

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081723\
 Data File : BF134826.D
 Acq On : 17 Aug 2023 20:01
 Operator : CG\JU
 Sample : 04045-04
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 350

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: BF134826.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.034	497	501	507	rVB	30395	35348	1.13%	0.152%
2	5.428	563	568	571	rBV	2842958	2724190	87.39%	11.698%
3	6.428	733	738	741	rBV	2713593	2707857	86.86%	11.628%
4	6.793	796	800	803	rBV	1014187	768936	24.67%	3.302%
5	7.351	890	895	898	rBV	1842632	1768363	56.73%	7.593%
6	8.069	1013	1017	1022	rBV	1232943	1009522	32.38%	4.335%
7	9.145	1196	1200	1204	rBV	3291097	3117381	100.00%	13.386%
8	9.263	1217	1220	1224	rBV	41303	35186	1.13%	0.151%
9	9.828	1312	1316	1319	rBV	1209252	1062911	34.10%	4.564%
10	10.616	1446	1450	1453	rBV	2033535	1730372	55.51%	7.430%
11	11.316	1565	1569	1571	rBV	1138542	945986	30.35%	4.062%
12	11.339	1571	1573	1576	rVV	149012	120769	3.87%	0.519%
13	11.386	1576	1581	1585	rVB	36679	42455	1.36%	0.182%
14	11.851	1656	1660	1665	rBV2	298450	286861	9.20%	1.232%
15	11.928	1670	1673	1676	rBV	41368	42172	1.35%	0.181%
16	12.533	1772	1776	1779	rBV	293608	280956	9.01%	1.206%
17	12.639	1789	1794	1804	rBV5	90090	130775	4.20%	0.562%
18	12.757	1806	1814	1818	rBV	258752	276469	8.87%	1.187%
19	12.910	1836	1840	1843	rBV	2720176	2294636	73.61%	9.853%
20	13.092	1868	1871	1874	rVB	43951	41123	1.32%	0.177%
21	13.192	1884	1888	1891	rBV	35781	36352	1.17%	0.156%
22	13.598	1954	1957	1961	rVB	32931	35515	1.14%	0.153%
23	13.710	1972	1976	1979	rBV2	37243	48742	1.56%	0.209%
24	13.816	1990	1994	1999	rBV2	117387	160569	5.15%	0.689%
25	13.963	2014	2019	2022	rBV2	912473	1004803	32.23%	4.315%
26	13.986	2022	2023	2030	rVB	182431	148258	4.76%	0.637%
27	14.351	2081	2085	2088	rVB	41741	41835	1.34%	0.180%
28	14.386	2088	2091	2095	rBV4	32799	38599	1.24%	0.166%
