

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050223\
 Data File : BF133195.D
 Acq On : 02 May 2023 18:22
 Operator : CG\JU
 Sample : 02572-03
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RT2343

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-BF042123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133195.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.928	479	483	489	rVB	61582	77321	1.78%	0.199%
2	5.340	549	553	557	rBV	4041037	4086691	94.24%	10.498%
3	6.369	723	728	731	rBV	4052777	4174535	96.26%	10.724%
4	6.728	786	789	793	rVB	1642146	1247200	28.76%	3.204%
5	7.292	880	885	888	rBV	2957788	2679635	61.79%	6.884%
6	8.016	1004	1008	1011	rBV	2031920	1690675	38.99%	4.343%
7	9.092	1186	1191	1194	rBV	5019516	4336631	100.00%	11.140%
8	9.763	1302	1305	1309	rBV	2130113	1772786	40.88%	4.554%
9	9.798	1309	1311	1314	rVB	72270	57920	1.34%	0.149%
10	10.310	1395	1398	1404	rBV	63663	57673	1.33%	0.148%
11	10.480	1423	1427	1430	rBV	978832	836963	19.30%	2.150%
12	10.551	1435	1439	1443	rBV	2636049	2558154	58.99%	6.572%
13	10.675	1457	1460	1465	rBV4	36282	49313	1.14%	0.127%
14	11.051	1521	1524	1529	rVB	62241	55729	1.29%	0.143%
15	11.245	1554	1557	1559	rBV	1952791	1616131	37.27%	4.152%
16	11.269	1559	1561	1565	rVV	767410	598504	13.80%	1.537%
