

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101521\
 Data File : BF125860.D
 Acq On : 15 Oct 2021 13:47
 Operator : JU/CG
 Sample : M4243-21
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 T4-COMP-(1-4)

Integration Parameters: rteint.p

Integrator: RTE

Smothing : 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-BF100721.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125860.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.422	392	397	404	rVB	51115	57841	1.52%	0.187%
2	5.051	499	504	511	rVB	94769	117273	3.08%	0.380%
3	5.451	567	572	575	rBV	2967770	2775543	72.80%	8.991%
4	6.463	738	744	747	rBV	2729198	2885749	75.69%	9.348%
5	6.834	803	807	810	rBV	1267332	972387	25.51%	3.150%
6	7.392	897	902	905	rBV	2112170	1881370	49.35%	6.095%
7	8.016	1004	1008	1020	rBV	242734	234822	6.16%	0.761%
8	8.110	1020	1024	1028	rBV	1466188	1328437	34.85%	4.304%
9	9.186	1202	1207	1210	rBV	4340919	3812399	100.00%	12.350%
10	9.863	1316	1322	1326	rBV	1779649	1554885	40.78%	5.037%
11	9.969	1332	1340	1344	rBV8	27756	83174	2.18%	0.269%
12	10.063	1353	1356	1361	rBV4	31746	55140	1.45%	0.179%
13	10.192	1361	1378	1380	rBV2	113911	428921	11.25%	1.390%
14	10.504	1428	1431	1435	rVB	48649	49909	1.31%	0.162%
15	10.651	1452	1456	1459	rBV	2233840	2004150	52.57%	6.493%
16	10.698	1461	1464	1469	rVV	345748	316520	8.30%	1.025%
17	11.345	1571	1574	1577	rBV	1578420	1432005	37.56%	4.639%
18	11.875	1661	1664	1666	rBV	567226	465365	12.21%	1.508%
19	12.557	1778	1780	1783	rVB	174674	128466	3.37%	0.416%
20	12.663	1793	1798	1805	rVB	993386	1304414	34.22%	4.226%
21	12.786	1817	1819	1821	rVB	165224	120573	3.16%	0.391%
22	12.933	1840	1844	1847	rBV	3707192	3245348	85.13%	10.513%
23	13.833	1994	1997	2003	rVB4	201848	291379	7.64%	0.944%
24	13.980	2013	2022	2025	rBV	1258013	1513957	39.71%	4.905%
25	14.186	2055	2057	2060	rBV	70462	63108	1.66%	0.204%
26	14.504	2108	2111	2114	rBV	93879	91027	2.39%	0.295%
27	14.551	2114	2119	2126	rVV	279881	558595	14.65%	1.810%
28	14.610	2126	2129	2134	rVB	139478	140951	3.70%	0.457%
29	14.833	2164	2167	2169	rBV	49078	57524	1.51%	0.186%
30	15.010	2194	2197	2205	rVB	78307	156327	4.10%	0.506%
31	15.110	2208	2214	2219	rVV2	187196	352057	9.23%	1.140%
32	15.310	2245	2248	2252	rVB	53792	69619	1.83%	0.226%
33	15.368	2255	2258	2261	rBV	58119	68831	1.81%	0.223%
34	15.433	2264	2269	2273	rBV	925006	1108310	29.07%	3.590%
35	15.757	2319	2324	2337	rVB2	119349	272290	7.14%	0.882%
36	16.133	2383	2388	2401	rBV8	147670	430244	11.29%	1.394%

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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-BF100721.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	16.504	2445	2451	2458	rBV2	68035	148151	3.89%	0.480%
38	16.862	2505	2512	2527	rVB5	105018	291626	7.65%	0.945%

