, dimethoxy-	74	C2H7BO2	004542-61-4	38
3	N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	28
4	Butane, 2-methoxy-2,3,3-trimethyl-	130	C8H18O	027705-21-1	23
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12

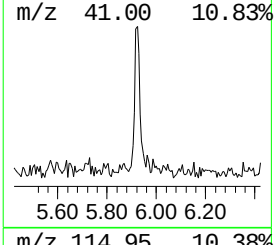


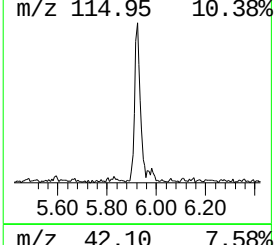


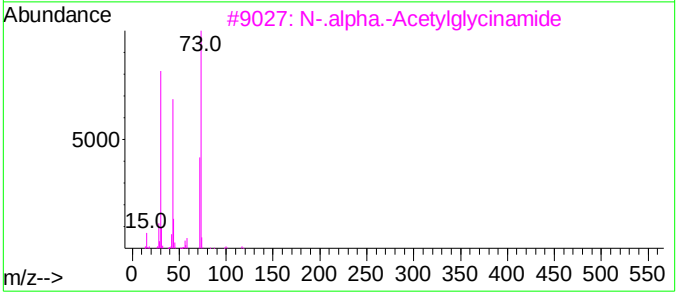


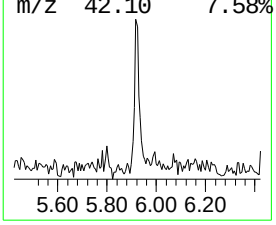












Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121821\
Data File : BP008504.D
Acq On : 18 Dec 2021 23:45
Operator : CG/JU
Sample : M5115-08
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-6

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

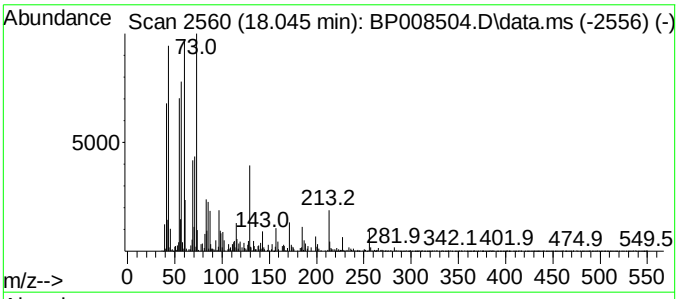
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

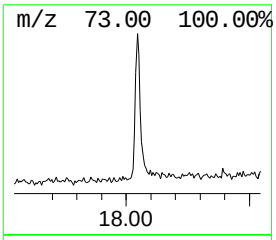
****

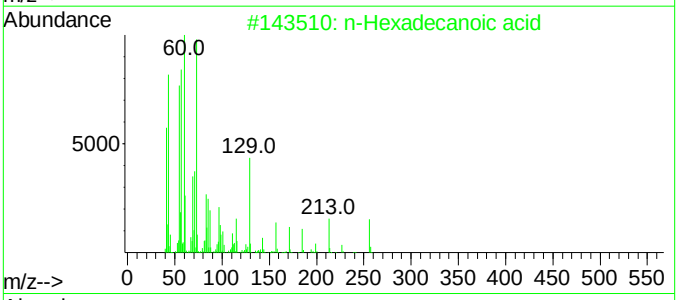
Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

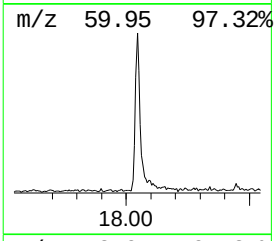
R.T.	EstConc	Area	Relative to ISTD	R.T.
18.045	4.38 ng	128443	Phenanthrene-d10	17.139

