

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042921\
 Data File : BP005417.D
 Acq On : 29 Apr 2021 19:31
 Operator : CG/JU
 Sample : M2196-05
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 WALL-D-4075-B

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: BP005417.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	356	364	380	rBV	531055	750912	32.01%	6.588%
2	6.817	626	634	648	rBV	486284	759377	32.37%	6.662%
3	7.622	765	771	781	rBV	118220	189021	8.06%	1.658%
4	8.787	962	969	988	rBV	285599	474770	20.24%	4.165%
5	10.416	1239	1246	1253	rBV	134084	228760	9.75%	2.007%
6	12.904	1661	1669	1681	rBV	789108	1116747	47.61%	9.798%
7	13.757	1809	1814	1822	rBV	15614	27599	1.18%	0.242%
8	14.293	1899	1905	1913	rBV	229812	327306	13.95%	2.872%
9	15.798	2154	2161	2173	rBV	829772	1179092	50.27%	10.345%
10	17.057	2369	2375	2381	rBV	320684	436644	18.61%	3.831%
11	17.963	2524	2529	2536	rBV2	114936	171585	7.31%	1.505%
12	19.086	2716	2720	2727	rVB	27387	40203	1.71%	0.353%
13	19.204	2736	2740	2748	rBV2	45762	64267	2.74%	0.564%
14	19.439	2777	2780	2790	rVB	37294	72095	3.07%	0.633%
15	19.639	2808	2814	2819	rBV	2073594	2345697	100.00%	20.580%
16	19.751	2825	2833	2851	rVB	151363	794965	33.89%	6.975%
17	20.263	2917	2920	2924	rBV3	58904	72746	3.10%	0.638%
18	20.845	3014	3019	3022	rBV	79851	130184	5.55%	1.142%
19	20.892	3022	3027	3032	rVV2	160020	335967	14.32%	2.948%
20	20.945	3032	3036	3044	rVV	445838	598103	25.50%	5.247%
21	21.163	3068	3073	3077	rBV	523132	656646	27.99%	5.761%
22	23.416	3450	3456	3464	rVB2	331707	625360	26.66%	5.487%

