

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120221\
 Data File : BP008189.D
 Acq On : 02 Dec 2021 13:25
 Operator : CG/JU
 Sample : PB141117BL
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 PB141117BL

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-BP112521.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP008189.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.393	402	409	422	rBV	2223769	3197634	76.94%	12.453%
2	6.987	672	680	701	rBV	1856632	3059214	73.61%	11.914%
3	7.799	811	818	827	rBV	400098	638832	15.37%	2.488%
4	8.963	1006	1016	1035	rBV	1140242	1938430	46.64%	7.549%
5	10.599	1285	1294	1306	rBV	456844	781877	18.81%	3.045%
6	13.075	1705	1715	1732	rBV	2451523	3733374	89.83%	14.539%
7	14.451	1942	1949	1963	rBV	589309	920964	22.16%	3.587%
8	15.951	2194	2204	2230	rBV	1589476	2599363	62.55%	10.123%
9	17.216	2412	2419	2434	rBV	623233	979370	23.57%	3.814%
10	19.492	2802	2806	2814	rBV	109424	134626	3.24%	0.524%
11	19.786	2850	2856	2866	rBV	3433110	4155839	100.00%	16.184%
12	20.516	2976	2980	2983	rBV	84880	93162	2.24%	0.363%
13	20.992	3056	3061	3065	rBV	73616	121404	2.92%	0.473%
14	21.045	3066	3070	3074	rVB	105065	144796	3.48%	0.564%
15	21.092	3074	3078	3086	rBV	308509	423208	10.18%	1.648%
16	21.316	3112	3116	3126	rVB	696857	891466	21.45%	3.472%
17	21.433	3131	3136	3147	rBV	737462	989961	23.82%	3.855%
18	23.721	3519	3525	3538	rVB2	417220	874672	21.05%	3.406%

Sum of corrected areas: 25678192

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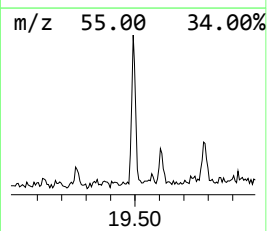
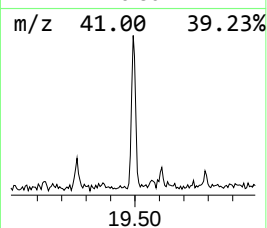
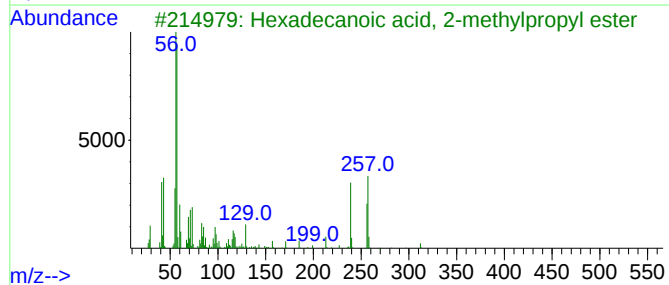
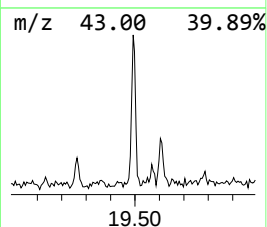
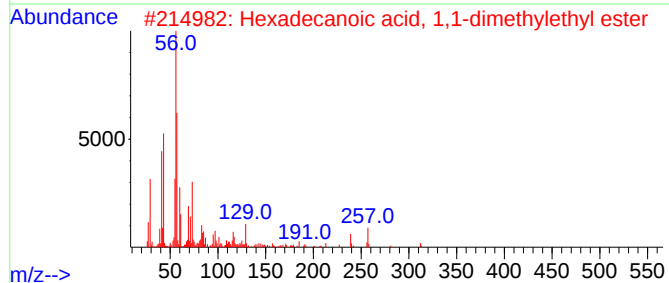
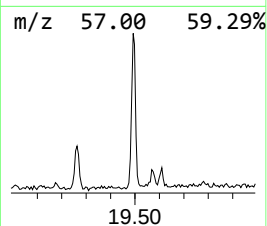
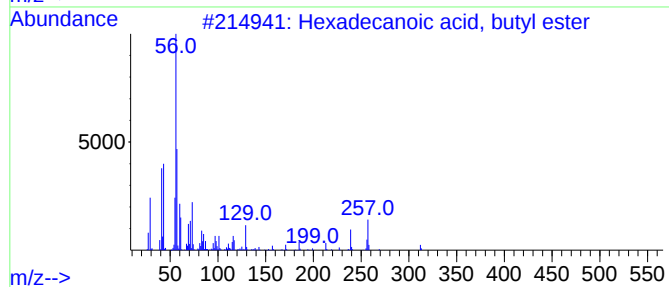
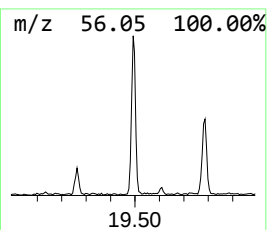
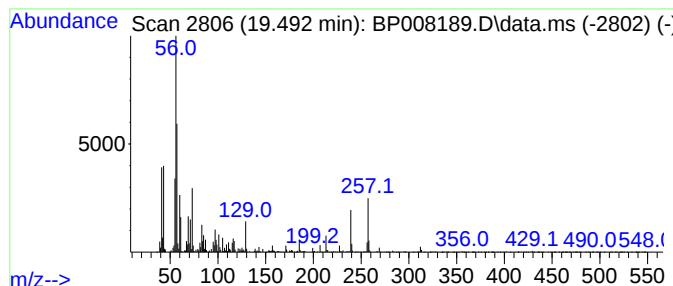
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Hexadecanoic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.492	3.02 ng	134626	Chrysene-d12	21.316

