

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP041221\
 Data File : BP005263.D
 Acq On : 12 Apr 2021 13:24
 Operator : CG/JU
 Sample : M1946-02
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 FS-SB10X

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-BP040921.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP005263.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.281	368	373	380	rVB	416437	591800	29.50%	4.617%
2	6.869	637	643	654	rVB	202683	332603	16.58%	2.595%
3	7.681	775	781	787	rVB	125306	190697	9.51%	1.488%
4	8.846	972	979	992	rVB	480650	758938	37.83%	5.921%
5	10.475	1248	1256	1262	rBV	138418	226200	11.28%	1.765%
6	12.963	1671	1679	1687	rBV	955417	1369239	68.25%	10.682%
7	13.810	1817	1823	1832	rBV	34798	49978	2.49%	0.390%
8	14.345	1908	1914	1920	rBV2	196500	287470	14.33%	2.243%
9	14.410	1920	1925	1934	rVB	40119	57921	2.89%	0.452%
10	15.169	2041	2054	2059	rBV	25983	52204	2.60%	0.407%
11	15.728	2139	2149	2158	rVB10	10846	28743	1.43%	0.224%
12	15.851	2158	2170	2179	rBV	830746	1142249	56.94%	8.911%
13	17.110	2378	2384	2390	rBV	250654	353585	17.63%	2.758%
14	18.016	2533	2538	2545	rBV	211798	314622	15.68%	2.454%
15	18.080	2545	2549	2554	rVB	34372	51469	2.57%	0.402%
16	19.033	2707	2711	2714	rBV	26230	27766	1.38%	0.217%
17	19.133	2722	2728	2735	rBV	39933	66757	3.33%	0.521%
18	19.257	2742	2749	2758	rBV2	115057	184731	9.21%	1.441%
19	19.486	2785	2788	2793	rVB	22097	28819	1.44%	0.225%
20	19.692	2817	2823	2828	rBV	1693885	2006148	100.00%	15.650%
21	20.169	2901	2904	2908	rBV2	29151	31912	1.59%	0.249%
22	20.369	2936	2938	2942	rVB2	25371	21125	1.05%	0.165%
23	20.433	2946	2949	2952	rVB	28926	28559	1.42%	0.223%
24	20.892	3021	3027	3031	rBV	406534	671389	33.47%	5.238%
25	20.945	3031	3036	3041	rVV	630992	1002872	49.99%	7.824%
26	20.998	3041	3045	3052	rVV	1611970	1774308	88.44%	13.842%
27	21.063	3053	3056	3063	rVB	104653	119381	5.95%	0.931%
28	21.121	3064	3066	3073	rVB	39291	45809	2.28%	0.357%
29	21.210	3076	3081	3085	rBV	381375	488820	24.37%	3.813%
30	21.333	3099	3102	3112	rVB2	44115	76371	3.81%	0.596%
31	23.492	3462	3469	3475	rVB	231832	436174	21.74%	3.403%

