

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042623\
 Data File : BF133087.D
 Acq On : 27 Apr 2023 02:39
 Operator : CG\JU
 Sample : 02423-11 2X
 Misc :
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SPE-1WC-23-04-18

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-BF042123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133087.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.693	266	273	278	rBV	48085	69183	2.23%	0.238%
2	4.904	476	479	487	rBV	77951	96867	3.13%	0.334%
3	5.340	549	553	559	rVB	1117092	975463	31.48%	3.360%
4	6.175	689	695	700	rBV3	49693	61110	1.97%	0.210%
5	6.369	725	728	733	rBV	1144593	1045890	33.75%	3.602%
6	6.739	787	791	794	rBV	2177415	1916522	61.84%	6.601%
7	7.139	856	859	869	rBV4	33641	56209	1.81%	0.194%
8	7.292	879	885	888	rBV	865939	740385	23.89%	2.550%
9	8.022	1005	1009	1012	rBV	3287289	2552659	82.37%	8.792%
10	8.733	1128	1130	1135	rVB	74795	60765	1.96%	0.209%
11	8.781	1135	1138	1144	rVB	109799	112079	3.62%	0.386%
12	9.092	1188	1191	1194	rVB	1670109	1275009	41.14%	4.392%
13	9.633	1278	1283	1287	rBV	70529	82784	2.67%	0.285%
14	9.775	1303	1307	1310	rVV	3013973	2415772	77.95%	8.321%
15	9.804	1310	1312	1319	rVB2	65899	71211	2.30%	0.245%
16	9.975	1338	1341	1346	rBV2	65688	65516	2.11%	0.226%
17	10.180	1372	1376	1379	rBV3	46135	59639	1.92%	0.205%
18	10.316	1397	1399	1406	rVB4	45856	54630	1.76%	0.188%
19	10.480	1423	1427	1430	rBV	239436	203617	6.57%	0.701%
20	10.557	1436	1440	1445	rBV	576390	498679	16.09%	1.718%
21	10.686	1459	1462	1466	rBV3	77246	114361	3.69%	0.394%
22	10.769	1473	1476	1478	rBV3	60057	62856	2.03%	0.217%
23	10.910	1496	1500	1502	rBV	826093	648563	20.93%	2.234%
24	11.257	1555	1559	1561	rBV	2417306	2150475	69.39%	7.407%
25	11.274	1561	1562	1565	rVV	477851	394528	12.73%	1.359%
26	11.327	1568	1571	1574	rVB	182226	179886	5.80%	0.620%
27	11.480	1595	1597	1600	rBV	82481	68993	2.23%	0.238%
28	11.792	1646	1650	1654	rBV2	616156	685107	22.11%	2.360%
29	12.069	1695	1697	1702	rVB	293692	282464	9.11%	0.973%
30	12.463	1762	1764	1768	rVB	703347	616230	19.88%	2.123%
31	12.580	1782	1784	1787	rBV	233708	231064	7.46%	0.796%
32	12.692	1801	1803	1806	rVB	696149	584358	18.86%	2.013%
33	12.839	1825	1828	1832	rBV	1081982	1001873	32.33%	3.451%
34	13.898	2004	2008	2011	rBV2	1610575	1805676	58.26%	6.219%
35	14.110	2041	2044	2049	rVB	2892363	2767675	89.31%	9.533%
36	14.262	2068	2070	2073	rVB	692287	609433	19.66%	2.099%

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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-BF042123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.333	2250	2252	2264	rVB	958647	1316079	42.47%	4.533%
38	16.339	2417	2423	2433	rVB	1711406	3099113	100.00%	10.675%

