

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061223\
 Data File : BF133706.D
 Acq On : 12 Jun 2023 16:19
 Operator : CG\JU
 Sample : 03047-04
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB33A

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-BF060923.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133706.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.040	498	502	508	rVB	22926	28957	1.62%	0.211%
2	5.445	566	571	574	rBV	1793681	1633524	91.27%	11.882%
3	6.463	738	744	747	rBV	1646761	1625447	90.82%	11.823%
4	6.834	803	807	810	rBV	558309	465216	25.99%	3.384%
5	7.392	898	902	905	rBV	1151278	1066613	59.59%	7.758%
6	8.116	1021	1025	1028	rBV	728459	563727	31.50%	4.100%
7	9.192	1204	1208	1211	rBV	2252494	1789836	100.00%	13.018%
8	9.869	1320	1323	1327	rBV	672880	542645	30.32%	3.947%
9	10.580	1438	1444	1447	rBV	84722	79102	4.42%	0.575%
10	10.657	1453	1457	1461	rBV	1052789	926558	51.77%	6.739%
11	11.304	1562	1567	1571	rBV5	13522	22903	1.28%	0.167%
12	11.357	1573	1576	1579	rVV	586632	483450	27.01%	3.516%
13	11.380	1579	1580	1583	rVB	61306	39655	2.22%	0.288%
14	11.851	1656	1660	1663	rBV3	23979	40210	2.25%	0.292%
15	11.886	1663	1666	1670	rVV	278711	242119	13.53%	1.761%
16	12.057	1693	1695	1704	rVB7	19693	28483	1.59%	0.207%
17	12.574	1779	1783	1785	rBV	147754	131029	7.32%	0.953%
18	12.668	1796	1799	1808	rBV	119119	136016	7.60%	0.989%
19	12.804	1817	1822	1825	rBV	111272	111489	6.23%	0.811%
20	12.951	1842	1847	1850	rVV	1333106	1266559	70.76%	9.212%
21	13.015	1854	1858	1862	rBV6	12600	24330	1.36%	0.177%
22	13.233	1892	1895	1898	rBV3	17731	21501	1.20%	0.156%
23	13.515	1939	1943	1946	rBV4	14807	22188	1.24%	0.161%
24	13.845	1996	1999	2006	rBV	168682	197332	11.03%	1.435%
25	14.004	2018	2026	2029	rBV	548620	660007	36.88%	4.801%
26	14.027	2029	2030	2038	rVB	107741	92702	5.18%	0.674%
27	14.168	2052	2054	2056	rBV	28528	26468	1.48%	0.193%
28	14.480	2104	2107	2112	rBV2	74844	112553	6.29%	0.819%
29	14.927	2180	2183	2186	rVB	102233	93910	5.25%	0.683%
30	15.039	2198	2202	2205	rBV	71977	103076	5.76%	0.750%
31	15.121	2212	2216	2218	rBV	89208	109911	6.14%	0.799%
32	15.145	2218	2220	2227	rVB	109340	143142	8.00%	1.041%
33	15.345	2251	2254	2259	rVB	43040	55179	3.08%	0.401%
34	15.404	2261	2264	2267	rVB	52675	56528	3.16%	0.411%
35	15.468	2270	2275	2279	rBV	415461	500412	27.96%	3.640%
36	15.698	2311	2314	2322	rVB5	36197	49401	2.76%	0.359%

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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-BF060923.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.939	2351	2355	2359	rVB2	60332	80849	4.52%	0.588%
38	15.992	2361	2364	2368	rVB4	26068	37949	2.12%	0.276%
39	16.733	2486	2490	2499	rVB4	66089	137437	7.68%	1.000%

