

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060223\
 Data File : BF133559.D
 Acq On : 02 Jun 2023 13:24
 Operator : CG\JU
 Sample : 02985-02
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PLYMOUTH-XRDS-001

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-BF052523.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133559.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.216	17	22	28	rBV	55133	73613	1.87%	0.270%
2	5.051	498	504	512	rVB	110866	151249	3.83%	0.554%
3	5.445	565	571	574	rBV	3370214	3518666	89.19%	12.882%
4	6.457	737	743	746	rBV	3238547	3598471	91.21%	13.175%
5	6.828	803	806	810	rBV	948971	770609	19.53%	2.821%
6	7.398	897	903	905	rBV	2395922	2323668	58.90%	8.507%
7	8.110	1021	1024	1027	rBV	1137285	1014551	25.72%	3.714%
8	9.192	1204	1208	1211	rBV	4636302	3945206	100.00%	14.444%
9	9.869	1319	1323	1326	rVB	1368262	1057872	26.81%	3.873%
10	10.586	1441	1445	1448	rBV	231180	198270	5.03%	0.726%
11	10.657	1453	1457	1460	rBV	2618209	2466739	62.52%	9.031%
12	11.357	1572	1576	1578	rBV	1259579	1101277	27.91%	4.032%
13	11.380	1578	1580	1583	rVV	281534	223614	5.67%	0.819%
14	11.427	1586	1588	1591	rVB	67875	53280	1.35%	0.195%
15	11.886	1663	1666	1670	rBV	208763	186678	4.73%	0.683%
16	11.969	1676	1680	1682	rBV2	60994	68793	1.74%	0.252%
17	12.568	1778	1782	1785	rBV	378725	313917	7.96%	1.149%
18	12.798	1814	1821	1823	rBV	297411	317080	8.04%	1.161%
19	12.951	1842	1847	1850	rBV	3302035	3383875	85.77%	12.389%
20	13.127	1874	1877	1880	rVB	44815	46241	1.17%	0.169%
21	13.192	1883	1888	1890	rBV3	35890	49685	1.26%	0.182%
22	13.915	2004	2011	2016	rBV9	40075	124599	3.16%	0.456%
23	13.998	2020	2025	2027	rVV2	841371	931558	23.61%	3.411%
24	14.021	2027	2029	2034	rVB	151253	131029	3.32%	0.480%