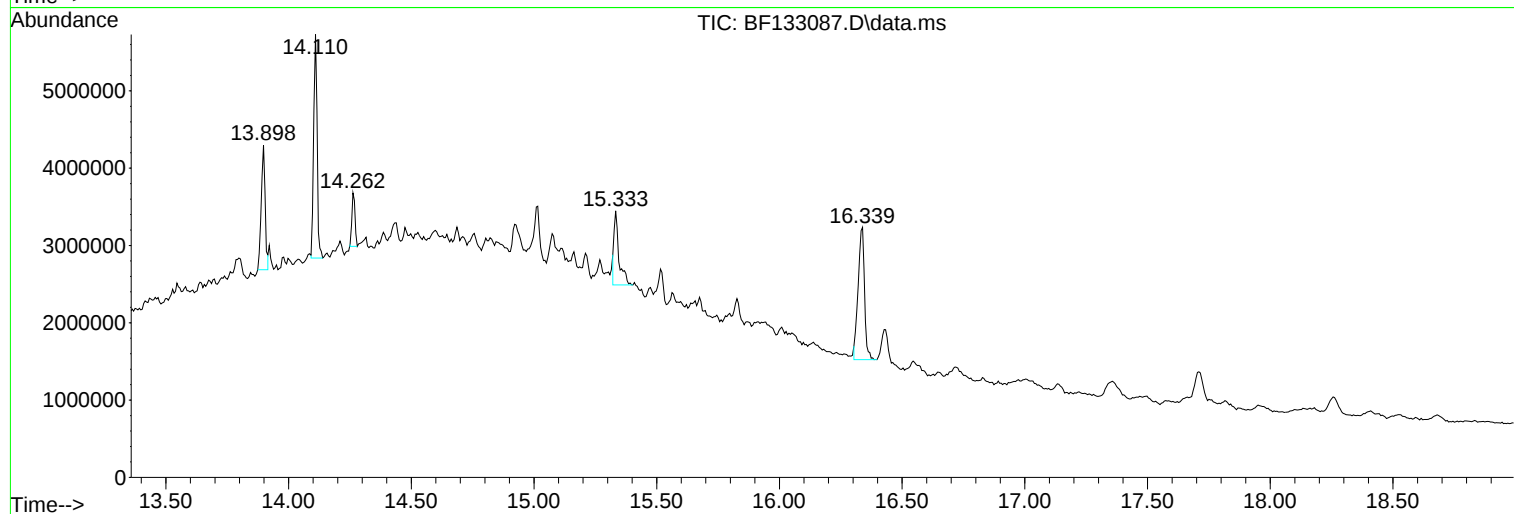
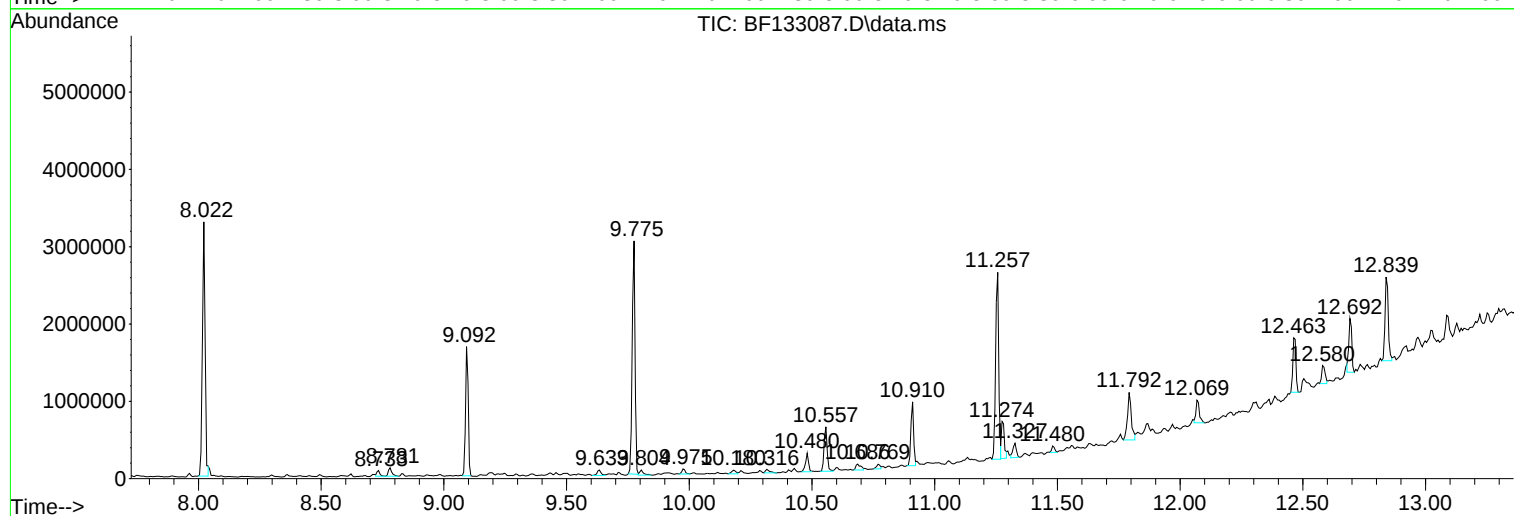
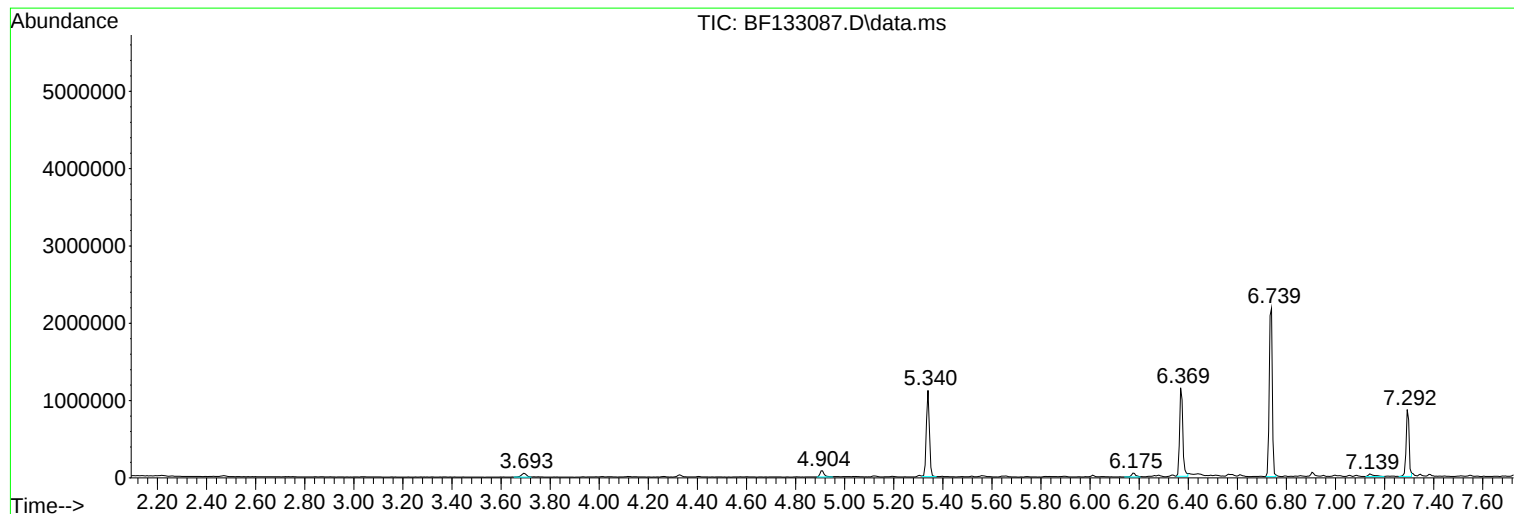
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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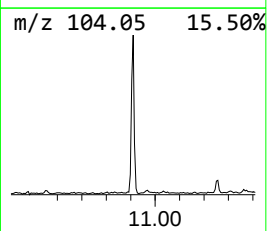
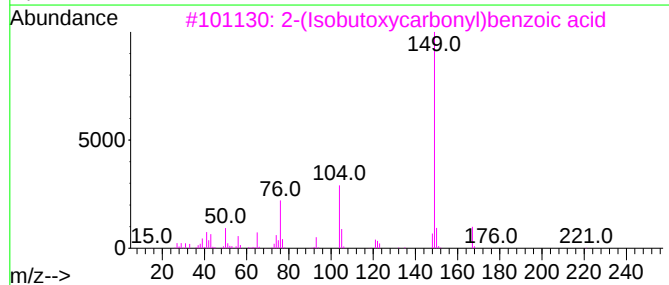
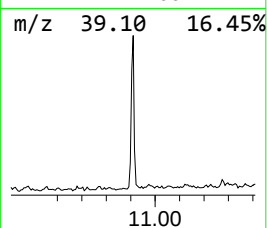
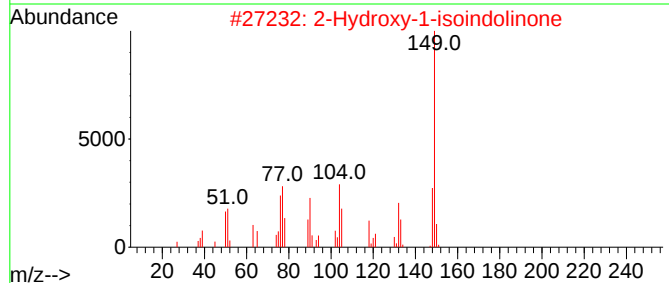
