

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061323\
 Data File : BF133734.D
 Acq On : 13 Jun 2023 16:52
 Operator : CG\JU
 Sample : 03069-04
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB35A

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: BF133734.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.040	498	502	508	rBV	35216	43602	2.94%	0.332%
2	5.446	567	571	574	rBV	1586278	1363695	91.85%	10.373%
3	6.457	739	743	746	rBV	1526718	1331192	89.66%	10.126%
4	6.663	774	778	781	rBV2	16593	19371	1.30%	0.147%
5	6.834	803	807	810	rBV	713967	569519	38.36%	4.332%
6	7.393	898	902	905	rBV	1116160	841214	56.66%	6.399%
7	8.116	1019	1025	1028	rBV	805743	644467	43.41%	4.902%
8	8.828	1143	1146	1151	rVB	29001	22638	1.52%	0.172%
9	8.928	1160	1163	1166	rBV	23981	20270	1.37%	0.154%
10	9.187	1204	1207	1211	rBV	1548102	1370542	92.31%	10.425%
11	9.528	1262	1265	1267	rBV	21897	19318	1.30%	0.147%
12	9.869	1320	1323	1327	rVV	706921	555141	37.39%	4.223%
13	9.898	1327	1328	1332	rVB2	18855	15863	1.07%	0.121%
14	10.075	1354	1358	1362	rBV	18007	17927	1.21%	0.136%
15	10.416	1412	1416	1422	rVB3	17934	23766	1.60%	0.181%
16	10.581	1440	1444	1450	rBV	103045	89972	6.06%	0.684%
17	10.657	1453	1457	1464	rBV	1001765	847160	57.06%	6.444%
18	10.786	1474	1479	1482	rBV2	20992	29089	1.96%	0.221%
19	11.222	1547	1553	1557	rBV5	12889	19432	1.31%	0.148%
20	11.357	1573	1576	1579	rBV	653121	600919	40.47%	4.571%
21	11.381	1579	1580	1584	rVV	135415	93511	6.30%	0.711%
22	11.433	1587	1589	1592	rVB	31553	25509	1.72%	0.194%
23	11.592	1610	1616	1618	rBV2	15060	20044	1.35%	0.152%
24	11.863	1656	1662	1663	rBV3	37618	48792	3.29%	0.371%
25	11.886	1663	1666	1671	rVB2	154628	152991	10.30%	1.164%
26	11.969	1678	1680	1683	rBV2	35542	34931	2.35%	0.266%
27	11.992	1683	1684	1689	rVB	25570	20803	1.40%	0.158%
28	12.063	1691	1696	1698	rBV5	16908	23357	1.57%	0.178%
29	12.157	1709	1712	1714	rBV	26456	25099	1.69%	0.191%
30	12.180	1714	1716	1720	rVB3	15704	16628	1.12%	0.126%
31	12.410	1752	1755	1758	rBV	33728	35681	2.40%	0.271%
32	12.445	1758	1761	1763	rVV2	25257	26920	1.81%	0.205%
33	12.498	1767	1770	1773	rBV2	20712	21824	1.47%	0.166%
34	12.575	1779	1783	1788	rBV	237604	206037	13.88%	1.567%
35	12.669	1797	1799	1802	rBV2	17561	16226	1.09%	0.123%
36	12.804	1817	1822	1828	rVV	185900	200369	13.50%	1.524%

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If leading or trailing edge < 100 prefer < Baseline drop else tangent >

