

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090523\
 Data File : BF135120.D
 Acq On : 06 Sep 2023 05:30
 Operator : CG\JU
 Sample : 04202-01
 Misc :
 ALS Vial : 31 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 C-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-BF083023.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135120.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.152	7	11	18	rVB	31401	39390	1.81%	0.240%
2	5.004	492	496	505	rVB	61720	78854	3.63%	0.480%
3	5.404	560	564	567	rBV	2193110	1965832	90.42%	11.967%
4	6.410	730	735	738	rBV	2046253	1948206	89.61%	11.860%
5	6.769	793	796	800	rBV	742574	608969	28.01%	3.707%
6	7.334	887	892	895	rBV	1430017	1258188	57.87%	7.659%
7	8.051	1009	1014	1017	rBV	945482	814450	37.46%	4.958%
8	9.128	1192	1197	1201	rBV	2412819	2174118	100.00%	13.235%
9	9.810	1308	1313	1316	rBV	929320	818562	37.65%	4.983%
10	10.598	1443	1447	1460	rBV	1203829	1103028	50.73%	6.715%
11	11.298	1563	1566	1569	rBV	823951	733700	33.75%	4.466%
12	11.322	1569	1570	1574	rVV	187536	124784	5.74%	0.760%
13	11.375	1574	1579	1582	rVB	43397	43072	1.98%	0.262%
14	11.833	1654	1657	1662	rBV	177302	191236	8.80%	1.164%
15	11.916	1668	1671	1673	rBV	32695	33424	1.54%	0.203%
16	12.357	1739	1746	1749	rBV	23733	25296	1.16%	0.154%
17	12.516	1770	1773	1777	rBV	251395	224288	10.32%	1.365%
18	12.569	1779	1782	1789	rVB2	37004	37972	1.75%	0.231%
19	12.627	1789	1792	1796	rBV5	29752	38286	1.76%	0.233%
20	12.727	1806	1809	1810	rBV2	73868	75840	3.49%	0.462%
21	12.745	1810	1812	1816	rVV	218056	206152	9.48%	1.255%
22	12.798	1819	1821	1827	rVB2	23473	27314	1.26%	0.166%
23	12.898	1834	1838	1841	rBV	2000946	1625298	74.76%	9.894%
24	12.969	1845	1850	1858	rBV5	20709	38950	1.79%	0.237%
25	13.080	1866	1869	1872	rVB	26562	26346	1.21%	0.160%
26	13.139	1872	1879	1882	rBV5	15035	28293	1.30%	0.172%
27	13.180	1882	1886	1890	rBV	36601	39375	1.81%	0.240%
28	13.274	1899	1902	1906	rBV2	16243	28193	1.30%	0.172%