29	14.451	2099	2102	2104	rBV4	31205	37549	1.20%	0.161%
30	14.551	2113	2119	2125	rBV5	43284	92797	2.98%	0.398%
31	14.604	2125	2128	2133	rBV2	70700	98485	3.16%	0.423%
32	14.651	2133	2136	2139	rBV4	26684	37116	1.19%	0.159%
33	14.833	2164	2167	2171	rVB2	39994	61668	1.98%	0.265%
34	15.004	2191	2196	2199	rBV	215715	321401	10.31%	1.380%
35	15.110	2210	2214	2217	rVB2	33655	41907	1.34%	0.180%
36	15.304	2243	2247	2253	rVB	128553	163315	5.24%	0.701%

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

37	15.368	2254	2258	2263	rBV	148129	180427	5.79%	0.775%
38	15.433	2264	2269	2277	rBV	754981	976483	31.32%	4.193%
39	15.933	2350	2354	2360	rBV	34212	63787	2.05%	0.274%
40	16.915	2516	2521	2529	rVB2	70480	144623	4.64%	0.621%
41	17.362	2590	2597	2602	rBV	61823	131786	4.23%	0.566%

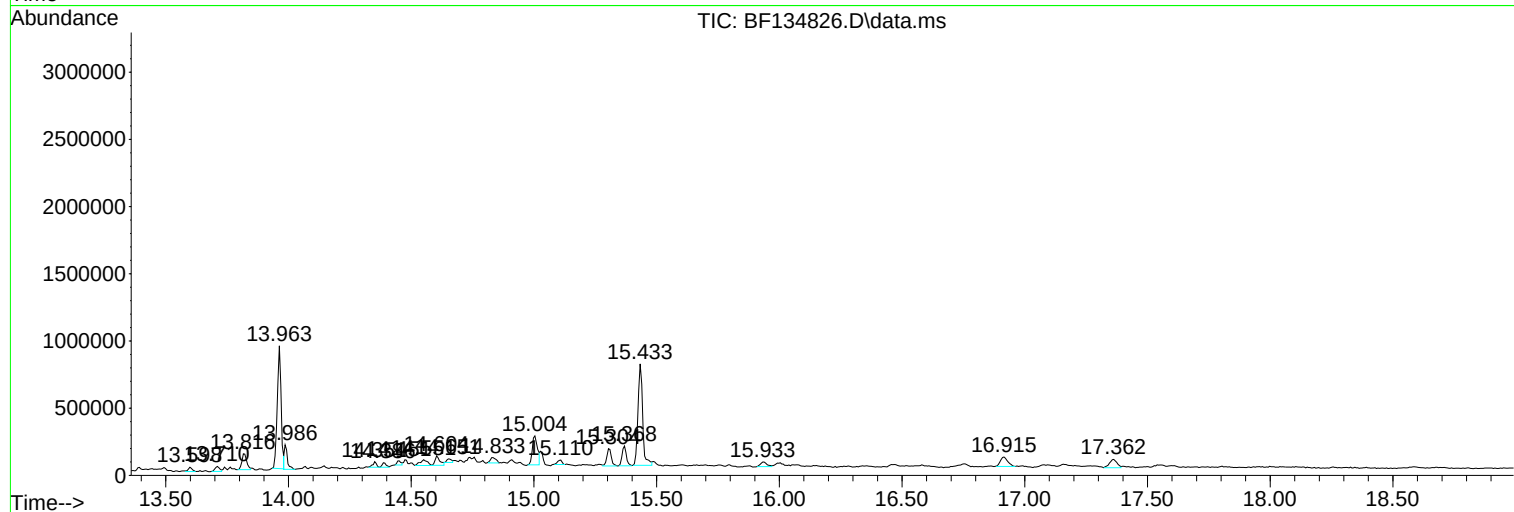
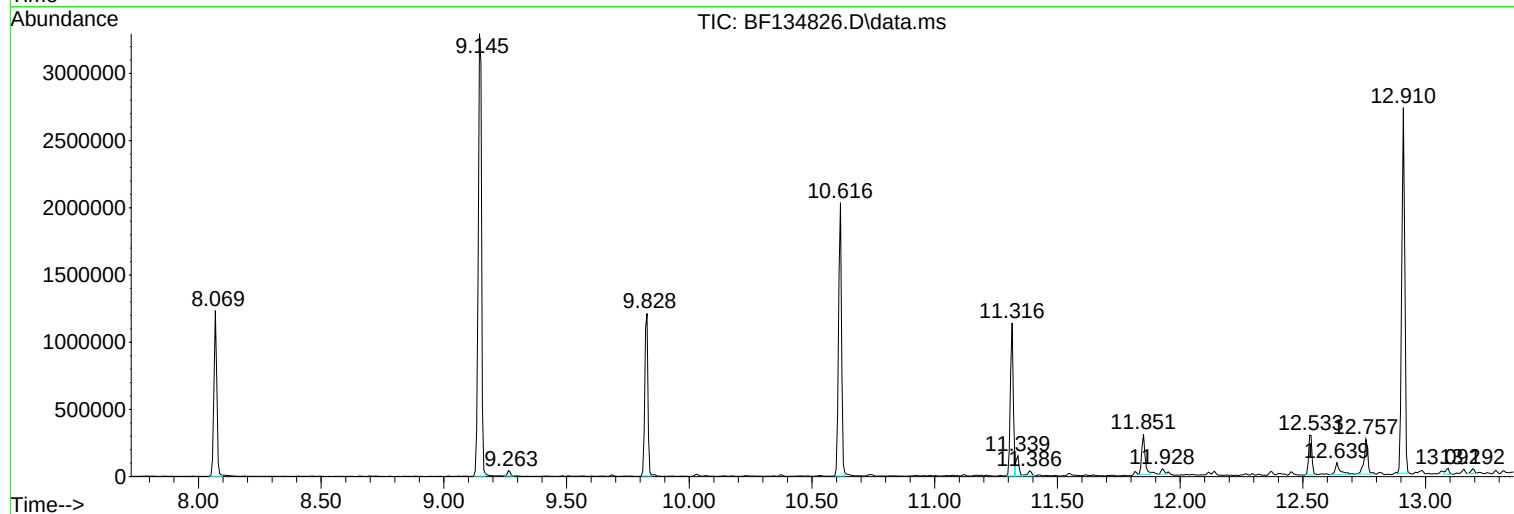
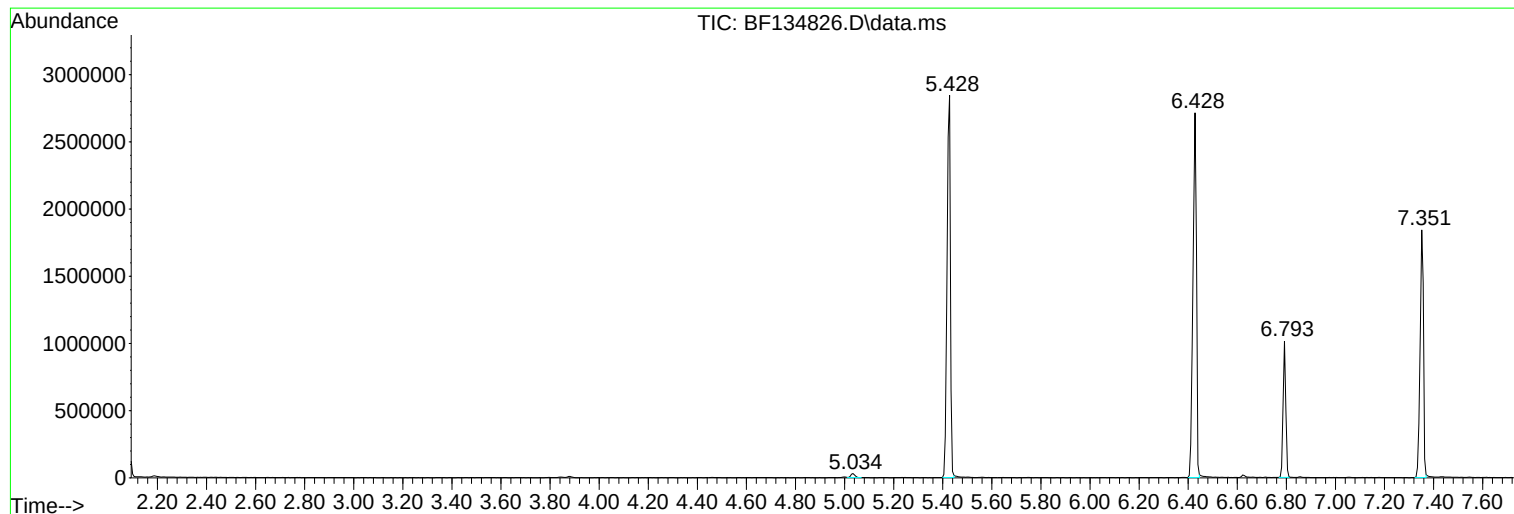