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37	12.857	1828	1831	1834	rVB2	17740	20062	1.35%	0.153%
38	12.951	1842	1847	1850	rBV	1567409	1484760	100.00%	11.294%
39	13.016	1855	1858	1866	rBV6	25581	50213	3.38%	0.382%
40	13.104	1871	1873	1875	rBV3	15512	16965	1.14%	0.129%
41	13.133	1875	1878	1880	rVB	41417	35969	2.42%	0.274%
42	13.180	1883	1886	1887	rBV	21070	16654	1.12%	0.127%
43	13.198	1887	1889	1891	rVV	27786	18957	1.28%	0.144%
44	13.233	1891	1895	1898	rVB2	28809	32924	2.22%	0.250%
45	13.363	1914	1917	1920	rBV3	17474	19287	1.30%	0.147%
46	13.639	1962	1964	1971	rBV	40473	40928	2.76%	0.311%
47	13.751	1981	1983	1986	rBV2	18651	15727	1.06%	0.120%
48	13.845	1996	1999	2007	rVB2	159899	195450	13.16%	1.487%
49	14.004	2021	2026	2029	rBV2	761230	773992	52.13%	5.888%
50	14.027	2029	2030	2033	rVB	108303	74783	5.04%	0.569%
51	14.169	2052	2054	2057	rVB2	28309	21507	1.45%	0.164%
52	14.392	2090	2092	2096	rVB2	32180	25797	1.74%	0.196%
53	14.480	2104	2107	2111	rBV3	53558	66422	4.47%	0.505%
54	14.927	2180	2183	2186	rBV	80543	74626	5.03%	0.568%
55	15.039	2199	2202	2206	rBV	76343	111416	7.50%	0.848%
56	15.116	2213	2215	2218	rVV2	52091	46166	3.11%	0.351%
57	15.145	2218	2220	2225	rVB2	44969	54855	3.69%	0.417%
58	15.404	2262	2264	2270	rVB	52249	53925	3.63%	0.410%
59	15.468	2271	2275	2285	rVB	392830	481112	32.40%	3.660%

