LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042921\
Data File : BP005418.D
Acq On : 29 Apr 2021 20:05
Operator : CG/JU
Sample : M2193-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : S-1

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-BP042921.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP005418.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.228	358	364	379	rBV	506581	722480	37.56%	7.269%
2	6.816	627	634	649	rBV	464610	735722	38.25%	7.402%
3	7.628	765	772	780	rBV	130455	208891	10.86%	2.102%
4	8.787	961	969	978	rBV	273343	456500	23.74%	4.593%
5	10.416	1237	1246	1262	rBV	145717	261403	13.59%	2.630%
6	12.904	1660	1669	1679	rBV	688809	995835	51.78%	10.019%
7	13.187	1709	1717	1723	rBV2	11916	20744	1.08%	0.209%
8	14.292	1898	1905	1915	rBV2	244827	364190	18.94%	3.664%
9	15.798	2153	2161	2173	rBV	787017	1119870	58.23%	11.267%
10	17.057	2369	2375	2385	rBV	332481	477472	24.83%	4.804%
11	17.963	2523	2529	2536	rBV2	77304	117995	6.13%	1.187%
12	19.204	2733	2740	2748	rBV5	30348	61585	3.20%	0.620%
13	19.639	2808	2814	2819	rBV	1663724	1923313	100.00%	19.351%
14	20.845	3013	3019	3021	rBV	81271	129409	6.73%	1.302%
15	20.892	3021	3027	3032	rVV2	153256	314684	16.36%	3.166%
16	20.945	3032	3036	3043	rVV	493743	617300	32.10%	6.211%
17	21.010	3045	3047	3054	rVB	28055	35346	1.84%	0.356%
18	21.163	3068	3073	3077	rBV	556893	691377	35.95%	6.956%
19	23.416	3449	3456	3464	rVB2	362718	684867	35.61%	6.891%

