

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080723\
 Data File : BF134645.D
 Acq On : 07 Aug 2023 10:21
 Operator : CG\JU
 Sample : 03891-03
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-2

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-BF080123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134645.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.204	13	20	28	rBV2	48922	77181	1.84%	0.218%
2	5.040	497	502	507	rVB	80699	107033	2.55%	0.302%
3	5.428	563	568	571	rBV	3786528	3713645	88.36%	10.480%
4	6.434	733	739	741	rBV	3324617	3778935	89.91%	10.664%
5	6.622	768	771	776	rBV	120108	109762	2.61%	0.310%
6	6.798	797	801	804	rBV	1448117	1170658	27.85%	3.304%
7	7.357	891	896	899	rBV	2638514	2378080	56.58%	6.711%
8	8.075	1013	1018	1021	rBV	1868610	1553684	36.97%	4.384%
9	9.151	1196	1201	1205	rBV	4520150	4203034	100.00%	11.861%
10	9.269	1218	1221	1225	rVB	59422	52637	1.25%	0.149%
11	9.827	1311	1316	1320	rBV	1897865	1678781	39.94%	4.737%
12	10.622	1446	1451	1454	rBV	2703595	2499314	59.46%	7.053%
13	11.316	1566	1569	1572	rBV	1782562	1720702	40.94%	4.856%
14	11.339	1572	1573	1577	rVV	660736	460888	10.97%	1.301%
15	11.392	1577	1582	1585	rVB	149523	138346	3.29%	0.390%
16	11.551	1603	1609	1611	rBV	64880	73412	1.75%	0.207%
17	11.821	1652	1655	1657	rBV	60081	50250	1.20%	0.142%
18	11.857	1657	1661	1665	rBV2	232081	264442	6.29%	0.746%
19	11.933	1670	1674	1676	rBV	108097	111188	2.65%	0.314%
20	12.121	1702	1706	1707	rBV	51649	52884	1.26%	0.149%
21	12.139	1707	1709	1713	rVB	88935	73438	1.75%	0.207%
22	12.457	1760	1763	1768	rVB2	46055	49390	1.18%	0.139%
23	12.533	1772	1776	1780	rVB	1101622	893871	21.27%	2.522%
24	12.763	1809	1815	1818	rBV	812350	833019	19.82%	2.351%
25	12.916	1837	1841	1844	rBV	4235907	3894270	92.65%	10.989%
26	12.986	1848	1853	1855	rBV2	43027	65900	1.57%	0.186%
27	13.092	1868	1871	1875	rVB	93160	89476	2.13%	0.252%
28	13.157	1879	1882	1885	rVV2	75168	61825	1.47%	0.174%
29	13.198	1886	1889	1891	rBV2	54809	53244	1.27%	0.150%
30	13.598	1955	1957	1965	rVB	59511	74074	1.76%	0.209%
31	13.710	1973	1976	1979	rBV2	62344	76471	1.82%	0.216%
32	13.739	1979	1981	1983	rBV	55043	48012	1.14%	0.135%
33	13.821	1993	1995	2000	rVB	191513	210168	5.00%	0.593%
34	13.962	2014	2019	2022	rBV2	1312482	1452098	34.55%	4.098%
35	13.992	2022	2024	2030	rVB	336072	280108	6.66%	0.790%
36	14.068	2035	2037	2040	rVB	56433	46653	1.11%	0.132%

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080723\
Data File : BF134645.D
Acq On : 07 Aug 2023 10:21
Operator : CG\JU
Sample : 03891-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-2

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-BF080123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.004	2192	2196	2199	rBV	314800	473547	11.27%	1.336%
38	15.304	2244	2247	2254	rVB	198348	249551	5.94%	0.704%
39	15.368	2255	2258	2261	rBV	250024	280833	6.68%	0.792%
40	15.433	2265	2269	2273	rVB	781487	949315	22.59%	2.679%
41	16.156	2389	2392	2400	rVB2	136699	257250	6.12%	0.726%
42	16.603	2464	2468	2475	rVB2	207546	370671	8.82%	1.046%
43	16.909	2517	2520	2529	rVB2	126446	242683	5.77%	0.685%
44	17.356	2593	2596	2608	rVB	99703	215667	5.13%	0.609%

