LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP041621\
Data File : BP005320.D
Acq On : 16 Apr 2021 15:58
Operator : CG/JU
Sample : M1998-12
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : SB-5C

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-BP041521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP005320.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.264	365	370	378	rVB	557859	783187	47.59%	8.656%
2	6.852	635	640	652	rVB	570540	888120	53.97%	9.816%
3	7.658	773	777	789	rVB	131230	215620	13.10%	2.383%
4	8.822	968	975	983	rBV	350024	543877	33.05%	6.011%
5	10.452	1245	1252	1257	rBV	124640	193957	11.79%	2.144%
6	12.934	1668	1674	1684	rBV	705687	956497	58.12%	10.572%
7	14.328	1904	1911	1923	rBV	220393	312548	18.99%	3.454%
8	15.828	2159	2166	2175	rBV	585811	822027	49.95%	9.085%
9	17.092	2374	2381	2386	rBV	277077	395002	24.00%	4.366%
10	17.992	2529	2534	2543	rBV2	93469	154666	9.40%	1.709%
11	19.116	2721	2725	2731	rVB4	10601	18095	1.10%	0.200%
12	19.233	2741	2745	2754	rBV4	33653	63240	3.84%	0.699%
13	19.492	2785	2789	2796	rVB	80468	109203	6.64%	1.207%
14	19.669	2814	2819	2827	rBV	1432846	1645592	100.00%	18.188%
15	19.939	2863	2865	2868	rBV4	13801	18696	1.14%	0.207%
16	20.622	2979	2981	2984	rBV3	17346	17792	1.08%	0.197%
17	20.874	3019	3024	3026	rBV	58931	87359	5.31%	0.966%
18	20.910	3026	3030	3037	rVV2	181543	362663	22.04%	4.008%
19	20.974	3037	3041	3049	rVV	300542	390153	23.71%	4.312%
20	21.192	3073	3078	3083	rBV	441276	565501	34.36%	6.250%
21	23.463	3458	3464	3474	rVB2	266975	503961	30.62%	5.570%