Sum of corrected areas: 9938983

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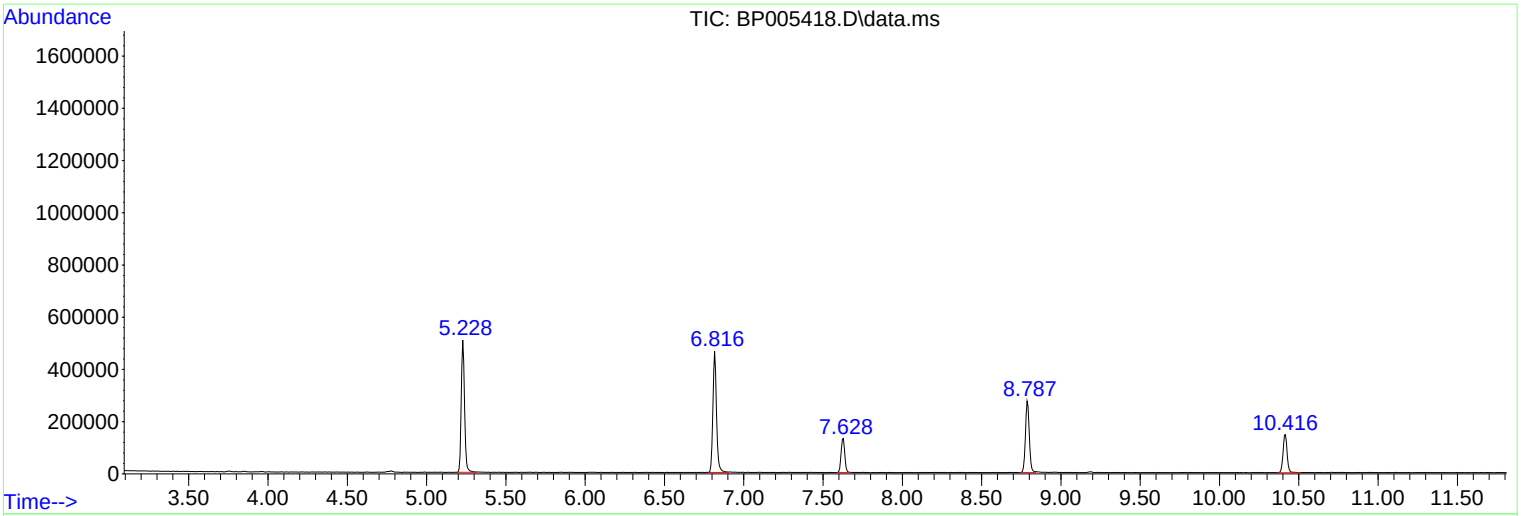
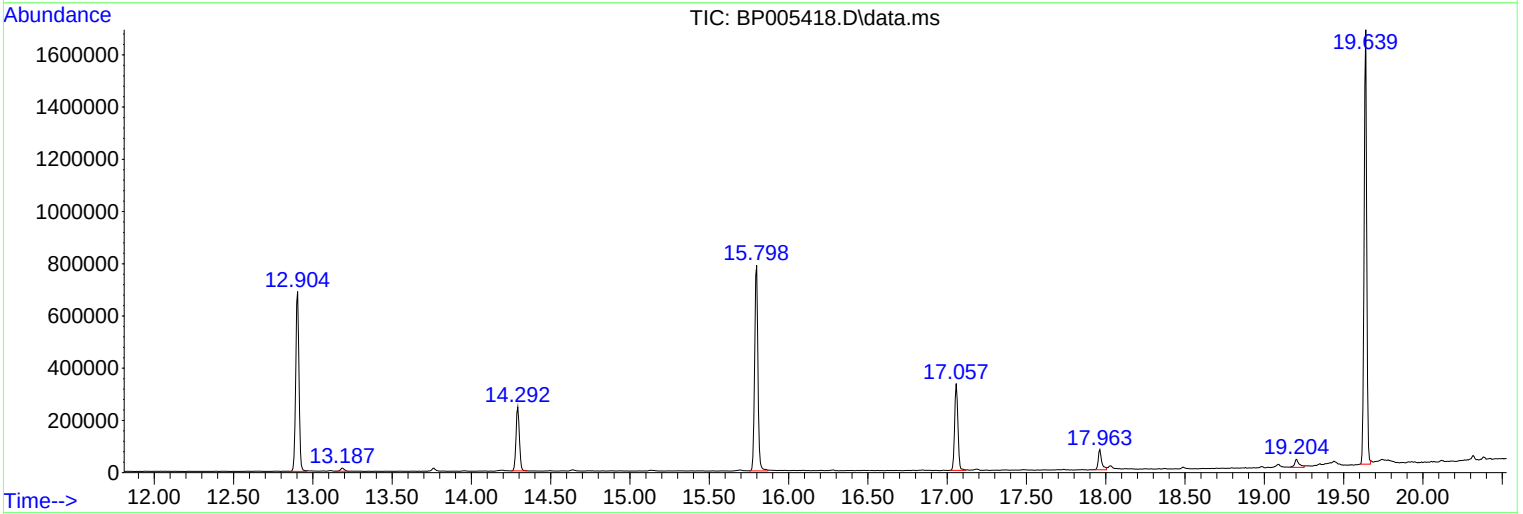
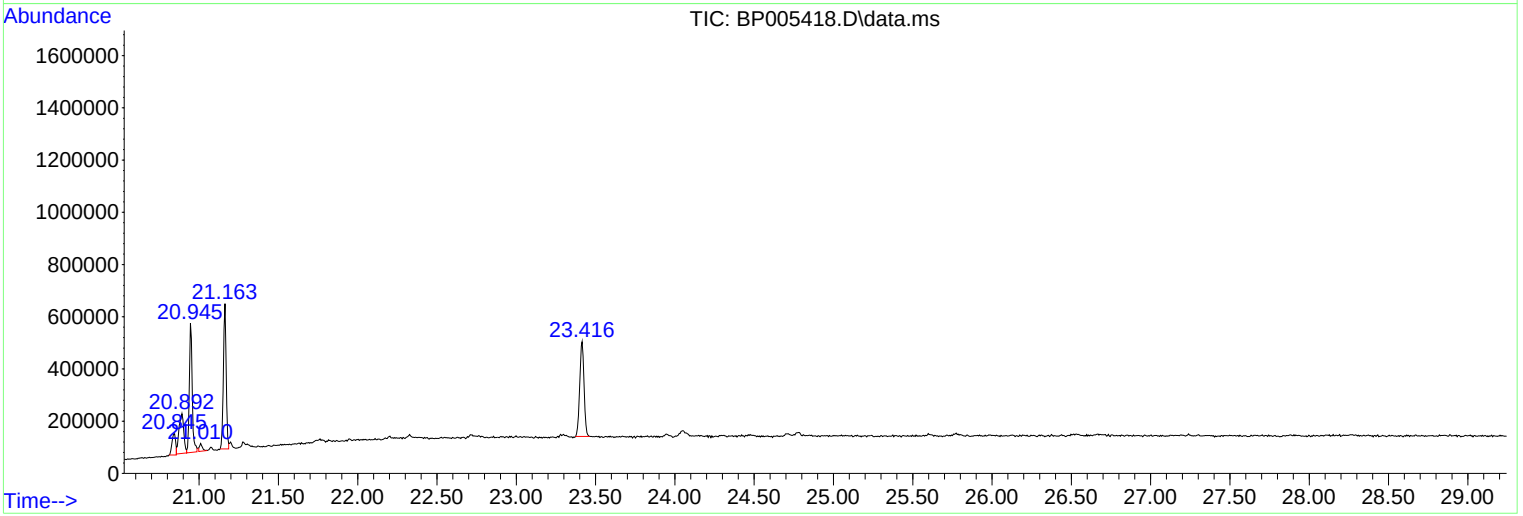
Instrument :
BNA_P
ClientSampleId :
S-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP042921.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 : BP005418.D
Acq On : 29 Apr 2021 20:05
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