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	98
2			Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	98
3			Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	91
4			Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	040482-05-1	35
5			Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	037910-65-9	35



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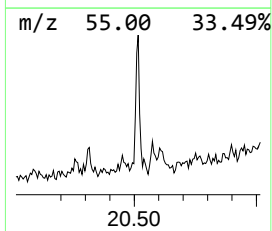
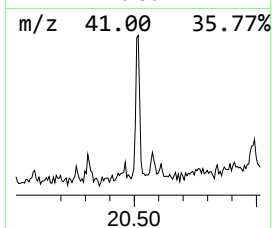
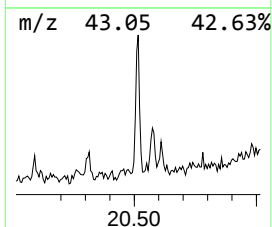
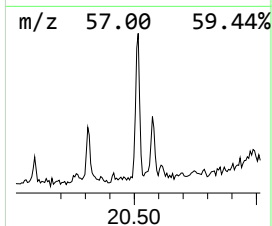
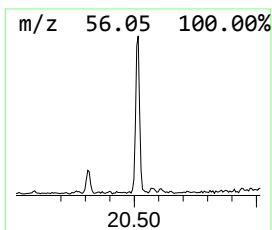
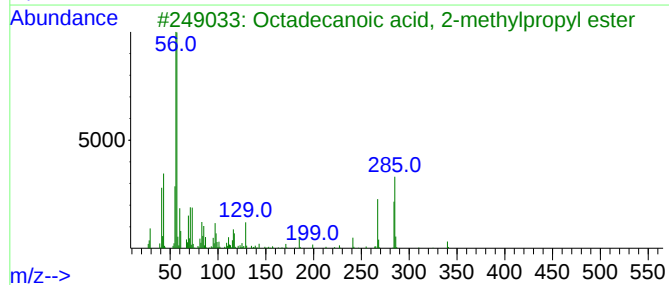
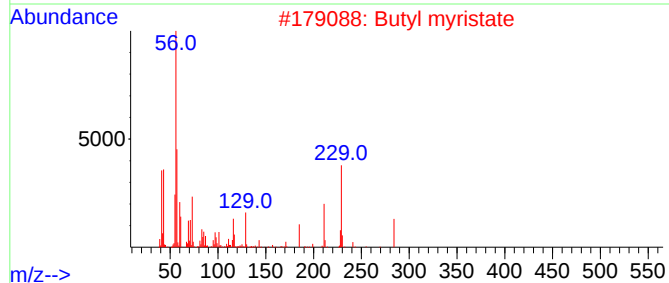
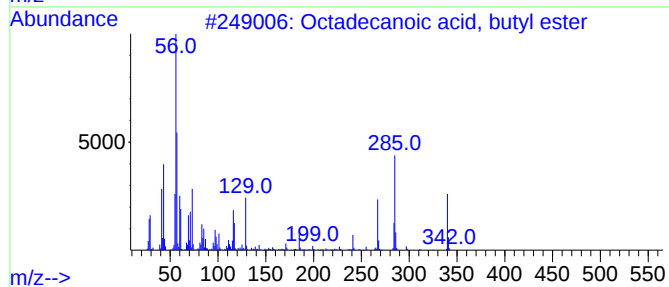
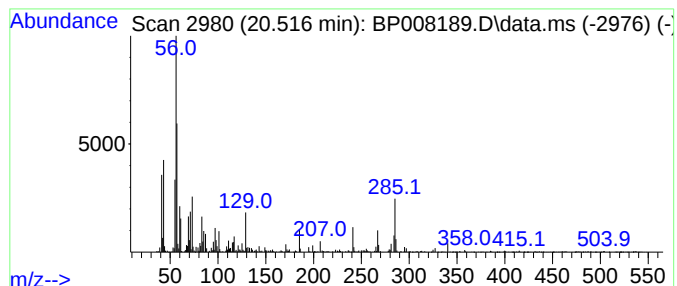
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Octadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.516	2.09 ng	93162	Chrysene-d12	21.316