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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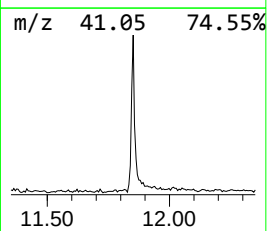
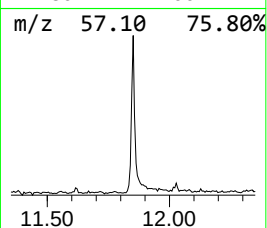
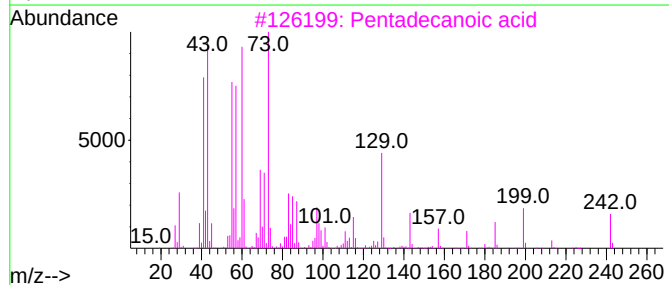
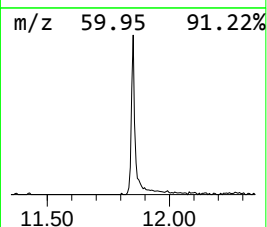
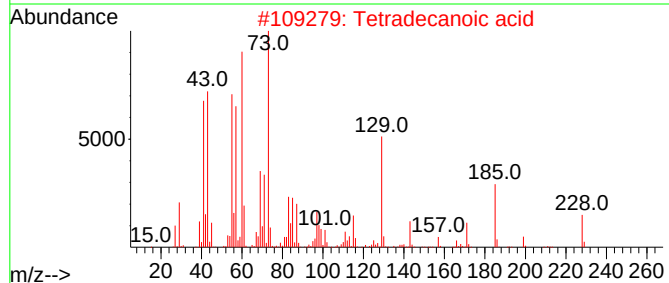
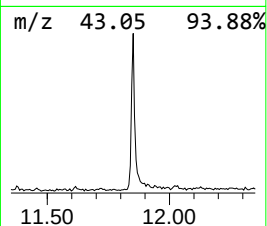
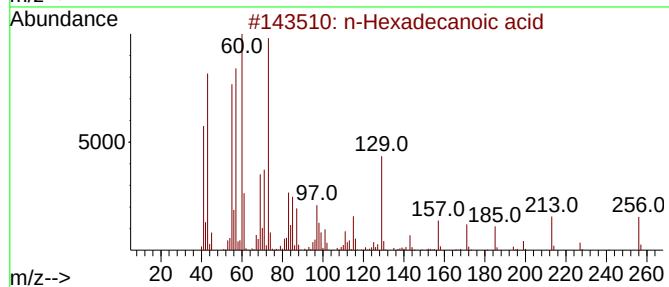
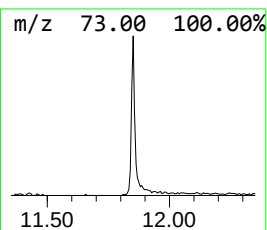
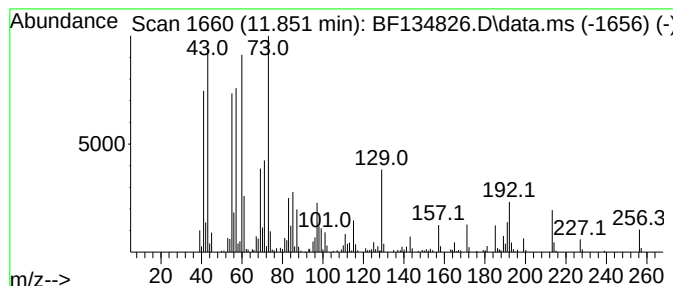
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.851	6.06 ng	286861	Phenanthrene-d10	11.316

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	92
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4		Tridecanoic acid	214	C13H26O2	000638-53-9	90
5		8-Methylnonanoic acid	172	C10H20O2	005963-14-4	43



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Misc :
ALS Vial : 11 Sample Multiplier: 1