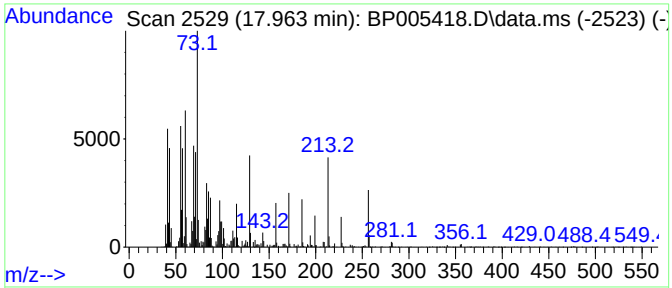
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

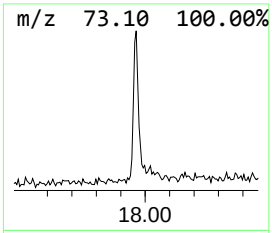
****

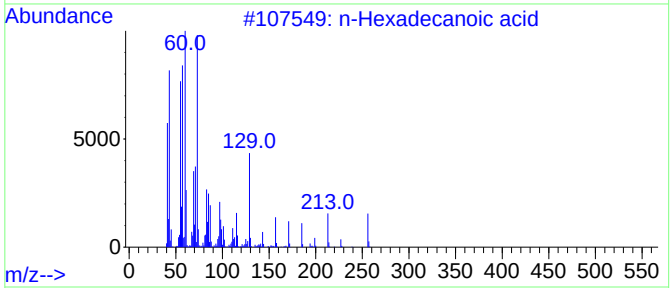
Peak Number 1 n-Hexadecanoic acid Concentration Rank 3

