

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP043021\
 Data File : BP005429.D
 Acq On : 30 Apr 2021 12:23
 Operator : CG/JU
 Sample : M2217-19
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 HTRCV2-GRAB-TS01-01

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: BP005429.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	376	rBV	402449	559749	1.57%	1.017%
2	6.817	625	634	645	rBV	363317	570107	1.60%	1.036%
3	8.787	961	969	976	rBV	228462	362654	1.02%	0.659%
4	12.899	1662	1668	1676	rBV	650159	946019	2.66%	1.719%
5	15.793	2155	2160	2169	rVB	711537	1007680	2.83%	1.831%
6	17.057	2369	2375	2379	rBV	345224	474555	1.33%	0.862%
7	17.969	2524	2530	2536	rBV	742520	1001475	2.82%	1.820%
8	18.028	2536	2540	2545	rBV	308821	420007	1.18%	0.763%
9	18.239	2564	2576	2581	rBV2	201834	569379	1.60%	1.035%
10	18.345	2587	2594	2605	rVB	336790	958826	2.70%	1.742%
11	19.086	2713	2720	2733	rBV	468035	767185	2.16%	1.394%
12	19.204	2736	2740	2750	rVB	400118	539373	1.52%	0.980%
13	19.410	2770	2775	2777	rBV	457766	611061	1.72%	1.110%
14	19.439	2777	2780	2789	rVB	524298	709207	1.99%	1.289%
15	19.657	2806	2817	2820	rBV	27155657	35559137	100.00%	64.608%
16	20.316	2925	2929	2935	rBV	852640	1019624	2.87%	1.853%
17	20.380	2936	2940	2944	rBV	451408	511023	1.44%	0.928%
18	20.839	3013	3018	3022	rBV	311452	485236	1.36%	0.882%
19	20.892	3022	3027	3032	rVB2	354827	682524	1.92%	1.240%
20	20.945	3032	3036	3042	rBV	1026834	1221425	3.43%	2.219%
21	21.075	3054	3058	3064	rBV	897665	951649	2.68%	1.729%
22	21.151	3066	3071	3076	rVV2	1174142	2172394	6.11%	3.947%
23	21.198	3076	3079	3089	rVB	957143	1267410	3.56%	2.303%
24	22.733	3333	3340	3343	rBV2	179867	422154	1.19%	0.767%
25	22.774	3343	3347	3353	rVB2	264844	476626	1.34%	0.866%
26	23.416	3450	3456	3465	rVB2	415913	771857	2.17%	1.402%

