

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022621\
 Data File : BF123316.D
 Acq On : 26 Feb 2021 22:30
 Operator : JU/CG
 Sample : M1499-01 2X
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 N-1

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-BF021921.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123316.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.463	570	574	595	rBV	1495357	1356808	79.57%	7.507%
2	6.475	742	746	761	rBV	1646261	1430652	83.91%	7.915%
3	6.845	806	809	813	rBV	975800	800824	46.97%	4.431%
4	7.410	901	905	917	rBV	973473	900635	52.82%	4.983%
5	8.133	1024	1028	1031	rBV	1313164	1068859	62.69%	5.914%
6	9.210	1207	1211	1214	rBV	1954320	1613269	94.62%	8.926%
7	9.604	1274	1278	1283	rBV	84349	82887	4.86%	0.459%
8	9.751	1300	1303	1307	rVB	63633	53532	3.14%	0.296%
9	9.892	1323	1327	1330	rBV	1414109	1235238	72.44%	6.834%
10	10.680	1457	1461	1469	rBV	1156637	1044700	61.27%	5.780%
11	10.810	1478	1483	1485	rVB4	21381	30119	1.77%	0.167%
12	11.245	1552	1557	1560	rBV4	15570	21236	1.25%	0.117%
13	11.380	1576	1580	1583	rBV	1608514	1316652	77.22%	7.285%
14	11.404	1583	1584	1586	rVB	74912	36544	2.14%	0.202%
15	11.457	1591	1593	1596	rVB	29593	26501	1.55%	0.147%
16	11.774	1643	1647	1650	rBV	312585	238940	14.01%	1.322%
17	11.839	1655	1658	1662	rBV3	17962	24354	1.43%	0.135%
18	11.880	1662	1665	1667	rVV	34178	32075	1.88%	0.177%
19	11.910	1667	1670	1677	rVV	215470	251972	14.78%	1.394%
20	11.992	1681	1684	1687	rVV3	42879	57310	3.36%	0.317%
21	12.016	1687	1688	1692	rVB	29624	24001	1.41%	0.133%
22	12.204	1718	1720	1724	rVB2	40490	37442	2.20%	0.207%
23	12.363	1743	1747	1750	rBV	138663	112654	6.61%	0.623%
24	12.421	1753	1757	1758	rBV	26357	32065	1.88%	0.177%
25	12.463	1761	1764	1766	rVV	1033121	841943	49.38%	4.658%
26	12.486	1766	1768	1773	rVB	733947	596553	34.99%	3.301%
27	12.568	1779	1782	1784	rBV	120356	93882	5.51%	0.519%
28	12.598	1784	1787	1790	rVV	109383	101005	5.92%	0.559%
29	12.698	1800	1804	1807	rBV2	58473	73040	4.28%	0.404%
30	12.763	1813	1815	1818	rBV	34748	31596	1.85%	0.175%
31	12.827	1821	1826	1828	rBV	128134	128191	7.52%	0.709%
32	12.968	1847	1850	1854	rVB	2083442	1705073	100.00%	9.434%
33	13.039	1860	1862	1867	rVB2	19477	27632	1.62%	0.153%
34	13.204	1887	1890	1892	rBV3	27862	30019	1.76%	0.166%
35	13.263	1897	1900	1903	rVB2	25161	27151	1.59%	0.150%
36	13.327	1908	1911	1913	rBV3	17066	22071	1.29%	0.122%

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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-BF021921.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.662	1966	1968	1972	rBV	32223	28173	1.65%	0.156%
38	13.880	2002	2005	2015	rBV5	87873	213039	12.49%	1.179%
39	14.027	2026	2030	2033	rBV	1047518	1037345	60.84%	5.739%
40	14.051	2033	2034	2039	rVB	72880	65139	3.82%	0.360%
41	14.451	2100	2102	2106	rBV4	27359	35891	2.10%	0.199%
42	14.498	2108	2110	2113	rVB	32750	34808	2.04%	0.193%
43	15.068	2204	2207	2216	rVB	91379	178682	10.48%	0.989%
44	15.374	2256	2259	2265	rVB	64319	83551	4.90%	0.462%
45	15.433	2267	2269	2275	rVB	66067	80281	4.71%	0.444%
46	15.504	2276	2281	2284	rBV	663093	809927	47.50%	4.481%