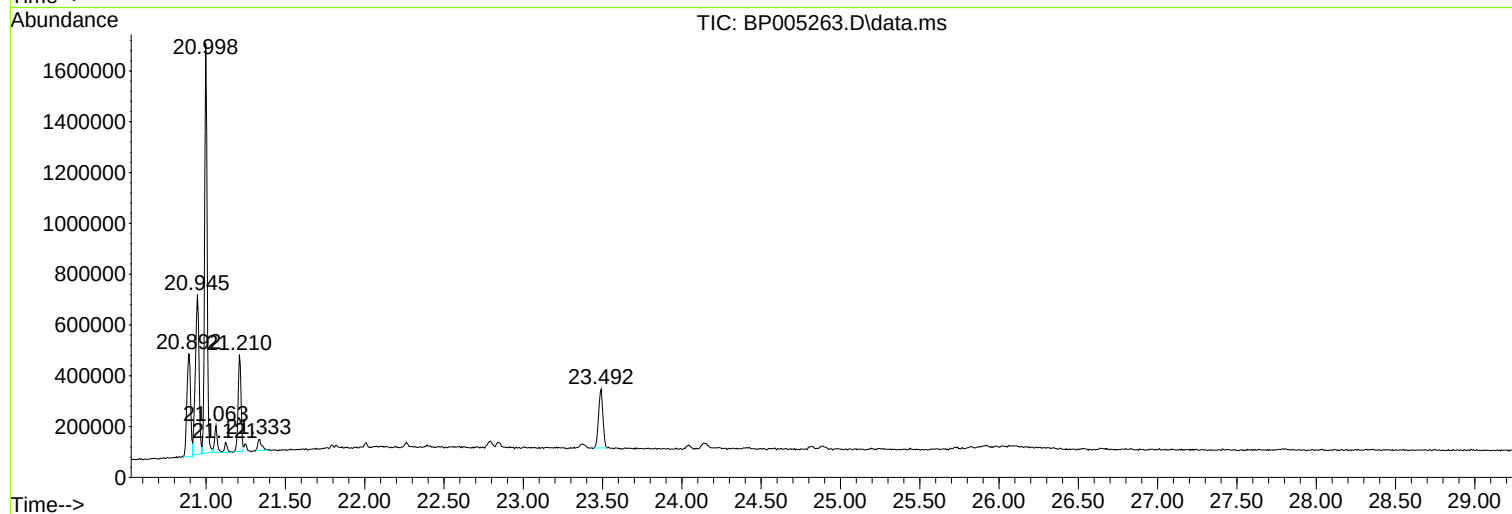
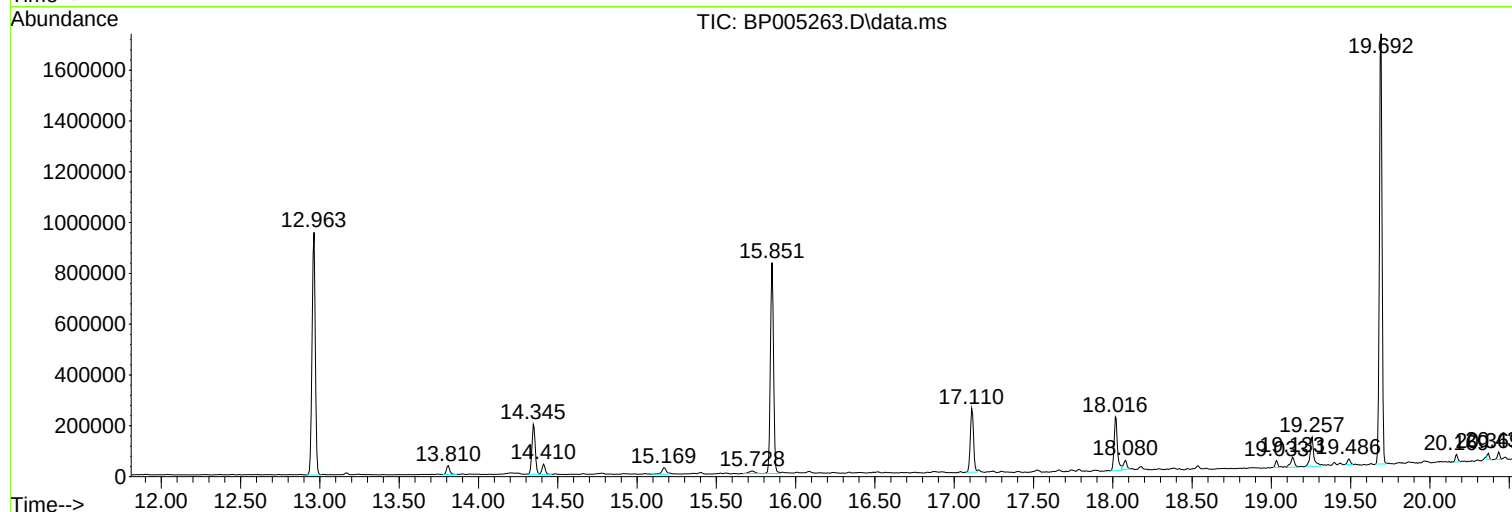
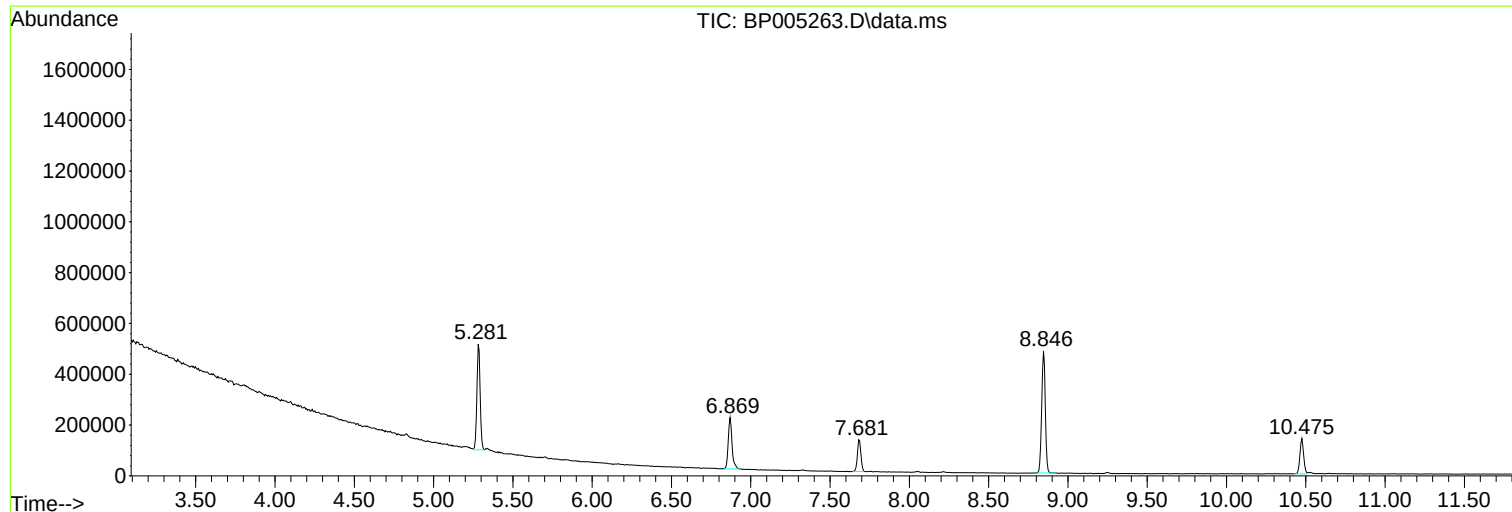
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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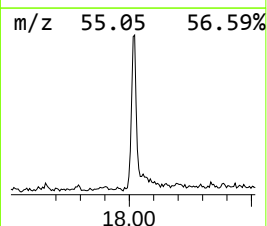
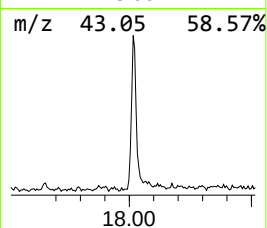
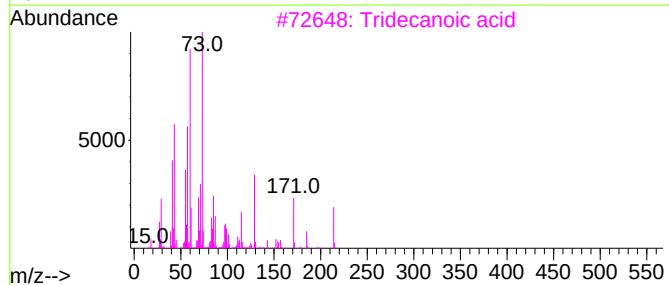
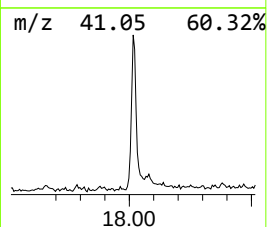
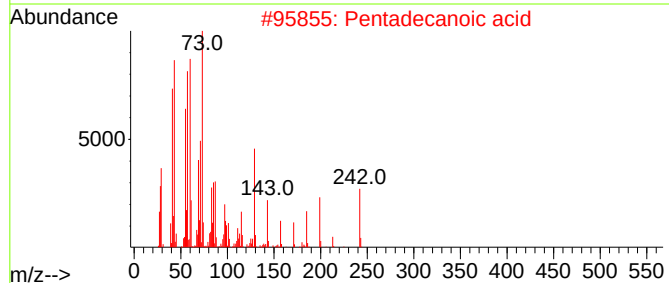
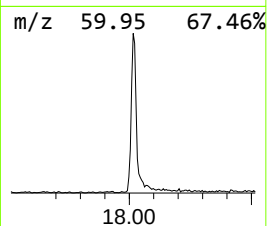
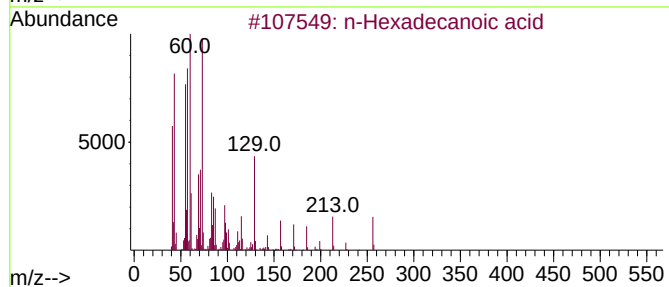
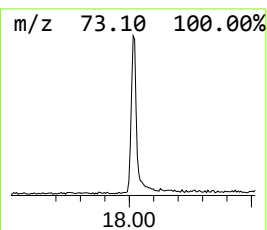
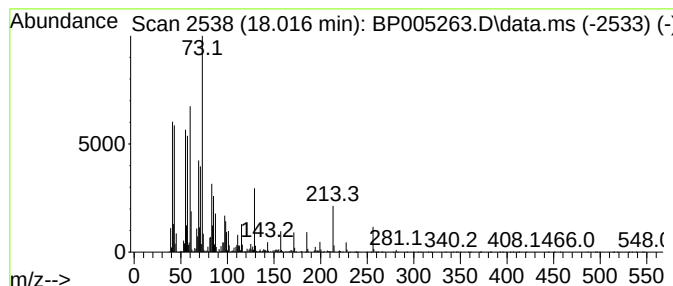
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
18.016	17.80 ng	314622	Phenanthrene-d10	17.110