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	78
2			Butyl myristate	284	C18H36O2	000110-36-1	68
3			Octadecanoic acid, 2-methylpropyl...	340	C22H44O2	000646-13-9	55
4			Cyclohexane, (1,1-dimethylethyl)-	140	C10H20	003178-22-1	45
5			1-Heptene, 2-methyl-	112	C8H16	015870-10-7	43



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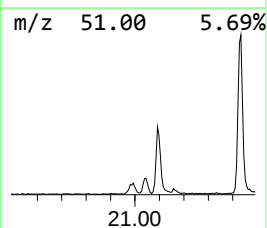
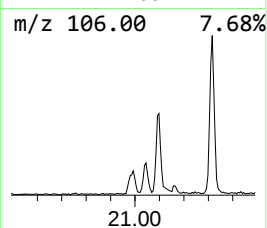
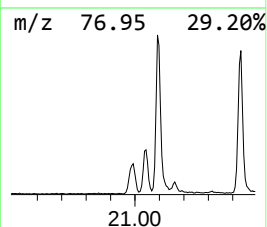
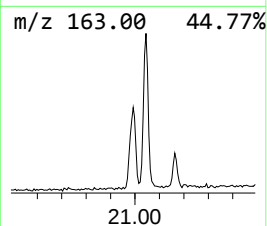
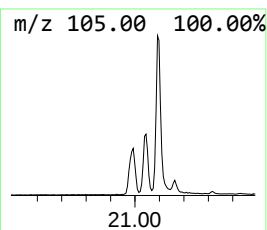
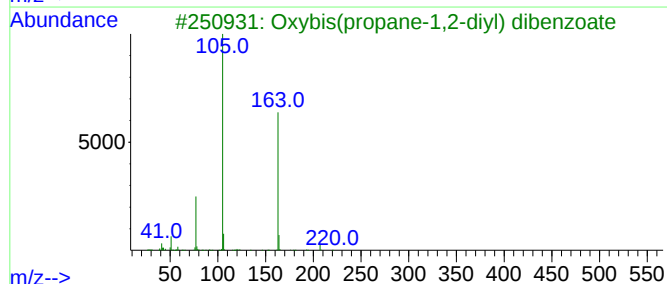
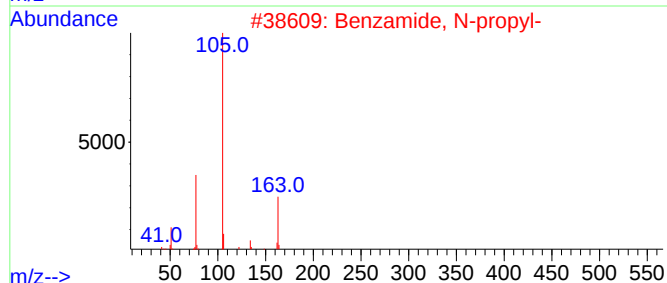
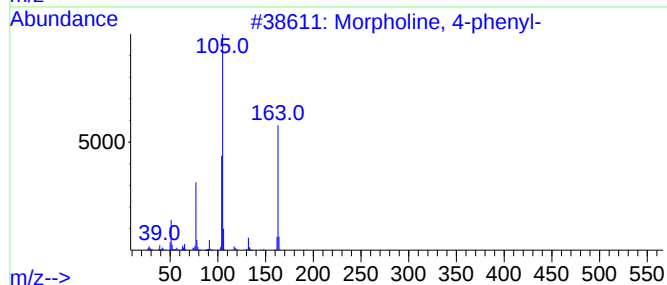
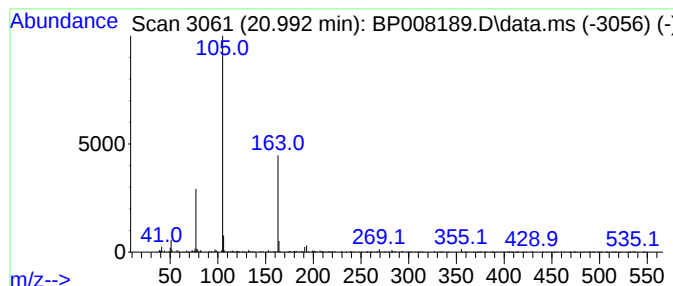
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.992	2.72 ng	121404	Chrysene-d12	21.316

