

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072123\
 Data File : BF134406.D
 Acq On : 21 Jul 2023 17:53
 Operator : CG\JU
 Sample : 03640-11
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP8

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-BF062623.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134406.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.146	3	10	18	rVB	189896	270782	15.49%	1.838%
2	5.093	507	511	520	rBV	23517	33648	1.92%	0.228%
3	5.481	572	577	597	rBV	1612991	1542468	88.24%	10.469%
4	6.481	742	747	750	rBV	1607167	1489287	85.20%	10.108%
5	6.834	804	807	816	rBV	459328	400196	22.89%	2.716%
6	7.404	899	904	915	rBV	1051536	985457	56.38%	6.688%
7	8.116	1021	1025	1028	rBV	649771	501651	28.70%	3.405%
8	9.192	1204	1208	1211	rBV	2308239	1747988	100.00%	11.864%
9	9.875	1320	1324	1327	rBV	641467	549128	31.41%	3.727%
10	10.669	1455	1459	1462	rBV	1396832	1168031	66.82%	7.928%
11	11.369	1574	1578	1580	rBV	659418	557045	31.87%	3.781%
12	11.392	1580	1582	1586	rVB	263295	195587	11.19%	1.327%
13	11.869	1660	1663	1665	rBV3	38650	46946	2.69%	0.319%
14	11.898	1665	1668	1676	rVV2	253334	240083	13.73%	1.629%
15	11.986	1680	1683	1685	rBV2	32661	30847	1.76%	0.209%
16	12.204	1717	1720	1725	rVB	50315	45635	2.61%	0.310%
17	12.592	1782	1786	1789	rBV	495879	435793	24.93%	2.958%
18	12.686	1800	1802	1807	rBV3	37723	40813	2.33%	0.277%
19	12.822	1819	1825	1829	rBV	379216	370771	21.21%	2.516%
20	12.963	1841	1849	1853	rBV	1552906	1536171	87.88%	10.426%
21	13.039	1858	1862	1866	rVB5	16010	24755	1.42%	0.168%
22	13.127	1874	1877	1879	rBV2	18290	22303	1.28%	0.151%
23	13.151	1879	1881	1884	rVB	30720	27681	1.58%	0.188%
24	13.257	1895	1899	1901	rBV2	23056	27318	1.56%	0.185%
25	13.669	1966	1969	1973	rVB	36313	33645	1.92%	0.228%
26	13.774	1984	1987	1990	rBV	36604	39473	2.26%	0.268%
27	13.874	2001	2004	2007	rVB2	32470	36509	2.09%	0.248%
