

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091423\
 Data File : BF135267.D
 Acq On : 14 Sep 2023 22:14
 Operator : CG\JU
 Sample : 04399-05
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 360

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-BF091123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135267.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.175	10	15	25	rVB2	24719	48892	1.52%	0.221%
2	5.016	494	498	506	rVB	34481	50727	1.57%	0.229%
3	5.404	559	564	567	rBV	3123090	2970793	92.18%	13.412%
4	6.410	729	735	738	rBV	2895127	2978322	92.41%	13.446%
5	6.763	791	795	798	rBV	958485	804449	24.96%	3.632%
6	7.328	885	891	894	rBV	1985799	1902933	59.04%	8.591%
7	8.039	1008	1012	1015	rBV	1250105	1003109	31.12%	4.529%
8	9.122	1190	1196	1199	rBV	3672662	3222990	100.00%	14.551%
9	9.798	1307	1311	1314	rBV	1243060	1011553	31.39%	4.567%
10	10.592	1441	1446	1449	rBV	1625024	1489138	46.20%	6.723%
11	11.286	1561	1564	1567	rBV	932223	863328	26.79%	3.898%
12	11.310	1567	1568	1573	rVB	88067	70568	2.19%	0.319%
13	11.822	1652	1655	1667	rBV	173091	201459	6.25%	0.910%
14	12.510	1768	1772	1775	rBV	211008	194990	6.05%	0.880%
15	12.616	1787	1790	1794	rBV3	37531	43993	1.36%	0.199%
16	12.739	1805	1811	1814	rBV	172029	166806	5.18%	0.753%
17	12.886	1832	1836	1839	rBV	2493191	2253681	69.93%	10.175%
18	13.068	1860	1867	1870	rVB2	24829	40613	1.26%	0.183%
19	13.133	1870	1878	1881	rBV3	24061	48241	1.50%	0.218%
20	13.810	1988	1993	2001	rBV5	82678	181319	5.63%	0.819%
21	13.945	2011	2016	2019	rBV	812850	794337	24.65%	3.586%
22	13.968	2019	2020	2026	rVB	100785	77075	2.39%	0.348%
23	14.045	2031	2033	2036	rVB2	36836	35480	1.10%	0.160%
24	14.457	2100	2103	2106	rBV2	59226	62957	1.95%	0.284%
25	14.586	2121	2125	2128	rBV	161431	176435	5.47%	0.797%
26	14.715	2143	2147	2153	rVB2	62566	138781	4.31%	0.627%
27	14.768	2153	2156	2158	rBV3	35434	39892	1.24%	0.180%
28	14.874	2172	2174	2178	rVB	49877	44871	1.39%	0.203%
29	14.986	2189	2193	2203	rVB	105870	194576	6.04%	0.878%
30	15.068	2204	2207	2210	rVB2	51950	48979	1.52%	0.221%
31	15.286	2241	2244	2251	rVB	59599	73083	2.27%	0.330%
32	15.351	2251	2255	2261	rBV	67405	95559	2.96%	0.431%
33	15.415	2261	2266	2270	rBV	530163	656325	20.36%	2.963%
34	15.651	2303	2306	2311	rVB5	33768	46974	1.46%	0.212%
35	15.892	2343	2347	2351	rVB2	54152	79196	2.46%	0.358%
36	16.886	2514	2516	2522	rVB3	25387	37300	1.16%	0.168%

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091423\
Data File : BF135267.D
Acq On : 14 Sep 2023 22:14
Operator : CG\JU
Sample : 04399-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
360

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-BF091123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