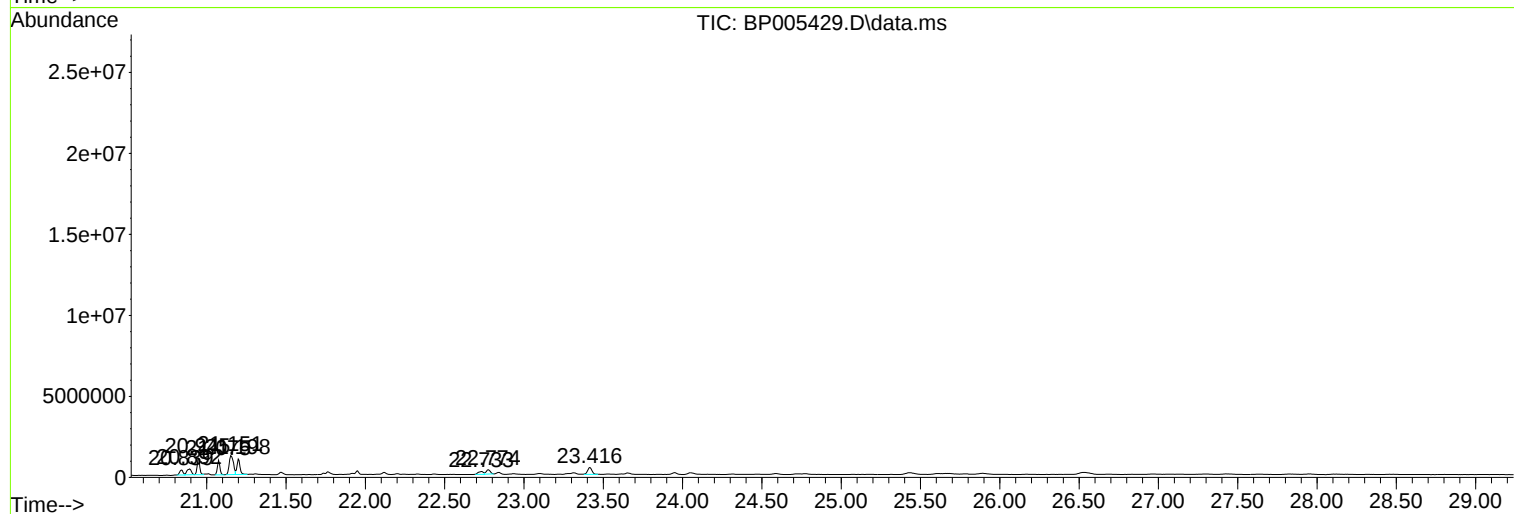
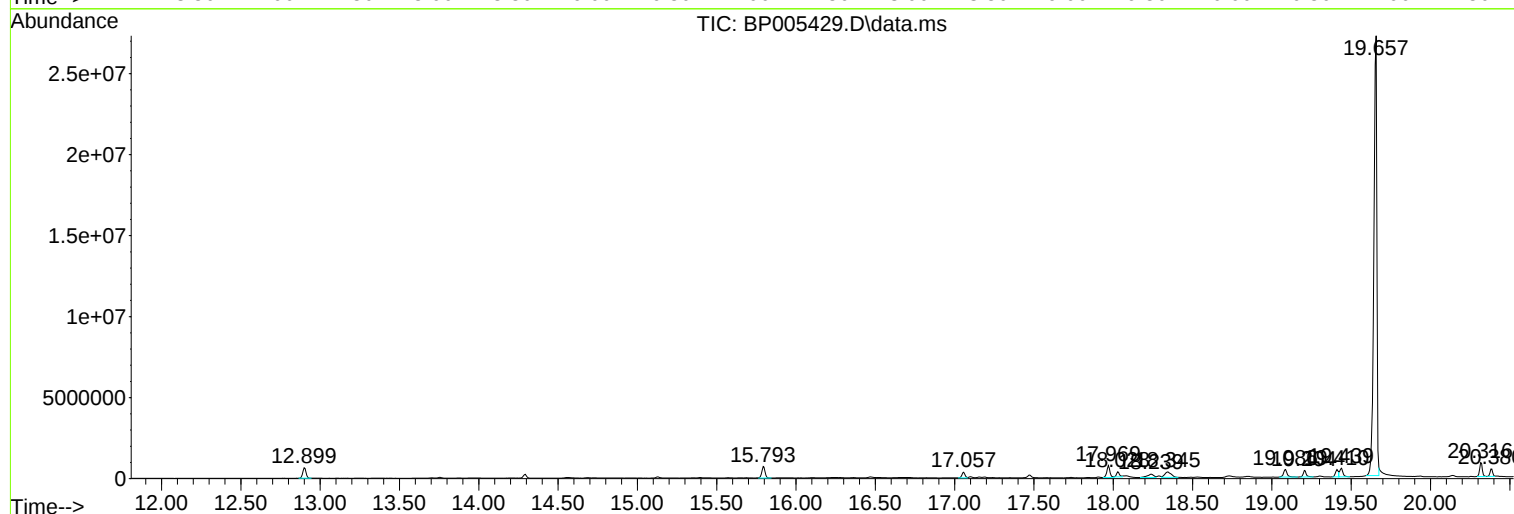
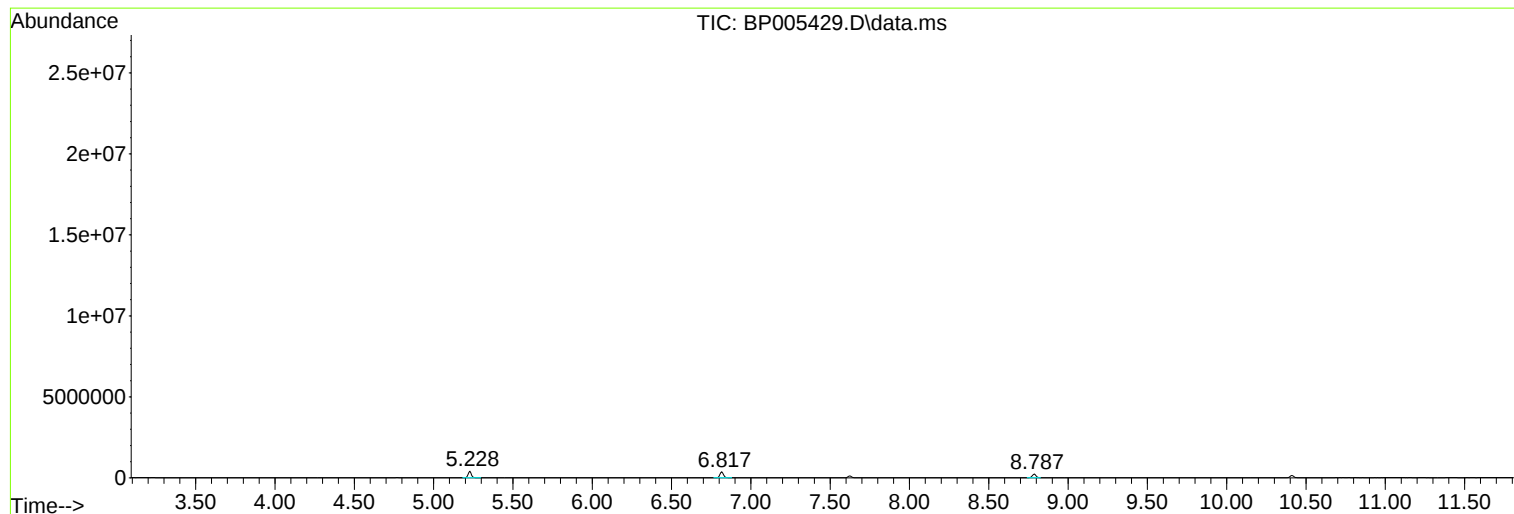
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ClientSampleId :
HTCRV2-GRAB-TS01-01

