

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020723\
 Data File : BF132343.D
 Acq On : 07 Feb 2023 14:23
 Operator : CG\JU
 Sample : 01442-01
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B-01-SB02

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-BF013123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132343.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.301	409	419	426	rBV	1179677	1759042	27.56%	3.505%
2	5.684	478	484	487	rBV	3848781	4232894	66.32%	8.435%
3	6.678	646	653	656	rBV	3345063	4223645	66.18%	8.417%
4	7.048	713	716	720	rBV	1152315	960146	15.04%	1.913%
5	7.619	807	813	816	rBV	2823782	2842737	44.54%	5.665%
6	7.819	816	847	850	rBV	1367564	6382338	100.00%	12.719%
7	8.336	931	935	938	rBV	1664777	1283470	20.11%	2.558%
8	9.413	1114	1118	1122	rBV	5783295	5538900	86.78%	11.038%
9	10.101	1231	1235	1238	rBV	1924149	1542893	24.17%	3.075%
10	10.172	1242	1247	1253	rBV	63031	85140	1.33%	0.170%
11	10.278	1259	1265	1269	rBV2	49535	83916	1.31%	0.167%
12	10.819	1353	1357	1360	rVB	1677872	1386143	21.72%	2.762%
13	10.895	1365	1370	1373	rBV	4683020	4377787	68.59%	8.724%
14	11.125	1405	1409	1412	rBV	197839	155791	2.44%	0.310%
15	11.377	1447	1452	1460	rBV2	46249	75185	1.18%	0.150%
16	11.595	1485	1489	1493	rBV	2005890	1694829	26.55%	3.377%
17	12.107	1569	1576	1592	rBV	1202639	1536465	24.07%	3.062%
18	12.813	1690	1696	1704	rBV2	83536	157046	2.46%	0.313%
19	12.895	1704	1710	1719	rBV	436844	472421	7.40%	0.941%
20	13.048	1731	1736	1746	rVB	272627	380027	5.95%	0.757%
21	13.195	1755	1761	1764	rVB	6299942	6306297	98.81%	12.567%
22	13.748	1844	1855	1858	rBV2	70702	115684	1.81%	0.231%
23	13.871	1872	1876	1883	rVB	123187	124769	1.95%	0.249%
24	14.077	1908	1911	1919	rBV	502769	789616	12.37%	1.574%
25	14.183	1923	1929	1933	rVV3	77785	193448	3.03%	0.385%
26	14.254	1937	1941	1944	rVV	1434815	1389891	21.78%	2.770%
27	14.277	1944	1945	1953	rVB	73271	69992	1.10%	0.139%
28	14.348	1953	1957	1962	rBV	149558	176164	2.76%	0.351%
29	14.460	1972	1976	1982	rVB	71192	89792	1.41%	0.179%
30	14.707	2015	2018	2020	rBV	59032	69409	1.09%	0.138%
31	14.730	2020	2022	2033	rVB4	75507	158461	2.48%	0.316%
32	15.130	2086	2090	2097	rVB	120003	136986	2.15%	0.273%
33	15.830	2203	2209	2213	rBV2	823352	1130978	17.72%	2.254%
34	16.742	2355	2364	2374	rBV2	39706	183268	2.87%	0.365%
35	16.895	2387	2390	2401	rVB6	34964	75904	1.19%	0.151%

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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-BF013123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