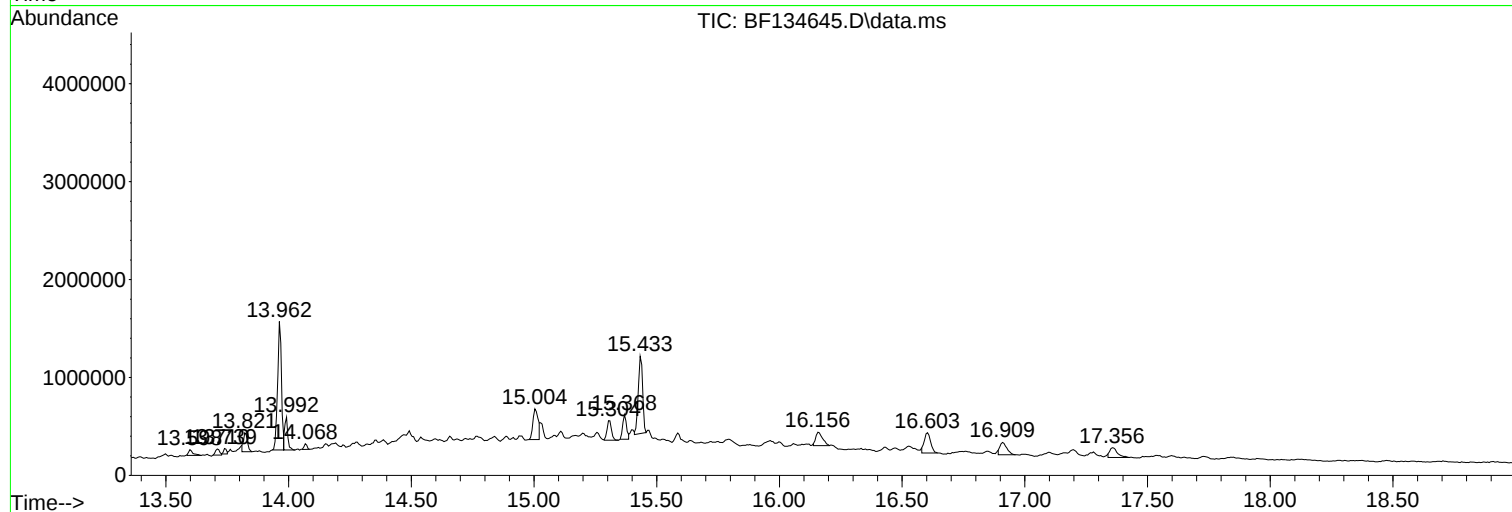
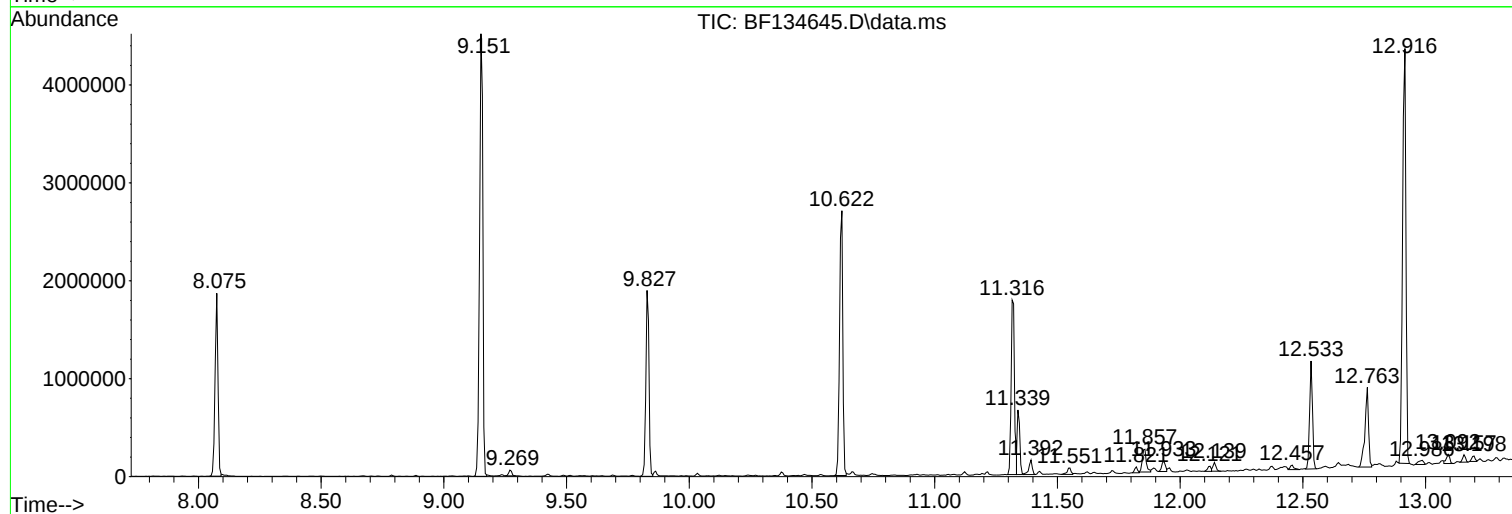