17	11.322	1565	1570	1573	rVB	160554	148433	3.42%	0.381%
18	11.474	1590	1596	1599	rBV2	75944	83098	1.92%	0.213%
19	11.745	1639	1642	1645	rBV	92499	90984	2.10%	0.234%
20	11.786	1645	1649	1652	rVV2	470195	507233	11.70%	1.303%
21	11.816	1652	1654	1658	rVV2	64269	88611	2.04%	0.228%
22	11.857	1658	1661	1664	rVV	169398	186657	4.30%	0.480%
23	11.880	1664	1665	1668	rVB	85950	49628	1.14%	0.127%
24	12.045	1690	1693	1694	rBV	69782	59000	1.36%	0.152%
25	12.063	1694	1696	1703	rVB2	117728	104579	2.41%	0.269%
26	12.192	1713	1718	1721	rBV2	40030	47876	1.10%	0.123%
27	12.298	1733	1736	1739	rBV	79414	75833	1.75%	0.195%
28	12.380	1747	1750	1755	rVB2	100290	95619	2.20%	0.246%
29	12.457	1759	1763	1767	rBV	1334446	1074697	24.78%	2.761%
30	12.686	1796	1802	1805	rBV	1119725	1083650	24.99%	2.784%
31	12.804	1819	1822	1823	rBV	69063	53496	1.23%	0.137%
32	12.833	1823	1827	1830	rVV	3632593	3162126	72.92%	8.123%
33	12.904	1834	1839	1842	rBV2	82396	115863	2.67%	0.298%
34	12.986	1851	1853	1855	rBV2	65742	71568	1.65%	0.184%
35	13.016	1855	1858	1861	rVB	123395	126062	2.91%	0.324%
36	13.080	1865	1869	1871	rBV2	118839	105528	2.43%	0.271%

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37	13.116	1871	1875	1878	rBV	129311	126071	2.91%	0.324%