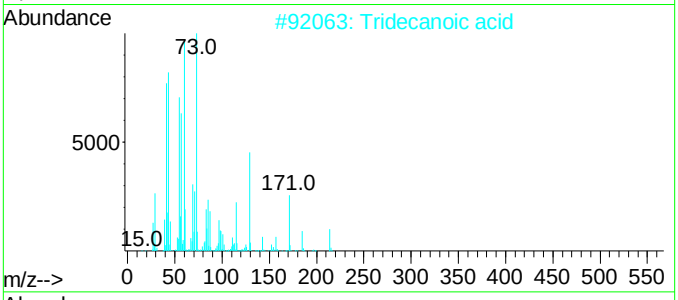
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5	n-Decanoic acid	172	C10H20O2	000334-48-5	64

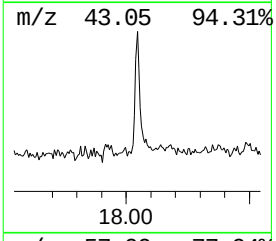


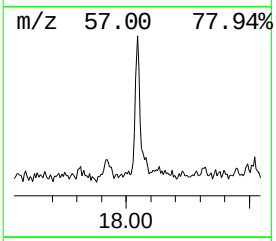


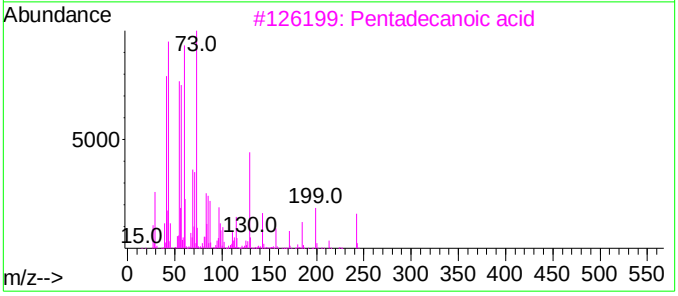


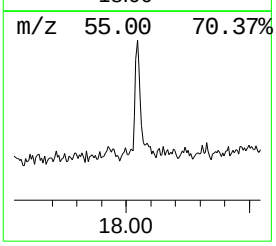












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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

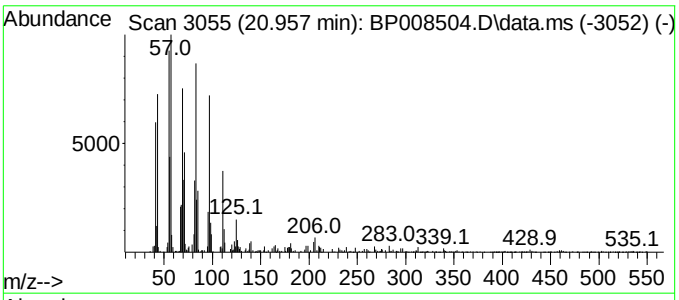
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

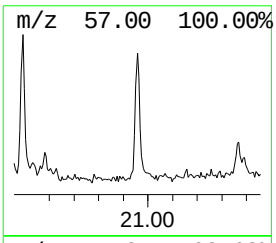
****

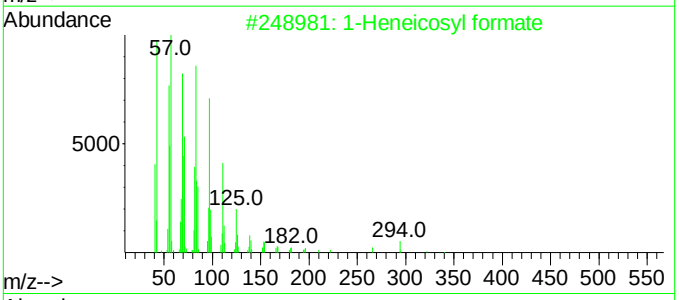
Peak Number 4 1-Heneicosyl formate Concentration Rank 5