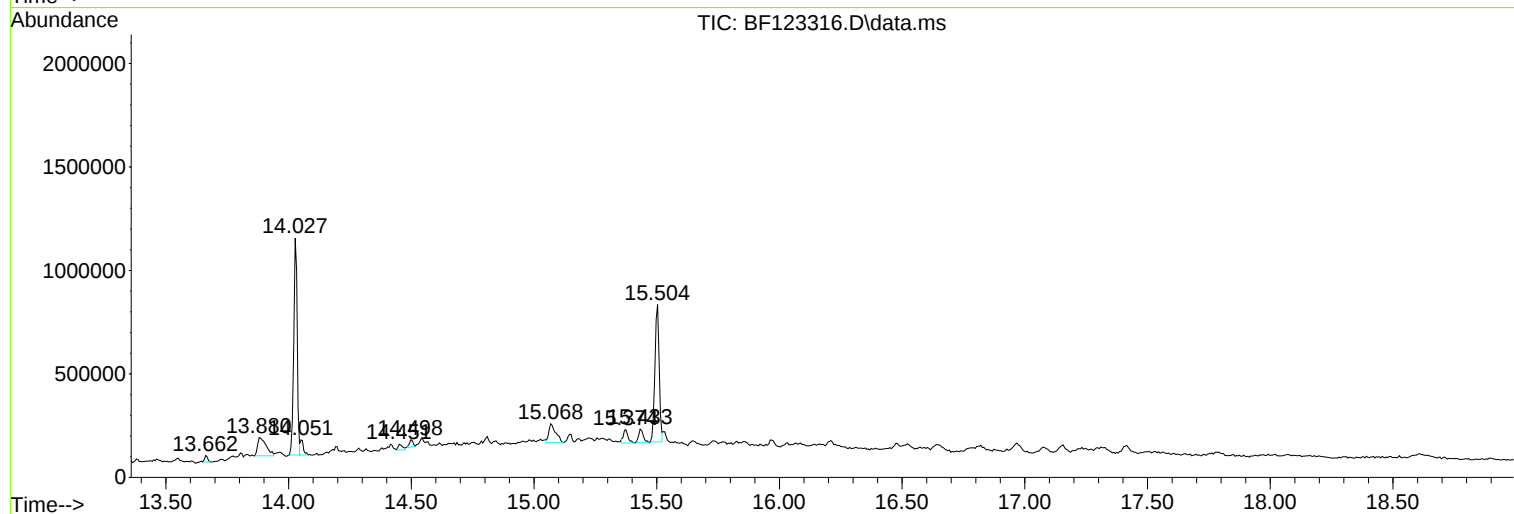
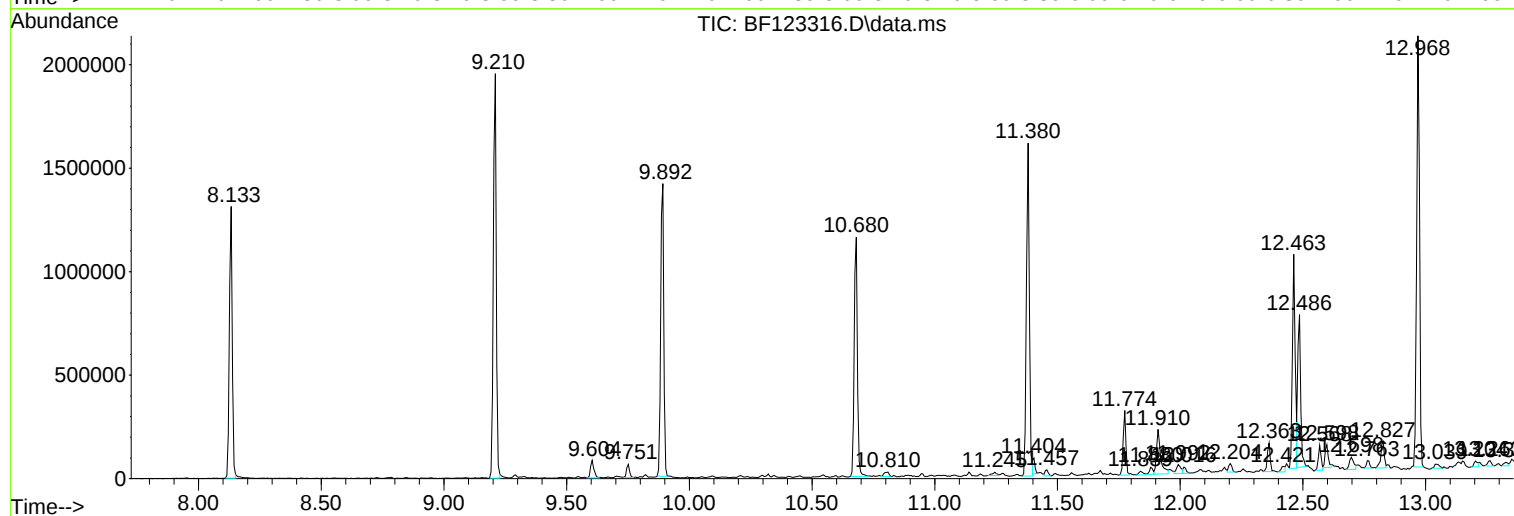
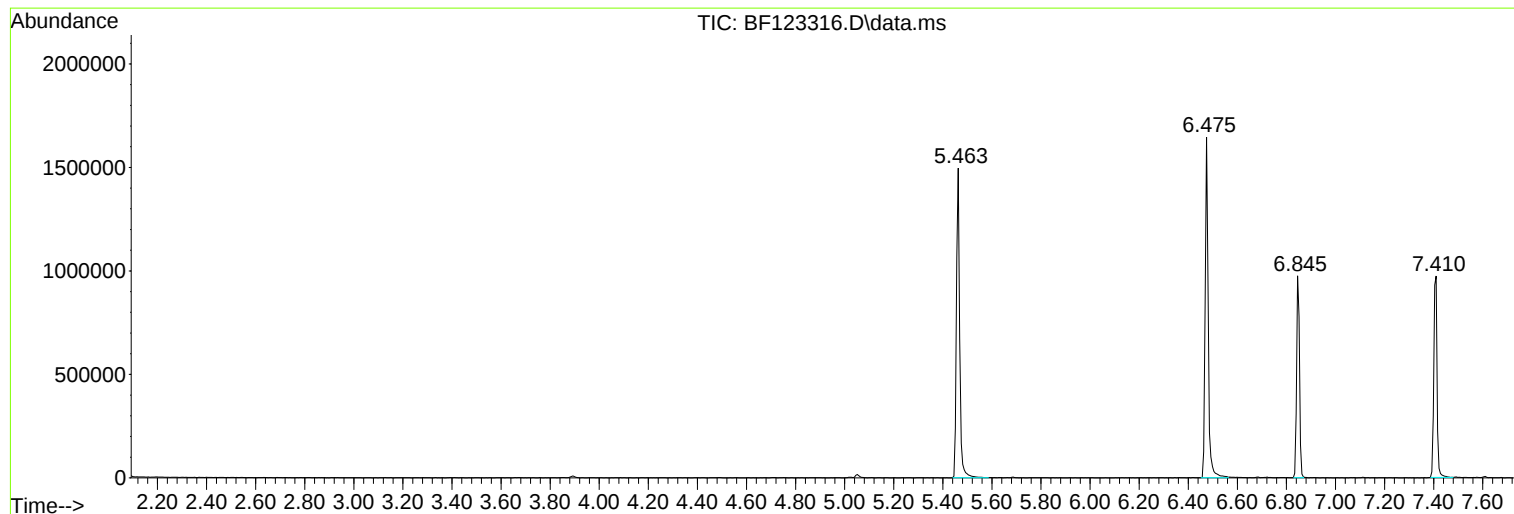
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF021921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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Misc :
ALS Vial : 14 Sample Multiplier: 1