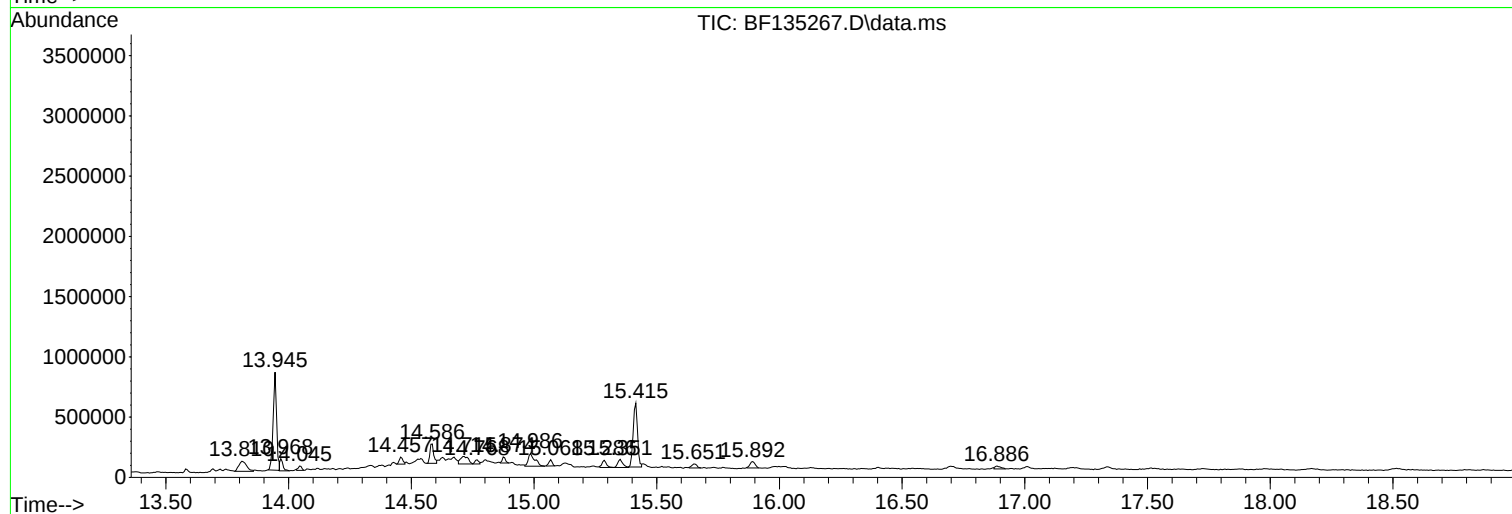
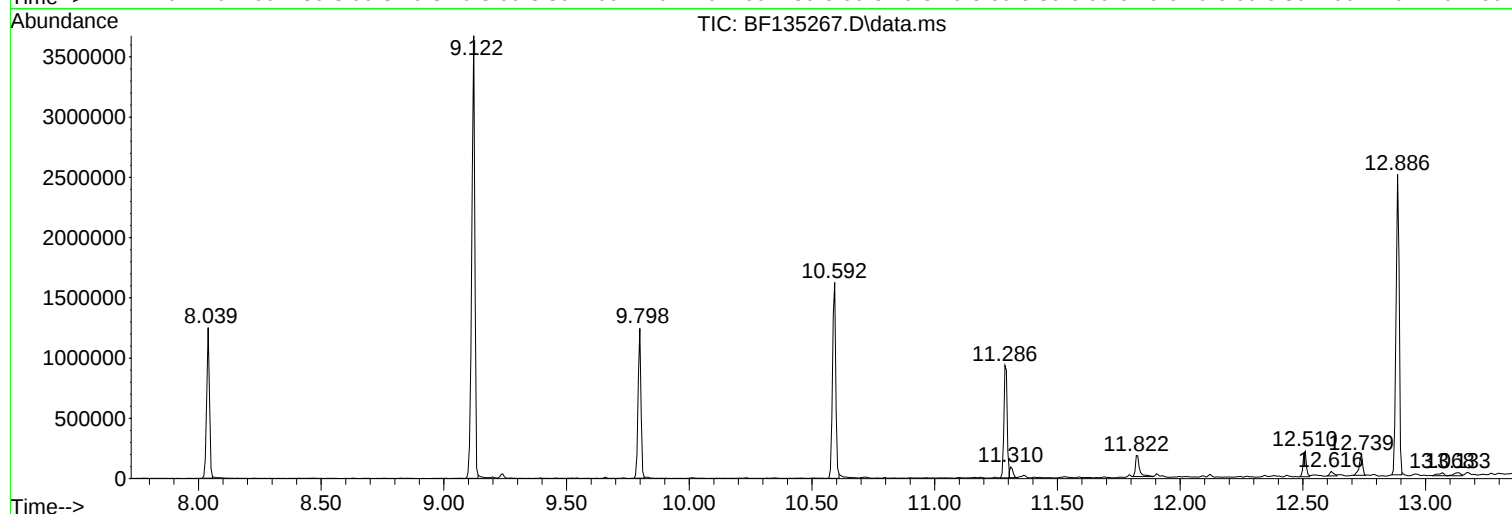
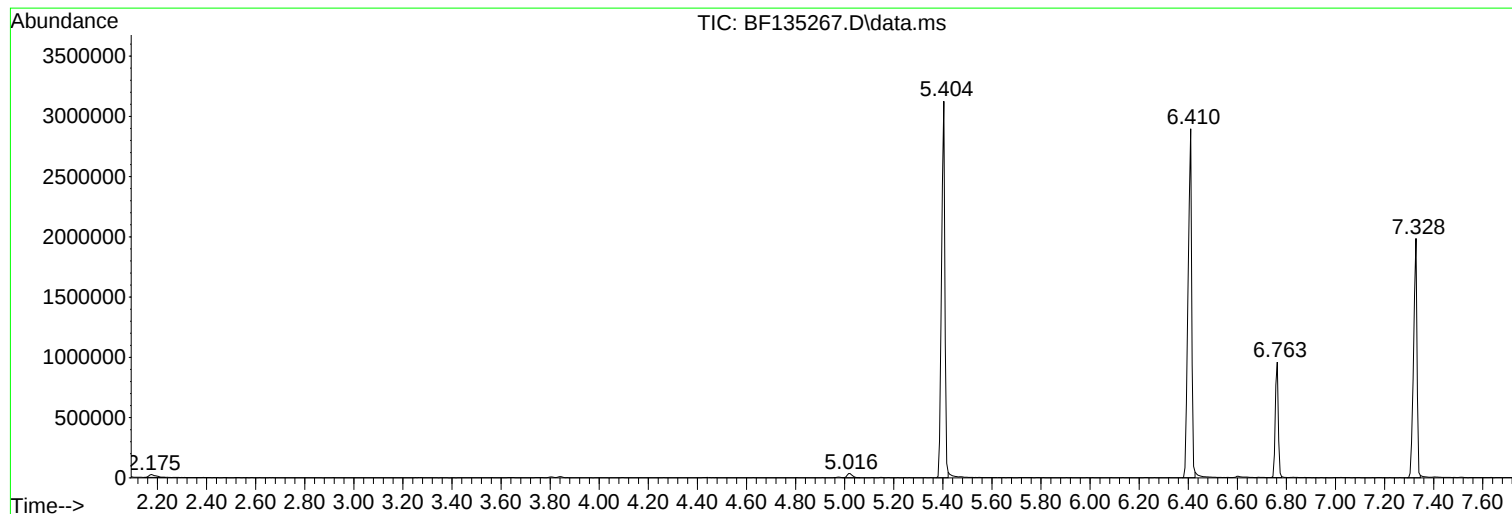
Sum of corrected areas: 22149724

