

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM111022\
 Data File : BM037447.D
 Acq On : 10 Nov 2022 12:31
 Operator : CG/JU
 Sample : N5469-03
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 SP-303-20221103

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_M\Methods\8270-BM102822.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM037447.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.387	384	391	404	rBV	1205948	1824346	2.95%	1.085%
2	6.993	658	664	675	rBV	720032	1176815	1.90%	0.700%
3	7.810	795	803	810	rBV	818513	1279998	2.07%	0.762%
4	8.981	994	1002	1017	rBV	2435791	3995692	6.46%	2.377%
5	10.610	1269	1279	1291	rBV	1023125	1746371	2.82%	1.039%
6	13.075	1690	1698	1710	rBV	5726521	8091951	13.08%	4.814%
7	14.445	1925	1931	1946	rBV	1447751	2098584	3.39%	1.249%
8	15.939	2178	2185	2201	rBV	2994151	4071560	6.58%	2.422%
9	16.404	2230	2264	2265	rBV	3323521	15527907	25.10%	9.238%
10	16.774	2298	2327	2349	rBV	6686000	40550828	65.55%	24.126%
11	17.068	2349	2377	2379	rBV	13871070	61861349	100.00%	36.805%
12	17.192	2393	2398	2405	rVB	1459870	2027273	3.28%	1.206%
13	17.333	2410	2422	2442	rVB	1373000	6254847	10.11%	3.721%
14	18.086	2545	2550	2559	rBV	1702180	2611177	4.22%	1.554%
15	18.645	2637	2645	2661	rVB2	220702	704426	1.14%	0.419%
16	19.362	2763	2767	2786	rBV	867043	1576307	2.55%	0.938%
17	19.815	2838	2844	2855	rVB	6286750	7727420	12.49%	4.597%
18	21.368	3104	3108	3112	rBV	1701342	2137848	3.46%	1.272%
19	21.415	3113	3116	3123	rVB	483664	702886	1.14%	0.418%
20	23.697	3499	3504	3511	rBV2	1119821	2112000	3.41%	1.257%