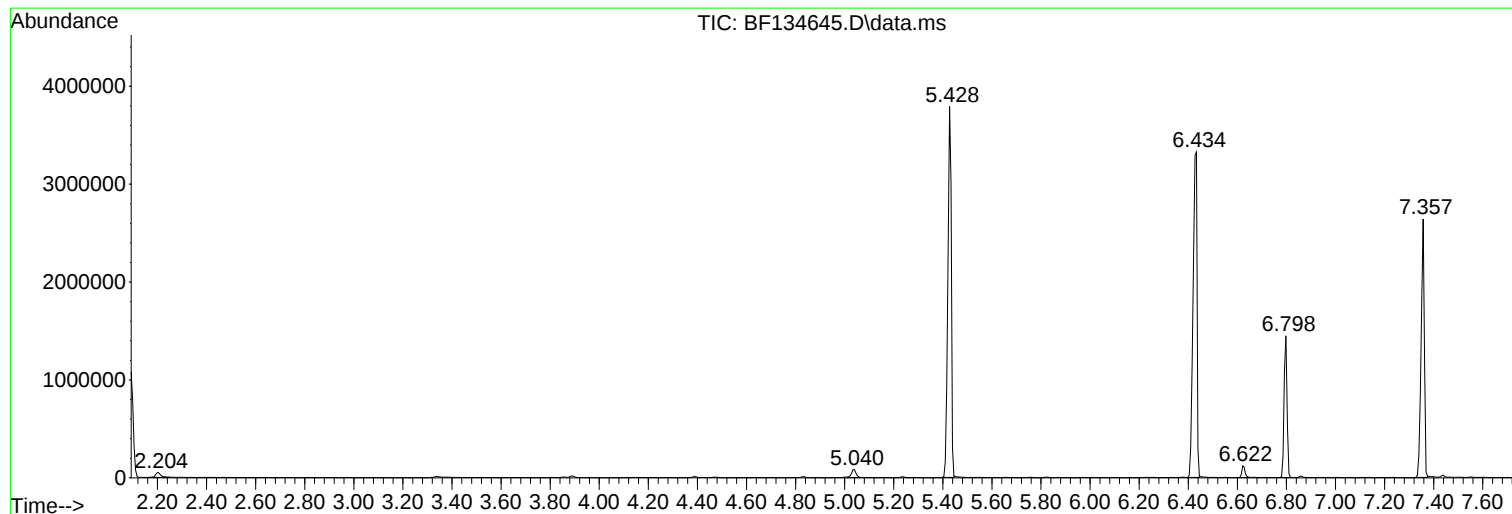
Sum of corrected areas: 35436390

