

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061523\
 Data File : BF133776.D
 Acq On : 15 Jun 2023 15:43
 Operator : CG\JU
 Sample : 03160-03 2X
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PNNL-B-0609-2

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-BF060923.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133776.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.146	6	10	15	rVB5	12648	17519	2.21%	0.210%
2	3.857	296	301	308	rBV2	5962	10021	1.27%	0.120%
3	5.028	496	500	507	rVB	26715	28759	3.64%	0.345%
4	5.434	565	569	578	rBV	765681	677941	85.70%	8.144%
5	6.451	738	742	745	rBV	830287	654684	82.76%	7.865%
6	6.828	803	806	810	rBV	720509	551256	69.68%	6.622%
7	7.387	898	901	910	rBV	503692	411124	51.97%	4.939%
8	8.110	1021	1024	1028	rBV	783289	636333	80.44%	7.644%
9	9.186	1203	1207	1210	rBV	965113	733458	92.72%	8.811%
10	9.869	1319	1323	1326	rBV	712620	603016	76.23%	7.244%
11	10.580	1439	1444	1447	rBV	40488	38489	4.87%	0.462%
12	10.651	1453	1456	1464	rBV	490958	430024	54.36%	5.166%
13	10.780	1473	1478	1482	rBV5	9022	11917	1.51%	0.143%
14	11.357	1572	1576	1578	rBV	701580	644665	81.49%	7.744%
15	11.375	1578	1579	1582	rVB	56860	43180	5.46%	0.519%
16	11.598	1613	1617	1621	rBV7	7028	15462	1.95%	0.186%
17	11.857	1658	1661	1662	rBV2	12538	11434	1.45%	0.137%
18	11.880	1662	1665	1670	rVB2	72791	77317	9.77%	0.929%
19	11.969	1677	1680	1682	rBV2	15580	18746	2.37%	0.225%
20	11.992	1682	1684	1688	rVB4	12198	12749	1.61%	0.153%
21	12.151	1709	1711	1714	rBV2	12481	12182	1.54%	0.146%
22	12.180	1714	1716	1721	rVB5	12184	10861	1.37%	0.130%
23	12.410	1752	1755	1757	rBV2	15187	15967	2.02%	0.192%
24	12.439	1757	1760	1766	rVB7	15011	26000	3.29%	0.312%
25	12.492	1766	1769	1773	rBV5	12178	14703	1.86%	0.177%
26	12.569	1779	1782	1786	rBV	184710	151064	19.10%	1.815%
27	12.669	1796	1799	1803	rBV5	23092	29908	3.78%	0.359%
28	12.763	1812	1815	1817	rBV2	18886	21115	2.67%	0.254%
29	12.798	1817	1821	1824	rVV	167277	143433	18.13%	1.723%
30	12.939	1842	1845	1849	rBV	881932	744187	94.07%	8.940%
31	13.127	1874	1877	1880	rVB2	24550	24500	3.10%	0.294%
32	13.227	1892	1894	1897	rBV2	16360	12004	1.52%	0.144%
33	13.468	1933	1935	1938	rBV4	23484	23804	3.01%	0.286%
34	13.633	1961	1963	1967	rBV2	23582	29239	3.70%	0.351%
35	13.845	1996	1999	2009	rBV2	68397	90290	11.41%	1.085%
36	13.998	2020	2025	2028	rBV	783107	791082	100.00%	9.503%

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061523\
Data File : BF133776.D
Acq On : 15 Jun 2023 15:43
Operator : CG\JU
Sample : 03160-03 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PNNL-B-0609-2

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

37	15.033	2198	2201	2204	rBV	80764	103628	13.10%	1.245%
38	15.462	2269	2274	2277	rBV	351496	452304	57.18%	5.433%