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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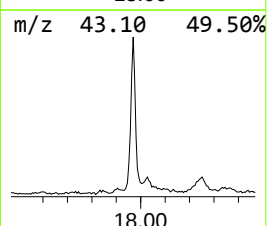
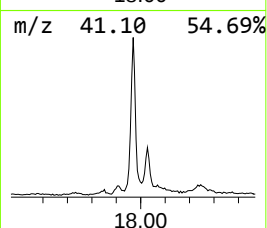
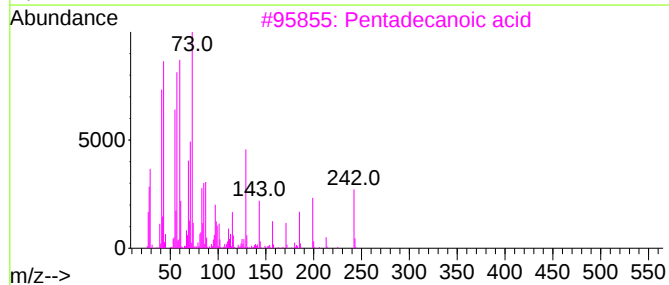
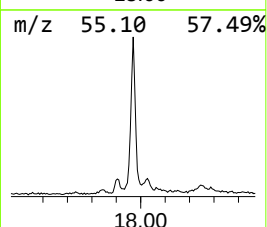
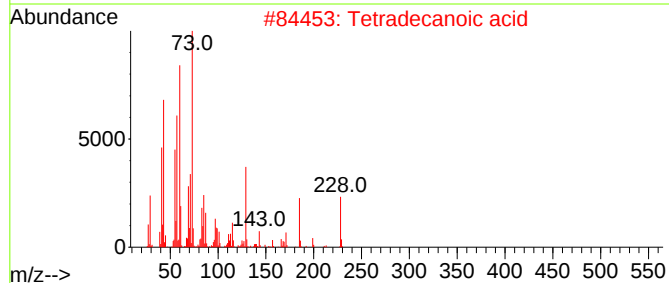
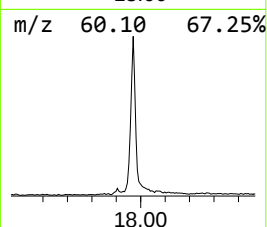
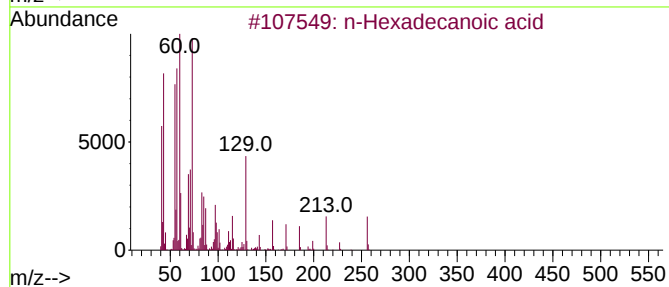
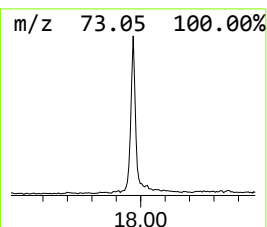
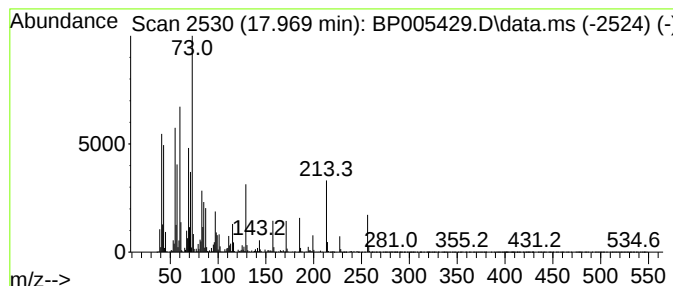
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.969	42.21 ng	1001480	Phenanthrene-d10	17.057

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	76
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	70
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	68
4			Tridecanoic acid	214	C13H26O2	000638-53-9	60
5			Undecanoic acid	186	C11H22O2	000112-37-8	40



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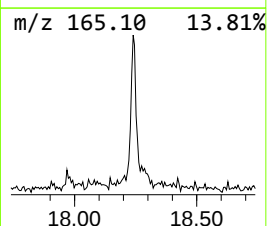
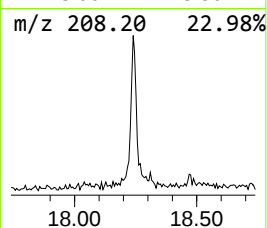
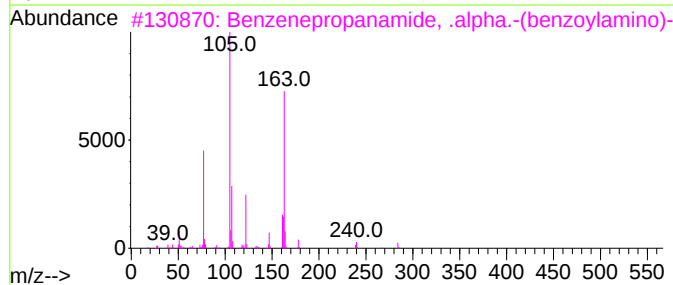
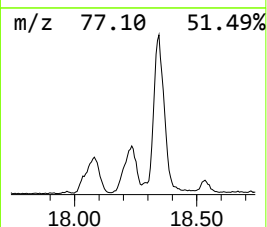
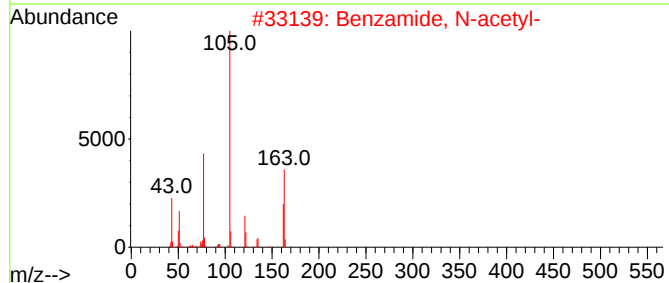
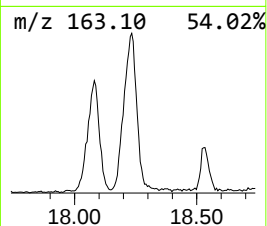
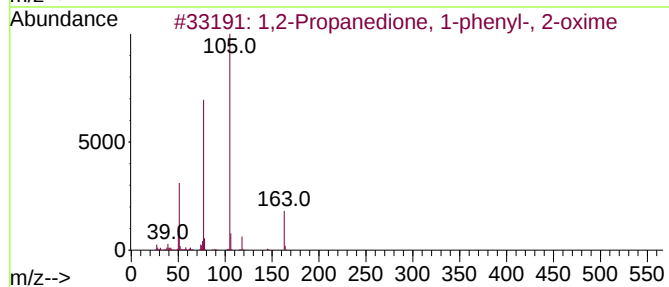
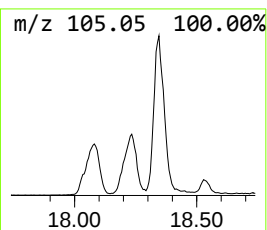
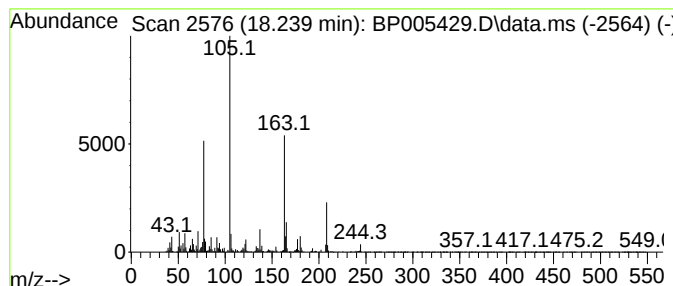
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown18.23 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.239	24.00 ng	569379	Phenanthrene-d10	17.057