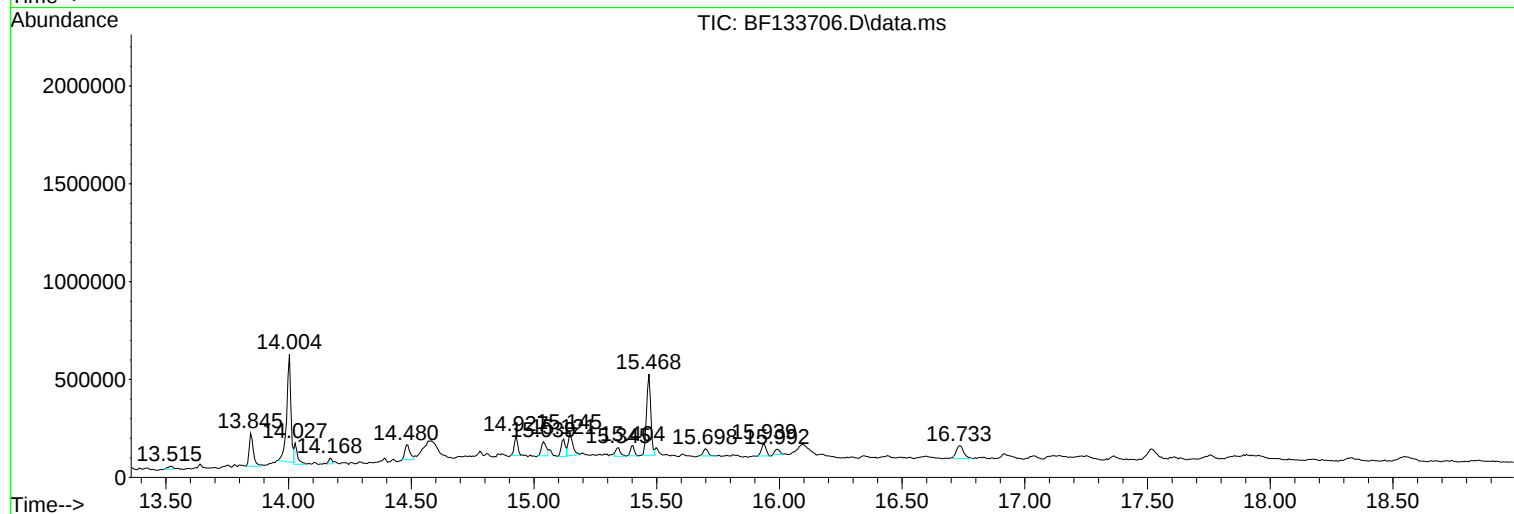
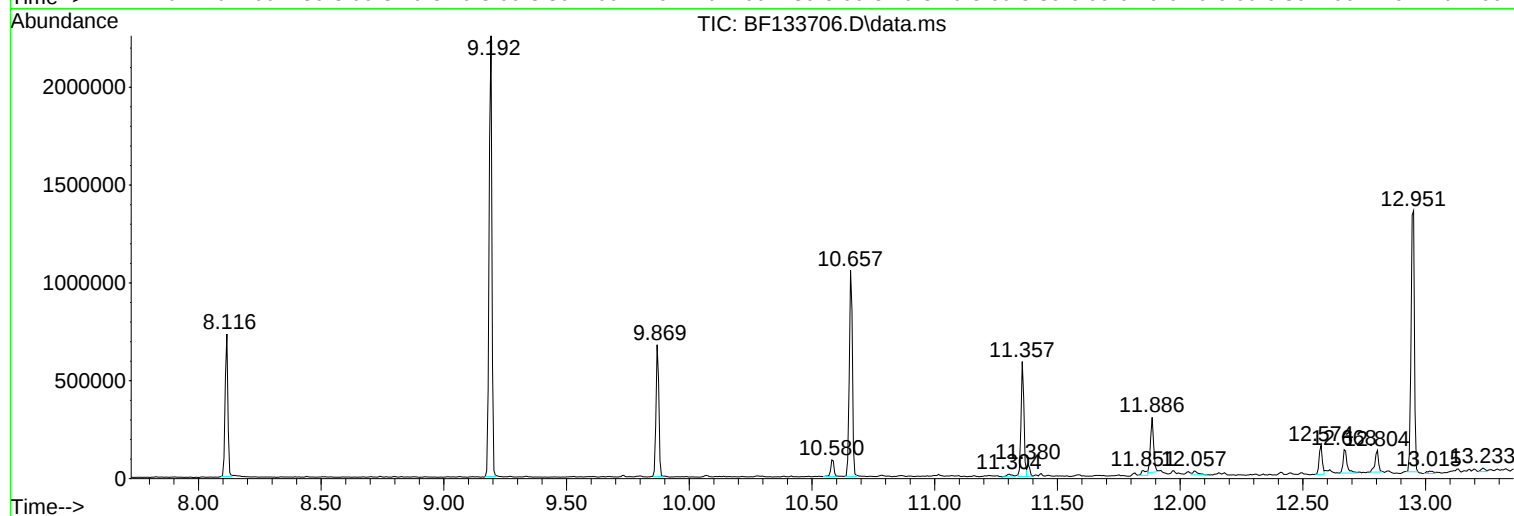
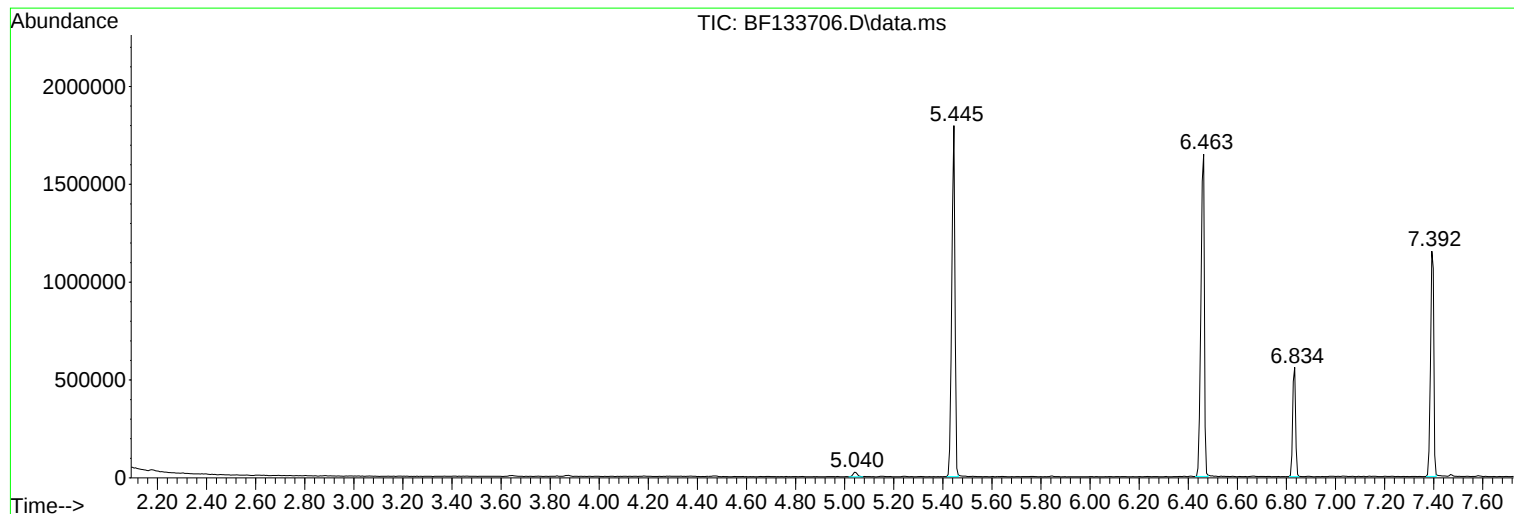
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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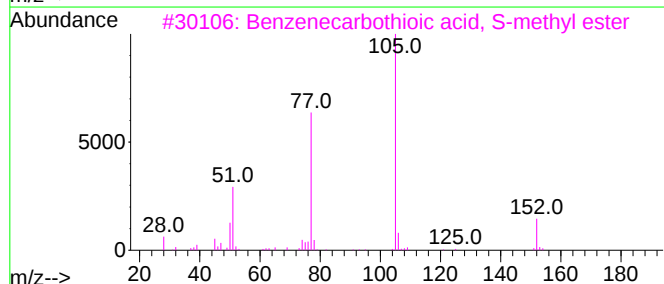
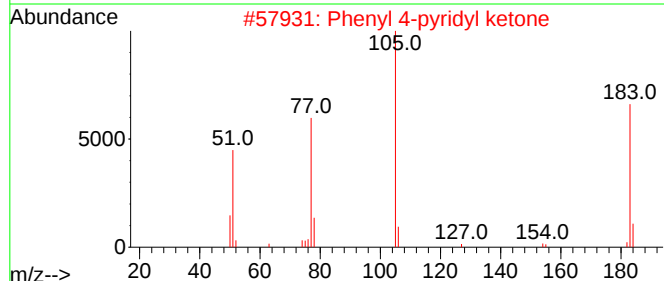
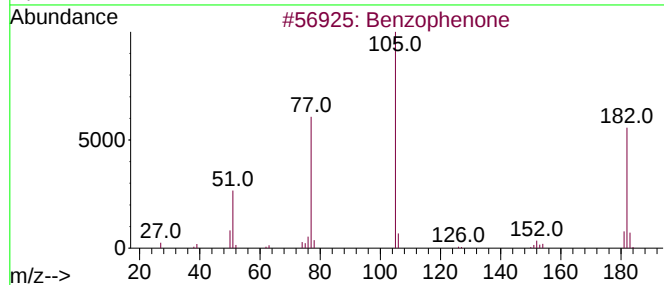
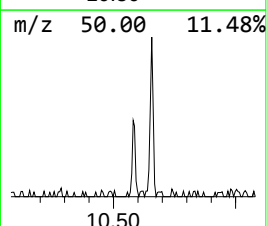
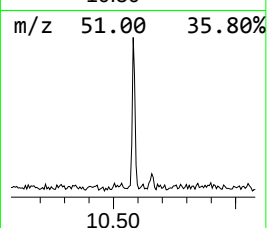
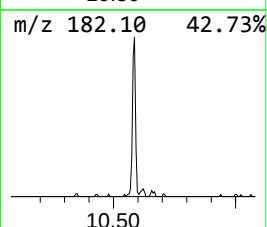
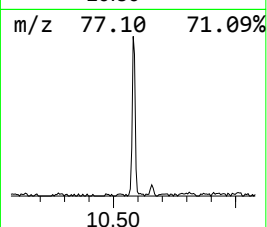
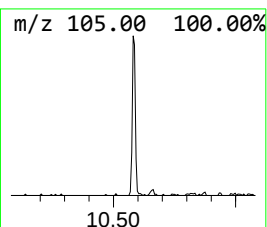
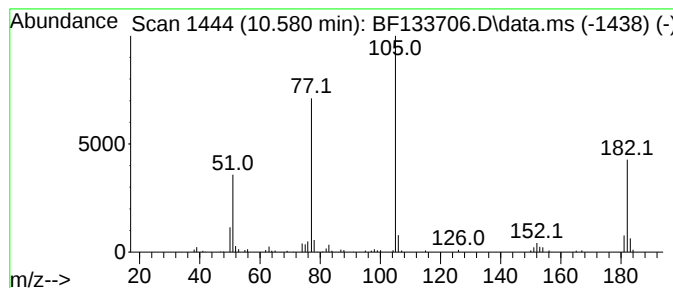
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Benzophenone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.580	2.92 ng	79102	Acenaphthene-d10	9.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	94
2			Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	58
3			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	52
4			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
5			Benzoyl bromide	184	C7H5BrO	000618-32-6	47