29	13.433	1926	1929	1932	rVB	33510	26486	1.22%	0.161%
30	13.480	1932	1937	1940	rBV5	21735	30622	1.41%	0.186%
31	13.592	1953	1956	1960	rVB	30154	28258	1.30%	0.172%
32	13.704	1970	1975	1978	rBV2	22321	33630	1.55%	0.205%
33	13.810	1989	1993	2001	rBV2	118523	183444	8.44%	1.117%
34	13.957	2010	2018	2020	rBV2	641073	712791	32.79%	4.339%
35	13.980	2020	2022	2025	rVB	108320	87841	4.04%	0.535%
36	14.127	2044	2047	2050	rBV3	22314	24034	1.11%	0.146%

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	14.345	2080	2084	2087	rBV	30657	30794	1.42%	0.187%
38	14.439	2096	2100	2103	rBV2	27558	29600	1.36%	0.180%
39	14.727	2146	2149	2154	rBV3	64659	96312	4.43%	0.586%
40	14.998	2190	2195	2198	rBV	75826	120797	5.56%	0.735%
41	15.298	2242	2246	2252	rVB	41751	52807	2.43%	0.321%
42	15.357	2252	2256	2262	rVB	56263	77673	3.57%	0.473%
43	15.421	2262	2267	2271	rBV	358565	468604	21.55%	2.853%
44	15.910	2346	2350	2354	rBV3	18716	24835	1.14%	0.151%
45	16.904	2514	2519	2527	rVB3	18702	41328	1.90%	0.252%