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1,2-Propanedione, 1-phenyl-, 2-o...	163	C9H9NO2	000119-51-7	47
2		Benzamide, N-acetyl-	163	C9H9NO2	001575-95-7	47
3		Benzenepropanamide, .alpha.-(ben...	284	C16H16N2O3	058690-81-6	38
4		Ethanone, 2-(2-methylpropoxy)-1,...	268	C18H20O2	022499-12-3	38
5		2-Propen-1-one, 1,2-diphenyl-	208	C15H12O	004452-11-3	38



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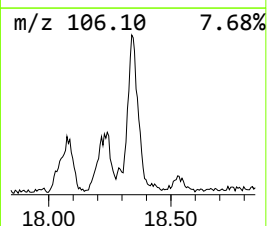
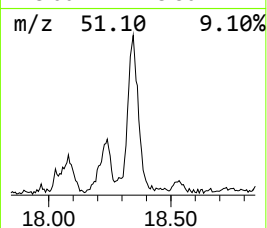
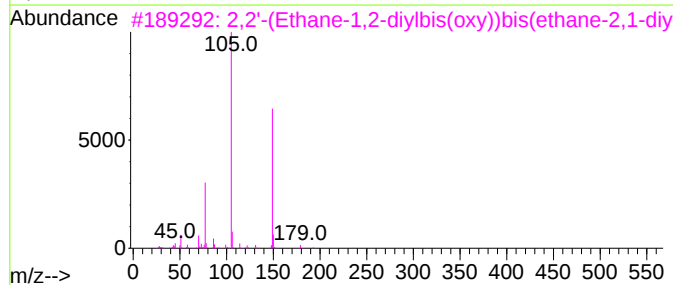
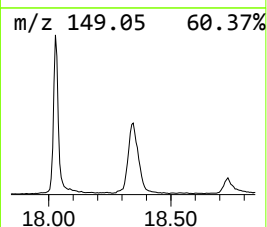
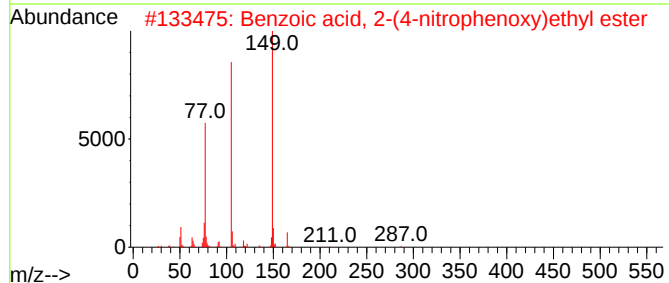
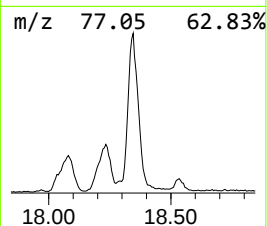
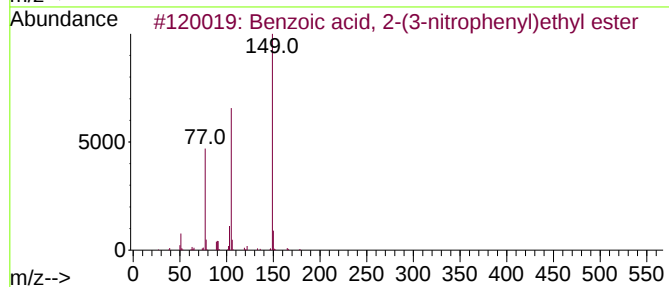
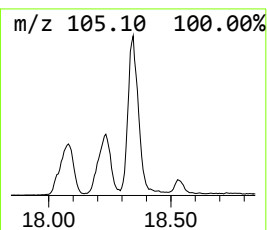
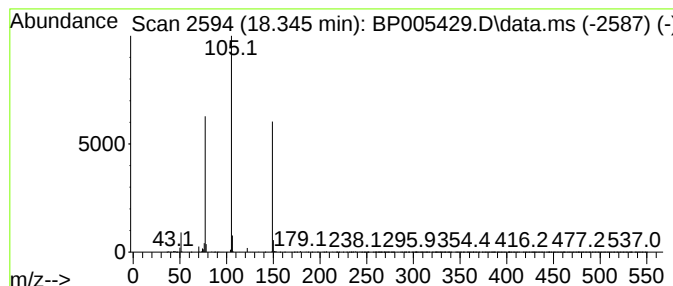
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.345	40.41 ng	958826	Phenanthrene-d10	17.057

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid, 2-(3-nitrophenyl)e...	271	C15H13NO4	1000368-22-4	78
2			Benzoic acid, 2-(4-nitrophenoxy)...	287	C15H13NO5	1000368-92-7	64
3			2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	56
4			Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	56
5			3-Benzoylamino-2-benzyl-butyric ...	311	C19H21NO3	1000193-12-7	56