25	14.474	2104	2106	2109	rBV2	52937	46230	1.17%	0.169%
26	15.027	2196	2200	2204	rBV	123851	197490	5.01%	0.723%
27	15.327	2248	2251	2257	rVB	84669	100772	2.55%	0.369%
28	15.392	2258	2262	2267	rBV	95258	113598	2.88%	0.416%
29	15.457	2268	2273	2277	rBV	613310	734028	18.61%	2.687%
30	16.892	2514	2517	2523	rVB3	39042	70878	1.80%	0.259%

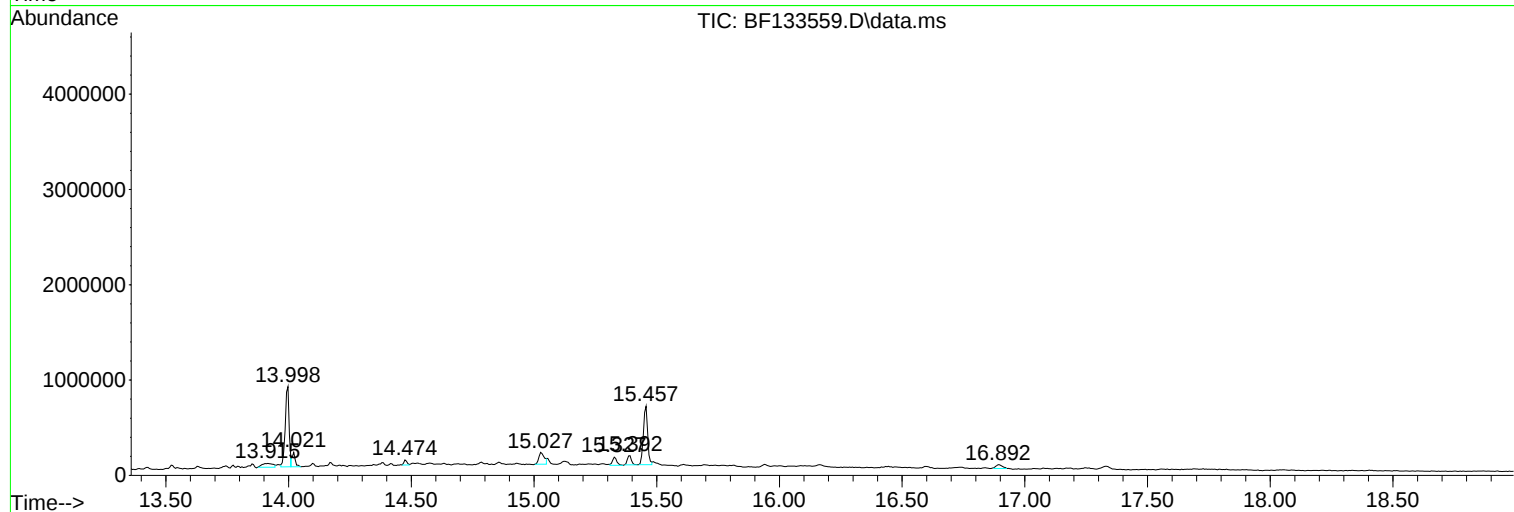
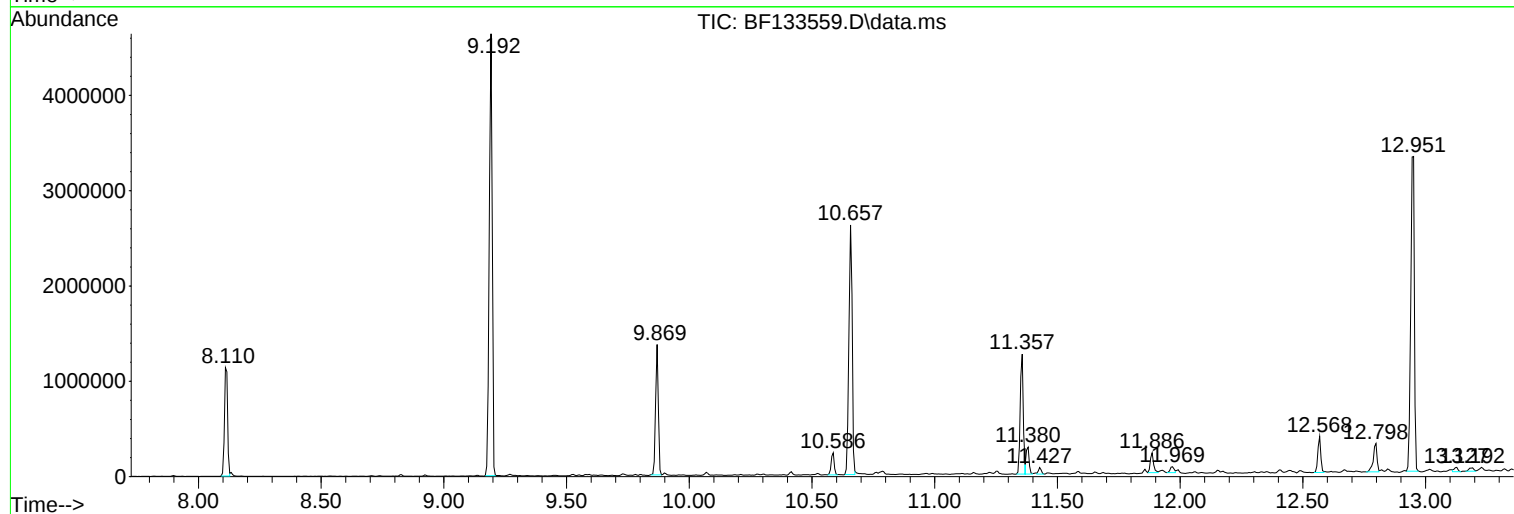
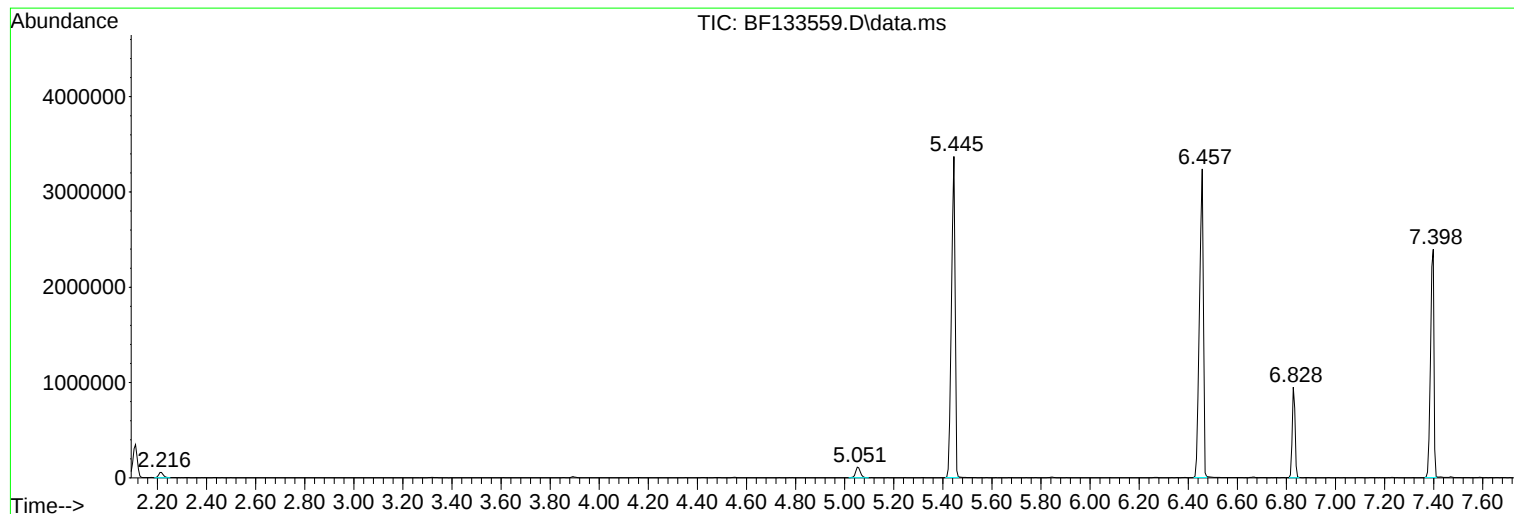
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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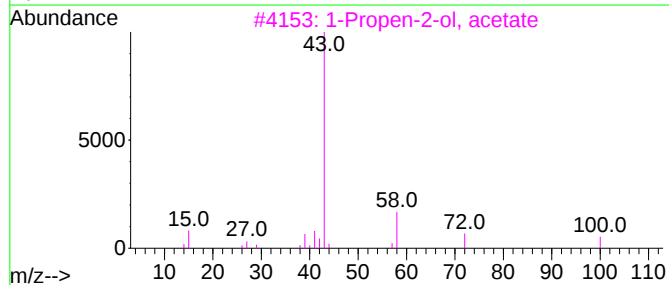
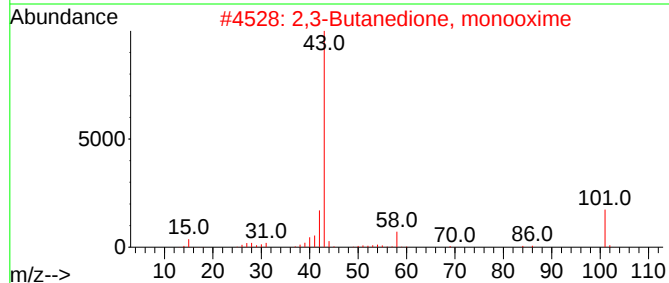
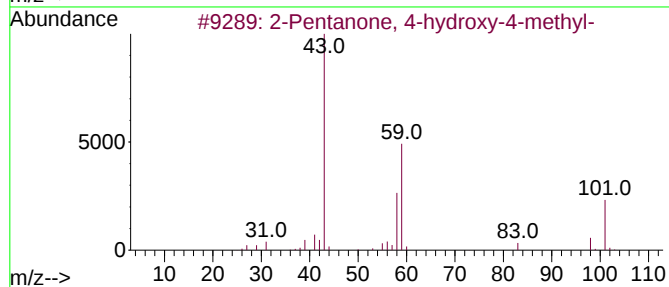
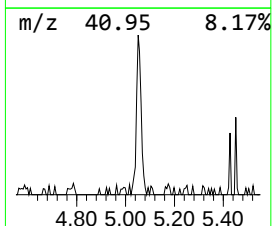
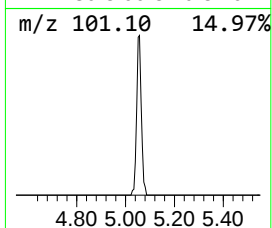
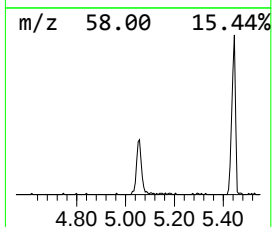
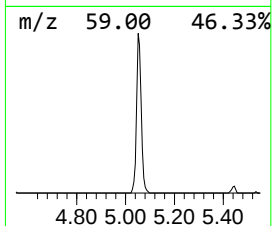
