LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042921\
Data File : BP005424.D
Acq On : 29 Apr 2021 23:29
Operator : CG/JU
Sample : M2222-06
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : TP-5A-COMP

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: BP005424.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	380	rBV	761226	1057370	33.46%	7.795%
2	6.817	627	634	650	rBV	706711	1100862	34.84%	8.116%
3	7.622	765	771	779	rBV	122112	191688	6.07%	1.413%
4	8.787	962	969	978	rBV	411734	685049	21.68%	5.050%
5	10.410	1237	1245	1257	rBV	137698	240753	7.62%	1.775%
6	12.904	1660	1669	1687	rBV	1201397	1695944	53.67%	12.503%
7	13.187	1710	1717	1724	rBV	127891	187585	5.94%	1.383%
8	13.757	1808	1814	1823	rBV	54433	88000	2.78%	0.649%
9	14.293	1898	1905	1914	rBV	234709	334994	10.60%	2.470%
10	15.798	2151	2161	2180	rBV	1214946	1725153	54.60%	12.718%
11	17.057	2368	2375	2380	rBV	316858	444061	14.05%	3.274%
12	17.963	2520	2529	2537	rBV3	77411	131287	4.15%	0.968%
13	19.086	2714	2720	2726	rBV	66330	98265	3.11%	0.724%
14	19.204	2734	2740	2745	rBV4	28101	48598	1.54%	0.358%
15	19.439	2771	2780	2789	rBV	63428	106302	3.36%	0.784%
16	19.639	2808	2814	2821	rBV	2905394	3159815	100.00%	23.294%
17	20.845	3013	3019	3022	rBV	58511	112435	3.56%	0.829%
18	20.892	3022	3027	3032	rVV2	118595	232982	7.37%	1.718%
19	20.945	3032	3036	3044	rVV	328312	391577	12.39%	2.887%
20	21.163	3067	3073	3077	rBV	534405	705250	22.32%	5.199%
21	21.198	3077	3079	3085	rVB	54094	61446	1.94%	0.453%
22	22.204	3246	3250	3254	rBV2	87875	114978	3.64%	0.848%
23	23.410	3449	3455	3462	rBV2	329908	650282	20.58%	4.794%