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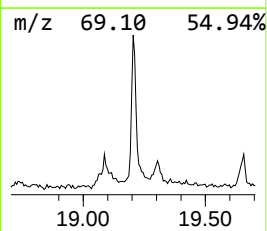
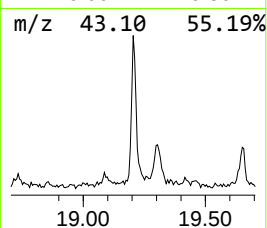
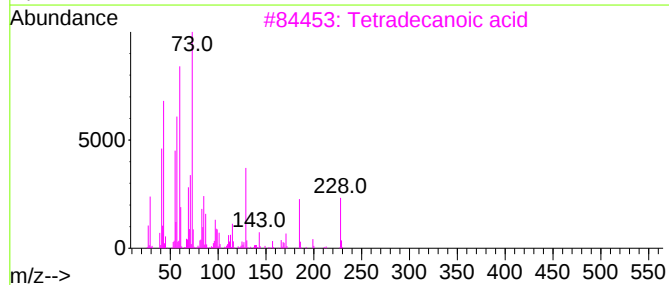
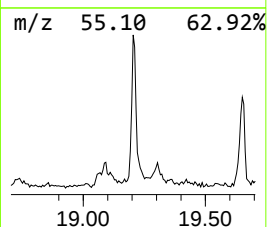
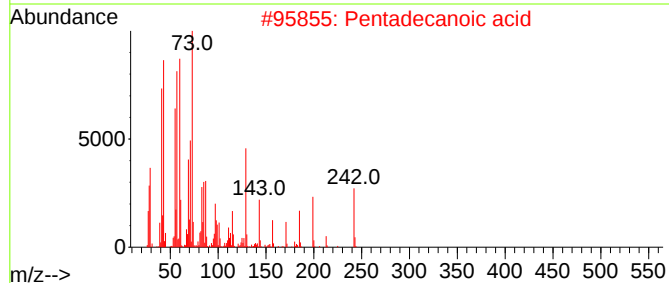
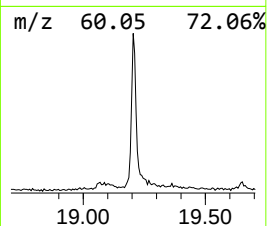
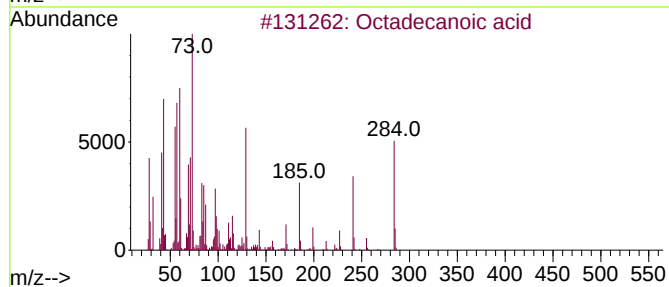
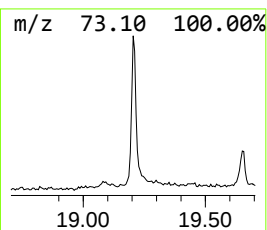
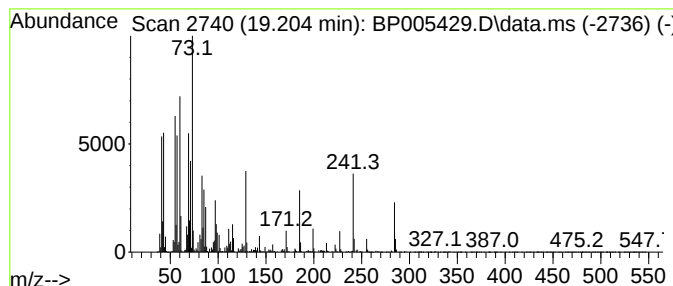
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Peak Number 4 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.204	4.97 ng	539373	Chrysene-d12	21.163

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	68
4			n-Decanoic acid	172	C10H20O2	000334-48-5	60
5			n-Decyl .alpha.-d-2-deoxyglucoside	304	C16H32O5	1000211-42-8	55