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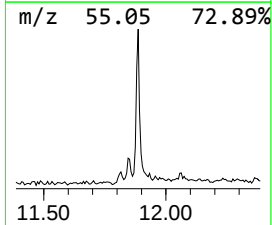
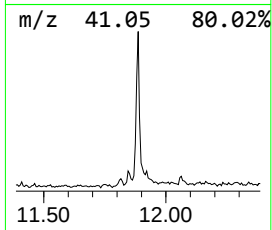
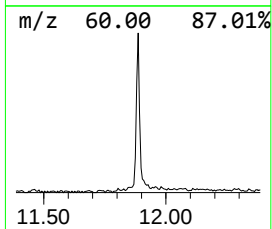
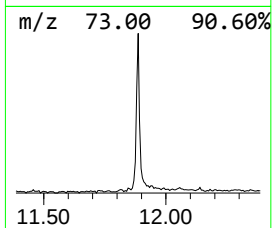
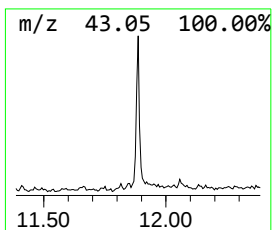
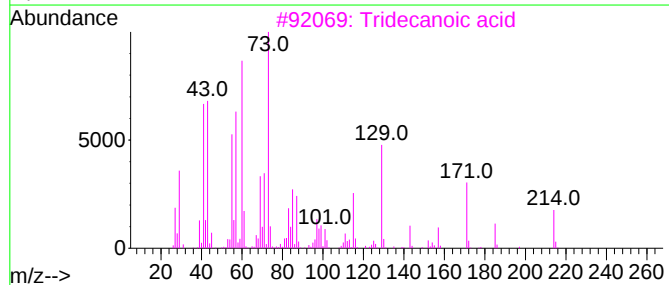
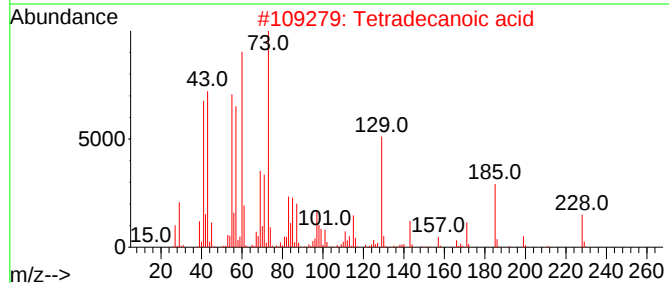
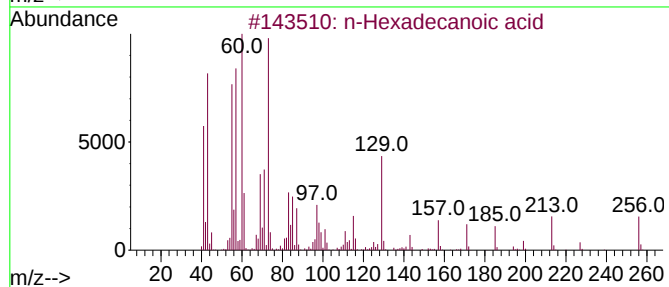
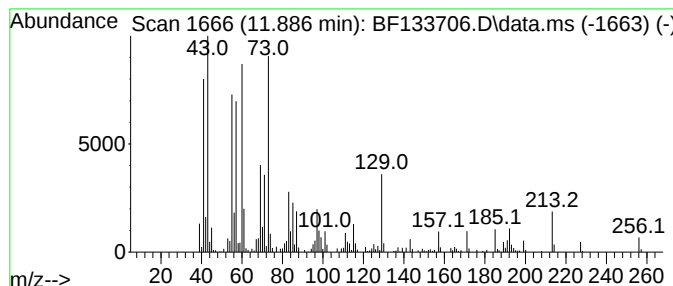
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.886	10.02 ng	242119	Phenanthrene-d10	11.357

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3			Tridecanoic acid	214	C13H26O2	000638-53-9	94
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
5			n-Decanoic acid	172	C10H20O2	000334-48-5	78



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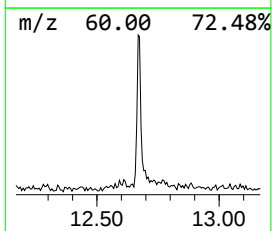
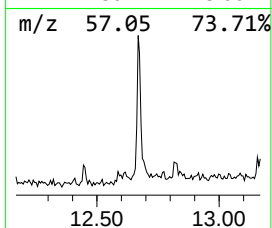
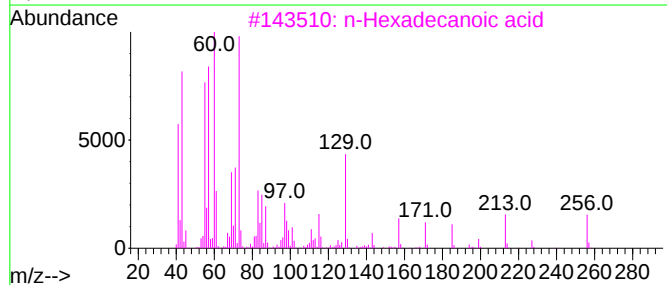
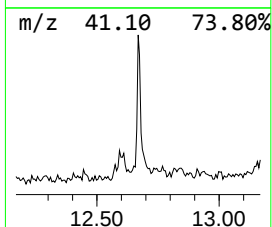
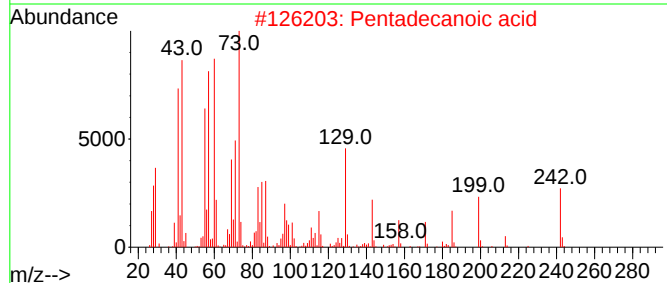
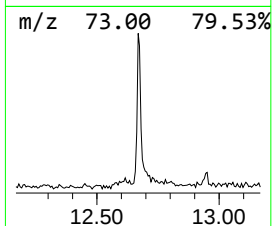
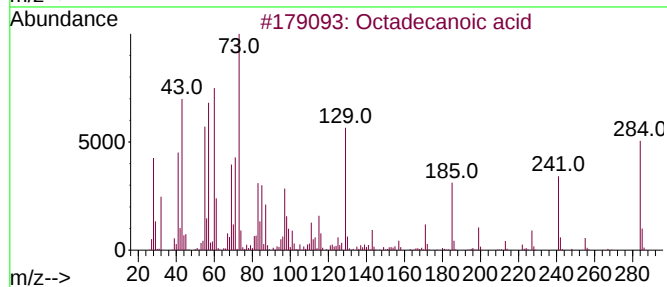
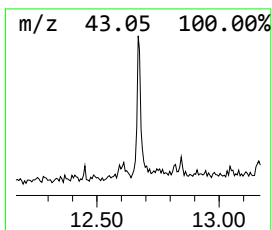
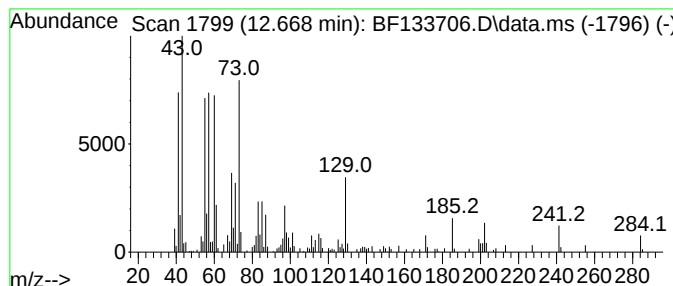
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.669	5.63 ng	136016	Phenanthrene-d10	11.357