Sum of corrected areas: 13564676

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042921\
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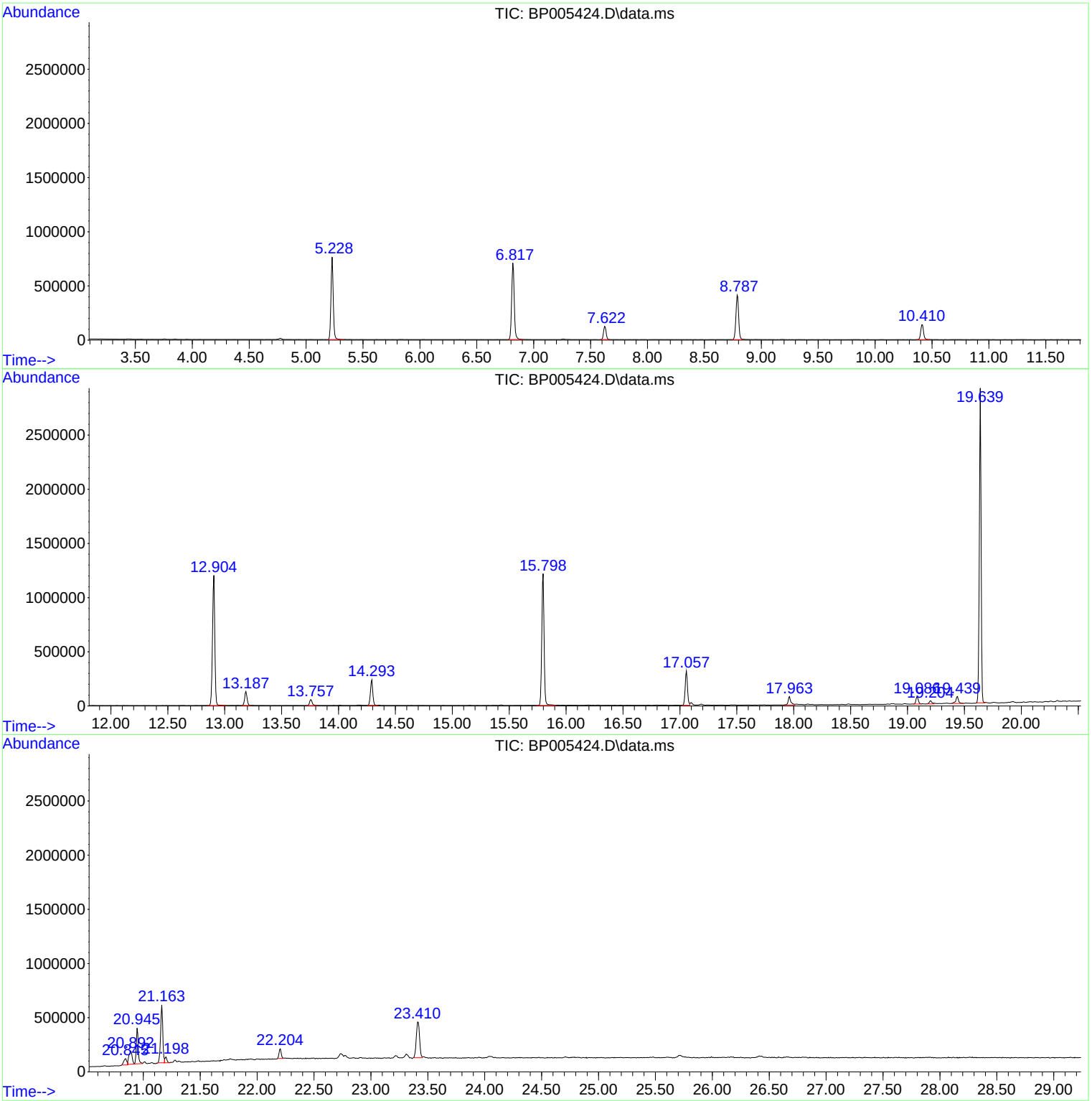
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP-5A-COMP

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 : BP005424.D
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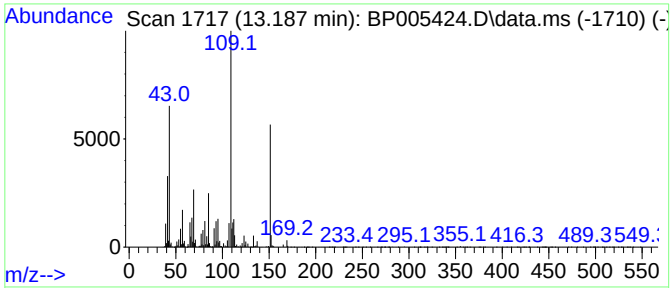
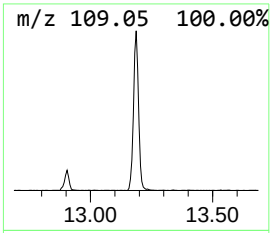
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

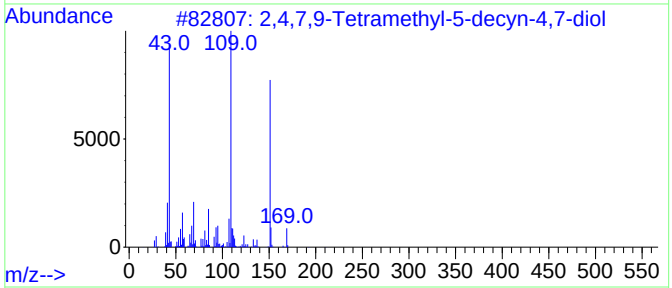
****
Peak Number 1 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 1