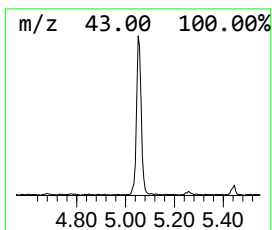
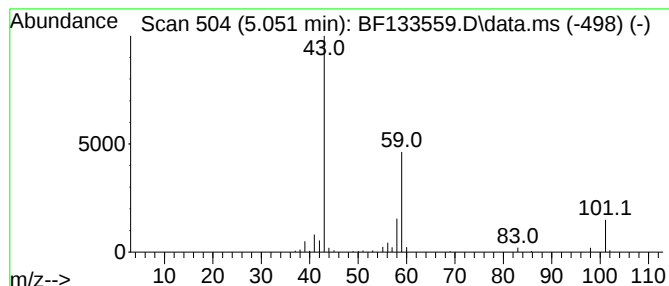
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.051	3.93 ng	151249	1,4-Dichlorobenzene-d4	6.828

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16		
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
4	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9		
5	2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9		



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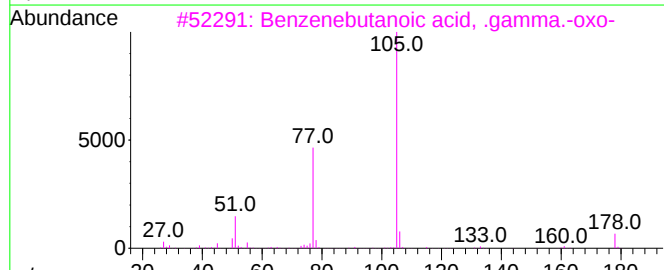
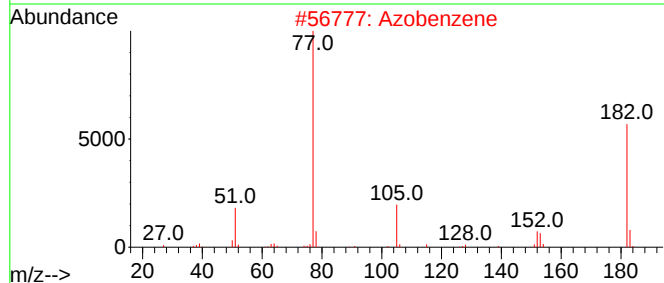
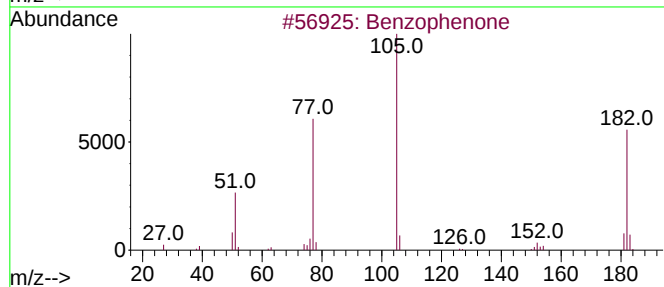
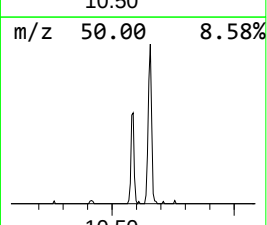
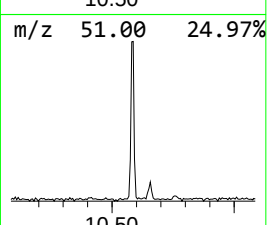
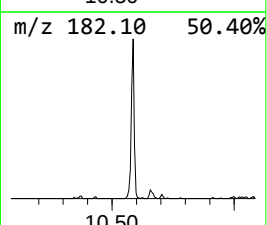
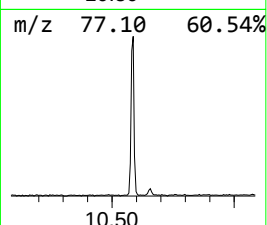
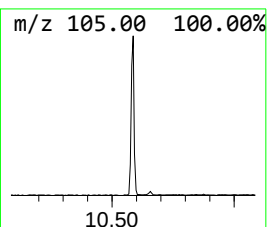
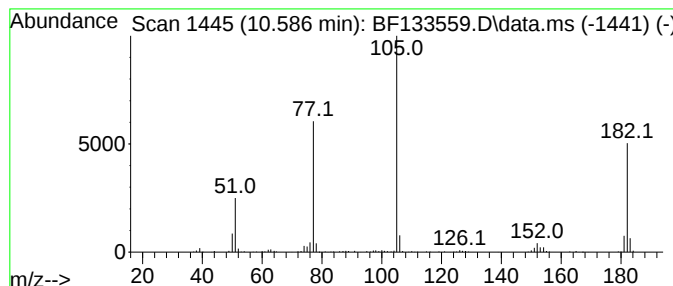