38	13.210	1888	1891	1894	rVB	74792	54225	1.25%	0.139%
39	13.239	1894	1896	1900	rBV2	57517	60836	1.40%	0.156%
40	13.515	1941	1943	1948	rVB	105213	103894	2.40%	0.267%
41	13.627	1958	1962	1965	rBV2	114870	160350	3.70%	0.412%
42	13.657	1965	1967	1969	rVV	63820	51579	1.19%	0.133%
43	13.680	1969	1971	1976	rVB2	61961	55920	1.29%	0.144%
44	13.721	1976	1978	1980	rBV	65618	54536	1.26%	0.140%
45	13.751	1980	1983	1984	rBV	85001	89776	2.07%	0.231%
46	13.880	2000	2005	2008	rBV2	1325228	1563552	36.05%	4.017%
47	13.904	2008	2009	2017	rVB	501699	396200	9.14%	1.018%
48	14.063	2034	2036	2039	rVB2	78761	67434	1.55%	0.173%
49	14.268	2069	2071	2073	rVB	83203	64915	1.50%	0.167%
50	14.304	2075	2077	2080	rVB2	82020	66757	1.54%	0.171%
51	14.362	2084	2087	2090	rBV2	86845	92059	2.12%	0.236%
52	14.392	2090	2092	2094	rBV2	54797	48613	1.12%	0.125%
53	14.733	2147	2150	2155	rBV3	105193	114854	2.65%	0.295%
54	14.898	2174	2178	2181	rBV	470831	679595	15.67%	1.746%
55	15.186	2223	2227	2232	rVB	254599	314911	7.26%	0.809%
56	15.239	2233	2236	2242	rBV	263898	317084	7.31%	0.815%
57	15.304	2243	2247	2250	rBV	970885	1050585	24.23%	2.699%
58	16.674	2476	2480	2487	rVB2	96792	166951	3.85%	0.429%

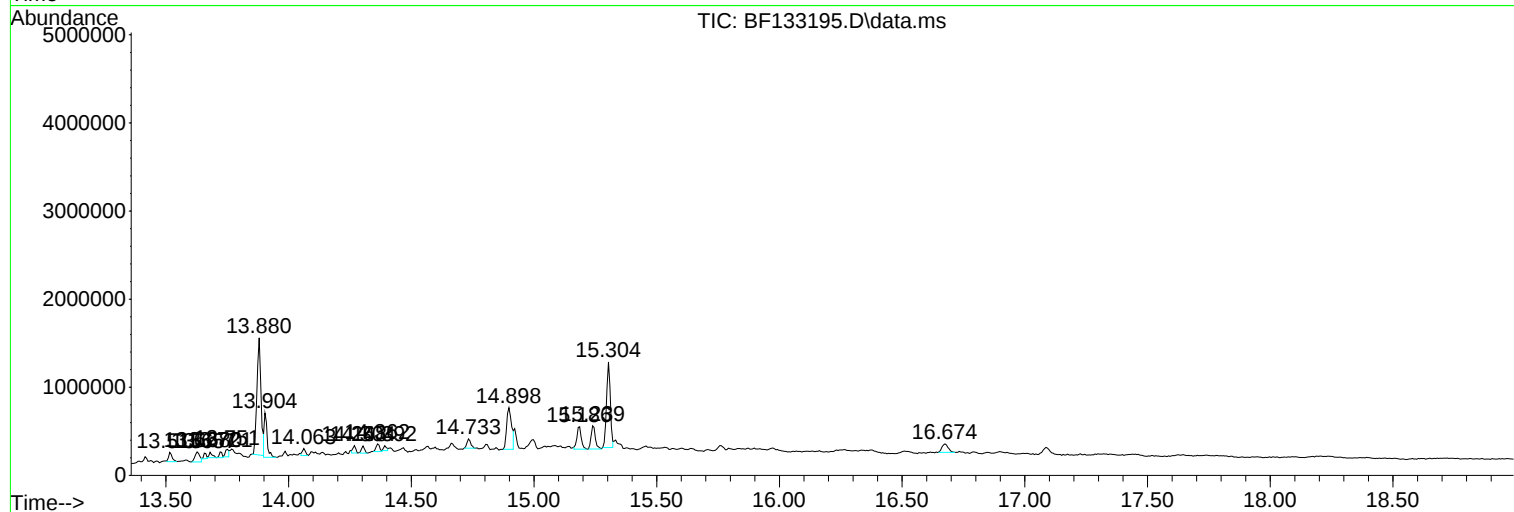
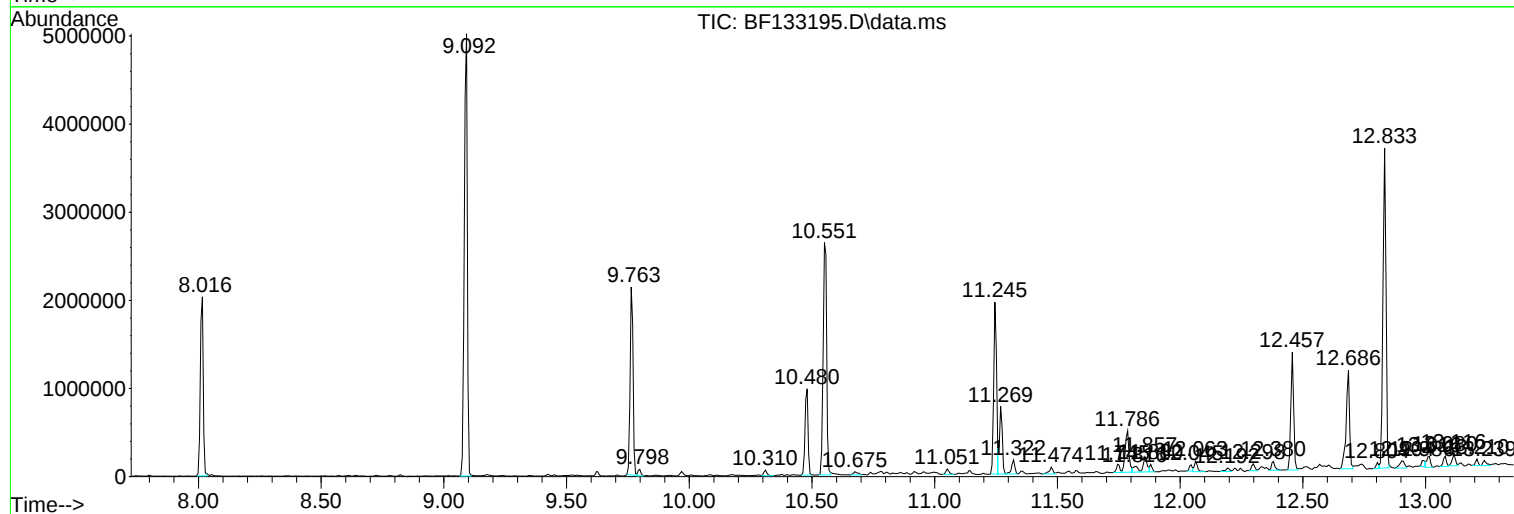