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080723\
Data File : BF134645.D
Acq On : 07 Aug 2023 10:21
Operator : CG\JU
Sample : 03891-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.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\BF080723\
Data File : BF134645.D
Acq On : 07 Aug 2023 10:21
Operator : CG\JU
Sample : 03891-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-2

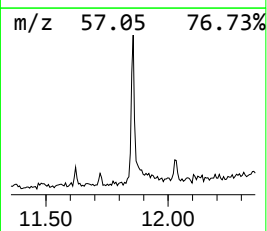
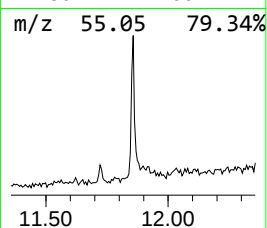
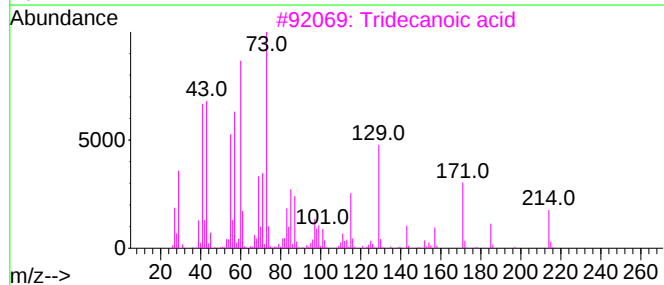
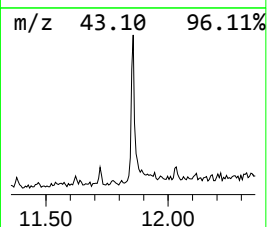
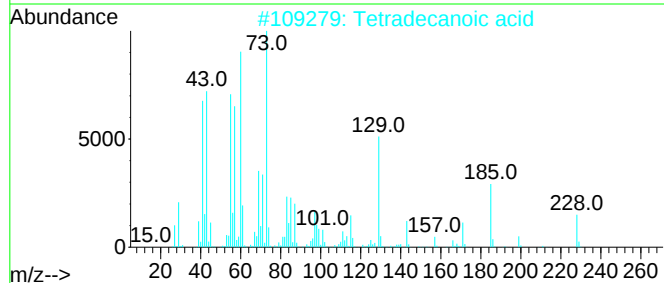
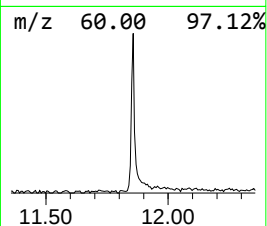
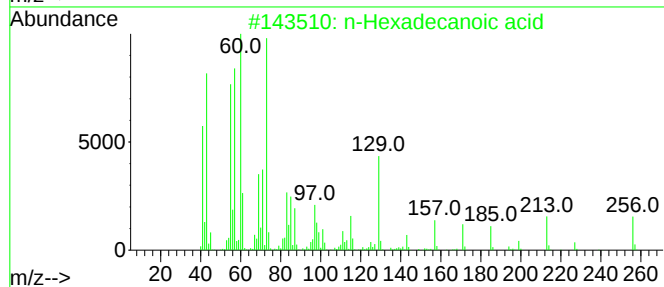
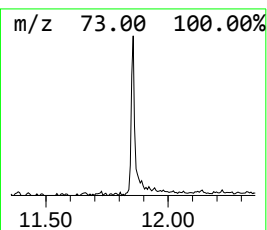
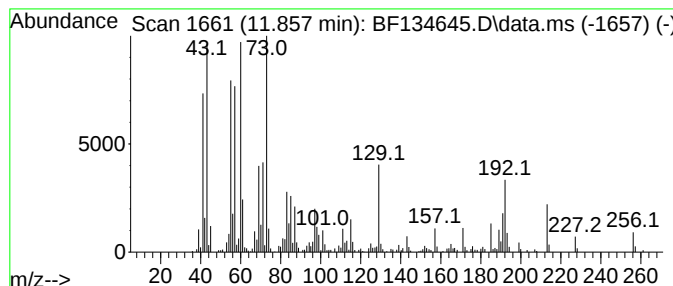
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.857	3.07 ng	264442	Phenanthrene-d10	11.322

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	97
3			Tridecanoic acid	214	C13H26O2	000638-53-9	92
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
5			n-Decanoic acid	172	C10H20O2	000334-48-5	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080723\
Data File : BF134645.D
Acq On : 07 Aug 2023 10:21
Operator : CG\JU
Sample : 03891-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