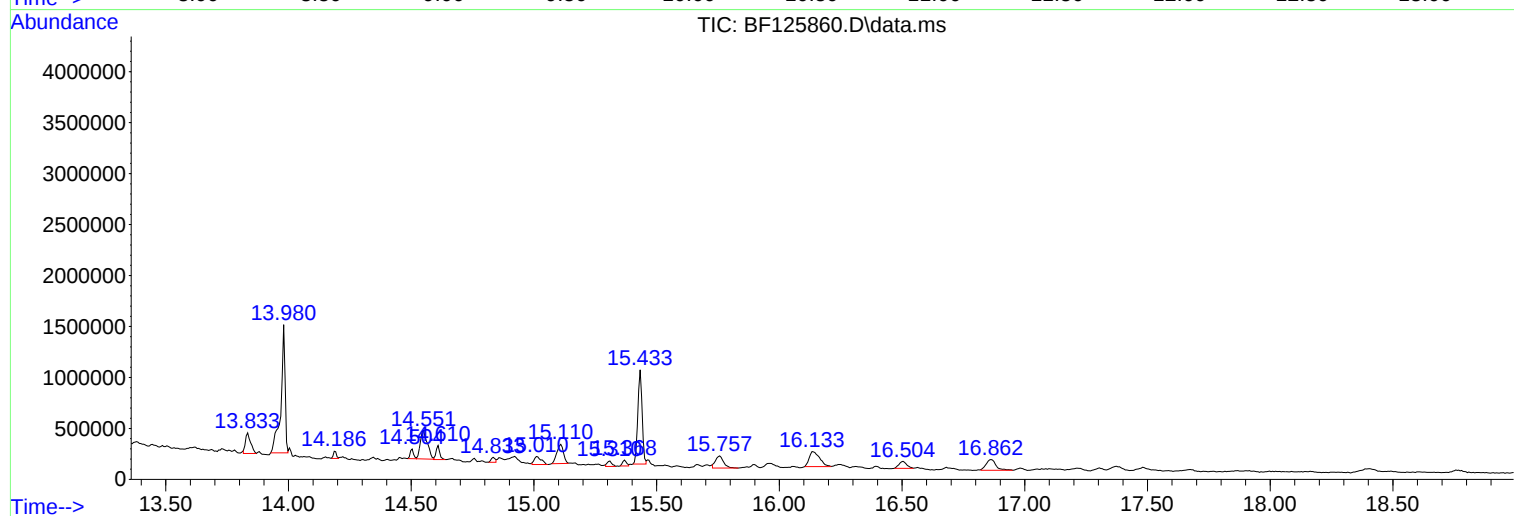
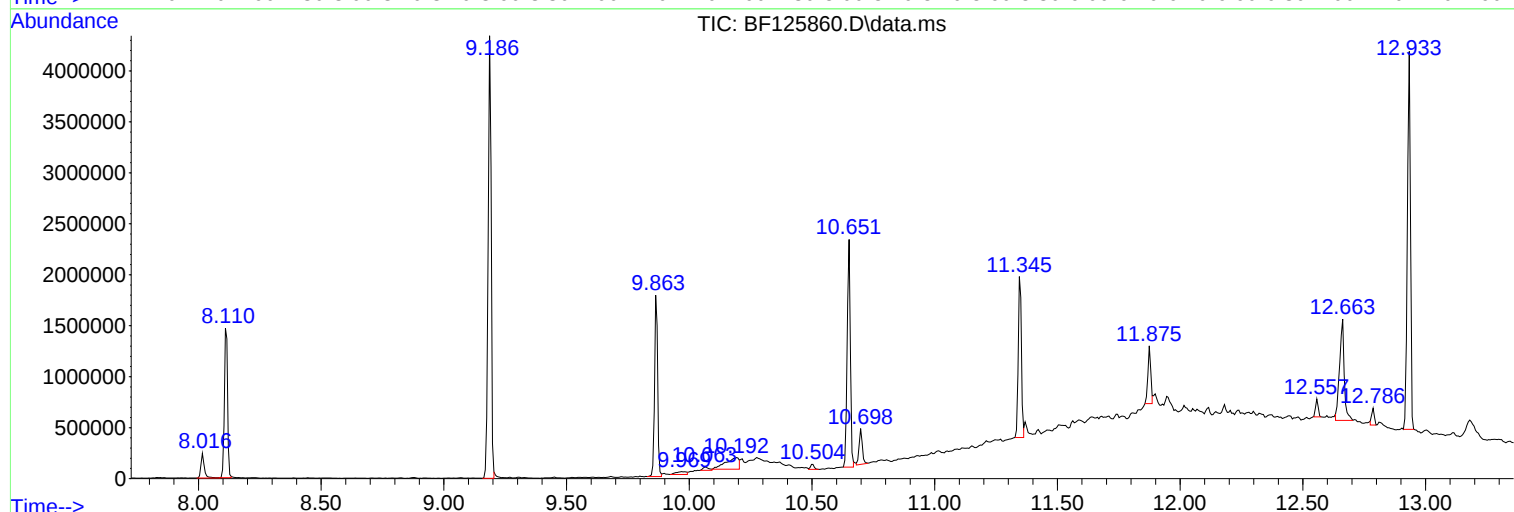
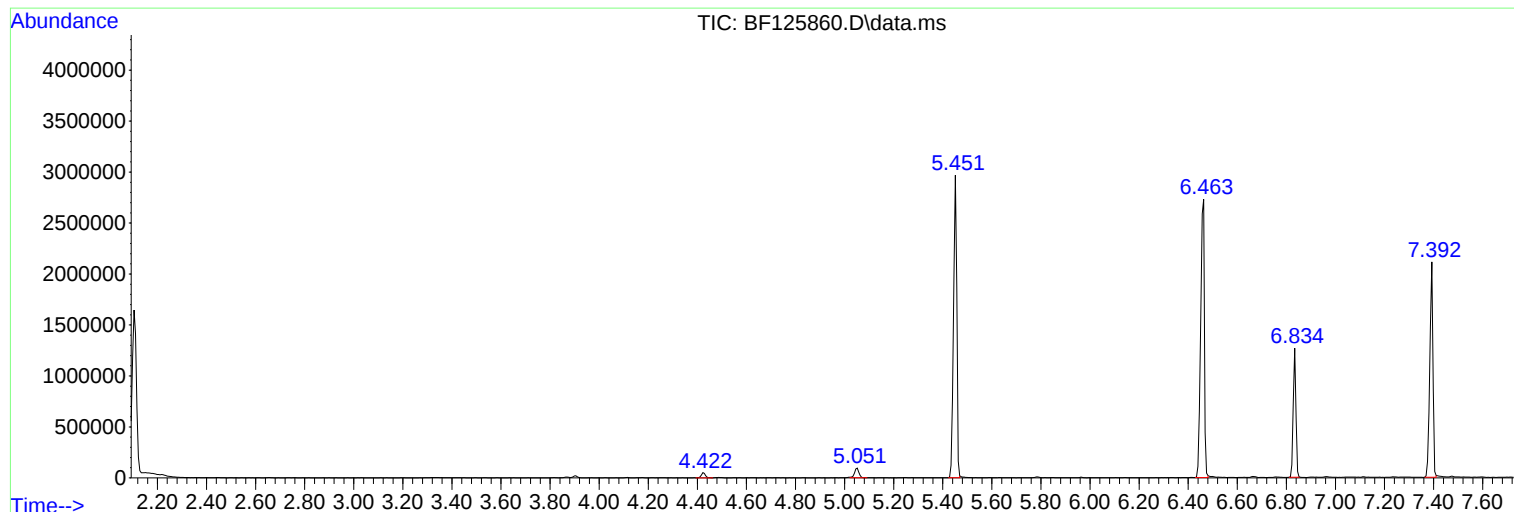
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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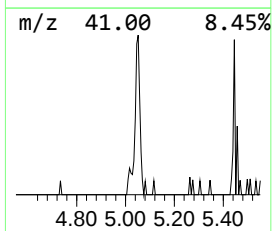
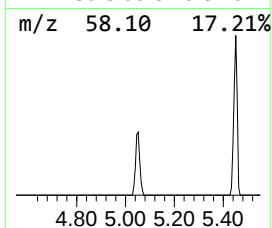
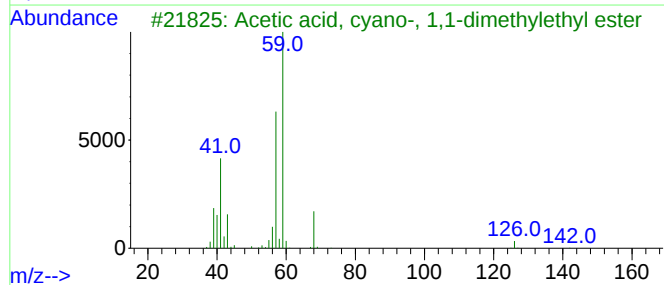
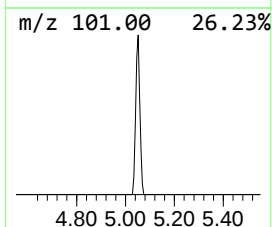
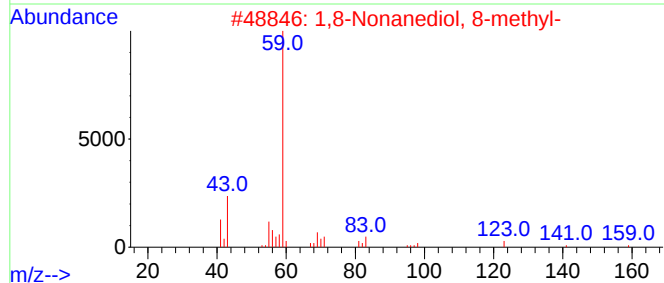
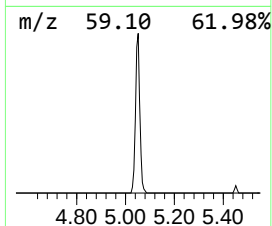
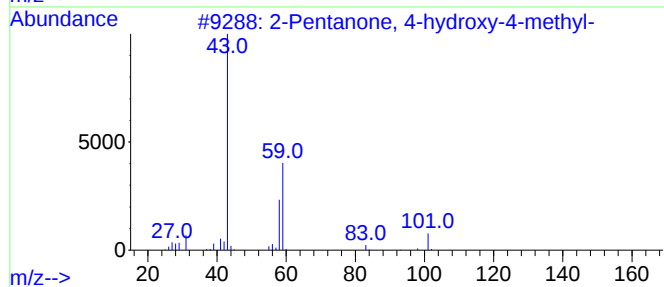
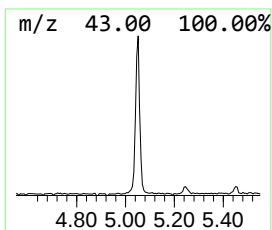
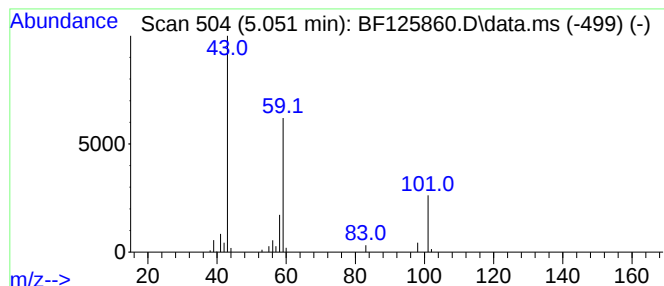
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.051	2.41 ng	117273	1,4-Dichlorobenzene-d4	6.834