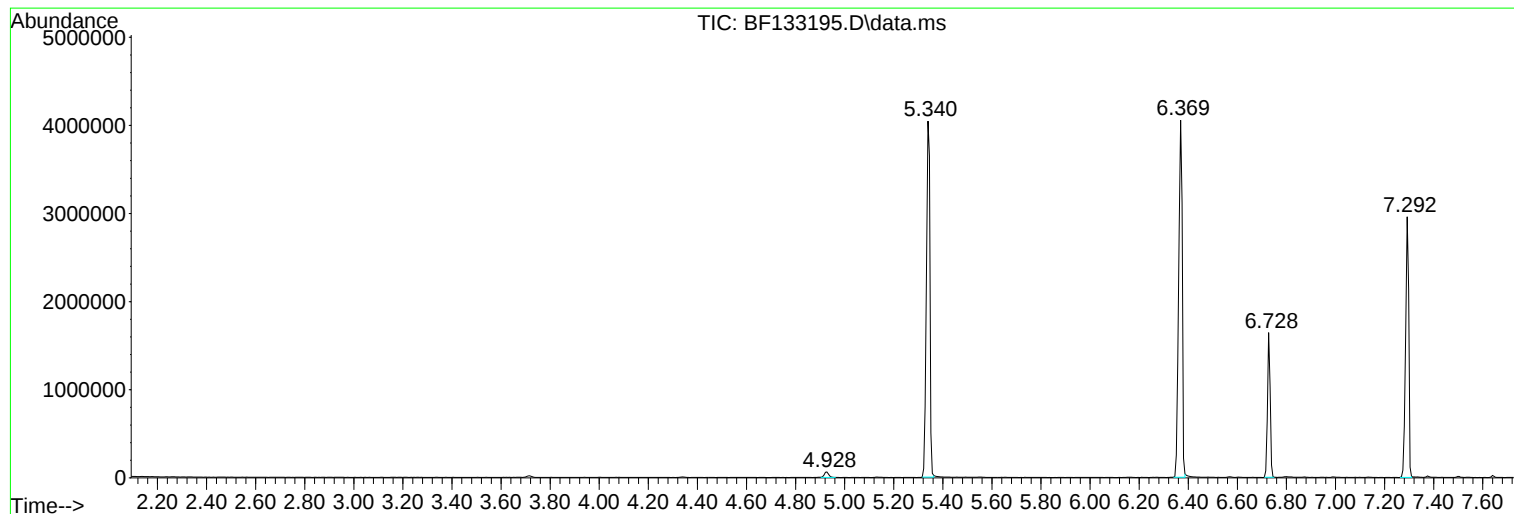
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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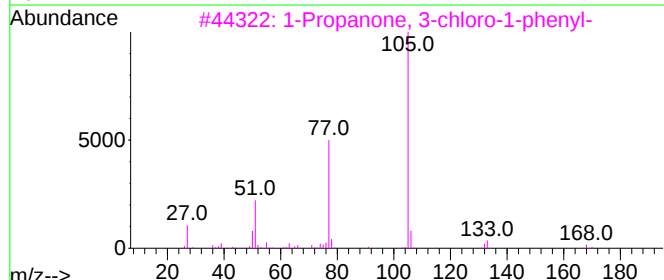
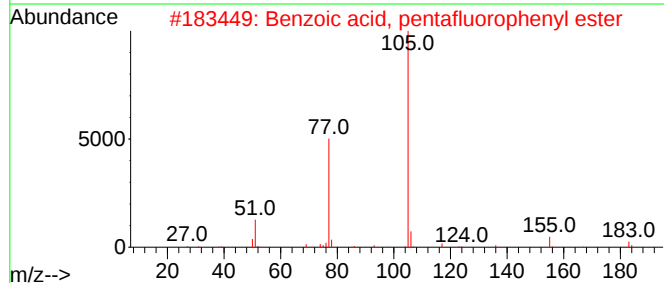
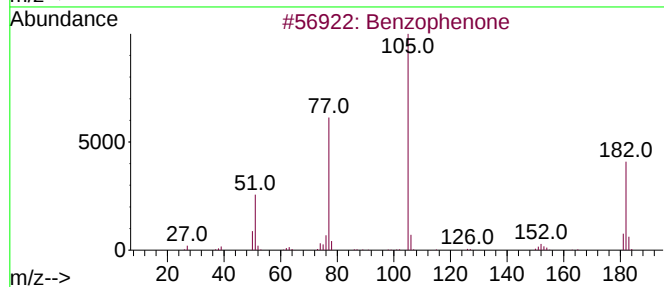
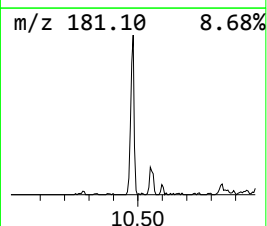
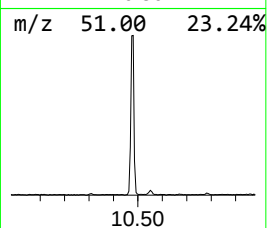
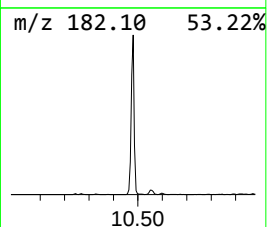
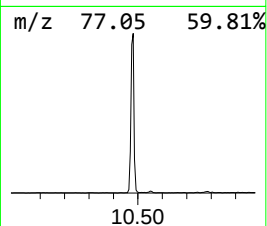
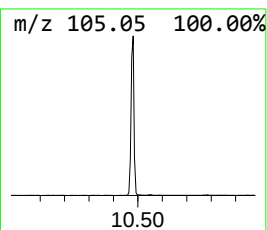
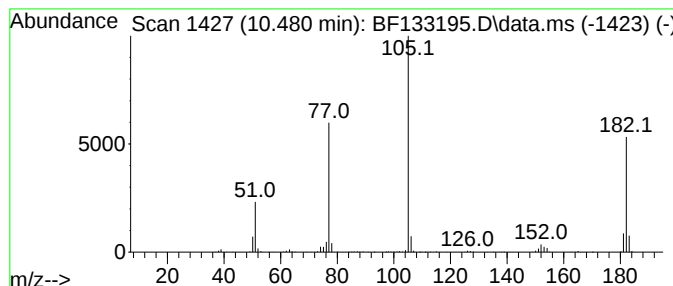
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Benzophenone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.480	9.44 ng	836963	Acenaphthene-d10	9.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Benzoic acid, pentafluorophenyl ...	288	C13H5F5O2	1000360-67-9	50
3			1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	47
4			Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47
5			N-Methylbenzamide, N-chlorodiflu...	247	C10H8ClF2NO2	1000446-98-2	47



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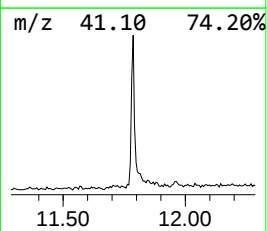
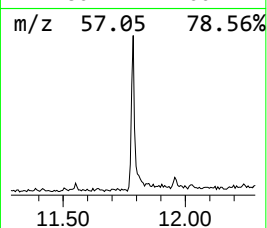
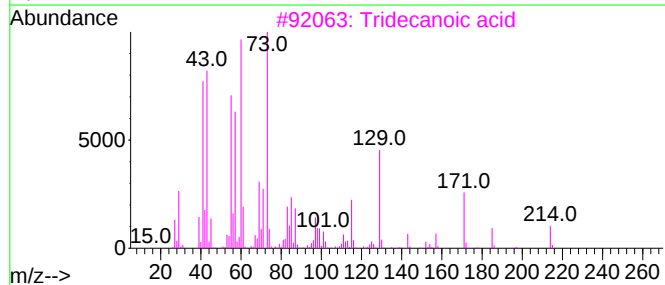
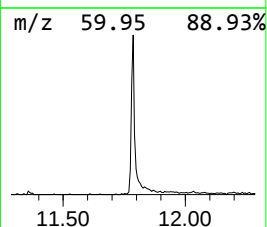
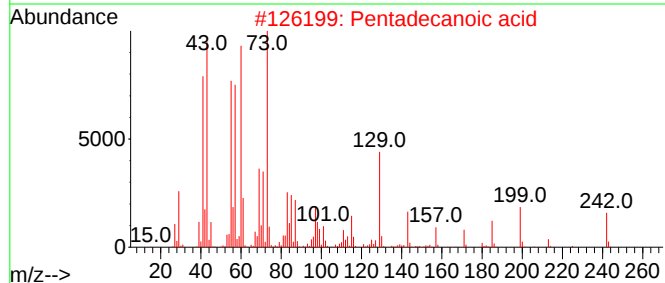