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	96
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	86
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	68
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5			n-Decanoic acid	172	C10H20O2	000334-48-5	49



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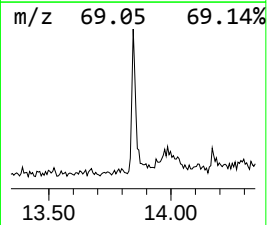
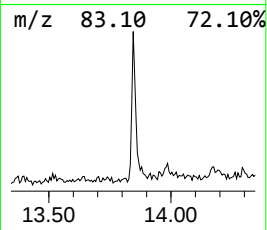
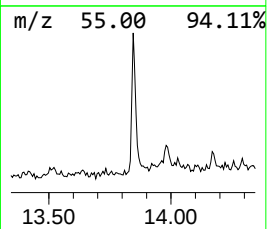
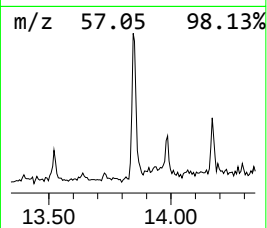
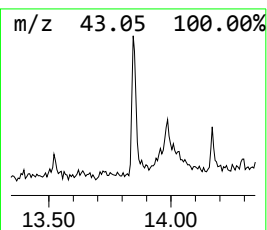
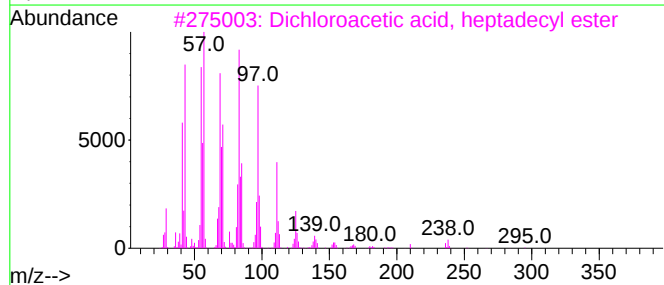
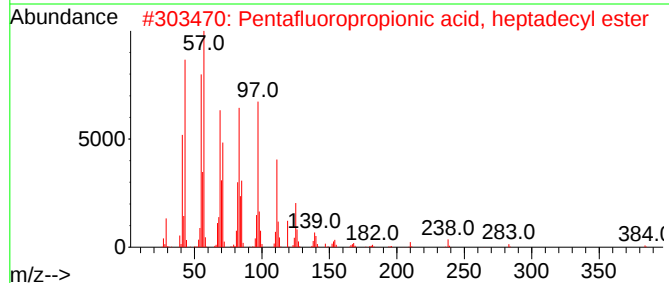
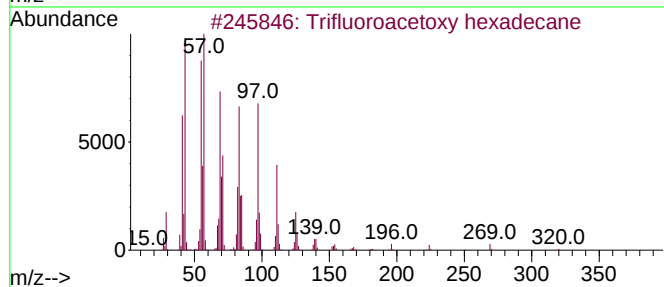
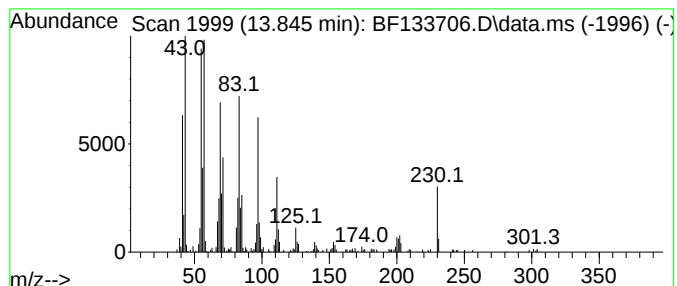
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Trifluoroacetoxy hexadecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.845	5.98 ng	197332	Chrysene-d12	14.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
2			Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	90
3			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	90
4			Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	90
5			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	90