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	64
3		Tridecanoic acid	214	C13H26O2	000638-53-9	52
4		Undecanoic acid	186	C11H22O2	000112-37-8	43
5		Undecane, 2-methyl-	170	C12H26	007045-71-8	20



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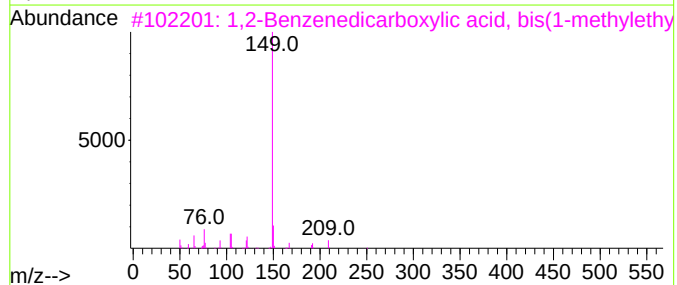
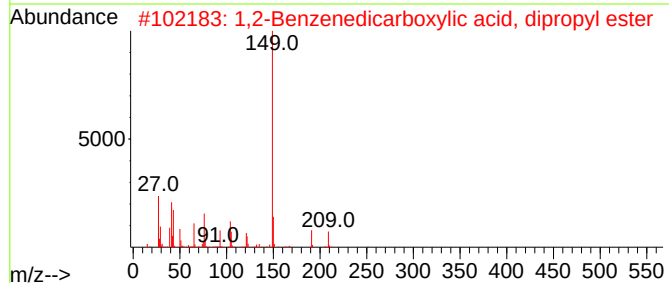
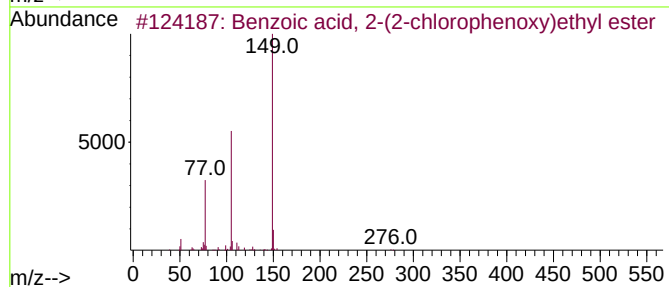
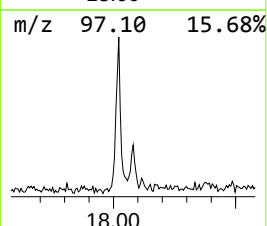
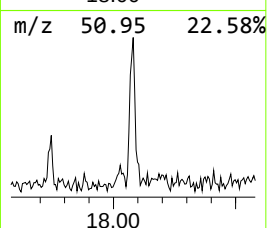
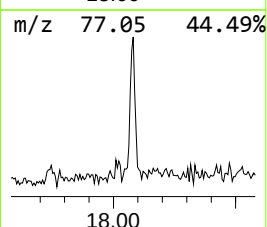
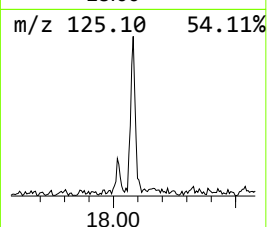
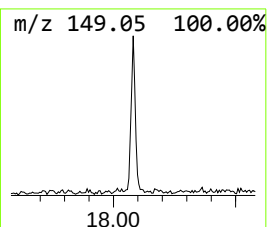
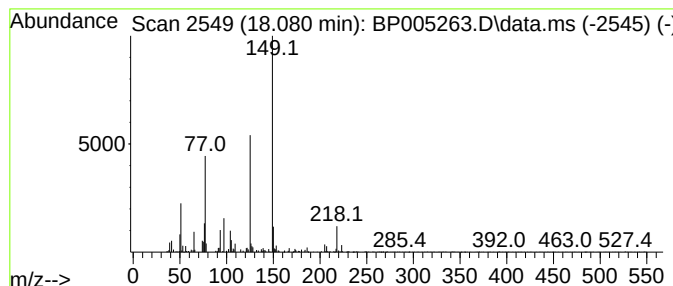
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown18.08 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.080	2.91 ng	51469	Phenanthrene-d10	17.110

