

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041522\
 Data File : BF127814.D
 Acq On : 15 Apr 2022 20:21
 Operator : CG\JU
 Sample : N2391-01 5X
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TR-06-041422

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_F\Methods\8270-BF040622.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF127814.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.563	553	557	560	rBV	644646	593519	6.44%	1.802%
2	6.563	723	727	730	rBV	679652	554225	6.01%	1.683%
3	6.945	788	792	796	rBV	995116	872950	9.47%	2.650%
4	7.504	883	887	891	rBV	442341	359888	3.90%	1.093%
5	8.234	1006	1011	1014	rBV	1162634	972208	10.55%	2.952%
6	9.304	1189	1193	1196	rBV	816526	605660	6.57%	1.839%
7	9.992	1306	1310	1313	rVB	1069026	928722	10.07%	2.820%
8	10.775	1440	1443	1447	rBV	381718	321188	3.48%	0.975%
9	11.480	1559	1563	1566	rBV	1167372	945804	10.26%	2.872%
10	11.639	1587	1590	1593	rBV	266525	207640	2.25%	0.630%
11	11.863	1625	1628	1632	rBV	2467648	2146799	23.29%	6.518%
12	11.998	1645	1651	1655	rBV2	696782	992961	10.77%	3.015%
13	12.039	1655	1658	1661	rVB	605081	485385	5.27%	1.474%
14	12.563	1742	1747	1749	rBV	7680965	9218193	100.00%	27.988%
15	12.580	1749	1750	1756	rVV2	5569696	4602484	49.93%	13.974%
16	12.657	1760	1763	1766	rBV	1224918	1119863	12.15%	3.400%
17	12.698	1766	1770	1781	rVV	1111683	1571106	17.04%	4.770%
18	12.786	1783	1785	1789	rVB3	97533	104693	1.14%	0.318%
19	12.927	1804	1809	1815	rVB	346746	369360	4.01%	1.121%
20	13.022	1822	1825	1828	rBV	125659	110010	1.19%	0.334%
21	13.069	1830	1833	1836	rVV	708298	553258	6.00%	1.680%
22	13.386	1885	1887	1890	rVB	126793	92350	1.00%	0.280%
23	13.921	1974	1978	1981	rVV	496624	622580	6.75%	1.890%
24	13.957	1981	1984	1990	rVB	685357	732589	7.95%	2.224%
25	14.057	1996	2001	2004	rBV2	156036	238373	2.59%	0.724%
26	14.127	2009	2013	2016	rVV	1059109	1053965	11.43%	3.200%
27	14.151	2016	2017	2021	rVB	150152	119403	1.30%	0.363%
28	15.192	2191	2194	2198	rBV	111040	168504	1.83%	0.512%
29	15.574	2257	2259	2266	rVB	91628	111104	1.21%	0.337%
30	15.645	2267	2271	2282	rVB	531967	800168	8.68%	2.429%
31	17.262	2539	2546	2560	rVB	669925	1361586	14.77%	4.134%