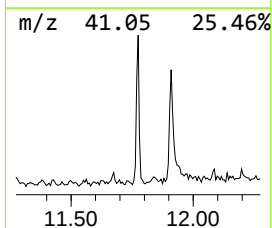
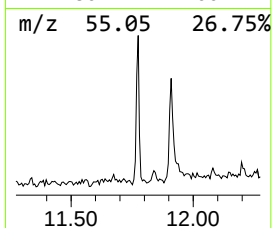
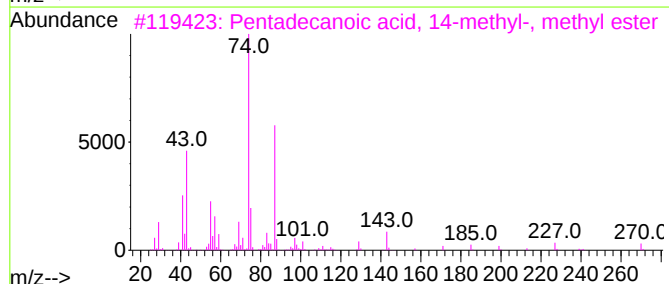
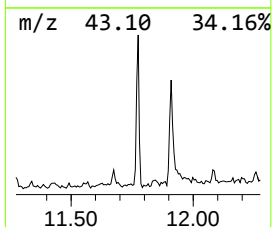
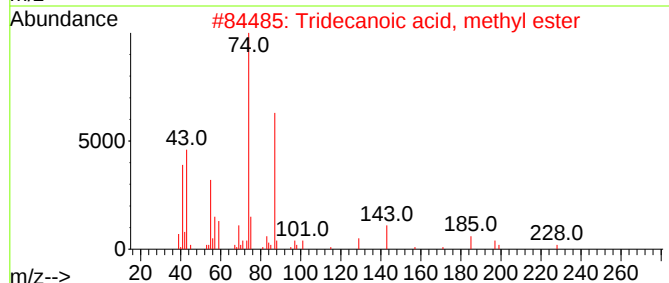
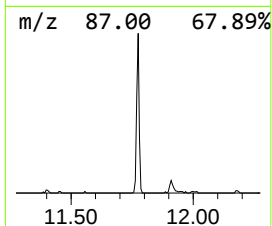
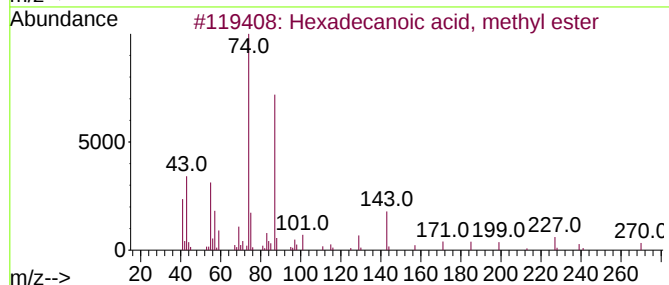
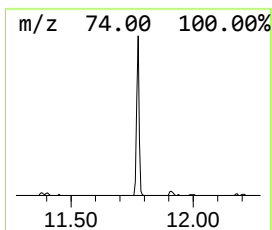
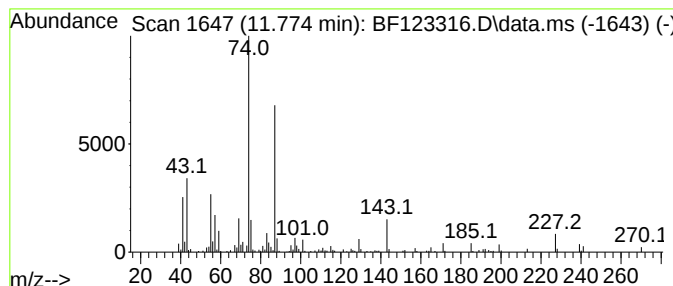
Instrument :
BNA_F
ClientSampleId :
N-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF021921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Hexadecanoic acid, methyl e... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.774	3.63 ng	238940	Phenanthrene-d10	11.380	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	99
2	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	93
3	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	87
4	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86
5	Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	86