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid, 2-(2-chlorophenoxy...	276	C15H13ClO3	1000368-25-9	47
2			1,2-Benzenedicarboxylic acid, di...	250	C14H18O4	000131-16-8	46
3			1,2-Benzenedicarboxylic acid, bi...	250	C14H18O4	000605-45-8	43
4			Benzoic acid, 2-(1-oxopropyl)-	178	C10H10O3	002360-45-4	43
5			Phthalic acid, cyclohexylmethyl ...	318	C19H26O4	1000309-08-6	38



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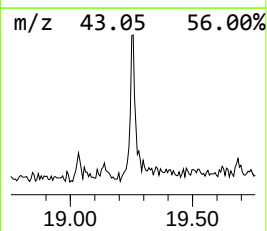
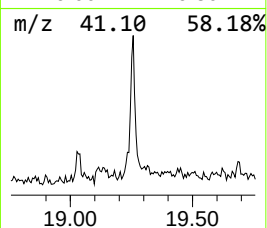
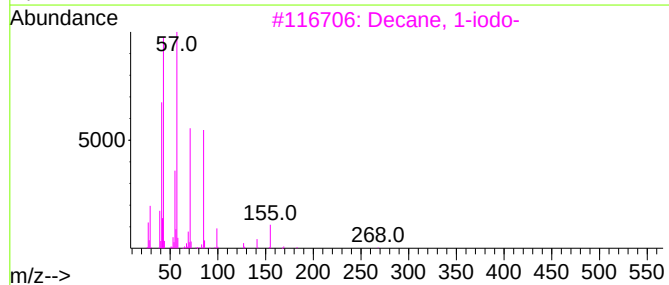
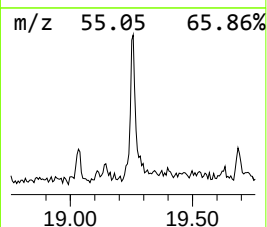
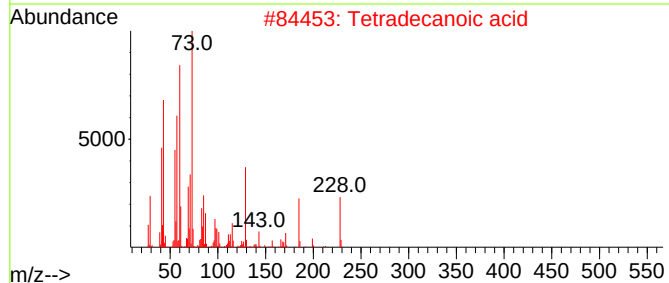
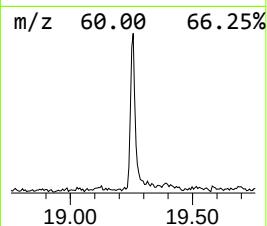
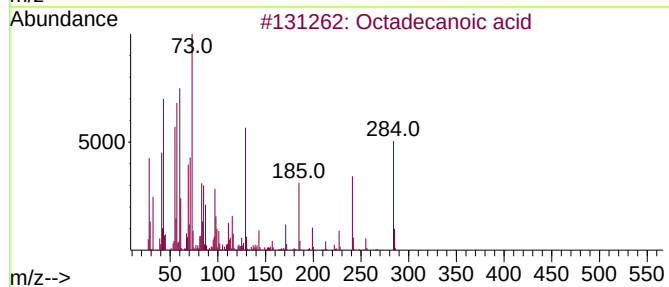
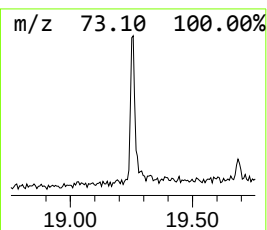
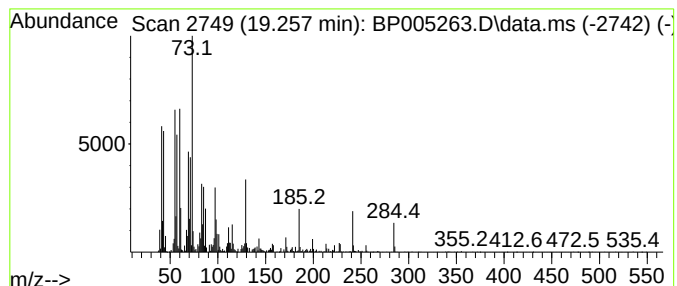
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Peak Number 4 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.257	7.56 ng	184731	Chrysene-d12	21.210