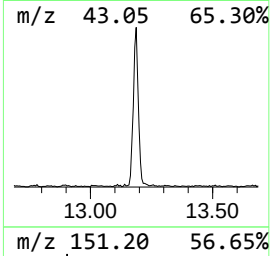
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.187	11.20 ng	187585	Acenaphthene-d10	14.293

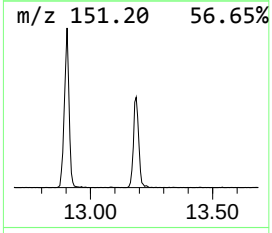
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	90
2	2-Propenal, 3-(2,2,6-trimethyl-7...	194	C12H18O2	055759-91-6	50
3	Metacetamol	151	C8H9NO2	000621-42-1	50
4	4-Pyridinemethanol, acetate (ester)	151	C8H9NO2	001007-48-3	50
5	Acetaminophen	151	C8H9NO2	000103-90-2	50

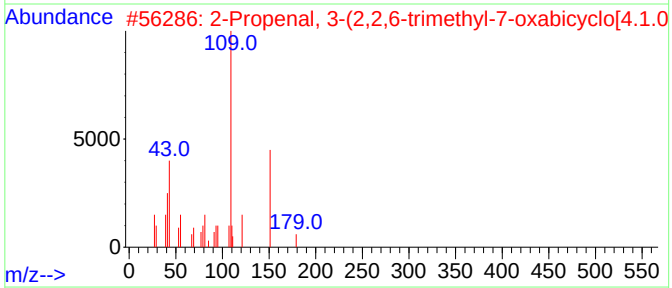


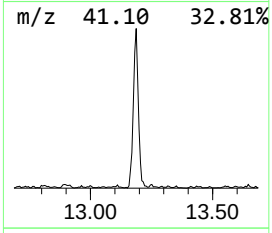


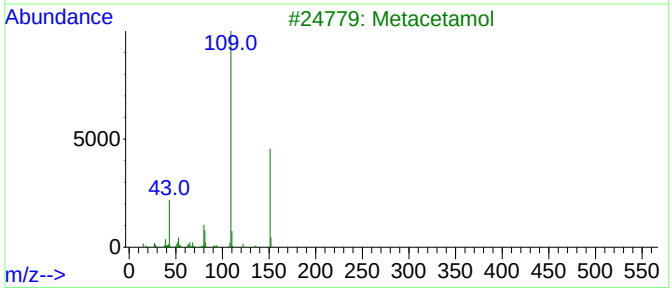


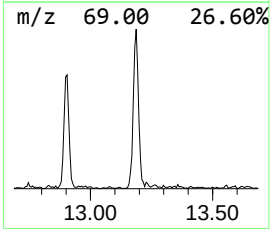












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Data File : BP005424.D
Acq On : 29 Apr 2021 23:29
Operator : CG/JU
Sample : M2222-06
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP-5A-COMP