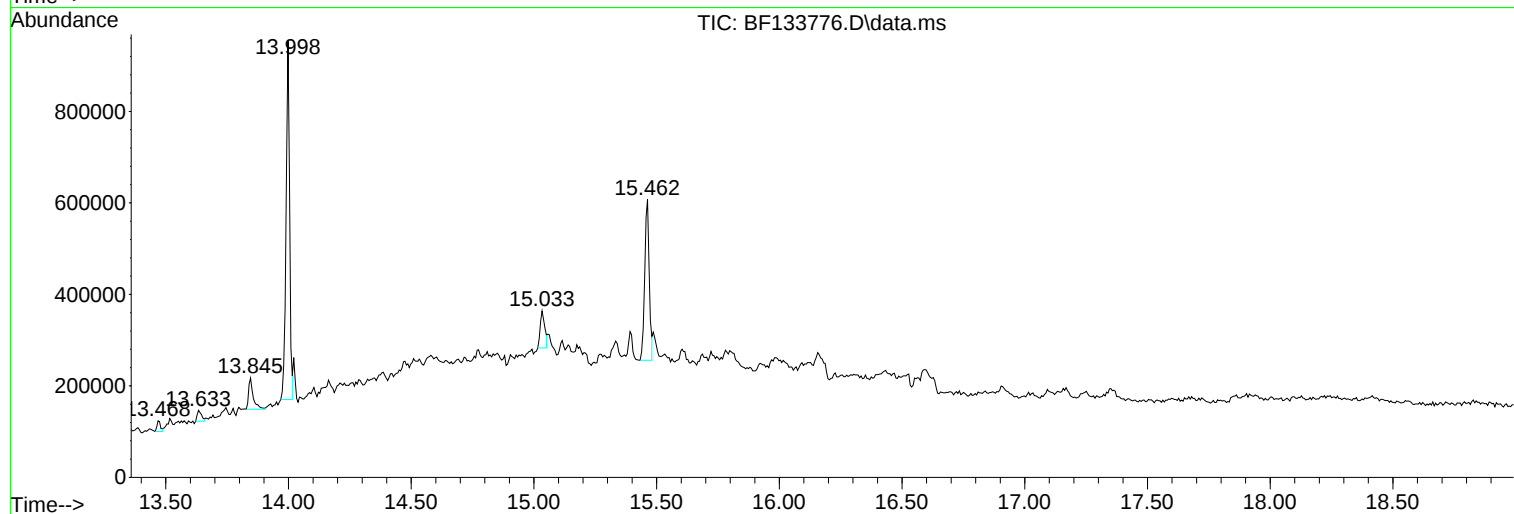
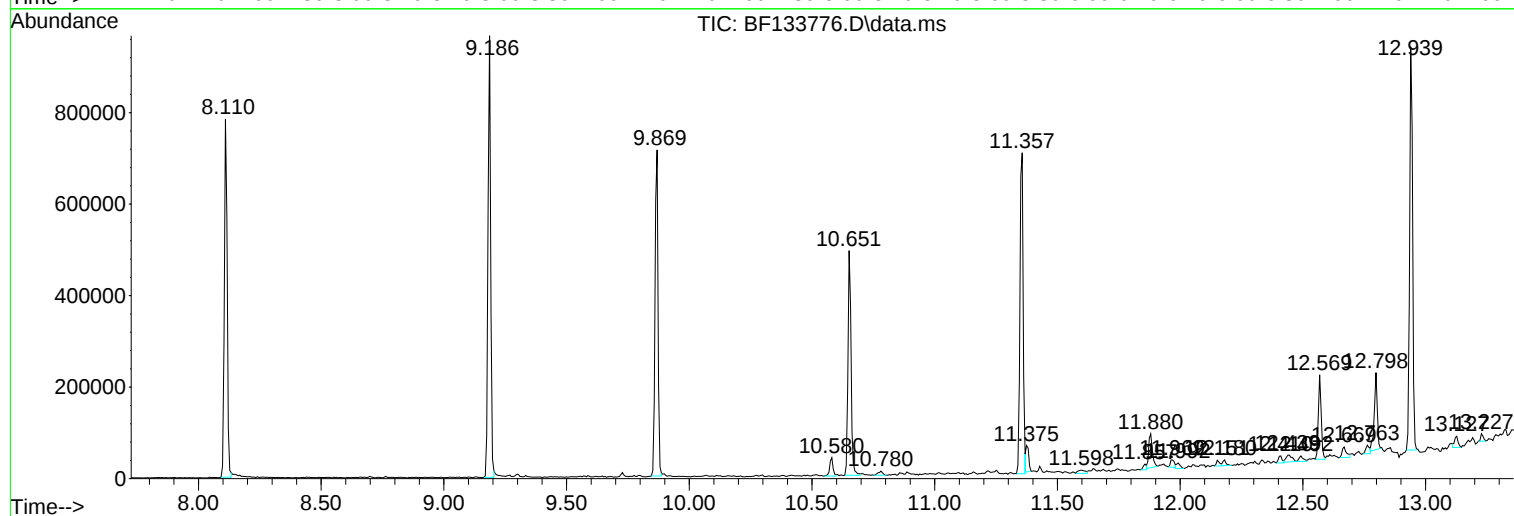