28	13.927	2007	2013	2015	rBV5	24809	49771	2.85%	0.338%
29	14.033	2023	2031	2033	rBV2	483305	575694	32.93%	3.907%
30	14.057	2033	2035	2043	rVB	194851	169728	9.71%	1.152%
31	14.133	2043	2048	2052	rBV3	21036	25557	1.46%	0.173%
32	14.186	2052	2057	2062	rBV7	27510	48465	2.77%	0.329%
33	14.421	2092	2097	2100	rVB	22994	25687	1.47%	0.174%
34	15.092	2207	2211	2215	rBV	174594	270294	15.46%	1.835%
35	15.404	2260	2264	2271	rVB	104285	137144	7.85%	0.931%
36	15.468	2271	2275	2281	rVB	112983	151727	8.68%	1.030%

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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-BF062623.M
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37	15.539	2282	2287	2292	rBV	321858	429418	24.57%	2.915%
38	16.010	2363	2367	2372	rBV4	20837	31780	1.82%	0.216%
39	16.527	2447	2455	2468	rBV4	37815	171781	9.83%	1.166%
40	17.080	2544	2549	2558	rVB2	53032	109607	6.27%	0.744%
41	17.551	2624	2629	2640	rVB2	47371	112790	6.45%	0.766%
42	17.809	2669	2673	2677	rBV6	12869	24346	1.39%	0.165%

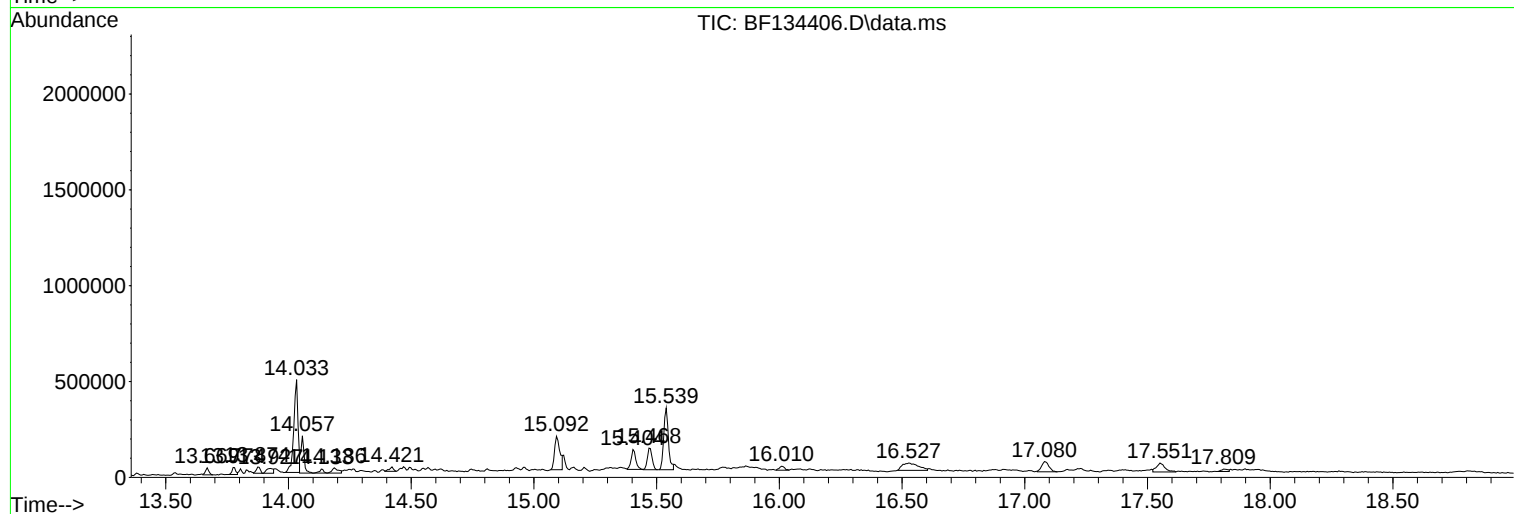
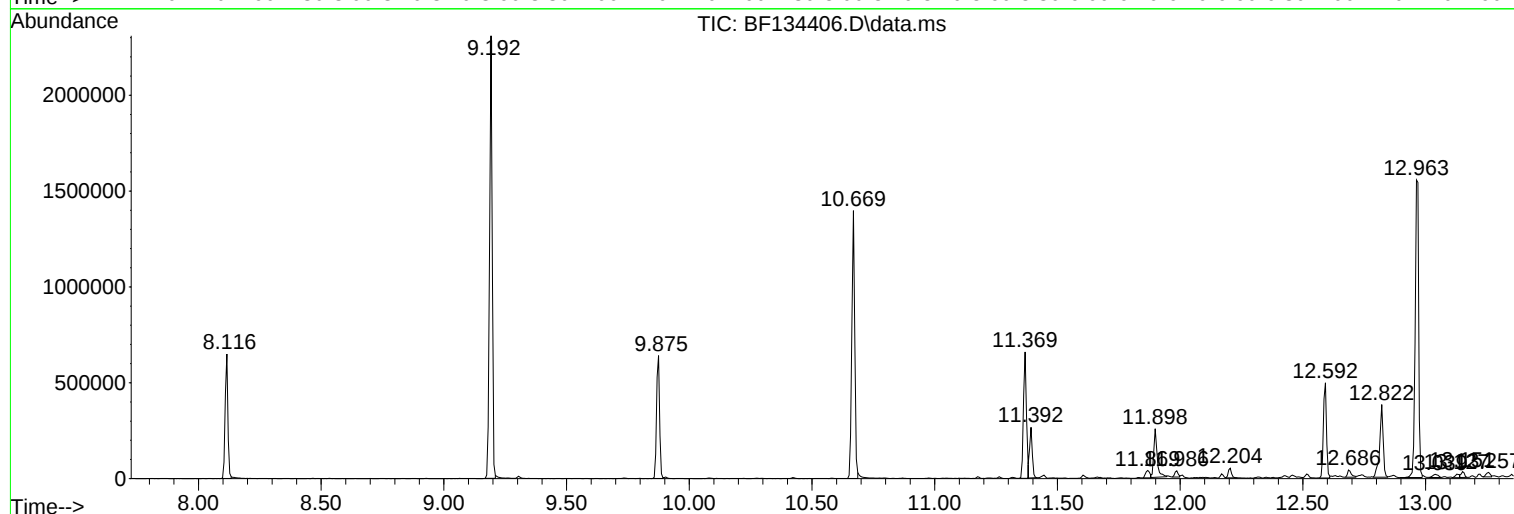
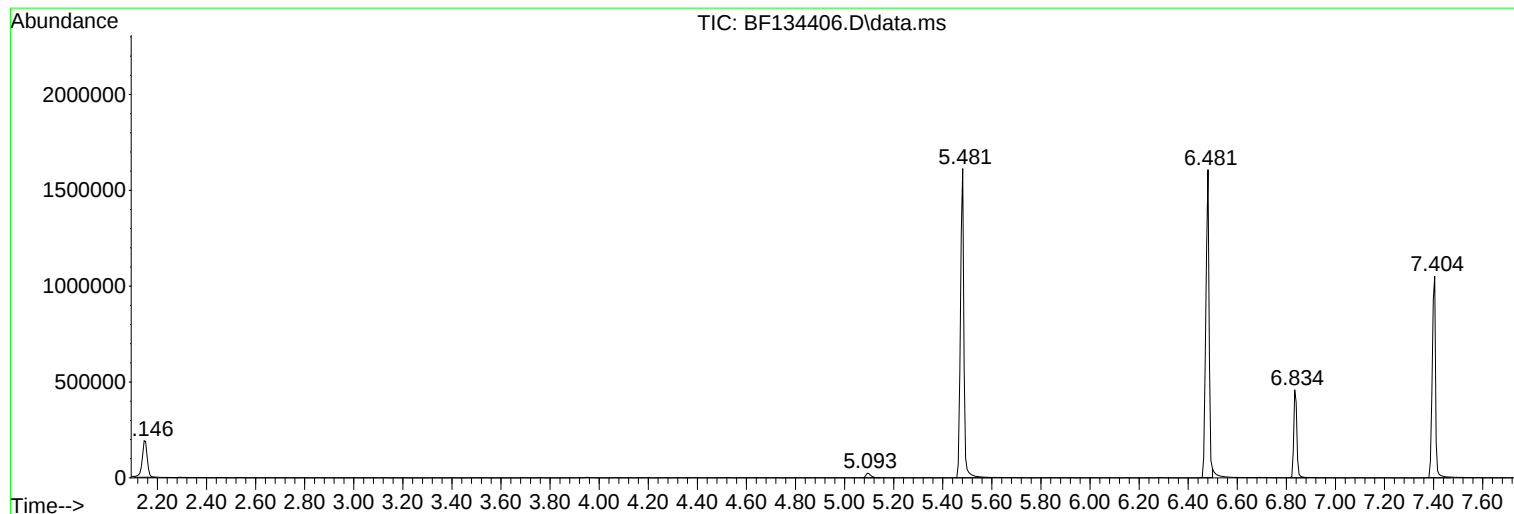
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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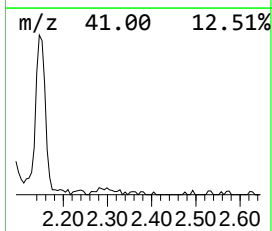
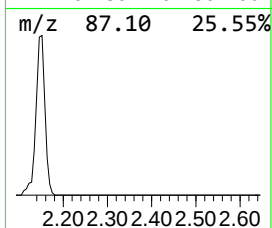
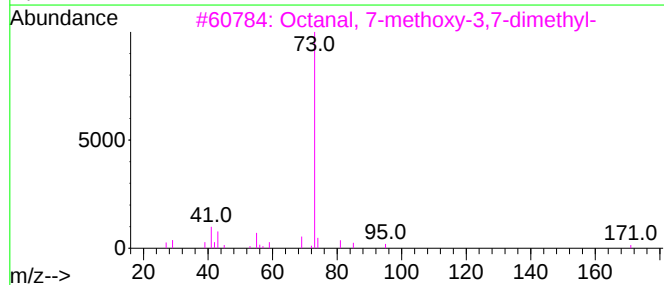
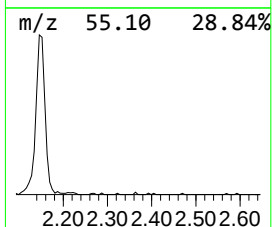
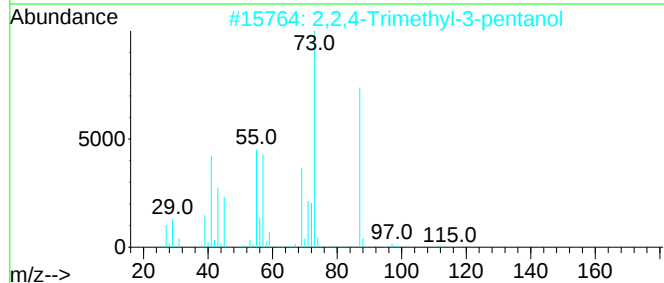
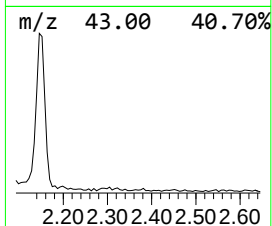
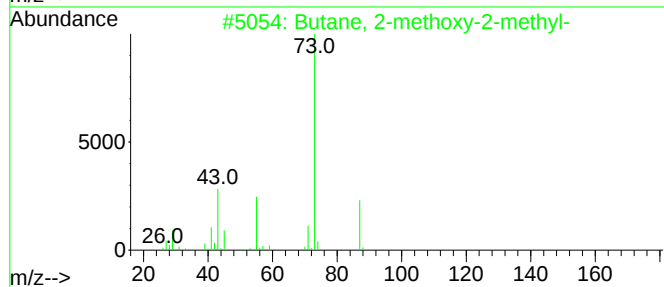
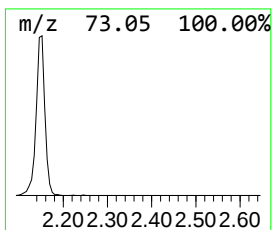
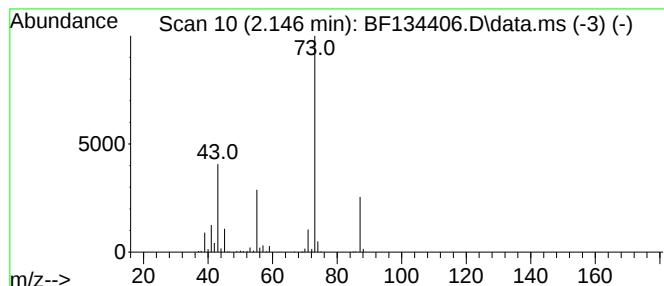
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.146	13.53 ng	270782	1,4-Dichlorobenzene-d4	6.834

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	17
4			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	17
5			Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9