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

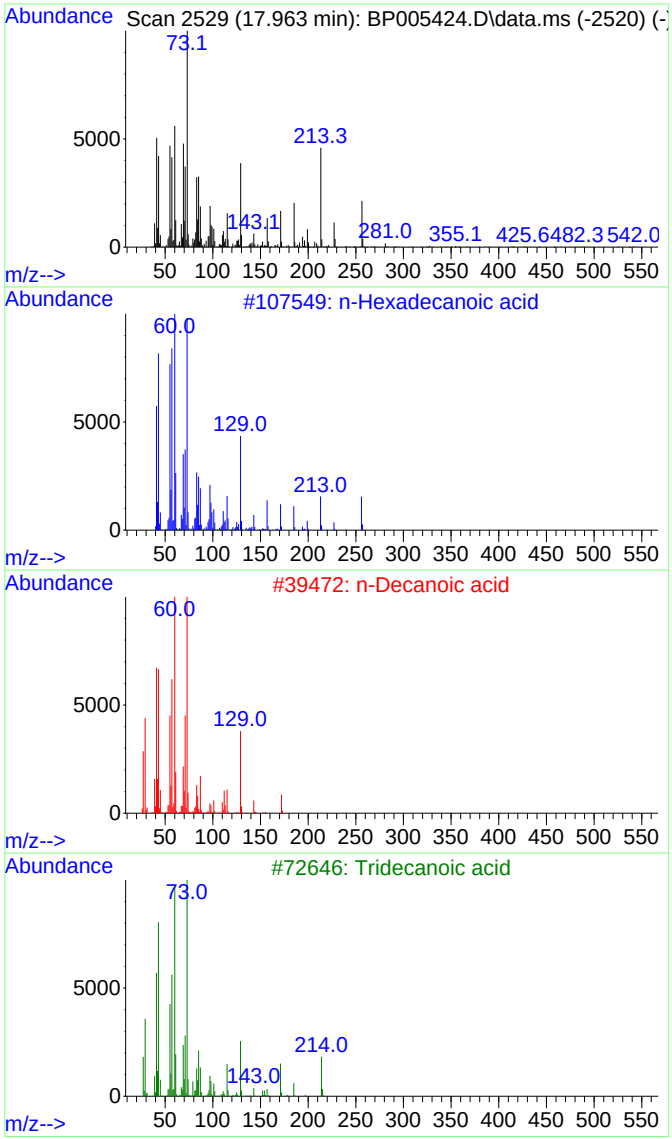
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

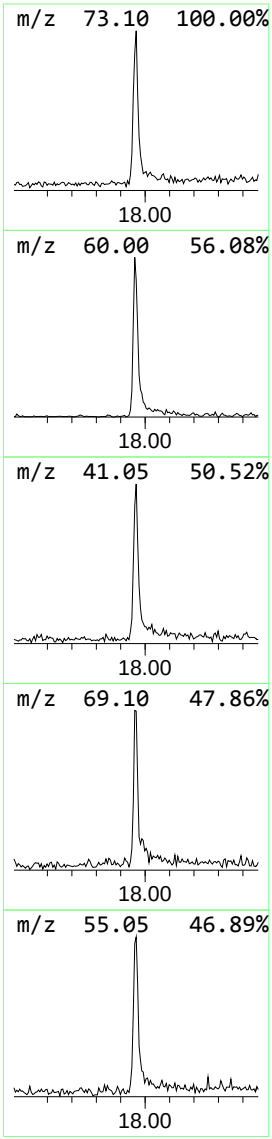
****

Peak Number 2 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.963	5.91 ng	131287	Phenanthrene-d10	17.057

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
2	n-Decanoic acid	172	C10H20O2	000334-48-5	52
3	Tridecanoic acid	214	C13H26O2	000638-53-9	46
4	Undecanoic acid	186	C11H22O2	000112-37-8	43
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	38