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Misc :
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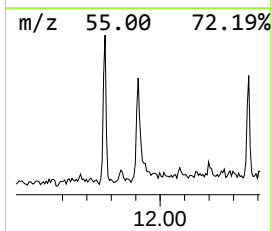
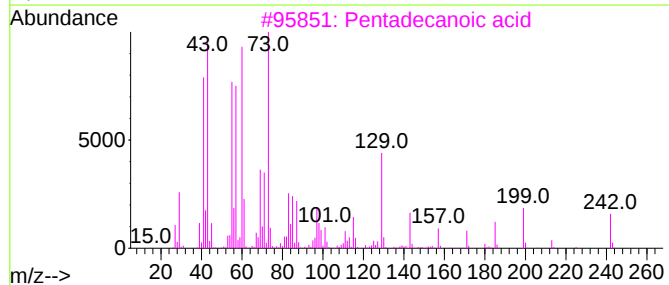
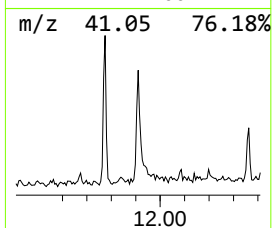
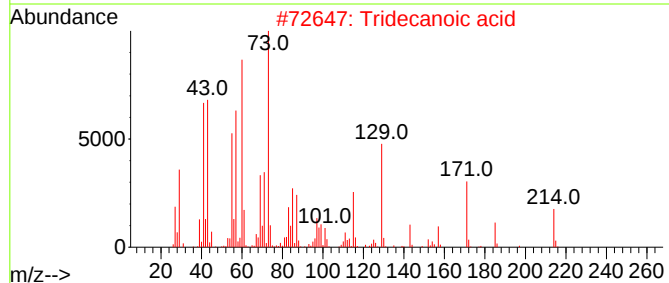
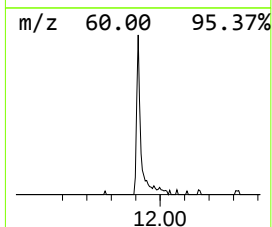
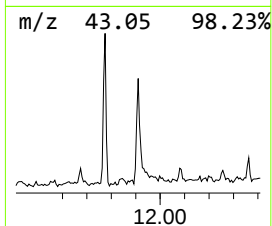
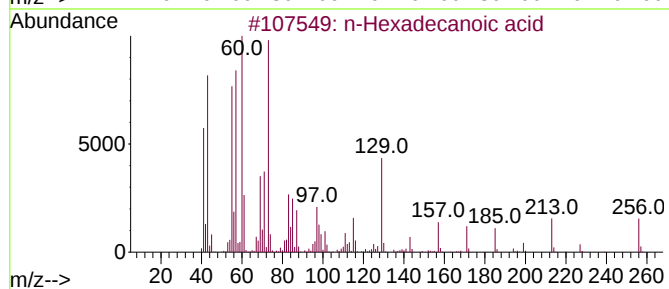
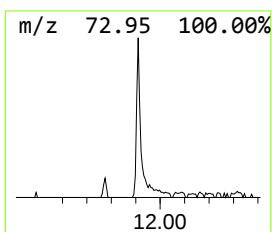
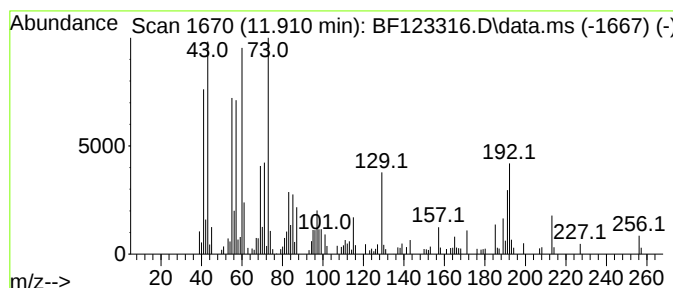
Instrument :
BNA_F
ClientSampled :
N-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF021921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.910	3.83 ng	251972	Phenanthrene-d10	11.380	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5	Nonanoic acid	158	C9H18O2	000112-05-0	38