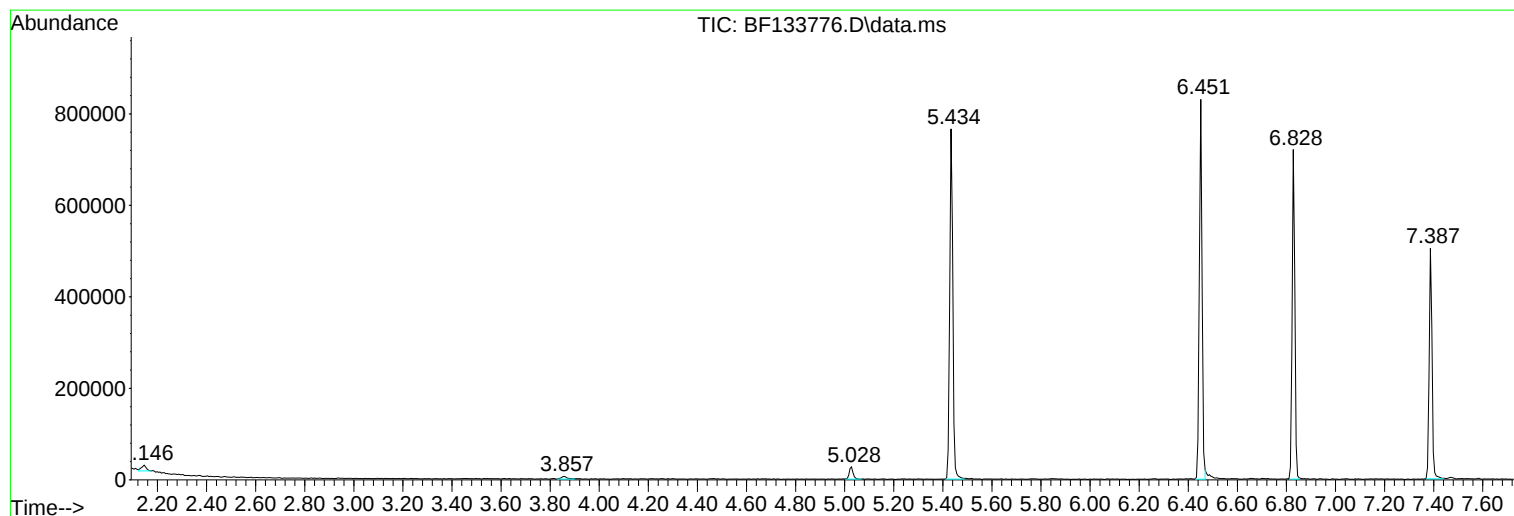
Sum of corrected areas: 8324365