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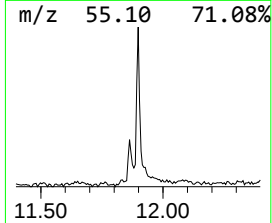
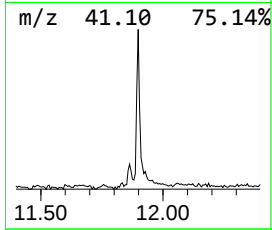
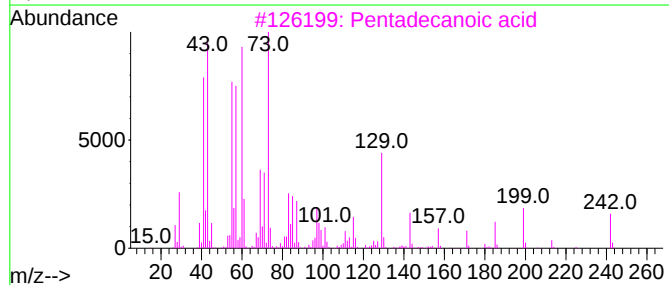
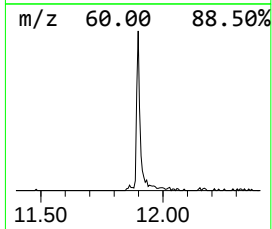
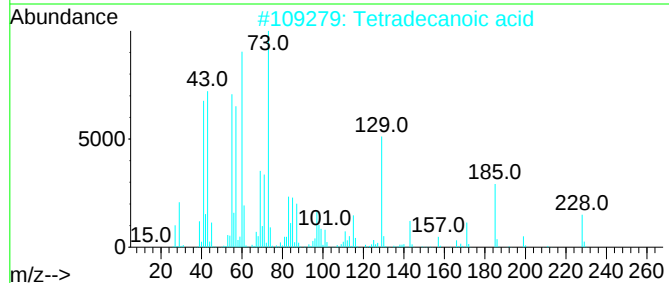
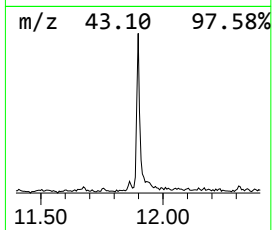
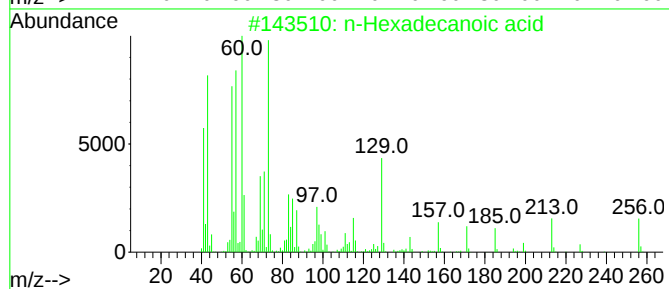
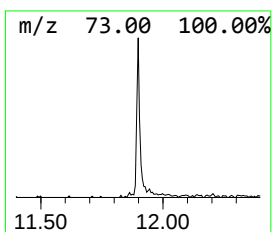
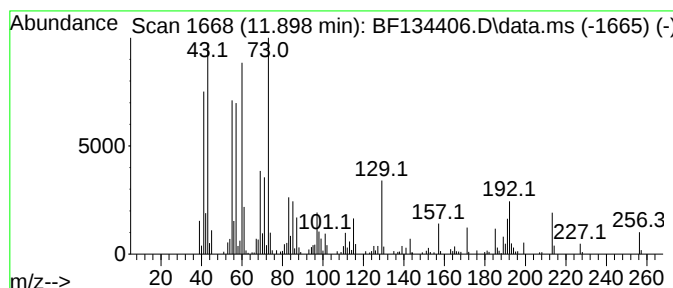
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.898	8.62 ng	240083	Phenanthrene-d10	11.369

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	95		
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	76		
4	Tridecanoic acid	214	C13H26O2	000638-53-9	64		
5	Undecanoic acid	186	C11H22O2	000112-37-8	58		



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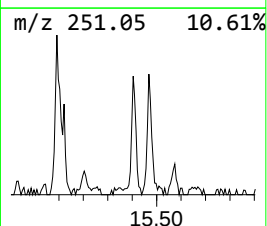
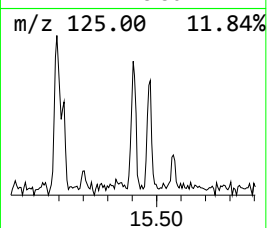
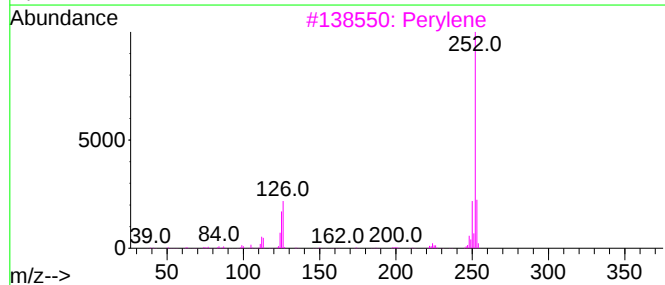
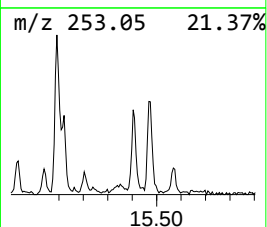
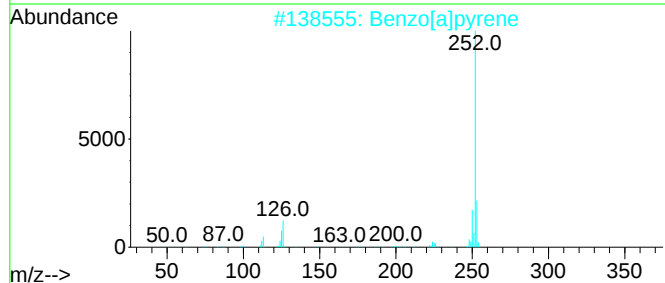