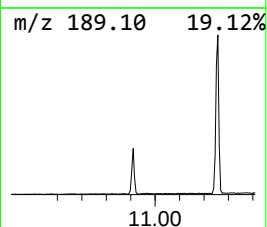
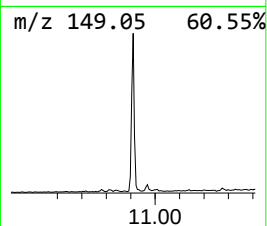
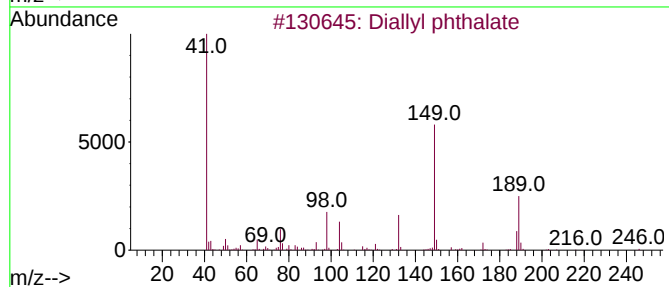
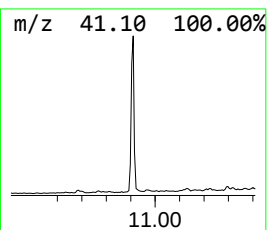
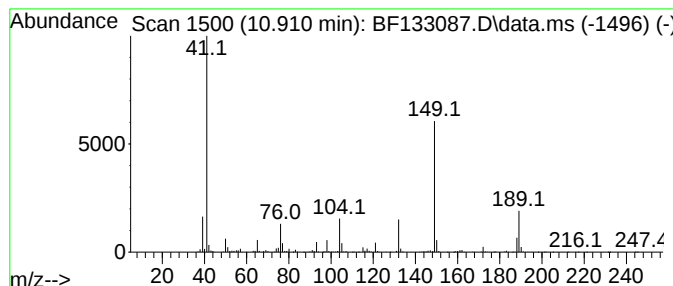
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Diallyl phthalate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.910	6.03 ng	648563	Phenanthrene-d10	11.257