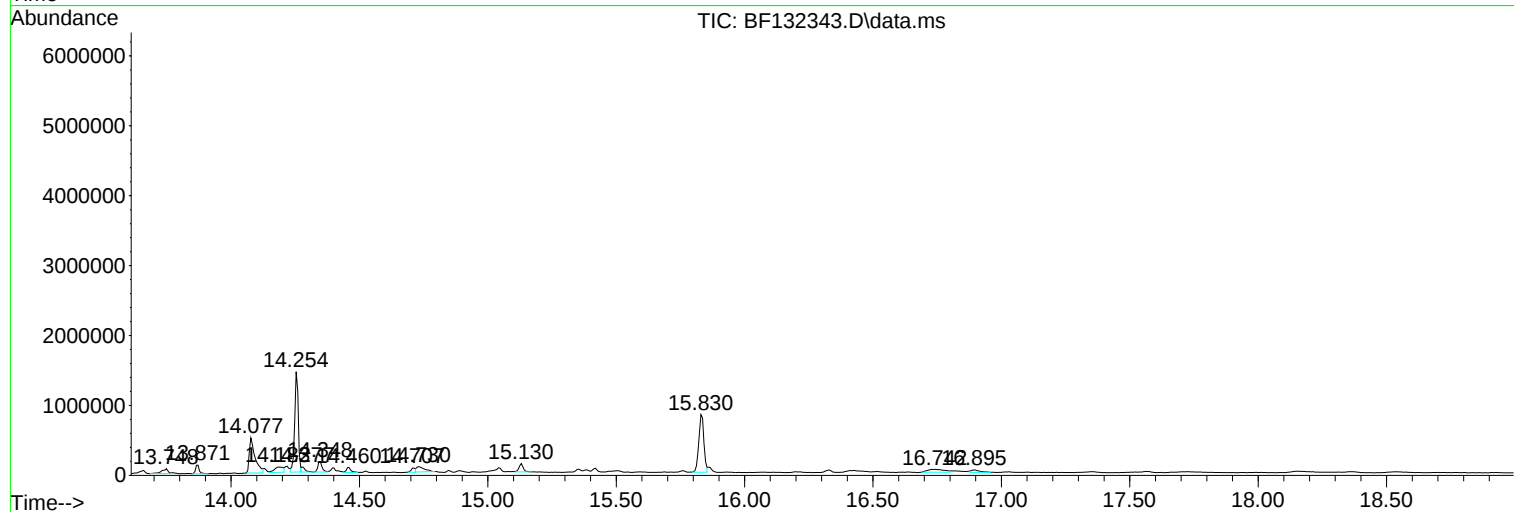
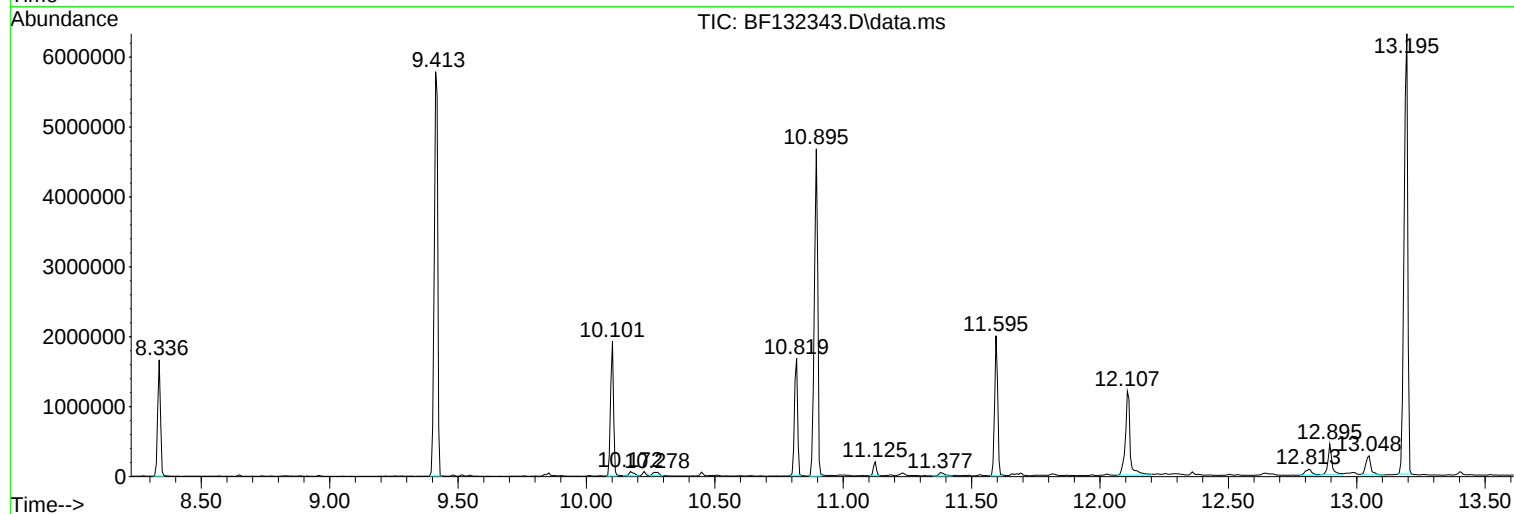
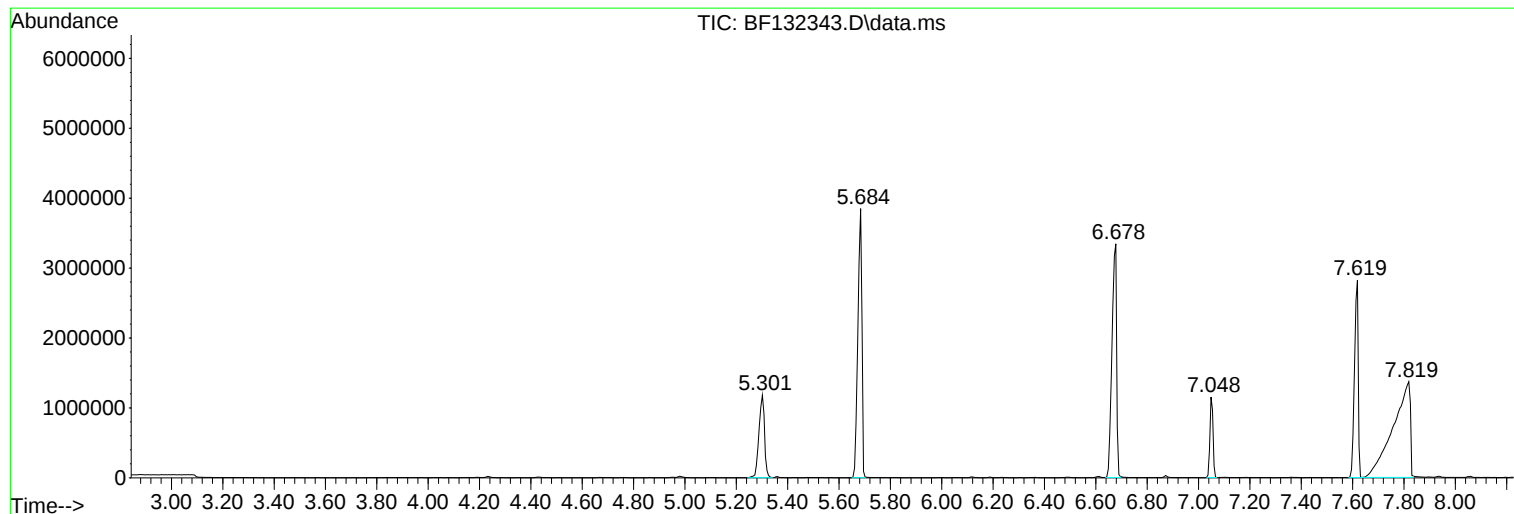
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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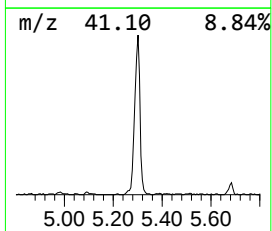
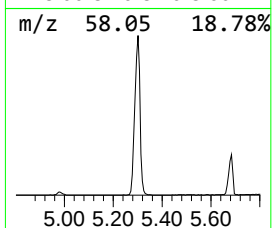
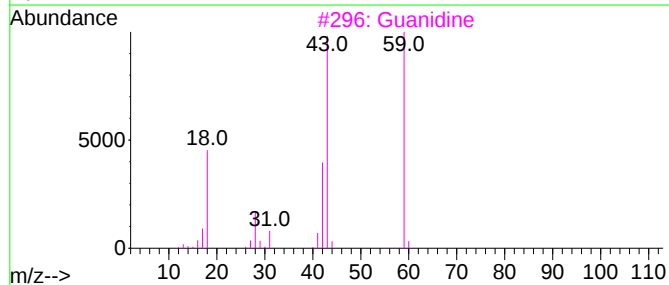
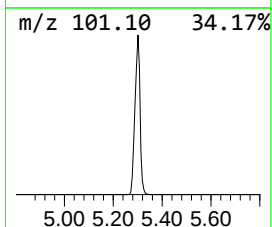
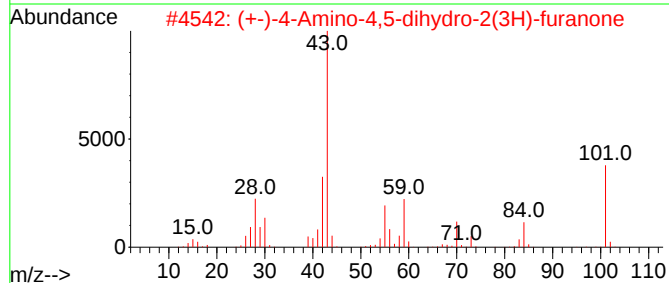
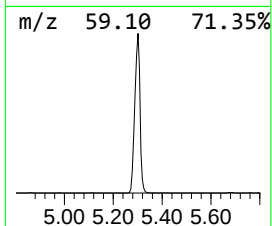
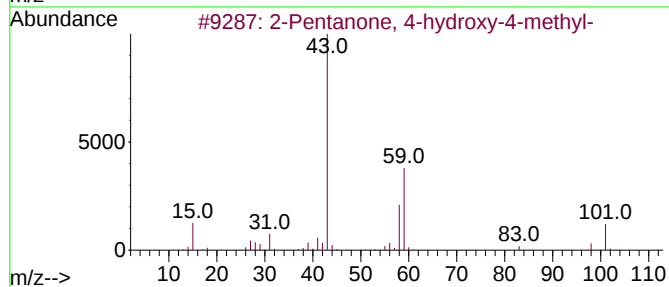
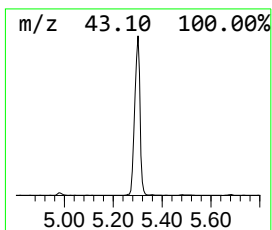
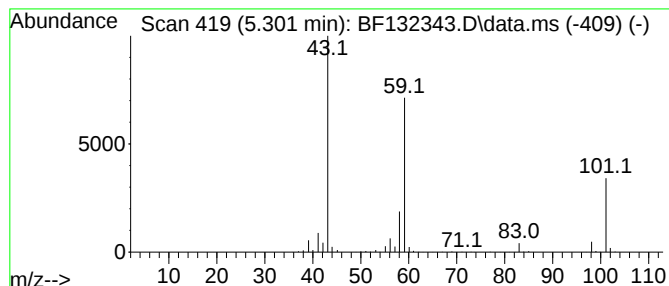
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.301	36.64 ng	1759040	1,4-Dichlorobenzene-d4	7.048