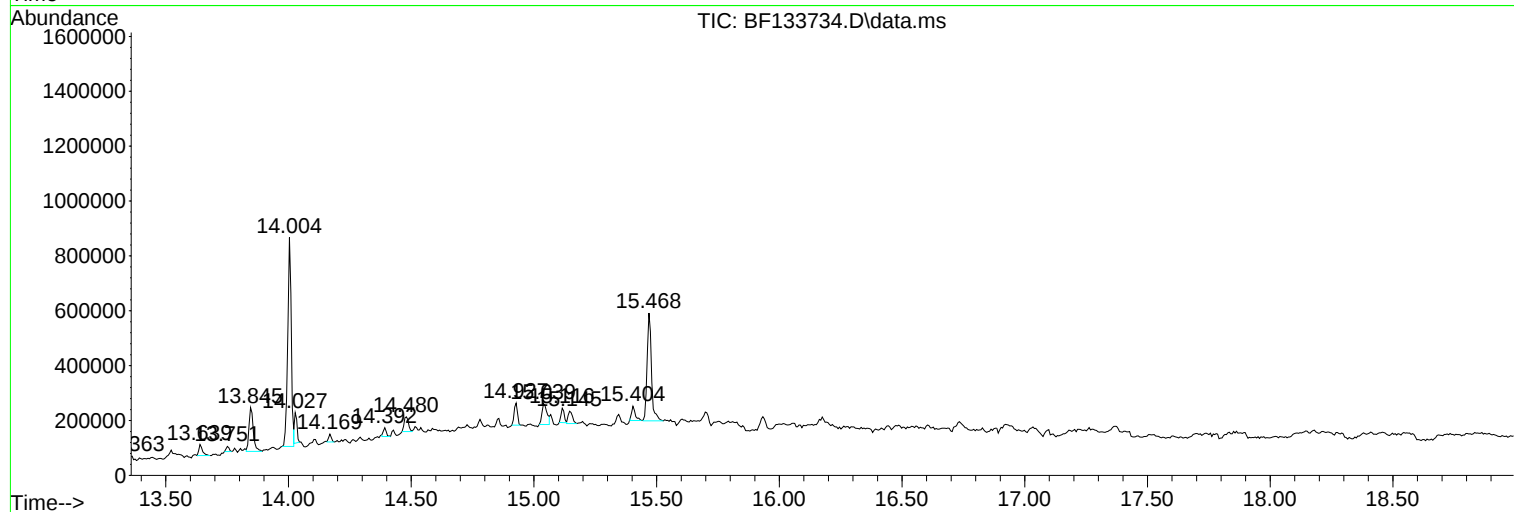
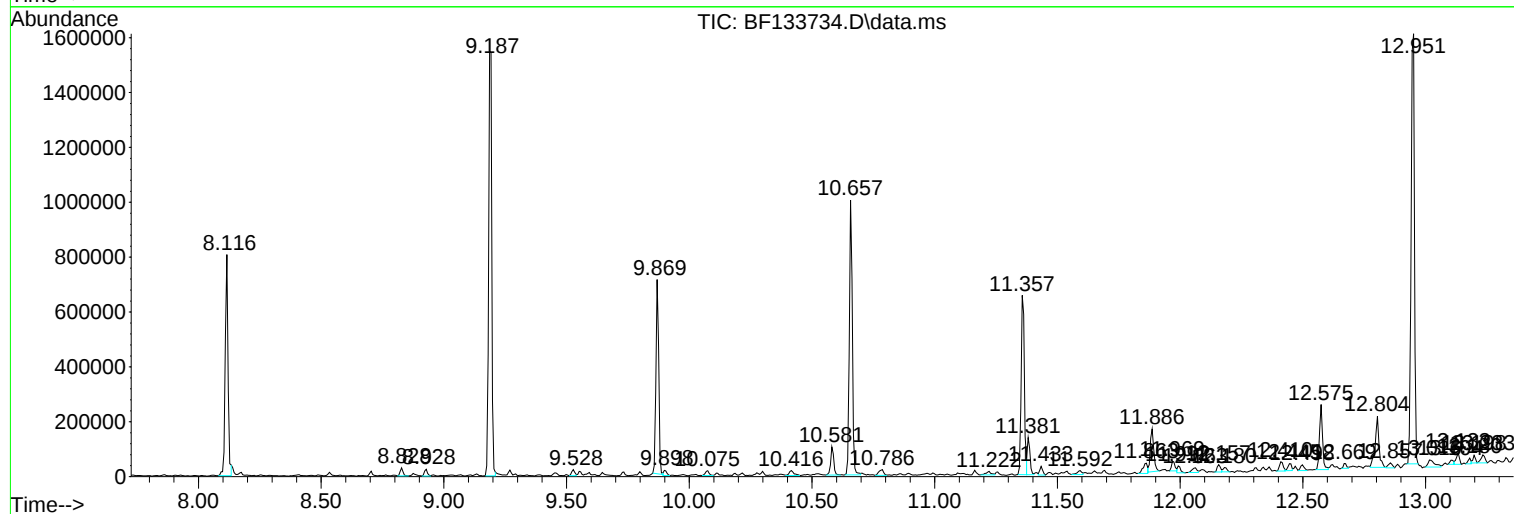
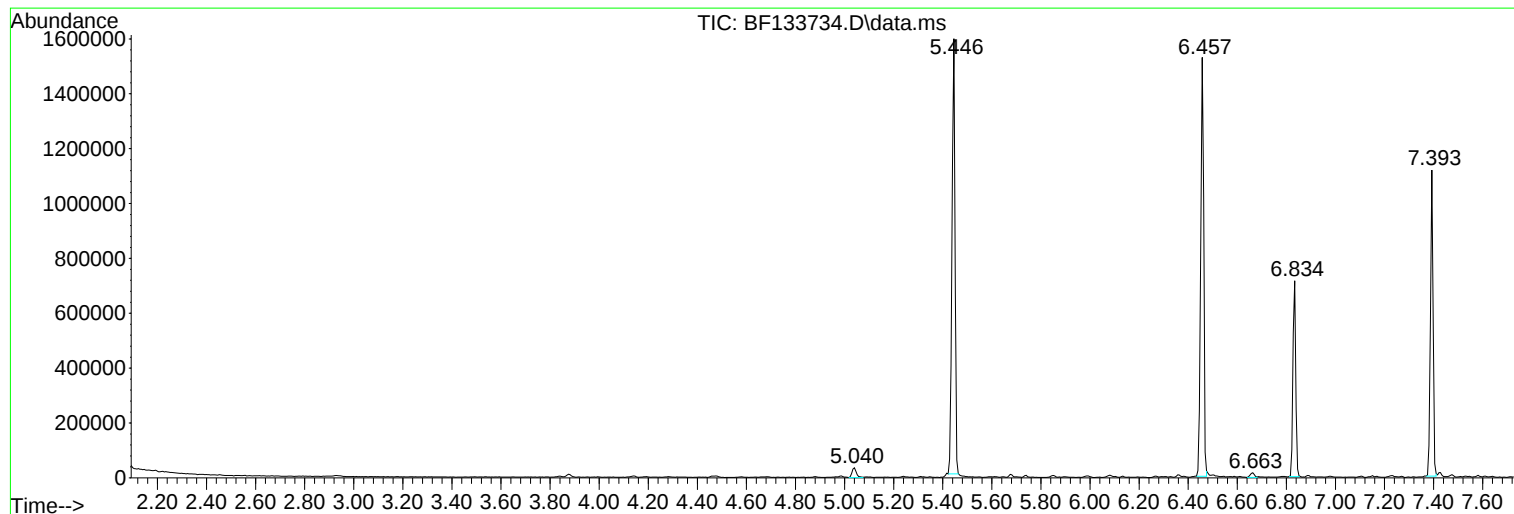
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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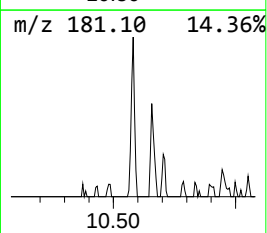
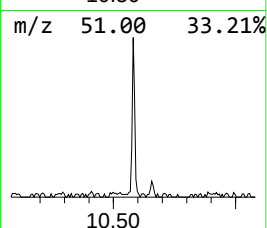
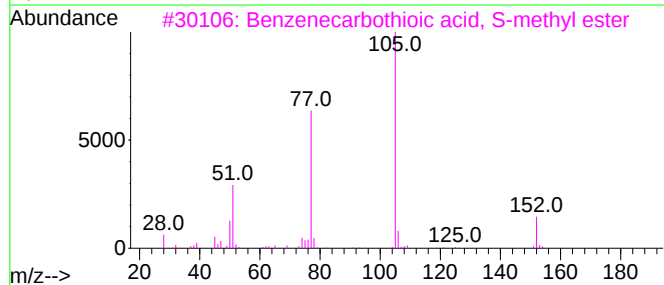
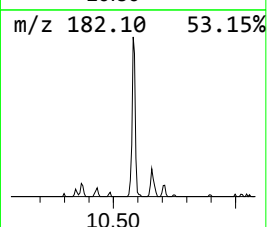
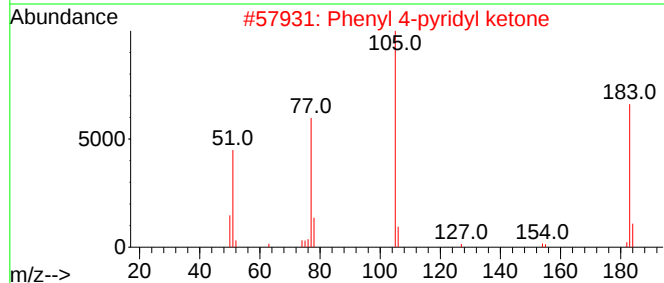
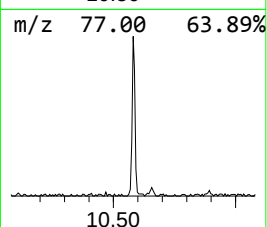