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	70
3			Decane, 1-iodo-	268	C10H21I	002050-77-3	45
4			n-Decanoic acid	172	C10H20O2	000334-48-5	41
5			Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	25



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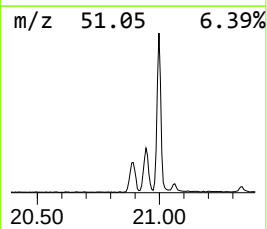
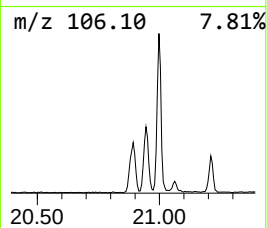
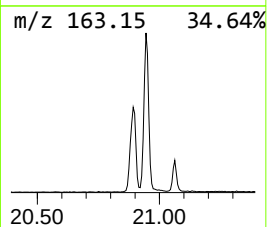
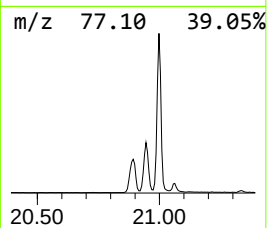
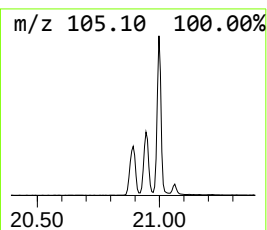
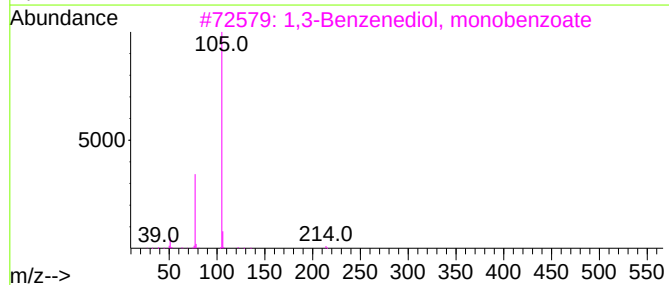
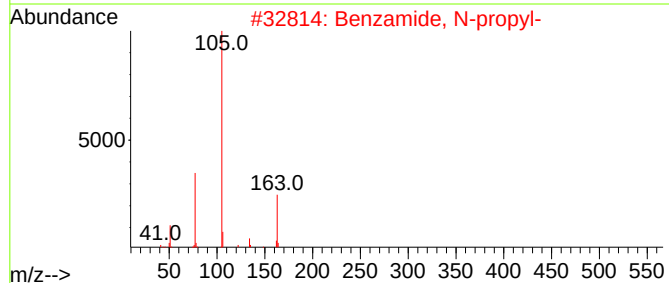
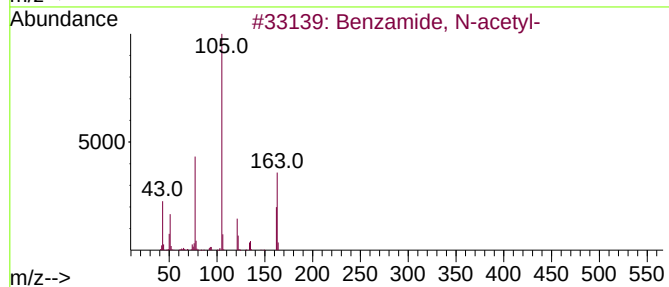
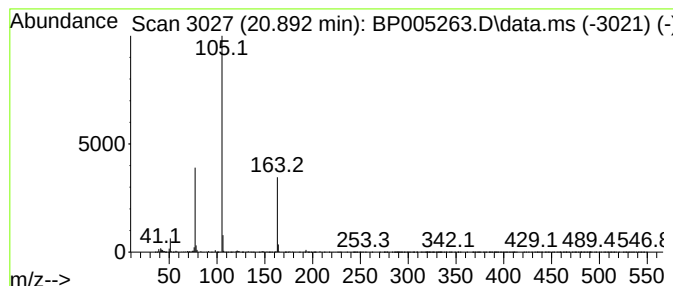
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Peak Number 5 Benzamide, N-acetyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.892	27.47 ng	671389	Chrysene-d12	21.210

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzamide, N-acetyl-	163	C9H9NO2	001575-95-7	80
2			Benzamide, N-propyl-	163	C10H13NO	010546-70-0	56
3			1,3-Benzenediol, monobenzoate	214	C13H10O3	000136-36-7	53
4			Benzoic acid, pentafluorophenyl ...	288	C13H5F5O2	1000360-67-9	53
5			Benzo[b]thiophene-3-carboxylic a...	343	C18H17NO4S	096334-43-9	53