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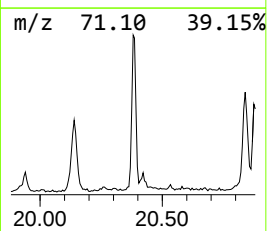
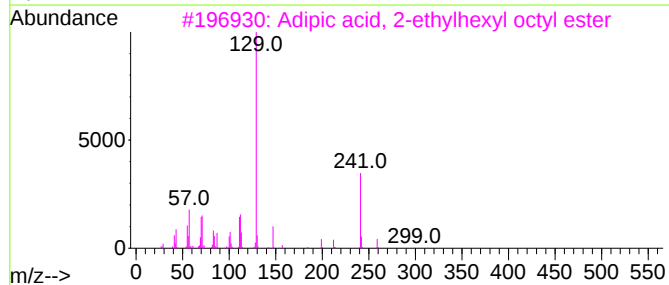
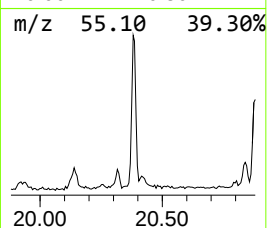
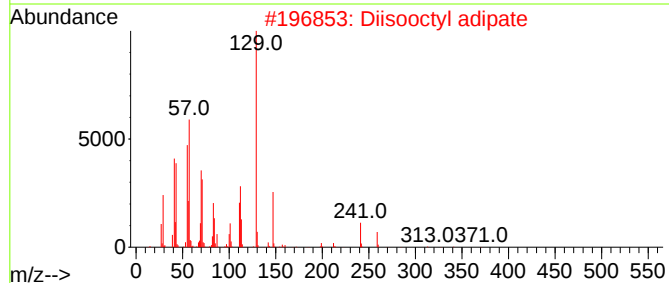
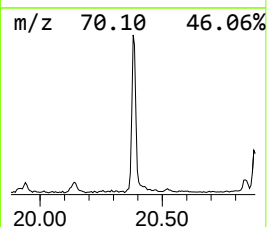
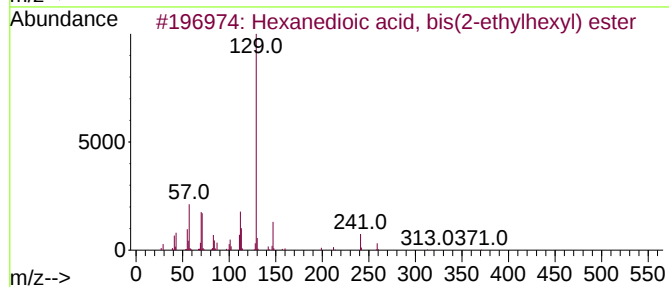
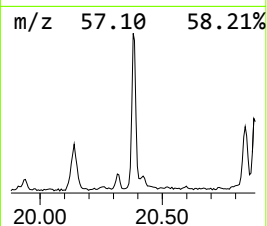
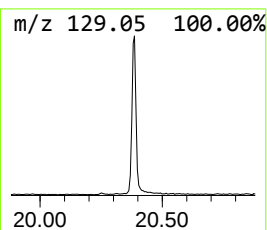
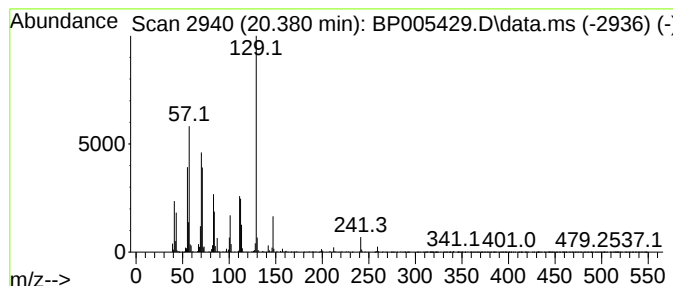
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Hexanedioic acid, bis(2-eth... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
20.381	4.70 ng	511023	Chrysene-d12	21.163	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	80
2	Diisooctyl adipate	370	C22H42O4	001330-86-5	72
3	Adipic acid, 2-ethylhexyl octyl ...	370	C22H42O4	1000324-48-6	59
4	Adipic acid, 2-pentyl octyl ester	328	C19H36O4	1000324-16-2	53
5	Hexanedioic acid, dioctyl ester	370	C22H42O4	000123-79-5	53



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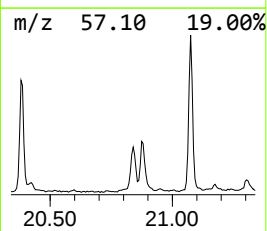
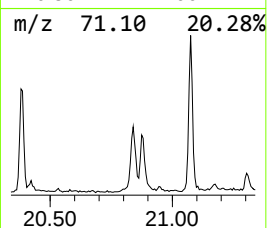
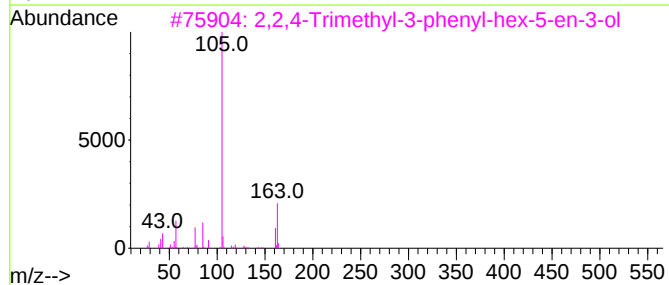
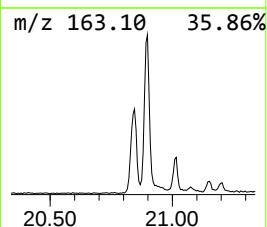
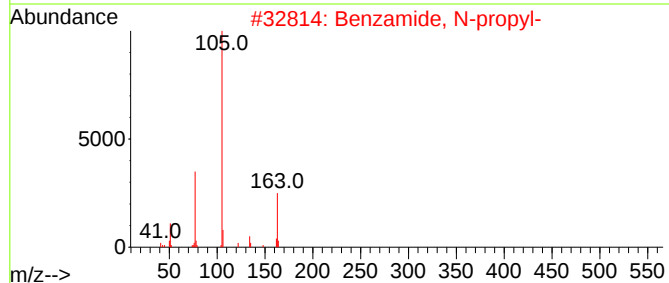
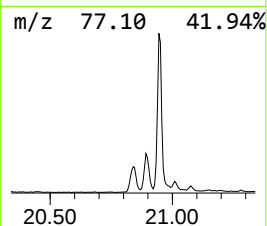
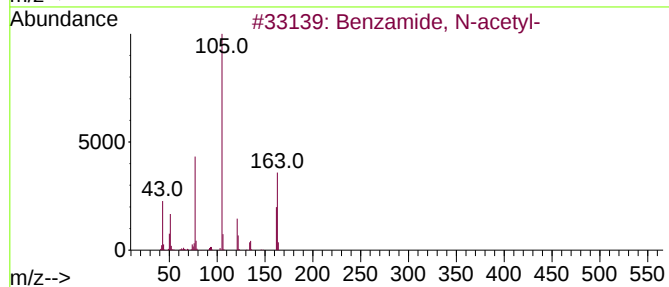
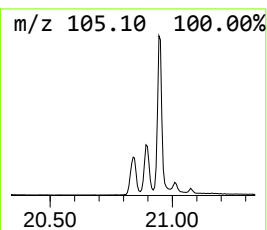
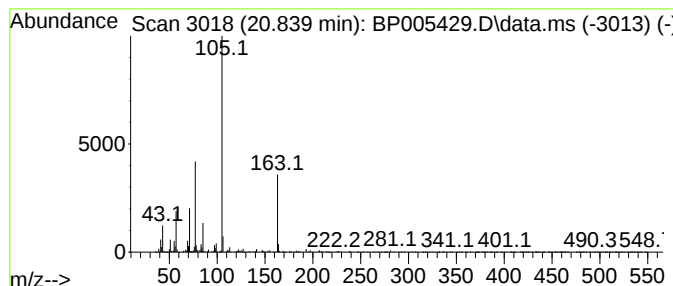
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP042921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Benzamide, N-acetyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.839	4.47 ng	485236	Chrysene-d12	21.163