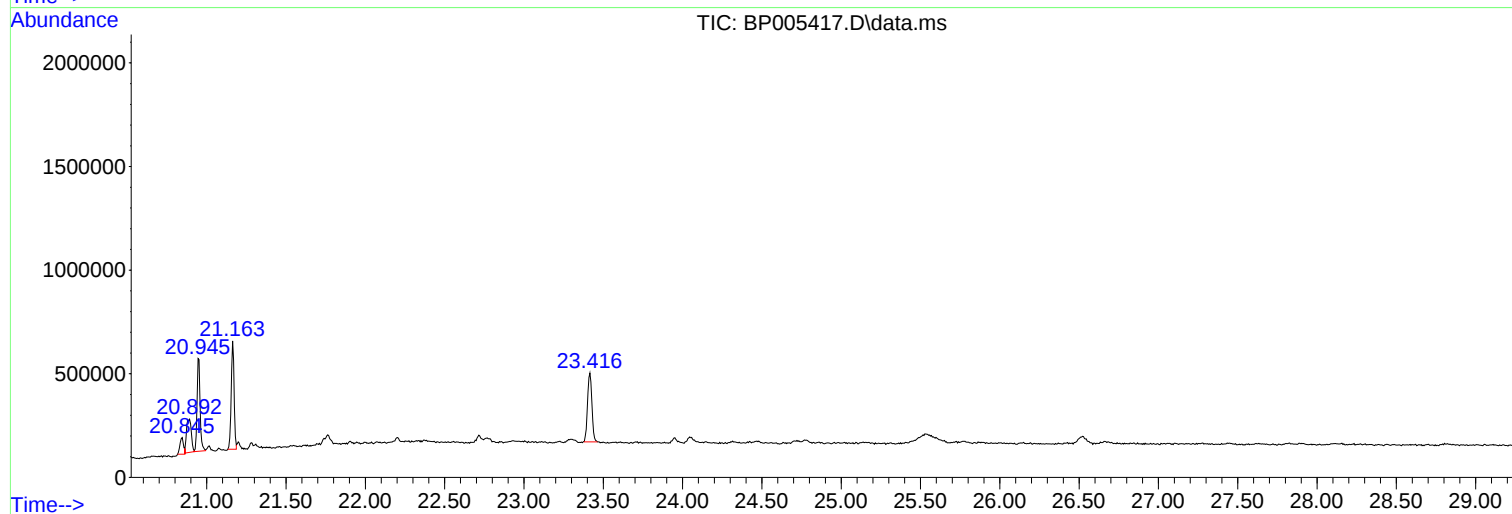
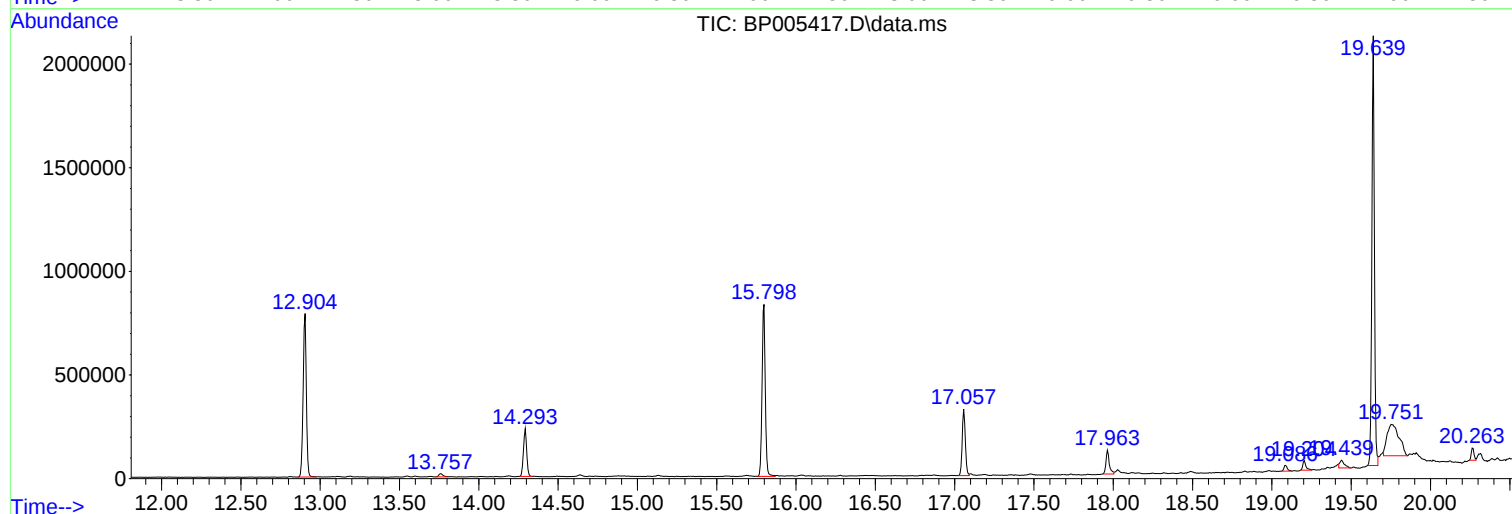
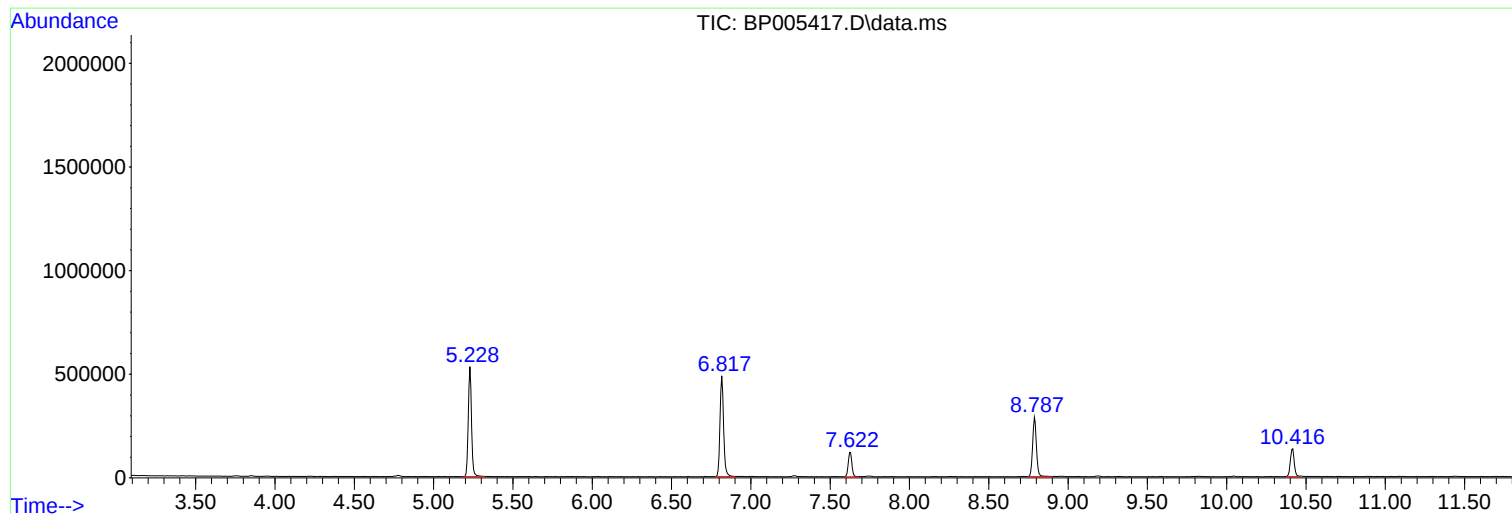
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ClientSampleId :
WALL-D-4075-B