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	23
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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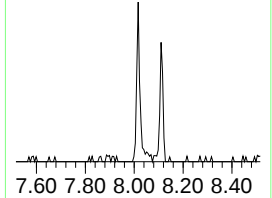
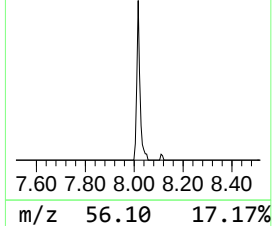
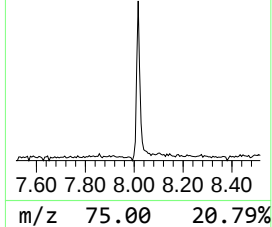
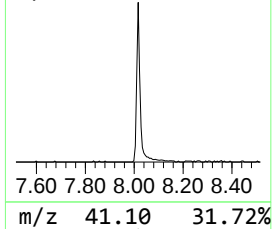
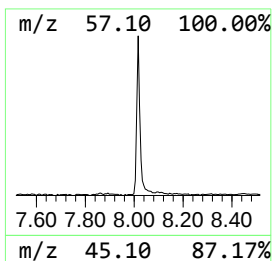
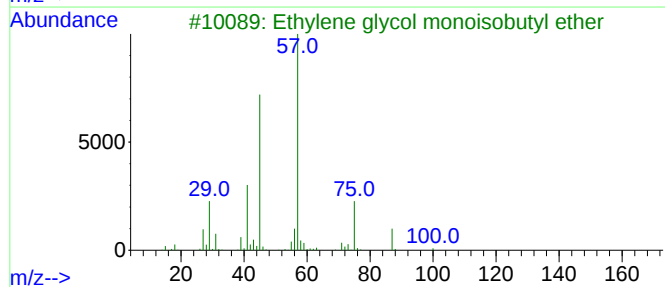
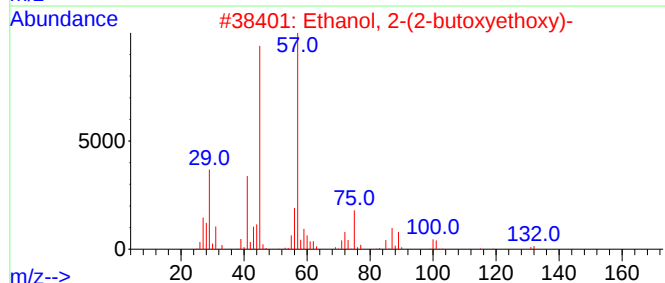
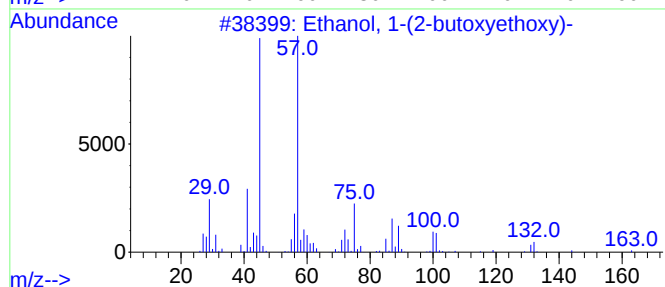
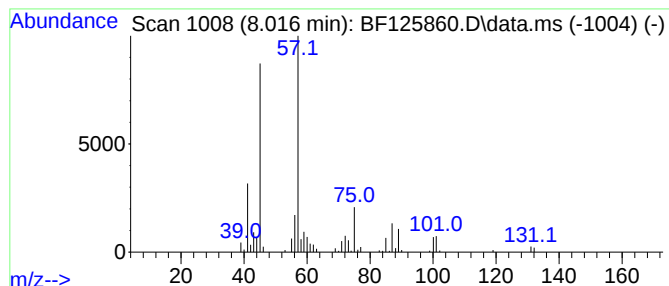
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Ethanol, 1-(2-butoxyethoxy)- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.016	3.54 ng	234822	Naphthalene-d8	8.110

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	90
2			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
3			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
4			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
5			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	52



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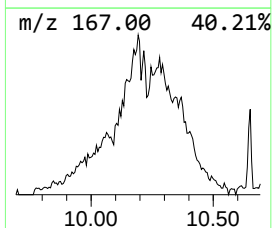
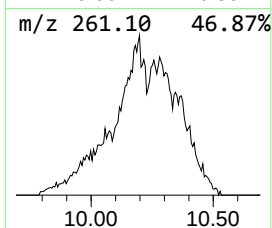
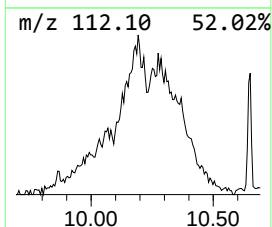
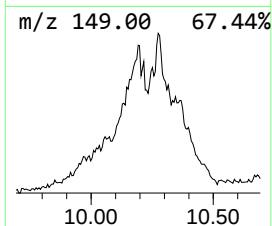
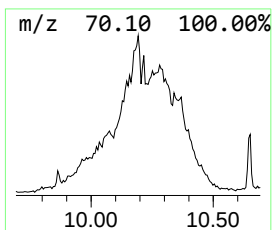
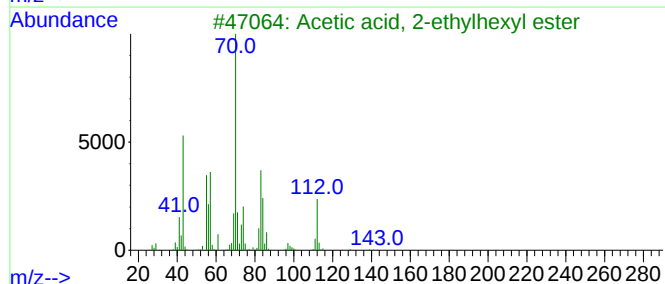
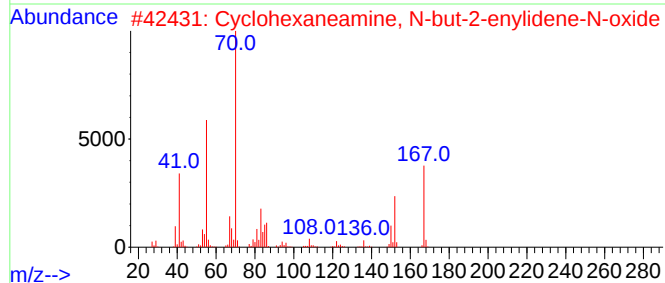
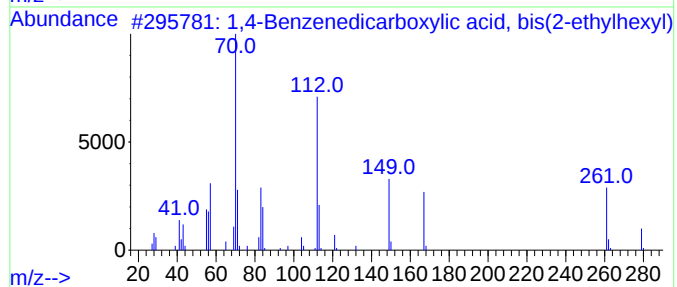
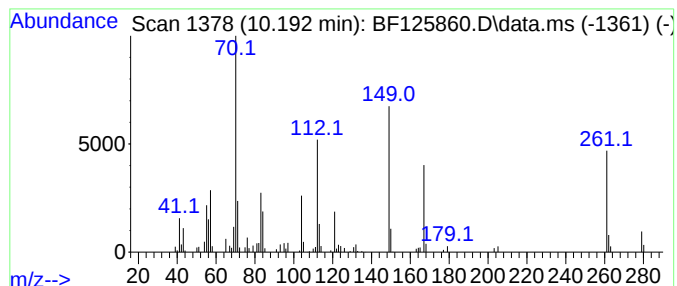
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown10.192 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.192	5.52 ng	428921	Acenaphthene-d10	9.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	38
2			Cyclohexanamine, N-but-2-enylid...	167	C10H17NO	068048-01-1	38
3			Acetic acid, 2-ethylhexyl ester	172	C10H20O2	000103-09-3	27
4			Phthalic acid, 6-ethyloct-3-yl 2...	418	C26H42O4	1000315-53-8	22
5			Phthalic acid, di(6-methylhept-2...	390	C24H38O4	1000377-97-3	22