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.586	3.75 ng	198270	Acenaphthene-d10	9.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Azobenzene	182	C12H10N2	000103-33-3	64
3			Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47
4			2-Benzoyl-4-bromo-5-methyl-1,2-o...	281	C11H8BrNO3	1000444-92-3	47
5			Vinyl benzoate	148	C9H8O2	000769-78-8	47



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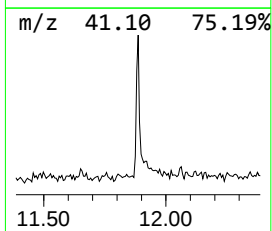
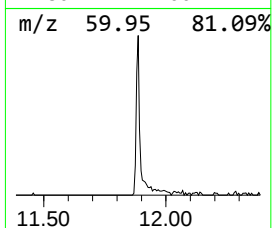
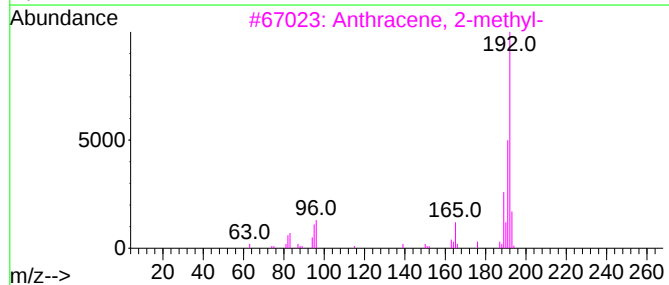
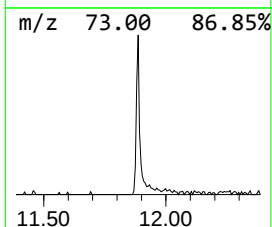
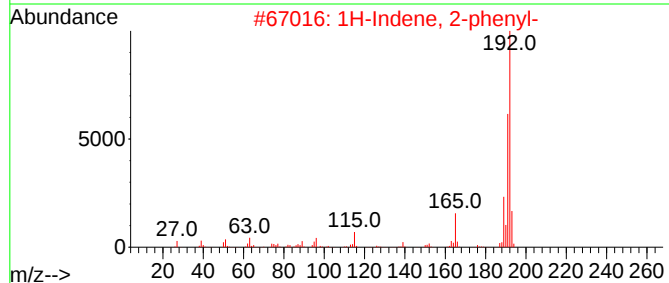
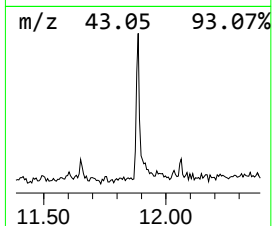
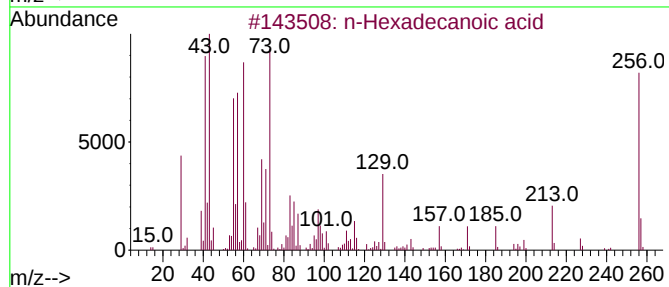
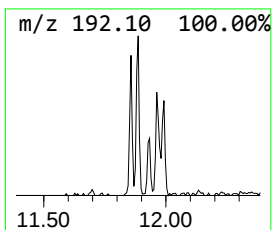
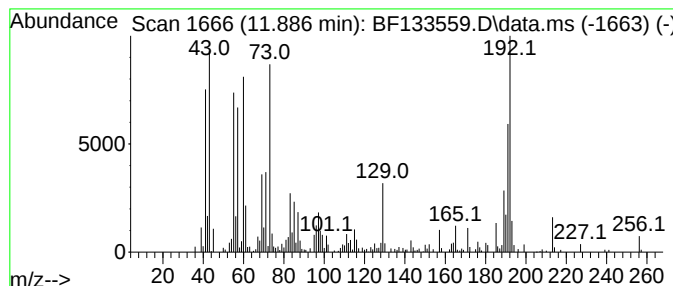
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.886	3.39 ng	186678	Phenanthrene-d10	11.357