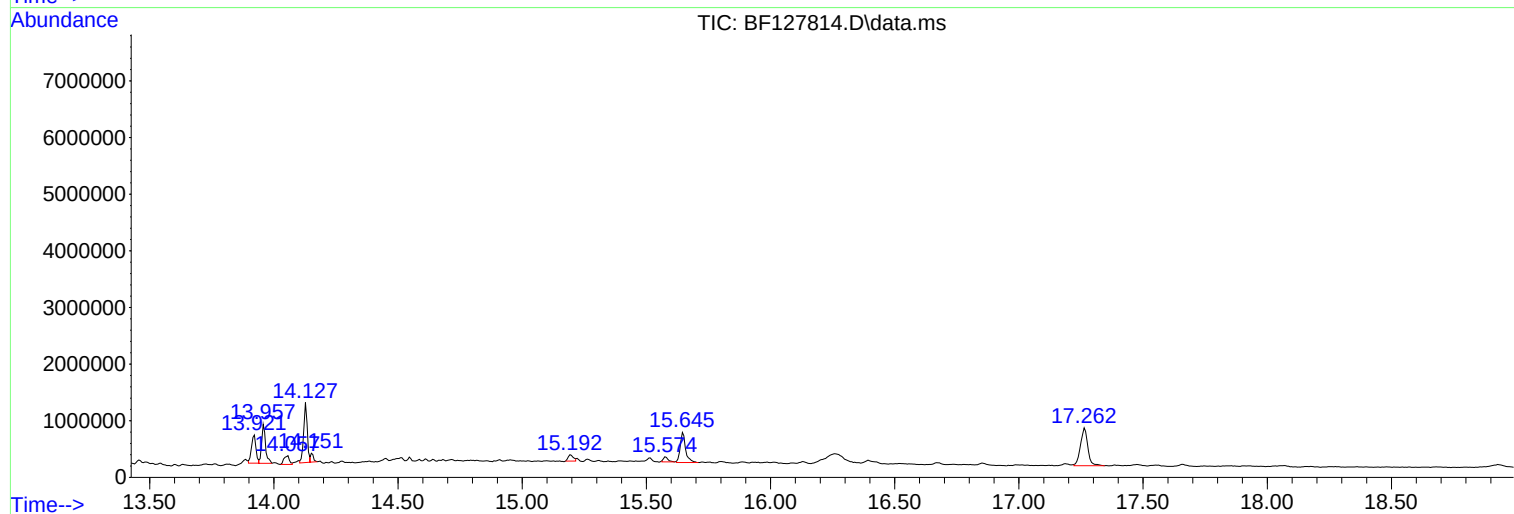
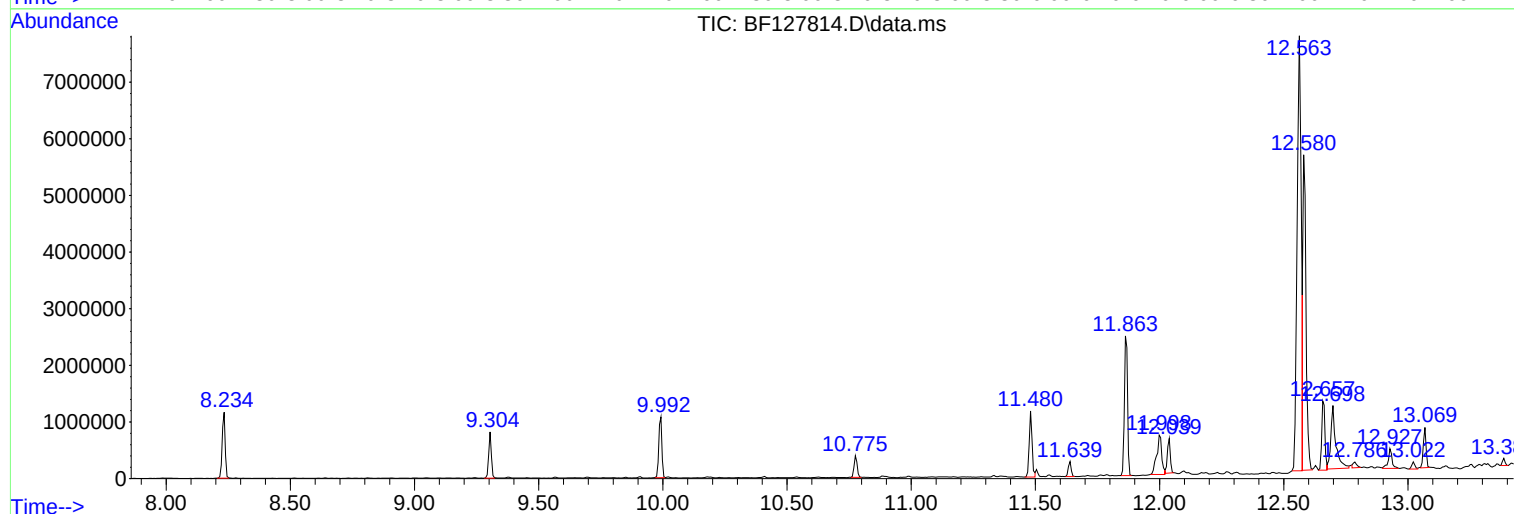
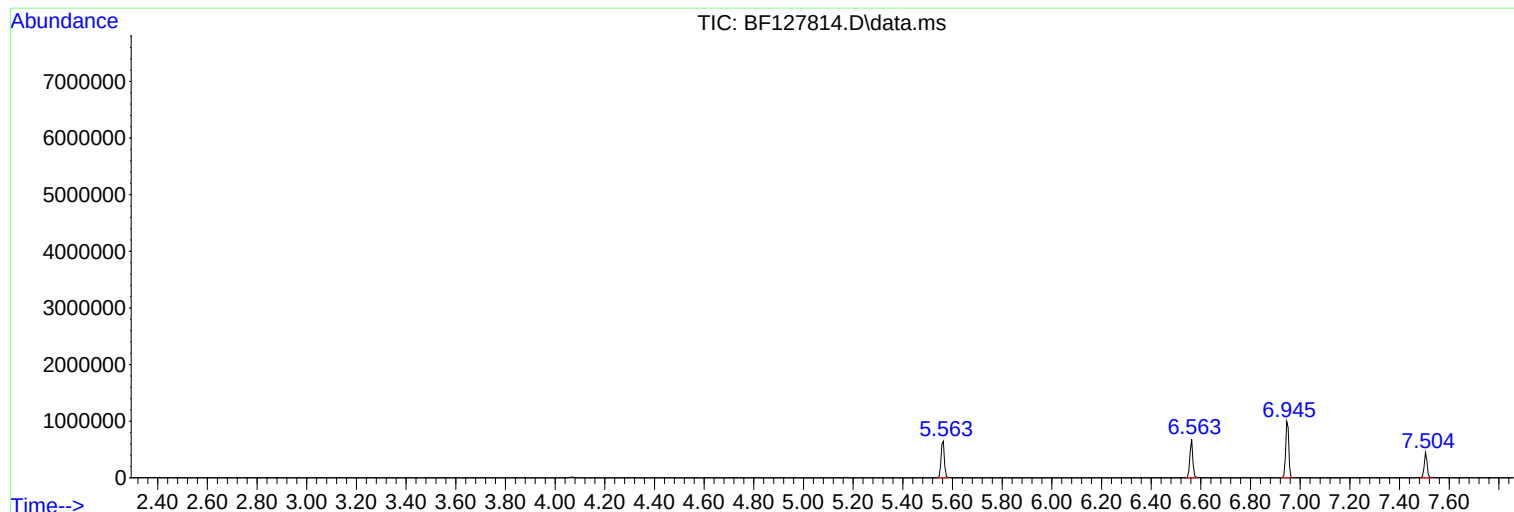
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF040622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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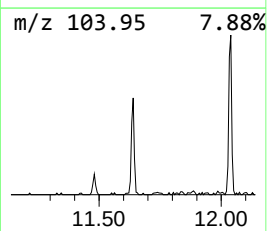
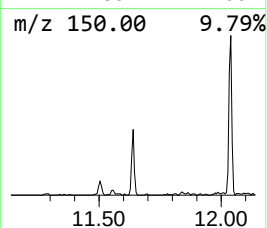
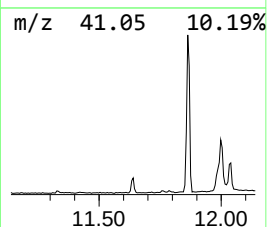
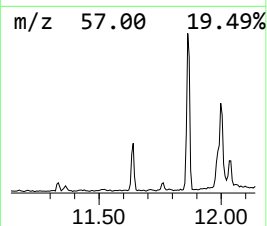
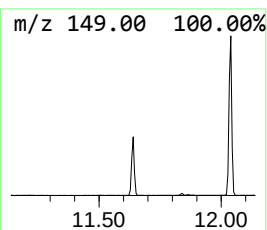
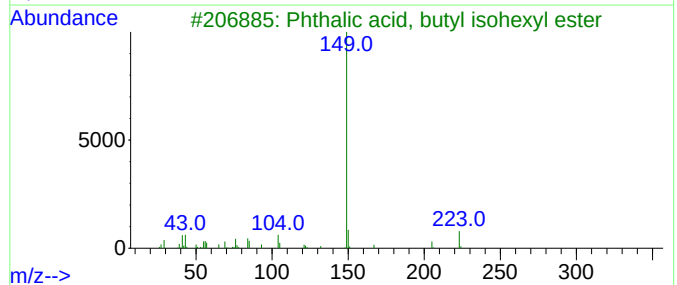
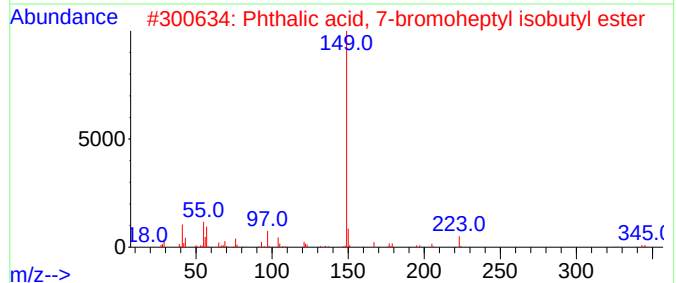
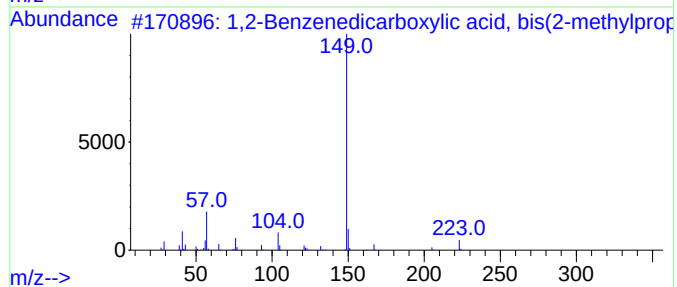
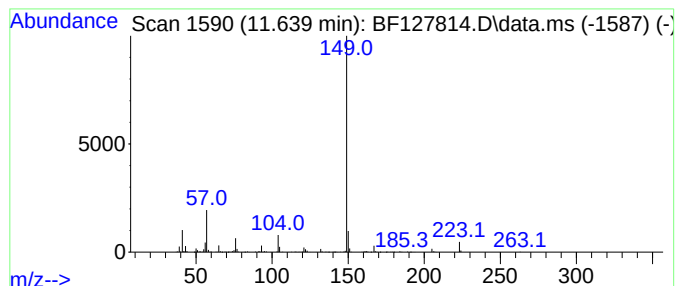
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 1,2-Benzenedicarboxylic aci... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.639	4.39 ng	207640	Phenanthrene-d10	11.480