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	47
3			Guanidine	59	CH5N3	000113-00-8	43
4			1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	23
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17



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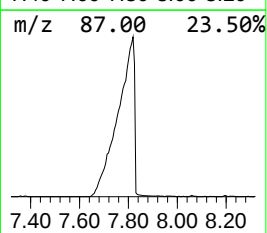
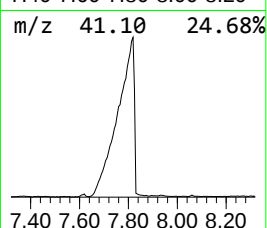
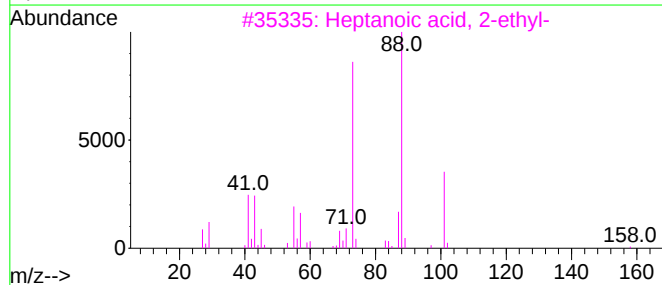
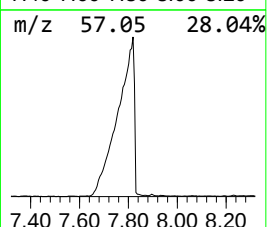
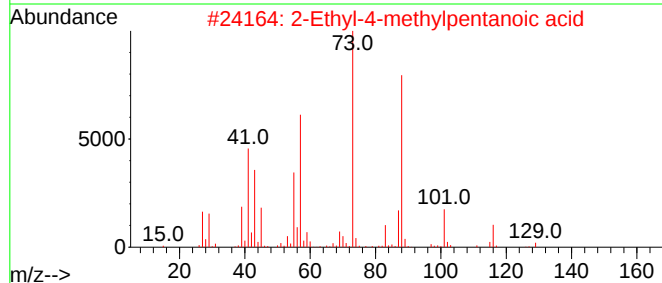
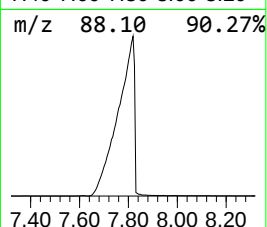
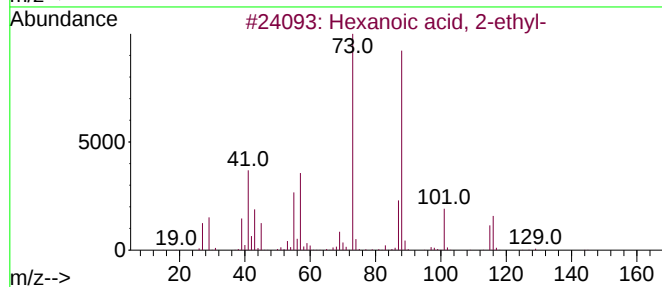
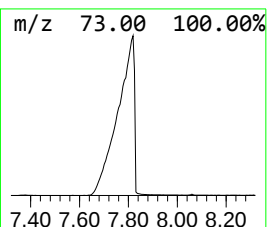
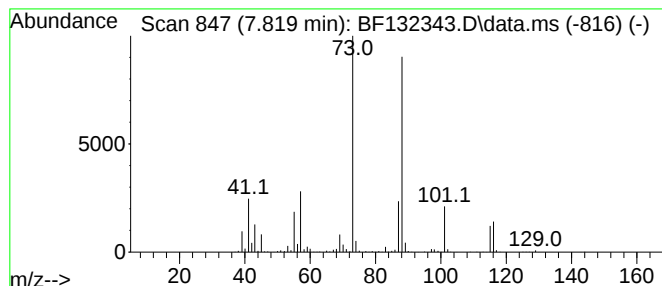
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Hexanoic acid, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.819	99.45 ng	6382340	Naphthalene-d8	8.336

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	90
2			2-Ethyl-4-methylpentanoic acid	144	C8H16O2	000108-81-6	64
3			Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	64
4			Acetic acid, diethyl-	116	C6H12O2	000088-09-5	50
5			Octanoic acid, 2-methyl-, methyl...	172	C10H20O2	002177-86-8	42



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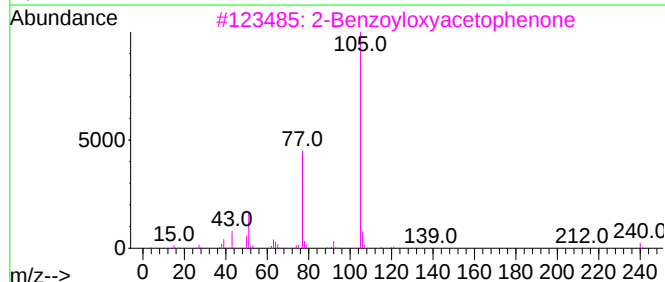
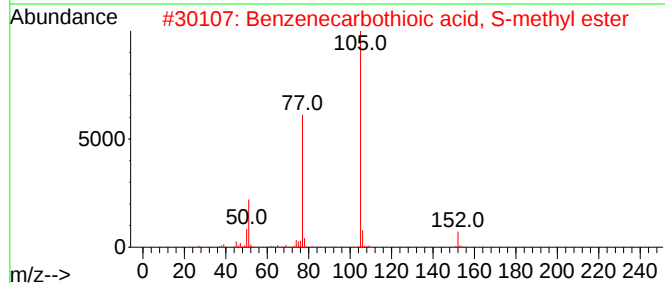
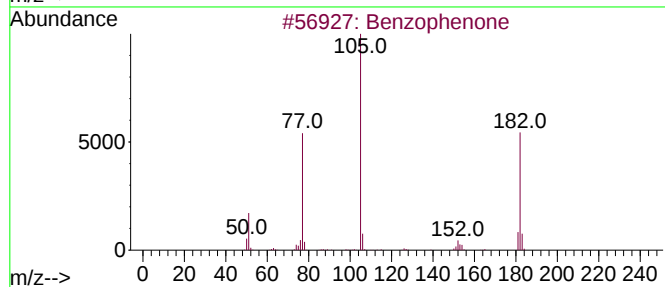
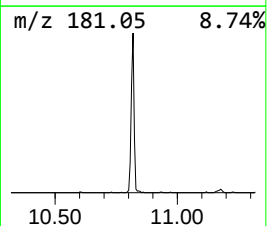
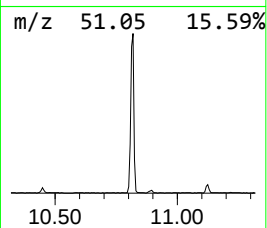
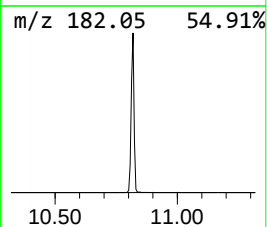
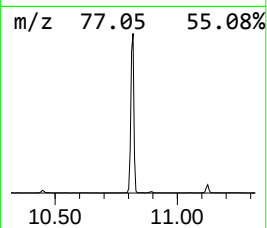
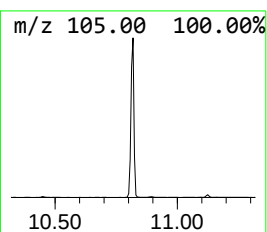
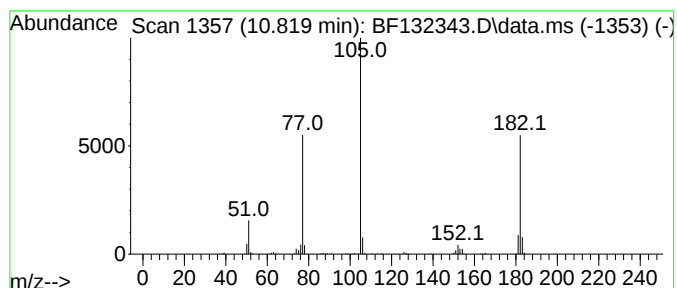
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.	
10.819	17.97 ng	1386140	Acenaphthene-d10		10.101	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Benzophenone		182	C13H10O	000119-61-9	96
2	Benzenecarbothioic acid, S-methy...		152	C8H8OS	005925-68-8	47
3	2-Benzoyloxyacetophenone		240	C15H12O3	004010-33-7	43
4	4-Nitrophenyl benzoate		243	C13H9NO4	000959-22-8	43
5	1,2-Propanedione, 1-phenyl-		148	C9H8O2	000579-07-7	43