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diallyl phthalate	246	C14H14O4	000131-17-9	64
2			2-Hydroxy-1-isoindolinone	149	C8H7NO2	1000289-12-0	58
3			2-(Isobutoxycarbonyl)benzoic acid	222	C12H14O4	030833-53-5	47
4			1H-Pyrrole-3-propanenitrile, 4-(...	189	C10H11N3O	103548-59-0	45
5			2-((Prop-2-ynyloxy)carbonyl)benz...	204	C11H8O4	006139-61-3	40



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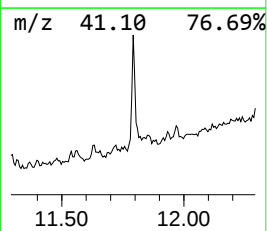
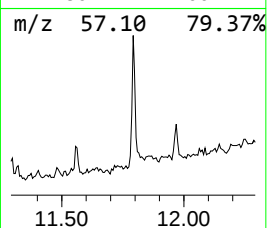
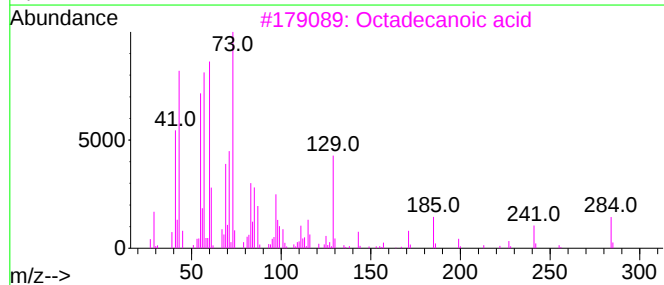
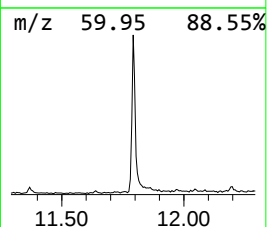
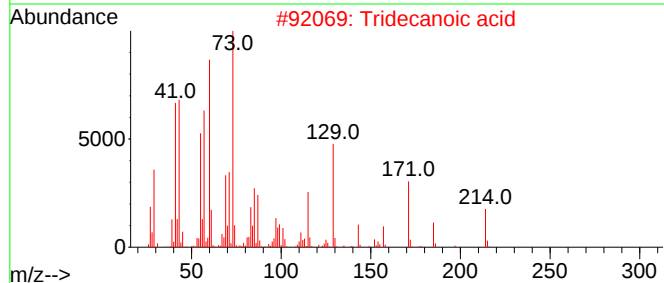
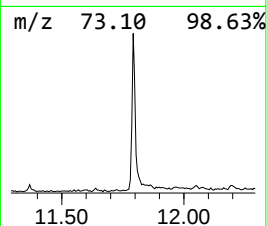
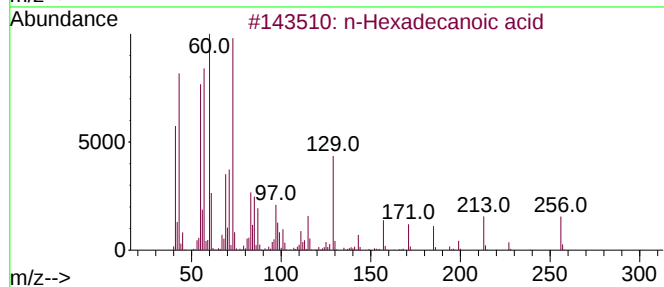
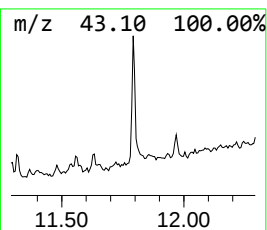
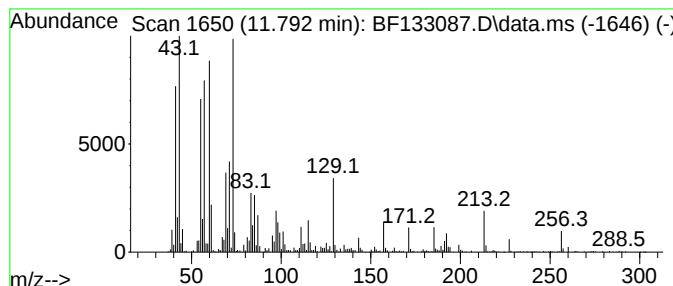
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.792	6.37 ng	685107	Phenanthrene-d10	11.257

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	93
3			Octadecanoic acid	284	C18H36O2	000057-11-4	93
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	92
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	76