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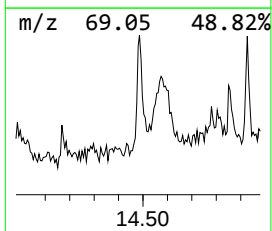
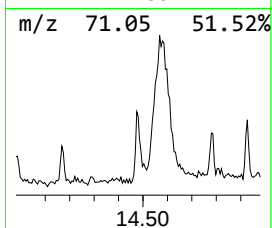
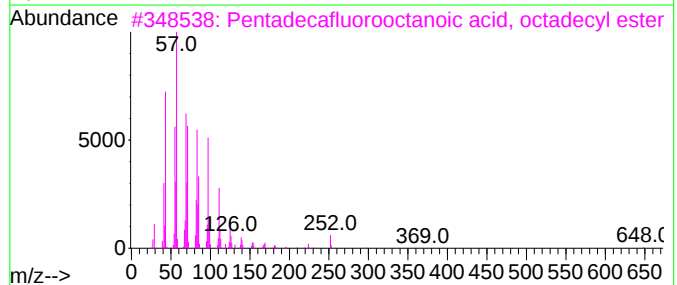
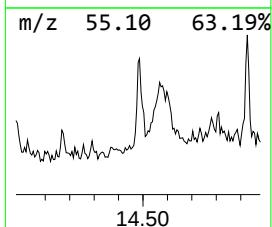
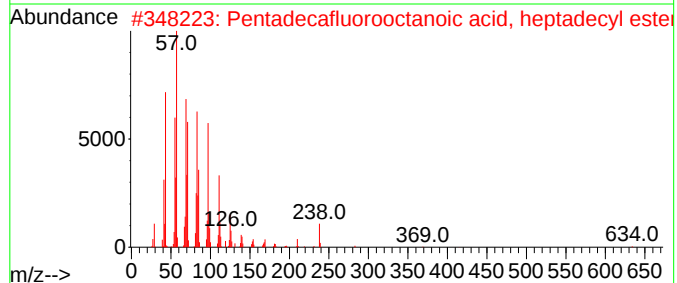
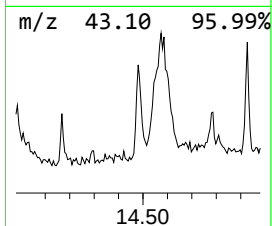
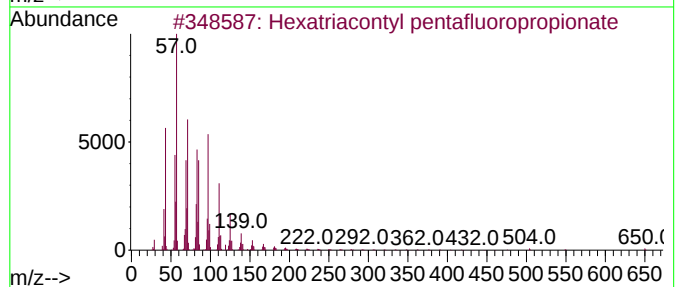
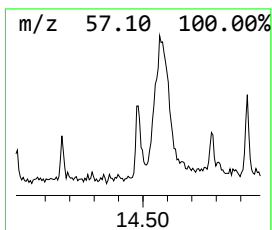
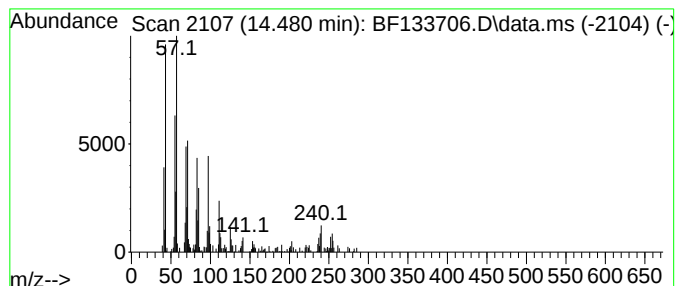
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Hexatriacontyl pentafluorop... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.480	3.41 ng	112553	Chrysene-d12	14.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexatriacontyl pentafluoropropio...	669	C39H73F5O2	1000351-89-0	87
2			Pentadecafluorooctanoic acid, he...	652	C25H35F15O2	1000406-04-7	87
3			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	87
4			Octatriacontyl pentafluoropropio...	697	C41H77F5O2	1000351-89-1	87
5			1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061223\
Data File : BF133706.D
Acq On : 12 Jun 2023 16:19
Operator : CG\JU
Sample : 03047-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

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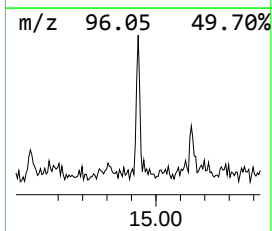
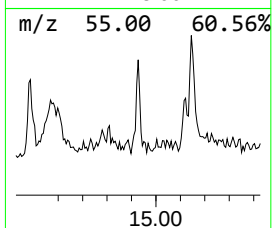
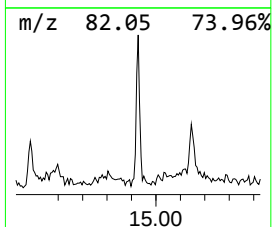
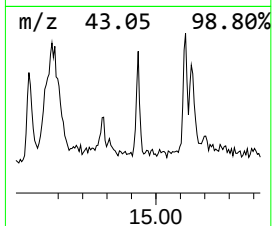
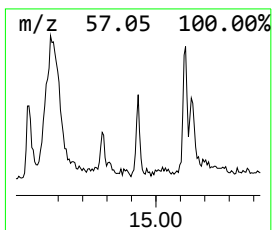
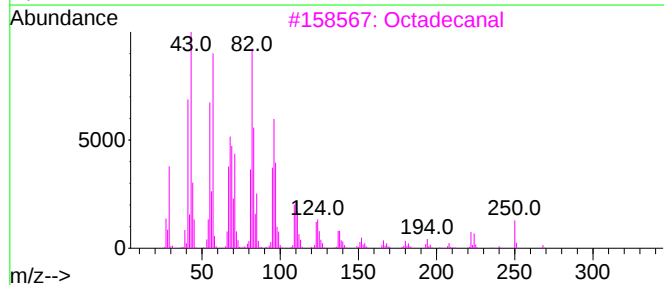
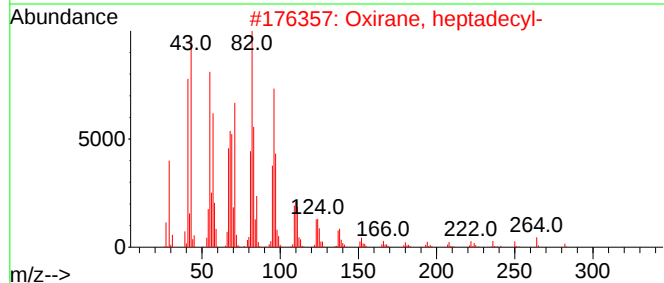
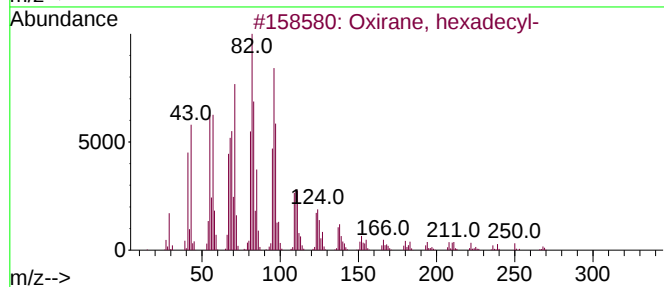
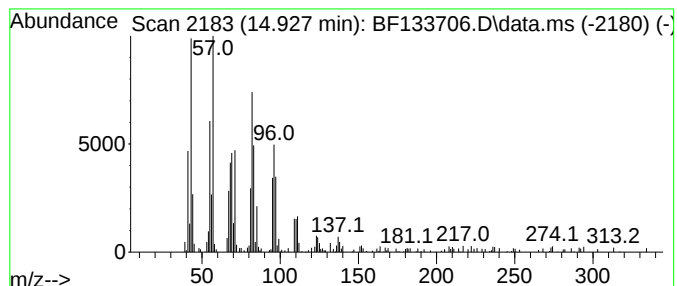
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Oxirane, hexadecyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.927	3.75 ng	93910	Perylene-d12	15.468

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxirane, hexadecyl-	268	C18H36O	007390-81-0	94
2			Oxirane, heptadecyl-	282	C19H38O	067860-04-2	93
3			Octadecanal	268	C18H36O	000638-66-4	93
4			Tetradecanal	212	C14H28O	000124-25-4	91
5			Pentadecanal	226	C15H30O	002765-11-9	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061223\
Data File : BF133706.D
Acq On : 12 Jun 2023 16:19
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Sample : 03047-04
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ALS Vial : 7 Sample Multiplier: 1