Sum of corrected areas: 9047756

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP041621\
Data File : BP005320.D
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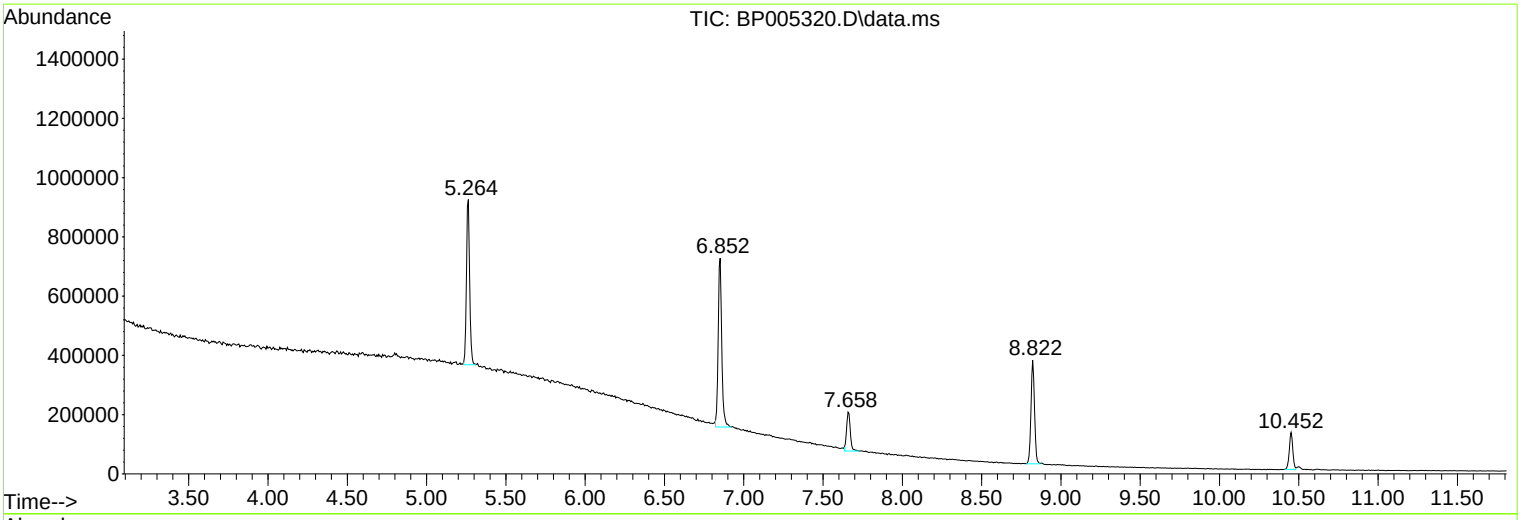
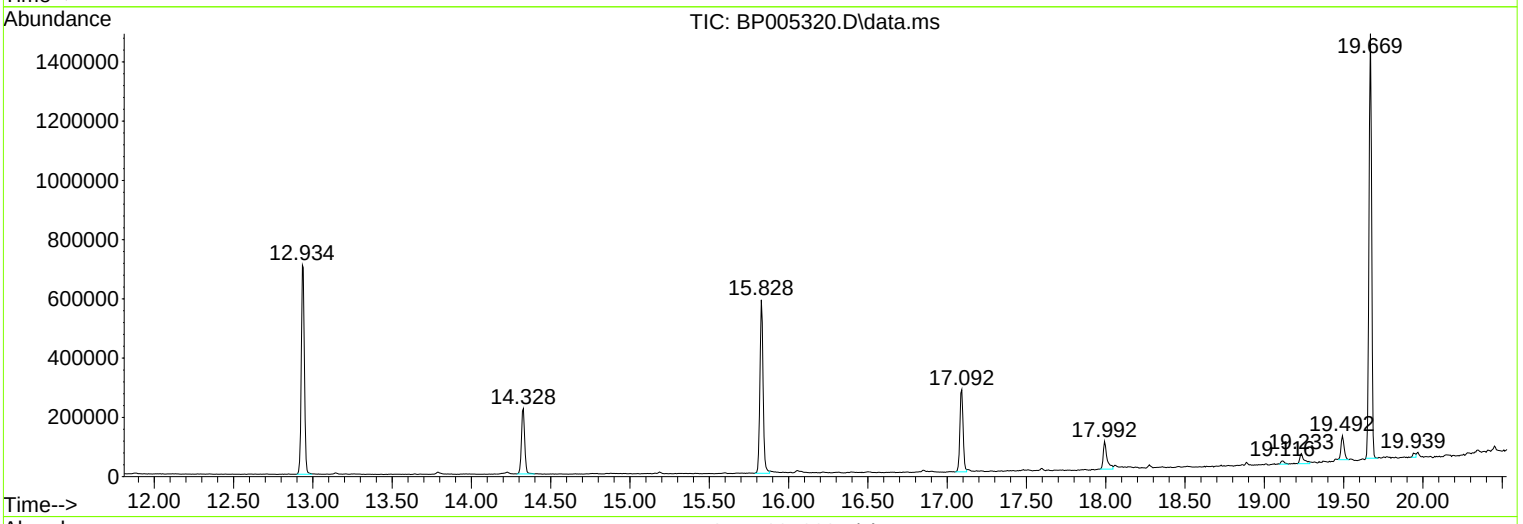
Sample : M1998-12
Misc :
ALS Vial : 12 Sample Multiplier: 1

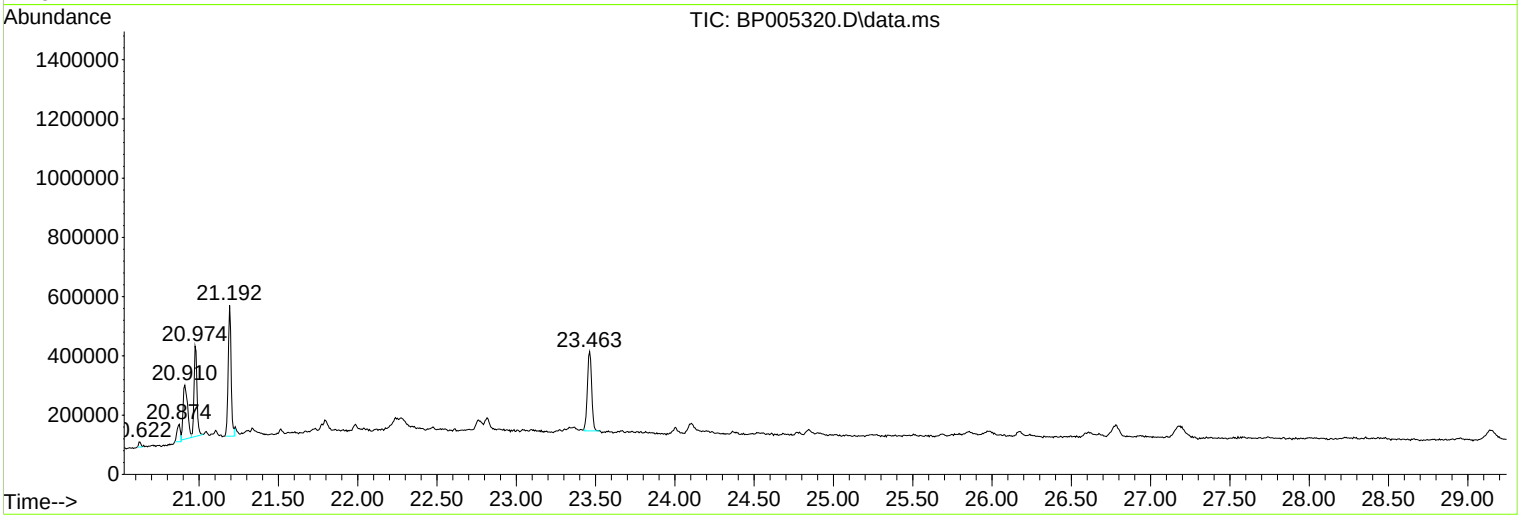
Instrument :
BNA_P
ClientSampleId :
SB-5C