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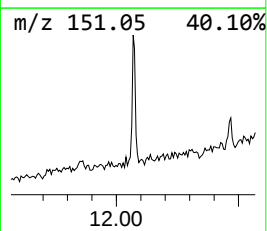
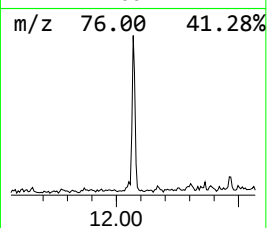
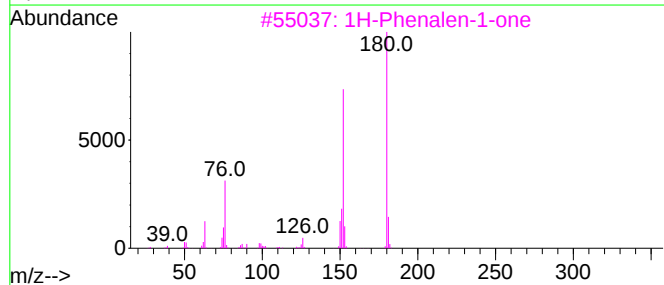
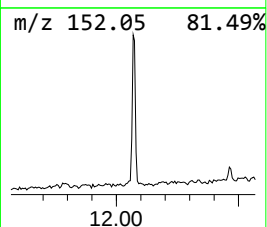
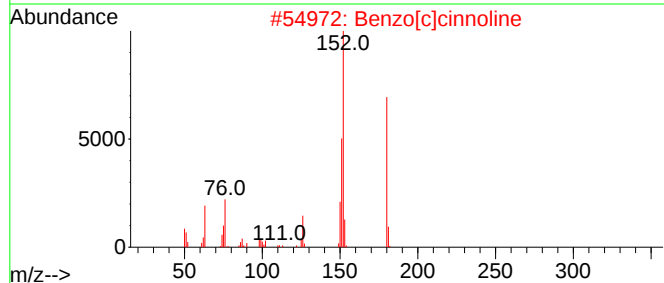
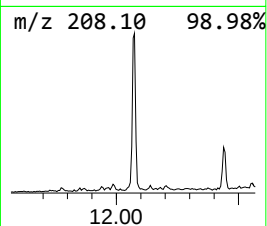
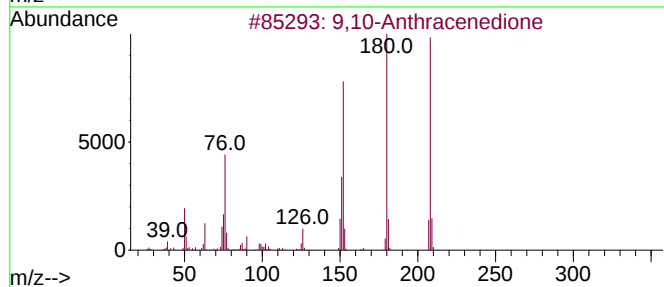
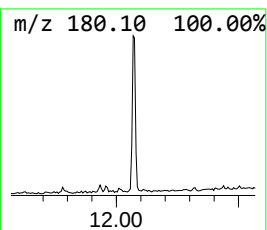
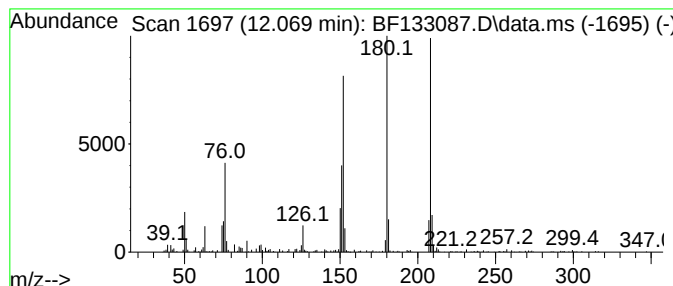
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 9,10-Anthracenedione Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.069	2.63 ng	282464	Phenanthrene-d10	11.257

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9,10-Anthracenedione	208	C14H8O2	000084-65-1	99
2			Benzo[c]cinnoline	180	C12H8N2	000230-17-1	64
3			1H-Phenalen-1-one	180	C13H8O	000548-39-0	60
4			9H-Fluoren-9-one	180	C13H8O	000486-25-9	58
5			Diphenic anhydride	224	C14H8O3	006050-13-1	52



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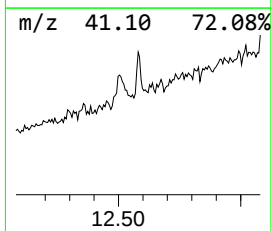
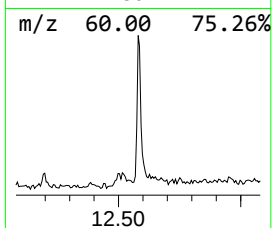
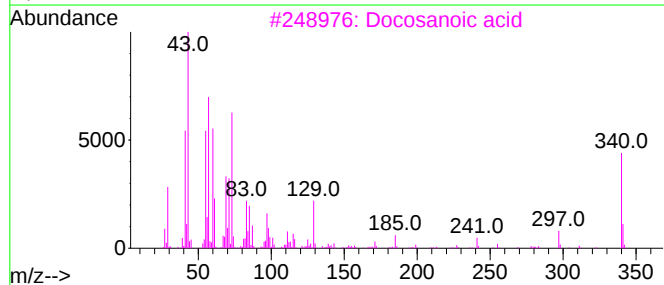
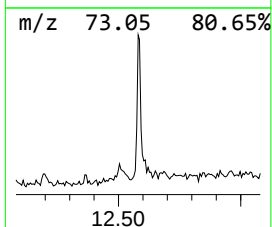
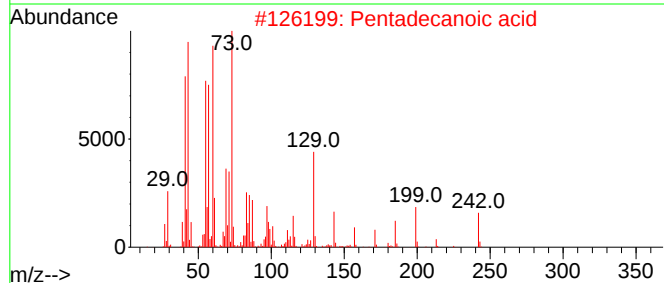
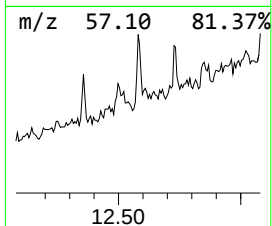
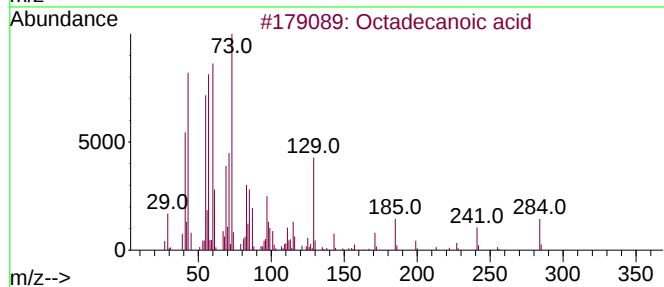
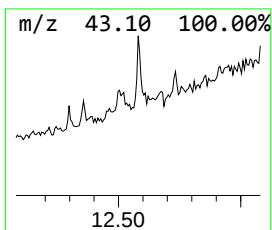
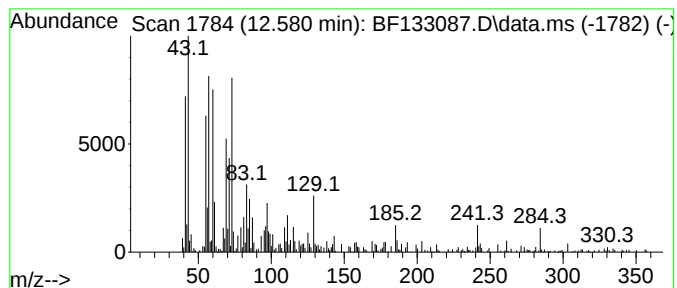
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.580	2.56 ng	231064	Chrysene-d12	13.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	98
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3			Docosanoic acid	340	C22H44O2	000112-85-6	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5			Undecanoic acid	186	C11H22O2	000112-37-8	64