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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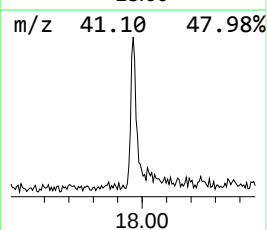
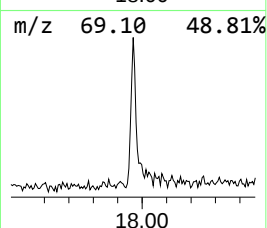
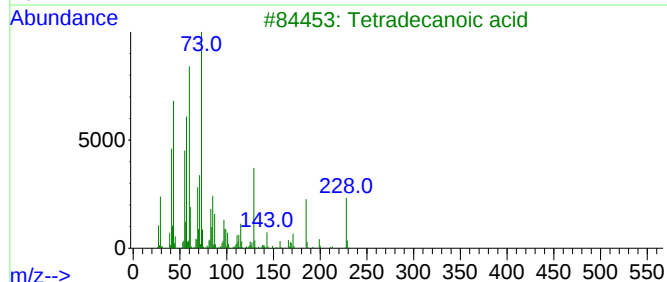
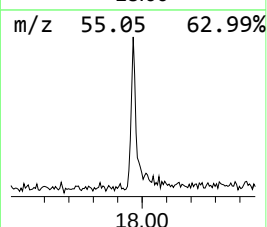
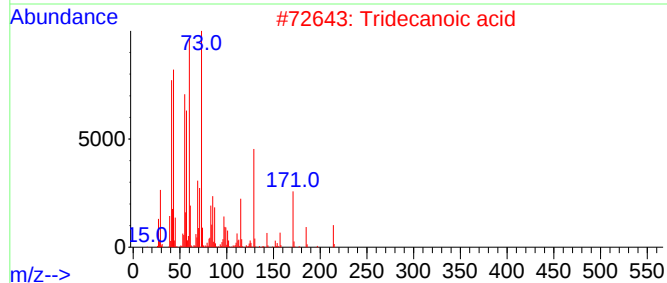
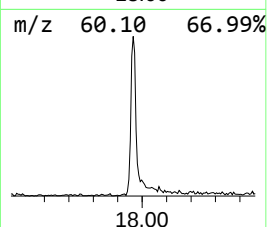
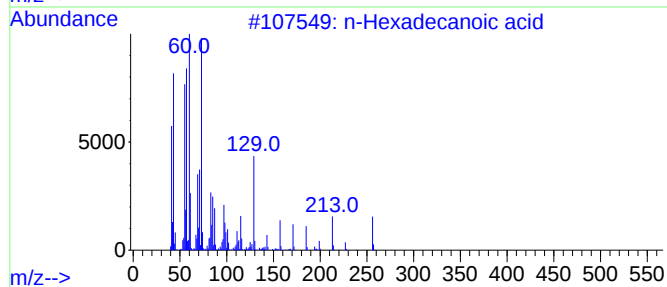
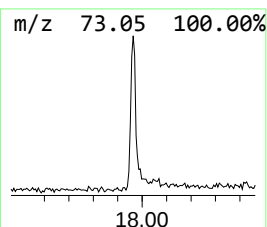
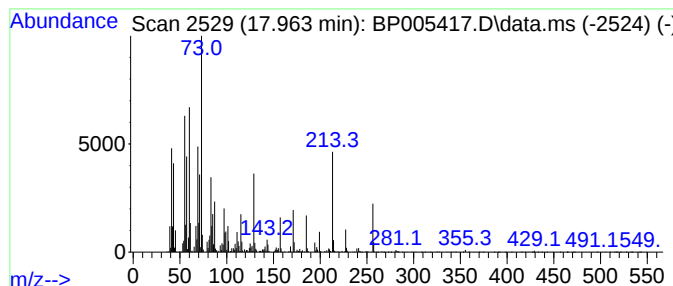
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.963	7.86 ng	171585	Phenanthrene-d10	17.057

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
2			Tridecanoic acid	214	C13H26O2	000638-53-9	86
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	46
4			n-Decanoic acid	172	C10H20O2	000334-48-5	42
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	35