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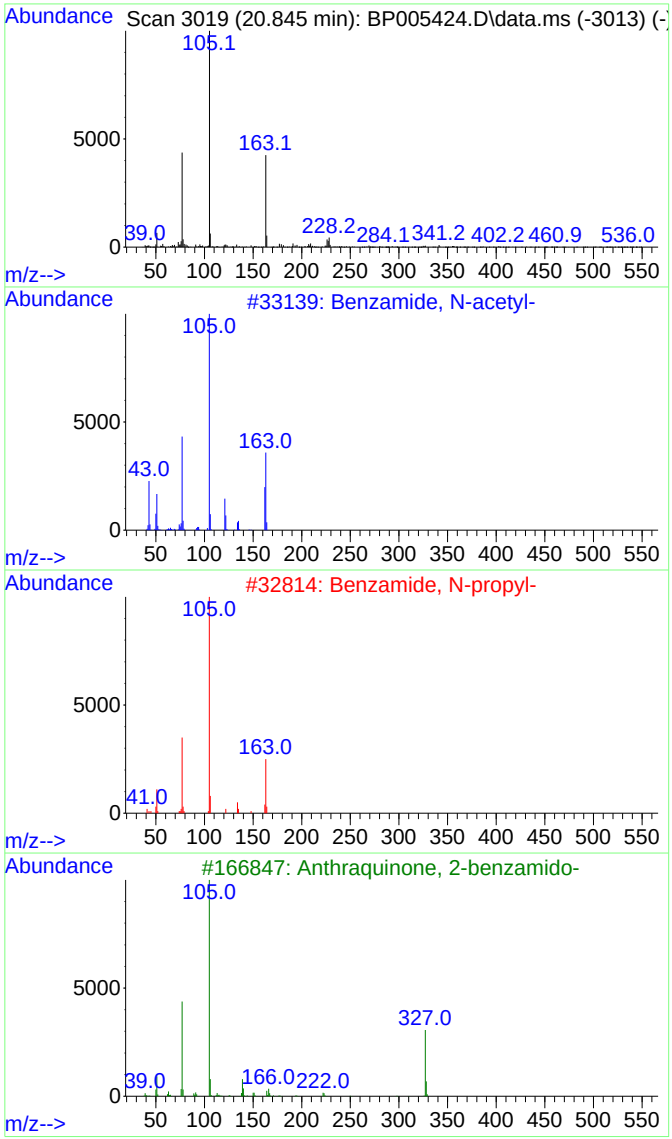
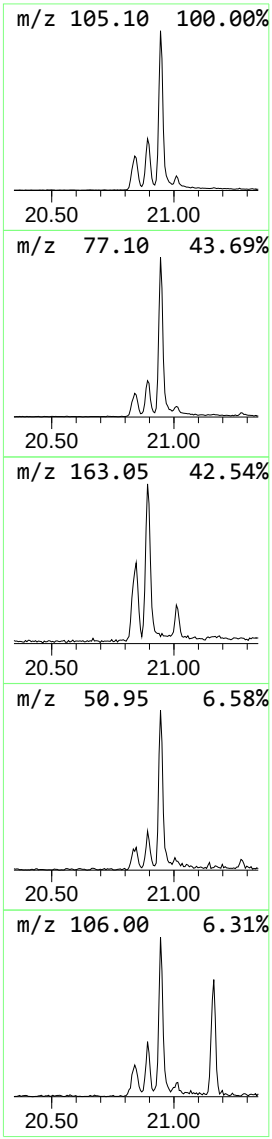
****

Peak Number 3 Benzamide, N-acetyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.845	3.19 ng	112435	Chrysene-d12	21.163

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzamide, N-acetyl-	163	C9H9NO2	001575-95-7	72
2	Benzamide, N-propyl-	163	C10H13NO	010546-70-0	50
3	Anthraquinone, 2-benzamido-	327	C21H13NO3	052869-18-8	38
4	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	37
5	2-Methoxyphenyl benzoate	228	C14H12O3	000531-37-3	32