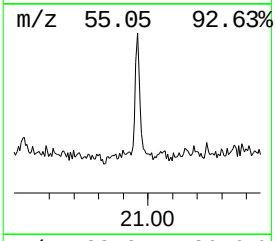
R.T.	EstConc	Area	Relative to ISTD	R.T.
20.957	2.24 ng	82190	Chrysene-d12	21.251

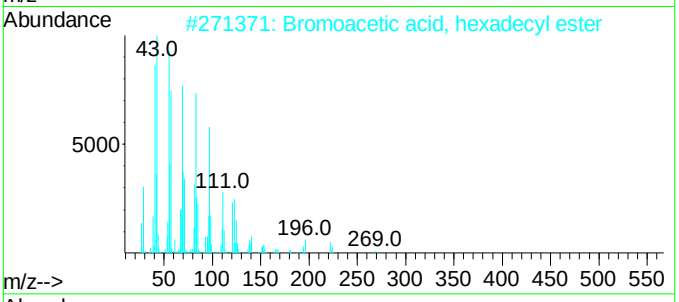
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
2	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	94
3	Cyclopentadecane	210	C15H30	000295-48-7	93
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	93
5	1-Tricosene	322	C23H46	018835-32-0	91

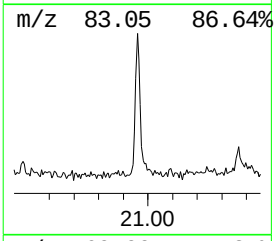


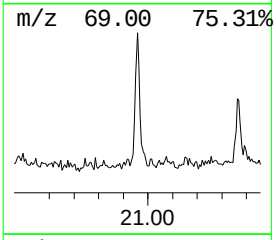


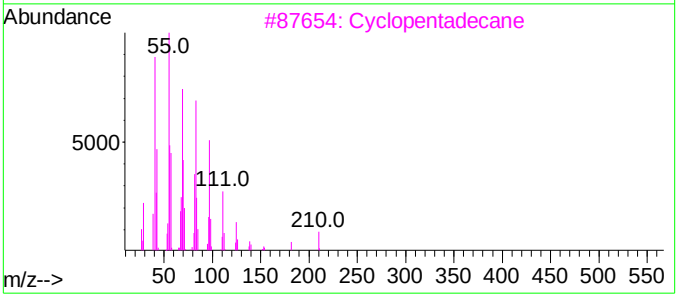


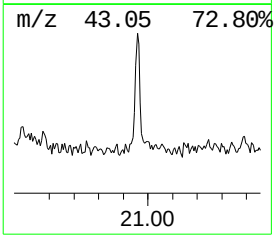












Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121821\
Data File : BP008504.D
Acq On : 18 Dec 2021 23:45
Operator : CG/JU
Sample : M5115-08
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-6

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

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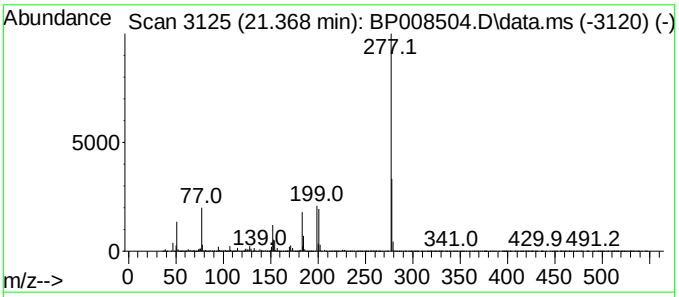
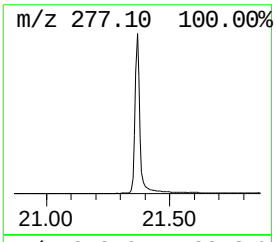
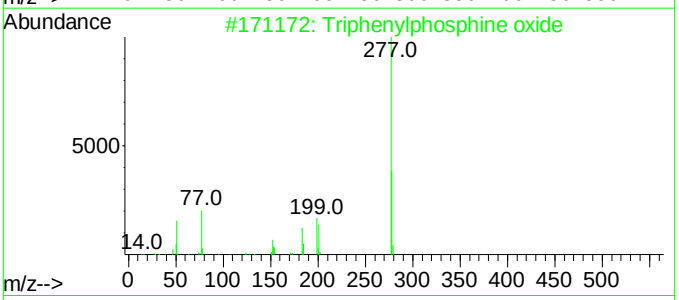
Peak Number 5 Triphenylphosphine oxide Concentration Rank 1