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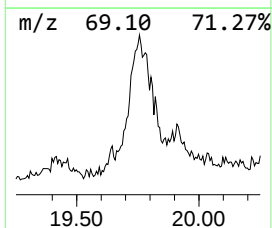
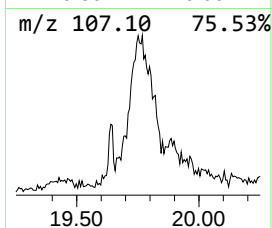
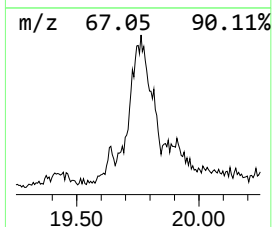
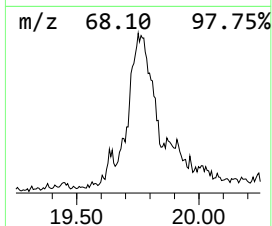
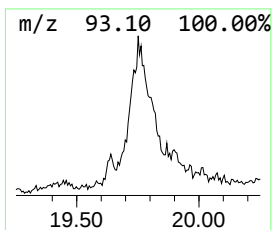
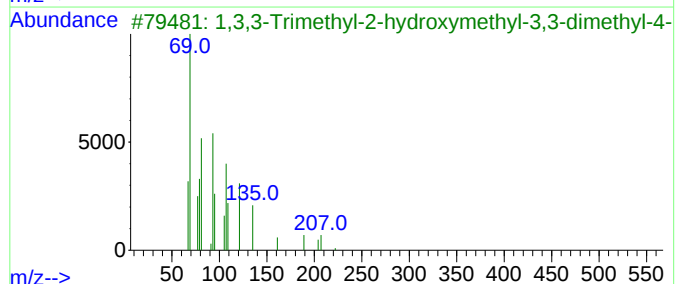
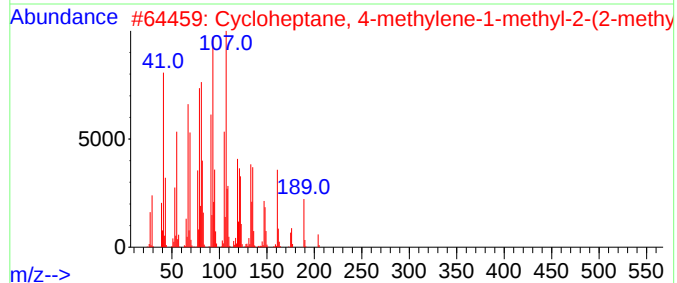
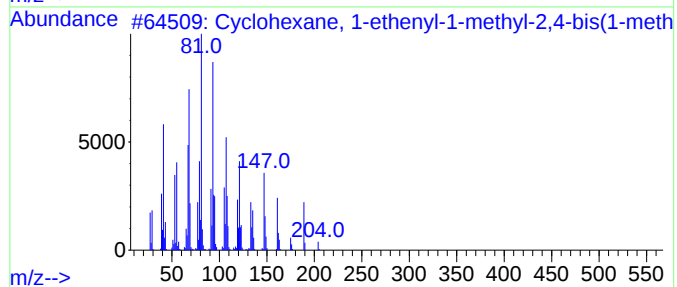
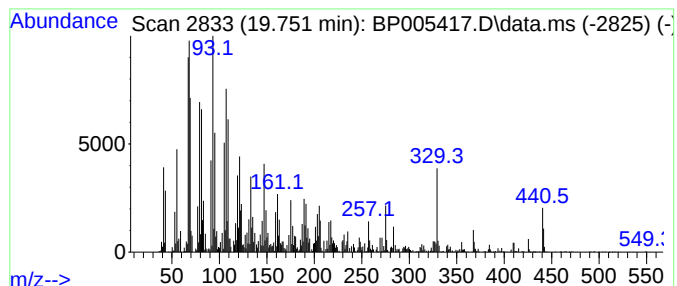
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ClientSampleId :
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Cyclohexane, 1-ethenyl-1-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.751	24.21 ng	794965	Chrysene-d12	21.163
Hit#	of 5	Tentative ID	MW MolForm	CAS# Qual
1		Cyclohexane, 1-ethenyl-1-methyl-...	204 C15H24	000515-13-9 83
2		Cycloheptane, 4-methylene-1-meth...	204 C15H24	1000159-38-5 41
3		1,3,3-Trimethyl-2-hydroxymethyl-...	222 C15H26O	1000144-10-7 38
4		6.beta.Bicyclo[4.3.0]nonane, 5.b...	332 C15H25I	1000195-85-9 35
5		Bicyclo[10.1.0]tridec-1-ene	178 C13H22	054766-91-5 27