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061523\
Data File : BF133776.D
Acq On : 15 Jun 2023 15:43
Operator : CG\JU
Sample : 03160-03 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PNNL-B-0609-2

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061523\
Data File : BF133776.D
Acq On : 15 Jun 2023 15:43
Operator : CG\JU
Sample : 03160-03 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PNNL-B-0609-2

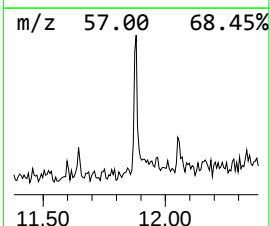
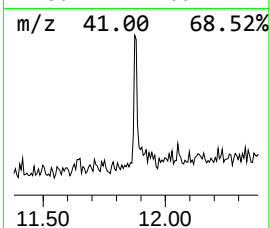
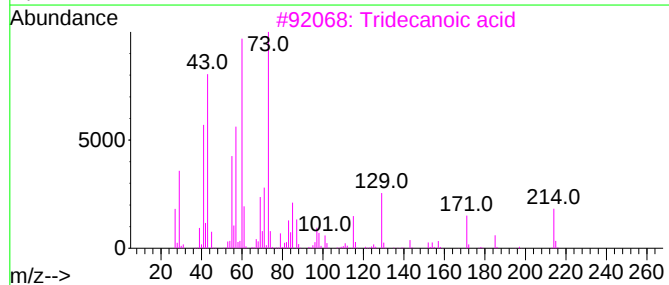
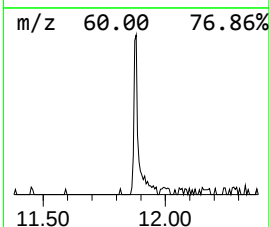
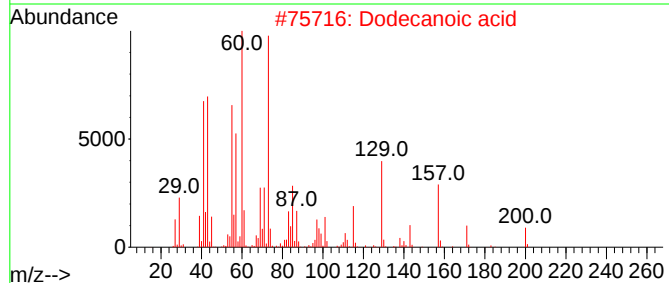
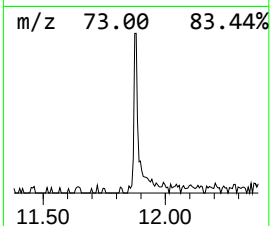
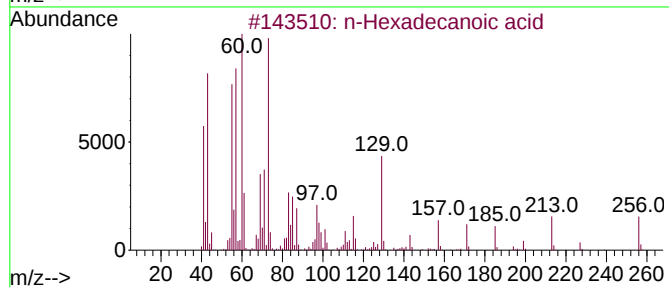
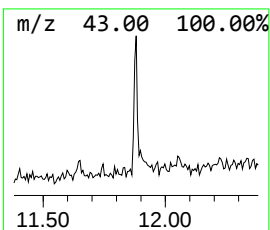
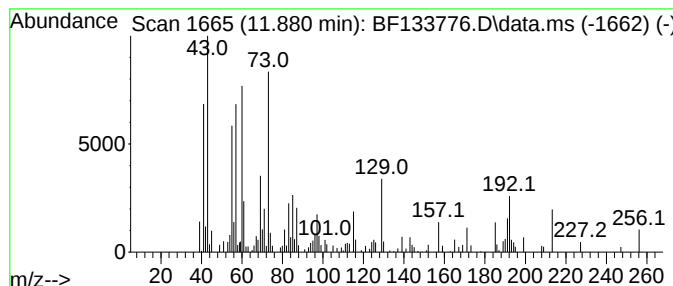
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.880	2.40 ng	77317	Phenanthrene-d10	11.357

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
2			Dodecanoic acid	200	C12H24O2	000143-07-7	50
3			Tridecanoic acid	214	C13H26O2	000638-53-9	50
4			Octanoic acid	144	C8H16O2	000124-07-2	50
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061523\
Data File : BF133776.D
Acq On : 15 Jun 2023 15:43
Operator : CG\JU
Sample : 03160-03 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PNNL-B-0609-2