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P







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Data File : BP005320.D
Acq On : 16 Apr 2021 15:58
Operator : CG/JU
Sample : M1998-12
Misc :
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Instrument :
BNA_P
ClientSampleId :
SB-5C

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

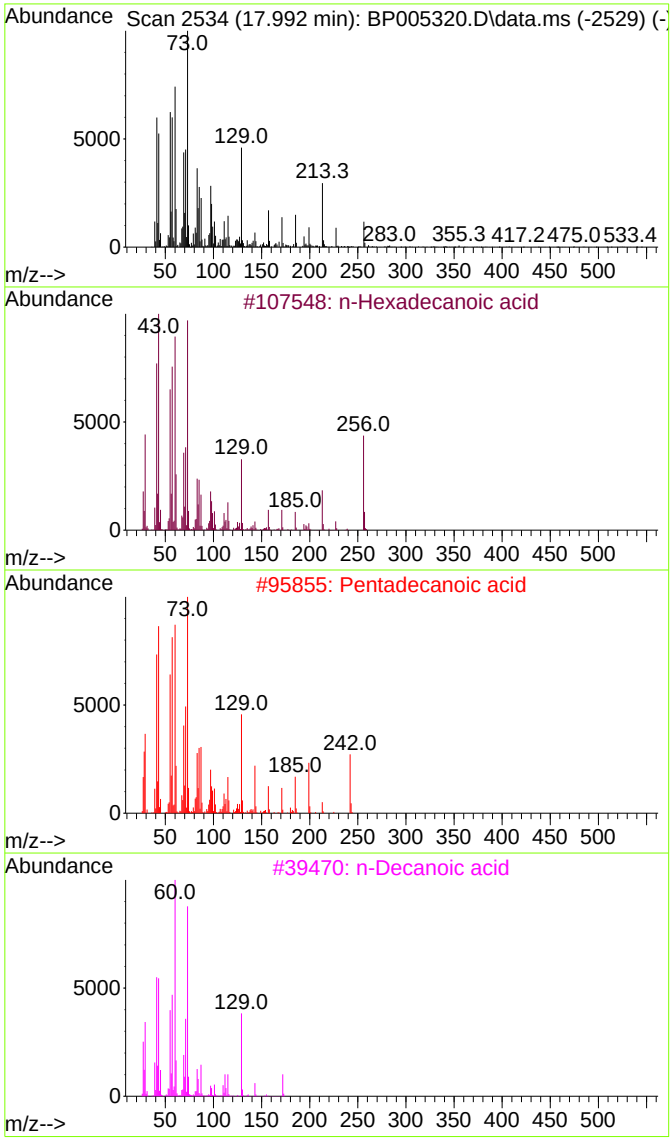
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