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091423\
Data File : BF135267.D
Acq On : 14 Sep 2023 22:14
Operator : CG\JU
Sample : 04399-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
360

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091423\
Data File : BF135267.D
Acq On : 14 Sep 2023 22:14
Operator : CG\JU
Sample : 04399-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
360

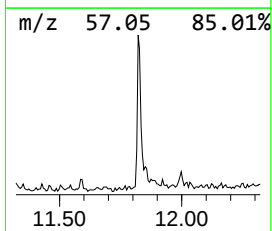
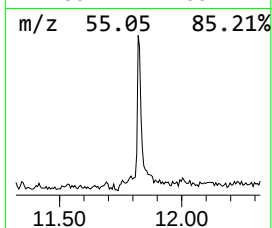
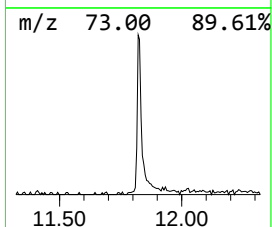
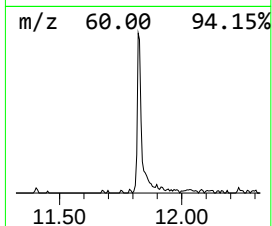
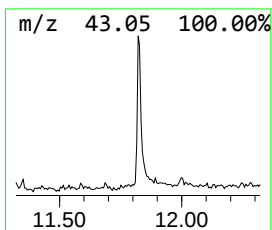
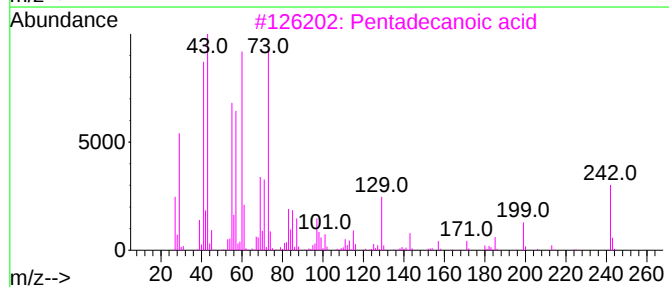
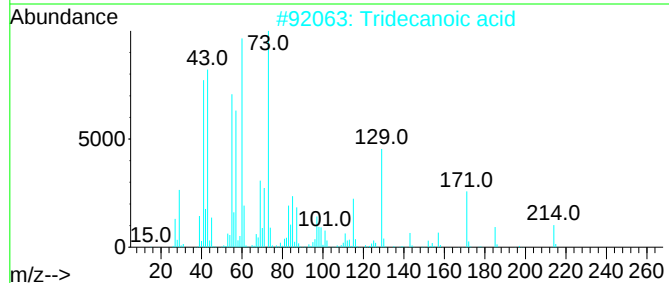
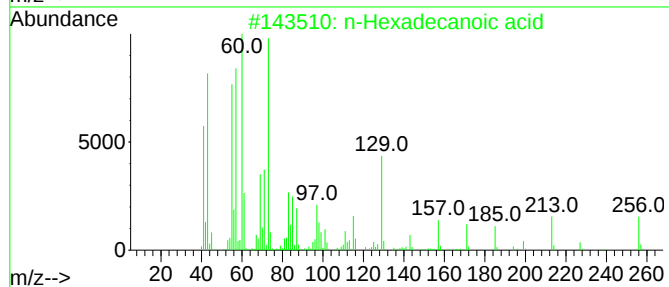
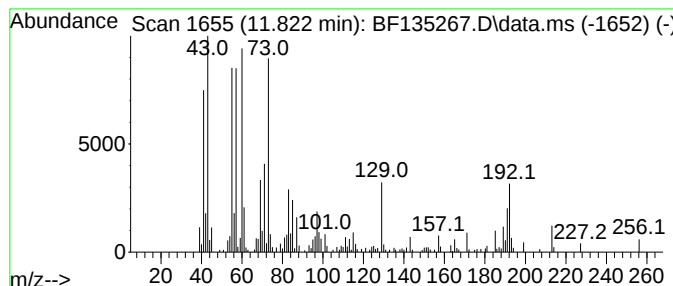
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.822	4.67 ng	201459	Phenanthrene-d10	11.286