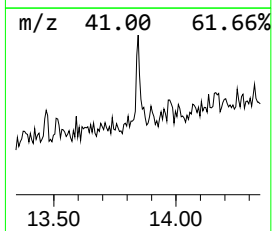
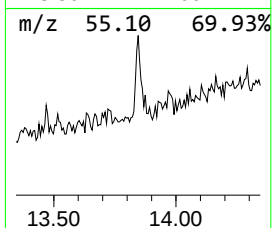
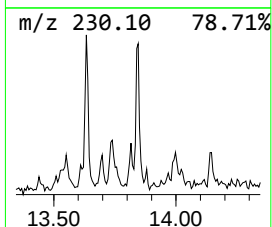
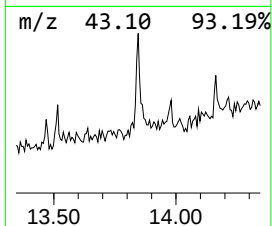
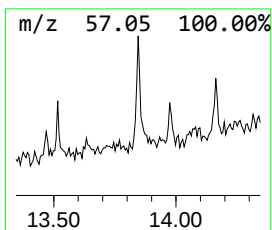
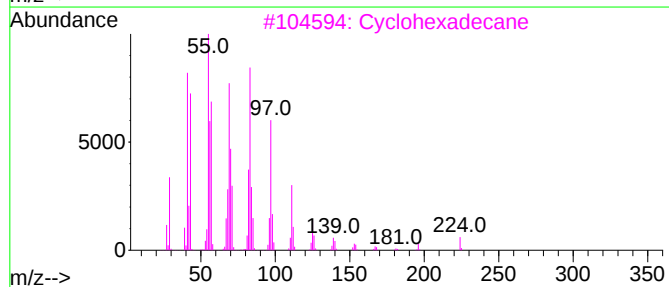
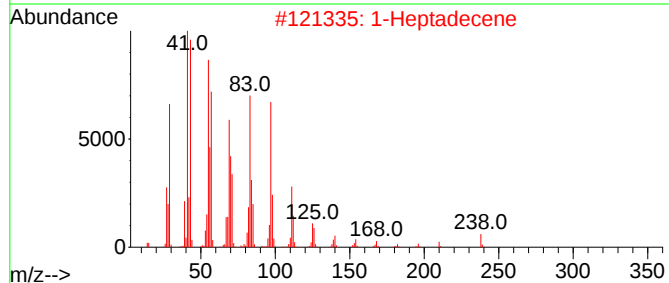
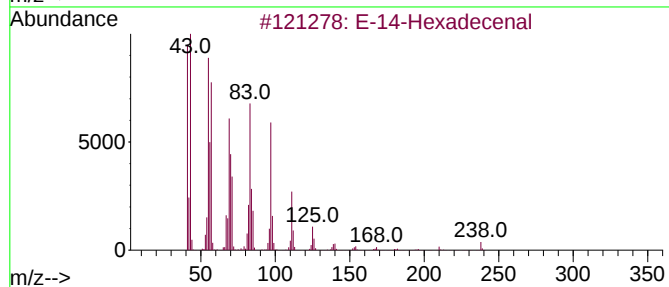
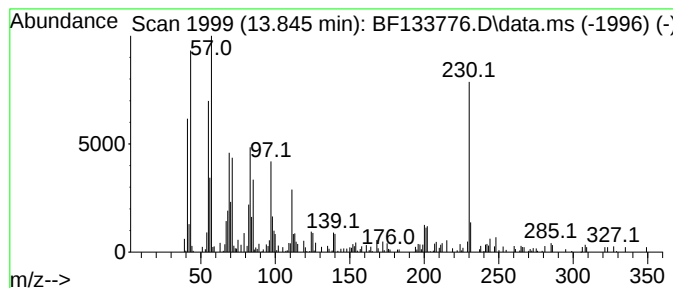
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 E-14-Hexadecenal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.845	2.28 ng	90290	Chrysene-d12	13.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	E-14-Hexadecenal			238	C16H30O	330207-53-9	83
2	1-Heptadecene			238	C17H34	006765-39-5	80
3	Cyclohexadecane			224	C16H32	000295-65-8	55
4	Dodecyl isobutyl carbonate			286	C17H34O3	959067-22-2	53
5	Heptadecyl heptafluorobutyrate			452	C21H35F7O2	959085-66-6	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061523\
Data File : BF133776.D
Acq On : 15 Jun 2023 15:43
Operator : CG\JU
Sample : 03160-03 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PNNL-B-0609-2

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Hexadecanoic ...	11.880	2.4	ng	77317	4	11.357	644665	20.0
E-14-Hexadecenal	13.845	2.3	ng	90290	5	13.998	791082	20.0