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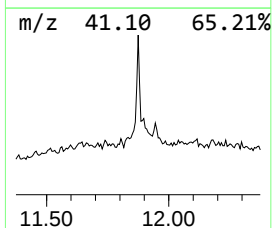
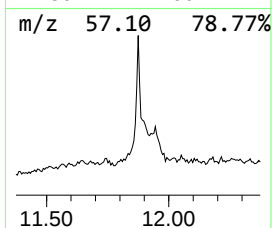
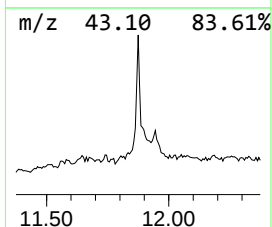
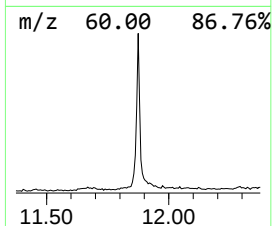
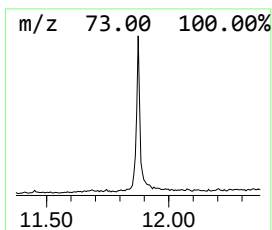
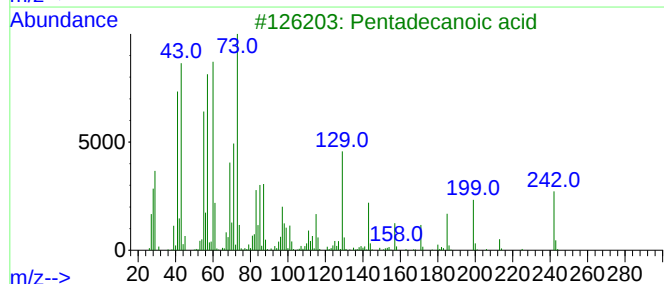
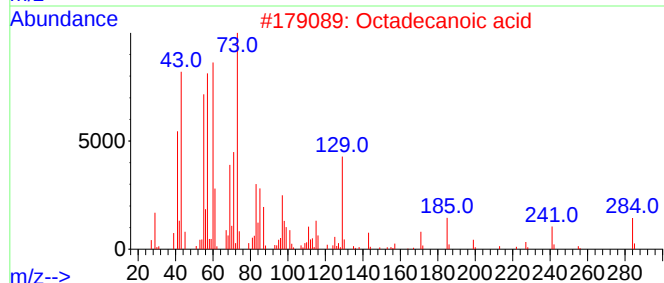
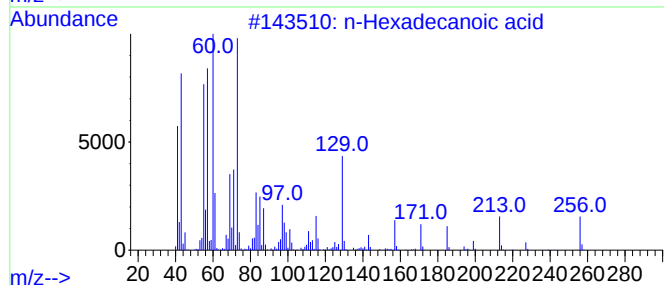
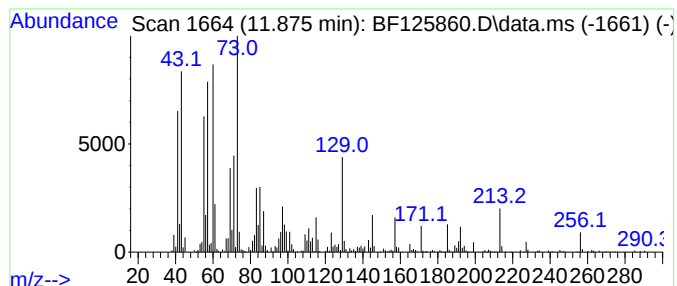
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.875	6.50 ng	465365	Phenanthrene-d10	11.345

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Octadecanoic acid	284	C18H36O2	000057-11-4	87
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4			Tridecanoic acid	214	C13H26O2	000638-53-9	76
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	70



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T4-COMP-(1-4)

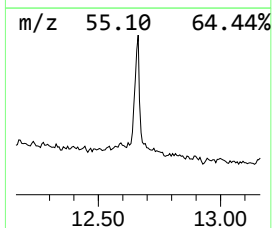
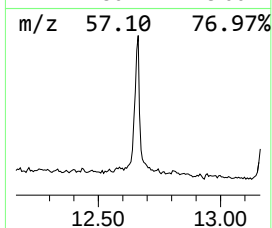
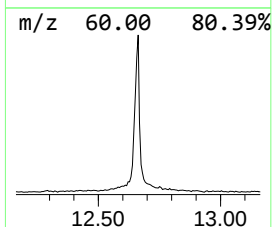
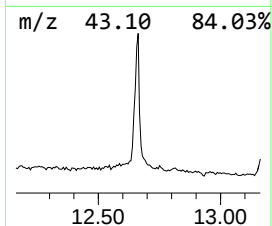
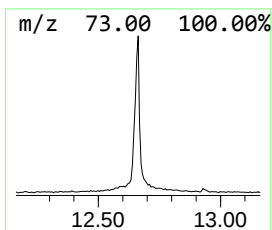
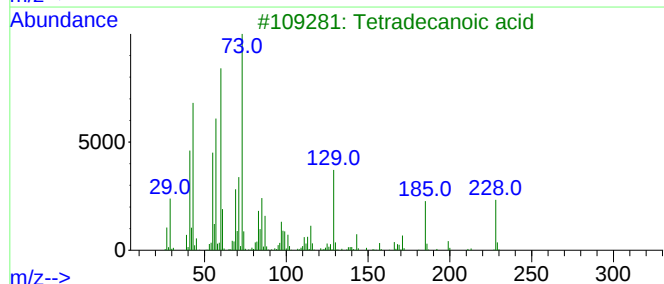
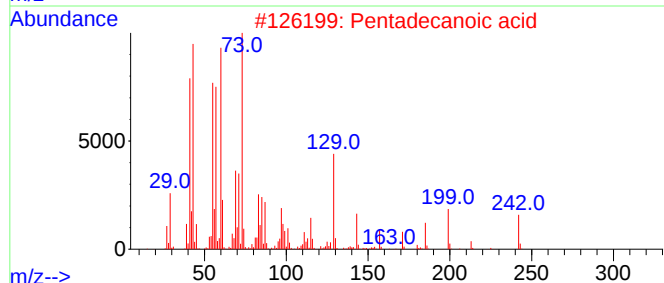
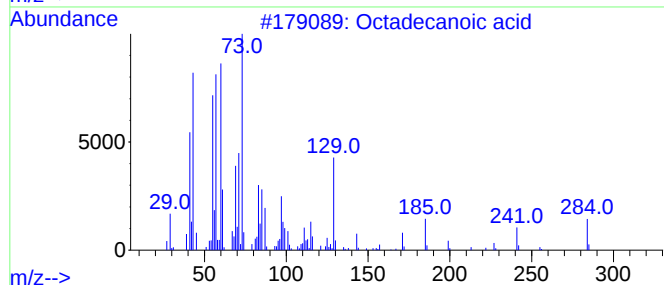
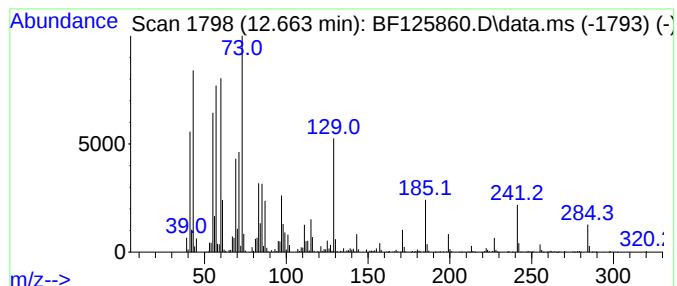
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Octadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.663	17.23 ng	1304410	Chrysene-d12	13.980