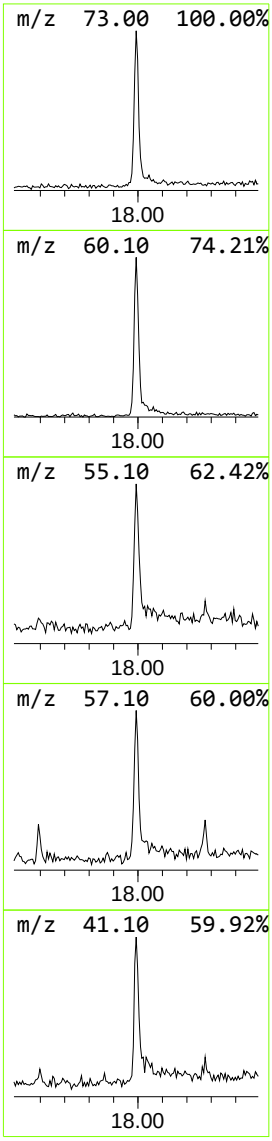
****

Peak Number 1 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.992	7.83 ng	154666	Phenanthrene-d10	17.092

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
3	n-Decanoic acid	172	C10H20O2	000334-48-5	70
4	Tridecanoic acid	214	C13H26O2	000638-53-9	68
5	Octadecanoic acid	284	C18H36O2	000057-11-4	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP041621\
Data File : BP005320.D
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Operator : CG/JU
Sample : M1998-12
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-5C

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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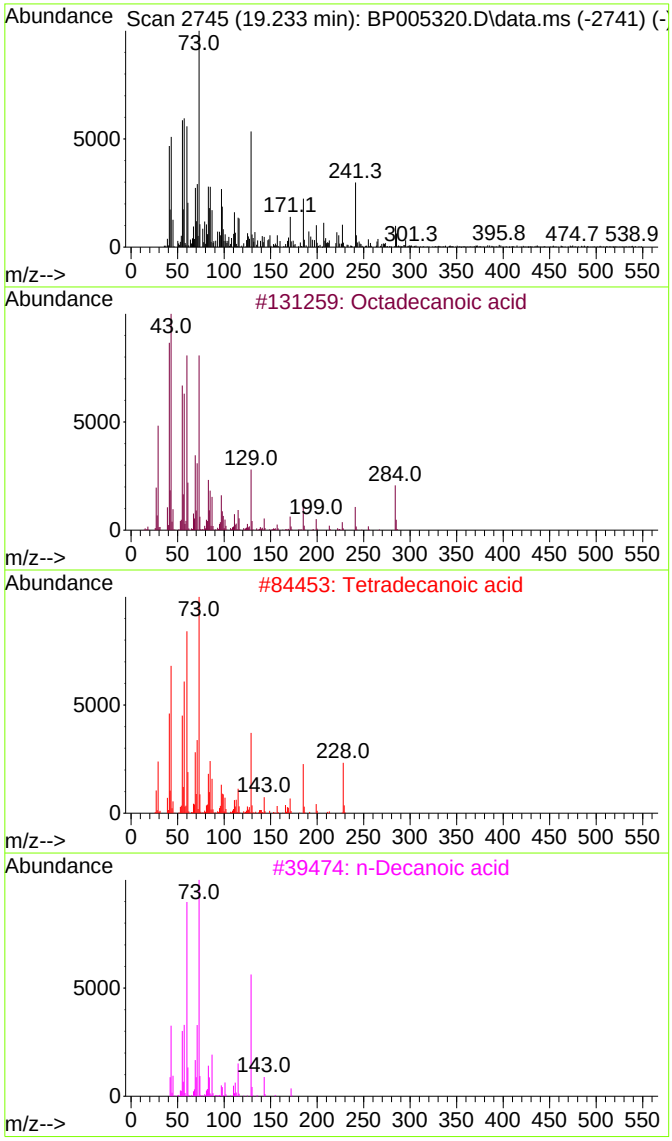
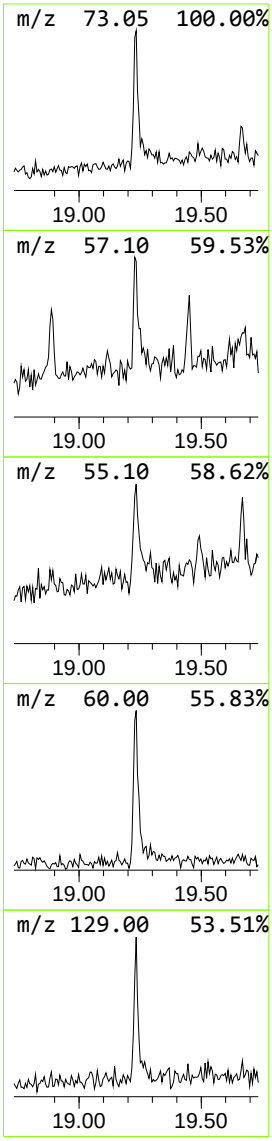
Peak Number 2 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.233	2.24 ng	63240	Chrysene-d12	21.192