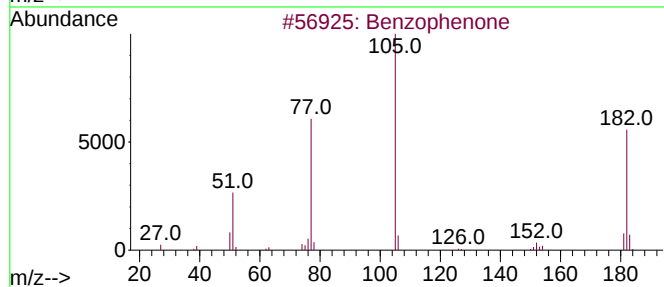
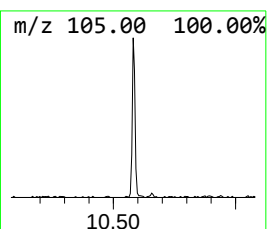
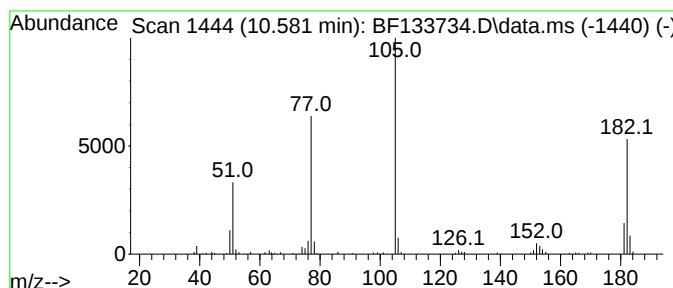
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.581	3.24 ng	89972	Acenaphthene-d10	9.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	60
3			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	43
4			Isopropyl phenyl ketone	148	C10H12O	000611-70-1	43
5			Vinyl benzoate	148	C9H8O2	000769-78-8	43