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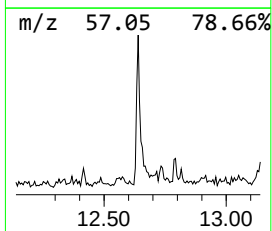
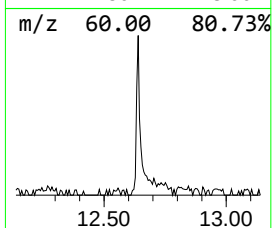
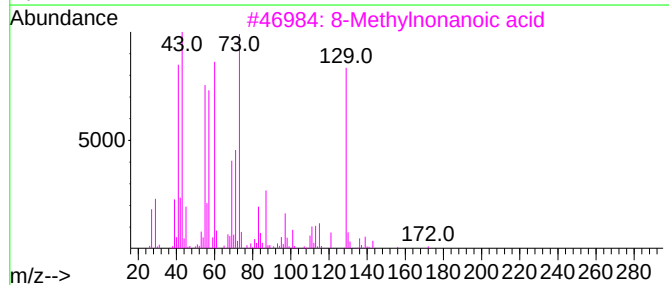
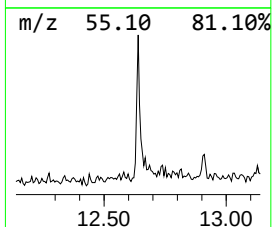
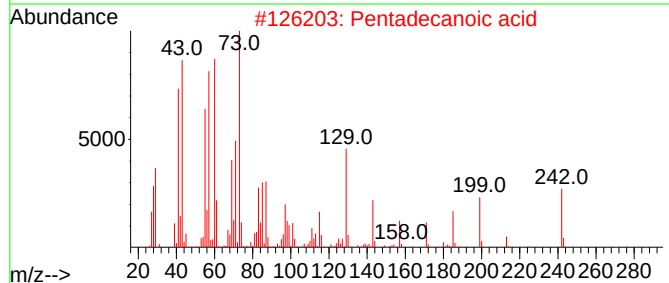
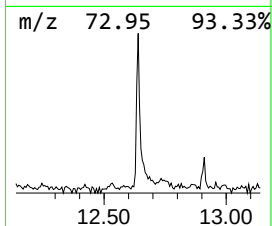
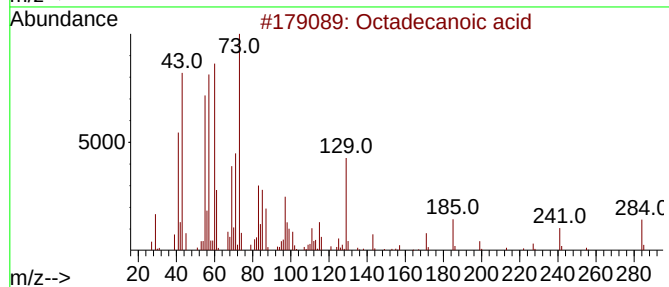
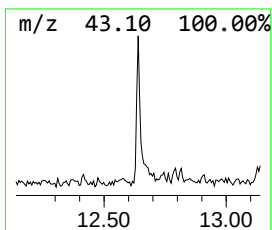
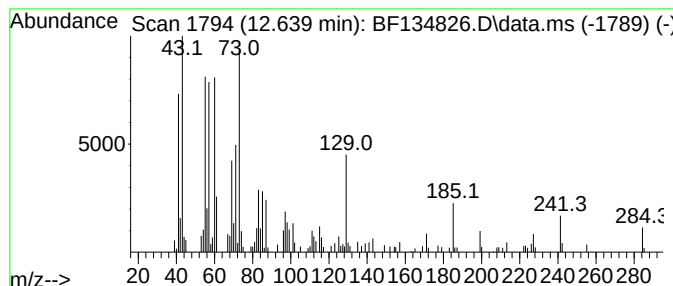
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.639	2.60 ng	130775	Chrysene-d12	13.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	70
4			n-Decanoic acid	172	C10H20O2	000334-48-5	68
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	49



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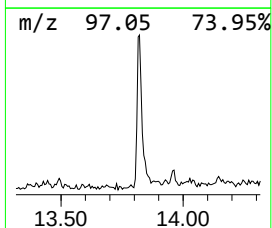
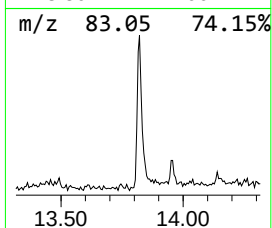
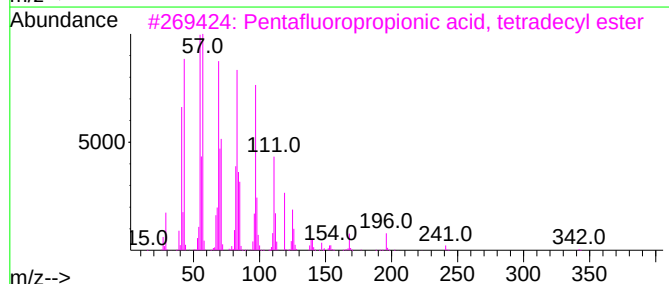
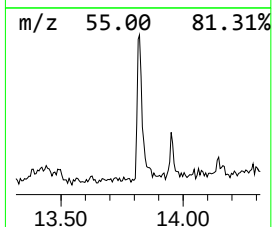
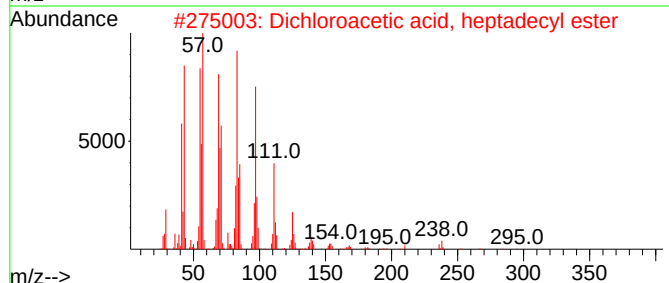
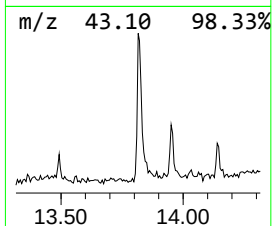