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	86
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	68
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5			Undecanoic acid	186	C11H22O2	000112-37-8	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091423\
Data File : BF135267.D
Acq On : 14 Sep 2023 22:14
Operator : CG\JU
Sample : 04399-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
360

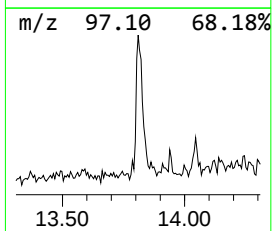
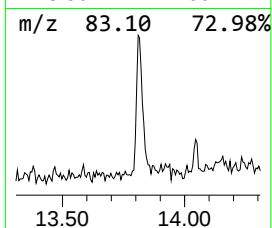
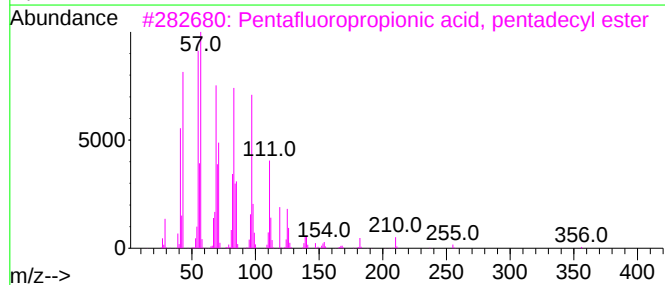
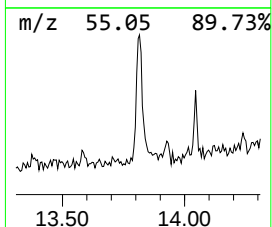
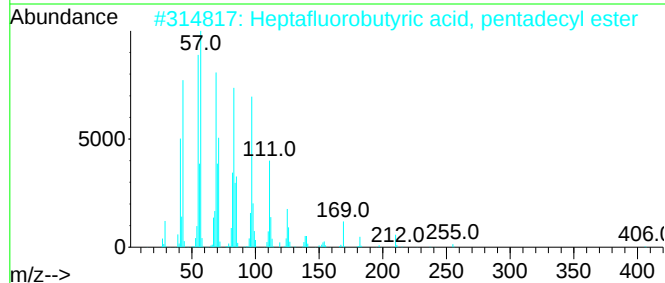
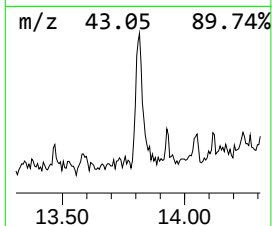
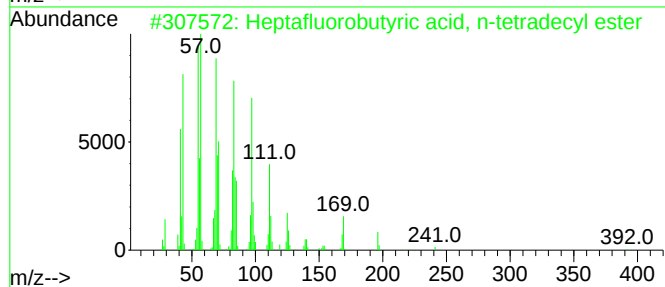
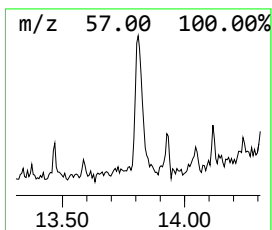
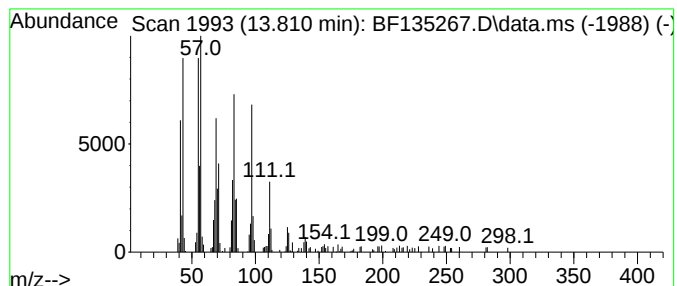
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Heptafluorobutyric acid, n-... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.810	4.57 ng	181319	Chrysene-d12	13.945