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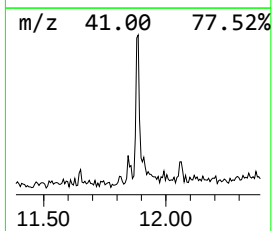
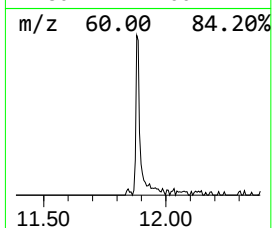
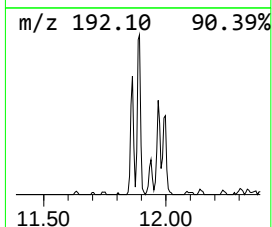
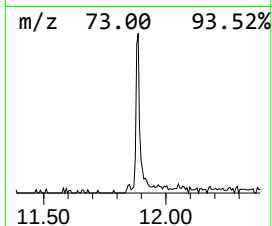
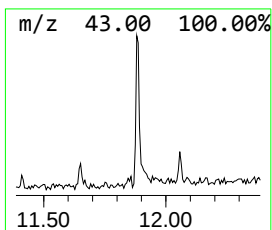
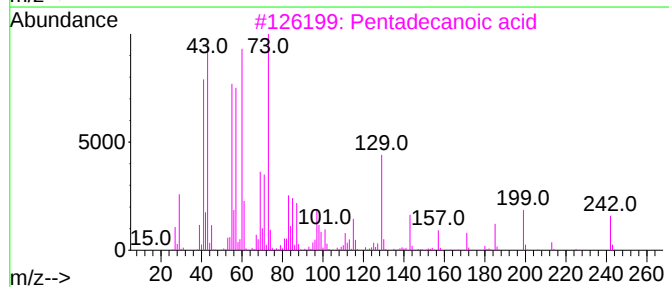
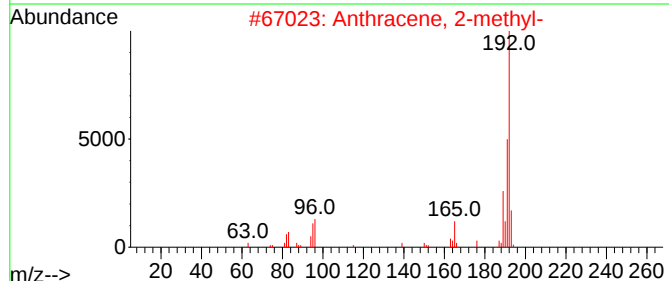
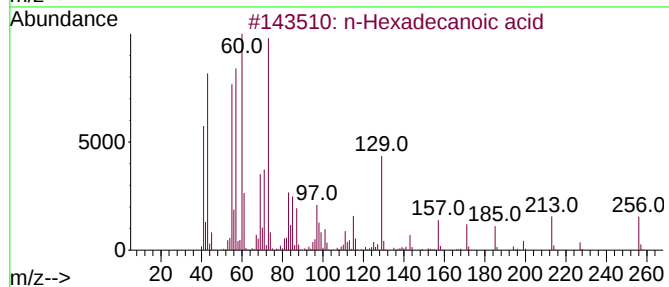
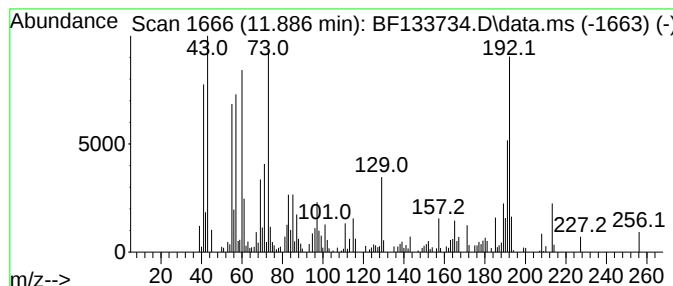
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.886	5.09 ng	152991	Phenanthrene-d10	11.357