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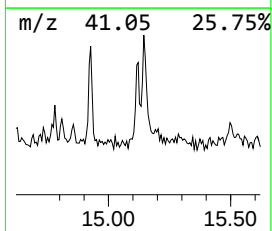
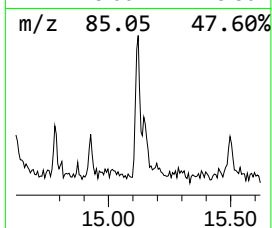
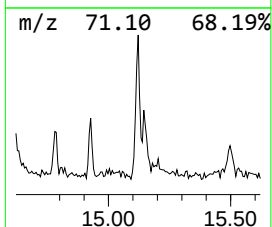
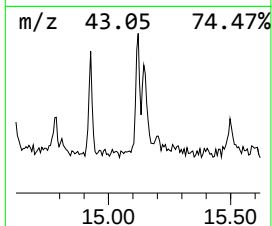
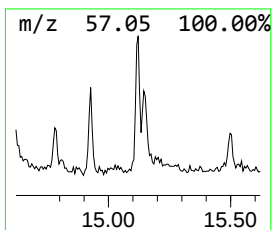
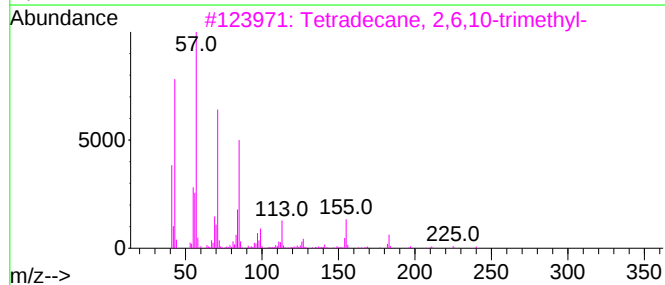
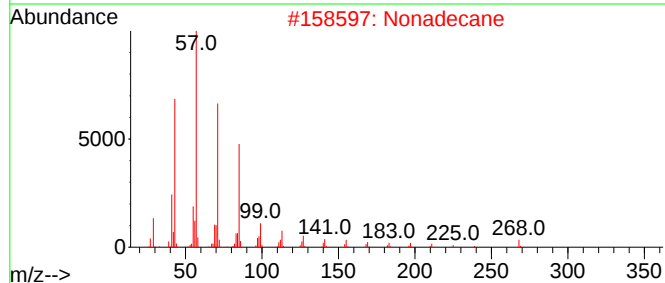
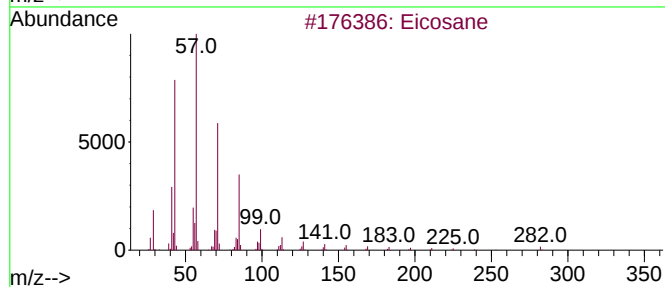
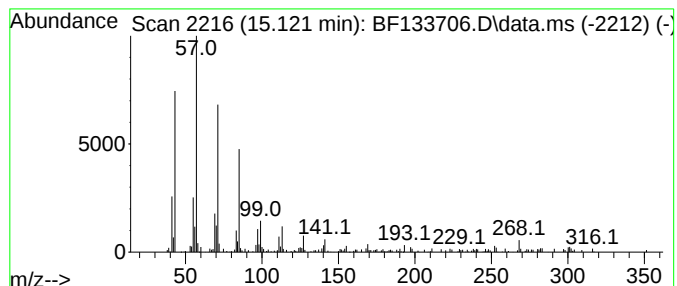
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.121	4.39 ng	109911	Perylene-d12	15.468

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	93
2			Nonadecane	268	C19H40	000629-92-5	93
3			Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	93
4			Hexacosane	366	C26H54	000630-01-3	90
5			Octacosane	394	C28H58	000630-02-4	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061223\
Data File : BF133706.D
Acq On : 12 Jun 2023 16:19
Operator : CG\JU
Sample : 03047-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

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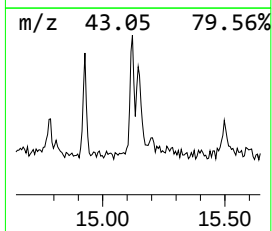
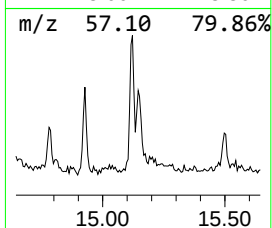
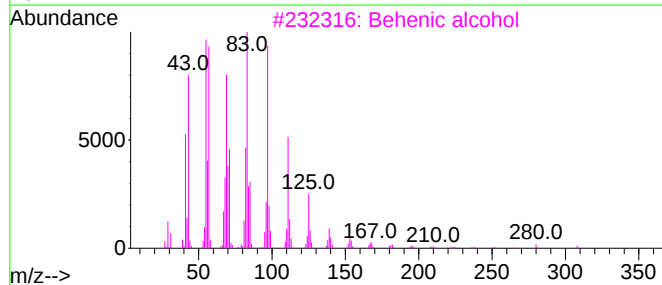
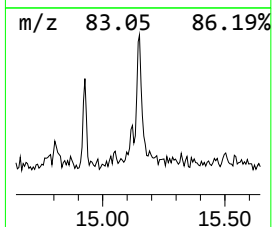
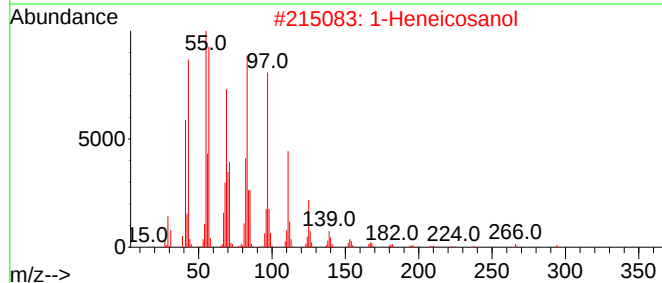
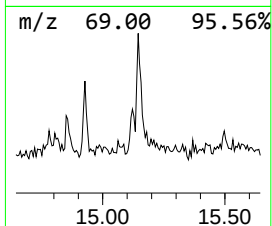
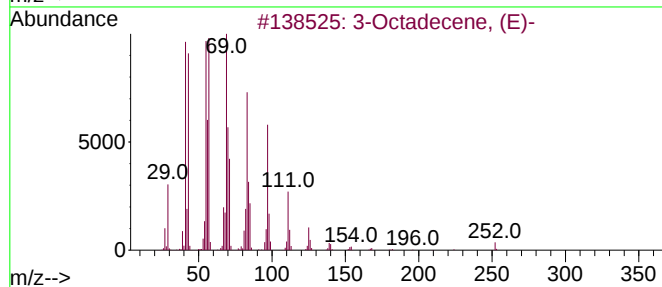
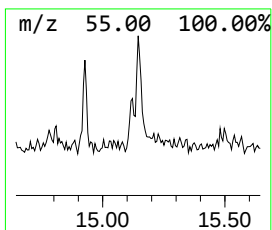
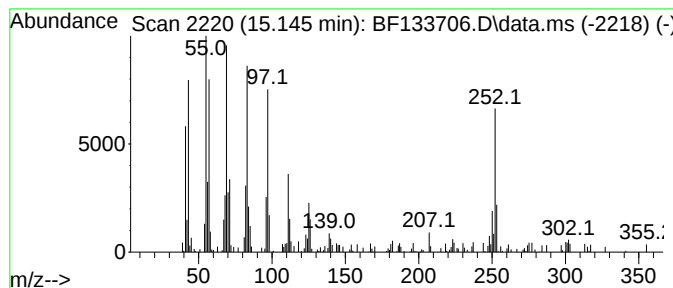
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 3-Octadecene, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.145	5.72 ng	143142	Perylene-d12	15.468