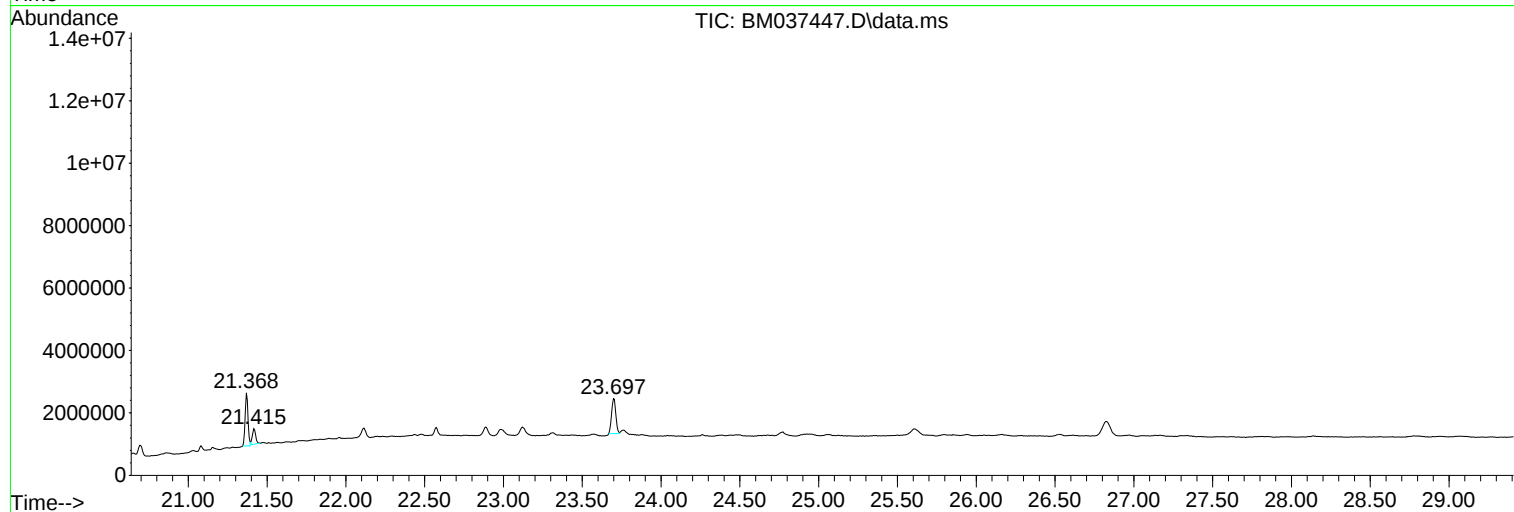
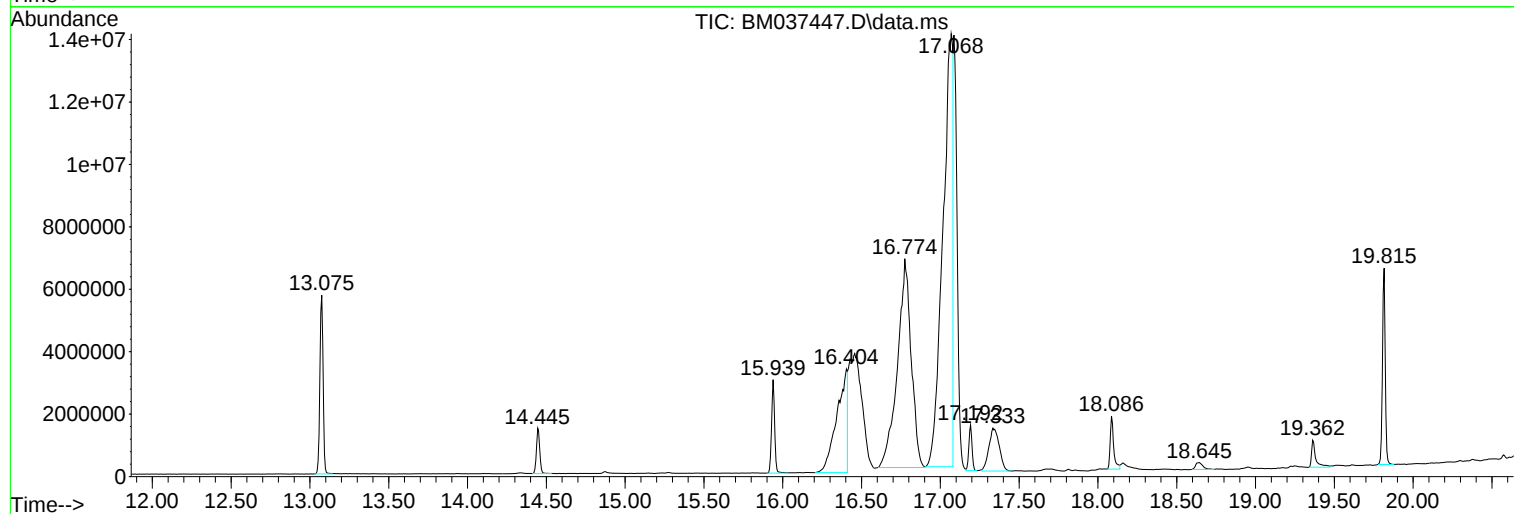
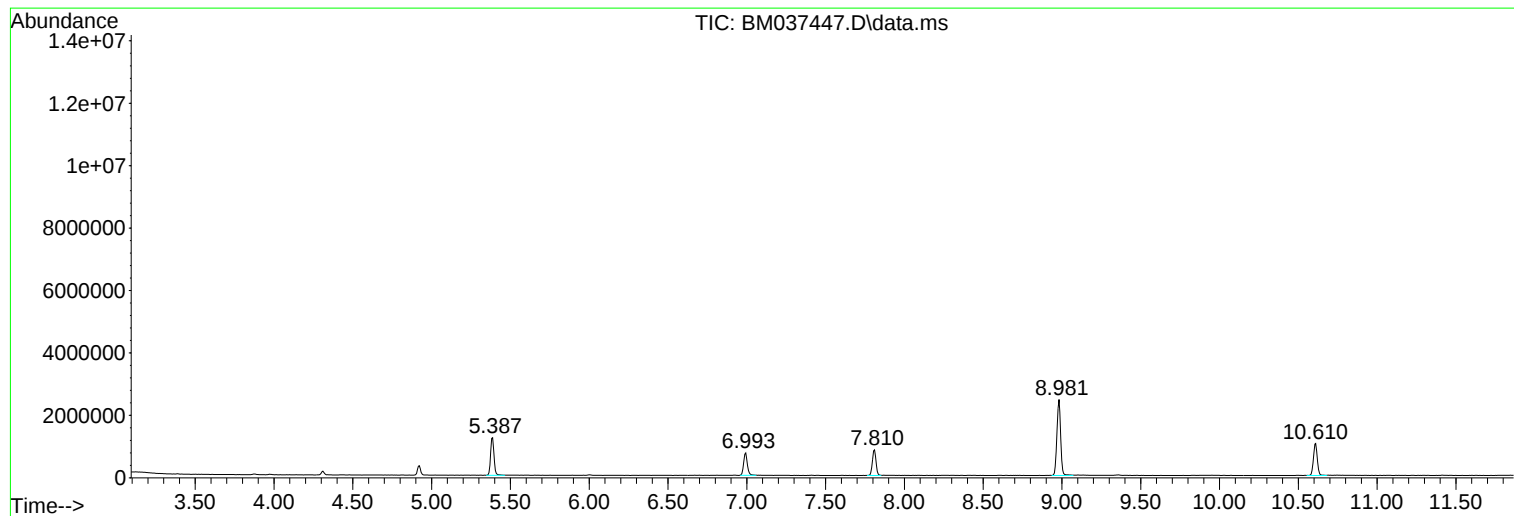
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Instrument :
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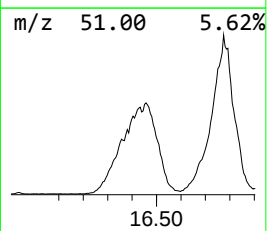
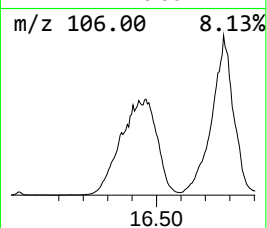
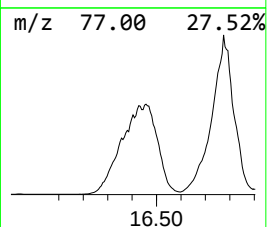
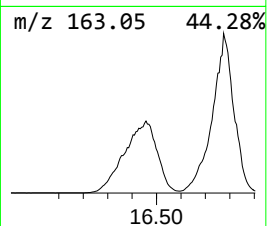