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	89
2			Anthracene, 2-methyl-	192	C15H12	000613-12-7	83
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	50
4			Anthracene, 1-methyl-	192	C15H12	000610-48-0	48
5			Tridecanoic acid	214	C13H26O2	000638-53-9	46



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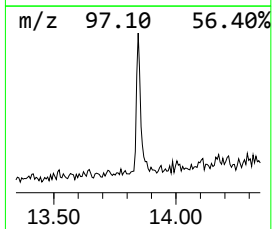
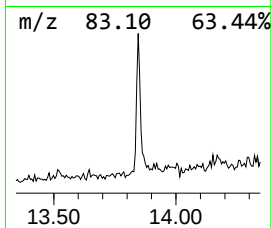
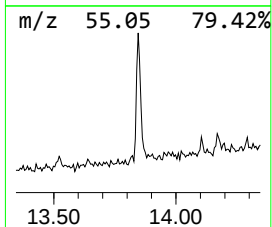
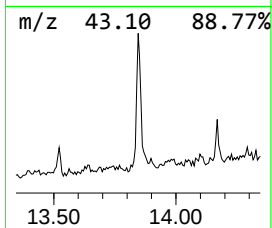
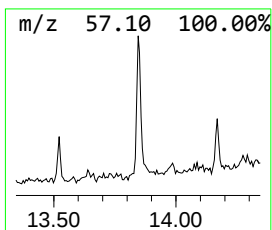
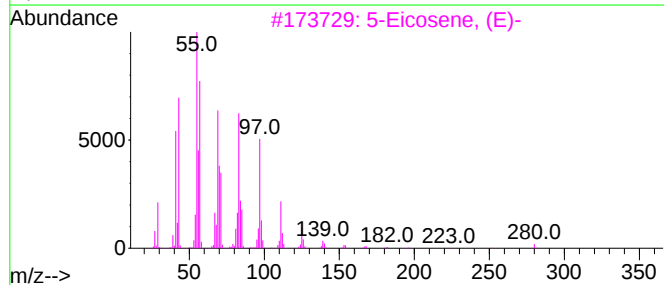
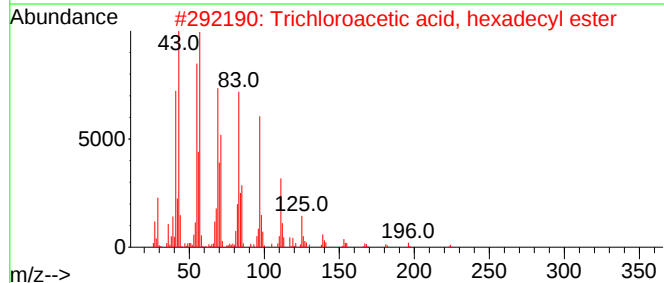
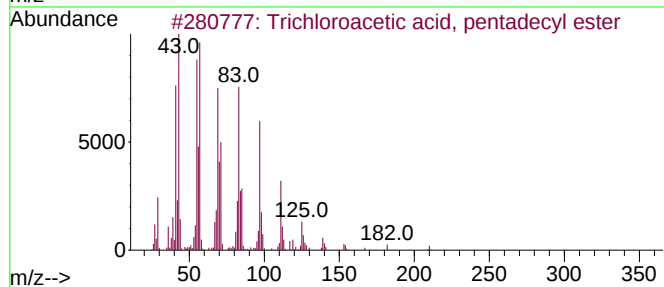
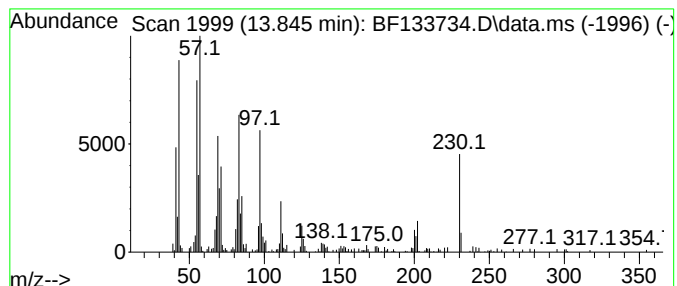
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Trichloroacetic acid, penta... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.845	5.05 ng	195450	Chrysene-d12	14.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	93
2			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	93
3			5-Eicosene, (E)-	280	C20H40	074685-30-6	93
4			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	93
5			1-Nonadecene	266	C19H38	018435-45-5	89