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	94
2			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
3			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
4			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
5			Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091423\
Data File : BF135267.D
Acq On : 14 Sep 2023 22:14
Operator : CG\JU
Sample : 04399-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

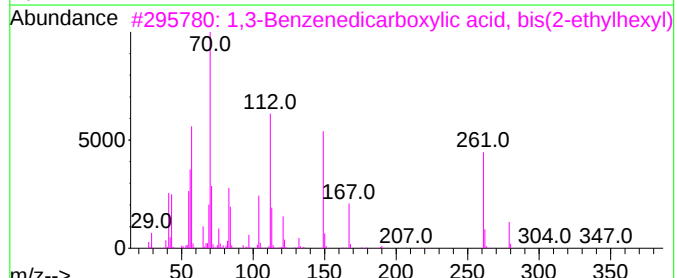
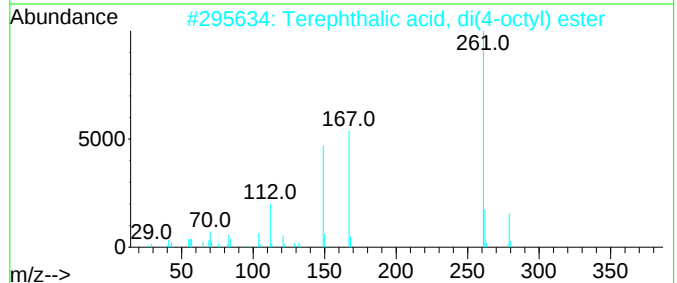
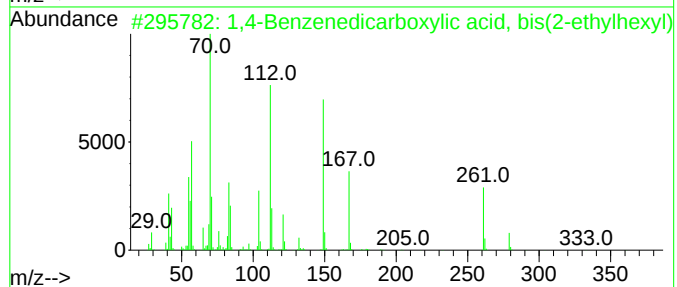
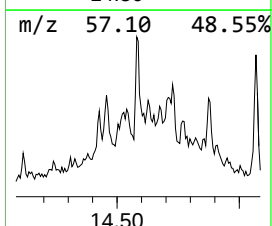
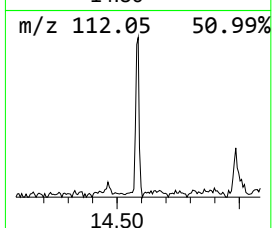
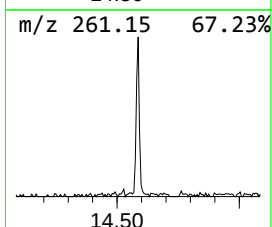
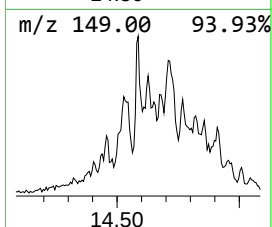
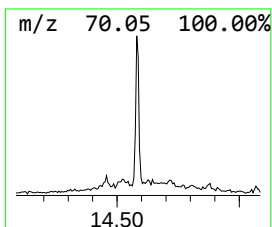
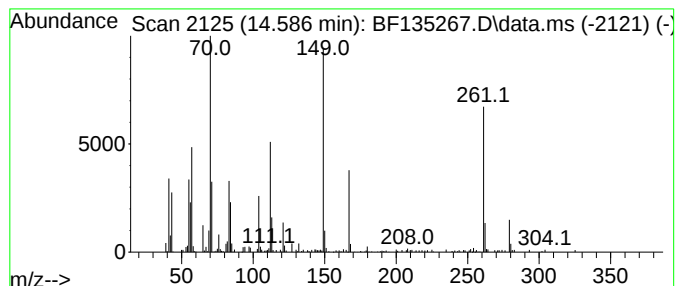
Instrument :
BNA_F
ClientSampleId :
360