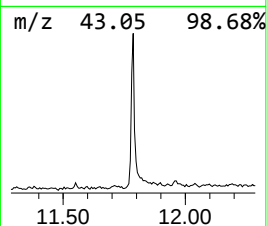
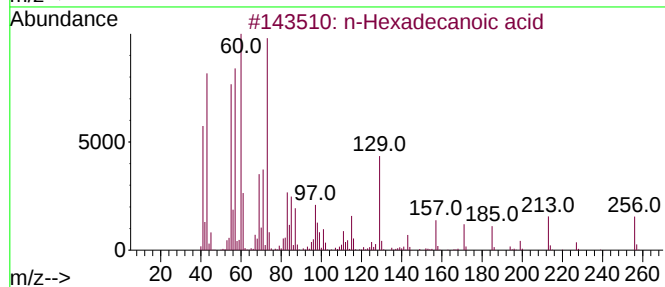
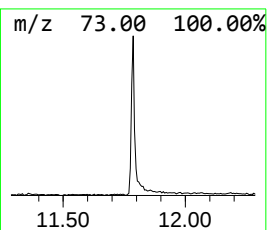
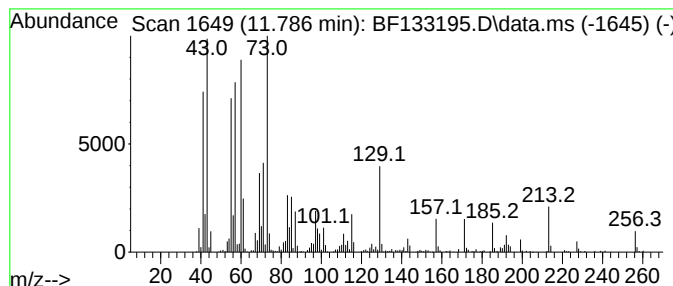
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.786	6.28 ng	507233	Phenanthrene-d10	11.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3			Tridecanoic acid	214	C13H26O2	000638-53-9	86
4			Undecanoic acid	186	C11H22O2	000112-37-8	81
5			n-Decanoic acid	172	C10H20O2	000334-48-5	70



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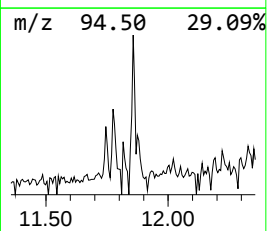
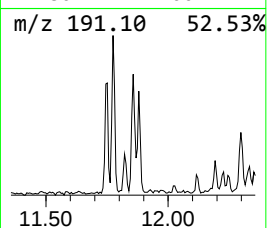
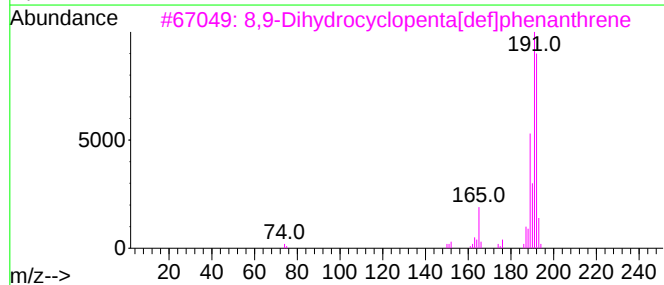
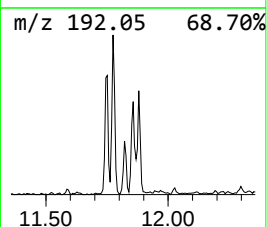
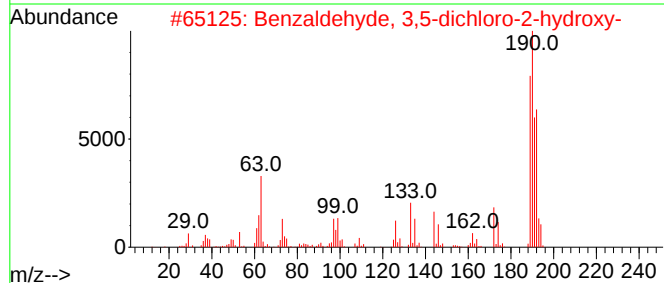
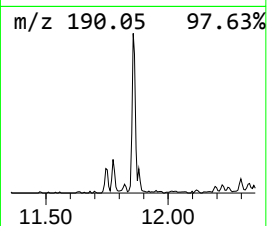
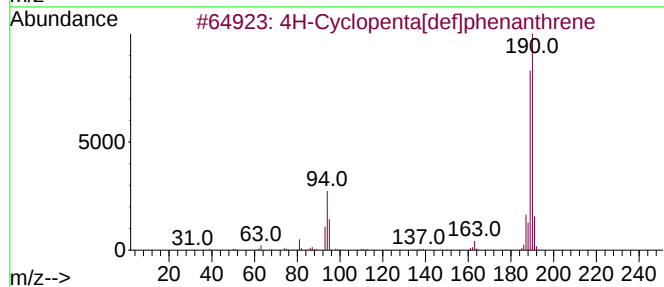
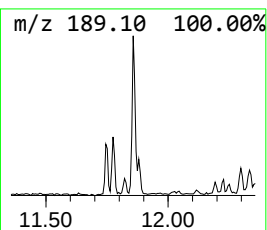
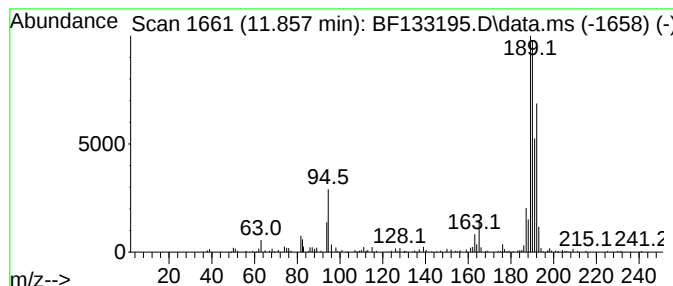
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 4H-Cyclopenta[def]phenanthrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.857	2.31 ng	186657	Phenanthrene-d10	11.245	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	64
2	Benzaldehyde, 3,5-dichloro-2-hyd...	190	C7H4Cl2O2	000090-60-8	64
3	8,9-Dihydrocyclopenta[def]phenan...	192	C15H12	027410-55-5	35