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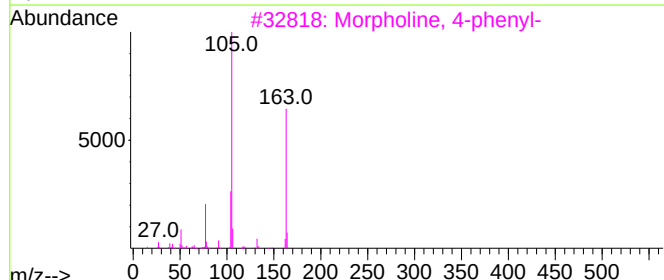
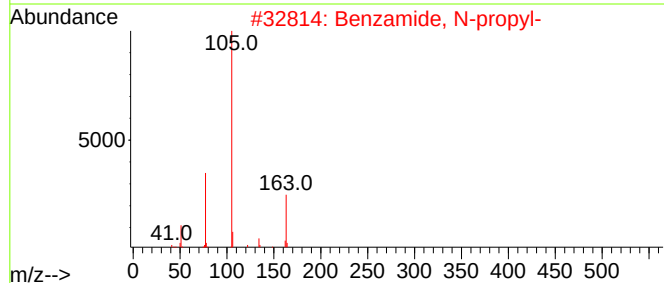
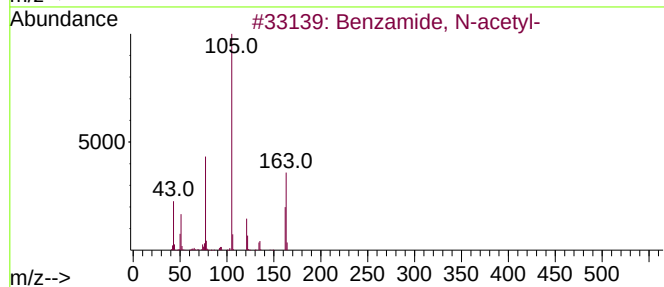
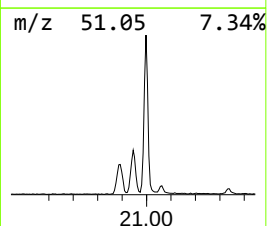
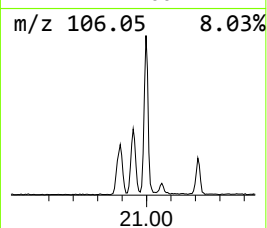
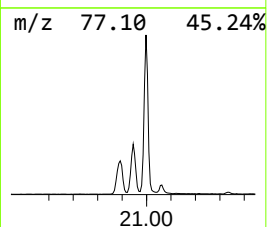
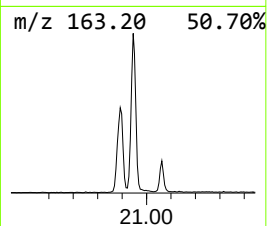
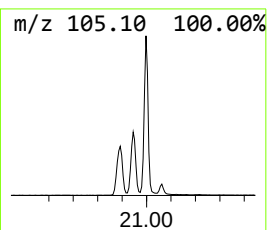
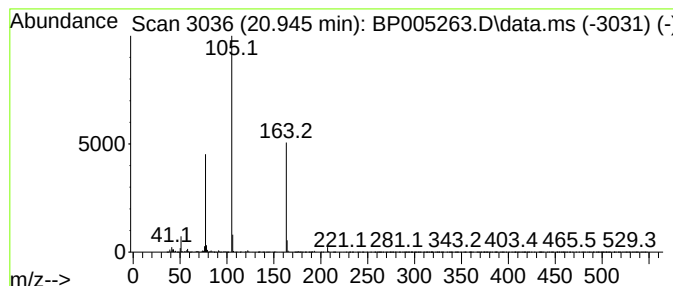
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Peak Number 6 Benzamide, N-propyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.945	41.03 ng	1002870	Chrysene-d12	21.210

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzamide, N-acetyl-	163	C9H9NO2	001575-95-7	64
2			Benzamide, N-propyl-	163	C10H13NO	010546-70-0	64
3			Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	50
4			Benzenepropanamide, .alpha.-(ben...	284	C16H16N2O3	058690-81-6	40
5			2-Pyrrolidinone, 3-hydroxy-4-met...	191	C11H13NO2	104194-17-4	40



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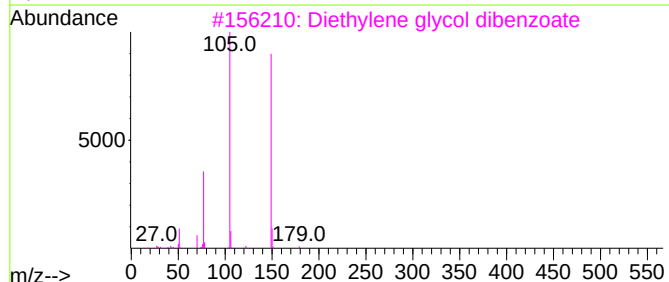
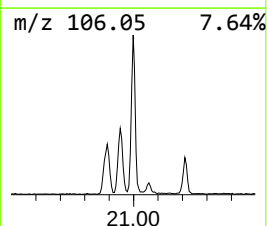
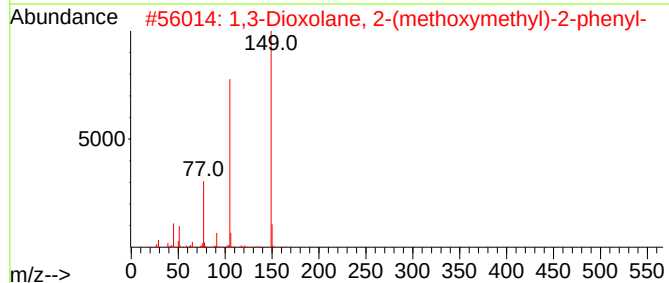
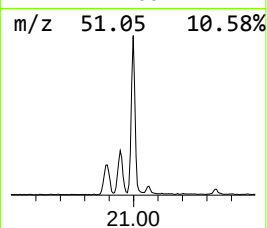
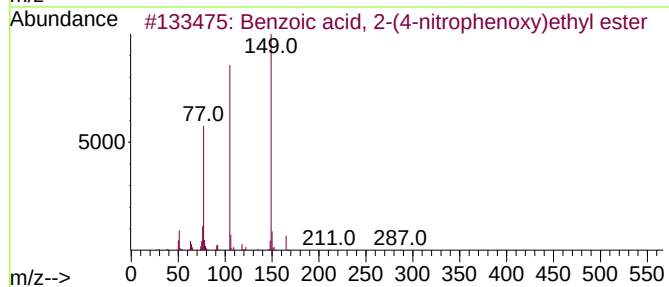
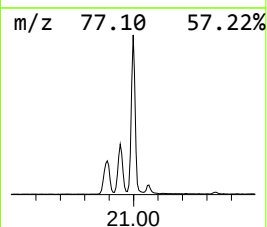
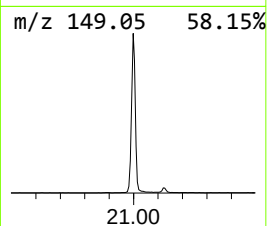
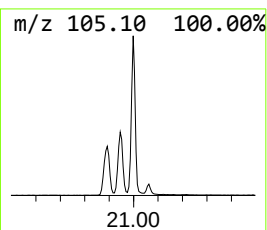
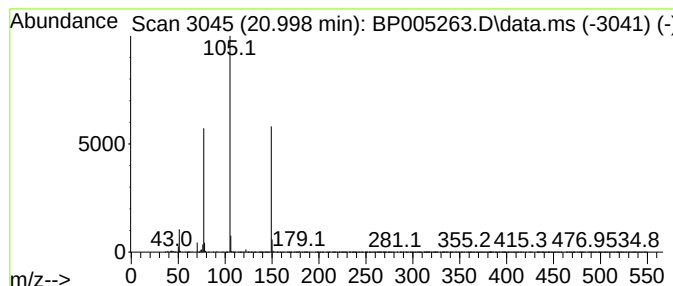
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Benzoic acid, 2-(4-nitrophe... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.998	72.60 ng	1774310	Chrysene-d12	21.210