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			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4			Oxalic acid, propyl tetradecyl e...	328	C19H36O4	1000309-26-7	25
5			Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	25



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Acq On : 15 Oct 2021 13:47
Operator : JU/CG
Sample : M4243-21
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
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ClientSampleId :
T4-COMP-(1-4)

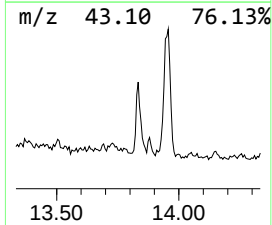
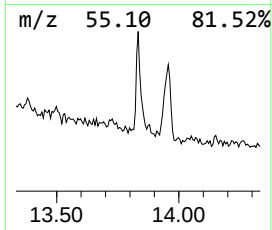
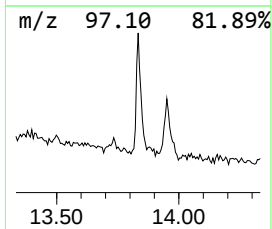
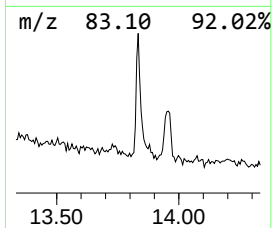
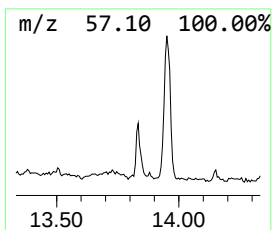
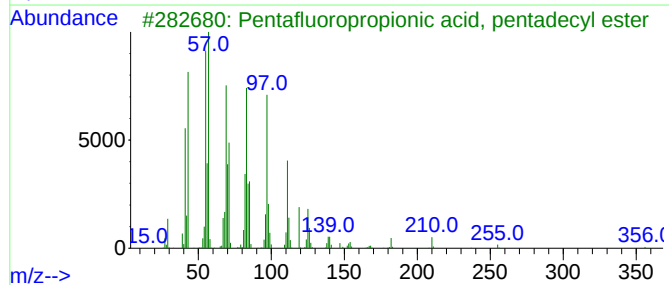
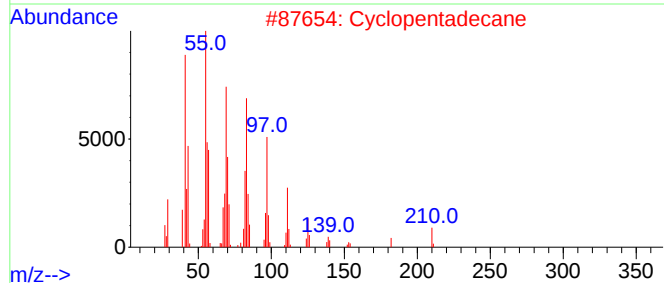
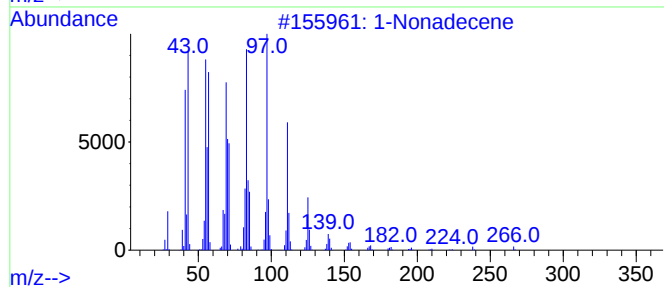
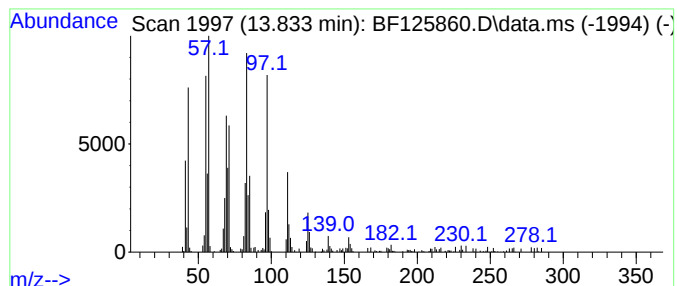
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Nonadecene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.833	3.85 ng	291379	Chrysene-d12	13.980

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene			266	C19H38	018435-45-5	98
2	Cyclopentadecane			210	C15H30	000295-48-7	97
3	Pentafluoropropionic acid, penta...			374	C18H31F5O2	959092-08-1	94
4	Heptafluorobutyric acid, hexadec...			438	C20H33F7O2	006385-15-5	94
5	Behenic alcohol			326	C22H46O	000661-19-8	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101521\
Data File : BF125860.D
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Instrument :
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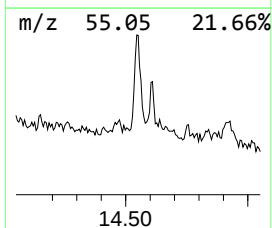
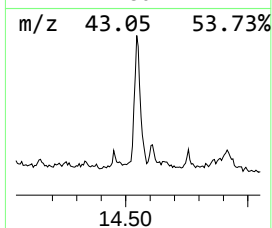
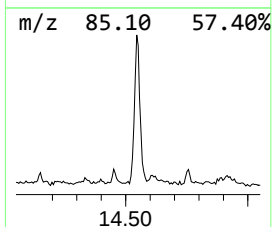
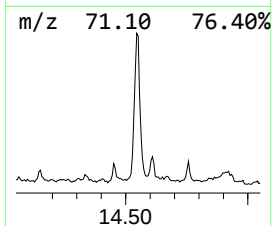
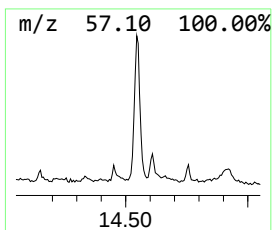
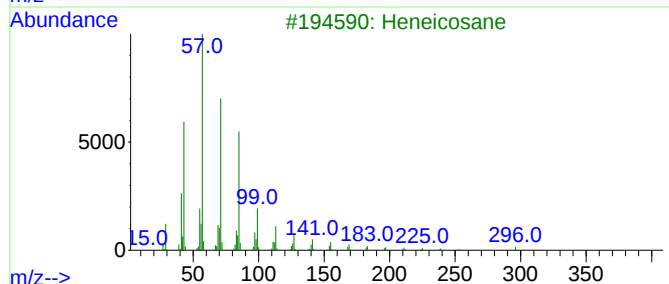
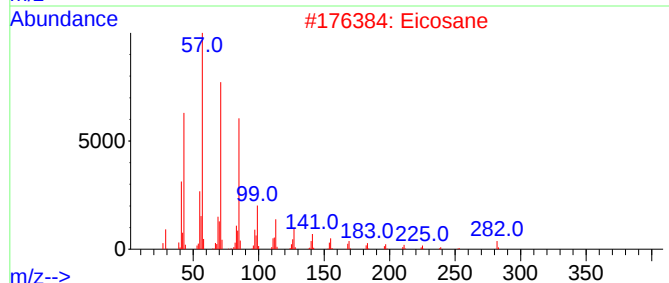
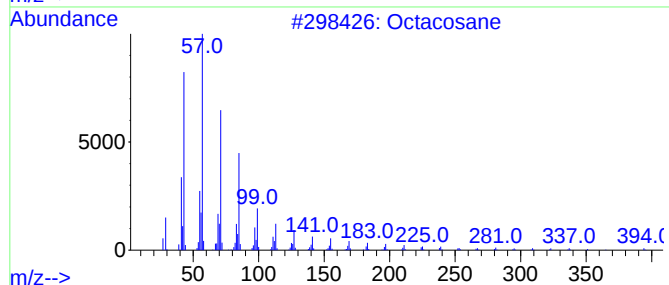
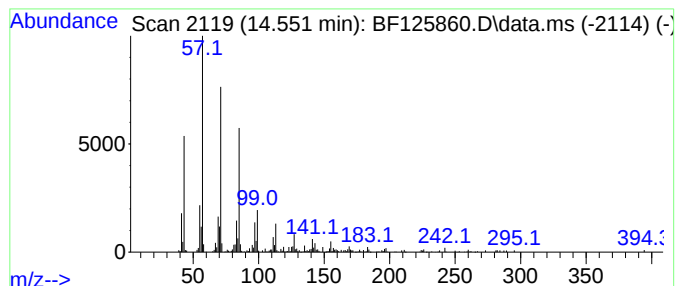
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.551	7.38 ng	558595	Chrysene-d12	13.980