4	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	35
5	Benzene, 1,1'-(2-cyclopropen-1-y...	192	C15H12	022825-21-4	30



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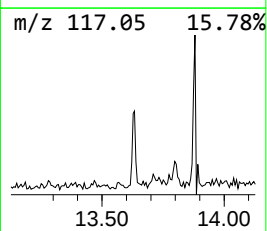
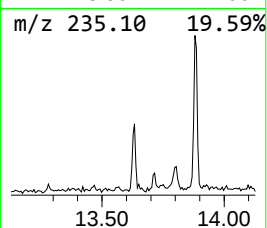
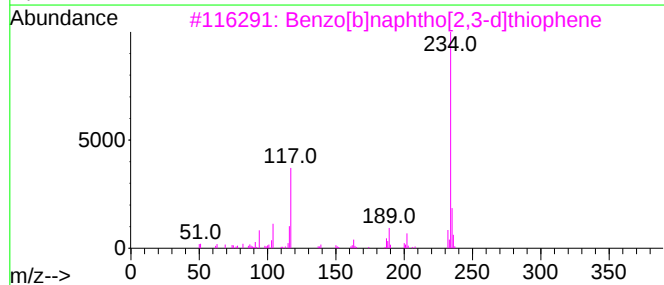
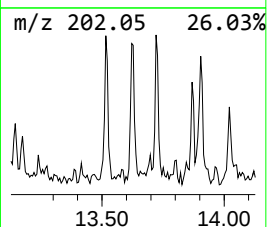
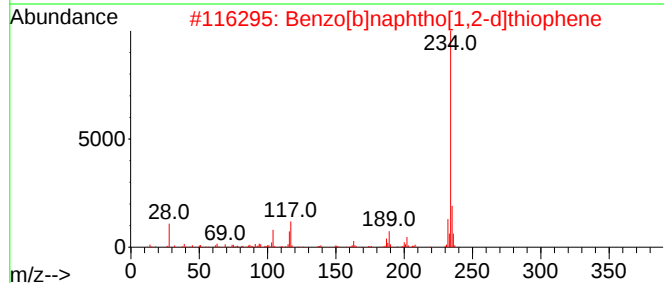
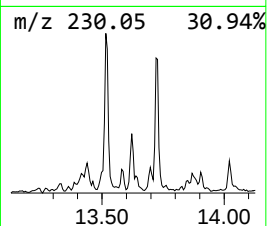
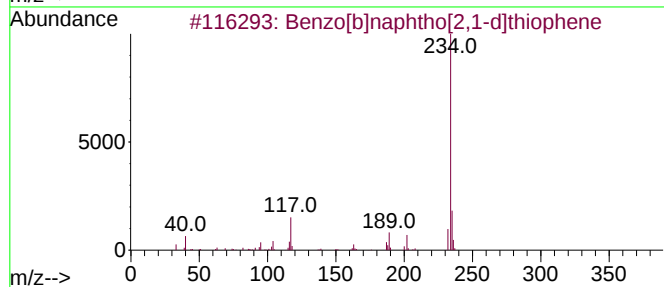
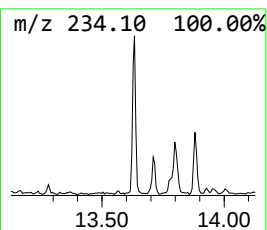
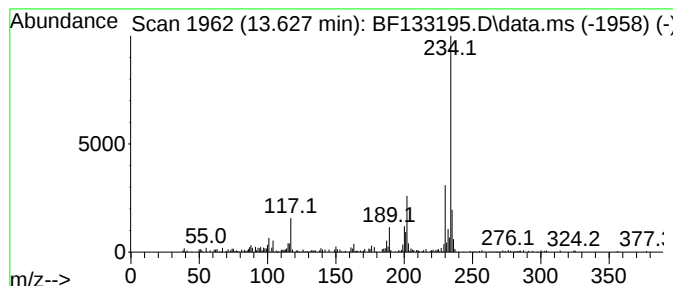
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Benzo[b]naphtho[2,1-d]thiop... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.627	2.05 ng	160350	Chrysene-d12	13.880

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[b]naphtho[2,1-d]thiophene	234	C16H10S	000239-35-0	86
2			Benzo[b]naphtho[1,2-d]thiophene	234	C16H10S	000205-43-6	64
3			Benzo[b]naphtho[2,3-d]thiophene	234	C16H10S	000243-46-9	62
4			3-(1H-benzimidazol-2-yl)-2H-inda...	234	C14H10N4	1097816-83-5	43
5			Thiazol-2-amine, 4-(1-adamantyl)-	234	C13H18N2S	019735-74-1	43



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ALS Vial : 18 Sample Multiplier: 1

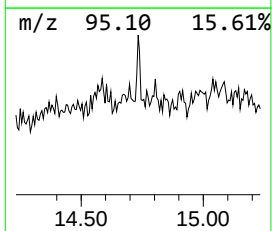
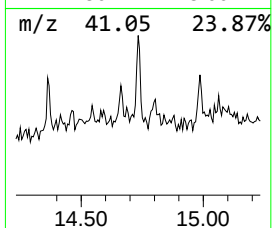