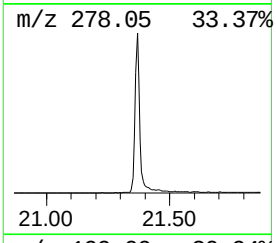
R.T.	EstConc	Area	Relative to ISTD	R.T.
21.369	53.35 ng	1958010	Chrysene-d12	21.251

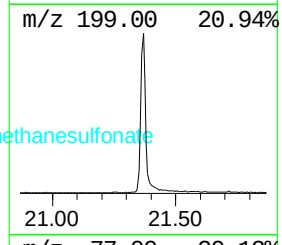
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	98
2	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	91
3	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	40
4	3-(3,4-Dichlorophenyl)-2-thioxo-...	277	C9H5Cl2NOS2	017046-34-3	32
5	Carbazol-1-one, 1,2,3,4-tetrahyd...	277	C18H15NO2	299962-12-2	9

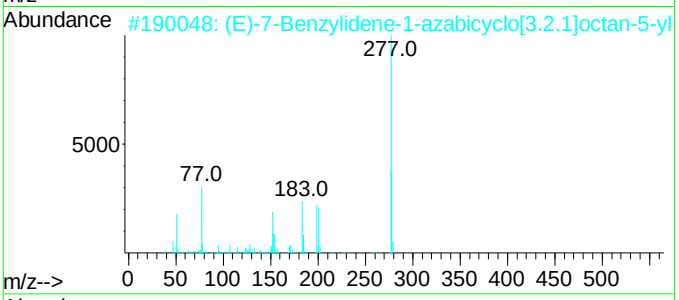


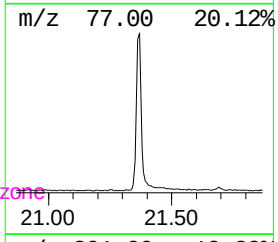


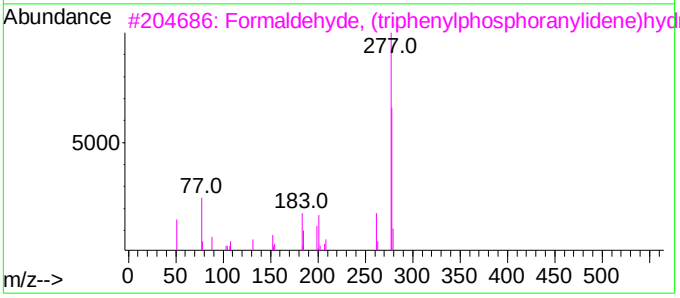


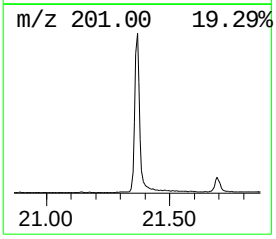












Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121821\
Data File : BP008504.D
Acq On : 18 Dec 2021 23:45
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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	12.3	ng	185016	1	7.722	301567	20.0
2-Pentanone, 4-...	5.922	3.8	ng	57232	1	7.722	301567	20.0
n-Hexadecanoic ...	18.045	4.4	ng	128443	4	17.139	586325	20.0
1-Heneicosyl fo...	20.957	2.2	ng	82190	5	21.251	734025	20.0
Triphenylphosph...	21.369	53.4	ng	1958010	5	21.251	734025	20.0