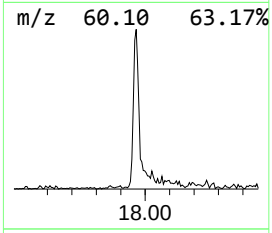
R.T.	EstConc	Area	Relative to ISTD	R.T.
17.963	4.94 ng	117995	Phenanthrene-d10	17.057

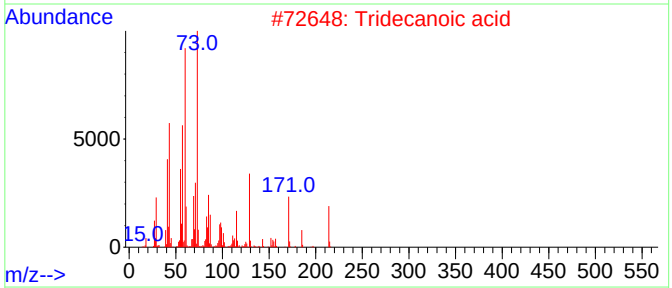
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2	Tridecanoic acid	214	C13H26O2	000638-53-9	55
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	49
4	Dodecanoic acid	200	C12H24O2	000143-07-7	46
5	Octadecanoic acid	284	C18H36O2	000057-11-4	38

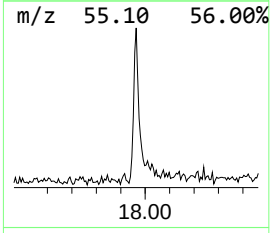


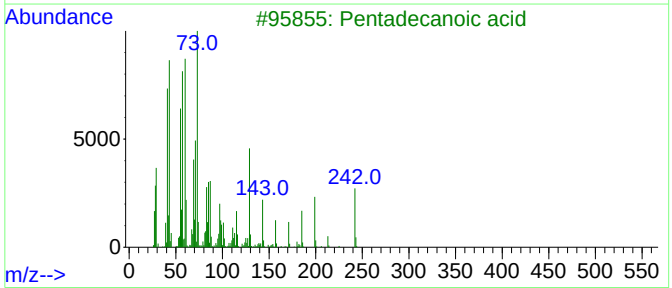


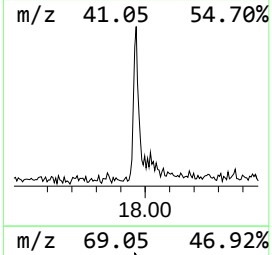


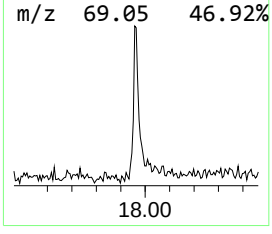












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Acq On : 29 Apr 2021 20:05
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Sample : M2193-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : S-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP042921.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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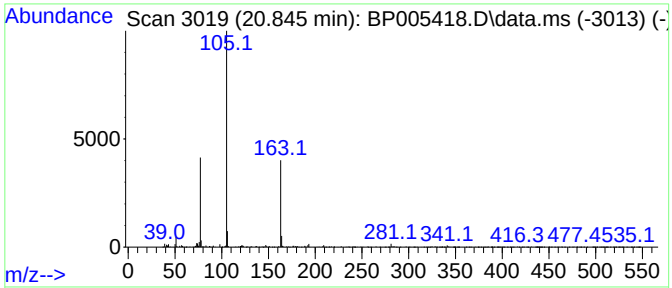
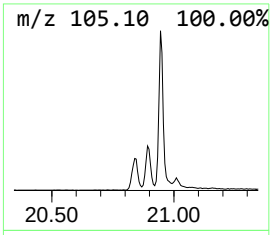
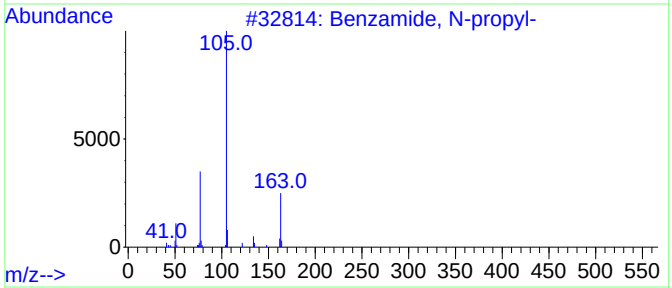
Peak Number 2 Benzamide, N-propyl- Concentration Rank 4