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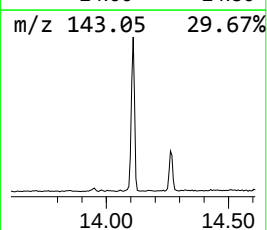
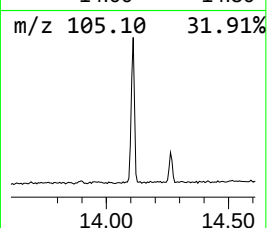
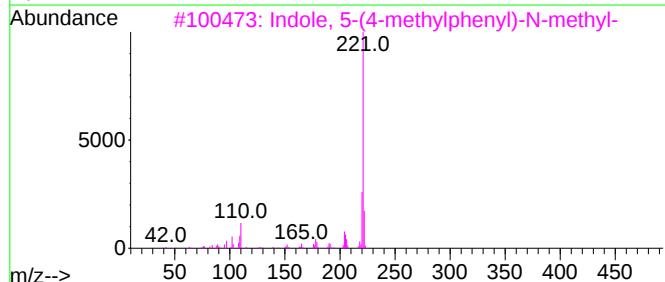
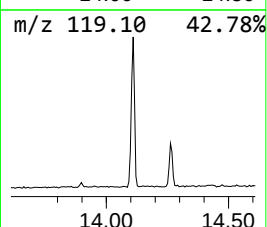
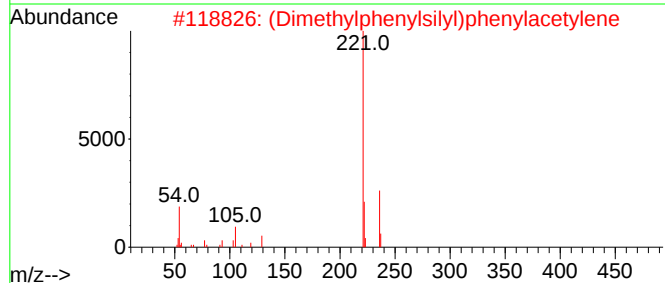
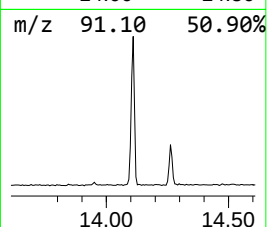
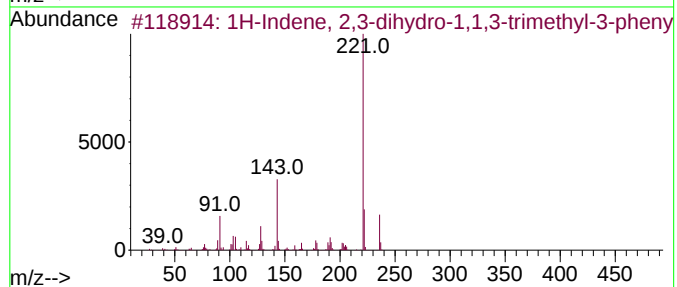
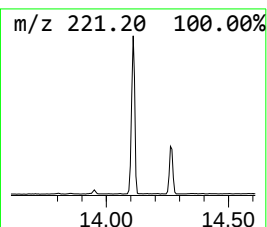
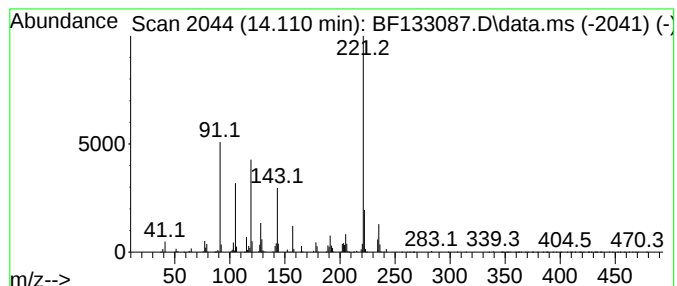
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown14.110 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.110	30.66 ng	2767680	Chrysene-d12	13.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Indene, 2,3-dihydro-1,1,3-tri...	236	C18H20	003910-35-8	47
2			(Dimethylphenylsilyl)phenylacety...	236	C16H16Si	1000434-31-1	43
3			Indole, 5-(4-methylphenyl)-N-met...	221	C16H15N	1000380-54-7	43
4			2-Pentene, 4-methyl-2,4-diphenyl-	236	C18H20	006258-73-7	40
5			Oxazole, 2,5-diphenyl-	221	C15H11NO	000092-71-7	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042623\
Data File : BF133087.D
Acq On : 27 Apr 2023 02:39
Operator : CG\JU
Sample : 02423-11 2X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SPE-1WC-23-04-18