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2			1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	80
3			Anthracene, 2-methyl-	192	C15H12	000613-12-7	60
4			Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	56
5			Anthracene, 1-methyl-	192	C15H12	000610-48-0	56



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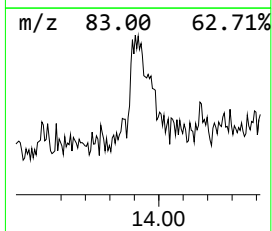
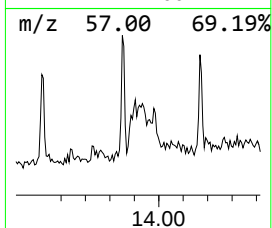
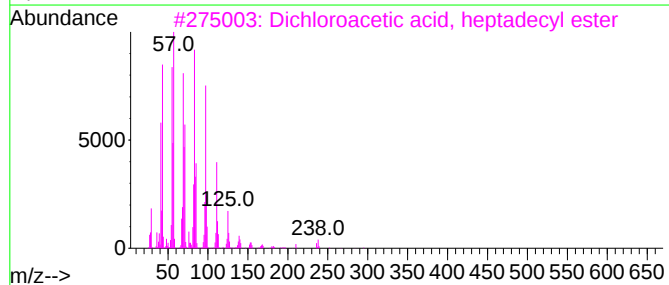
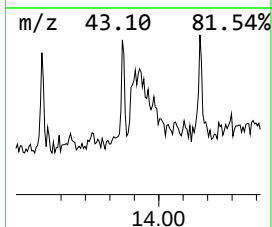
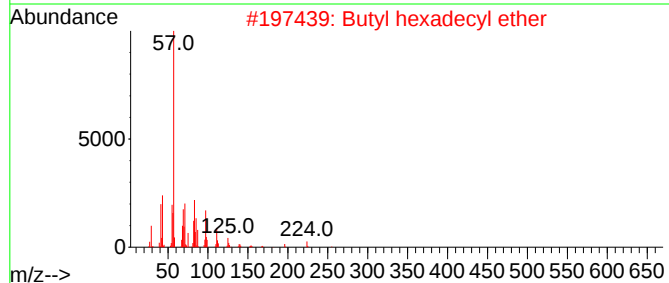
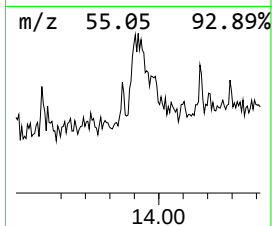
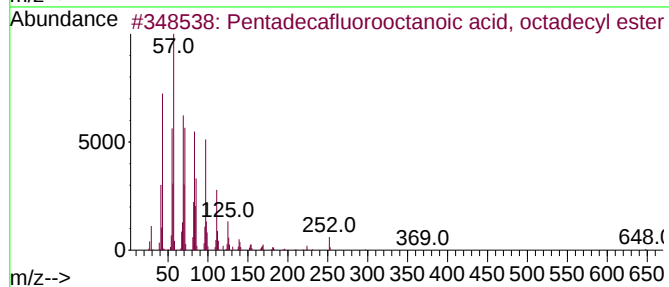
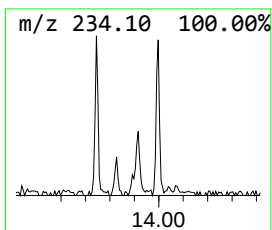
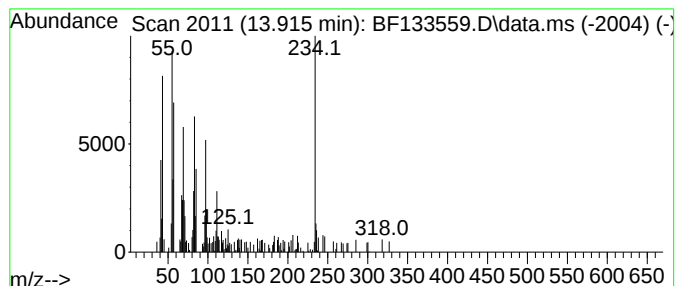