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Data File : BP005424.D
Acq On : 29 Apr 2021 23:29
Operator : CG/JU
Sample : M2222-06
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP042921.M
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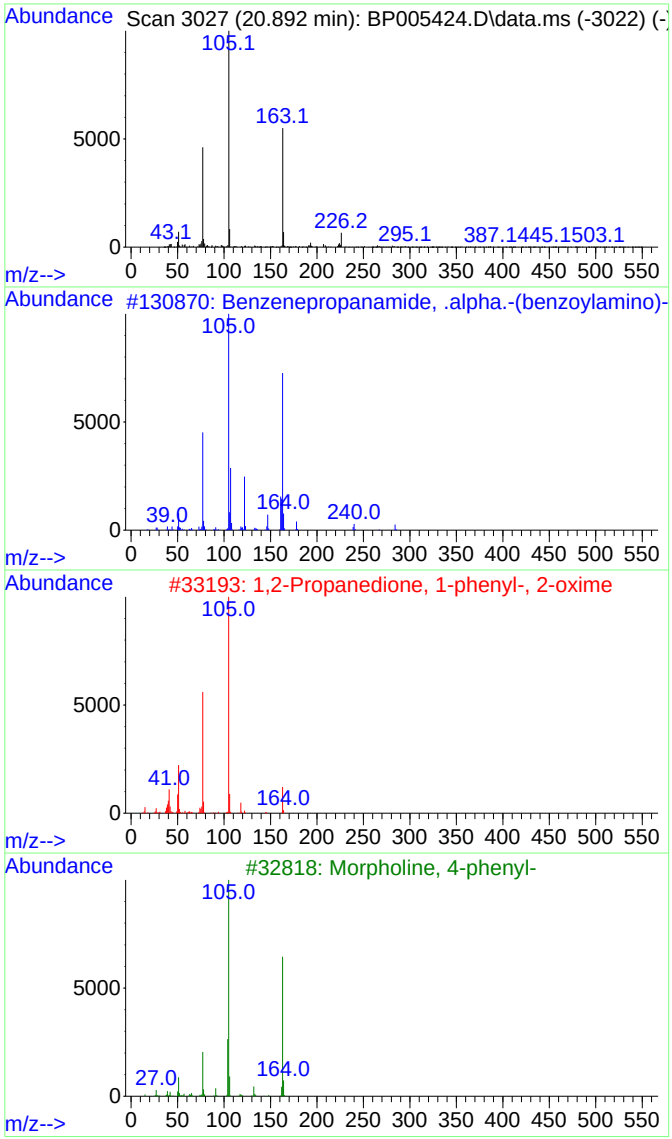
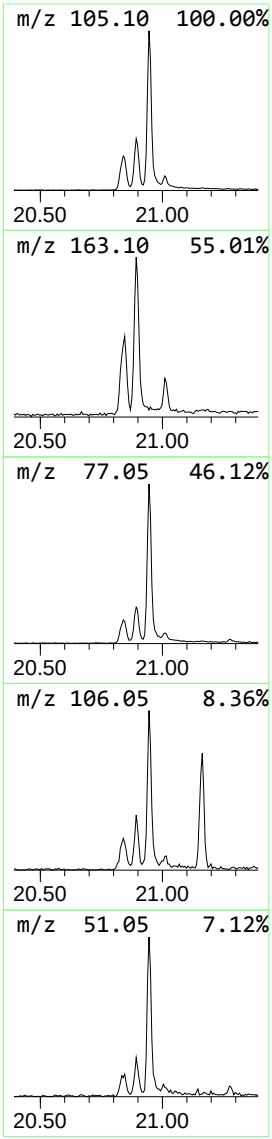
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Benzenepropanamide, .alpha.... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.892	6.61 ng	232982	Chrysene-d12	21.163

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenepropanamide, .alpha.-(ben...	284	C16H16N2O3	058690-81-6	56
2	1,2-Propanedione, 1-phenyl-, 2-o...	163	C9H9NO2	000119-51-7	50
3	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	42
4	2-Pyrrolidinone, 3-hydroxy-4-met...	191	C11H13NO2	104194-17-4	40
5	Biphenyl, 4,4'-dibenzoyloxy-	394	C26H18O4	1000294-15-4	38





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Sample : M2222-06
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : TP-5A-COMP