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,2-Benzenedicarboxylic acid, bi...	278	C16H22O4	000084-69-5	91
2			Phthalic acid, 7-bromoheptyl iso...	398	C19H27BrO4	1000415-51-7	90
3			Phthalic acid, butyl isohexyl ester	306	C18H26O4	1000309-03-6	90
4			Dibutyl phthalate	278	C16H22O4	000084-74-2	86
5			Phthalic acid, decyl isobutyl ester	362	C22H34O4	1000308-94-2	83



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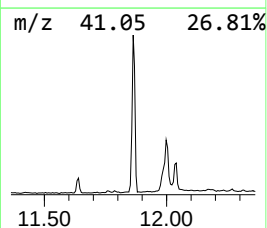
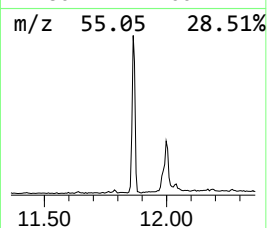
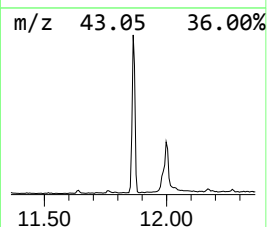
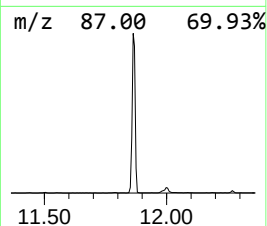
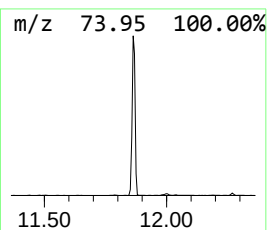
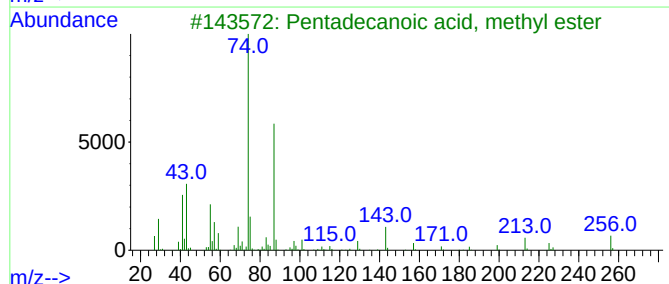
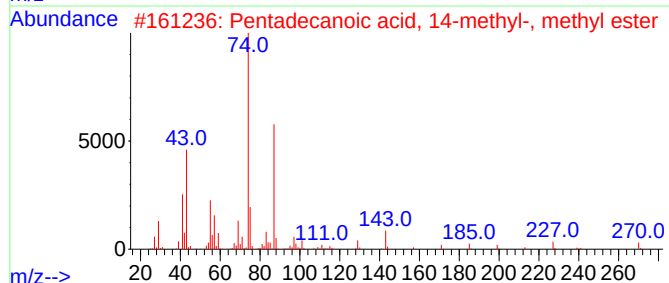
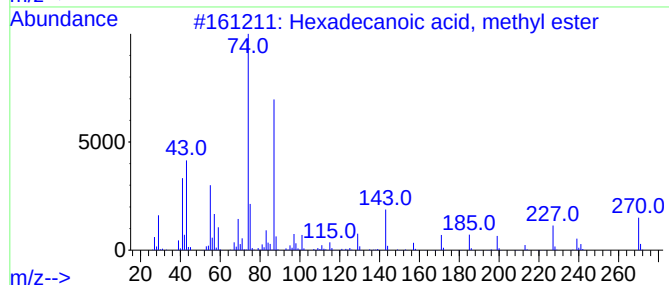
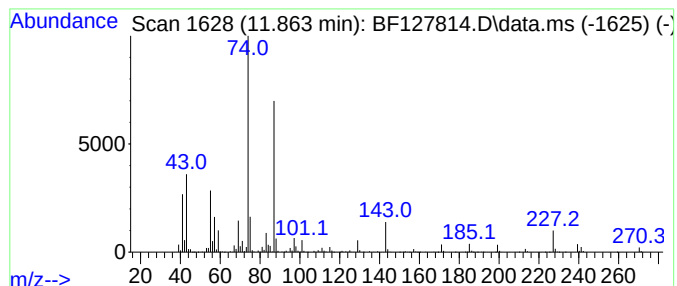
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Hexadecanoic acid, methyl e... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.863	45.40 ng	2146800	Phenanthrene-d10	11.480