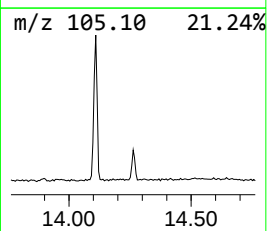
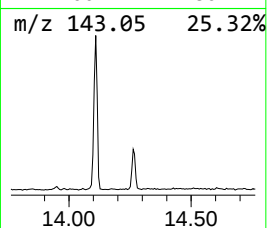
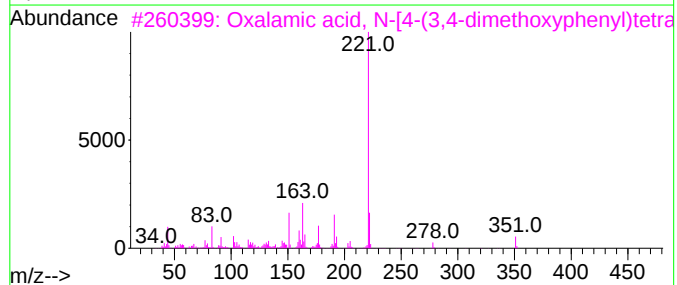
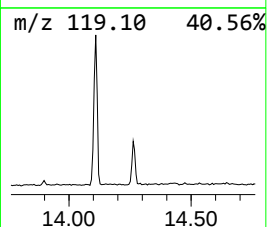
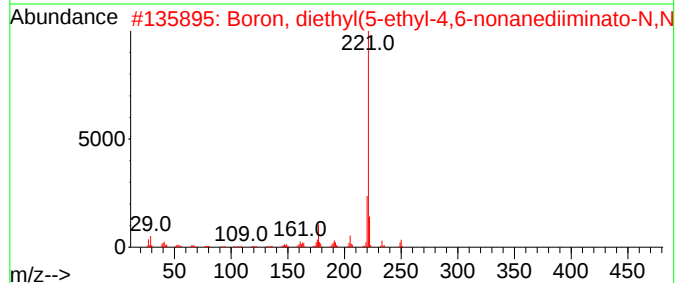
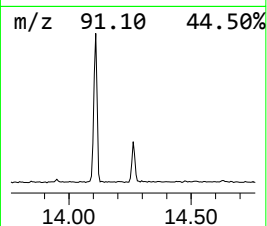
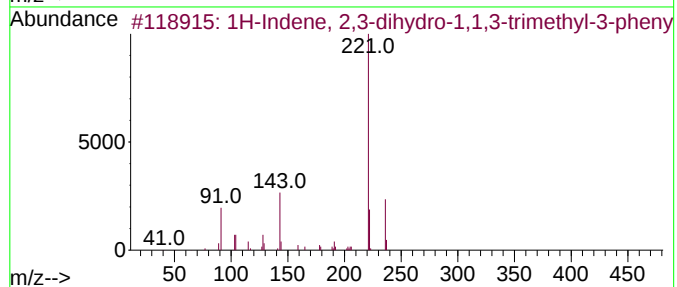
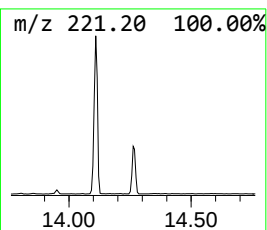
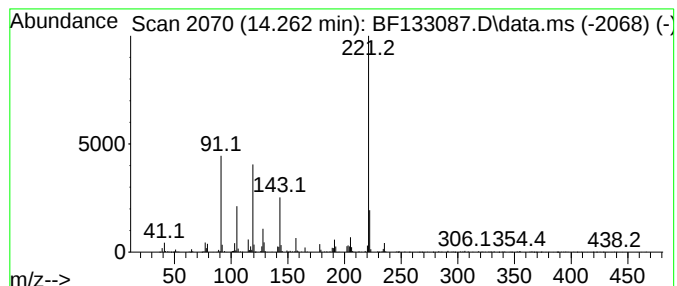
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown14.262 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.262	6.75 ng	609433	Chrysene-d12	13.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Indene, 2,3-dihydro-1,1,3-tri...	236	C18H20	003910-35-8	40
2			Boron, diethyl(5-ethyl-4,6-nonan...	250	C15H31BN2	136705-03-8	38
3			Oxalamic acid, N-[4-(3,4-dimetho...	351	C18H25N06	1000295-43-8	38
4			Indole, 5-(4-methylphenyl)-N-met...	221	C16H15N	1000380-54-7	32
5			benzonitrile, 4-[2-(4-chlorophen...	360	C19H13ClN6	1000398-49-8	32



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042623\
Data File : BF133087.D
Acq On : 27 Apr 2023 02:39
Operator : CG\JU
Sample : 02423-11 2X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SPE-1WC-23-04-18