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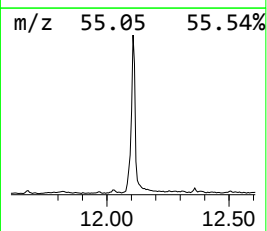
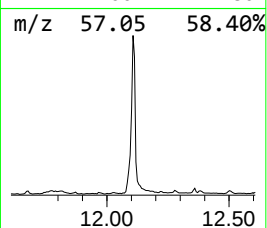
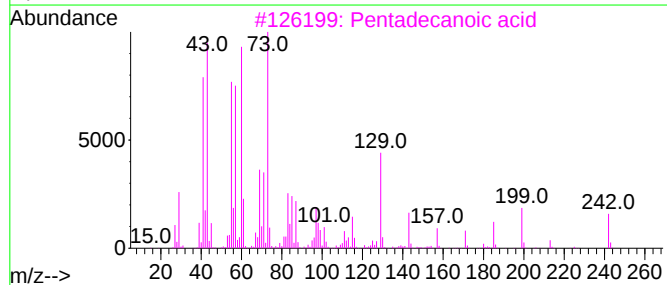
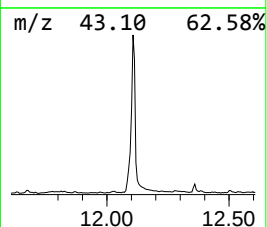
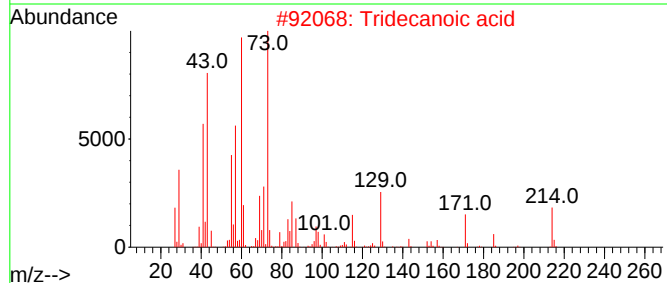
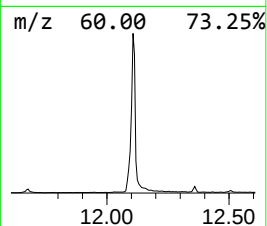
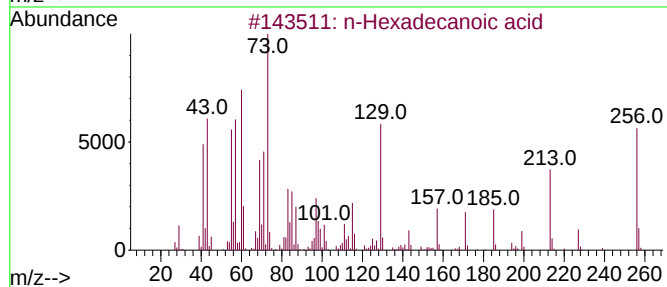
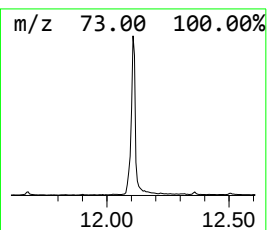
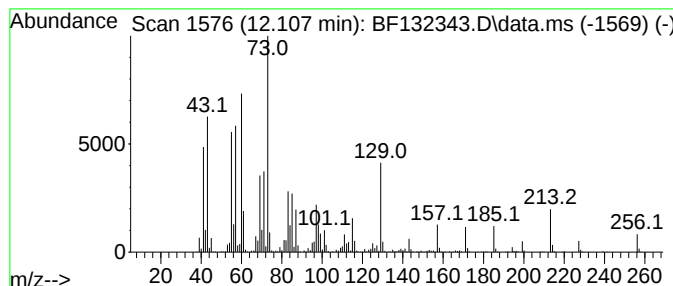
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.		
12.107	18.13 ng	1536470	Phenanthrene-d10	11.595		
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	89
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5		Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NO5	029926-41-8	38



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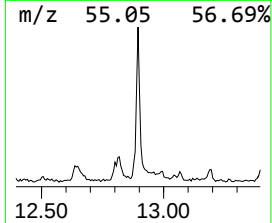
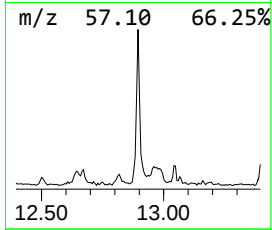
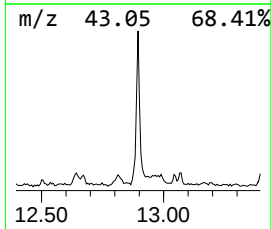
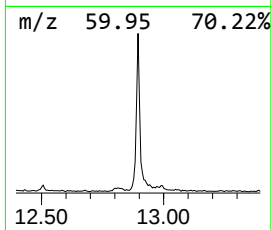
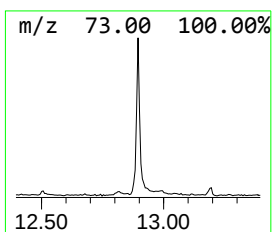
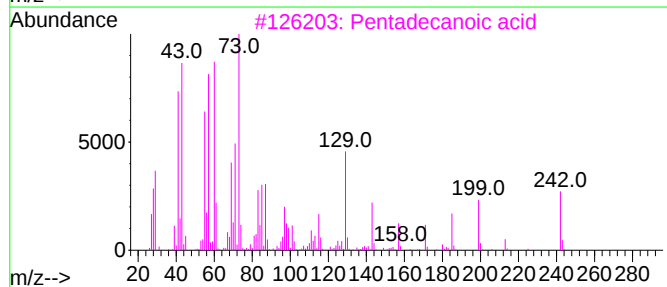
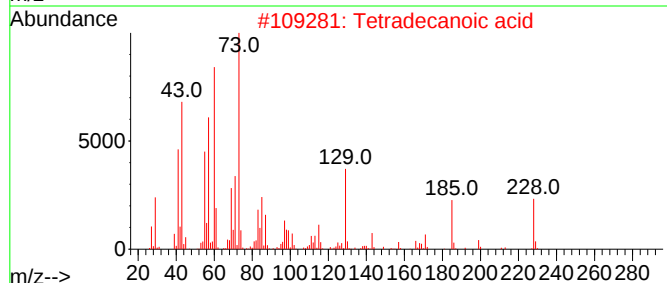
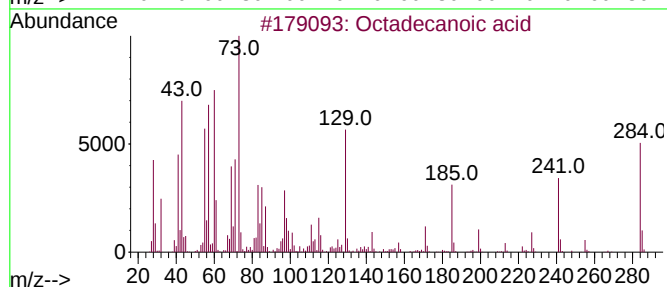
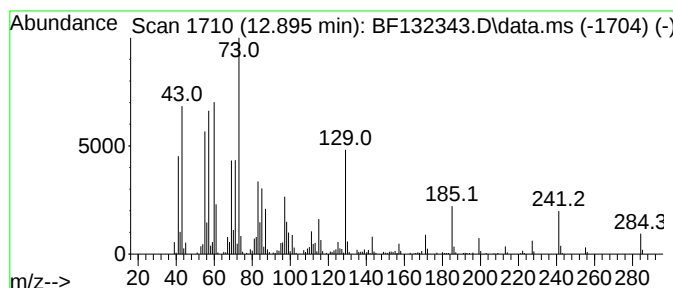
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.895	5.57 ng	472421	Phenanthrene-d10	11.595