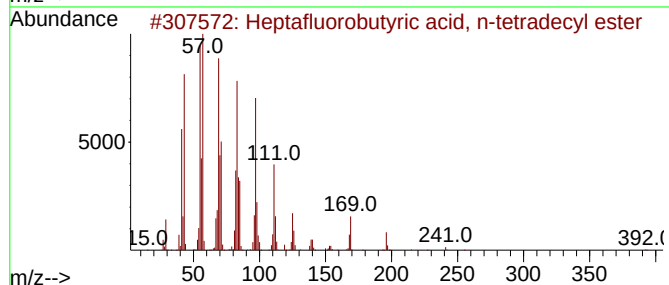
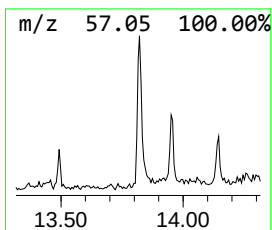
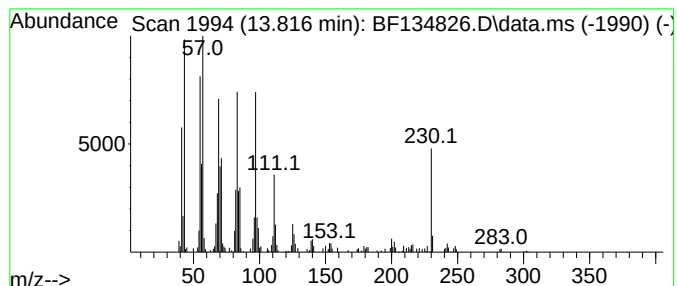
Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Heptafluorobutyric acid, n-... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.816	3.20 ng	160569	Chrysene-d12		13.963	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, n-tetra...		410	C18H29F7O2	007365-36-8	93
2	Dichloroacetic acid, heptadecyl ...		366	C19H36Cl2O2	1000282-98-2	93
3	Pentafluoropropionic acid, tetra...		360	C17H29F5O2	006222-06-6	93
4	Pentafluoropropionic acid, penta...		374	C18H31F5O2	959092-08-1	91
5	Heptafluorobutyric acid, pentade...		424	C19H31F7O2	959261-23-5	91



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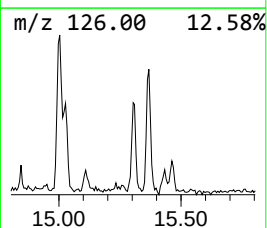
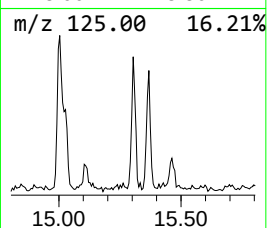
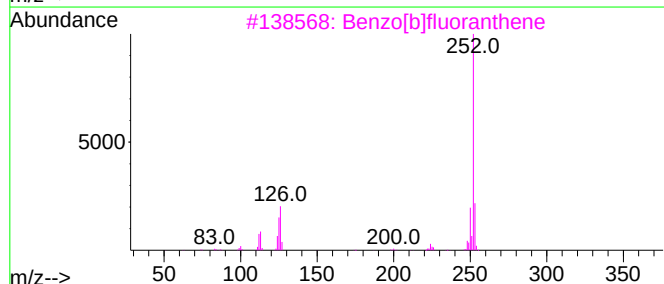
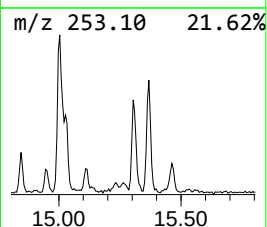
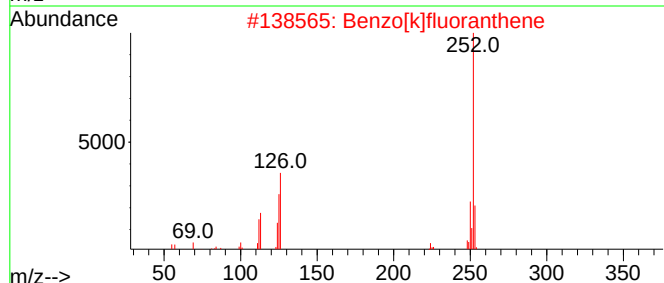