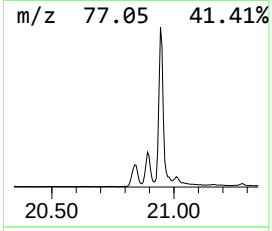
R.T.	EstConc	Area	Relative to ISTD	R.T.
20.845	3.74 ng	129409	Chrysene-d12	21.163

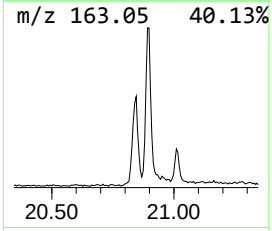
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzamide, N-propyl-	163	C10H13NO	010546-70-0	78
2	(3-Phenyloxiran-2-yl)methyl benz...	254	C16H14O3	1000366-96-1	64
3	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	43
4	2-Pyrrolidinone, 3-hydroxy-4-met...	191	C11H13NO2	104194-17-4	43
5	Benzamide, N-acetyl-	163	C9H9NO2	001575-95-7	36

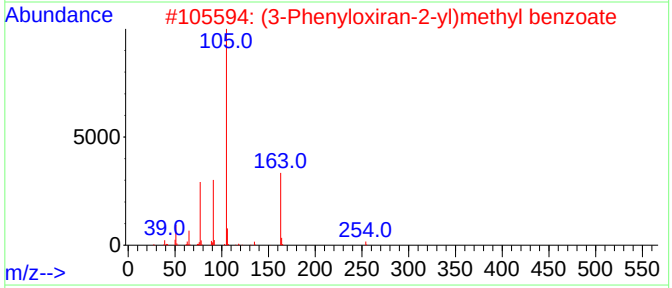


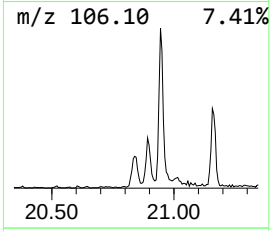


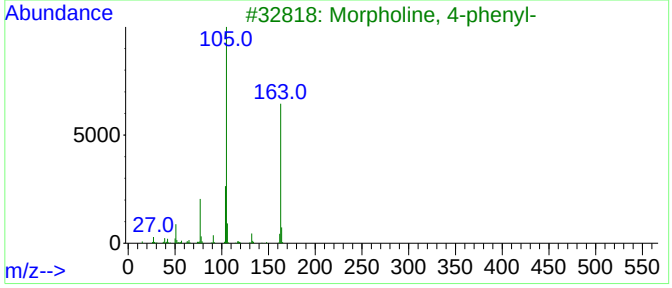


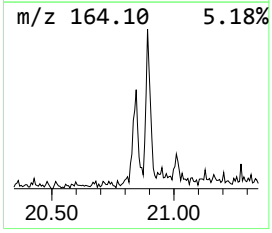












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Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : S-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP042921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