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	89
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	89
4			Tridecanoic acid	214	C13H26O2	000638-53-9	62
5			n-Decanoic acid	172	C10H20O2	000334-48-5	38



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Data File : BF132343.D
Acq On : 07 Feb 2023 14:23
Operator : CG\JU
Sample : 01442-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

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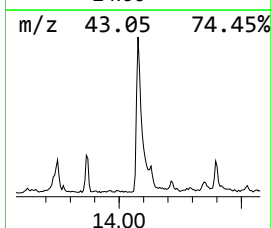
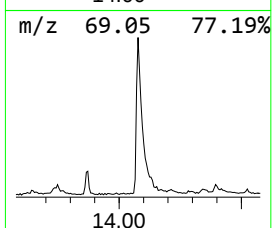
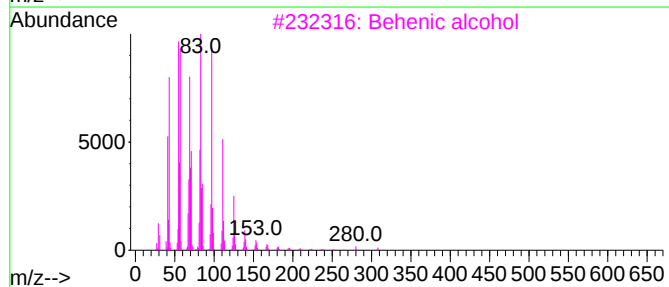
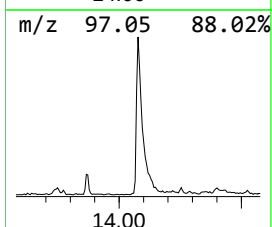
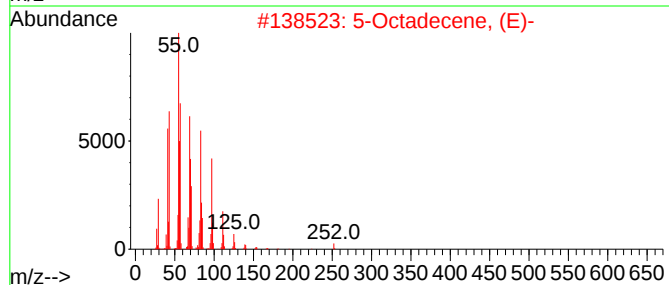
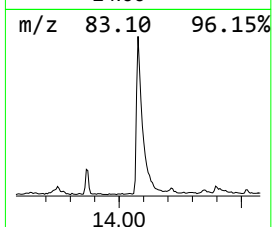
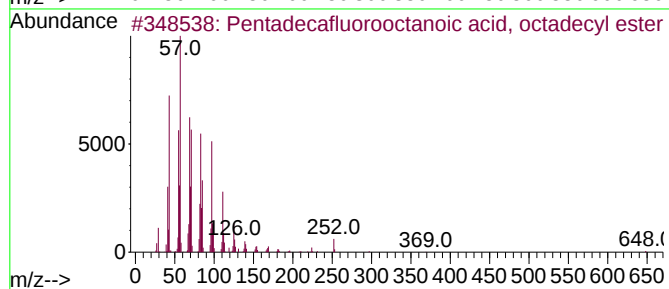
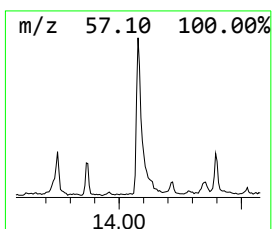
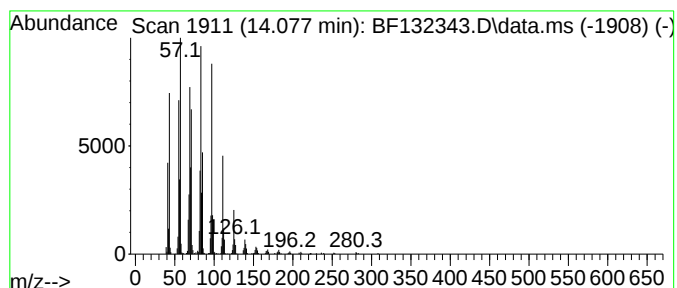
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Pentadecafluorooctanoic aci... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.077	11.36 ng	789616	Chrysene-d12	14.254