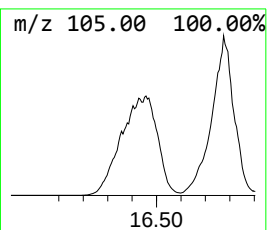
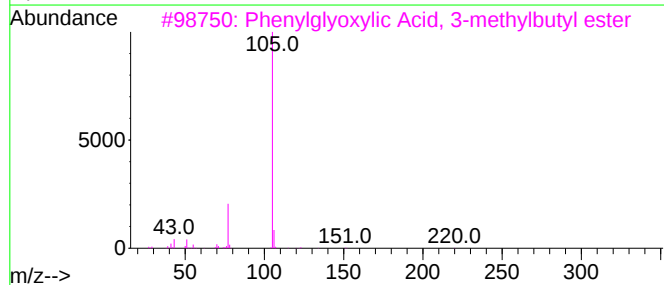
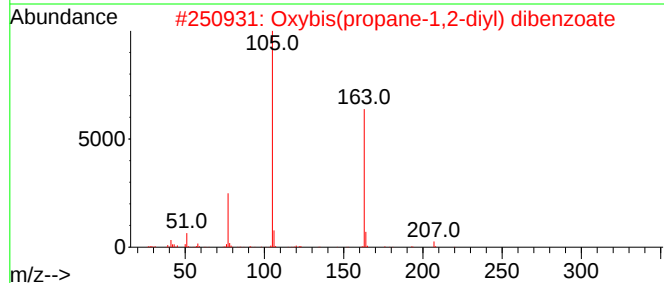
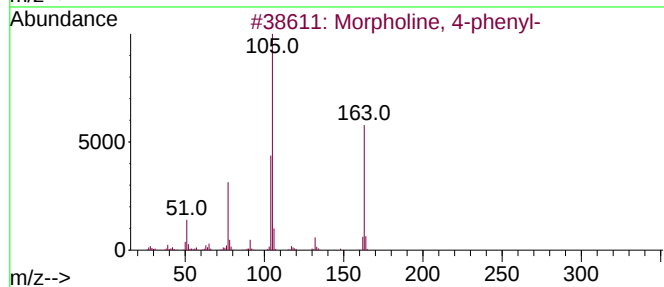
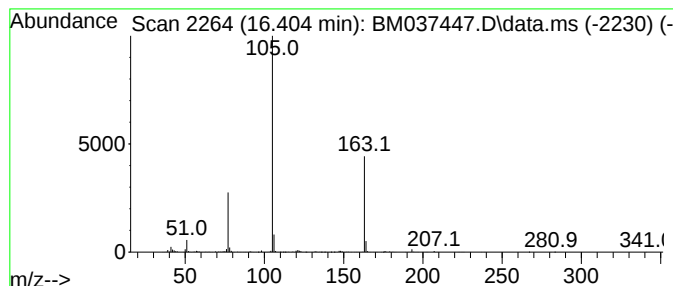
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Morpholine, 4-phenyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.404	153.19 ng	15527900	Phenanthrene-d10	17.192