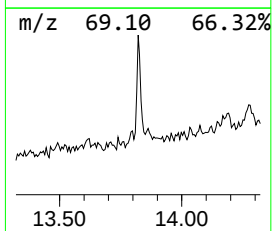
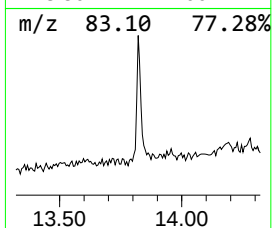
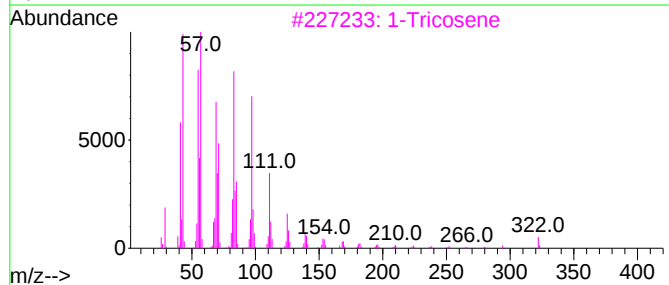
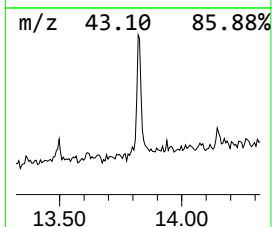
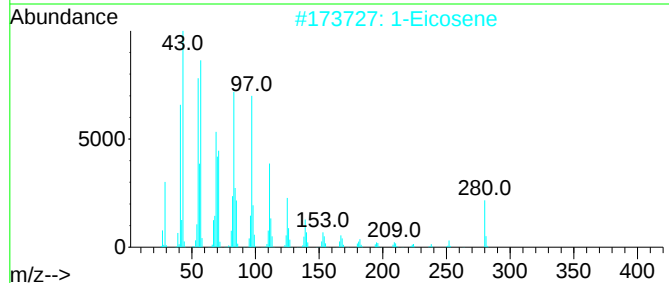
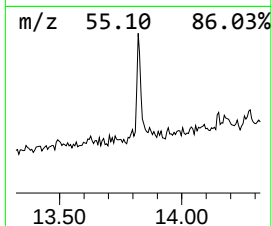
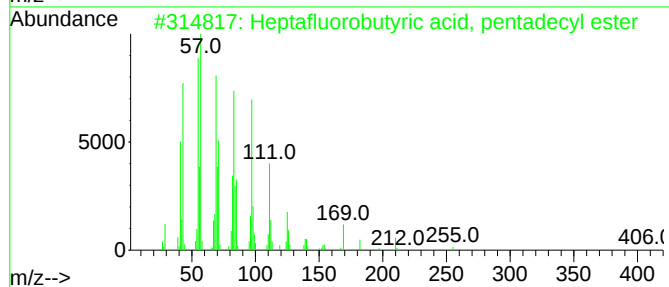
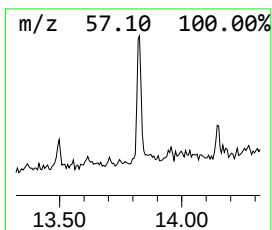
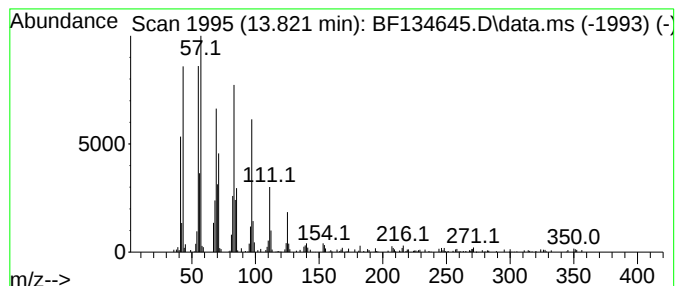
Instrument :
BNA_F
ClientSampleId :
TP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.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, pe... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.821	2.89 ng	210168	Chrysene-d12	13.963	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
2	1-Eicosene	280	C20H40	003452-07-1	91
3	1-Tricosene	322	C23H46	018835-32-0	91
4	1-Hexacosene	364	C26H52	018835-33-1	91
5	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080723\
Data File : BF134645.D
Acq On : 07 Aug 2023 10:21
Operator : CG\JU
Sample : 03891-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-2