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	96
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	89
3	n-Decanoic acid	172	C10H20O2	000334-48-5	38
4	Tetracosanoic acid	368	C24H48O2	000557-59-5	35
5	L-Lyxose	150	C5H10O5	001949-78-6	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP041621\
Data File : BP005320.D
Acq On : 16 Apr 2021 15:58
Operator : CG/JU
Sample : M1998-12
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-5C

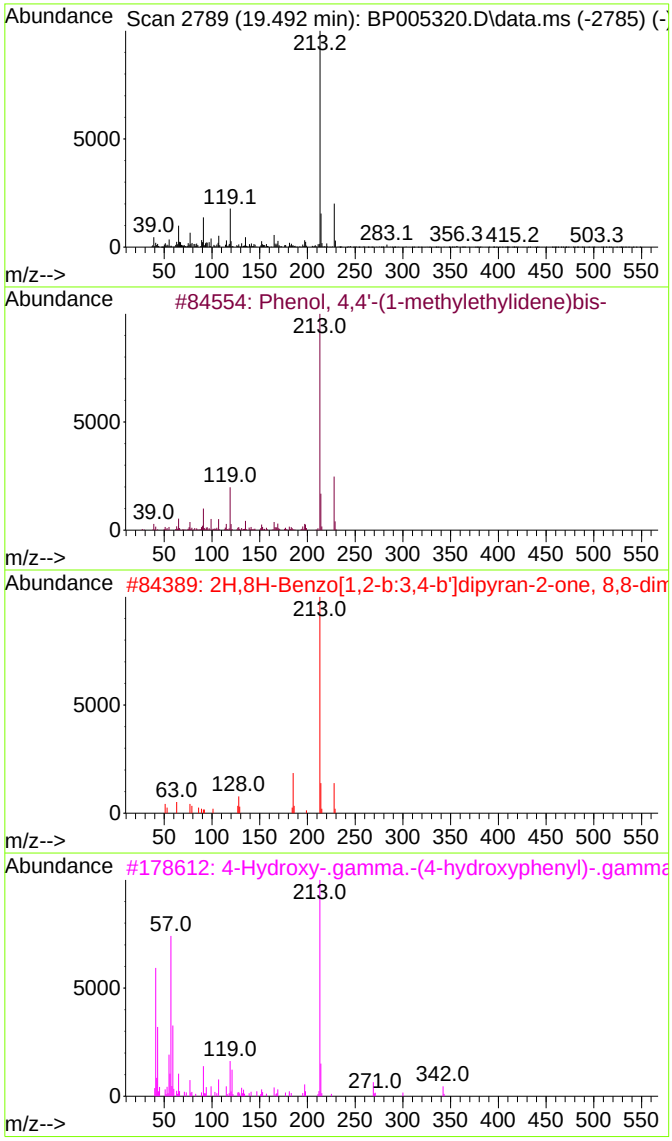
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

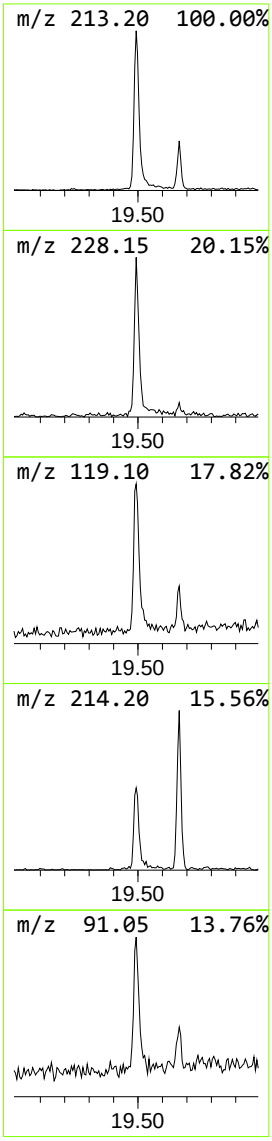
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Phenol, 4,4'-(1-methylethyl... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.492	3.86 ng	109203	Chrysene-d12	21.192

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	98
2	2H,8H-Benzo[1,2-b:3,4-b']dipyran...	228	C14H12O3	000523-59-1	59
3	4-Hydroxy-.gamma.-(4-hydroxyphen...	342	C21H26O4	138721-52-5	59
4	Carbanilic acid, p-phenyl-	213	C13H11NO2	004474-53-7	58
5	2,2'-Bis(p-acetoxyphenyl)propane	312	C19H20O4	010192-62-8	45