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Octadecene, (E)-	252	C18H36	007206-19-1	72
2		1-Heneicosanol	312	C21H44O	015594-90-8	60
3		Behenic alcohol	326	C22H46O	000661-19-8	60
4		1-Tridecene	182	C13H26	002437-56-1	58
5		Cetene	224	C16H32	000629-73-2	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061223\
Data File : BF133706.D
Acq On : 12 Jun 2023 16:19
Operator : CG\JU
Sample : 03047-04
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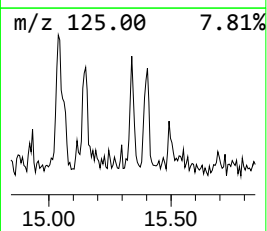
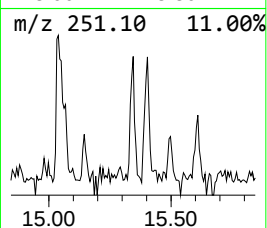
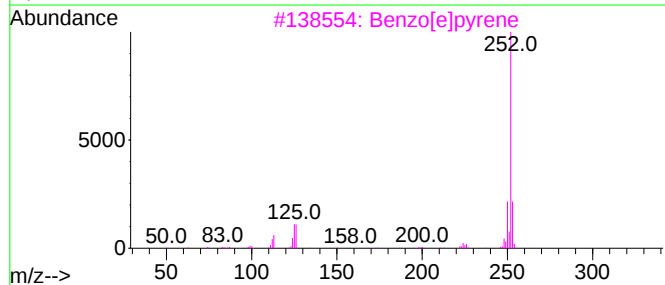
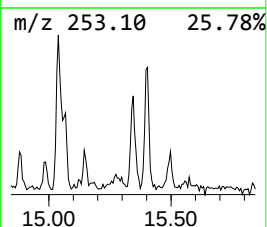
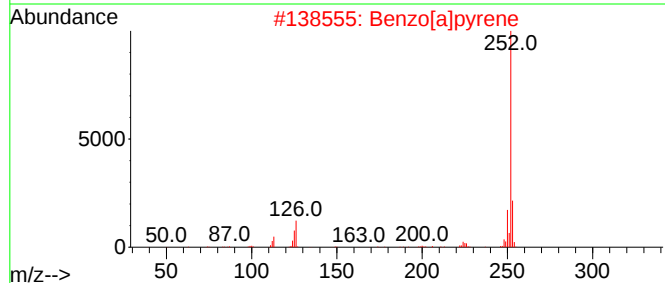
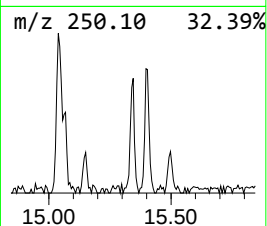
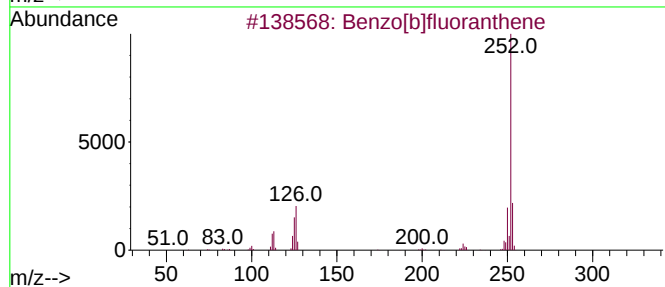
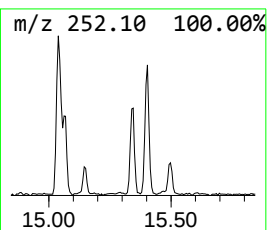
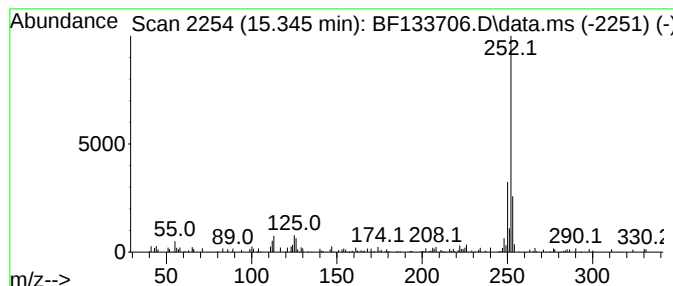
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Benzo[e]pyrene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.345	2.21 ng	55179	Perylene-d12	15.468

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[b]fluoranthene	252	C20H12	000205-99-2	93
2			Benzo[a]pyrene	252	C20H12	000050-32-8	90
3			Benzo[e]pyrene	252	C20H12	000192-97-2	90
4			(1-Cyclopentenyl)ferrocene	252	C15H16Fe	012260-67-2	78
5			Perylene	252	C20H12	000198-55-0	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061223\
Data File : BF133706.D
Acq On : 12 Jun 2023 16:19
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Sample : 03047-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

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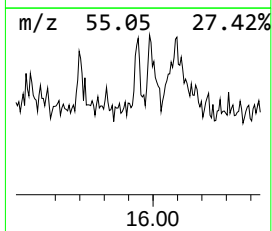
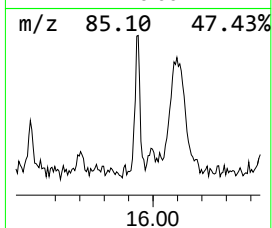
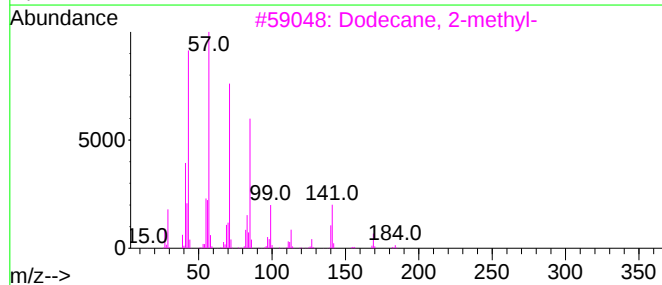
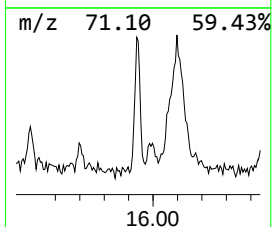
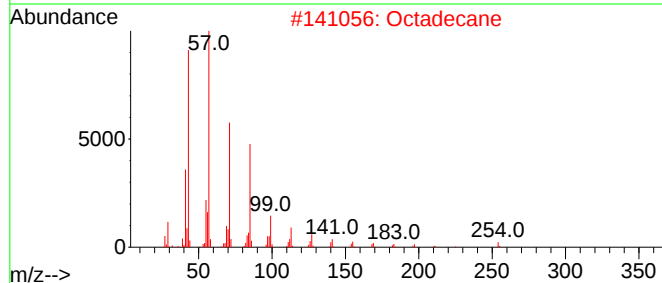
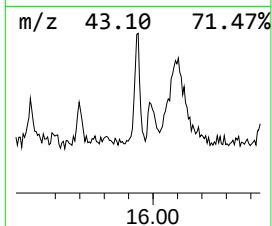
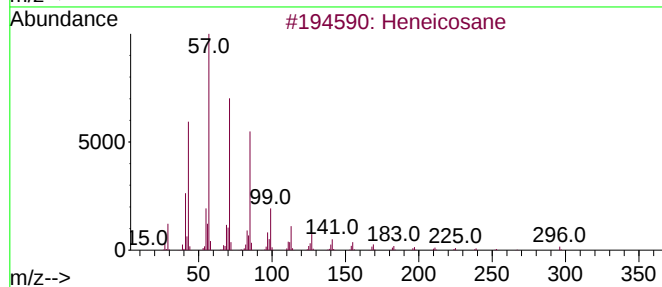
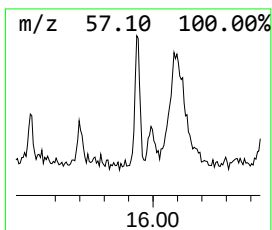
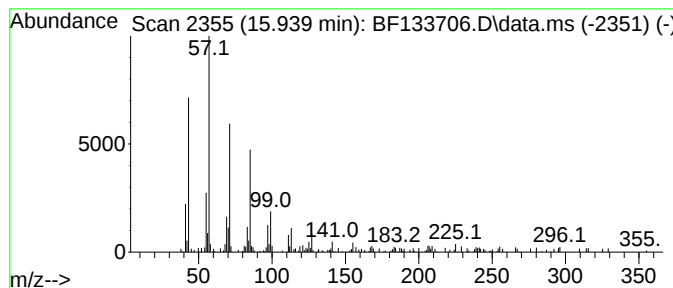
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.939	3.23 ng	80849	Perylene-d12	15.468