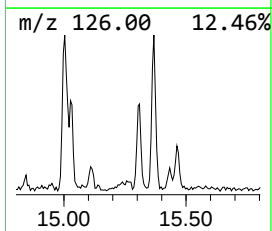
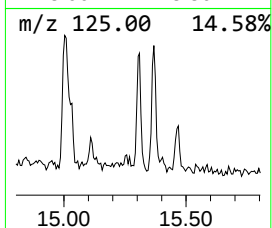
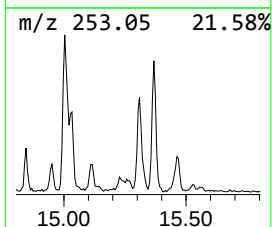
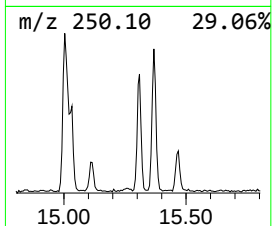
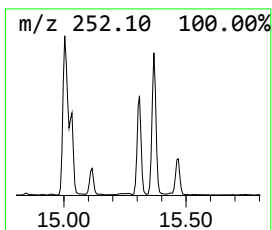
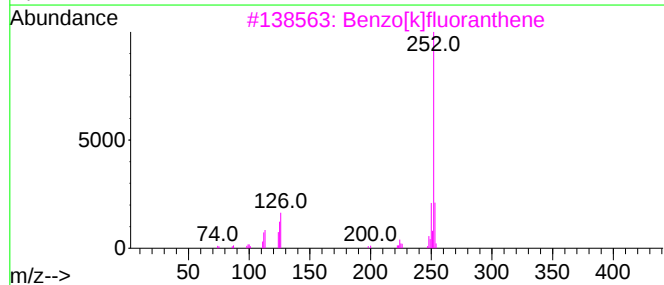
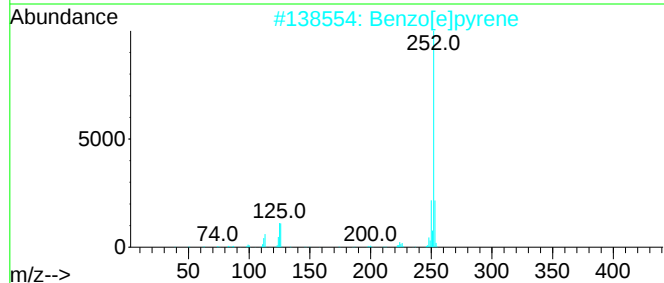
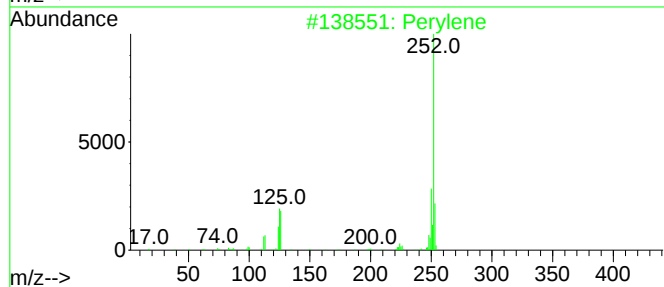
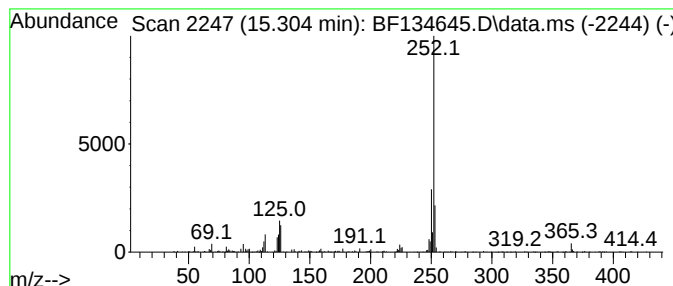
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Perylene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.304	5.26 ng	249551	Perylene-d12	15.433

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Perylene	252	C20H12	000198-55-0	99
2			Benzo[e]pyrene	252	C20H12	000192-97-2	98
3			Benzo[k]fluoranthene	252	C20H12	000207-08-9	97
4			Benzo[a]pyrene	252	C20H12	000050-32-8	97
5			Benzo[b]fluoranthene	252	C20H12	000205-99-2	96



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080723\
Data File : BF134645.D
Acq On : 07 Aug 2023 10:21
Operator : CG\JU
Sample : 03891-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