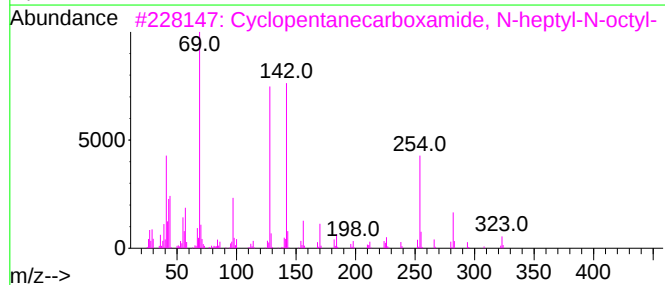
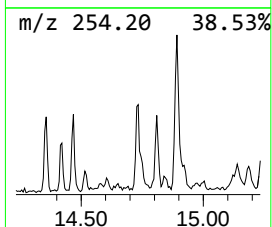
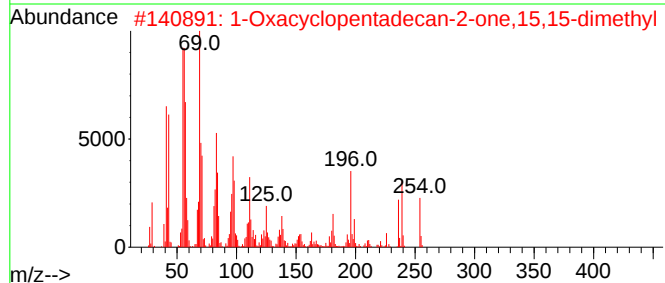
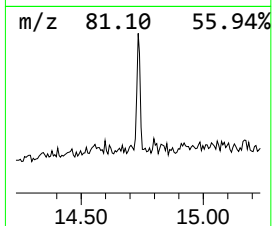
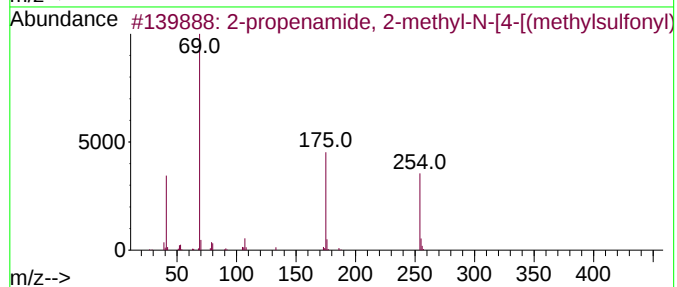
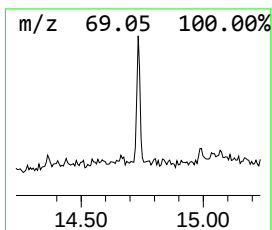
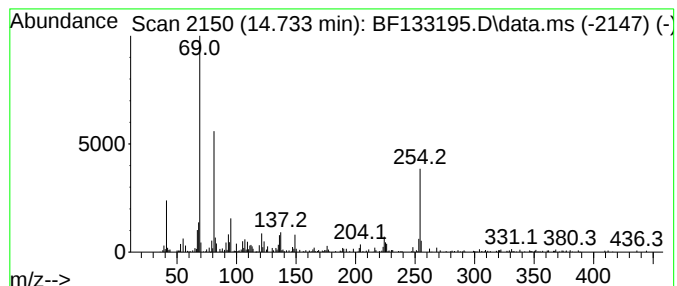
Instrument :
BNA_F
ClientSampleId :
RT2343

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 2-propenamide, 2-methyl-N-[... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.733	2.19 ng	114854	Perylene-d12	15.304	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-propenamide, 2-methyl-N-[4-[(m...	254	C11H14N2O3S	1000401-43-5	68
2	1-Oxacyclopentadecan-2-one,15,15...	254	C16H30O2	1000196-63-1	38
3	Cyclopentanecarboxamide, N-hepty...	323	C21H41NO	1000308-61-4	38
4	1,3-Hexanedione, 4,4,5,5,6,6-h...	322	C10H5F7O2S	000559-94-4	23
5	2-propenoic acid, 2-methyl-, 2-[...	255	C11H13NO4S	1000401-47-0	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050223\
Data File : BF133195.D
Acq On : 02 May 2023 18:22
Operator : CG\JU
Sample : 02572-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RT2343

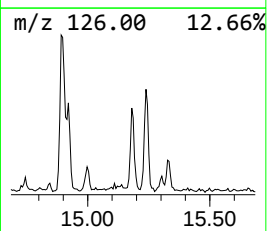
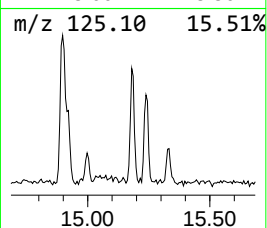
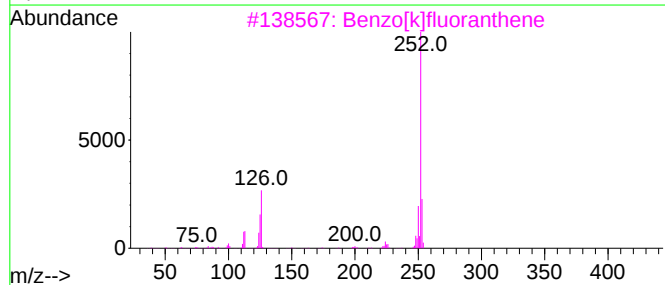
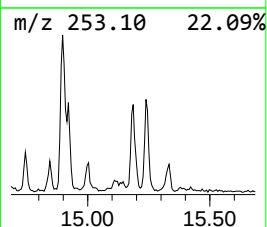