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid, 2-(4-nitrophenoxy)...	287	C15H13NO5	1000368-92-7	78
2			1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	64
3			Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	59
4			Benzoic acid, 2-(3-nitrophenyl)e...	271	C15H13NO4	1000368-22-4	50
5			2-(2-(2-Methoxyethoxy)ethoxy)eth...	268	C14H20O5	1000366-99-1	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP041221\
Data File : BP005263.D
Acq On : 12 Apr 2021 13:24
Operator : CG/JU
Sample : M1946-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
FS-SB10X

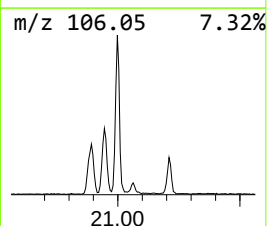
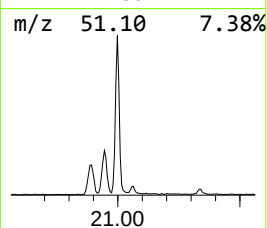
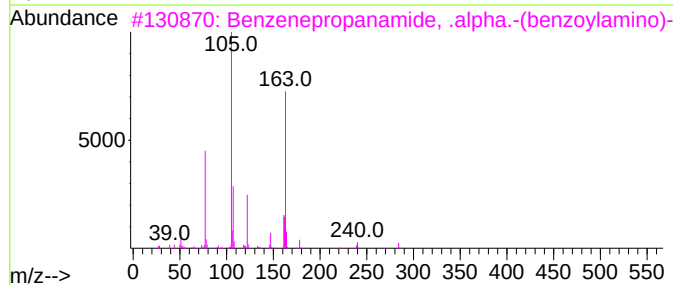
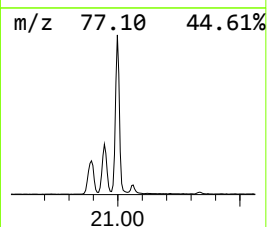
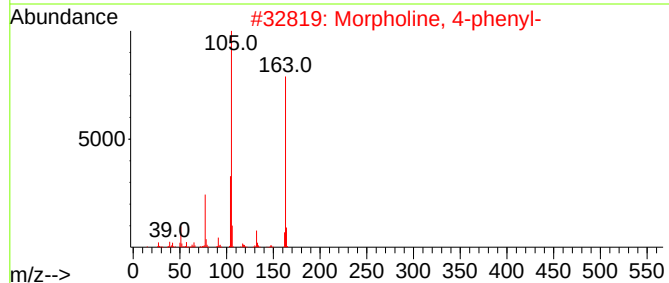
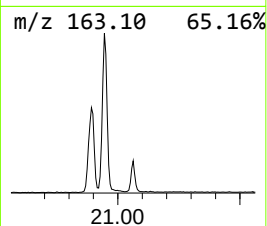
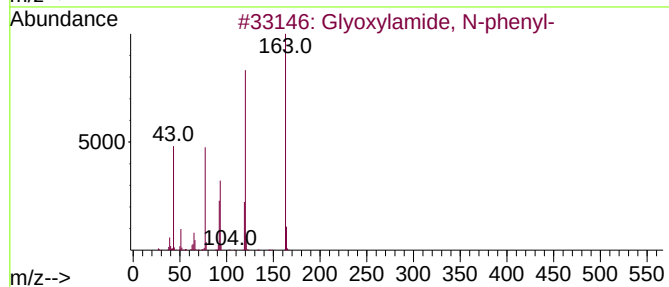
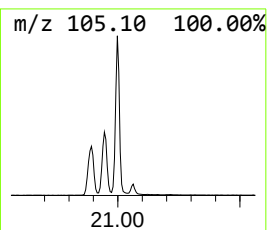
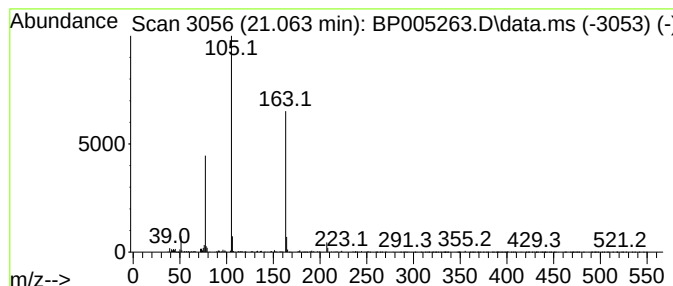
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Glyoxylamide, N-phenyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.063	4.88 ng	119381	Chrysene-d12	21.210