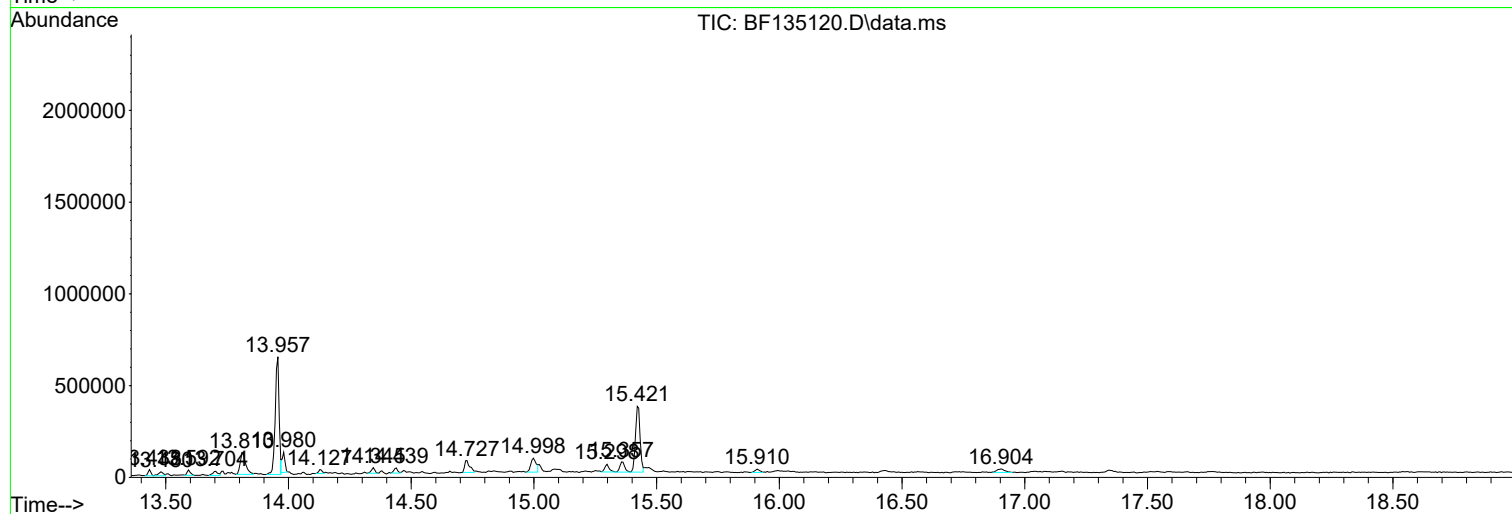
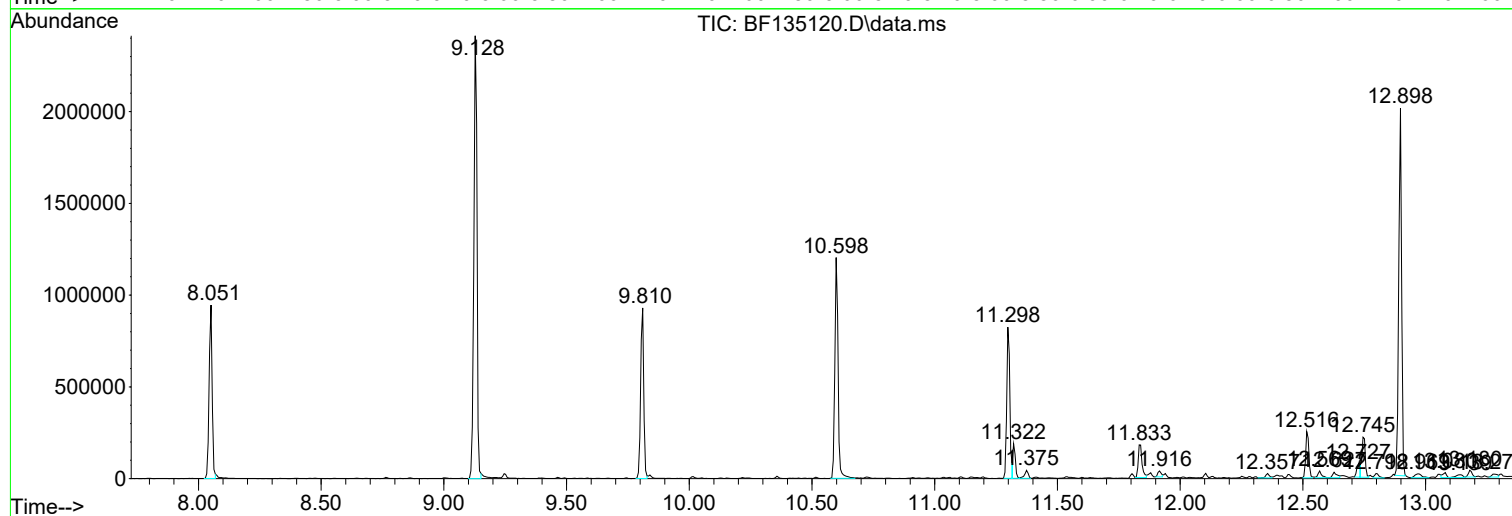
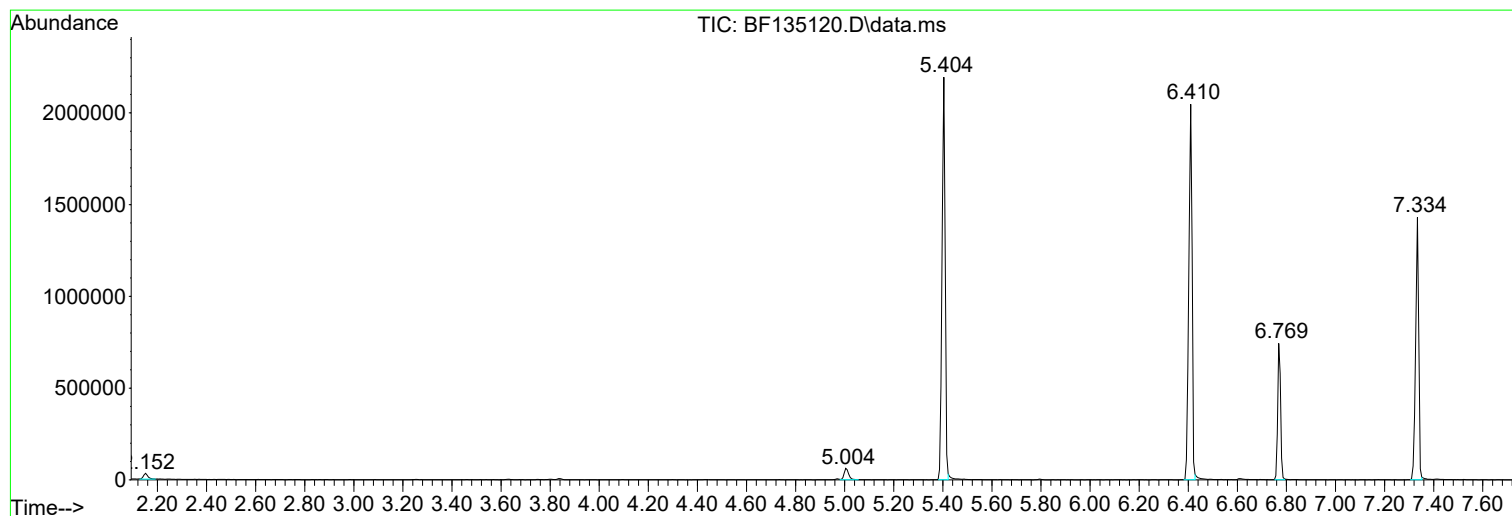
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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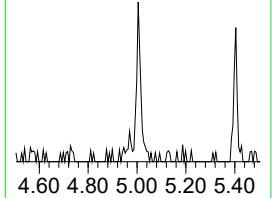
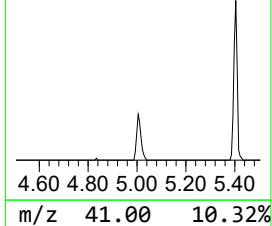
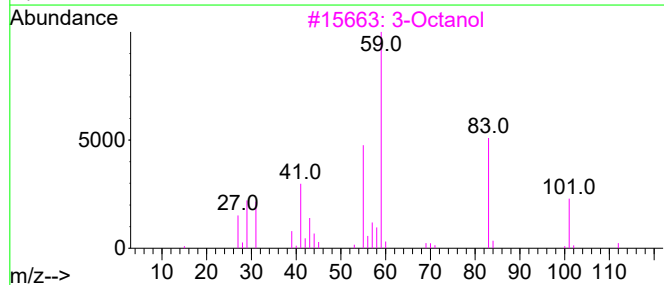
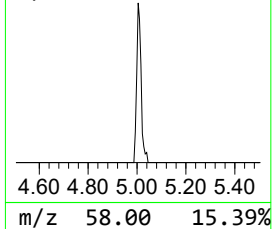
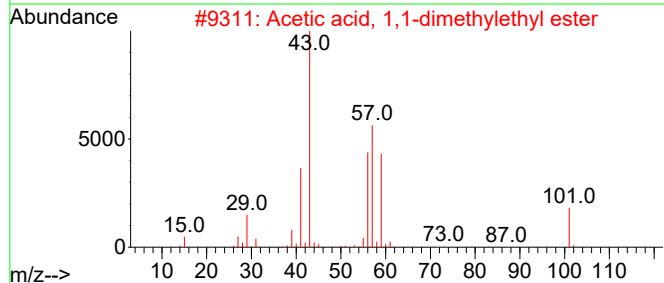
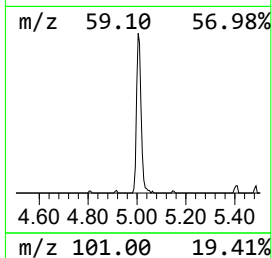
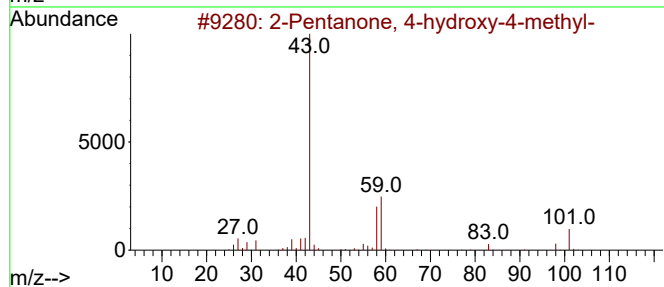
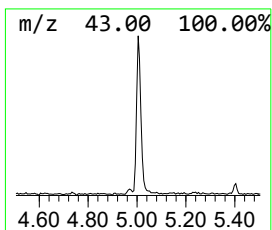
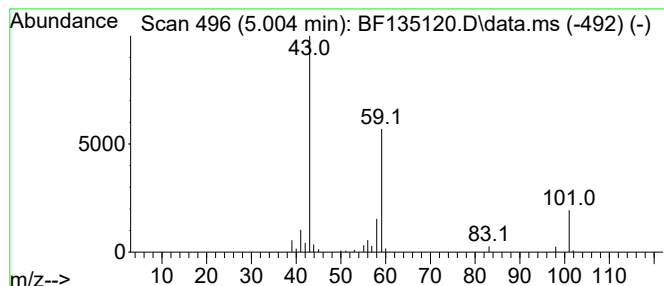
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.004	2.59 ng	78854	1,4-Dichlorobenzene-d4	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39		
3	3-Octanol	130	C8H18O	000589-98-0	33		
4	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	23		
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		



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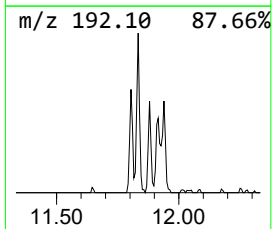