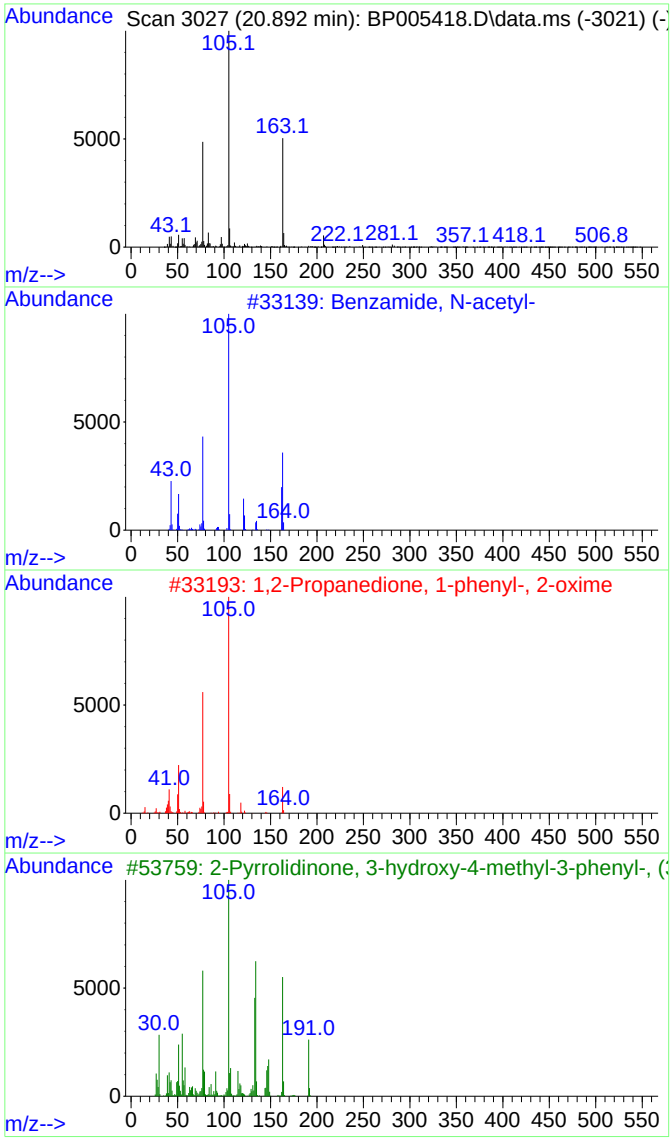
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

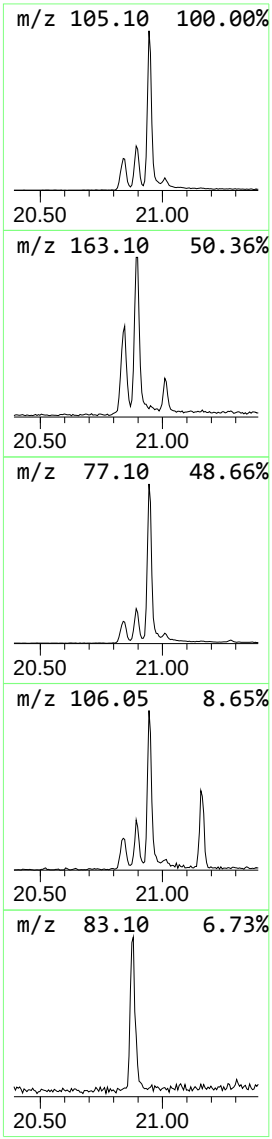
****

Peak Number 3 Benzamide, N-acetyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.892	9.10 ng	314684	Chrysene-d12	21.163

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzamide, N-acetyl-	163	C9H9NO2	001575-95-7	72
2	1,2-Propanedione, 1-phenyl-, 2-o...	163	C9H9NO2	000119-51-7	53
3	2-Pyrrolidinone, 3-hydroxy-4-met...	191	C11H13NO2	104194-17-4	40
4	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	37
5	Phthalic acid, 2,6-dimethoxyphen...	316	C17H16O6	1000315-74-1	33





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Instrument : BNA_P
ClientSampleId : S-1