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	64
2			Benzamide, N-propyl-	163	C10H13NO	010546-70-0	64
3			Oxybis(propane-1,2-diyl) dibenzoate	342	C20H22O5	000094-03-1	53
4			(3-Phenyloxiran-2-yl)methyl benz...	254	C16H14O3	1000366-96-1	39
5			Ethyl 4-(benzoylamino)benzoate	269	C16H15NO3	000736-40-3	27



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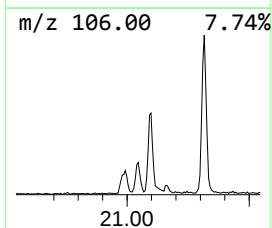
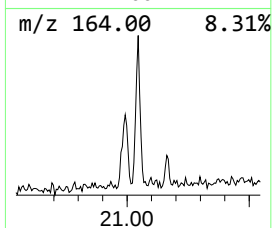
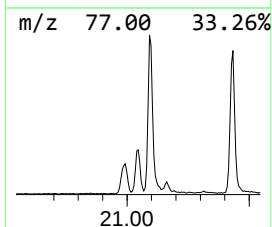
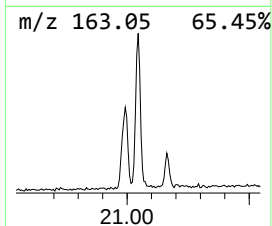
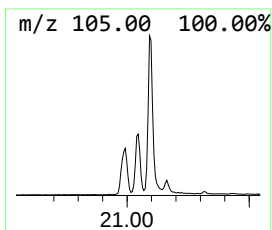
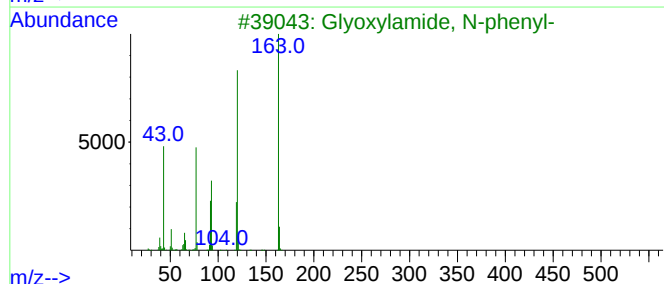
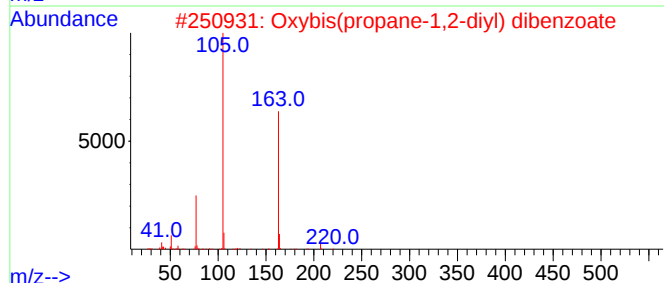
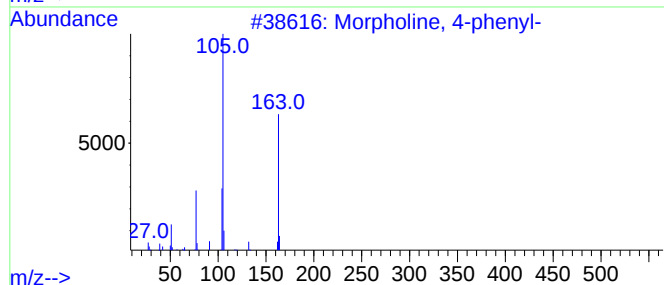
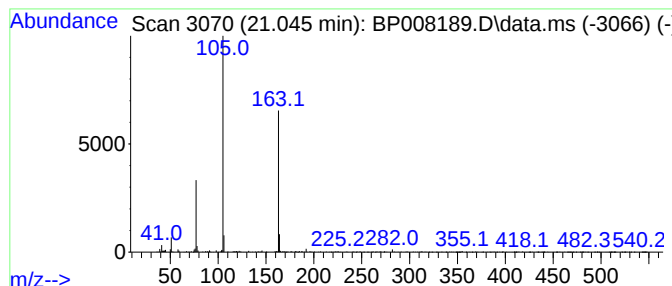
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Morpholine, 4-phenyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.045	3.25 ng	144796	Chrysene-d12	21.316

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	72
2			Oxybis(propane-1,2-diyl) dibenzoate	342	C20H22O5	000094-03-1	56
3			Glyoxylamide, N-phenyl-	163	C9H9NO2	032331-52-5	47
4			Benzenepropanamide, .alpha.-(ben...	284	C16H16N2O3	058690-81-6	45
5			1-Propanol, 2-[2-(benzoyloxy)pro...	342	C20H22O5	020109-39-1	40