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
2		5-Octadecene, (E)-	252	C18H36	007206-21-5	93
3		Behenic alcohol	326	C22H46O	000661-19-8	93
4		1-Hexacosene	364	C26H52	018835-33-1	93
5		1-Heneicosyl formate	340	C22H44O2	077899-03-7	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020723\
Data File : BF132343.D
Acq On : 07 Feb 2023 14:23
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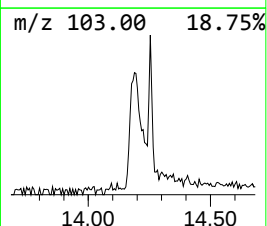
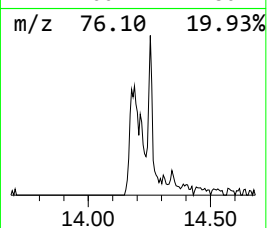
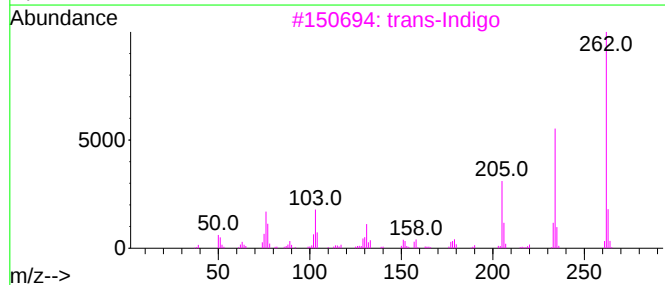
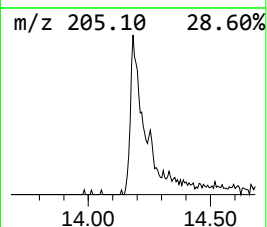
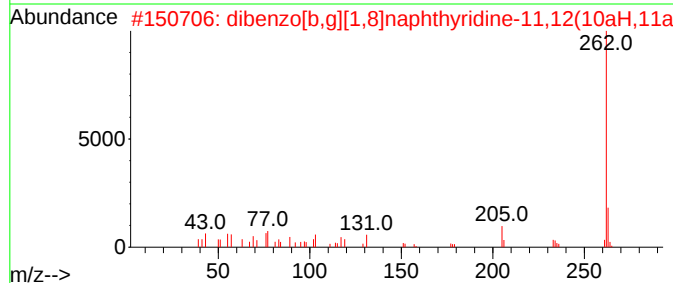
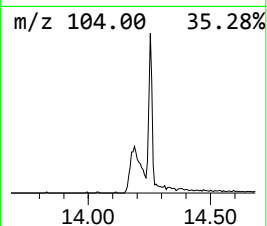
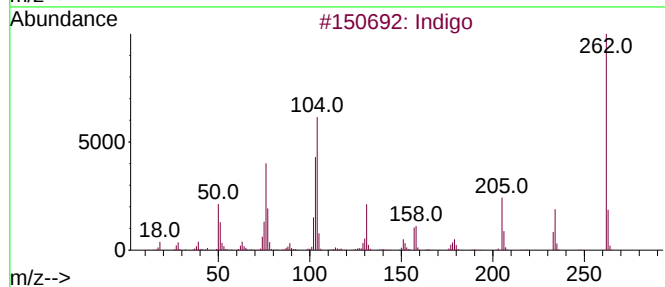
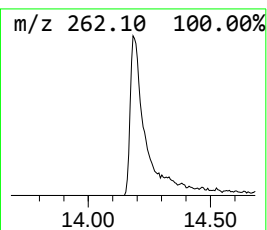
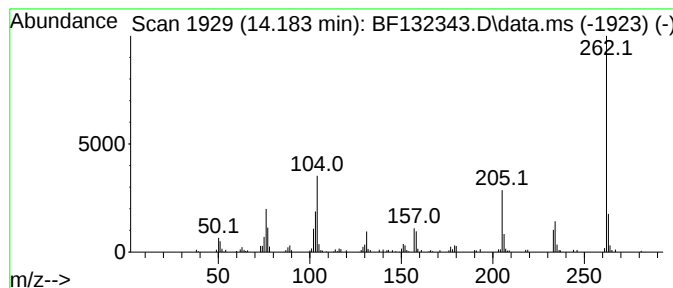
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Indigo Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.183	2.78 ng	193448	Chrysene-d12	14.254

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indigo	262	C16H10N2O2	000482-89-3	97
2			dibenzo[b,g][1,8]naphthyridine-1...	262	C16H10N2O2	1000396-82-0	70
3			trans-Indigo	262	C16H10N2O2	064784-13-0	58
4			1,2,3,6,7,8,9,10,11,12-Decahydro...	262	C20H22	092387-50-3	52
5			Benzo[g]naphtho[1,8-bc][1,5]diox...	262	C18H14O2	052826-35-4	50



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Data File : BF132343.D
Acq On : 07 Feb 2023 14:23
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Misc :
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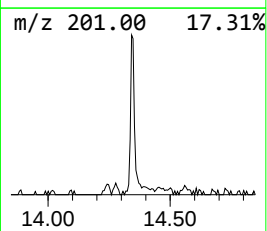
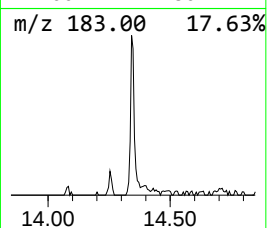
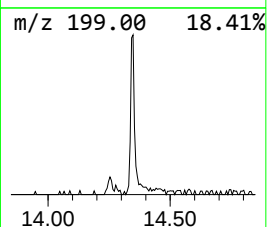
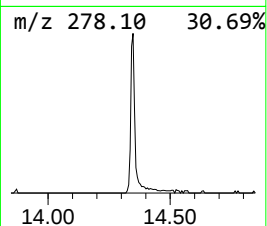
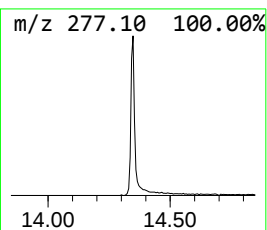
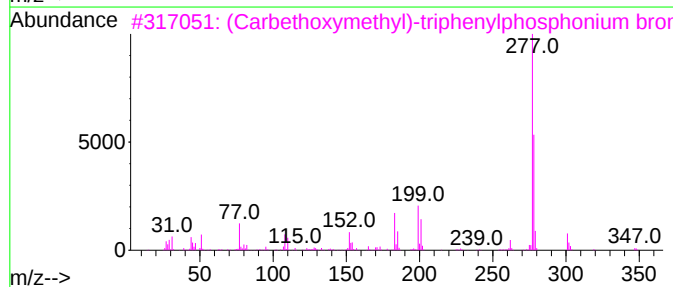
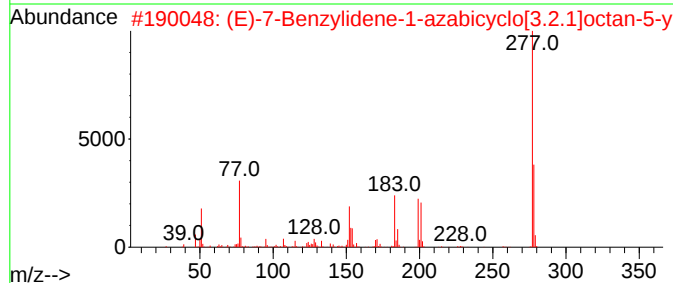
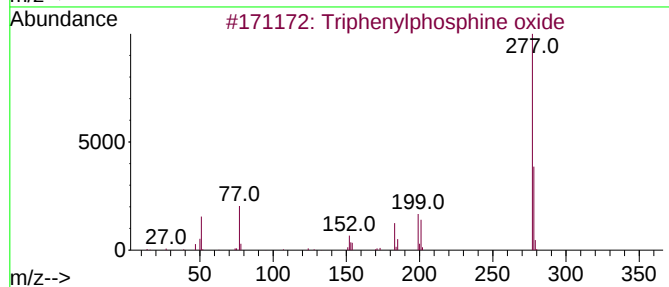
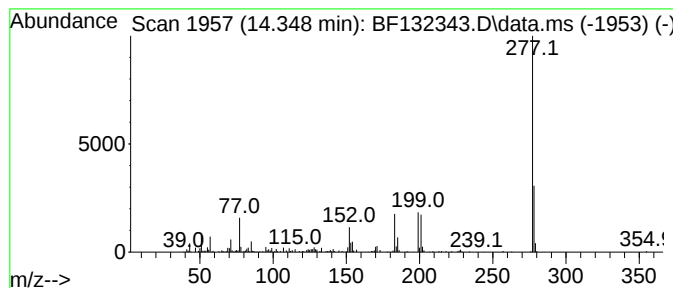
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Triphenylphosphine oxide Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.348	2.53 ng	176164	Chrysene-d12	14.254