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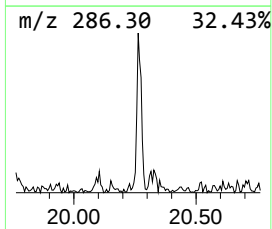
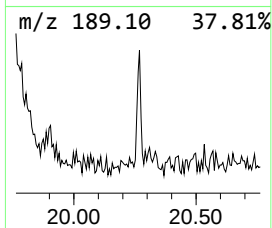
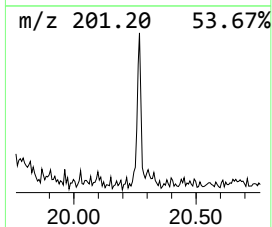
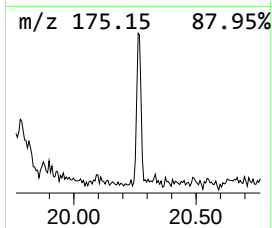
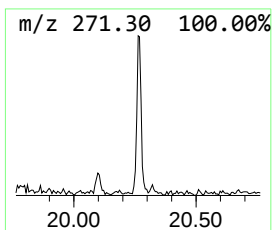
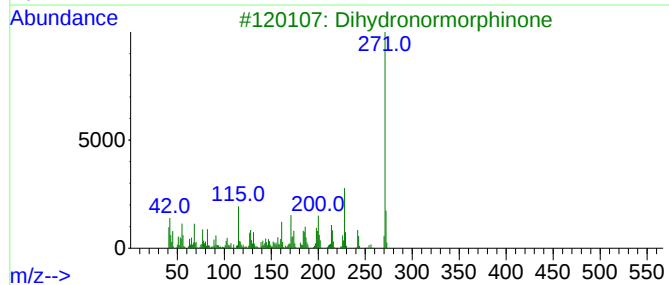
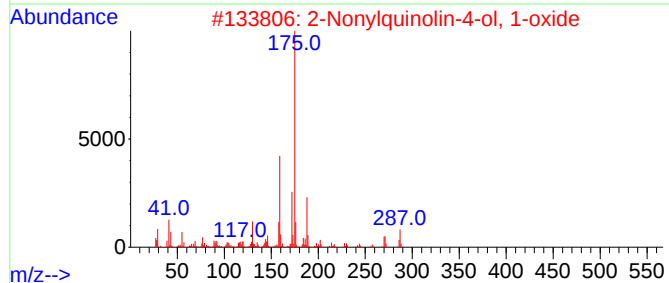
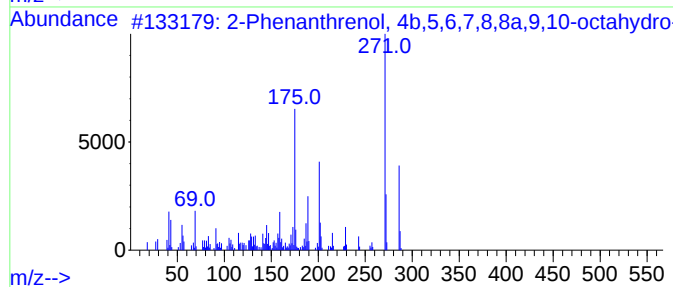
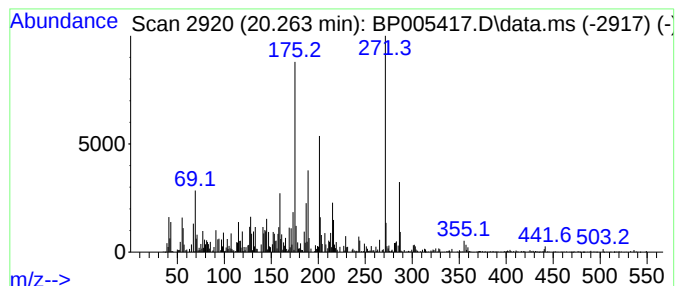
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 2-Phenanthrenol, 4b,5,6,7,8... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.263	2.22 ng	72746	Chrysene-d12	21.163

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Phenanthrenol, 4b,5,6,7,8,8a,9...	286	C20H30O	000511-15-9	87
2		2-Nonylquinolin-4-ol, 1-oxide	287	C18H25NO2	000316-66-5	38
3		Dihydronormorphine	271	C16H17NO3	014696-23-2	35
4		Pyrrrolidine, 1-[5-(1,3-benzodiox...	271	C16H17NO3	025924-78-1	35
5		2,2-Bis(4'-methoxyphenyl)-2-etho...	286	C18H22O3	1000283-53-7	27