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	91
2			Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	87
3			Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86
4			Methyl 11-methyl-dodecanoate	228	C14H28O2	1000336-45-1	80
5			Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	80



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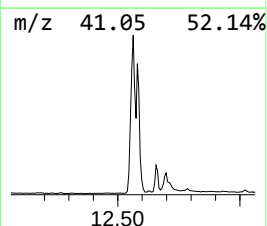
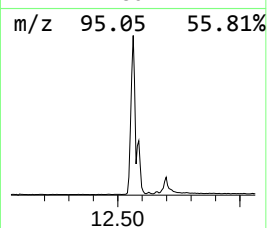
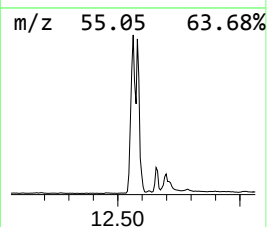
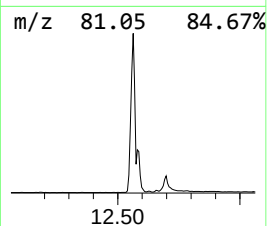
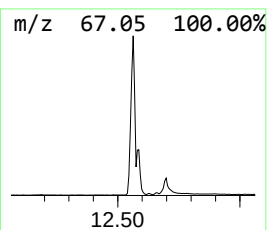
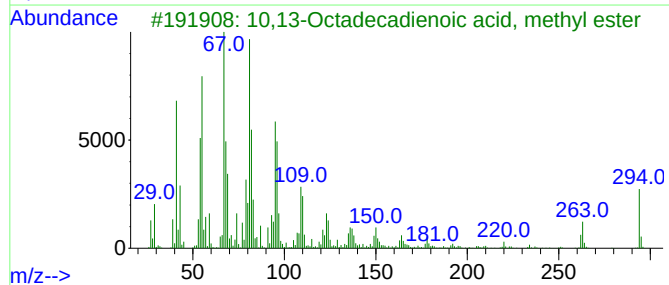
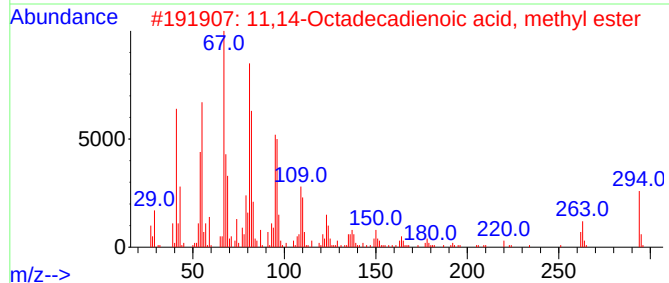
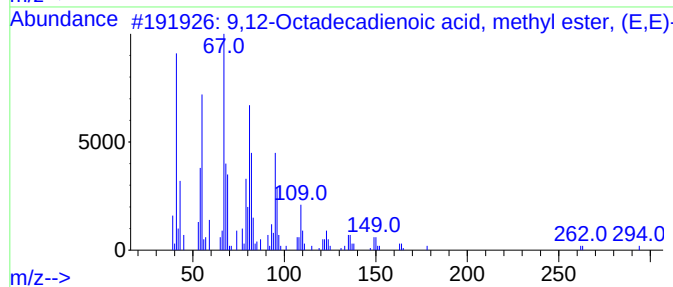
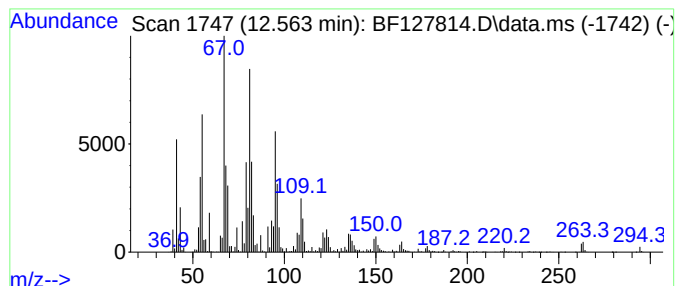
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Peak Number 3 9,12-Octadecadienoic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.563	194.93 ng	9218190	Phenanthrene-d10	11.480

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99		
2	11,14-Octadecadienoic acid, meth...	294	C19H34O2	056554-61-1	98		
3	10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	98		
4	Methyl 10-trans,12-cis-octadecad...	294	C19H34O2	1000336-44-2	98		
5	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	97		