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	C15H19N03S	1000483-83-4	91
3			(Carbethoxymethyl)-triphenylphos...	428	C22H22BrO2P	001530-45-6	45
4			2-Phenyl-6-(trifluoromethyl)-1H-...	277	C15H10F3NO	1000387-59-3	42
5			5-Methyl-8-phenylfuro[3',2':5,6]...	277	C16H11N3O2	1000460-07-9	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020723\
Data File : BF132343.D
Acq On : 07 Feb 2023 14:23
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ClientSampleId :
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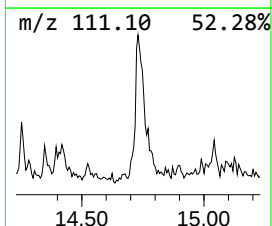
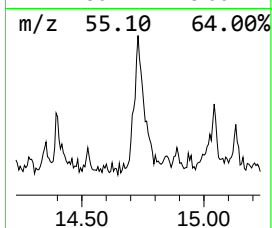
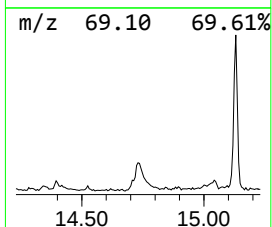
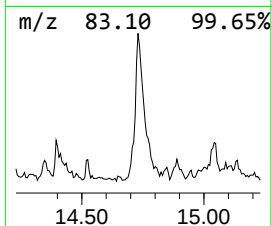
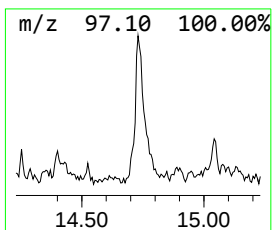
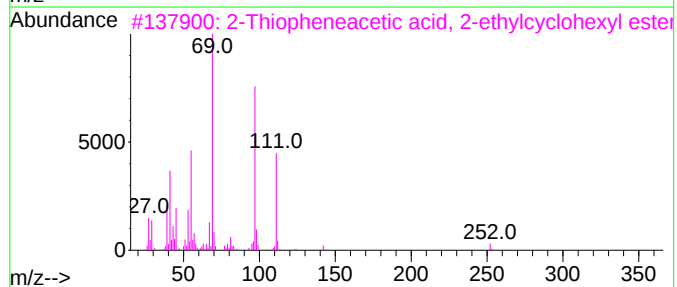
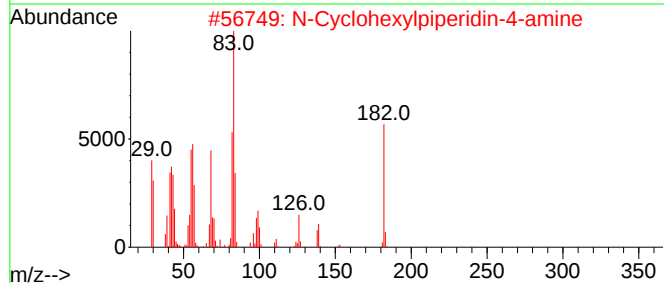
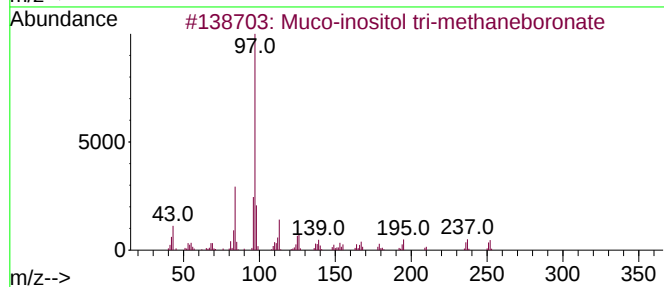
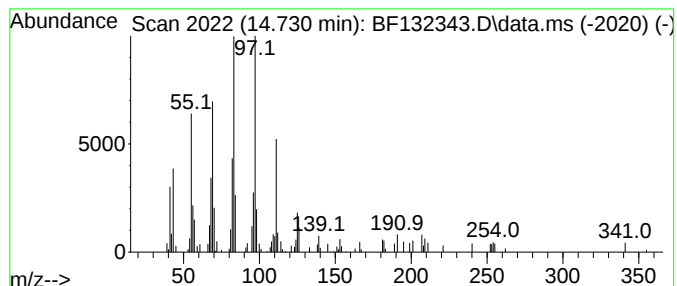
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown14.730 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.730	2.28 ng	158461	Chrysene-d12	14.254

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Muco-inositol tri-methaneboronate	252	C9H15B3O6	1000064-40-0	46
2			N-Cyclohexylpiperidin-4-amine	182	C11H22N2	852486-61-4	43
3			2-Thiopheneacetic acid, 2-ethylc...	252	C14H20O2S	1000278-96-1	38
4			Cyclohexanecarboxylic acid, (1H-...	195	C8H13N5O	1000310-78-1	30
5			Heptylcyclohexane	182	C13H26	005617-41-4	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020723\
Data File : BF132343.D
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Misc :
ALS Vial : 4 Sample Multiplier: 1

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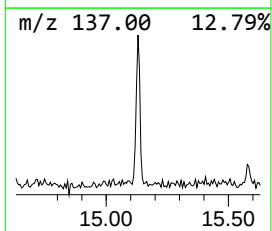
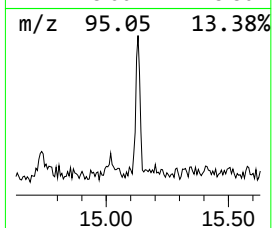
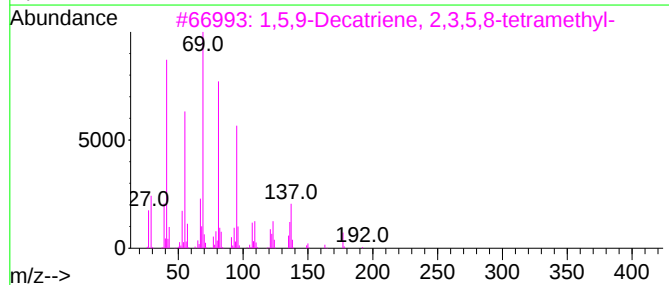
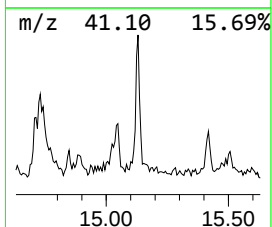
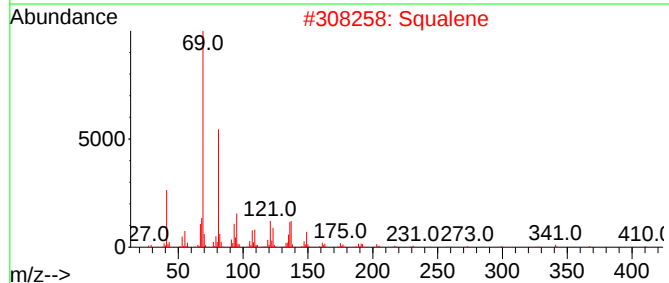
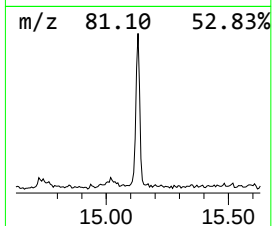
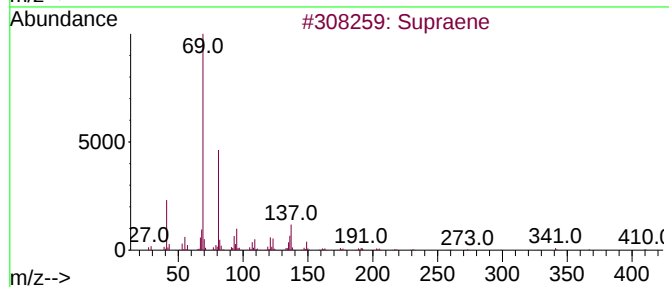
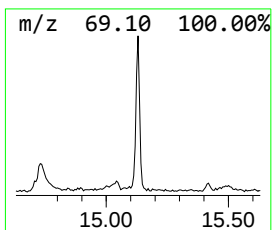
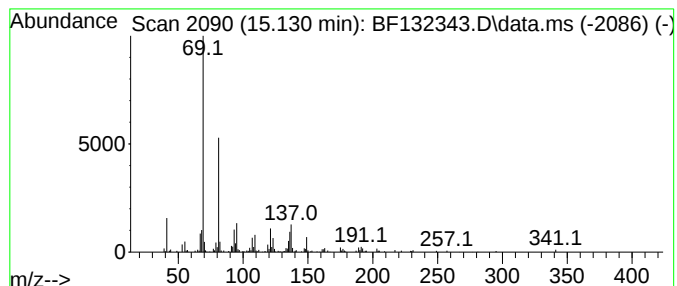
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Supraene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.130	2.42 ng	136986	Perylene-d12	15.830