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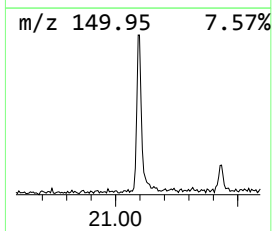
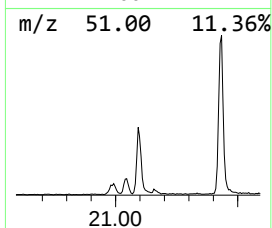
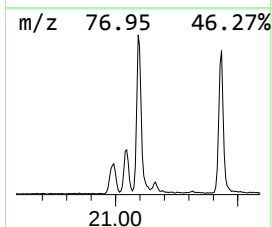
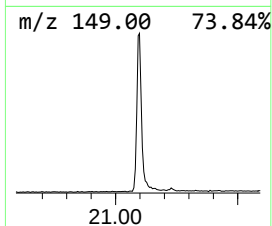
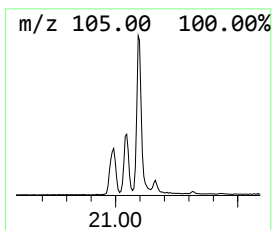
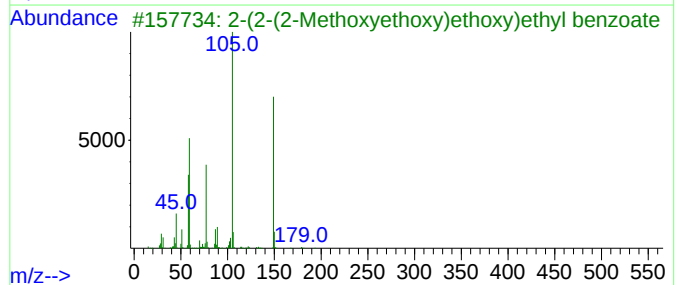
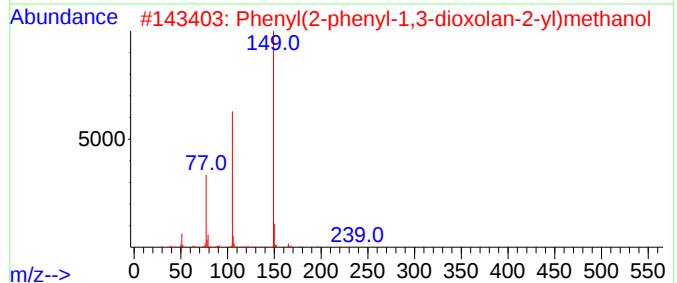
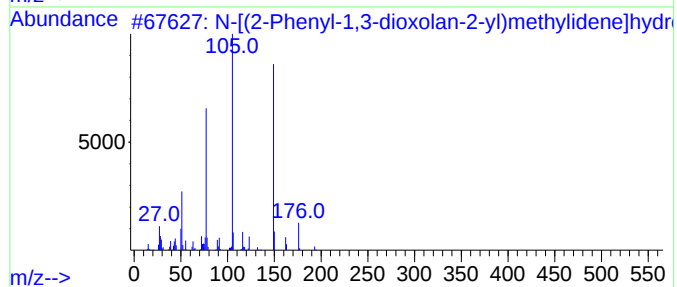
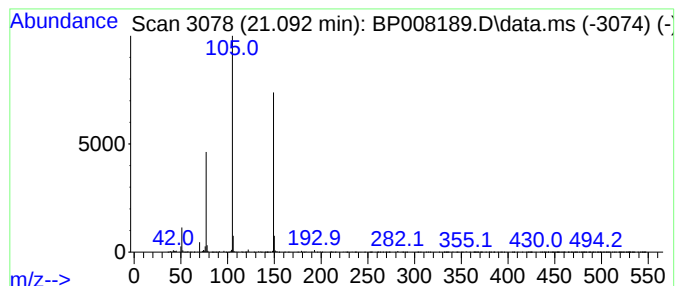
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 N-[(2-Phenyl-1,3-dioxolan-2-yl)methylidene]hydr Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.092	9.49 ng	423208	Chrysene-d12	21.316

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			N-[(2-Phenyl-1,3-dioxolan-2-yl)methylidene]hydr	193	C10H11NO3	1000411-48-9	83
2			Phenyl(2-phenyl-1,3-dioxolan-2-yl)methanol	256	C16H16O3	005694-69-9	78
3			2-(2-(2-Methoxyethoxy)ethoxy)ethyl benzoate	268	C14H20O5	1000366-99-1	74
4			2,2'-(Ethane-1,2-diylbis(oxy))bis(2-phenyl-1,3-dioxolan-2-yl)methanol	358	C20H22O6	1000366-99-4	74
5			Ethanol, 2-(4-phenoxyphenoxy)-, ...	334	C21H18O4	055191-59-8	72