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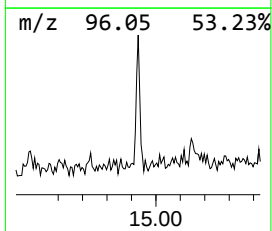
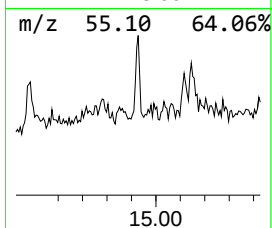
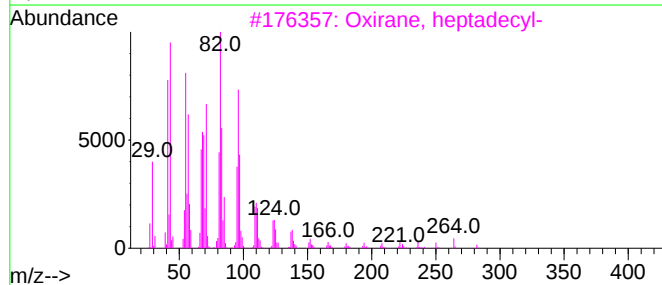
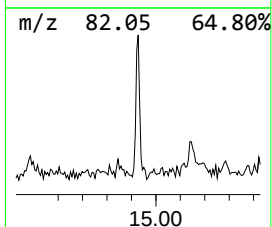
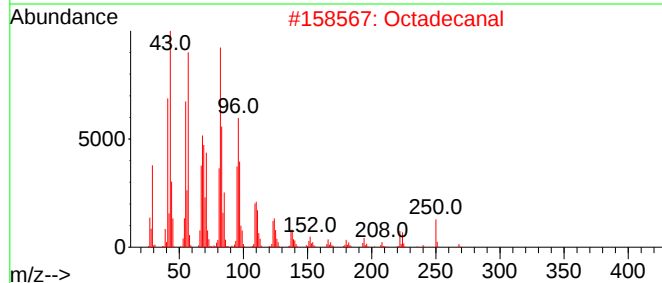
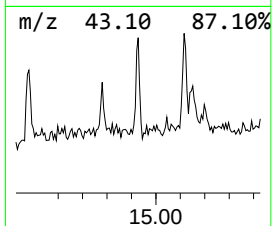
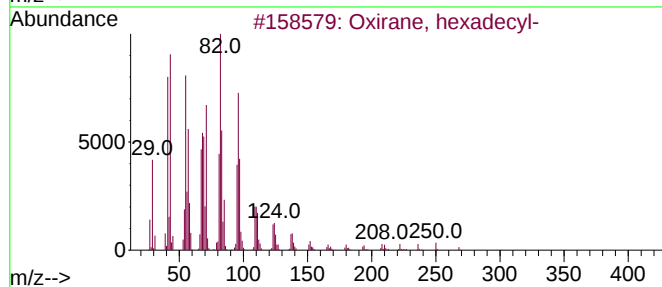
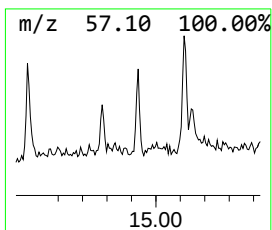
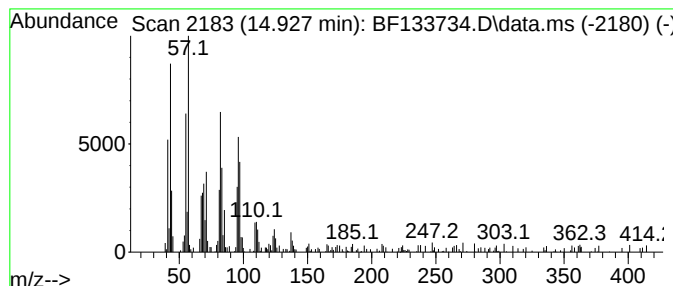
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Oxirane, hexadecyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.927	3.10 ng	74626	Perylene-d12	15.469

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxirane, hexadecyl-	268	C18H36O	007390-81-0	94
2			Octadecanal	268	C18H36O	000638-66-4	83
3			Oxirane, heptadecyl-	282	C19H38O	067860-04-2	81
4			1,19-Eicosadiene	278	C20H38	014811-95-1	76
5			1,16-Hexadecanediol	258	C16H34O2	007735-42-4	76



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Misc :
ALS Vial : 15 Sample Multiplier: 1