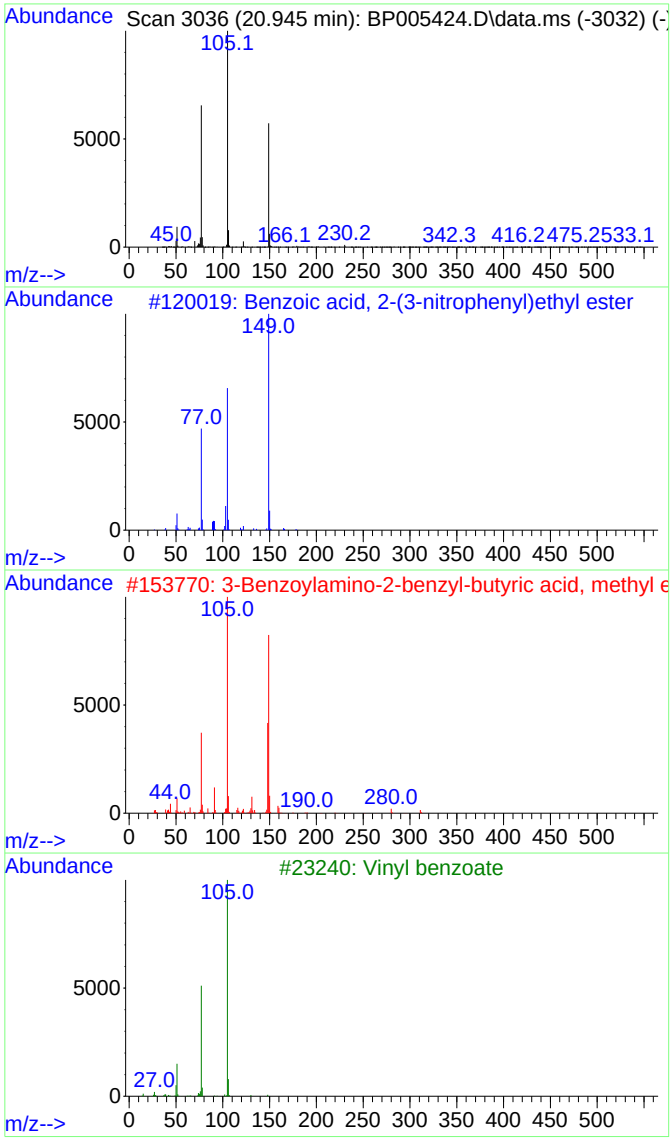
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP042921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

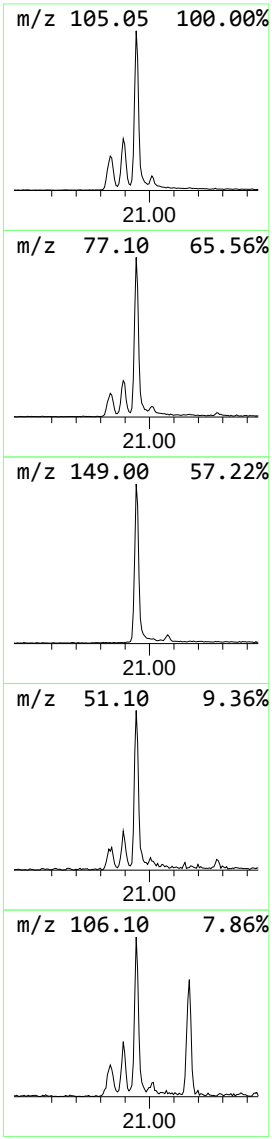
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Benzoic acid, 2-(3-nitrophe... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.945	11.10 ng	391577	Chrysene-d12	21.163

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, 2-(3-nitrophenyl)e...	271	C15H13NO4	1000368-22-4	72
2	3-Benzoylamino-2-benzyl-butyric ...	311	C19H21NO3	1000193-12-7	56
3	Vinyl benzoate	148	C9H8O2	000769-78-8	47
4	Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	47
5	Phenacyl thiocyanate	177	C9H7NOS	005399-30-4	47