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP041621\
Data File : BP005320.D
Acq On : 16 Apr 2021 15:58
Operator : CG/JU
Sample : M1998-12
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : SB-5C

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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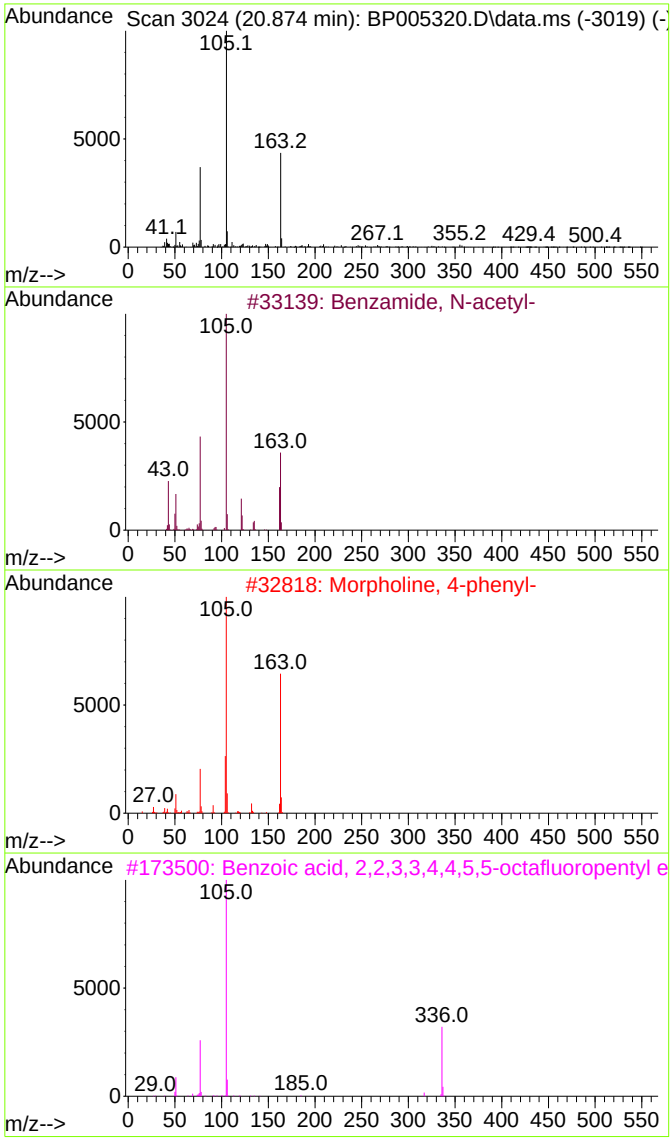
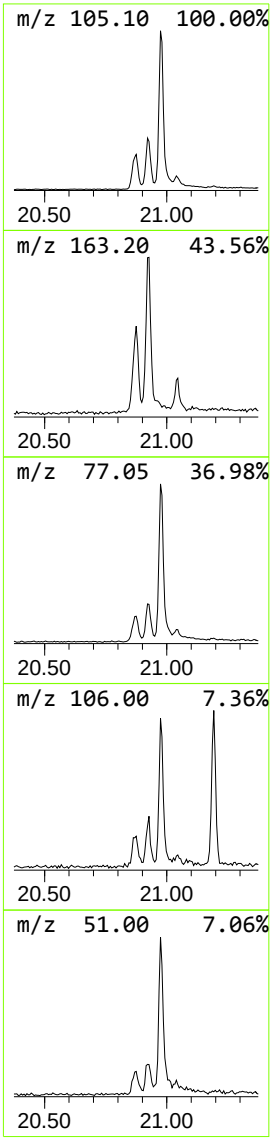
Peak Number 4 Benzamide, N-acetyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.875	3.09 ng	87359	Chrysene-d12	21.192

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzamide, N-acetyl-	163	C9H9NO2	001575-95-7	72
2	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	53
3	Benzoic acid, 2,2,3,3,4,4,5,5-oc...	336	C12H8F8O2	1000360-67-6	27
4	Anthraquinone, 2-benzamido-	327	C21H13NO3	052869-18-8	25
5	Propenoic acid, 2-benzoylamino-3...	355	C20H21NO5	274691-51-9	25





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Acq On : 16 Apr 2021 15:58
Operator : CG/JU
Sample : M1998-12
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : SB-5C