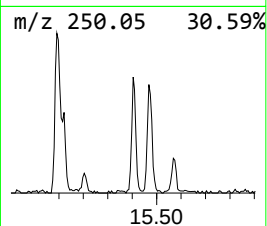
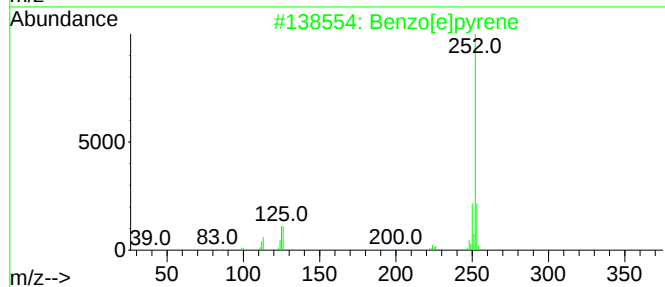
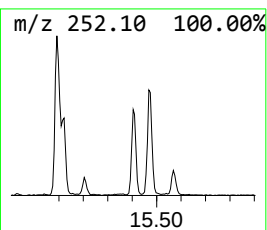
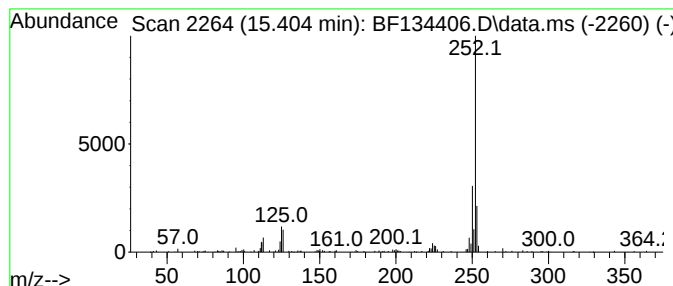
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Benzo[e]pyrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.404	6.39 ng	137144	Perylene-d12	15.539

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	96
2			Benzo[a]pyrene	252	C20H12	000050-32-8	93
3			Perylene	252	C20H12	000198-55-0	93
4			Benzo[b]fluoranthene	252	C20H12	000205-99-2	93
5			Benzo[k]fluoranthene	252	C20H12	000207-08-9	91



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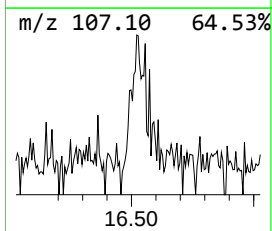
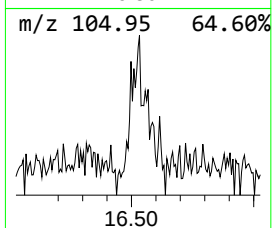
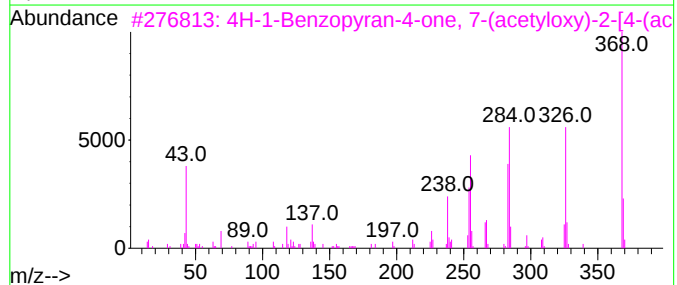
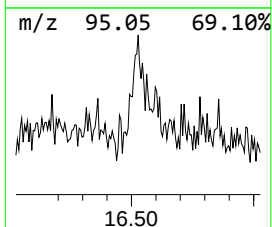
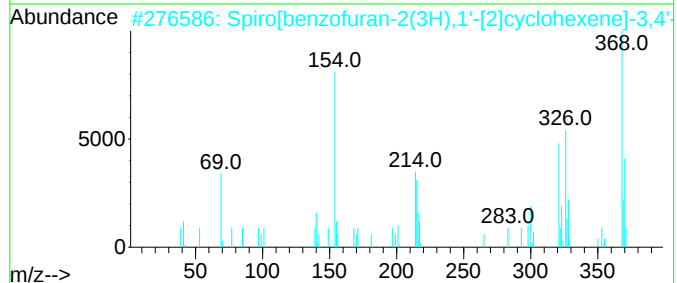
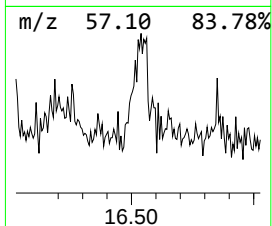
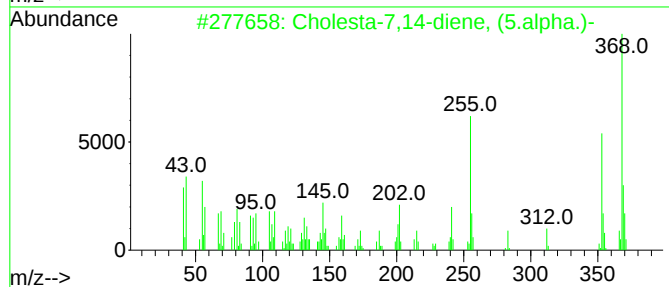
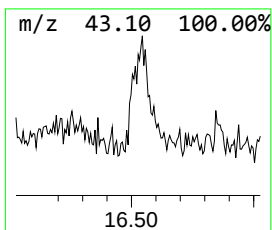