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	50
3			Phenylglyoxylic Acid, 3-methylbu...	220	C13H16O3	1000453-46-1	38
4			4-(Benzoyloxy)benzoic acid	242	C14H10O4	028547-23-1	38
5			Isopropyl phenyl ketone	148	C10H12O	000611-70-1	38



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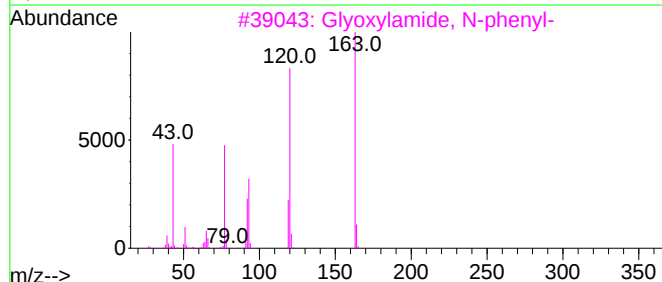
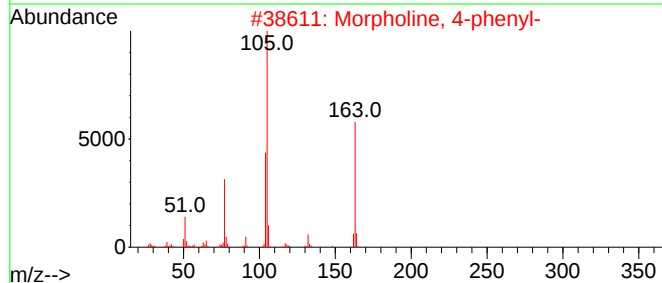
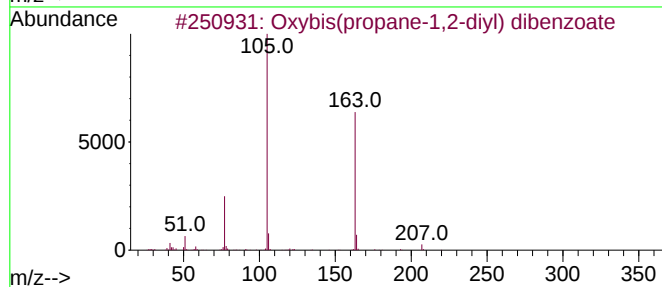
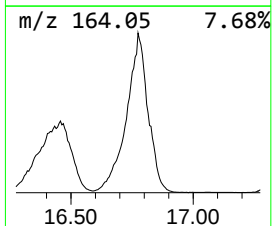
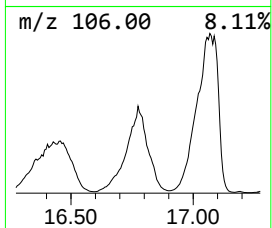
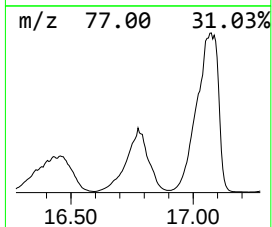
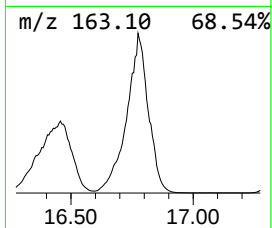
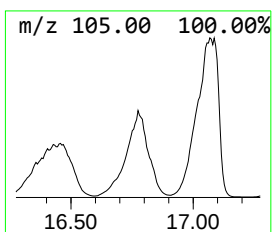
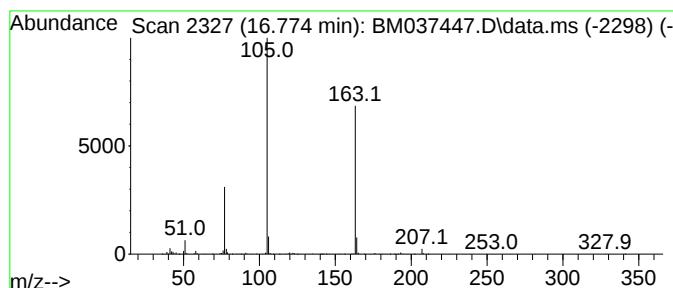
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Oxybis(propene-1,2-diyl) di... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.774	400.05 ng	40550800	Phenanthrene-d10	17.192

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxybis(propene-1,2-diyl) dibenzoate	342	C20H22O5	000094-03-1	91
2			Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	72
3			Glyoxylamide, N-phenyl-	163	C9H9NO2	032331-52-5	50
4			.delta.2-1,3,4-Oxadiazolin-5-one...	163	C7H5N3O2	002845-82-1	43
5			Benzeneacetic acid, .alpha.-oxo-...	178	C10H10O3	001603-79-8	38