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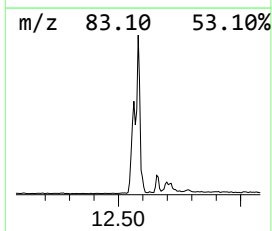
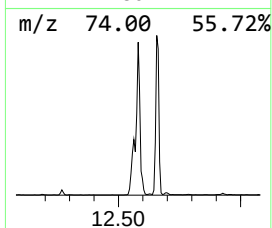
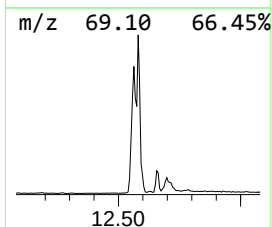
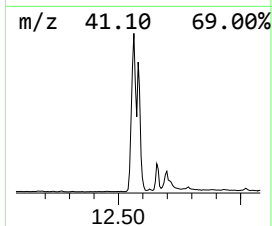
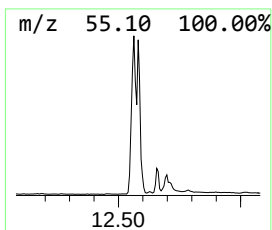
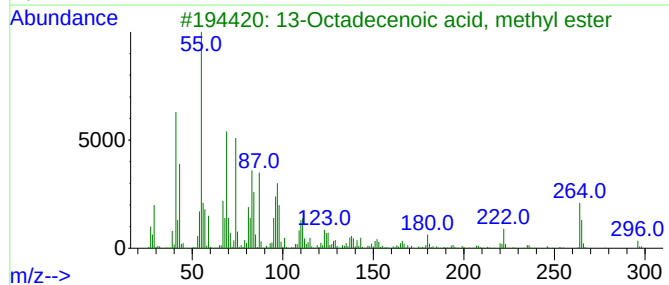
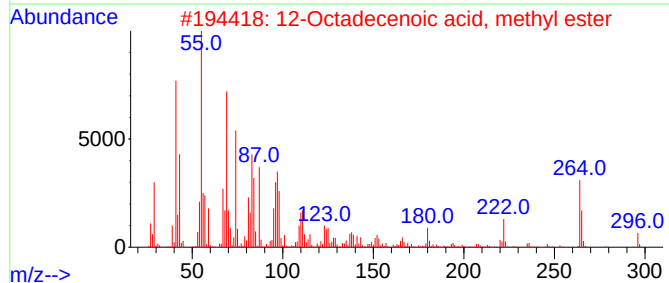
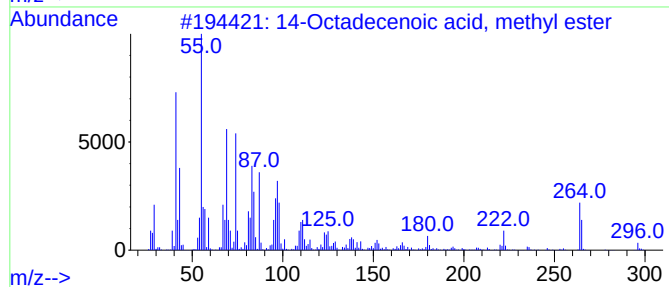
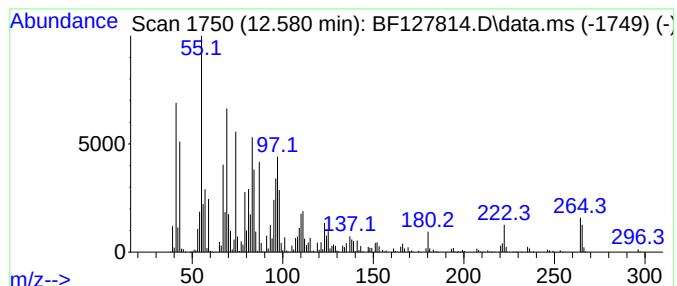
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 14-Octadecenoic acid, methyl... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.580	97.32 ng	4602480	Phenanthrene-d10		11.480	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	14-Octadecenoic acid, methyl ester		296	C19H36O2	056554-48-4	99
2	12-Octadecenoic acid, methyl ester		296	C19H36O2	056554-46-2	99
3	13-Octadecenoic acid, methyl ester		296	C19H36O2	056554-47-3	99
4	15-Octadecenoic acid, methyl ester		296	C19H36O2	004764-72-1	99
5	6-Octadecenoic acid, methyl ester		296	C19H36O2	052355-31-4	99



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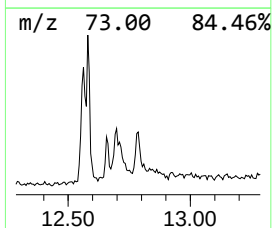
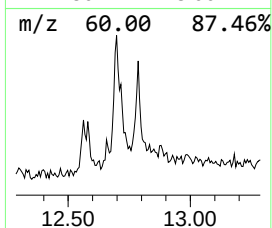
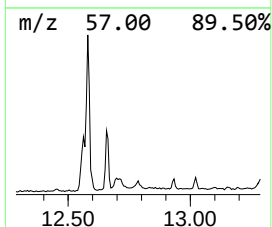
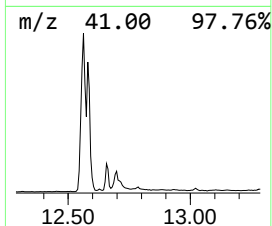
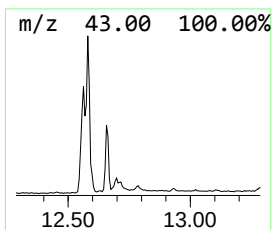
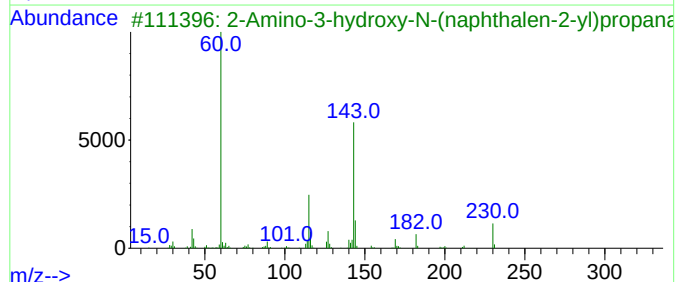
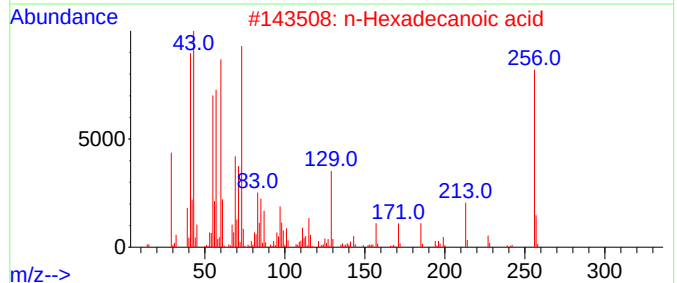
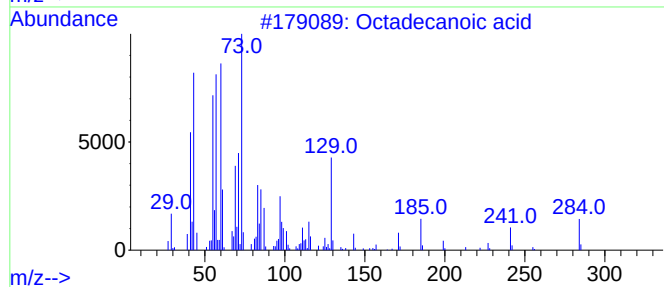
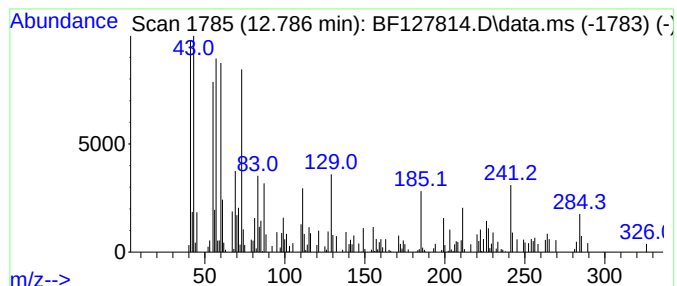
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Peak Number 5 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.786	2.21 ng	104693	Phenanthrene-d10	11.480