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 1,4-Benzenedicarboxylic aci... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.		
14.586	4.44 ng	176435	Chrysene-d12	13.945		
Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	70
2		Terephthalic acid, di(4-octyl) e...	390	C24H38O4	1000323-74-2	58
3		1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	49
4		Terephthalic acid, 2-ethylhexyl ...	390	C24H38O4	1000324-00-5	38
5		Bis(2-ethylhexyl) phthalate	390	C24H38O4	000117-81-7	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091423\
Data File : BF135267.D
Acq On : 14 Sep 2023 22:14
Operator : CG\JU
Sample : 04399-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
360

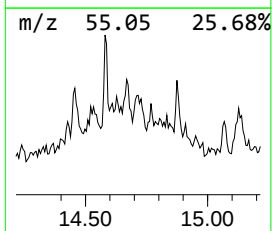
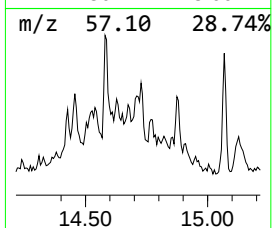
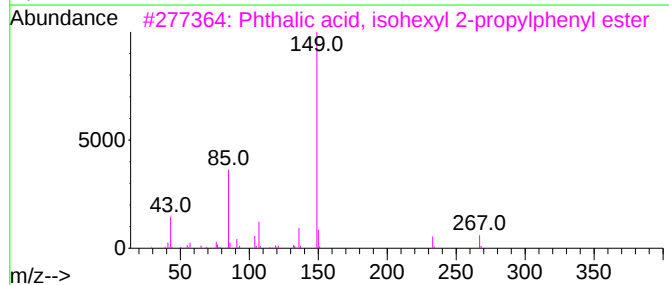
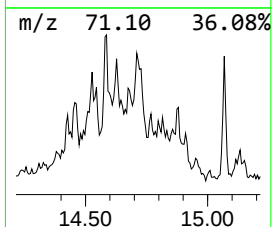
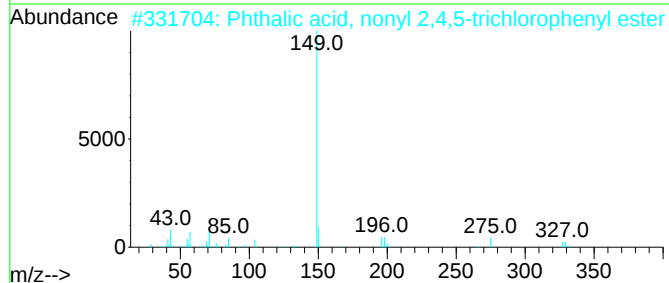
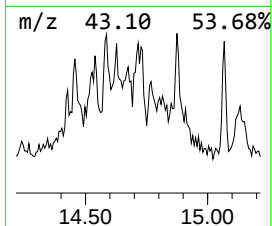
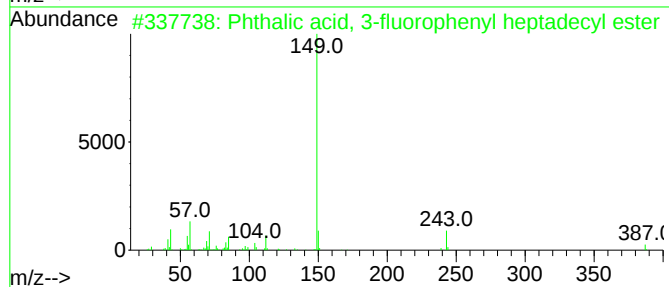
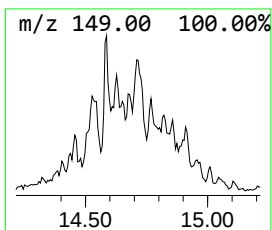
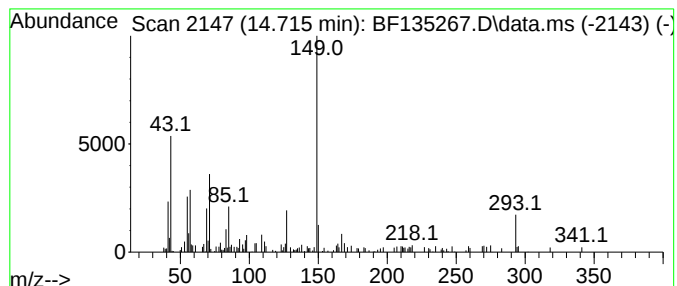
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Phthalic acid, 3-fluorophen... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.715	4.23 ng	138781	Perylene-d12	15.415

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phthalic acid, 3-fluorophenyl he...	498	C31H43F04	1000356-66-2	59
2			Phthalic acid, nonyl 2,4,5-trich...	470	C23H25Cl3O4	1010357-04-9	59
3			Phthalic acid, isohexyl 2-propyl...	368	C23H28O4	1000357-02-1	50
4			Phthalic acid, hexyl trans-hex-3...	332	C20H28O4	1010360-48-4	50
5			Phthalic acid, 2,4-dimethylpent...	446	C28H46O4	1000356-85-2	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091423\
Data File : BF135267.D
Acq On : 14 Sep 2023 22:14
Operator : CG\JU
Sample : 04399-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
360