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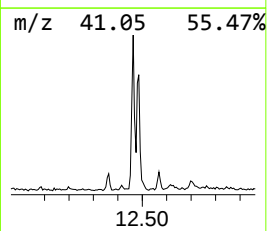
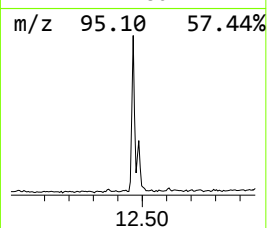
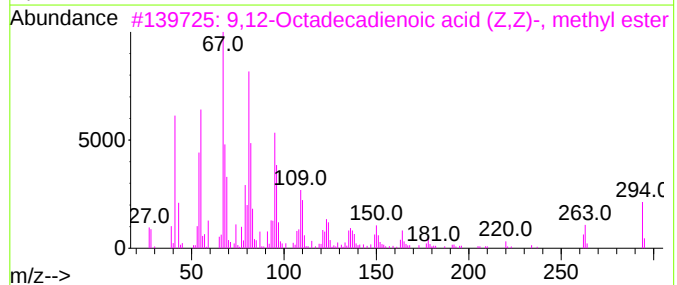
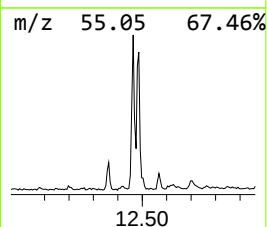
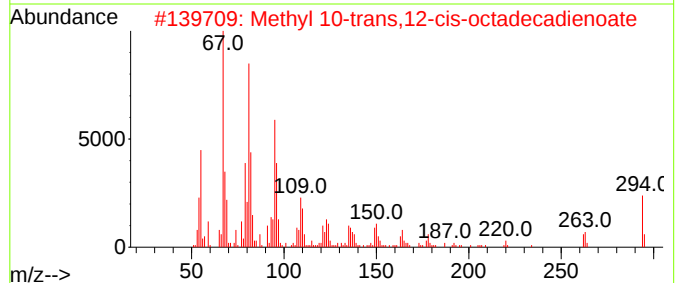
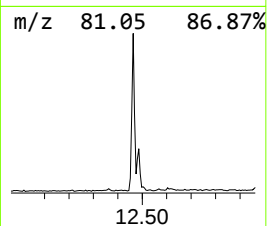
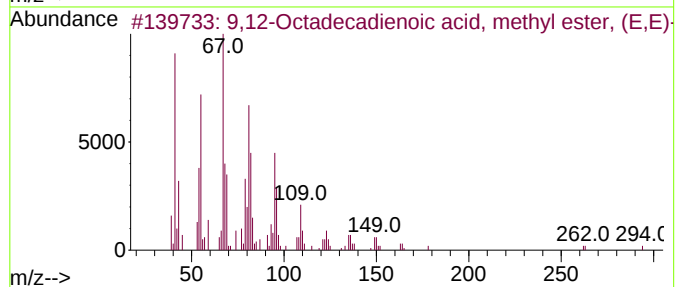
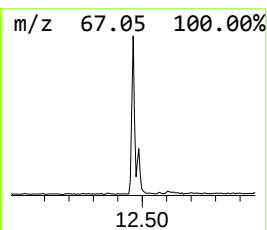
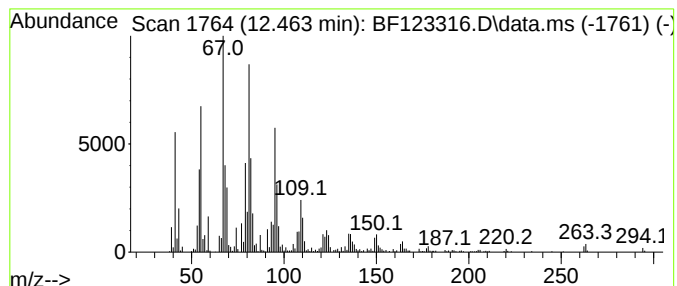
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.463	12.79 ng	841943	Phenanthrene-d10		11.380	
Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
2		Methyl 10-trans,12-cis-octadecad...	294	C19H34O2	1000336-44-2	99
3		9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99
4		10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	99
5		Methyl 7,12-octadecadienoate	294	C19H34O2	1000336-43-8	98



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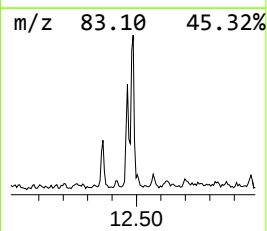
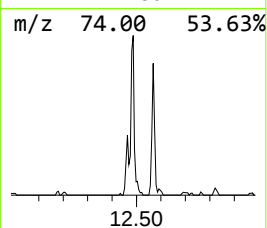
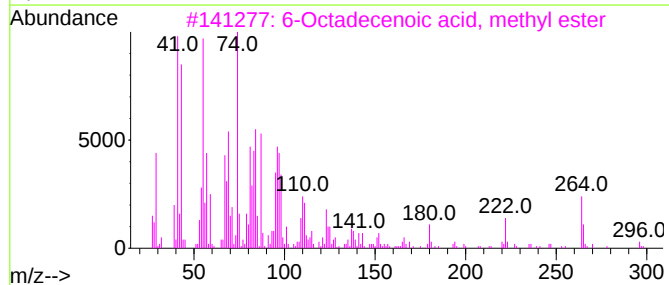
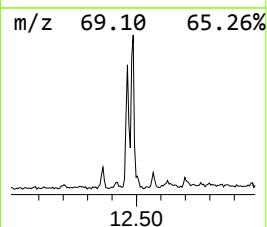
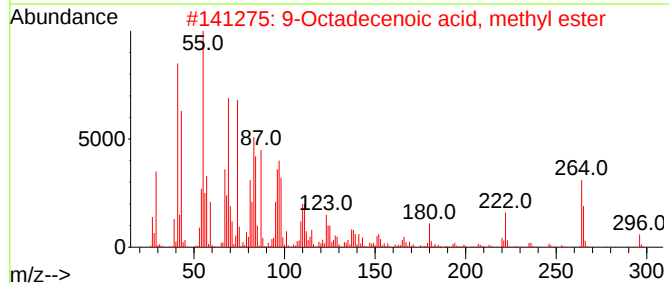
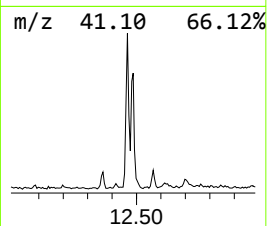
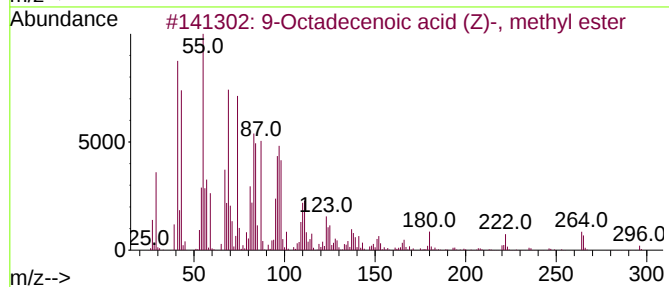
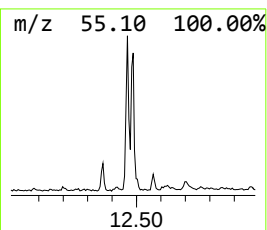
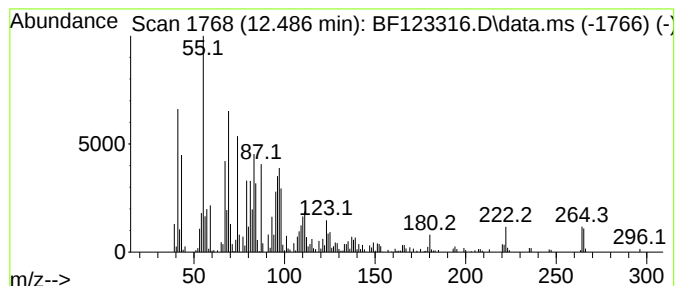
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 9-Octadecenoic acid (Z)-, m... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.486	9.06 ng	596553	Phenanthrene-d10	11.380