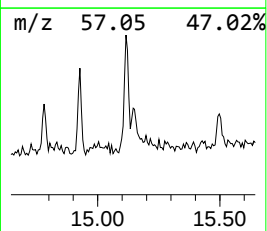
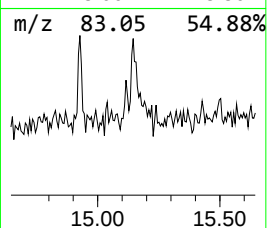
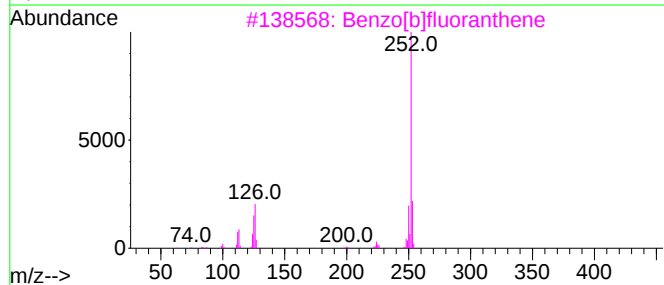
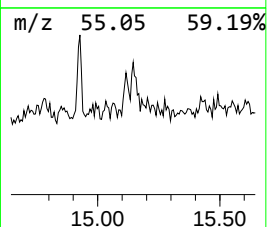
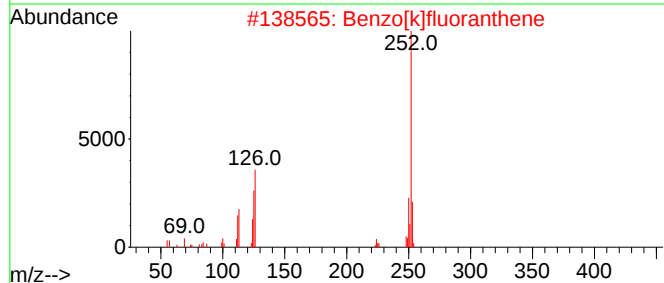
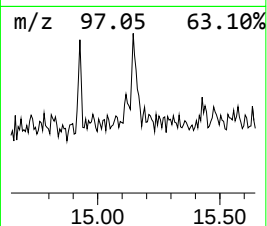
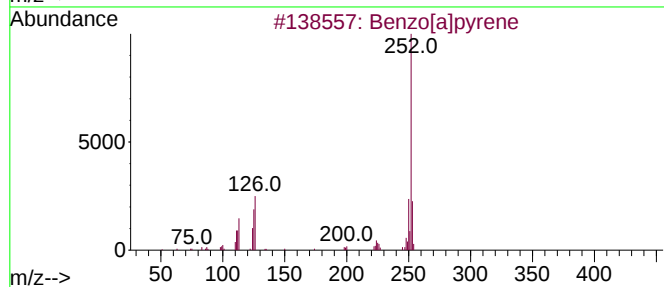
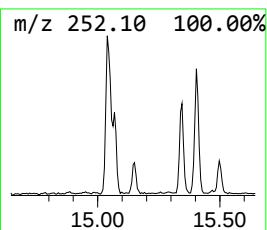
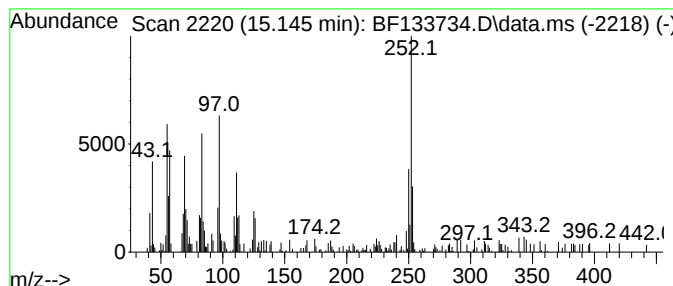
Instrument :
BNA_F
ClientSampleId :
SB35A

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 5 unknown15.145 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.145	2.28 ng	54855	Perylene-d12	15.469	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[a]pyrene	252	C20H12	000050-32-8	50
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	45
3	Benzo[b]fluoranthene	252	C20H12	000205-99-2	45
4	Benzo[e]pyrene	252	C20H12	000192-97-2	43
5	1-Phenyl-3-(4-methoxyphenyl)-2-p...	252	C16H16N2O	003314-43-0	41



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061323\
Data File : BF133734.D
Acq On : 13 Jun 2023 16:52
Operator : CG\JU
Sample : 03069-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB35A

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
Benzophenone	10.581	3.2	ng	89972	3	9.869	555141	20.0
n-Hexadecanoic ...	11.886	5.1	ng	152991	4	11.357	600919	20.0
Trichloroacetic...	13.845	5.0	ng	195450	5	14.004	773992	20.0
Oxirane, hexade...	14.927	3.1	ng	74626	6	15.469	481112	20.0
unknown15.145	15.145	2.3	ng	54855	6	15.469	481112	20.0