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzamide, N-acetyl-	163	C9H9NO2	001575-95-7	50
2			Benzamide, N-propyl-	163	C10H13NO	010546-70-0	47
3			2,2,4-Trimethyl-3-phenyl-hex-5-e...	218	C15H22O	066534-36-9	43
4			Ethanone, 2-(2-methylpropoxy)-1,...	268	C18H20O2	022499-12-3	42
5			Vinyl benzoate	148	C9H8O2	000769-78-8	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP043021\
Data File : BP005429.D
Acq On : 30 Apr 2021 12:23
Operator : CG/JU
Sample : M2217-19
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
HTCRV2-GRAB-TS01-01

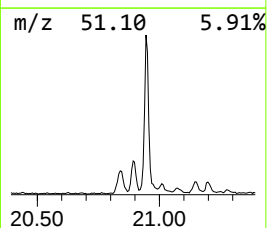
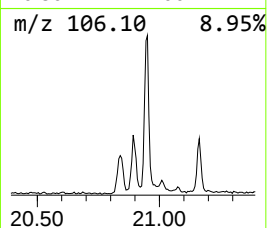
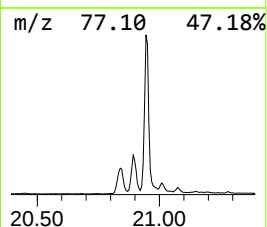
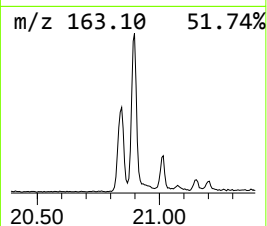
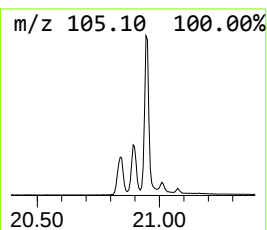
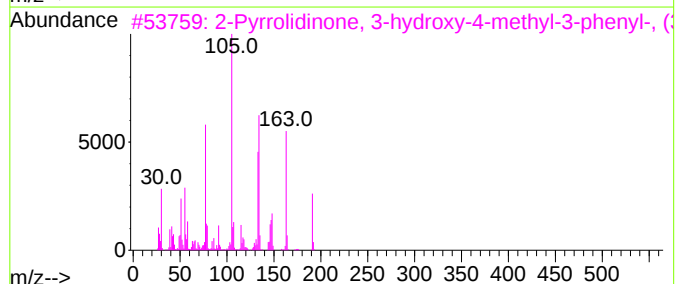
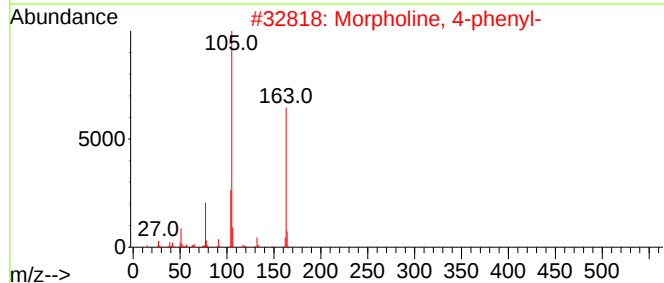
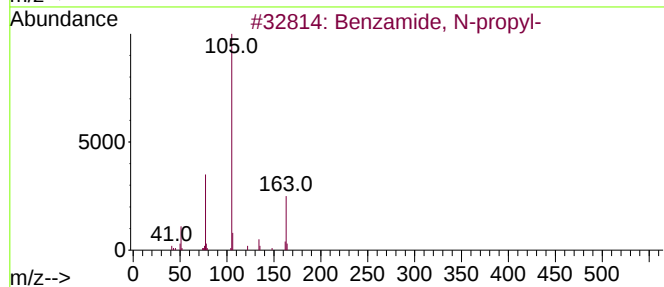
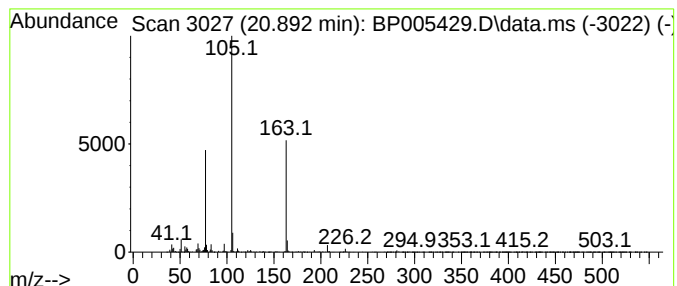
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP042921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Benzamide, N-propyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.892	6.28 ng	682524	Chrysene-d12	21.163

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzamide, N-propyl-	163	C10H13NO	010546-70-0	56
2			Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	47
3			2-Pyrrolidinone, 3-hydroxy-4-met...	191	C11H13NO2	104194-17-4	40
4			Benzenepropanamide, .alpha.-(ben...	284	C16H16N2O3	058690-81-6	40
5			Phthalic acid, 4-chloro-3-methyl...	304	C16H13ClO4	1000315-71-2	33