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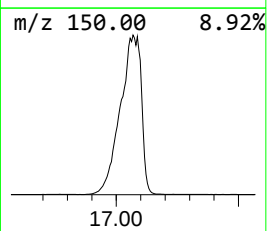
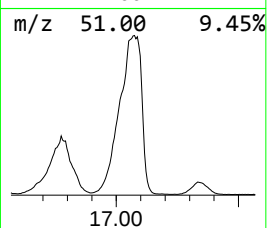
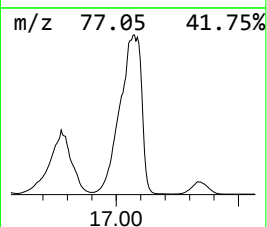
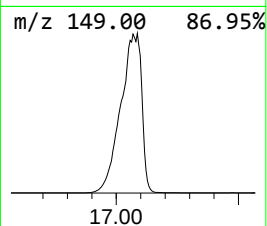
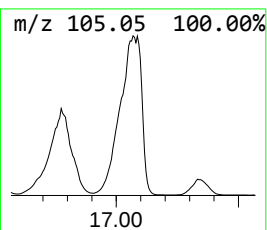
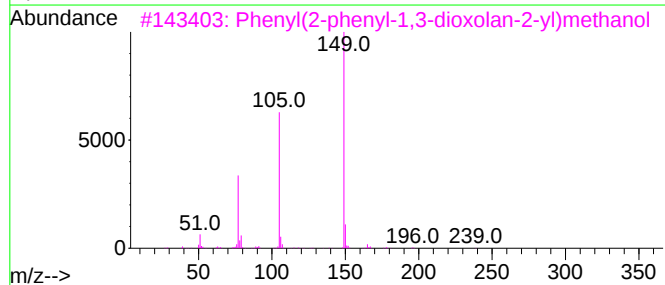
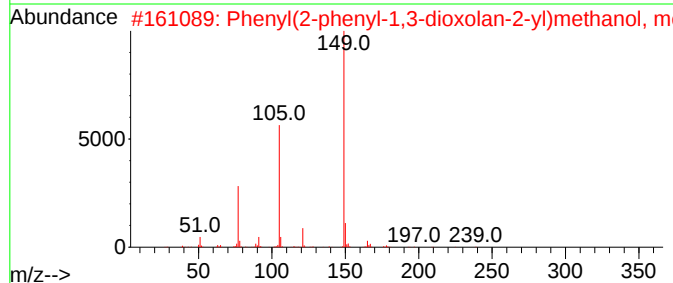
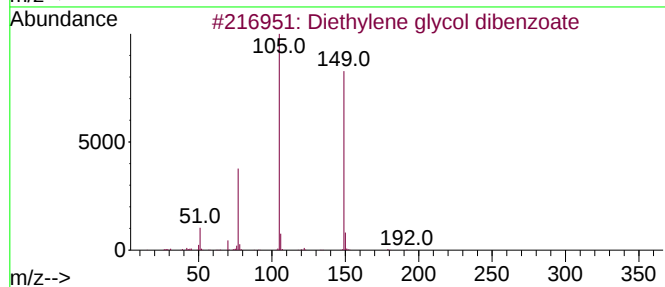
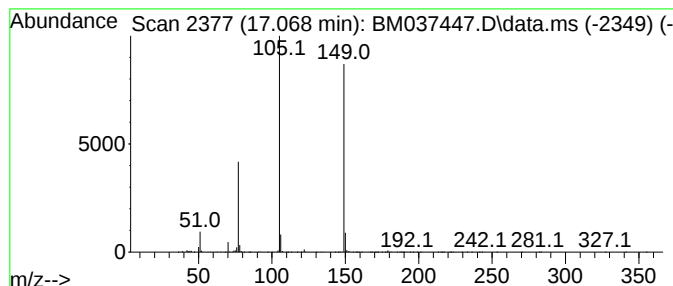
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Diethylene glycol dibenzoate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.069	610.29 ng	61861300	Phenanthrene-d10	17.192

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	91
2			Phenyl(2-phenyl-1,3-dioxolan-2-y...	270	C17H18O3	1000507-07-6	78
3			Phenyl(2-phenyl-1,3-dioxolan-2-y...	256	C16H16O3	005694-69-9	78
4			Benzoic acid, 2-(3-nitrophenyl)e...	271	C15H13NO4	1000368-22-4	72
5			2-(2-Carboxyvinyl)pyridine, trans	149	C8H7NO2	007340-22-9	49



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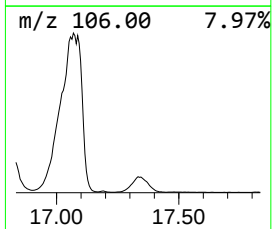
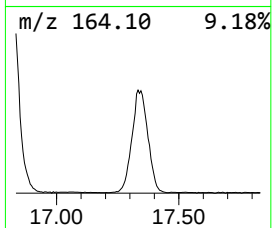
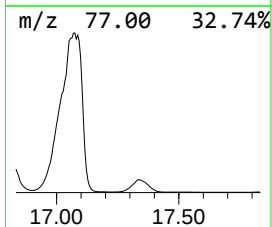
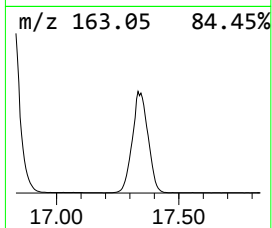
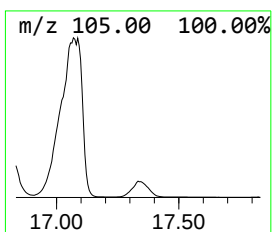
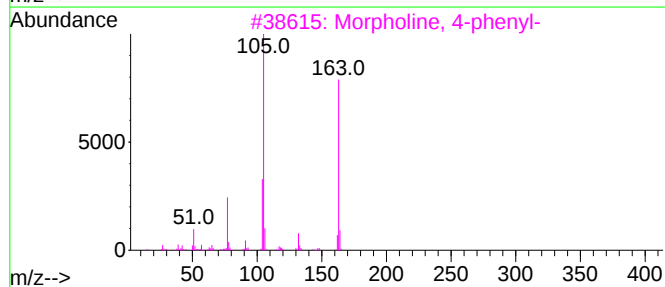
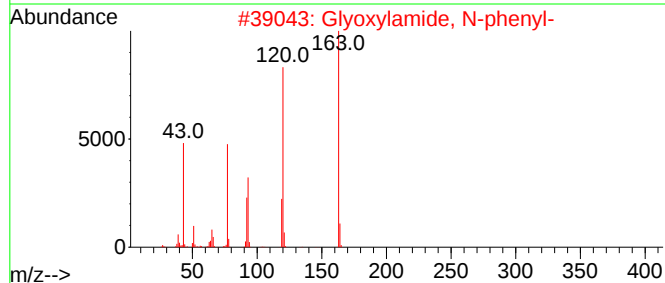
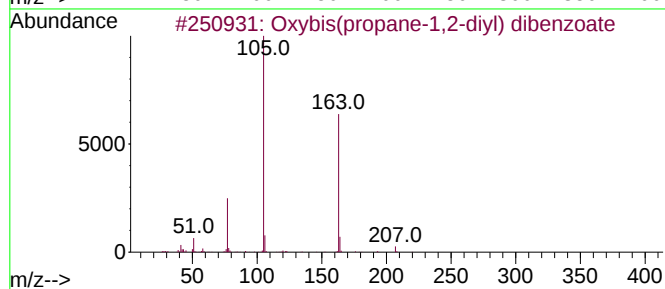
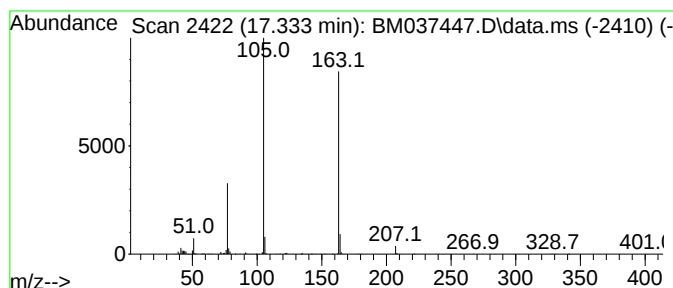
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Glyoxylamide, N-phenyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.	
17.333	61.71 ng	6254850	Phenanthrene-d10		17.192	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxybis(propane-1,2-diyl)	dibenzoate	342	C20H22O5	000094-03-1	90
2	Glyoxylamide, N-phenyl-		163	C9H9NO2	032331-52-5	59
3	Morpholine, 4-phenyl-		163	C10H13NO	000092-53-5	56
4	.delta.2-1,3,4-Oxadiazolin-5-one...		163	C7H5N3O2	002845-82-1	50
5	4-Nitrophenyl benzoate		243	C13H9NO4	000959-22-8	22