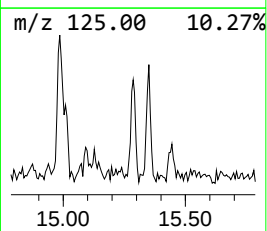
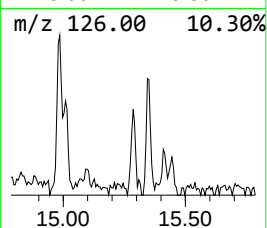
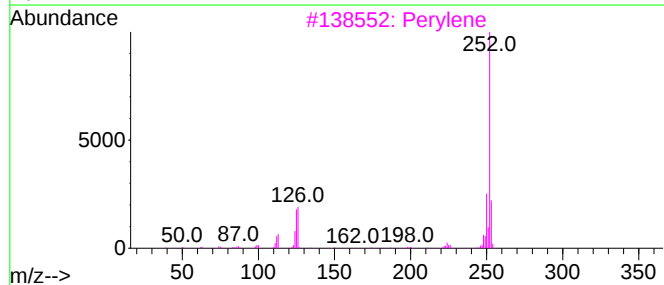
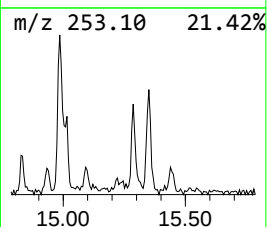
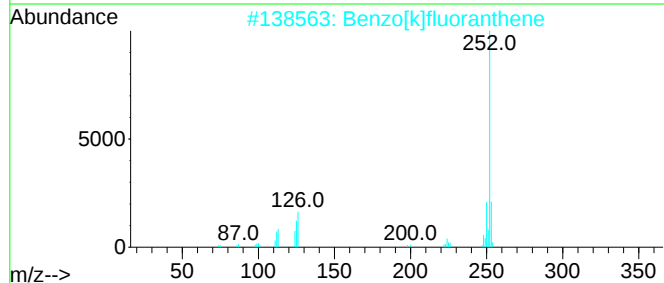
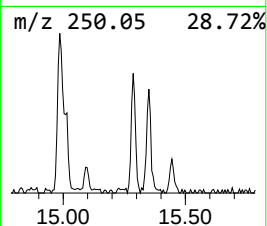
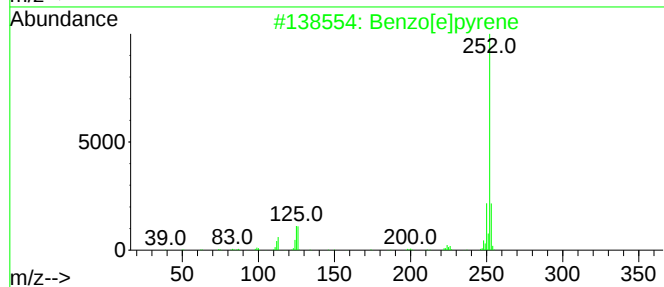
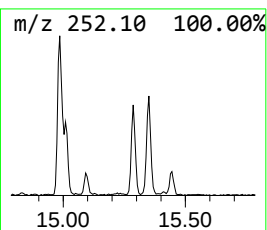
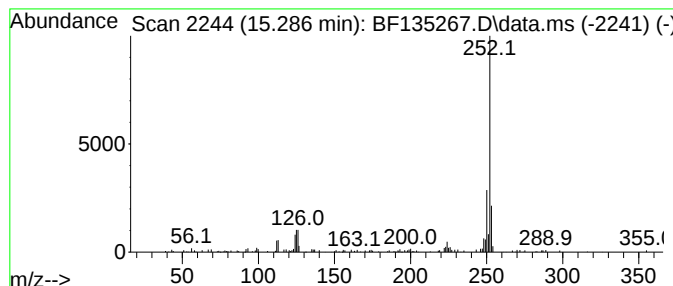
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Benzo[e]pyrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.286	2.23 ng	73083	Perylene-d12	15.415

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	97
2			Benzo[k]fluoranthene	252	C20H12	000207-08-9	96
3			Perylene	252	C20H12	000198-55-0	94
4			Benzo[j]fluoranthene	252	C20H12	000205-82-3	93
5			Benzo[b]fluoranthene	252	C20H12	000205-99-2	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091423\
Data File : BF135267.D
Acq On : 14 Sep 2023 22:14
Operator : CG\JU
Sample : 04399-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
360