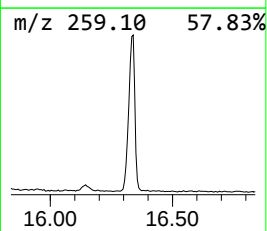
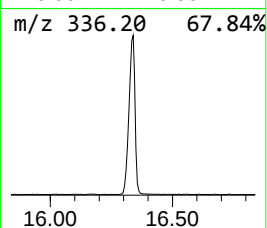
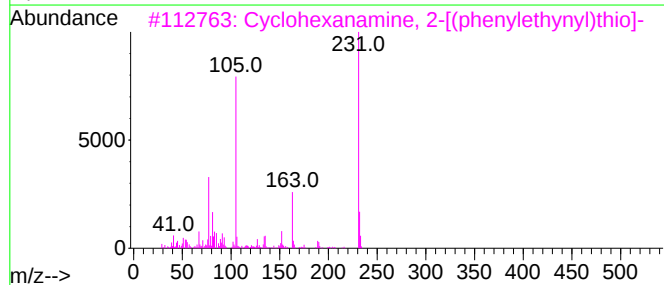
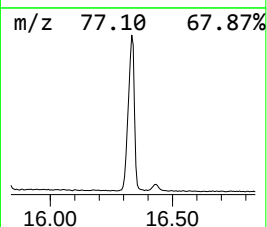
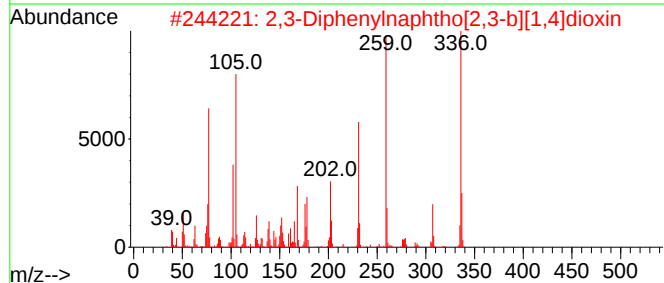
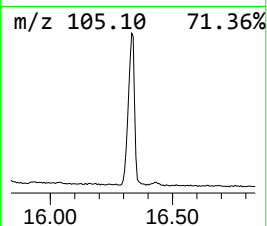
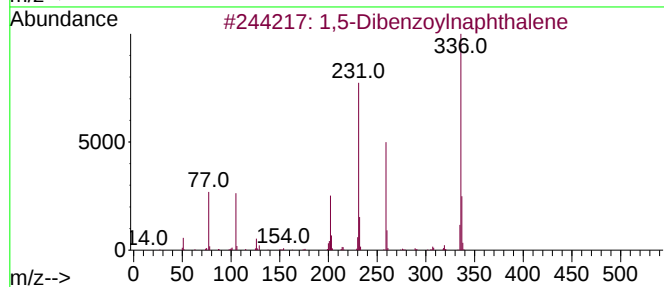
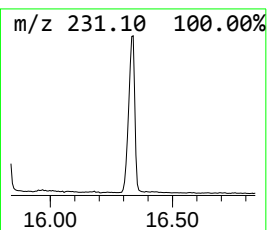
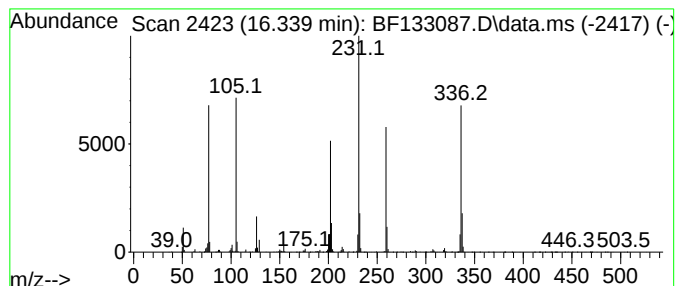
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1,5-Dibenzoylnaphthalene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.339	47.10 ng	3099110	Perylene-d12	15.333

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,5-Dibenzoylnaphthalene	336	C24H16O2	000083-80-7	99
2			2,3-Diphenylnaphtho[2,3-b][1,4]d...	336	C24H16O2	091201-57-9	46
3			Cyclohexanamine, 2-[(phenylethyn...	231	C14H17NS	1000327-34-1	27
4			Ethyl 5-oxo-1-phenyl-4-phenylazo...	336	C18H16N4O3	007171-33-7	22
5			Benzene, 1-nitro-4-(phenylthio)-	231	C12H9NO2S	000952-97-6	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042623\
Data File : BF133087.D
Acq On : 27 Apr 2023 02:39
Operator : CG\JU
Sample : 02423-11 2X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SPE-1WC-23-04-18

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.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
Diallyl phthalate	10.910	6.0	ng	648563	4	11.257	2150480	20.0
n-Hexadecanoic ...	11.792	6.4	ng	685107	4	11.257	2150480	20.0
9,10-Anthracene...	12.069	2.6	ng	282464	4	11.257	2150480	20.0
Octadecanoic acid	12.580	2.6	ng	231064	5	13.898	1805680	20.0
unknown14.110	14.110	30.7	ng	2767680	5	13.898	1805680	20.0
unknown14.262	14.262	6.8	ng	609433	5	13.898	1805680	20.0
1,5-Dibenzoylna...	16.339	47.1	ng	3099110	6	15.333	1316080	20.0