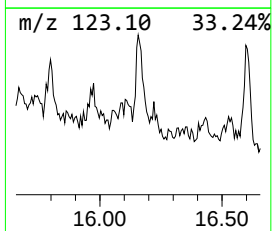
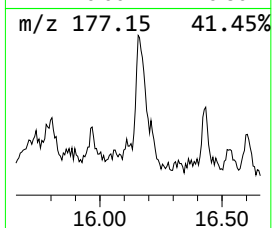
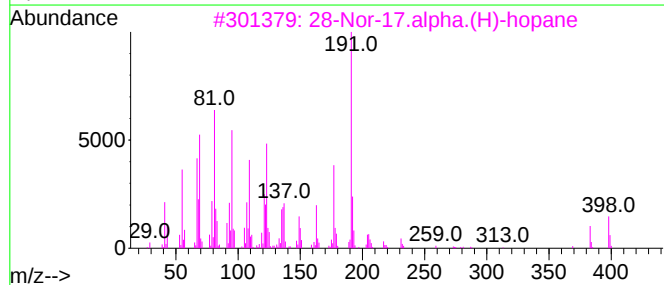
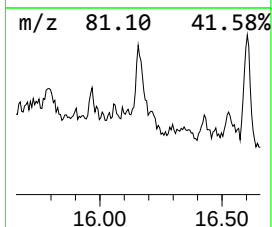
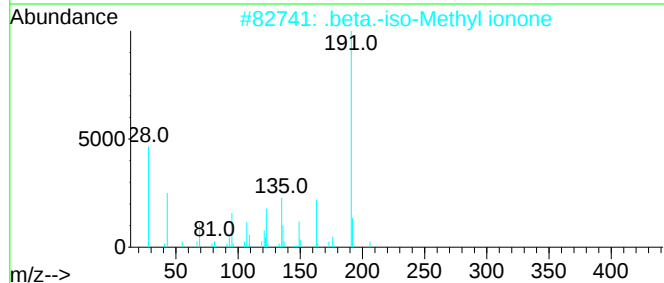
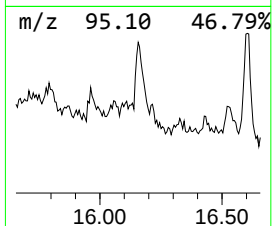
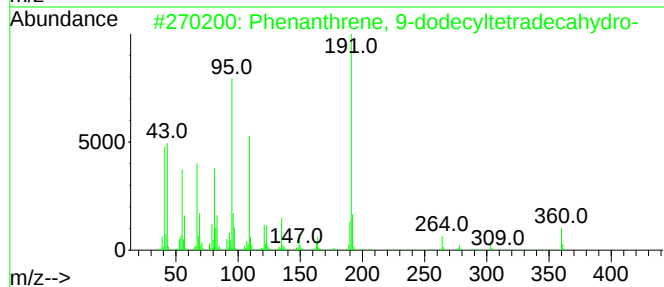
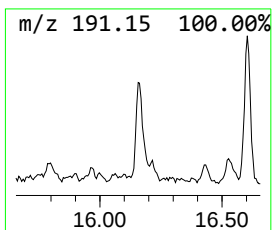
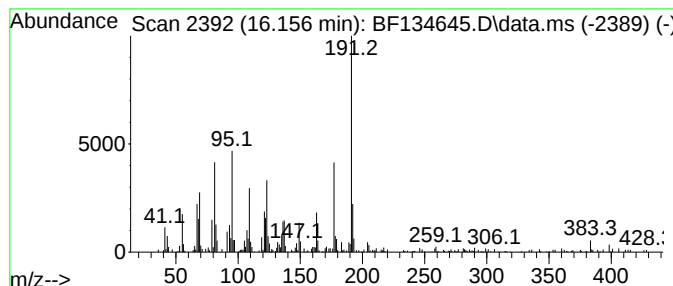
Instrument :
BNA_F
ClientSampleId :
TP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Phenanthrene, 9-dodecyltetra... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.157	5.42 ng	257250	Perylene-d12	15.433	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 9-dodecyltetradeca...	360	C26H48	055334-01-5	50
2	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	47
3	28-Nor-17.alpha.(H)-hopane	398	C29H50	053584-60-4	45
4	5-(p-Aminophenyl)-2-thiazolamine	191	C9H9N3S	090349-87-4	30
5	3-Buten-2-one, 4-(2,5,6,6-tetram...	206	C14H22O	000079-70-9	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080723\
Data File : BF134645.D
Acq On : 07 Aug 2023 10:21
Operator : CG\JU
Sample : 03891-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-2