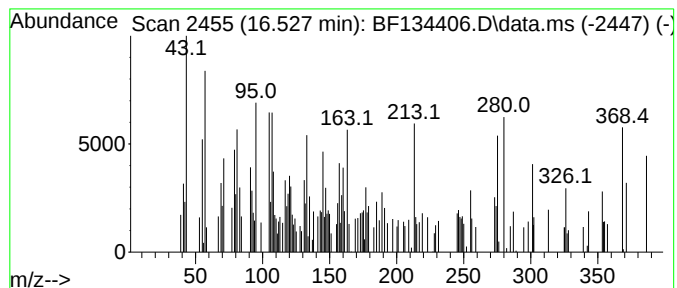
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown16.527 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.527	8.00 ng	171781	Perylene-d12	15.539

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cholesta-7,14-diene, (5.alpha.)-	368	C27H44	054482-39-2	45
2			Spiro[benzofuran-2(3H),1'-[2]cyc...	368	C17H17C10S5	026881-62-9	11
3			4H-1-Benzopyran-4-one, 7-(acetyl...	368	C20H16O7	029376-69-0	11
4			Benzoic acid, 2-(3-cyano-4,6-dim...	326	C18H18N2O2S	330472-70-3	11
5			Sinapinic acid, 2TMS derivative	368	C17H28O5Si2	027750-80-7	10



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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
Butane, 2-metho...	2.146	13.5	ng	270782	1	6.834	400196	20.0
n-Hexadecanoic ...	11.898	8.6	ng	240083	4	11.369	557045	20.0
Benzo[e]pyrene	15.404	6.4	ng	137144	6	15.539	429418	20.0
unknown16.527	16.527	8.0	ng	171781	6	15.539	429418	20.0