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	60
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	45
3			2-Amino-3-hydroxy-N-(naphthalen-...	230	C13H14N2O2	091806-63-2	42
4			n-Decanoic acid	172	C10H20O2	000334-48-5	41
5			Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NO5	029926-41-8	35



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TR-06-041422

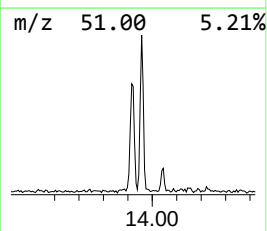
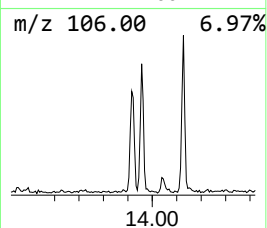
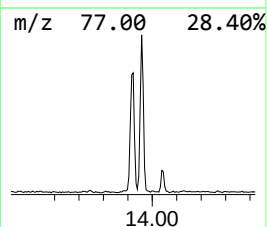
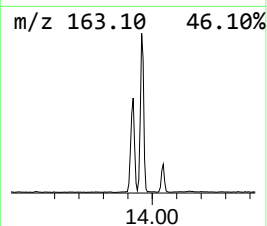
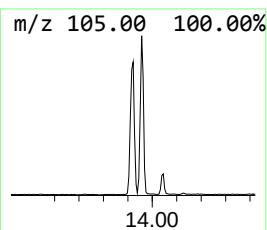
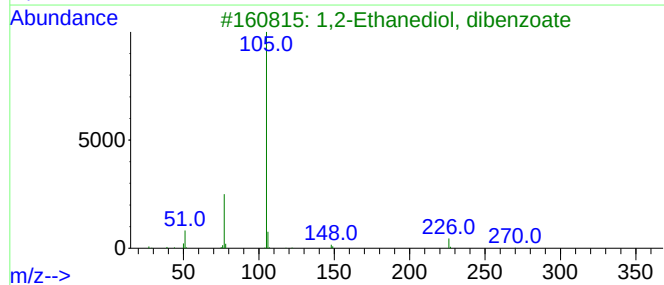
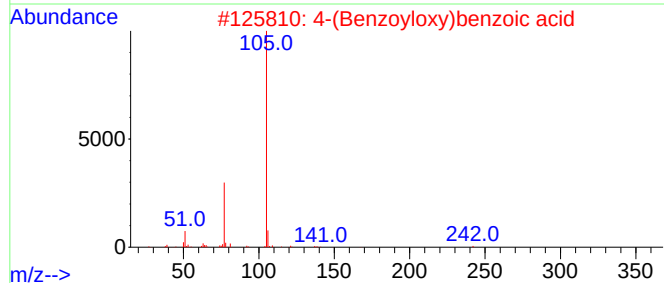
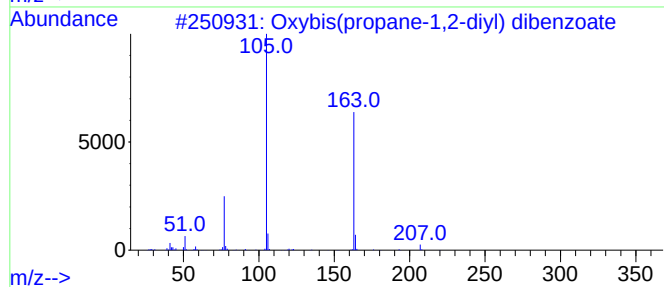
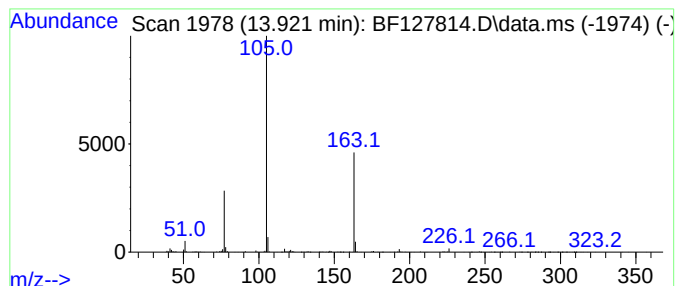
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Oxybis(propene-1,2-diyl) di... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.922	11.81 ng	622580	Chrysene-d12	14.127

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxybis(propene-1,2-diyl) dibenzoate	342	C20H22O5	000094-03-1	59
2			4-(Benzoyloxy)benzoic acid	242	C14H10O4	028547-23-1	35
3			1,2-Ethanediol, dibenzoate	270	C16H14O4	000094-49-5	35
4			Benzoic acid, 3-ethylphenyl ester	226	C15H14O2	1000360-68-3	35
5			Benzoic acid, 3-formylphenyl ester	226	C14H10O3	033696-06-9	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041522\
Data File : BF127814.D
Acq On : 15 Apr 2022 20:21
Operator : CG\JU
Sample : N2391-01 5X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-06-041422