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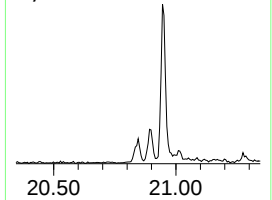
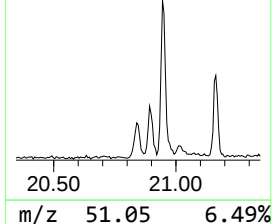
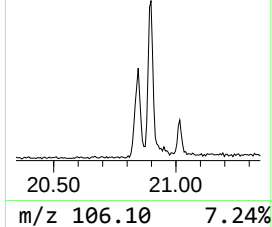
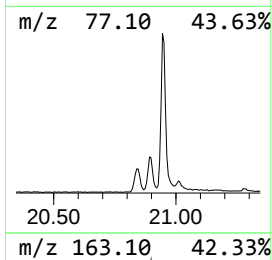
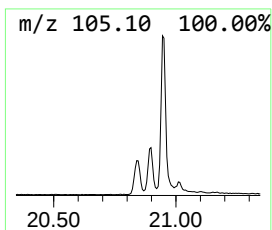
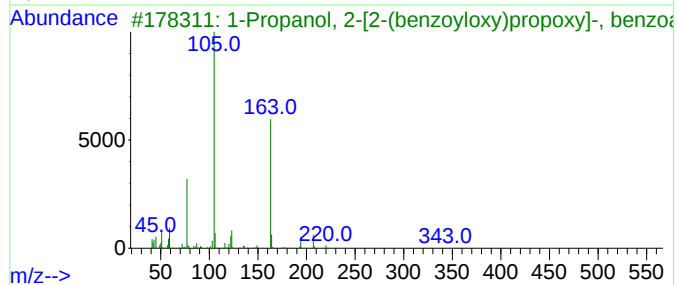
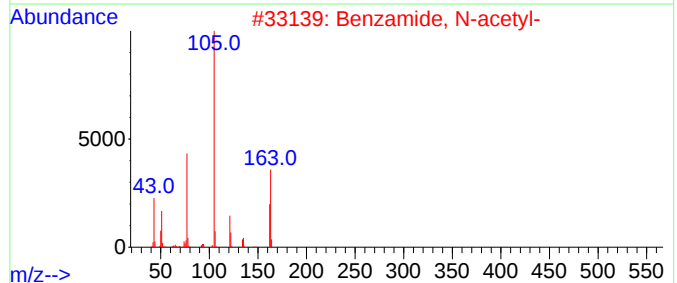
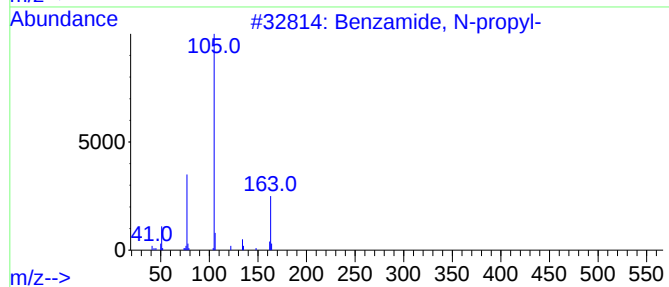
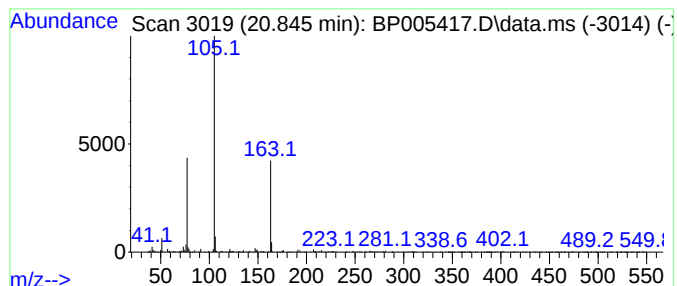
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Peak Number 5 Benzamide, N-propyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.845	3.97 ng	130184	Chrysene-d12	21.163

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzamide, N-propyl-	163	C10H13NO	010546-70-0	78
2			Benzamide, N-acetyl-	163	C9H9NO2	001575-95-7	64
3			1-Propanol, 2-[2-(benzoyloxy)pro...	342	C20H22O5	020109-39-1	56
4			Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	43
5			Biphenyl, 4,4'-dibenzoyloxy-	394	C26H18O4	1000294-15-4	37