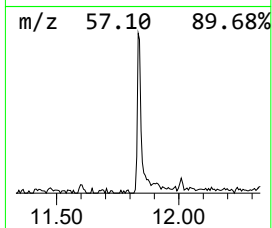
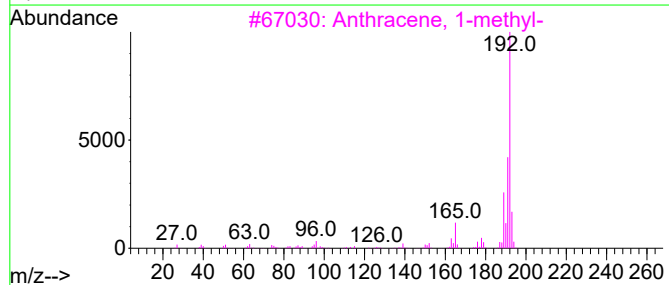
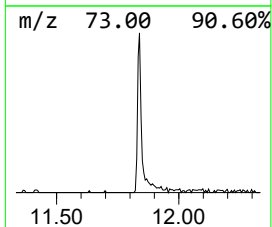
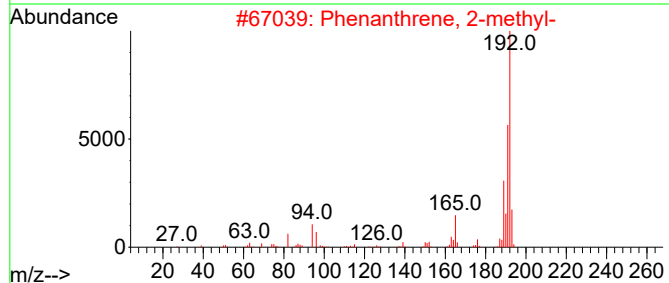
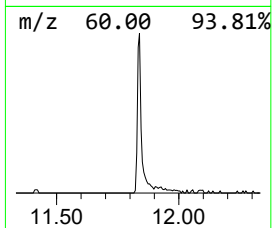
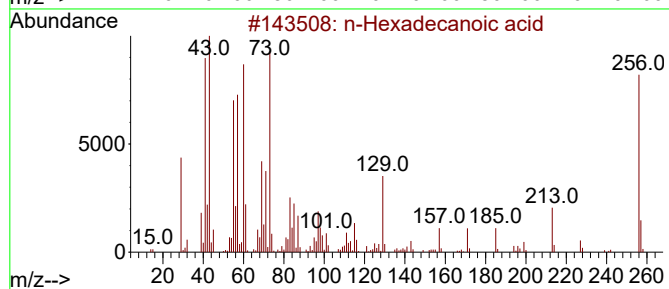
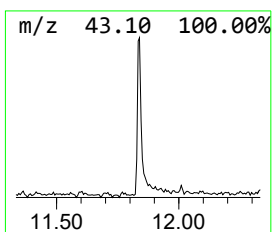
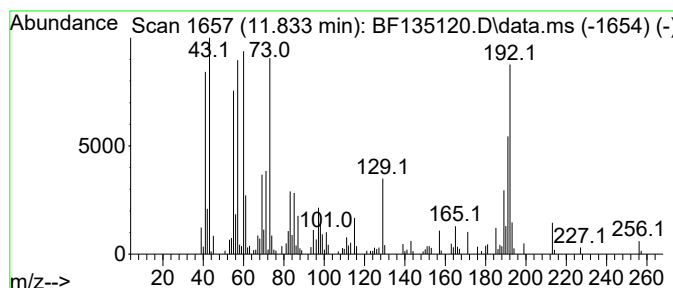
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.833	5.21 ng	191236	Phenanthrene-d10	11.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2			Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	91
3			Anthracene, 1-methyl-	192	C15H12	000610-48-0	68
4			Anthracene, 9-methyl-	192	C15H12	000779-02-2	66
5			Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	64



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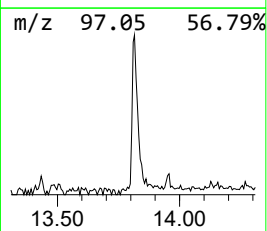
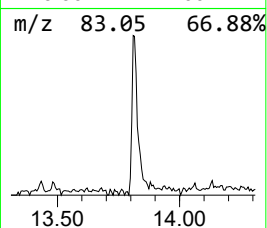
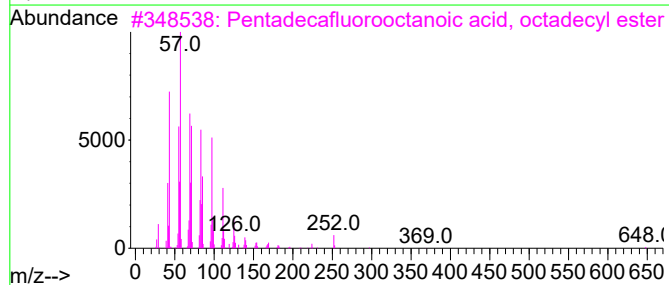
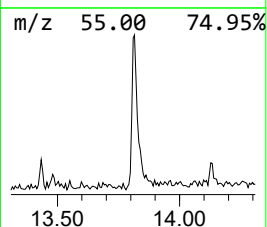