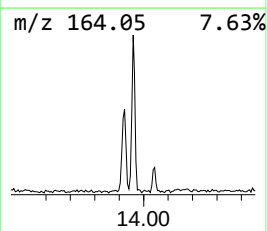
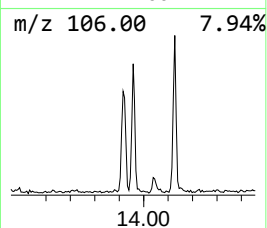
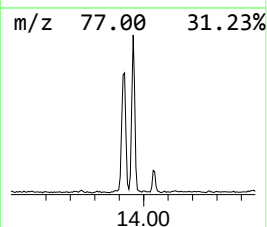
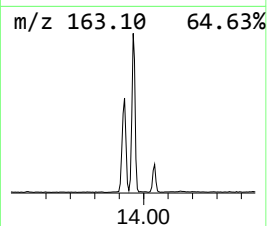
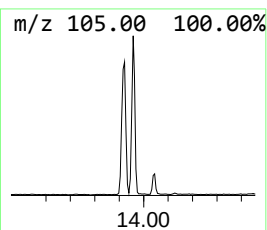
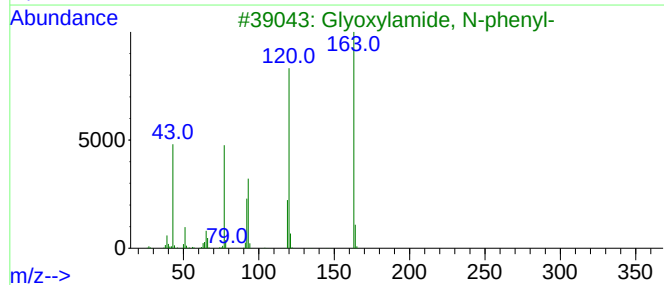
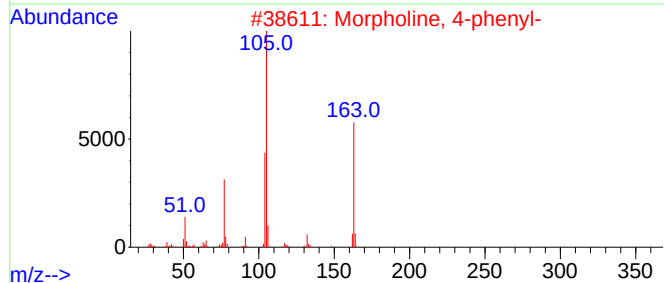
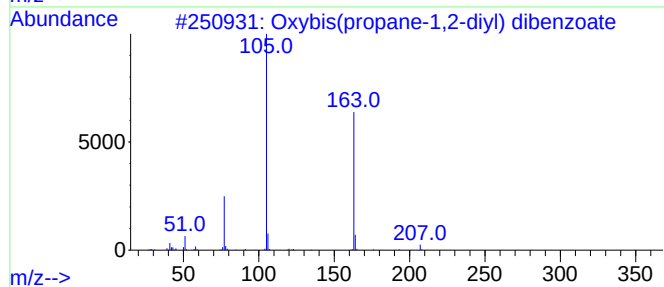
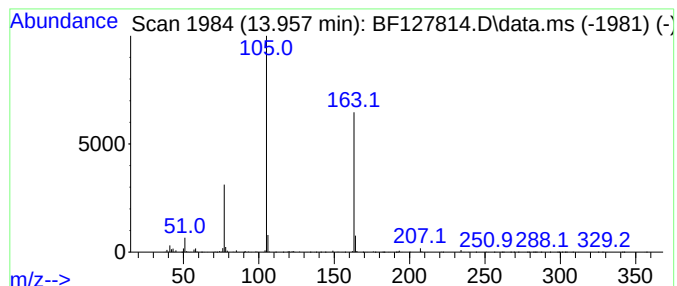
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Morpholine, 4-phenyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.957	13.90 ng	732589	Chrysene-d12	14.127

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxybis(propene-1,2-diyl) dibenzoate	342	C20H22O5	000094-03-1	86
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			Glyoxylic acid, phenyl-, (2'-ace...	268	C16H12O4	166538-12-1	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041522\
Data File : BF127814.D
Acq On : 15 Apr 2022 20:21
Operator : CG\JU
Sample : N2391-01 5X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-06-041422

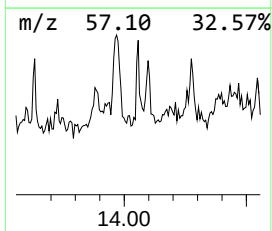
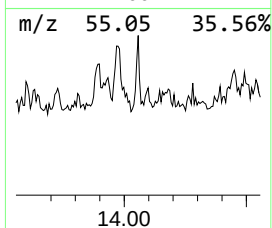
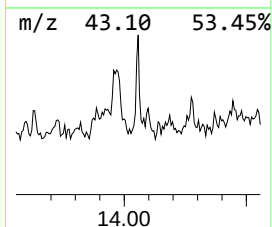
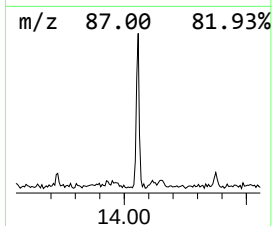
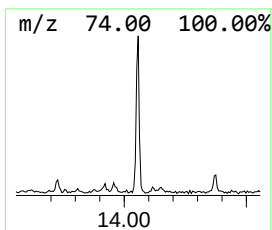
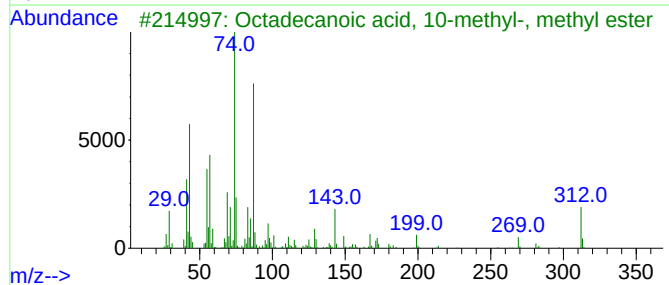
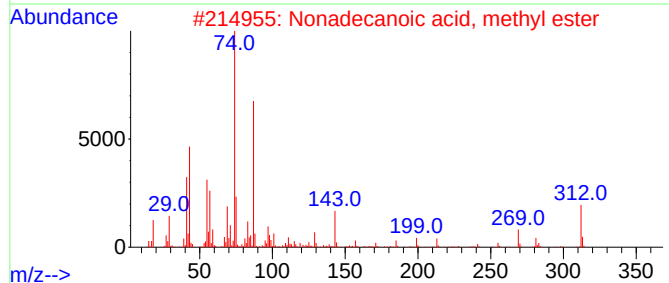
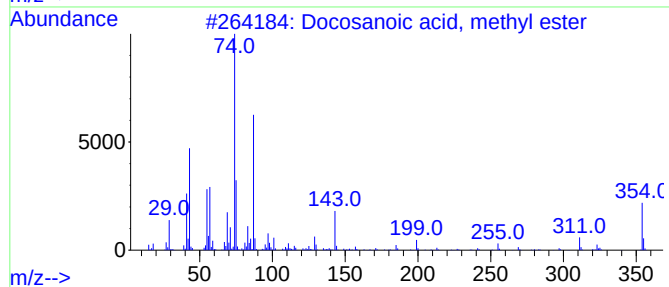
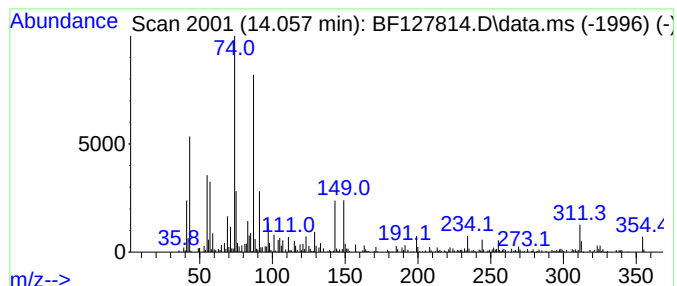
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Docosanoic acid, methyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.057	4.52 ng	238373	Chrysene-d12	14.127