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Peak Number 4 unknown13.916 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.916	2.68 ng	124599	Chrysene-d12	13.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	49
2			Butyl hexadecyl ether	298	C20H42O	1010406-40-5	46
3			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	45
4			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	41
5			Benzo[b]1,4-dioxan-2-ol, 2-(2-th...	234	C12H10O3S	312614-85-0	41



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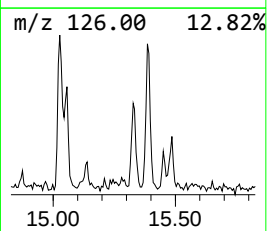
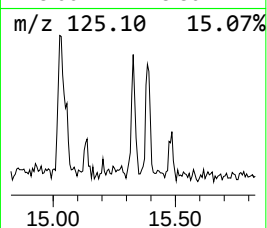
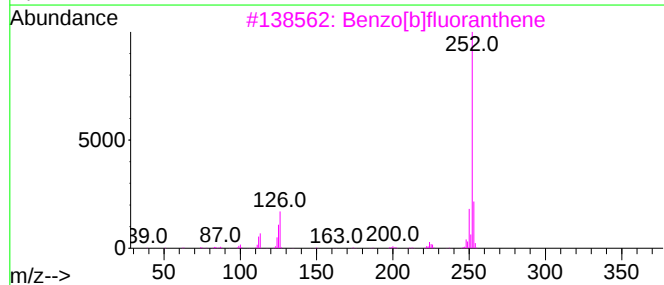
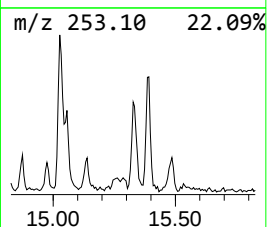
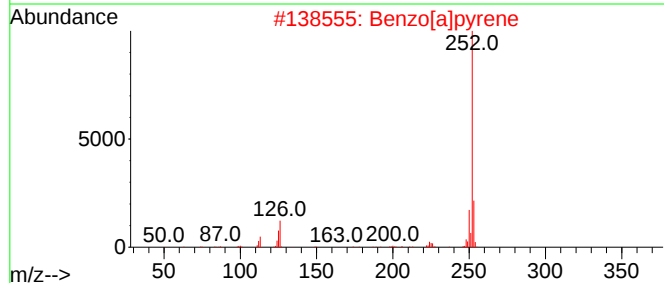
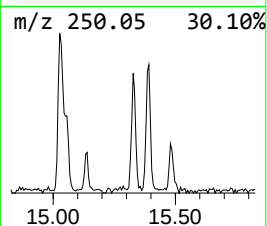
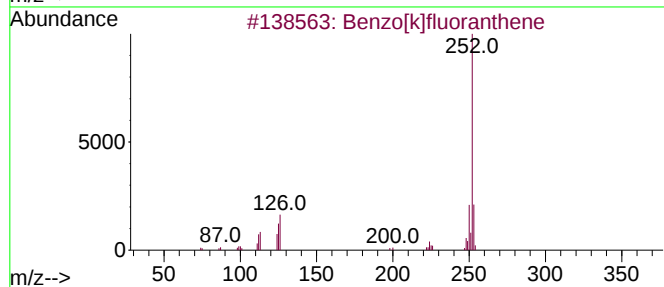
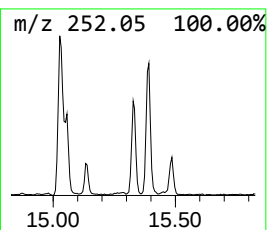
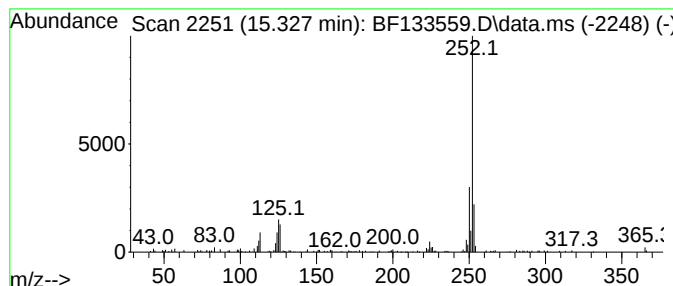
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Peak Number 5 Benzo[e]pyrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.327	2.75 ng	100772	Perylene-d12	15.457

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[k]fluoranthene	252	C20H12	000207-08-9	98
2			Benzo[a]pyrene	252	C20H12	000050-32-8	96
3			Benzo[b]fluoranthene	252	C20H12	000205-99-2	96
4			Benzo[e]pyrene	252	C20H12	000192-97-2	94
5			Benzo[j]fluoranthene	252	C20H12	000205-82-3	93



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PLYMOUTH-XRDS-001

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052523.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-...	5.051	3.9	ng	151249	1	6.828	770609	20.0
Benzophenone	10.586	3.8	ng	198270	3	9.869	1057870	20.0
n-Hexadecanoic ...	11.886	3.4	ng	186678	4	11.357	1101280	20.0
unknown13.916	13.916	2.7	ng	124599	5	13.998	931558	20.0
Benzo[e]pyrene	15.327	2.8	ng	100772	6	15.457	734028	20.0