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	95
2			Eicosane	282	C20H42	000112-95-8	95
3			Heneicosane	296	C21H44	000629-94-7	91
4			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
5			Docosane, 11-butyl-	366	C26H54	013475-76-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101521\
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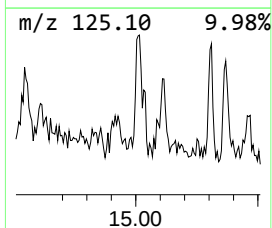
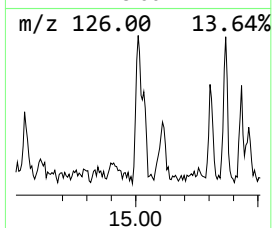
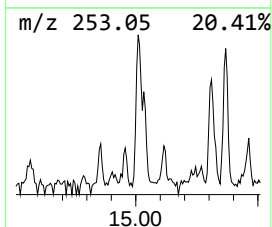
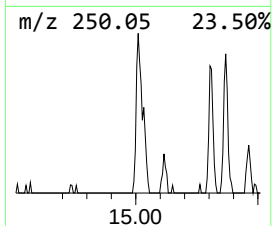
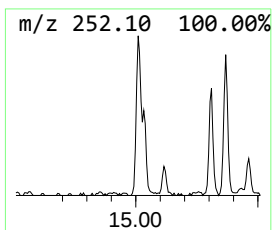
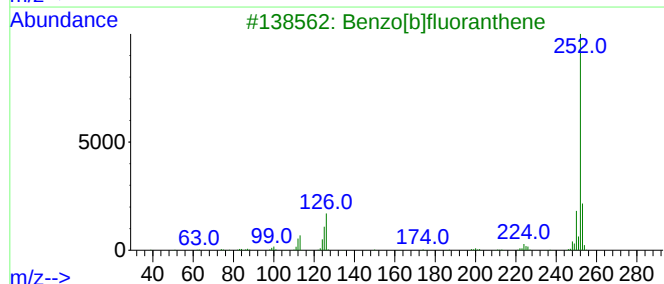
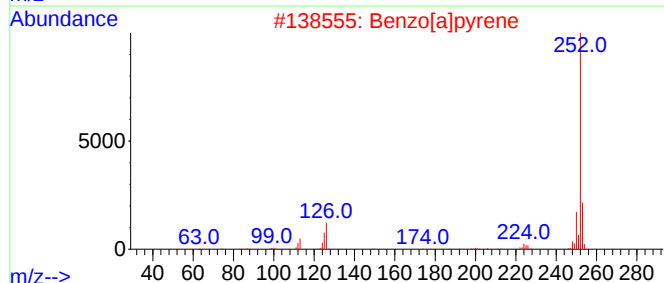
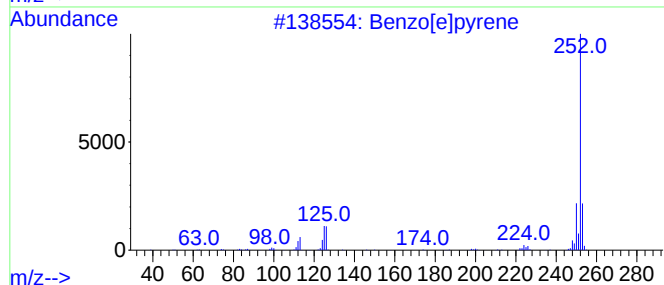
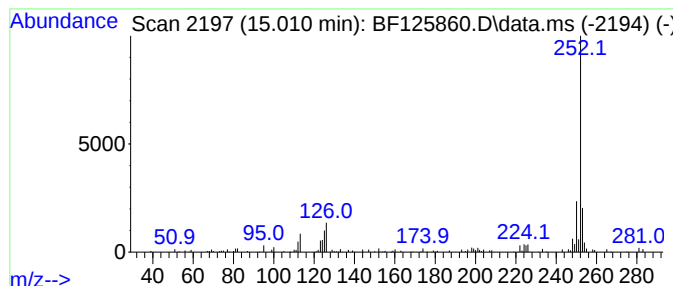
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Benzo[e]pyrene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.010	2.82 ng	156327	Perylene-d12	15.433

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	95
2			Benzo[a]pyrene	252	C20H12	000050-32-8	95
3			Benzo[b]fluoranthene	252	C20H12	000205-99-2	95
4			Benzo[k]fluoranthene	252	C20H12	000207-08-9	90
5			Perylene	252	C20H12	000198-55-0	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101521\
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Acq On : 15 Oct 2021 13:47
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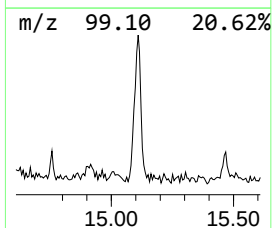
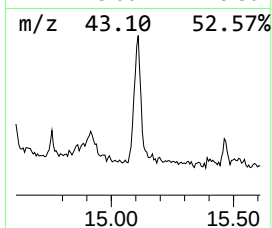
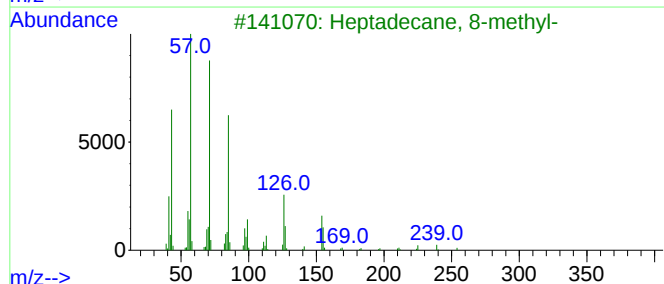
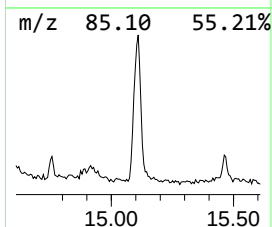
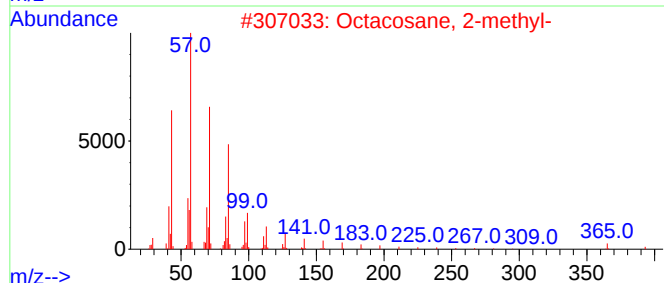
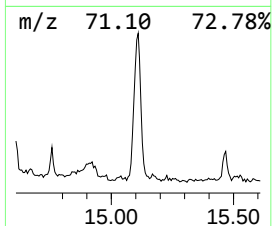
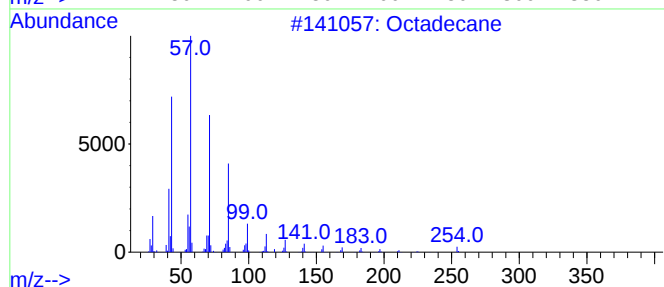
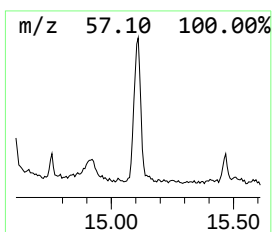
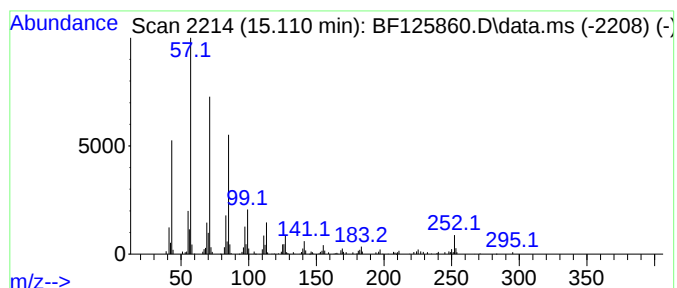
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.110	6.35 ng	352057	Perylene-d12	15.433