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

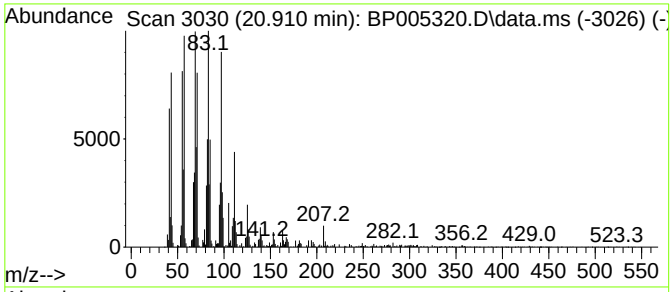
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

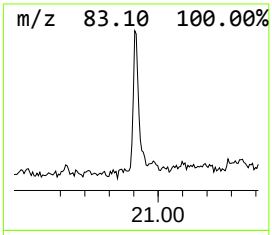
****

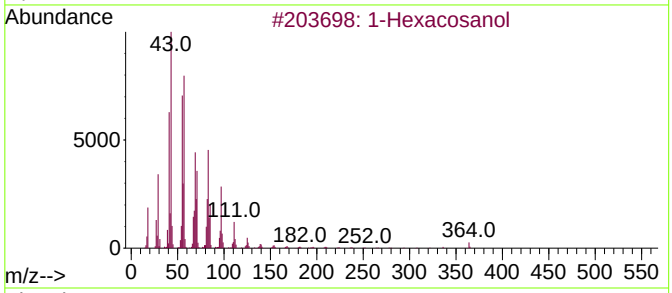
Peak Number 5 1-Hexacosanol Concentration Rank 2

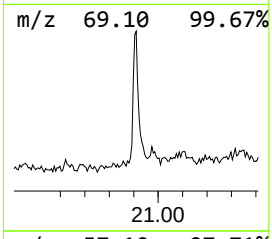
R.T.	EstConc	Area	Relative to ISTD	R.T.
20.910	12.83 ng	362663	Chrysene-d12	21.192

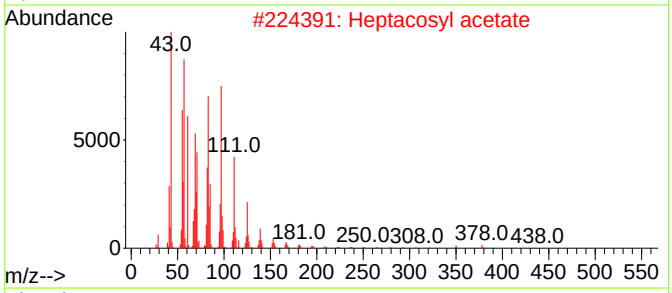
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosanol	382	C26H54O	000506-52-5	91
2	Heptacosyl acetate	438	C29H58O2	1000351-78-2	91
3	Cetene	224	C16H32	000629-73-2	90
4	1-Heneicosyl formate	340	C22H44O2	077899-03-7	90
5	1-Docosanol, methyl ether	340	C23H48O	1000333-91-9	89