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99
2			9-Octadecenoic acid, methyl ester	296	C19H36O2	002462-84-2	99
3			6-Octadecenoic acid, methyl ester	296	C19H36O2	052355-31-4	99
4			cis-13-Octadecenoic acid, methyl...	296	C19H36O2	1000333-58-3	99
5			9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	99



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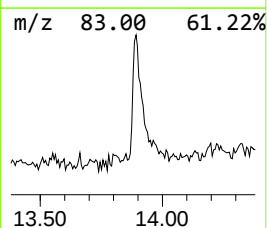
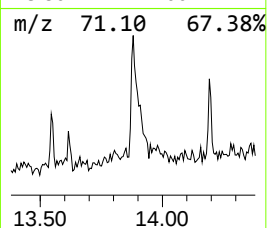
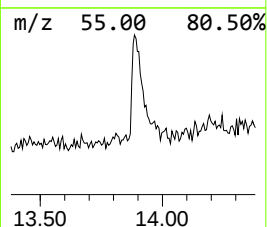
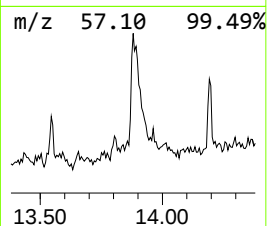
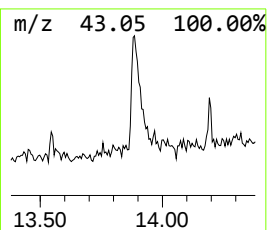
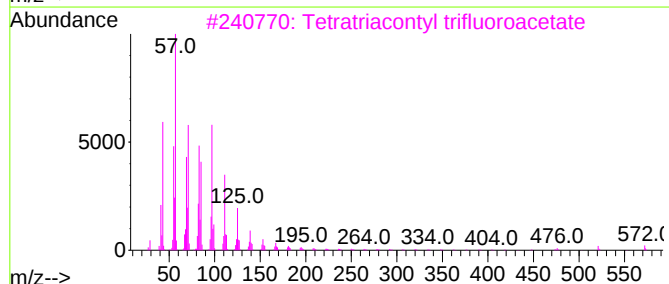
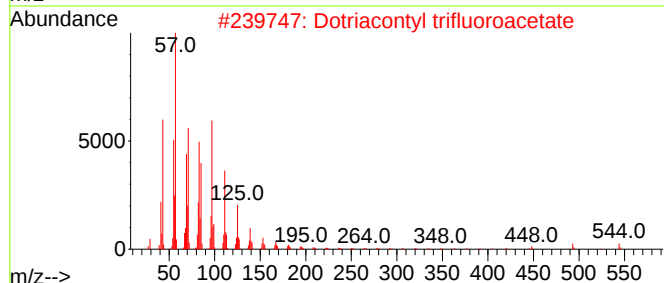
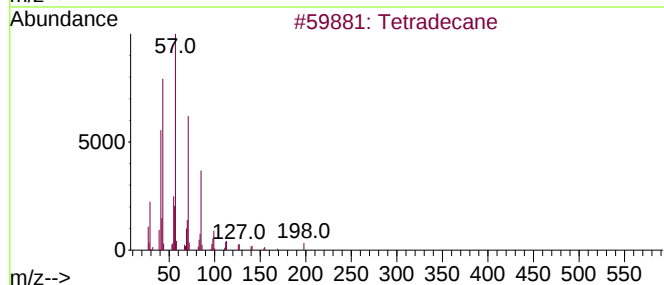
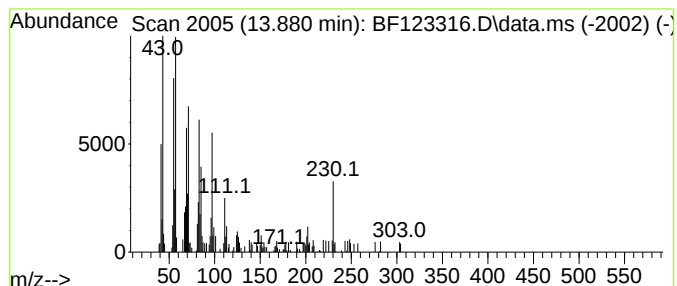
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF021921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Tetradecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.880	4.11 ng	213039	Chrysene-d12	14.027