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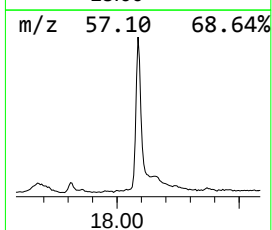
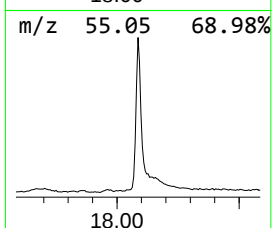
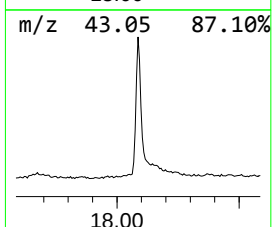
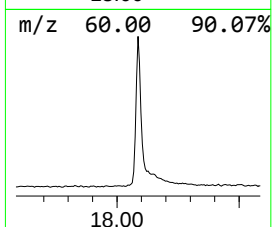
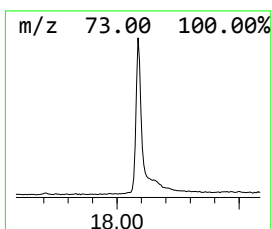
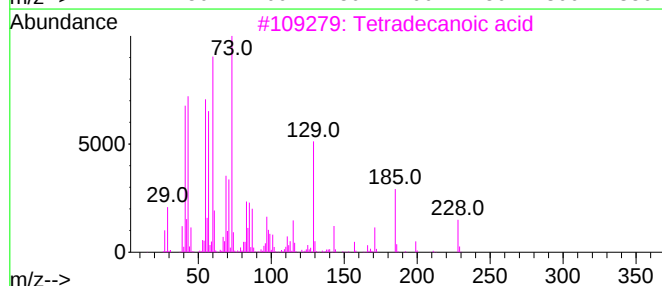
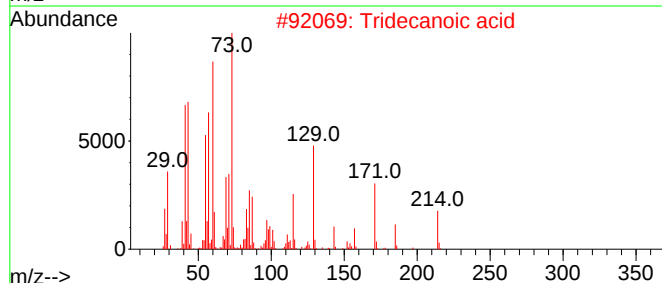
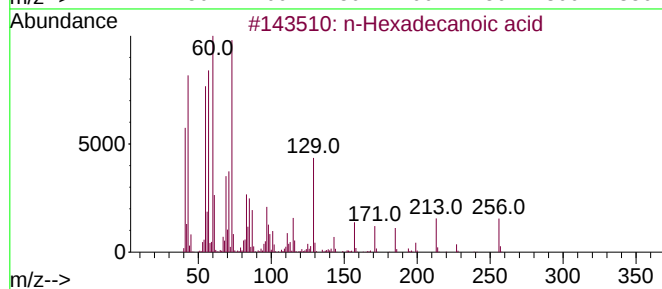
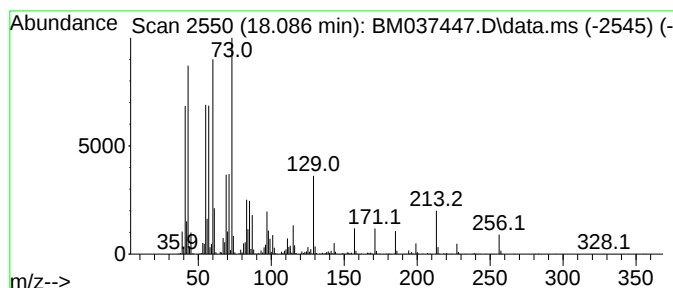
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.086	25.76 ng	2611180	Phenanthrene-d10	17.192	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	94
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
5	Undecanoic acid	186	C11H22O2	000112-37-8	53