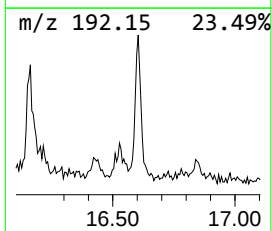
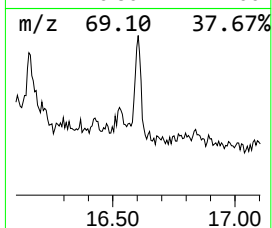
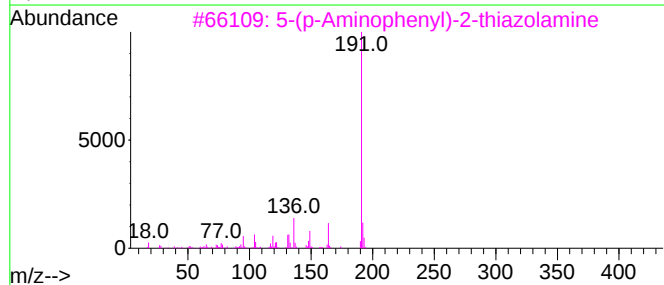
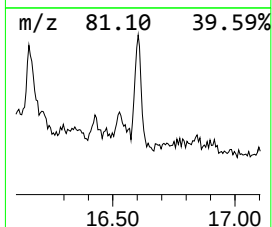
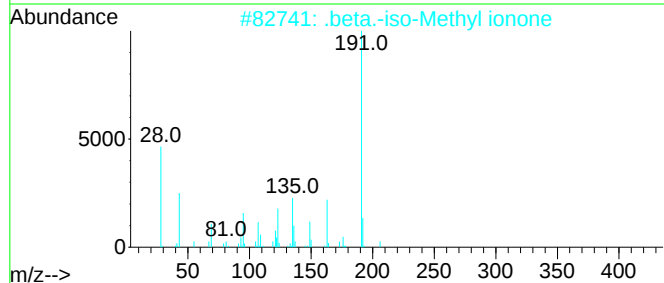
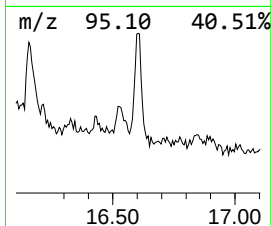
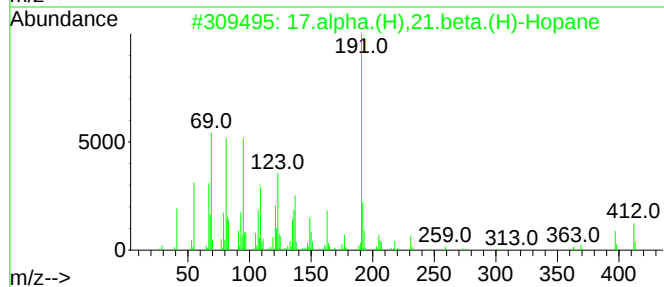
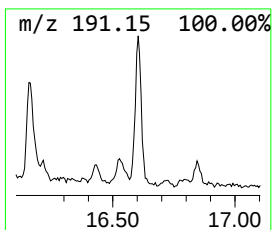
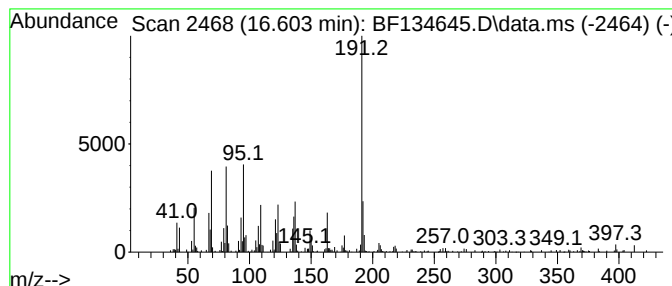
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 17.alpha.(H),21.beta.(H)-Ho... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.604	7.81 ng	370671	Perylene-d12	15.433

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			17.alpha.(H),21.beta.(H)-Hopane	412	C30H52	013849-96-2	97
2			.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	53
3			5-(p-Aminophenyl)-2-thiazolamine	191	C9H9N3S	090349-87-4	38
4			2,3,4,5-Tetramethylacetanilide	191	C12H17NO	1000432-93-7	38
5			1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080723\
Data File : BF134645.D
Acq On : 07 Aug 2023 10:21
Operator : CG\JU
Sample : 03891-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.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 ...	11.857	3.1	ng	264442	4	11.322	1720700	20.0
Heptafluorobuty...	13.821	2.9	ng	210168	5	13.963	1452100	20.0
Perylene	15.304	5.3	ng	249551	6	15.433	949315	20.0
Phenanthrene, 9...	16.157	5.4	ng	257250	6	15.433	949315	20.0
17.alpha.(H),21...	16.604	7.8	ng	370671	6	15.433	949315	20.0