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecane	198	C14H30	000629-59-4	70
2			Dotriacontyl trifluoroacetate	562	C34H65F3O2	1000351-75-4	70
3			Tetratriacontyl trifluoroacetate	591	C36H69F3O2	1000351-75-3	70
4			Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	70
5			Dotriacontyl heptafluorobutyrate	662	C36H65F7O2	1000351-84-2	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022621\
Data File : BF123316.D
Acq On : 26 Feb 2021 22:30
Operator : JU/CG
Sample : M1499-01 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
N-1

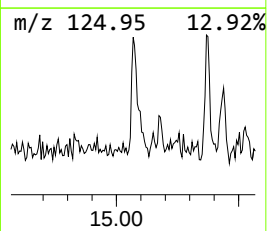
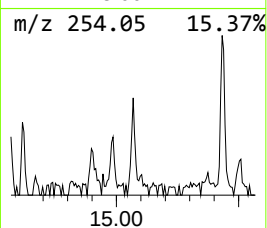
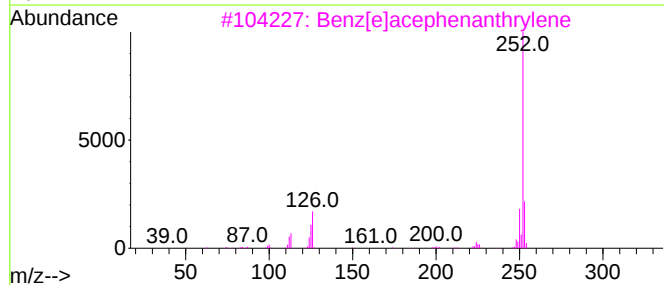
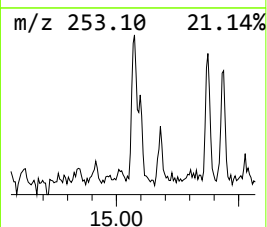
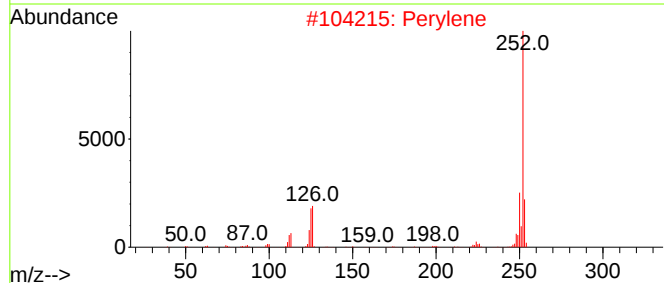
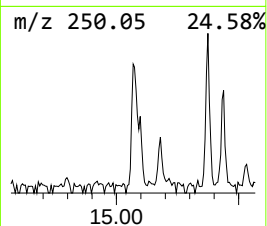
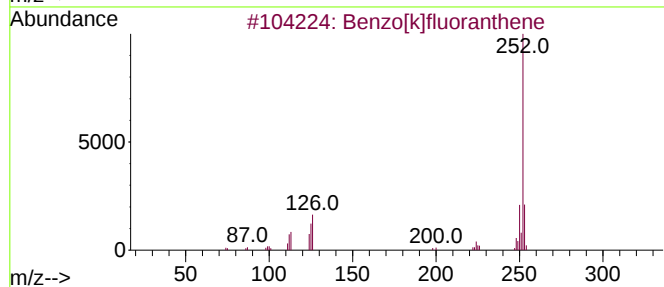
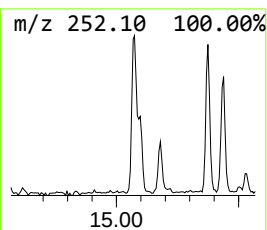
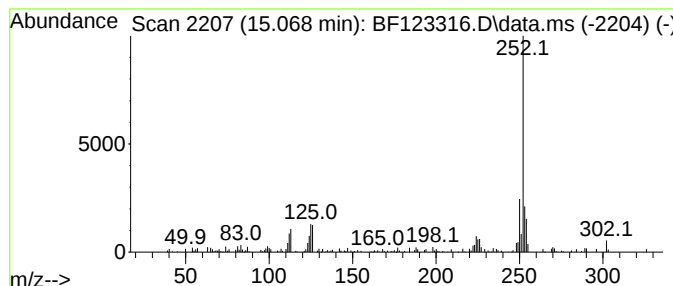
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Perylene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.068	4.41 ng	178682	Perylene-d12	15.504