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane	254	C18H38	000593-45-3	95
2			Octacosane, 2-methyl-	408	C29H60	001560-98-1	90
3			Heptadecane, 8-methyl-	254	C18H38	013287-23-5	90
4			Heneicosane	296	C21H44	000629-94-7	87
5			Sulfurous acid, butyl undecyl ester	292	C15H32O3S	1000309-17-8	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101521\
Data File : BF125860.D
Acq On : 15 Oct 2021 13:47
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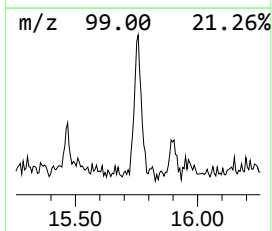
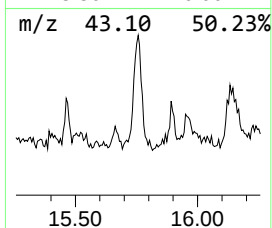
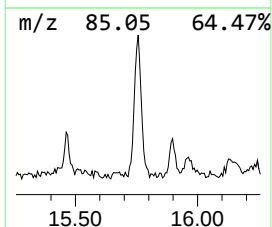
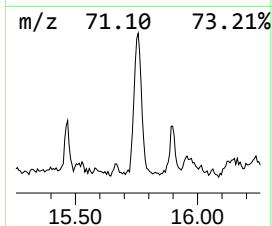
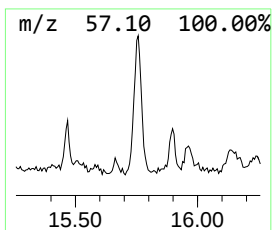
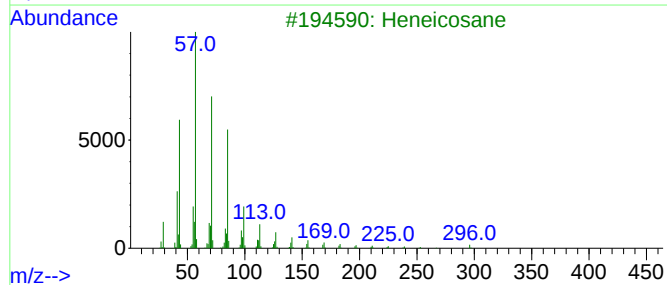
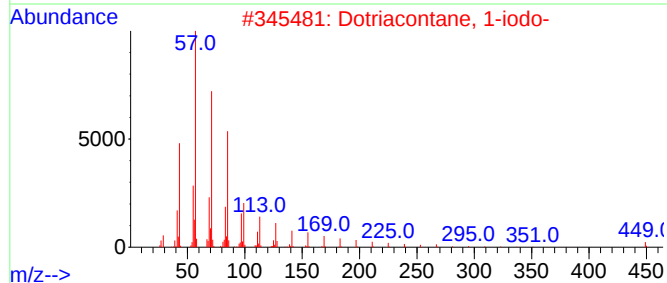
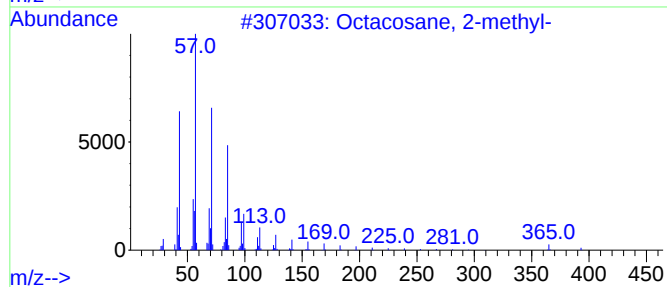
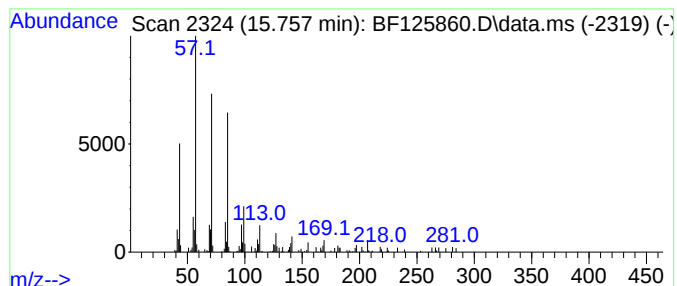
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octacosane, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.757	4.91 ng	272290	Perylene-d12	15.433