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Docosanoic acid, methyl ester	354	C23H46O2	000929-77-1	96
2			Nonadecanoic acid, methyl ester	312	C20H40O2	001731-94-8	93
3			Octadecanoic acid, 10-methyl-, m...	312	C20H40O2	002490-19-9	81
4			Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	74
5			Methyl stearate	298	C19H38O2	000112-61-8	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041522\
Data File : BF127814.D
Acq On : 15 Apr 2022 20:21
Operator : CG\JU
Sample : N2391-01 5X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
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ClientSampleId :
TR-06-041422

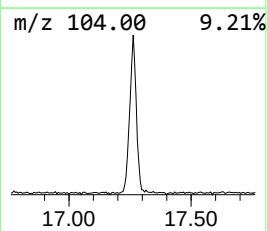
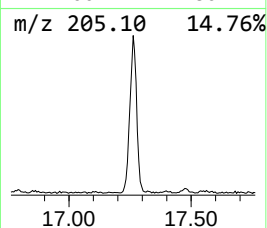
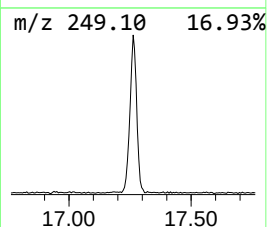
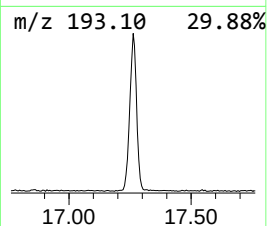
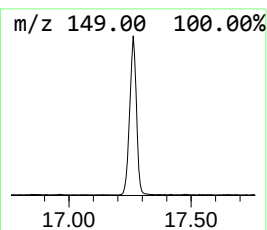
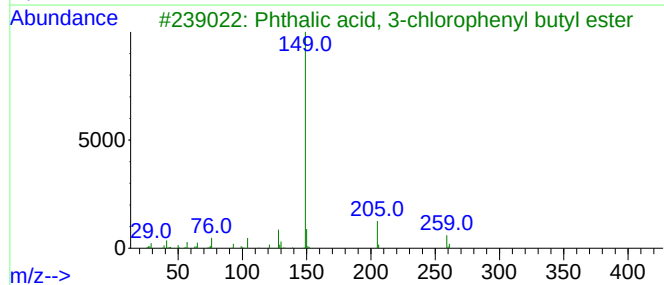
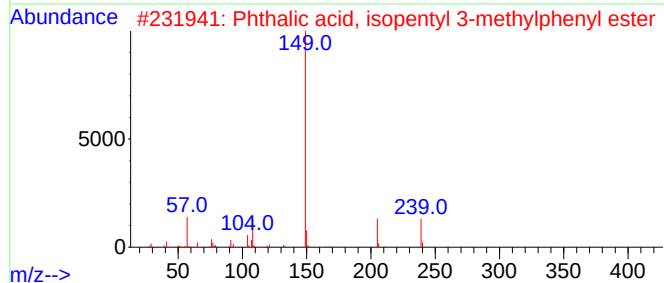
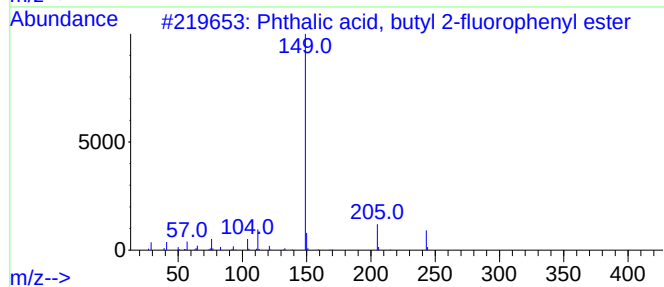
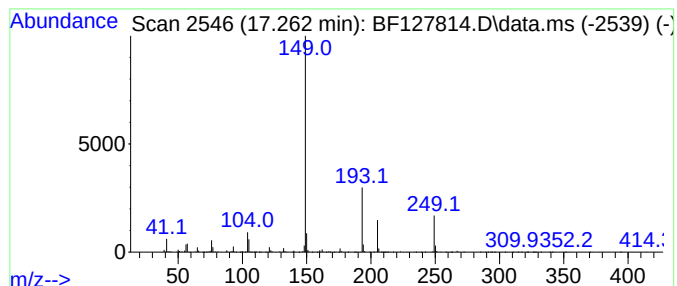
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Phthalic acid, butyl 2-fluo... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.262	34.03 ng	1361590	Perylene-d12	15.645

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phthalic acid, butyl 2-fluorophe...	316	C18H17F04	1000360-51-3	59
2			Phthalic acid, isopentyl 3-methy...	326	C20H22O4	1000315-37-2	59
3			Phthalic acid, 3-chlorophenyl bu...	332	C18H17ClO4	1000308-96-6	59
4			Phthalic acid, 3-ethylphenyl iso...	326	C20H22O4	1000357-07-7	59
5			Phthalic acid, butyl 2,4,5-trich...	400	C18H15Cl3O4	1000357-04-4	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041522\
Data File : BF127814.D
Acq On : 15 Apr 2022 20:21
Operator : CG\JU
Sample : N2391-01 5X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-06-041422

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF040622.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
1,2-Benzenedica...	11.639	4.4	ng	207640	4	11.480	945804	20.0
Hexadecanoic ac...	11.863	45.4	ng	2146800	4	11.480	945804	20.0
9,12-Octadecadi...	12.563	194.9	ng	9218190	4	11.480	945804	20.0
14-Octadecenoic...	12.580	97.3	ng	4602480	4	11.480	945804	20.0
Octadecanoic acid	12.786	2.2	ng	104693	4	11.480	945804	20.0
Oxybis(propane-...	13.922	11.8	ng	622580	5	14.127	1053970	20.0
Morpholine, 4-p...	13.957	13.9	ng	732589	5	14.127	1053970	20.0
Docosanoic acid...	14.057	4.5	ng	238373	5	14.127	1053970	20.0
Phthalic acid, ...	17.262	34.0	ng	1361590	6	15.645	800168	20.0