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[k]fluoranthene	252	C20H12	000207-08-9	95
2			Perylene	252	C20H12	000198-55-0	89
3			Benz[e]acephenanthrylene	252	C20H12	000205-99-2	76
4			Benzo[a]pyrene	252	C20H12	000050-32-8	76
5			Benzo[e]pyrene	252	C20H12	000192-97-2	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022621\
Data File : BF123316.D
Acq On : 26 Feb 2021 22:30
Operator : JU/CG
Sample : M1499-01 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
N-1

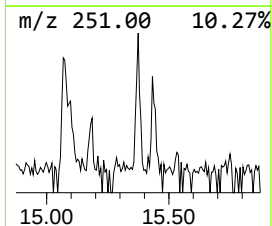
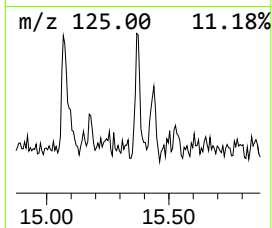
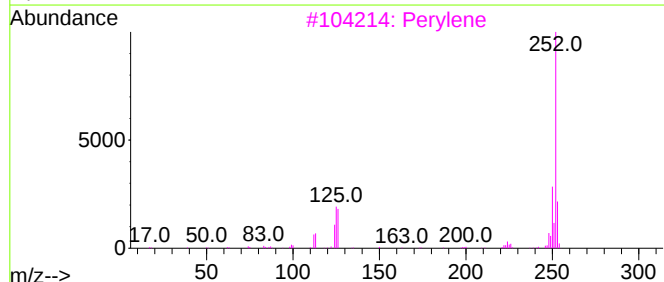
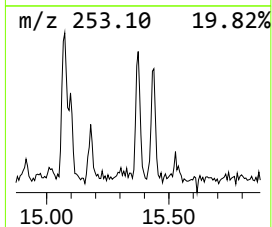
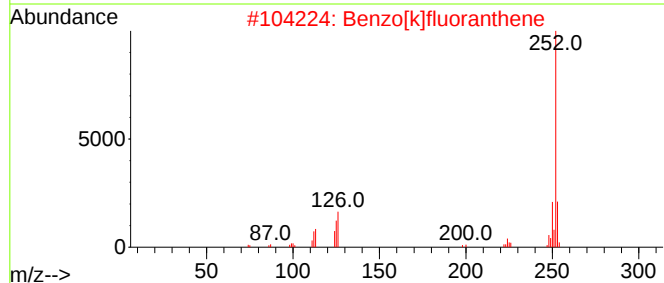
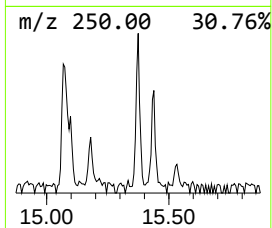
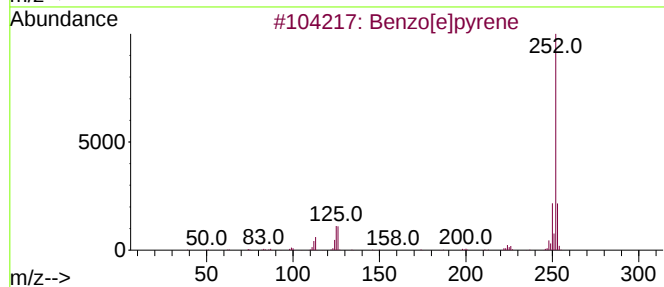
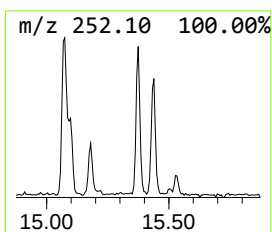
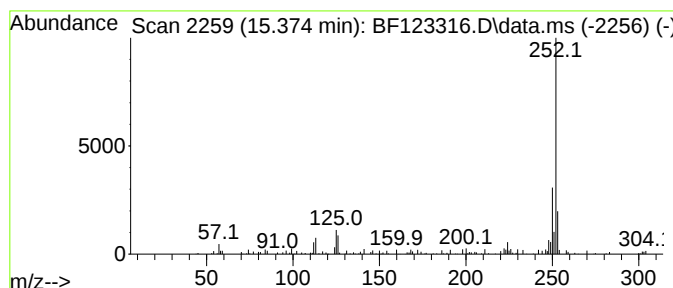
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Benzo[e]pyrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.374	2.06 ng	83551	Perylene-d12	15.504

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	93
2			Benzo[k]fluoranthene	252	C20H12	000207-08-9	90
3			Perylene	252	C20H12	000198-55-0	89
4			Benzo[a]pyrene	252	C20H12	000050-32-8	81
5			Benzo[j]fluoranthene	252	C20H12	000205-82-3	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022621\
Data File : BF123316.D
Acq On : 26 Feb 2021 22:30
Operator : JU/CG
Sample : M1499-01 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
N-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF021921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Hexadecanoic ac...	11.774	3.6	ng	238940	4	11.380	1316650	20.0
n-Hexadecanoic ...	11.910	3.8	ng	251972	4	11.380	1316650	20.0
9,12-Octadecadi...	12.463	12.8	ng	841943	4	11.380	1316650	20.0
9-Octadecenoic ...	12.486	9.1	ng	596553	4	11.380	1316650	20.0
Tetradecane	13.880	4.1	ng	213039	5	14.027	1037350	20.0
Perylene	15.068	4.4	ng	178682	6	15.504	809927	20.0
Benzo[e]pyrene	15.374	2.1	ng	83551	6	15.504	809927	20.0