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	99
2			Octadecane	254	C18H38	000593-45-3	93
3			Dodecane, 2-methyl-	184	C13H28	001560-97-0	90
4			Hexatriacontane	507	C36H74	000630-06-8	87
5			Tridecane, 7-hexyl-	268	C19H40	007225-66-3	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061223\
Data File : BF133706.D
Acq On : 12 Jun 2023 16:19
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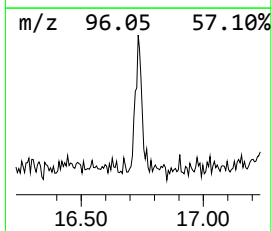
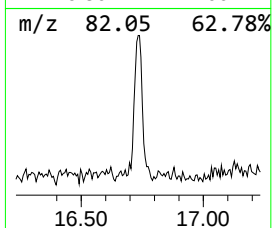
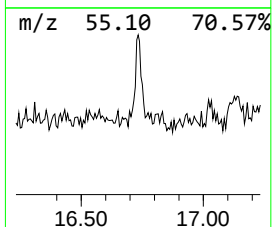
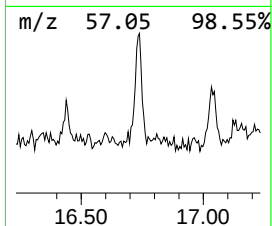
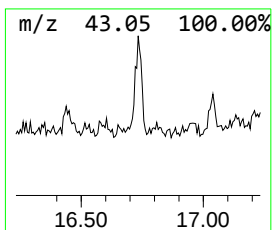
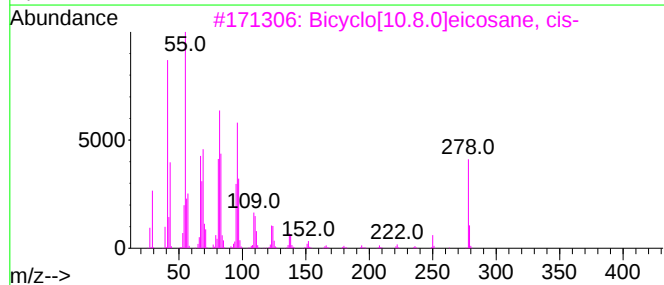
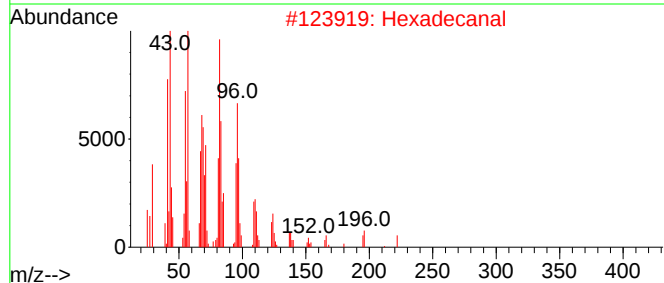
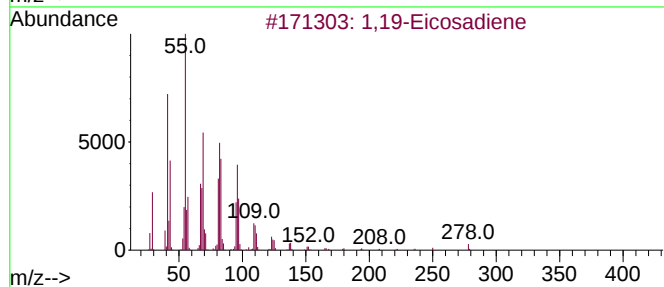
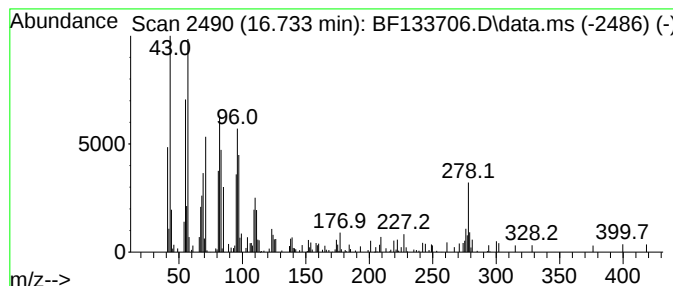
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 1,19-Eicosadiene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.733	5.49 ng	137437	Perylene-d12	15.468

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,19-Eicosadiene			278	C20H38	014811-95-1	70
2	Hexadecanal			240	C16H32O	000629-80-1	68
3	Bicyclo[10.8.0]eicosane, cis-			278	C20H38	1000155-82-2	64
4	Oxirane, hexadecyl-			268	C18H36O	007390-81-0	62
5	1,15-Hexadecadiene			222	C16H30	021964-51-2	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061223\
Data File : BF133706.D
Acq On : 12 Jun 2023 16:19
Operator : CG\JU
Sample : 03047-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.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
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n-Hexadecanoic ...	11.886	10.0	ng	242119	4	11.357	483450	20.0
Octadecanoic acid	12.669	5.6	ng	136016	4	11.357	483450	20.0
Trifluoroacetox...	13.845	6.0	ng	197332	5	14.004	660007	20.0
Hexatriacontyl ...	14.480	3.4	ng	112553	5	14.004	660007	20.0
Oxirane, hexade...	14.927	3.8	ng	93910	6	15.468	500412	20.0
Eicosane	15.121	4.4	ng	109911	6	15.468	500412	20.0
3-Octadecene, (E)-	15.145	5.7	ng	143142	6	15.468	500412	20.0
Benzo[e]pyrene	15.345	2.2	ng	55179	6	15.468	500412	20.0
Heneicosane	15.939	3.2	ng	80849	6	15.468	500412	20.0
1,19-Eicosadiene	16.733	5.5	ng	137437	6	15.468	500412	20.0