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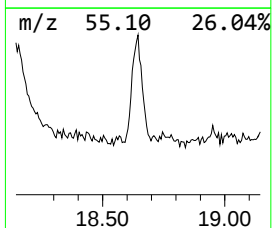
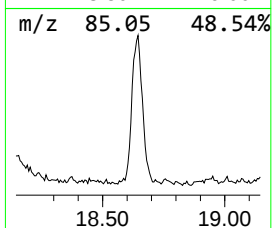
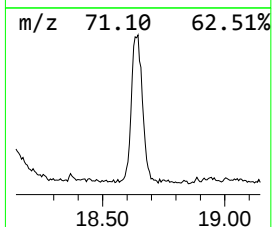
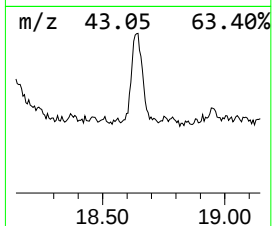
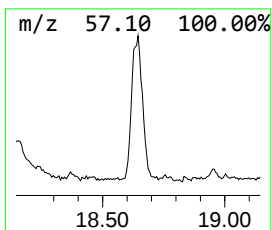
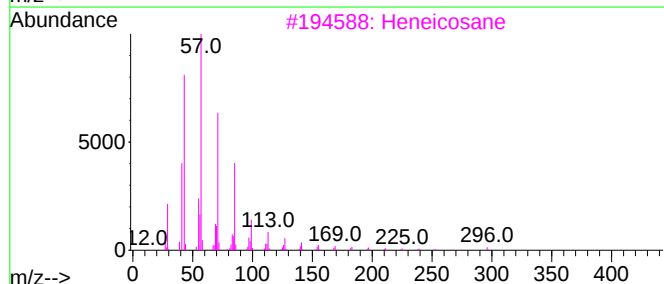
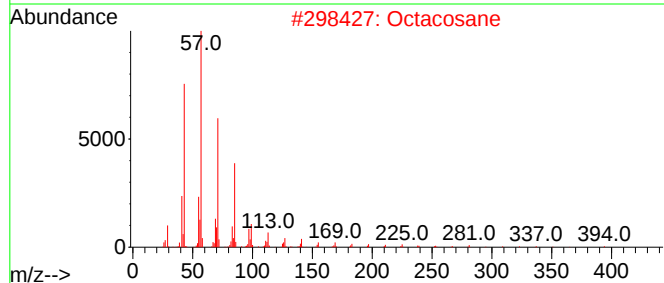
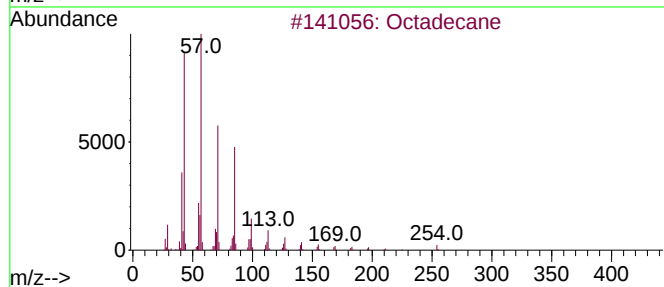
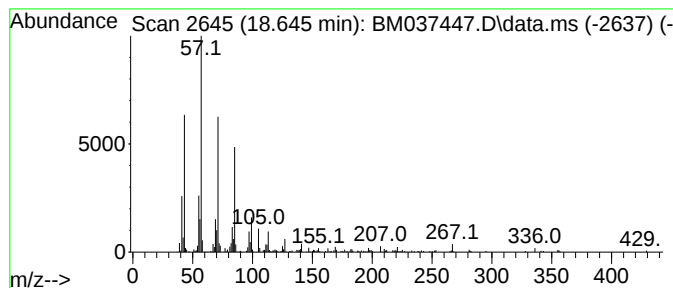
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.645	6.95 ng	704426	Phenanthrene-d10	17.192

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane	254	C18H38	000593-45-3	90
2			Octacosane	394	C28H58	000630-02-4	90
3			Heneicosane	296	C21H44	000629-94-7	90
4			Hexacosane	366	C26H54	000630-01-3	90
5			Eicosane	282	C20H42	000112-95-8	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM111022\
Data File : BM037447.D
Acq On : 10 Nov 2022 12:31
Operator : CG/JU
Sample : N5469-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SP-303-20221103