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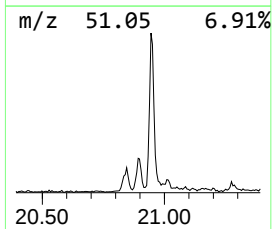
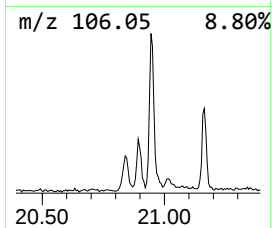
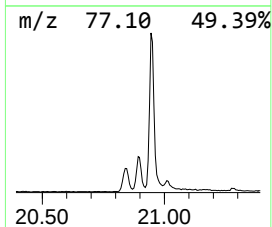
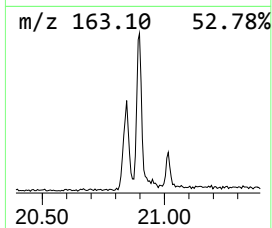
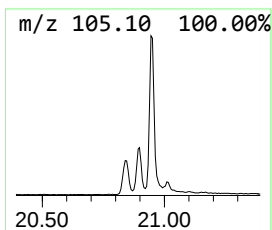
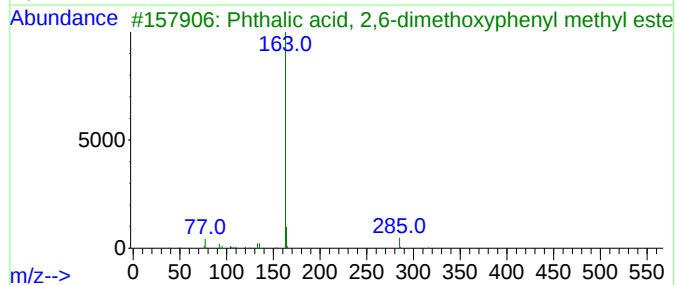
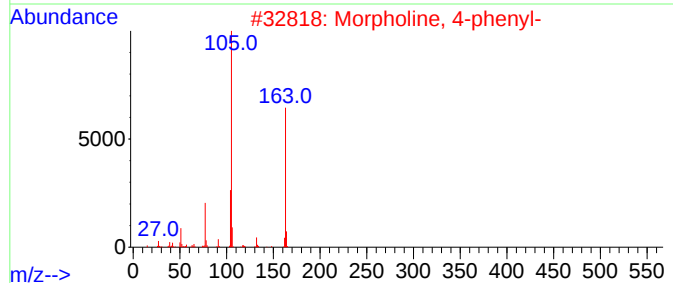
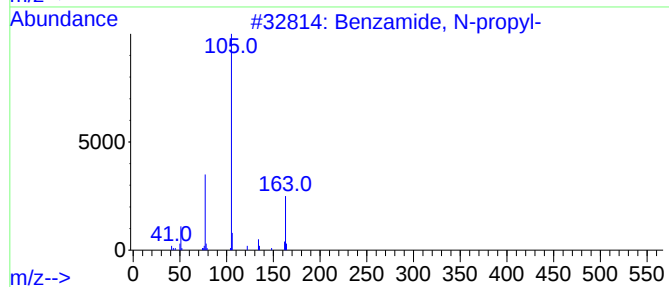
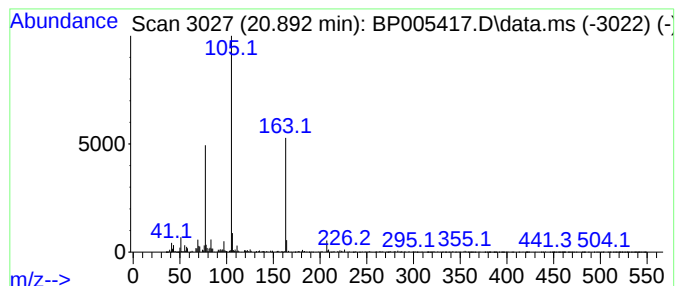
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 unknown20.892 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.892	10.23 ng	335967	Chrysene-d12	21.163

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzamide, N-propyl-	163	C10H13NO	010546-70-0	72
2			Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	47
3			Phthalic acid, 2,6-dimethoxyphen...	316	C17H16O6	1000315-74-1	40
4			2-Pyrrolidinone, 3-hydroxy-4-met...	191	C11H13NO2	104194-17-4	40
5			Biphenyl, 4,4'-dibenzoyloxy-	394	C26H18O4	1000294-15-4	32