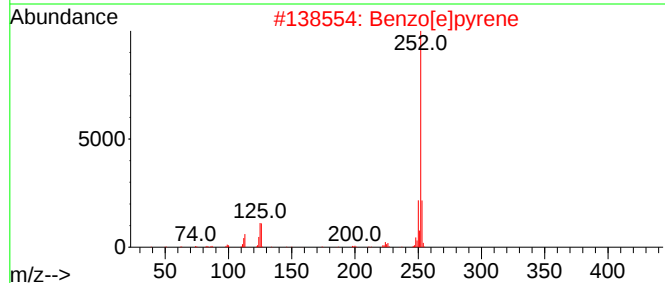
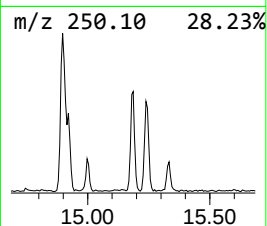
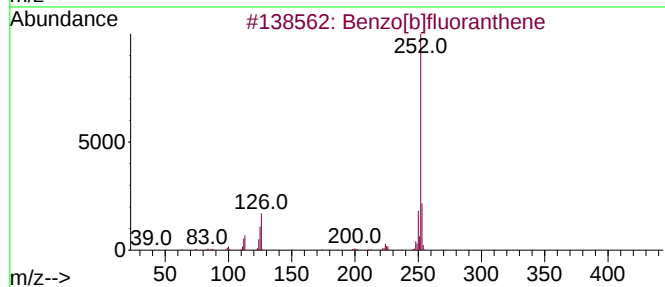
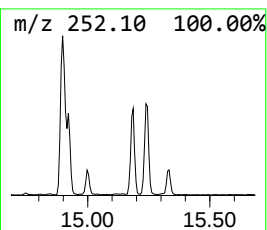
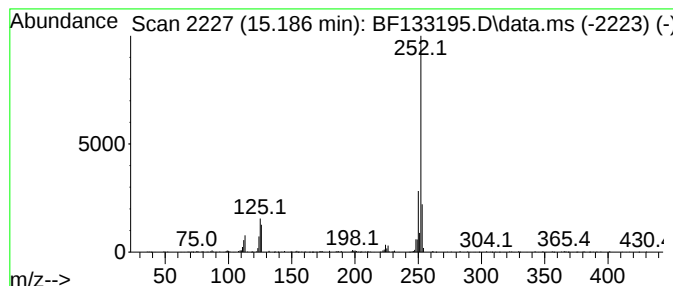
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Benzo[e]pyrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.186	5.99 ng	314911	Perylene-d12	15.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[b]fluoranthene	252	C20H12	000205-99-2	96
2			Benzo[e]pyrene	252	C20H12	000192-97-2	94
3			Benzo[k]fluoranthene	252	C20H12	000207-08-9	93
4			Perylene	252	C20H12	000198-55-0	93
5			Benzo[a]pyrene	252	C20H12	000050-32-8	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050223\
Data File : BF133195.D
Acq On : 02 May 2023 18:22
Operator : CG\JU
Sample : 02572-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RT2343

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Benzophenone	10.480	9.4	ng	836963	3	9.763	1772790	20.0
n-Hexadecanoic ...	11.786	6.3	ng	507233	4	11.245	1616130	20.0
4H-Cyclopenta[d...]	11.857	2.3	ng	186657	4	11.245	1616130	20.0
Benzo[b]naphtho...	13.627	2.0	ng	160350	5	13.880	1563550	20.0
2-propenamide, ...	14.733	2.2	ng	114854	6	15.304	1050590	20.0
Benzo[e]pyrene	15.186	6.0	ng	314911	6	15.304	1050590	20.0