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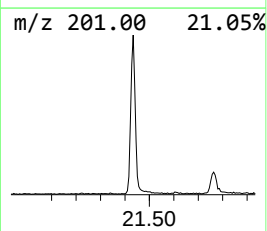
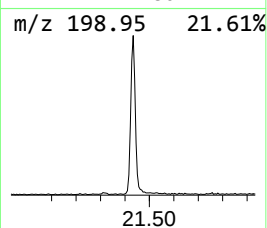
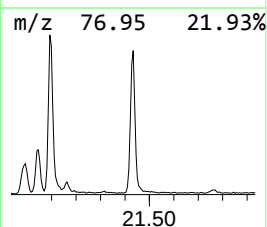
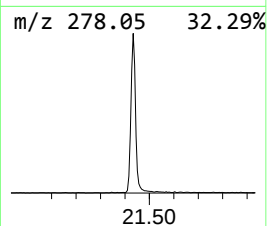
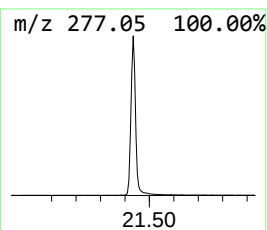
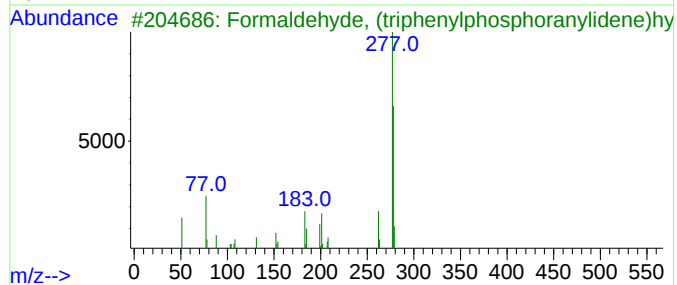
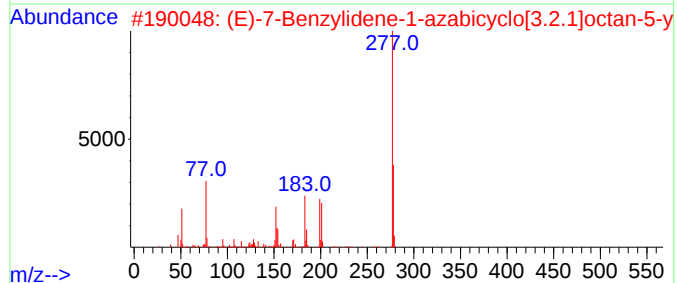
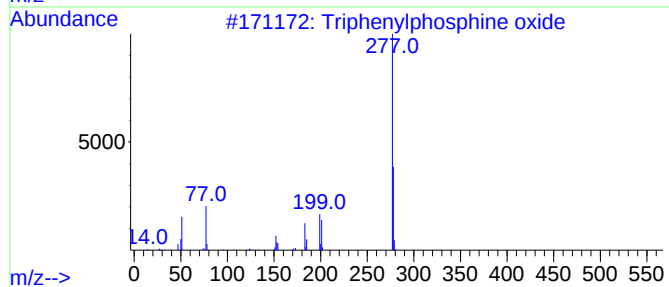
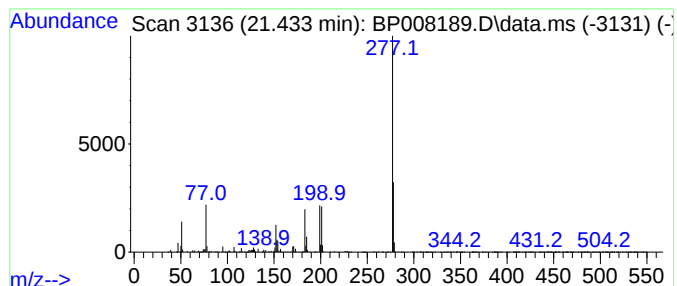
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Triphenylphosphine oxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.433	22.21 ng	989961	Chrysene-d12	21.316

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	94
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19NO3S	1000483-83-4	64
3			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	50
4			1H-Indole-3-acetic acid, 5-[(tri...	277	C14H19NO3Si	072101-35-0	17
5			5-quinolinol, 8-[2-(3,5-dimethyl...	277	C17H15N3O	1000397-10-2	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120221\
Data File : BP008189.D
Acq On : 02 Dec 2021 13:25
Operator : CG/JU
Sample : PB141117BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PB141117BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Hexadecanoic ac...	19.492	3.0	ng	134626	5	21.316	891466	20.0
Octadecanoic ac...	20.516	2.1	ng	93162	5	21.316	891466	20.0
Benzamide, N-pr...	20.992	2.7	ng	121404	5	21.316	891466	20.0
Morpholine, 4-p...	21.045	3.3	ng	144796	5	21.316	891466	20.0
N-[(2-Phenyl-1,...	21.092	9.5	ng	423208	5	21.316	891466	20.0
Triphenylphosph...	21.433	22.2	ng	989961	5	21.316	891466	20.0