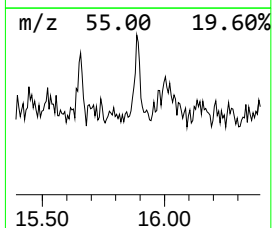
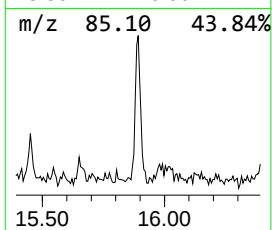
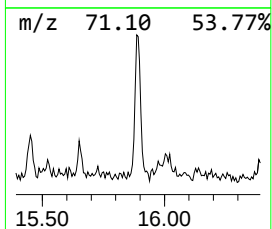
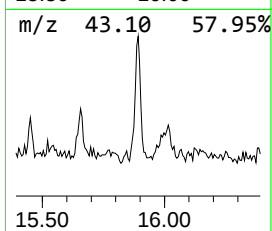
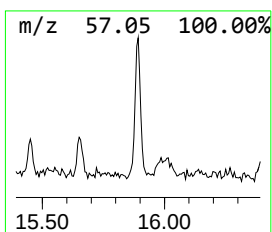
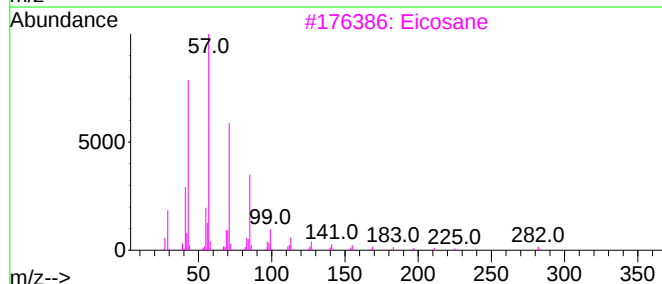
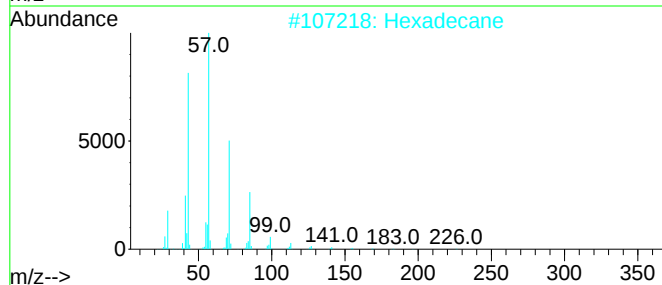
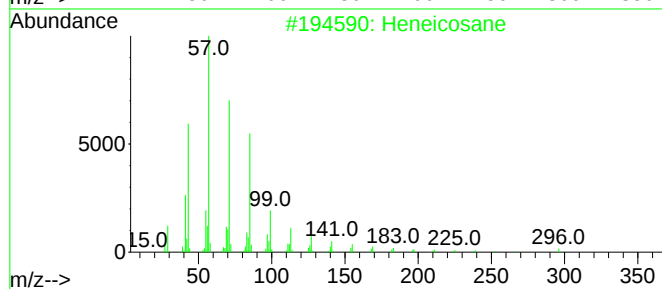
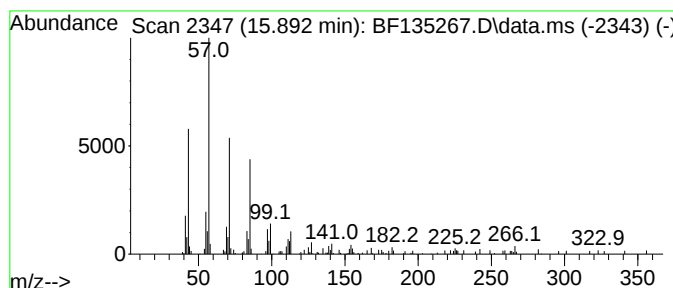
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.892	2.41 ng	79196	Perylene-d12	15.415

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	98
2	Hexadecane	226	C16H34	000544-76-3	94
3	Eicosane	282	C20H42	000112-95-8	91
4	Hexacosane	366	C26H54	000630-01-3	90
5	Octacosane	394	C28H58	000630-02-4	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091423\
Data File : BF135267.D
Acq On : 14 Sep 2023 22:14
Operator : CG\JU
Sample : 04399-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
360

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Hexadecanoic ...	11.822	4.7	ng	201459	4	11.286	863328	20.0
Heptafluorobuty...	13.810	4.6	ng	181319	5	13.945	794337	20.0
1,4-Benzenedica...	14.586	4.4	ng	176435	5	13.945	794337	20.0
Phthalic acid, ...	14.715	4.2	ng	138781	6	15.415	656325	20.0
Benzo[e]pyrene	15.286	2.2	ng	73083	6	15.415	656325	20.0
Heneicosane	15.892	2.4	ng	79196	6	15.415	656325	20.0