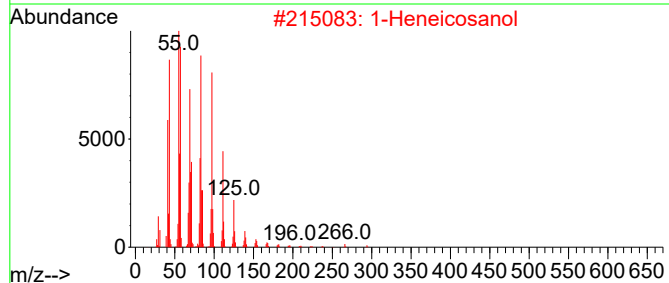
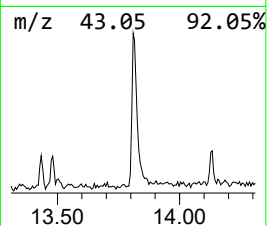
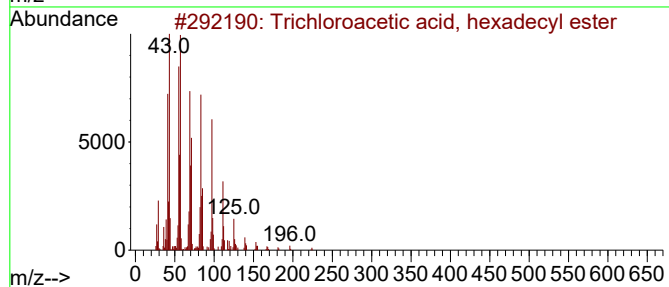
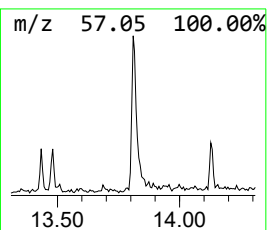
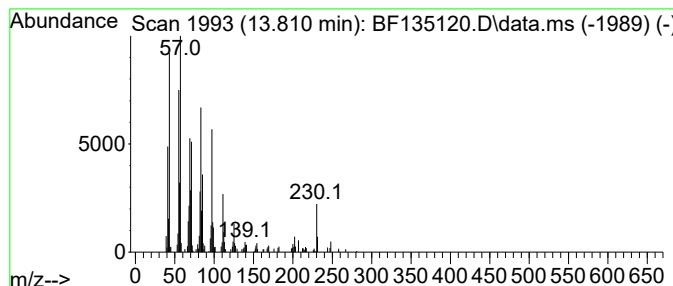
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Trichloroacetic acid, hexad... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.810	5.15 ng	183444	Chrysene-d12	13.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	93
2			1-Heneicosanol	312	C21H44O	015594-90-8	93
3			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	91
4			1-Hexacosanol	382	C26H54O	000506-52-5	87
5			1-Heptacosanol	396	C27H56O	002004-39-9	87



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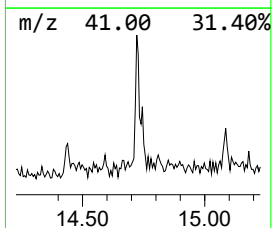
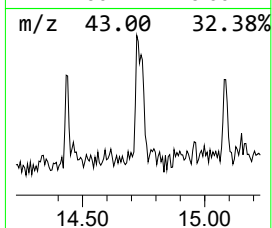
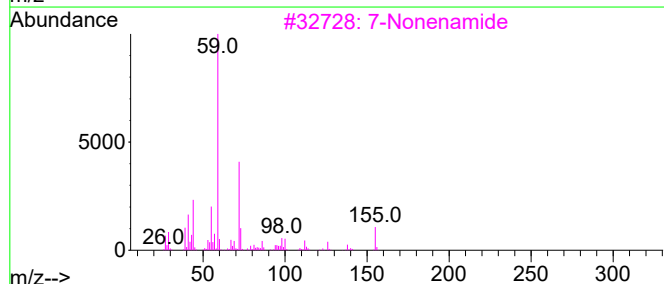
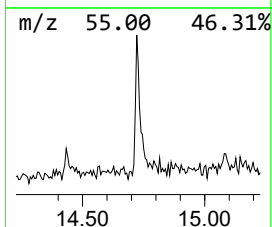
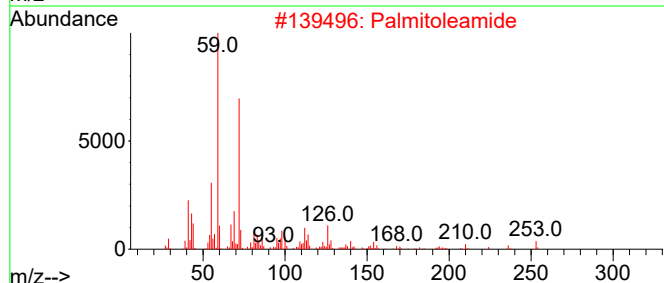
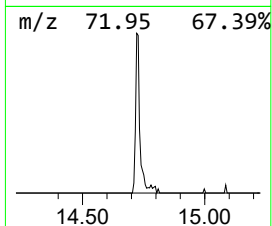
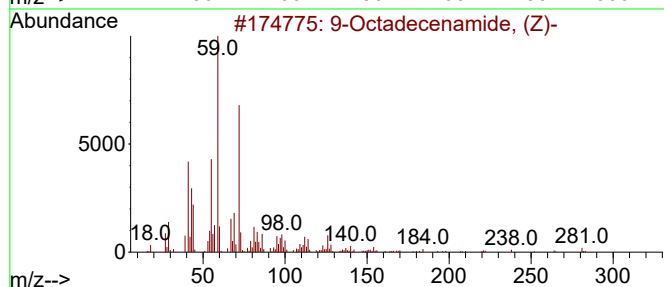