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP043021\
Data File : BP005429.D
Acq On : 30 Apr 2021 12:23
Operator : CG/JU
Sample : M2217-19
Misc :
ALS Vial : 5 Sample Multiplier: 1

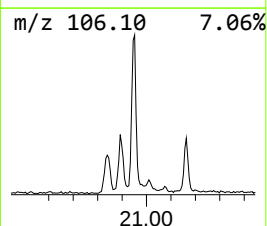
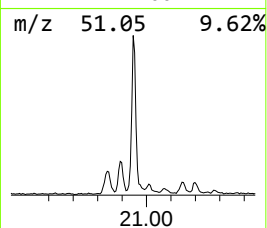
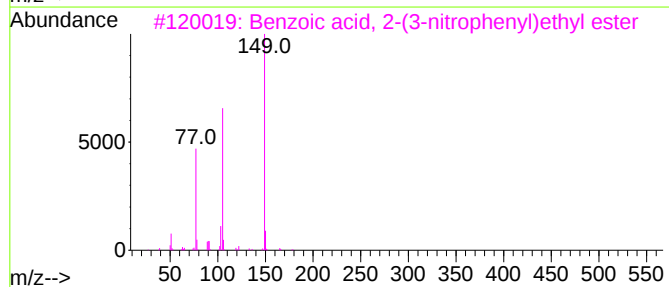
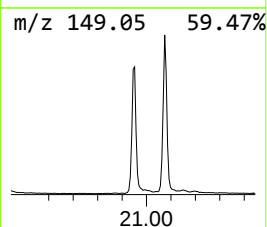
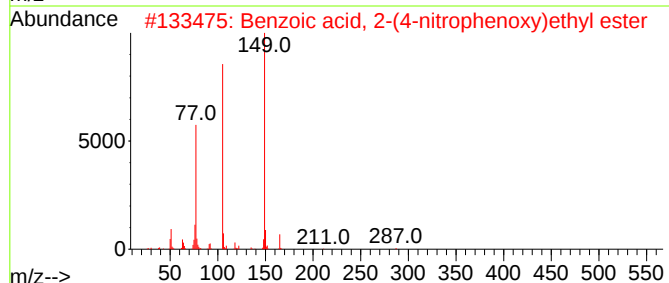
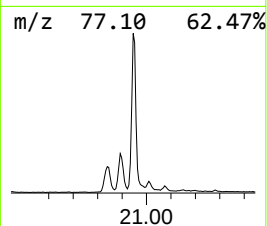
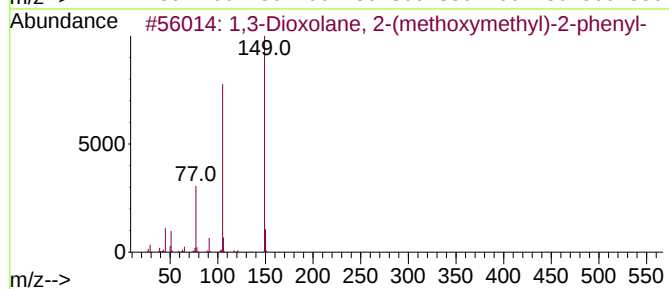
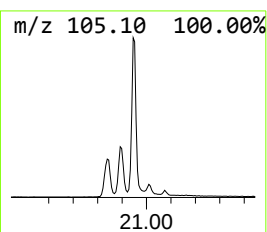
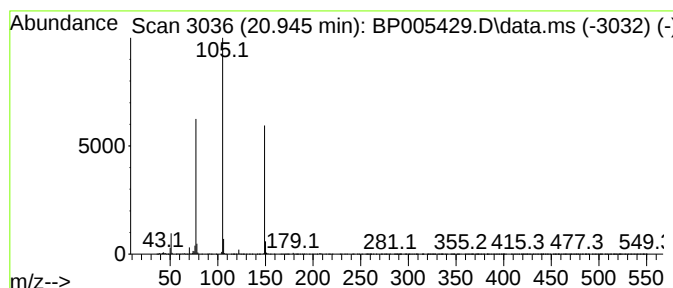
Instrument :
BNA_P
ClientSampleId :
HTCRV2-GRAB-TS01-01

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 8 1,3-Dioxolane, 2-(methoxyme... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
20.945	11.24 ng	1221430	Chrysene-d12	21.163	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	64
2	Benzoic acid, 2-(4-nitrophenoxy)...	287	C15H13NO5	1000368-92-7	64
3	Benzoic acid, 2-(3-nitrophenyl)e...	271	C15H13NO4	1000368-22-4	56
4	3-Benzoylamino-2-benzyl-butyric ...	311	C19H21NO3	1000193-12-7	56
5	2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	56



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP043021\
Data File : BP005429.D
Acq On : 30 Apr 2021 12:23
Operator : CG/JU
Sample : M2217-19
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
HTCRV2-GRAB-TS01-01

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 ...	17.969	42.2	ng	1001480	4	17.057	474555	20.0
unknown18.23	18.239	24.0	ng	569379	4	17.057	474555	20.0
Benzoic acid, 2...	18.345	40.4	ng	958826	4	17.057	474555	20.0
Octadecanoic acid	19.204	5.0	ng	539373	5	21.163	2172390	20.0
Hexanedioic aci...	20.381	4.7	ng	511023	5	21.163	2172390	20.0
Benzamide, N-ac...	20.839	4.5	ng	485236	5	21.163	2172390	20.0
Benzamide, N-pr...	20.892	6.3	ng	682524	5	21.163	2172390	20.0
1,3-Dioxolane, ...	20.945	11.2	ng	1221430	5	21.163	2172390	20.0