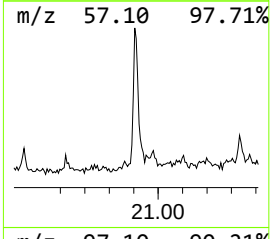


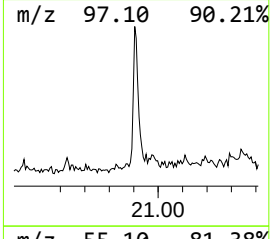


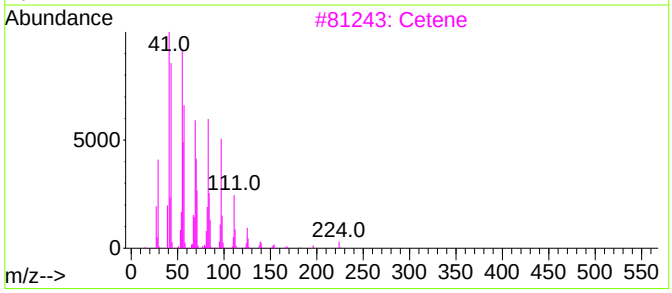


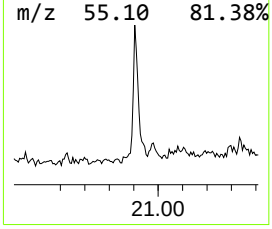












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ClientSampleId :
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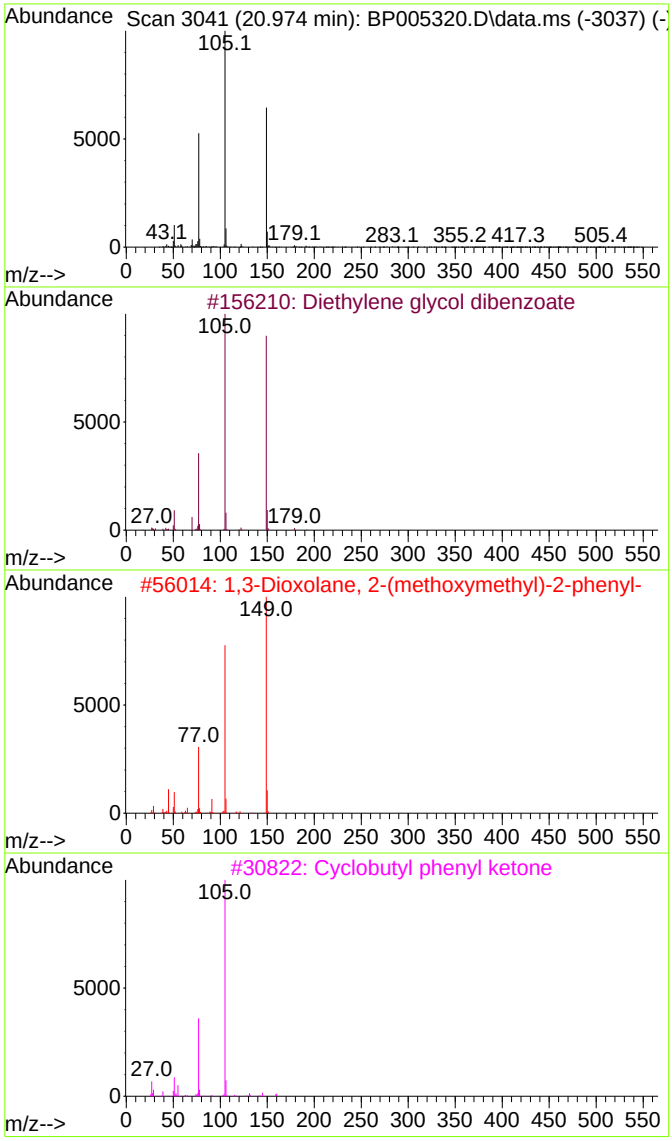
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

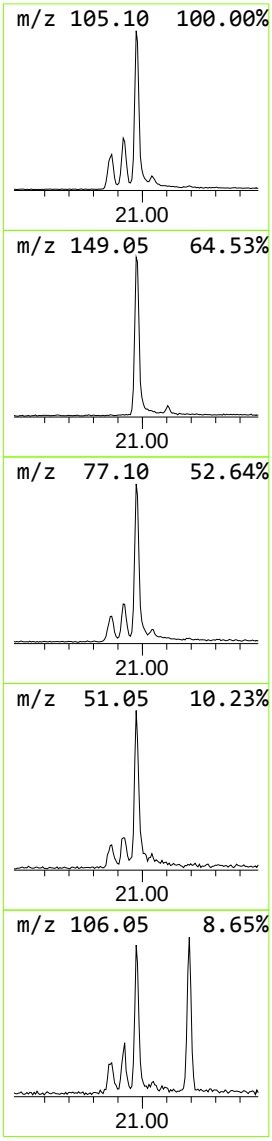
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Diethylene glycol dibenzoate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.974	13.80 ng	390153	Chrysene-d12	21.192

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	64
2	1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	59
3	Cyclobutyl phenyl ketone	160	C11H12O	005407-98-7	47
4	1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	47
5	Benzoylformic acid	150	C8H6O3	000611-73-4	47





Tentatively Identified Compound (LSC) summary

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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
n-Hexadecanoic ...	17.992	7.8	ng	154666	4	17.092	395002	20.0
Octadecanoic acid	19.233	2.2	ng	63240	5	21.192	565501	20.0
Phenol, 4,4'-(1...	19.492	3.9	ng	109203	5	21.192	565501	20.0
Benzamide, N-ac...	20.875	3.1	ng	87359	5	21.192	565501	20.0
1-Hexacosanol	20.910	12.8	ng	362663	5	21.192	565501	20.0
Diethylene glyc...	20.974	13.8	ng	390153	5	21.192	565501	20.0