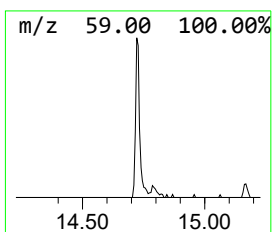
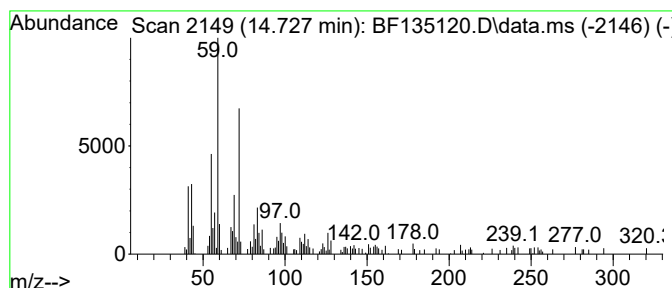
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 9-Octadecenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.727	4.11 ng	96312	Perylene-d12	15.421	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	94
2	Palmitoleamide	253	C16H31NO	106010-22-4	80
3	7-Nonenamide	155	C9H17NO	090949-53-4	72
4	Acetic acid, cyanohydroxyimino-,...	128	C4H4N2O3	061295-92-9	38
5	9-Octadecenamide	281	C18H35NO	003322-62-1	38



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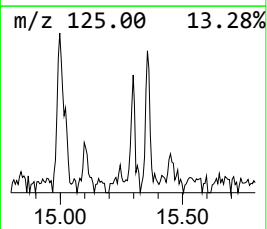
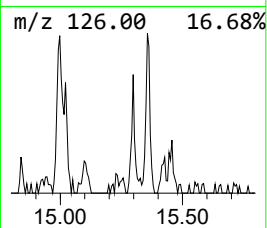
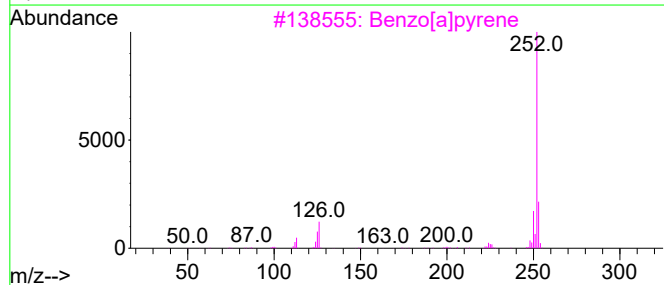
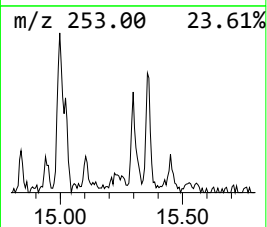
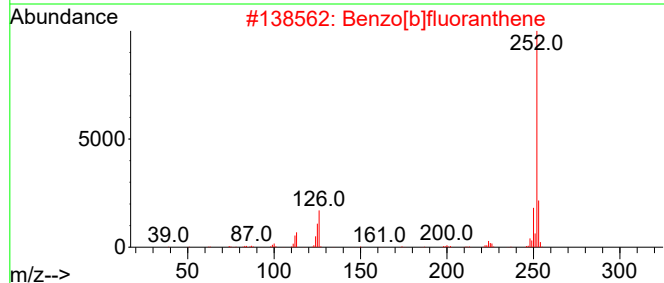
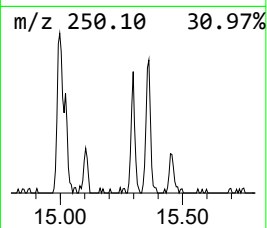
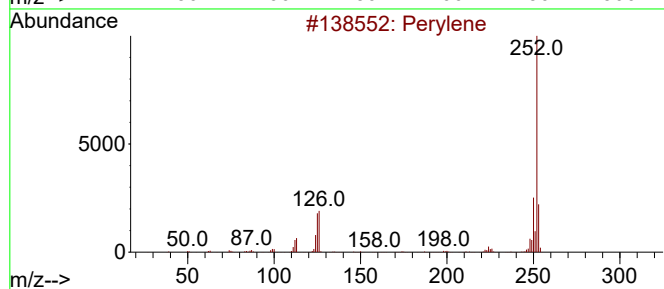
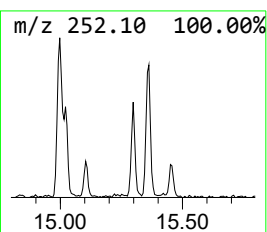
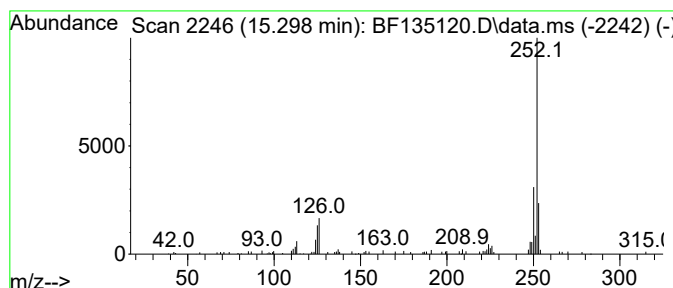
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Perylene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.298	2.25 ng	52807	Perylene-d12	15.421

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Perylene	252	C20H12	000198-55-0	95
2			Benzo[b]fluoranthene	252	C20H12	000205-99-2	95
3			Benzo[a]pyrene	252	C20H12	000050-32-8	94
4			Benzo[e]pyrene	252	C20H12	000192-97-2	94
5			Benzo[j]fluoranthene	252	C20H12	000205-82-3	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090523\
Data File : BF135120.D
Acq On : 06 Sep 2023 05:30
Operator : CG\JU
Sample : 04202-01
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
C-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083023.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
2-Pentanone, 4-...	5.004	2.6	ng	78854	1	6.769	608969	20.0
n-Hexadecanoic ...	11.833	5.2	ng	191236	4	11.298	733700	20.0
Trichloroacetic...	13.810	5.2	ng	183444	5	13.957	712791	20.0
9-Octadecenamid...	14.727	4.1	ng	96312	6	15.421	468604	20.0
Perylene	15.298	2.3	ng	52807	6	15.421	468604	20.0