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Supraene	410	C30H50	007683-64-9	91
2		Squalene	410	C30H50	000111-02-4	91
3		1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	74
4		1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	72
5		Farnesol isomer a	222	C15H26O	1000108-92-4	68



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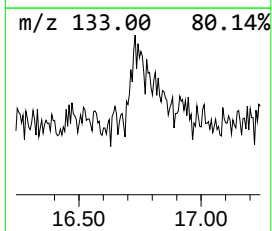
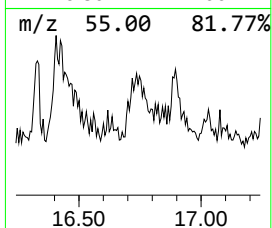
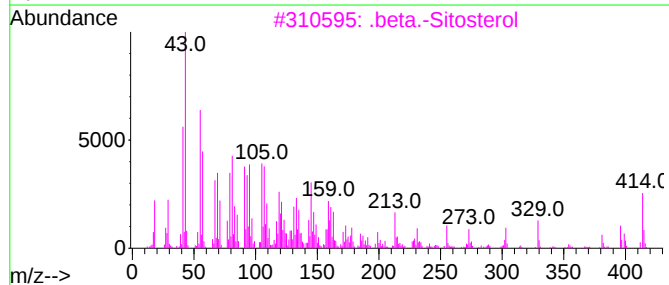
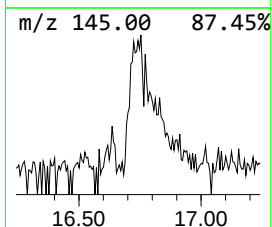
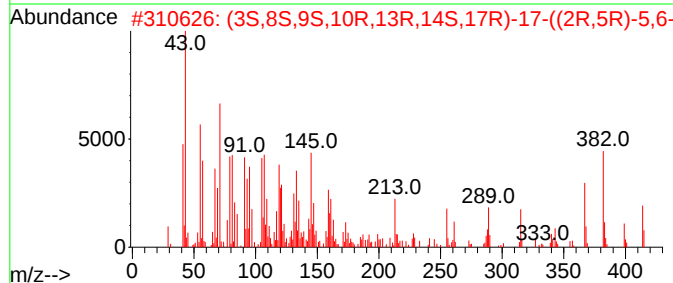
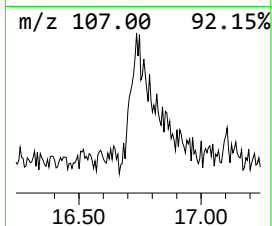
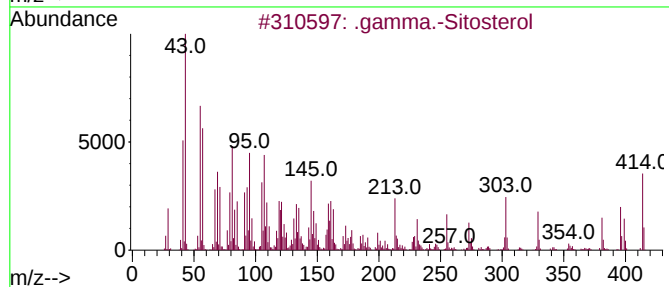
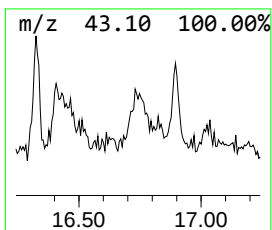
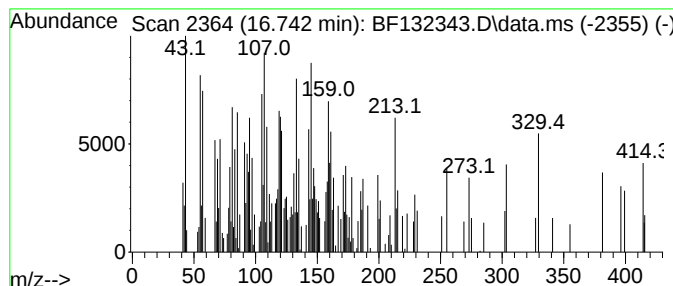
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 .gamma.-Sitosterol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.742	3.24 ng	183268	Perylene-d12	15.830
Hit#	of 5	Tentative ID	MW MolForm	CAS# Qual
1		.gamma.-Sitosterol	414 C29H50O	000083-47-6 90
2		(3S,8S,9S,10R,13R,14S,17R)-17-((...)	414 C29H50O	029365-29-5 83
3		.beta.-Sitosterol	414 C29H50O	000083-46-5 70
4		Cholest-5-ene, 3-ethoxy-, (3.bet...	414 C29H50O	000986-19-6 43
5		17-(1,5-Dimethylhexyl)-10,13-dim...	414 C29H50O	1000210-86-9 25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020723\
Data File : BF132343.D
Acq On : 07 Feb 2023 14:23
Operator : CG\JU
Sample : 01442-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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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
2-Pentanone, 4-...	5.301	36.6	ng	1759040	1	7.048	960146	20.0
Hexanoic acid, ...	7.819	99.5	ng	6382340	2	8.336	1283470	20.0
Benzophenone	10.819	18.0	ng	1386140	3	10.101	1542890	20.0
n-Hexadecanoic ...	12.107	18.1	ng	1536470	4	11.595	1694830	20.0
Octadecanoic acid	12.895	5.6	ng	472421	4	11.595	1694830	20.0
Pentadecafluoro...	14.077	11.4	ng	789616	5	14.254	1389890	20.0
Indigo	14.183	2.8	ng	193448	5	14.254	1389890	20.0
Triphenylphosph...	14.348	2.5	ng	176164	5	14.254	1389890	20.0
unknown14.730	14.730	2.3	ng	158461	5	14.254	1389890	20.0
Supraene	15.130	2.4	ng	136986	6	15.830	1130980	20.0
.gamma.-Sitosterol	16.742	3.2	ng	183268	6	15.830	1130980	20.0