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Glyoxylamide, N-phenyl-	163	C9H9NO2	032331-52-5	50
2			Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	47
3			Benzenepropanamide, .alpha.-(ben...	284	C16H16N2O3	058690-81-6	40
4			Benzamide, N-(2,3-dihydro-6-benz...	395	C24H17N3O3	186965-74-2	38
5			1-Propanol, 2-[2-(benzoyloxy)pro...	342	C20H22O5	020109-39-1	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP041221\
Data File : BP005263.D
Acq On : 12 Apr 2021 13:24
Operator : CG/JU
Sample : M1946-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
FS-SB10X

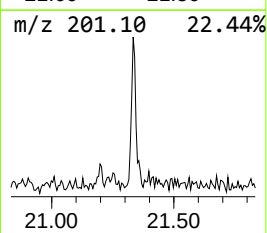
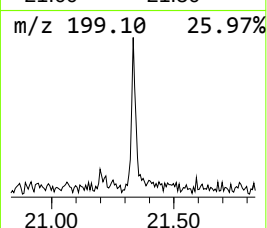
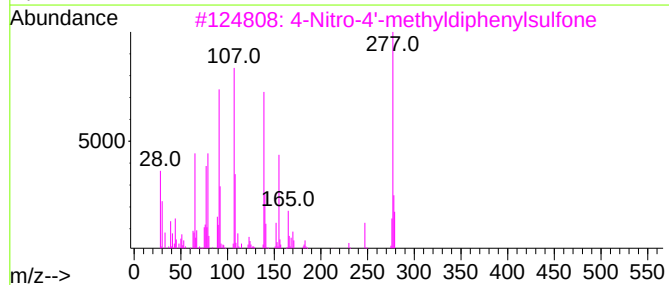
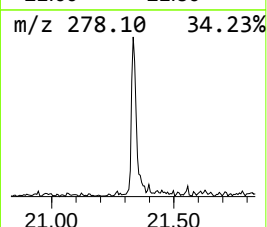
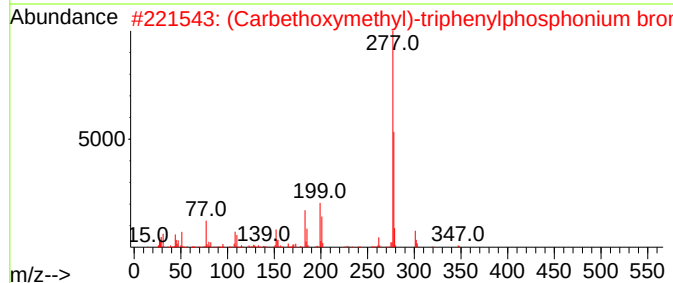
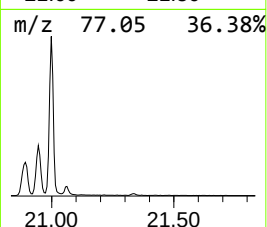
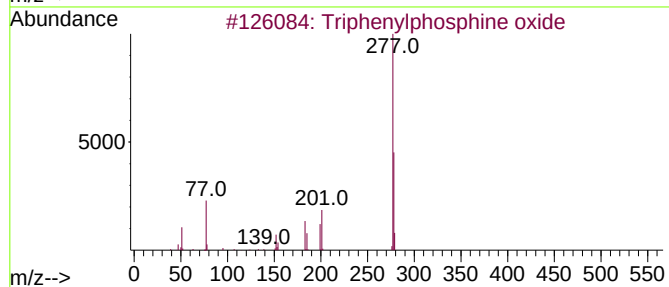
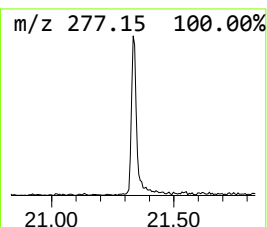
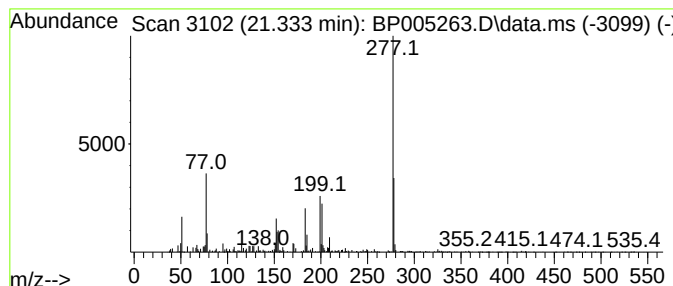
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP040921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Triphenylphosphine oxide Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.333	3.12 ng	76371	Chrysene-d12	21.210

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	74
2			(Carbethoxymethyl)-triphenylphos...	428	C22H22BrO2P	001530-45-6	42
3			4-Nitro-4'-methyldiphenylsulfone	277	C13H11NO4S	004094-37-5	38
4			Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	32
5			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	28



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP041221\
Data File : BP005263.D
Acq On : 12 Apr 2021 13:24
Operator : CG/JU
Sample : M1946-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
FS-SB10X

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP040921.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 ...	18.016	17.8	ng	314622	4	17.110	353585	20.0
unknown18.08	18.080	2.9	ng	51469	4	17.110	353585	20.0
Octadecanoic acid	19.257	7.6	ng	184731	5	21.210	488820	20.0
Benzamide, N-ac...	20.892	27.5	ng	671389	5	21.210	488820	20.0
Benzamide, N-pr...	20.945	41.0	ng	1002870	5	21.210	488820	20.0
Benzoic acid, 2...	20.998	72.6	ng	1774310	5	21.210	488820	20.0
Glyoxylamide, N...	21.063	4.9	ng	119381	5	21.210	488820	20.0
Triphenylphosph...	21.333	3.1	ng	76371	5	21.210	488820	20.0