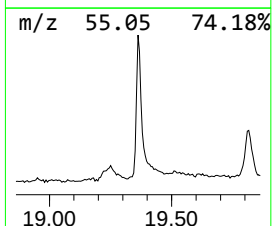
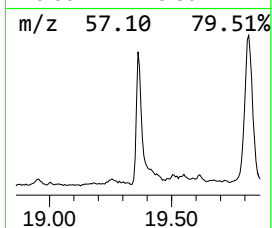
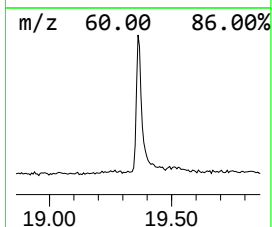
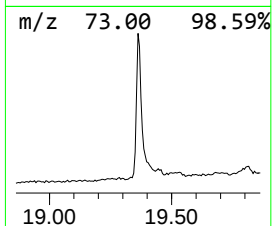
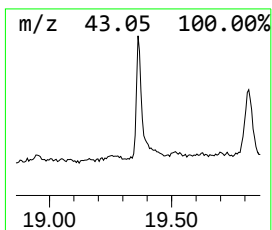
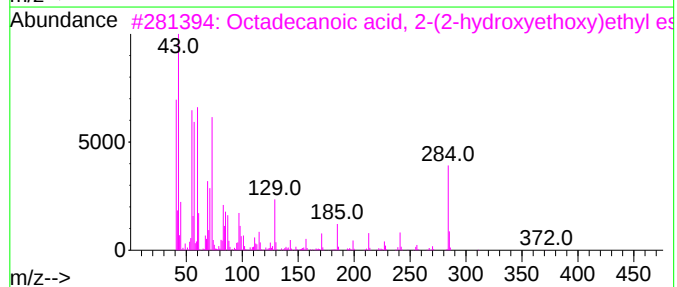
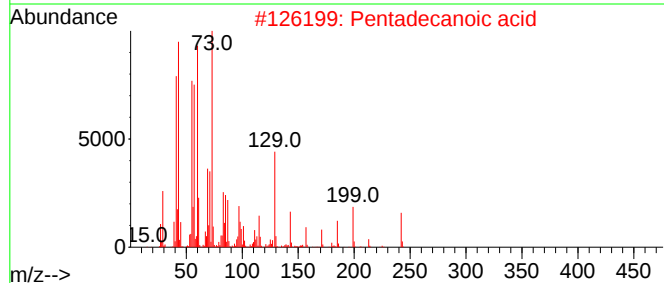
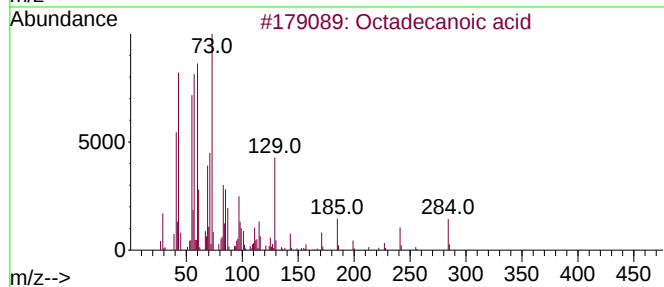
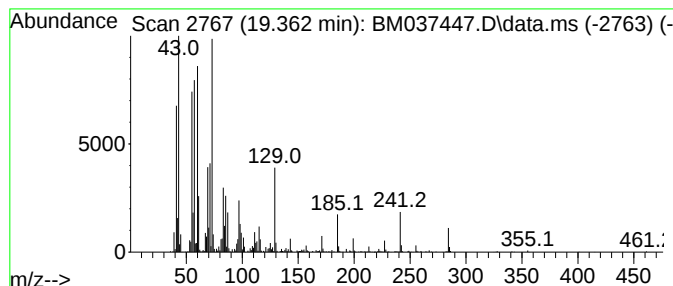
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.362	14.75 ng	1576310	Chrysene-d12	21.368

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	91
3			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	86
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5			n-Decanoic acid	172	C10H20O2	000334-48-5	62



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM111022\
Data File : BM037447.D
Acq On : 10 Nov 2022 12:31
Operator : CG/JU
Sample : N5469-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SP-303-20221103

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102822.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
Morpholine, 4-p...	16.404	153.2	ng	15527900	4	17.192	2027270	20.0
Oxybis(propane-...	16.774	400.1	ng	40550800	4	17.192	2027270	20.0
Diethylene glyc...	17.069	610.3	ng	61861300	4	17.192	2027270	20.0
Glyoxylamide, N...	17.333	61.7	ng	6254850	4	17.192	2027270	20.0
n-Hexadecanoic ...	18.086	25.8	ng	2611180	4	17.192	2027270	20.0
Octadecane	18.645	7.0	ng	704426	4	17.192	2027270	20.0
Octadecanoic acid	19.362	14.8	ng	1576310	5	21.368	2137850	20.0