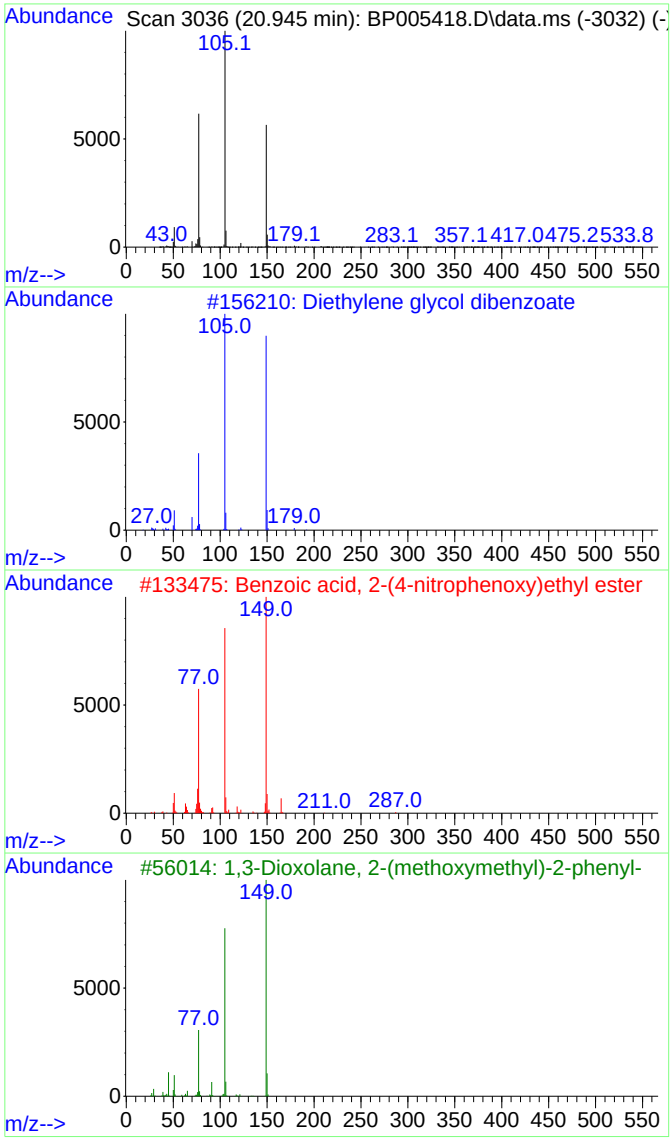
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP042921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

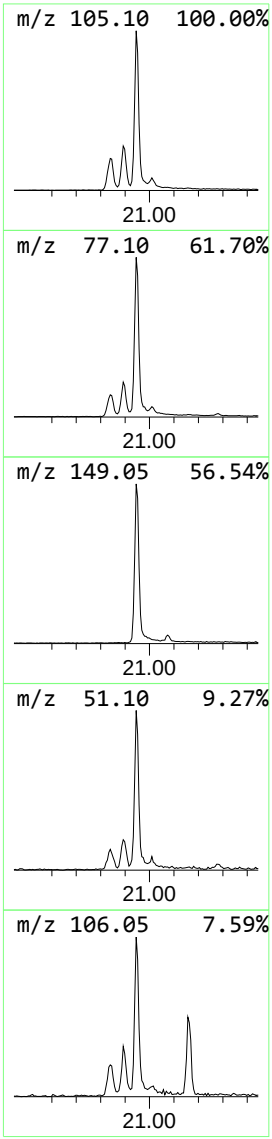
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Diethylene glycol dibenzoate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.945	17.86 ng	617300	Chrysene-d12	21.163

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	78
2	Benzoic acid, 2-(4-nitrophenoxy)...	287	C15H13NO5	1000368-92-7	64
3	1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	64
4	2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	56
5	Benzoic acid, 2-(3-nitrophenyl)e...	271	C15H13NO4	1000368-22-4	56





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 ...	17.963	4.9	ng	117995	4	17.057	477472	20.0
Benzamide, N-pr...	20.845	3.7	ng	129409	5	21.163	691377	20.0
Benzamide, N-ac...	20.892	9.1	ng	314684	5	21.163	691377	20.0
Diethylene glyc...	20.945	17.9	ng	617300	5	21.163	691377	20.0