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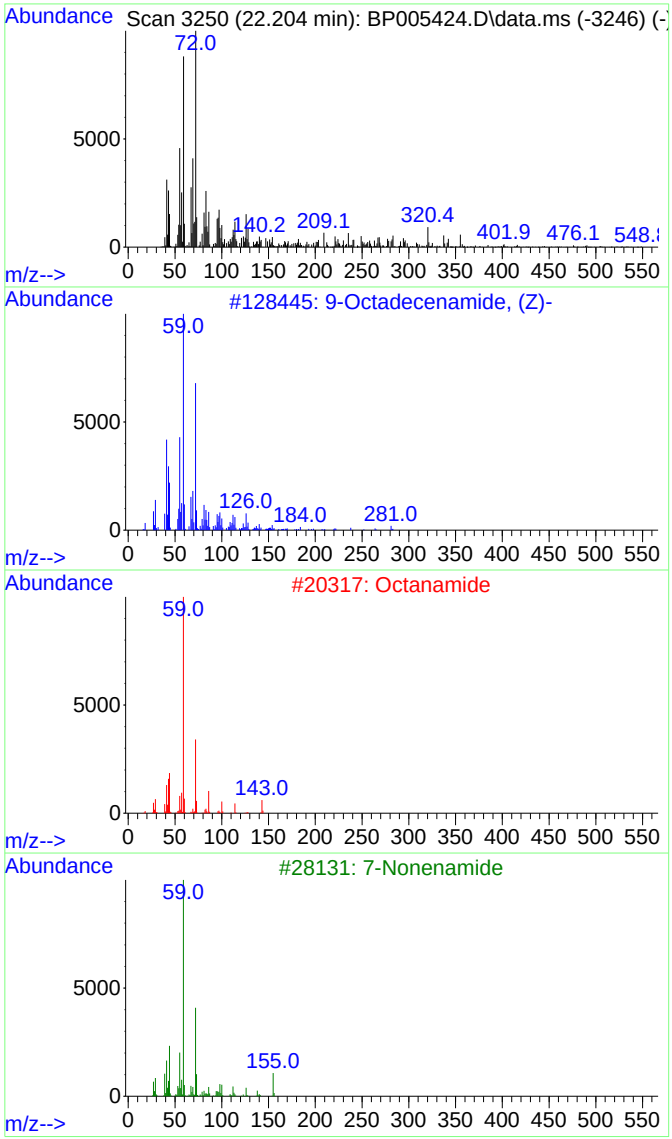
TIC Integration Parameters: LSCINT.P

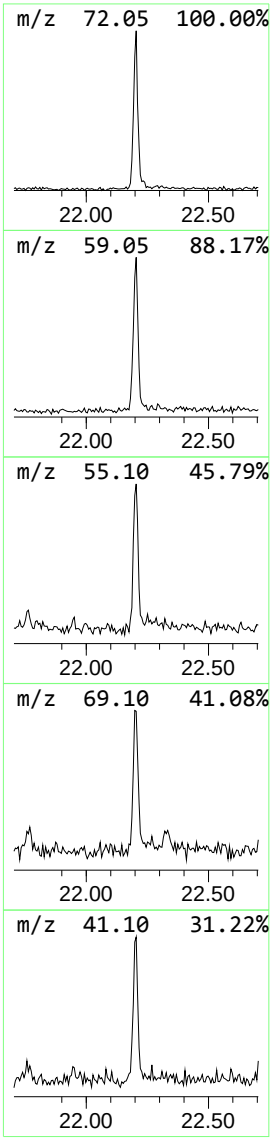
****

Peak Number 6 9-Octadecenamide, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.204	3.26 ng	114978	Chrysene-d12	21.163

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	60
2	Octanamide	143	C8H17NO	000629-01-6	50
3	7-Nonenamide	155	C9H17NO	090949-53-4	47
4	trans-13-Docosenamide	337	C22H43NO	010436-09-6	47
5	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	46





Tentatively Identified Compound (LSC) summary

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					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2,4,7,9-Tetrame...	13.187	11.2	ng	187585	3	14.293	334994	20.0
n-Hexadecanoic ...	17.963	5.9	ng	131287	4	17.057	444061	20.0
Benzamide, N-ac...	20.845	3.2	ng	112435	5	21.163	705250	20.0
Benzenepropanam...	20.892	6.6	ng	232982	5	21.163	705250	20.0
Benzoic acid, 2...	20.945	11.1	ng	391577	5	21.163	705250	20.0
9-Octadecenamid...	22.204	3.3	ng	114978	5	21.163	705250	20.0