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
2			Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	90
3			Heneicosane	296	C21H44	000629-94-7	90
4			Tridecane, 3-methyl-	198	C14H30	006418-41-3	86
5			Pentacosane	352	C25H52	000629-99-2	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101521\
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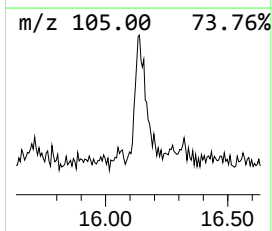
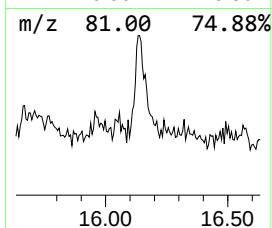
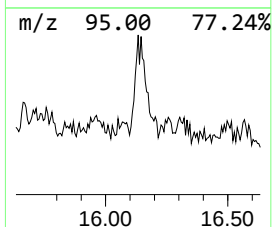
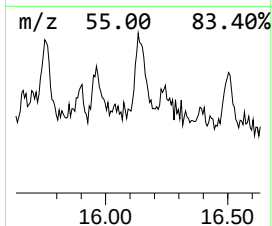
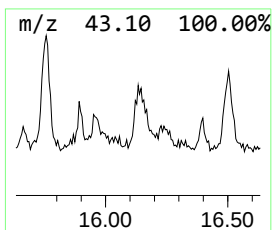
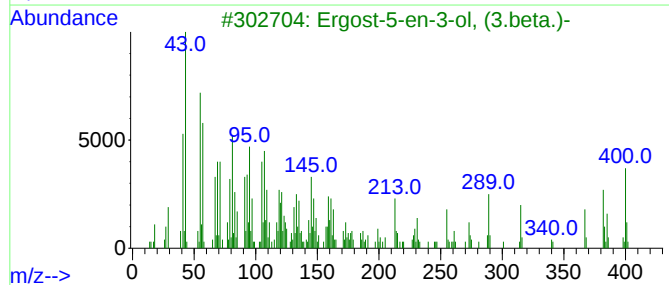
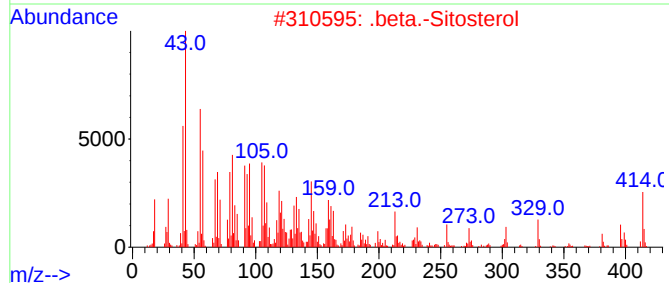
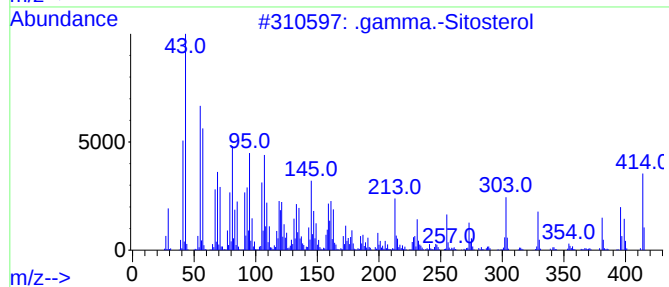
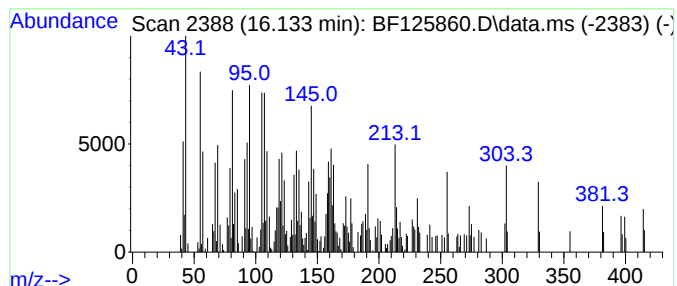
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 .gamma.-Sitosterol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
16.133	7.76 ng	430244	Perylene-d12		15.433	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	.gamma.-Sitosterol		414	C29H50O	000083-47-6	99
2	.beta.-Sitosterol		414	C29H50O	000083-46-5	91
3	Ergost-5-en-3-ol, (3.beta.)-		400	C28H48O	004651-51-8	53
4	Campesterol		400	C28H48O	000474-62-4	49
5	5-Cholestene-3-ol, 24-methyl-		400	C28H48O	290299-12-6	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101521\
Data File : BF125860.D
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ALS Vial : 4 Sample Multiplier: 1

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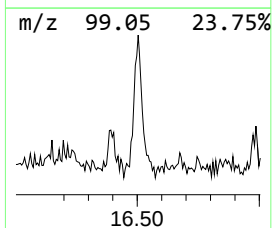
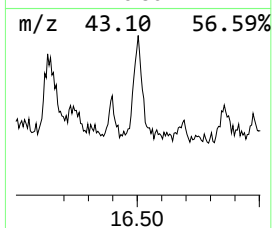
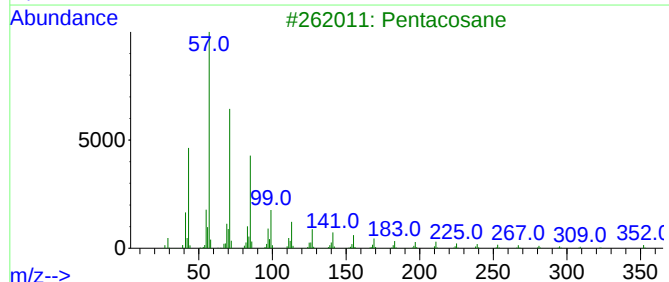
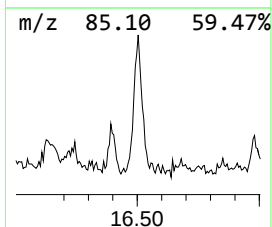
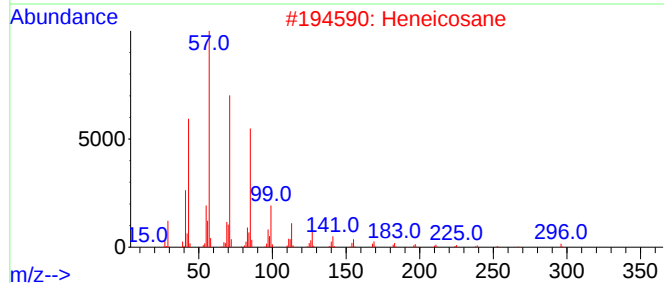
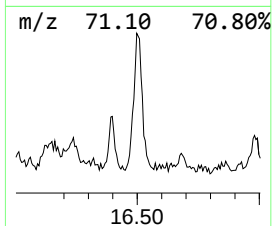
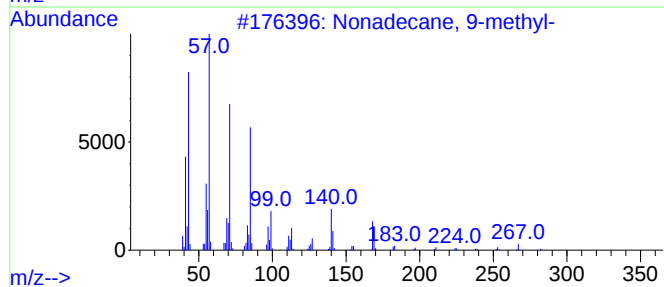
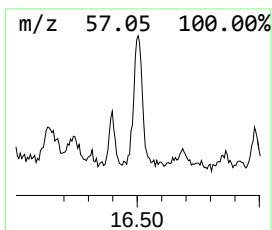
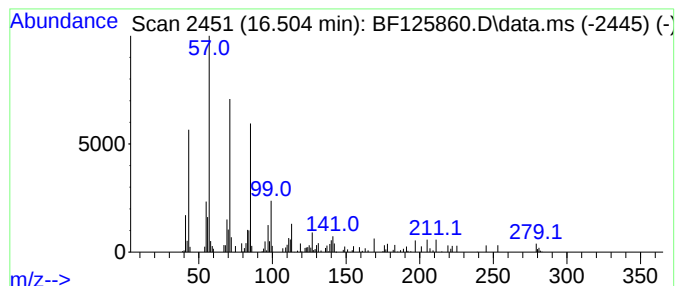
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Nonadecane, 9-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.504	2.67 ng	148151	Perylene-d12	15.433

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane, 9-methyl-	282	C20H42	013287-24-6	94
2			Heneicosane	296	C21H44	000629-94-7	91
3			Pentacosane	352	C25H52	000629-99-2	91
4			Triacontane	422	C30H62	000638-68-6	91
5			Octacosane	394	C28H58	000630-02-4	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101521\
Data File : BF125860.D
Acq On : 15 Oct 2021 13:47
Operator : JU/CG
Sample : M4243-21
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
T4-COMP-(1-4)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.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
2-Pentanone, 4-...	5.051	2.4	ng	117273	1	6.834	972387	20.0
Ethanol, 1-(2-b...	8.016	3.5	ng	234822	2	8.110	1328440	20.0
unknown10.192	10.192	5.5	ng	428921	3	9.863	1554890	20.0
n-Hexadecanoic ...	11.875	6.5	ng	465365	4	11.345	1432010	20.0
Octadecanoic acid	12.663	17.2	ng	1304410	5	13.980	1513960	20.0
1-Nonadecene	13.833	3.9	ng	291379	5	13.980	1513960	20.0
Octacosane	14.551	7.4	ng	558595	5	13.980	1513960	20.0
Benzo[e]pyrene	15.010	2.8	ng	156327	6	15.433	1108310	20.0
Octadecane	15.110	6.3	ng	352057	6	15.433	1108310	20.0
Octacosane, 2-m...	15.757	4.9	ng	272290	6	15.433	1108310	20.0
.gamma.-Sitosterol	16.133	7.8	ng	430244	6	15.433	1108310	20.0
Nonadecane, 9-m...	16.504	2.7	ng	148151	6	15.433	1108310	20.0