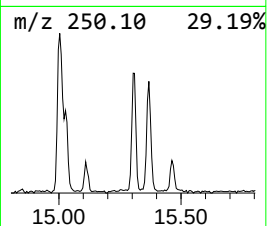
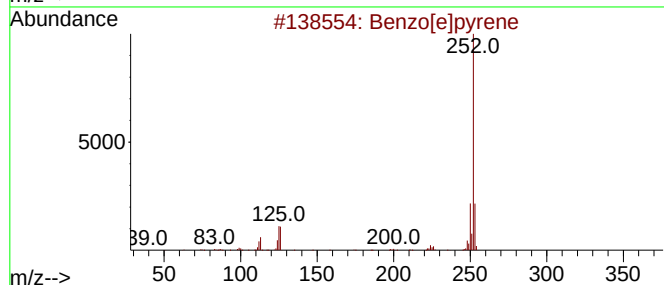
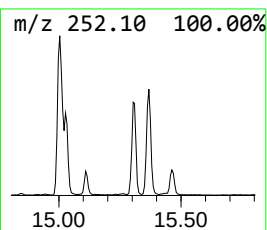
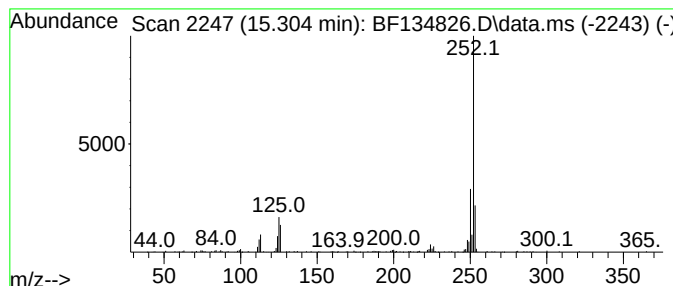
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzo[e]pyrene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.304	3.34 ng	163315	Perylene-d12	15.433

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	98
2			Benzo[k]fluoranthene	252	C20H12	000207-08-9	95
3			Benzo[b]fluoranthene	252	C20H12	000205-99-2	94
4			Benzo[j]fluoranthene	252	C20H12	000205-82-3	91
5			Benzo[a]pyrene	252	C20H12	000050-32-8	91



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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 ...	11.851	6.1	ng	286861	4	11.316	945986	20.0
Octadecanoic acid	12.639	2.6	ng	130775	5	13.963	1004800	20.0
Heptafluorobuty...	13.816	3.2	ng	160569	5	13.963	1004800	20.0
Benzo[e]pyrene	15.304	3.3	ng	163315	6	15.433	976483	20.0