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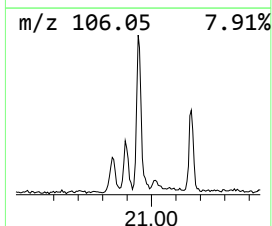
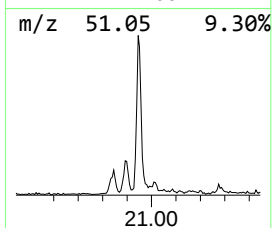
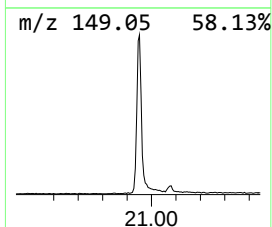
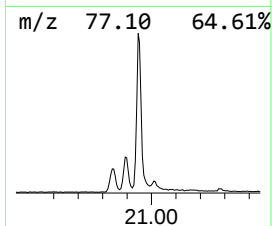
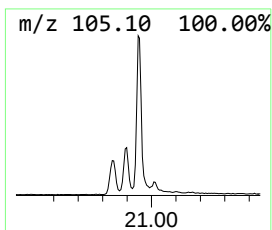
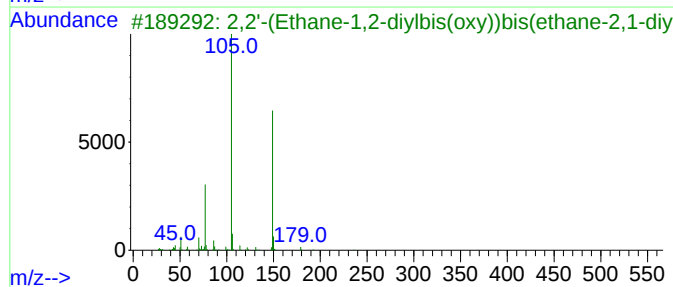
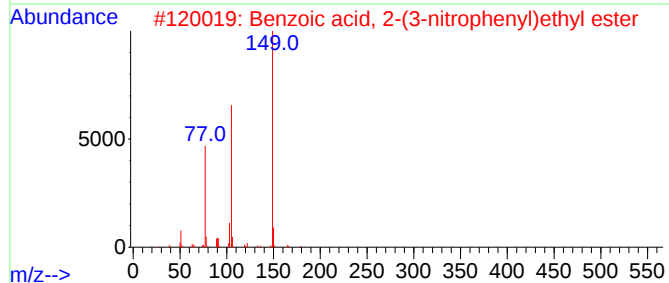
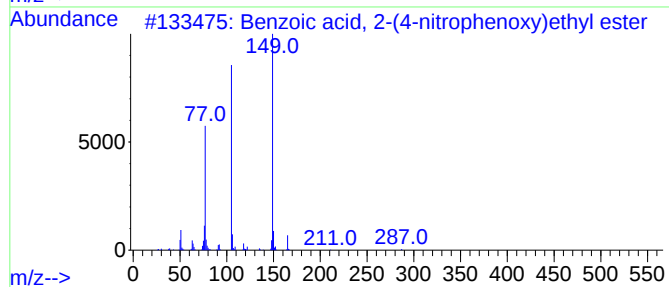
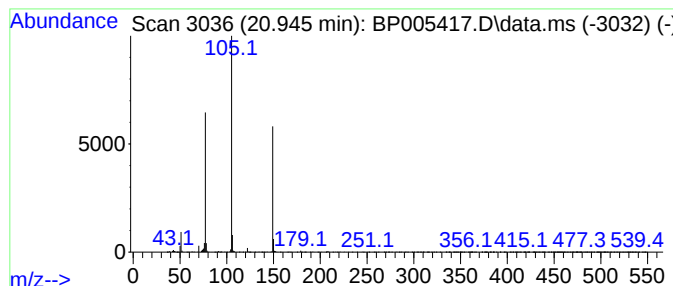
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP042921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Benzoic acid, 2-(4-nitrophe... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.945	18.22 ng	598103	Chrysene-d12	21.163

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid, 2-(4-nitrophenoxy)...	287	C15H13NO5	1000368-92-7	78
2			Benzoic acid, 2-(3-nitrophenyl)e...	271	C15H13NO4	1000368-22-4	64
3			2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	64
4			1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	64
5			3-Benzoylamino-2-benzyl-butyr...	311	C19H21NO3	1000193-12-7	56



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042921\
Data File : BP005417.D
Acq On : 29 Apr 2021 19:31
Operator : CG/JU
Sample : M2196-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
WALL-D-4075-B

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Hexadecanoic ...	17.963	7.9	ng	171585	4	17.057	436644	20.0
Cyclohexane, 1-...	19.751	24.2	ng	794965	5	21.163	656646	20.0
2-Phenanthrenol...	20.263	2.2	ng	72746	5	21.163	656646	20.0
Benzamide, N-pr...	20.845	4.0	ng	130184	5	21.163	656646	20.0
unknown20.892	20.892	10.2	ng	335967	5	21.163	656646	20.0
Benzoic acid, 2...	20.945	18.2	ng	598103	5	21.163	656646	20.0