

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100923\
 Data File : BF135673.D
 Acq On : 10 Oct 2023 02:48
 Operator : CG\JU
 Sample : 04609-05
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-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-BF091123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135673.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.963	485	489	506	rVB	282953	383047	15.88%	2.106%
2	5.375	555	559	577	rBV	2159521	2227930	92.35%	12.249%
3	6.387	728	731	752	rBV	2141406	2329447	96.56%	12.808%
4	6.740	787	791	800	rBV	740511	668881	27.73%	3.678%
5	7.304	883	887	898	rBV	1648232	1477804	61.26%	8.125%
6	8.016	1005	1008	1022	rVB	1010089	861949	35.73%	4.739%
7	9.098	1187	1192	1195	rBV	2602950	2412535	100.00%	13.264%
8	9.216	1208	1212	1216	rVB2	38040	37462	1.55%	0.206%
9	9.775	1303	1307	1311	rBV	1024038	859404	35.62%	4.725%
10	10.569	1438	1442	1457	rBV	1371741	1274259	52.82%	7.006%
11	11.269	1558	1561	1564	rBV	928919	767362	31.81%	4.219%
12	11.292	1564	1565	1570	rVB	115741	74535	3.09%	0.410%
13	11.775	1644	1647	1650	rBV2	27248	28538	1.18%	0.157%
14	11.804	1650	1652	1663	rVV2	202769	225362	9.34%	1.239%
15	11.886	1663	1666	1669	rBV2	36965	32376	1.34%	0.178%
16	12.492	1765	1769	1773	rVB	248483	204951	8.50%	1.127%
17	12.598	1784	1787	1792	rBV2	39133	58118	2.41%	0.320%
18	12.722	1802	1808	1813	rBV	219564	218845	9.07%	1.203%
19	12.769	1813	1816	1823	rVB4	14563	26821	1.11%	0.147%
20	12.863	1828	1832	1836	rBV	1793490	1722596	71.40%	9.471%
21	12.939	1842	1845	1850	rBV4	17844	30863	1.28%	0.170%
22	13.057	1862	1865	1869	rVB2	27470	29207	1.21%	0.161%
23	13.157	1878	1882	1887	rBV3	28516	35491	1.47%	0.195%
24	13.439	1926	1930	1933	rBV3	25352	25788	1.07%	0.142%
25	13.769	1982	1986	1988	rBV3	29976	36796	1.53%	0.202%
26	13.851	1994	2000	2007	rBV8	30763	90091	3.73%	0.495%
27	13.933	2009	2014	2017	rVV2	605336	728564	30.20%	4.006%
28	13.957	2017	2018	2023	rVB	120691	81369	3.37%	0.447%
29	14.092	2038	2041	2044	rBV2	39503	37985	1.57%	0.209%
30	14.321	2075	2080	2084	rBV3	29739	42219	1.75%	0.232%
31	14.398	2089	2093	2095	rBV3	43585	46795	1.94%	0.257%
32	14.698	2141	2144	2150	rBV3	25213	30050	1.25%	0.165%
33	14.980	2188	2192	2194	rBV	96881	140094	5.81%	0.770%
34	15.033	2199	2201	2207	rVB4	42437	50348	2.09%	0.277%
35	15.092	2207	2211	2213	rBV3	19925	29005	1.20%	0.159%
36	15.280	2239	2243	2248	rBV	53795	72129	2.99%	0.397%

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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-BF091123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.339	2250	2253	2259	rVV	80718	115864	4.80%	0.637%
38	15.398	2259	2263	2273	rVB	392439	551905	22.88%	3.034%
39	15.845	2336	2339	2343	rVB2	25325	35175	1.46%	0.193%
40	16.904	2513	2519	2523	rBV2	28931	57457	2.38%	0.316%
41	17.357	2592	2596	2600	rBV3	17881	28519	1.18%	0.157%

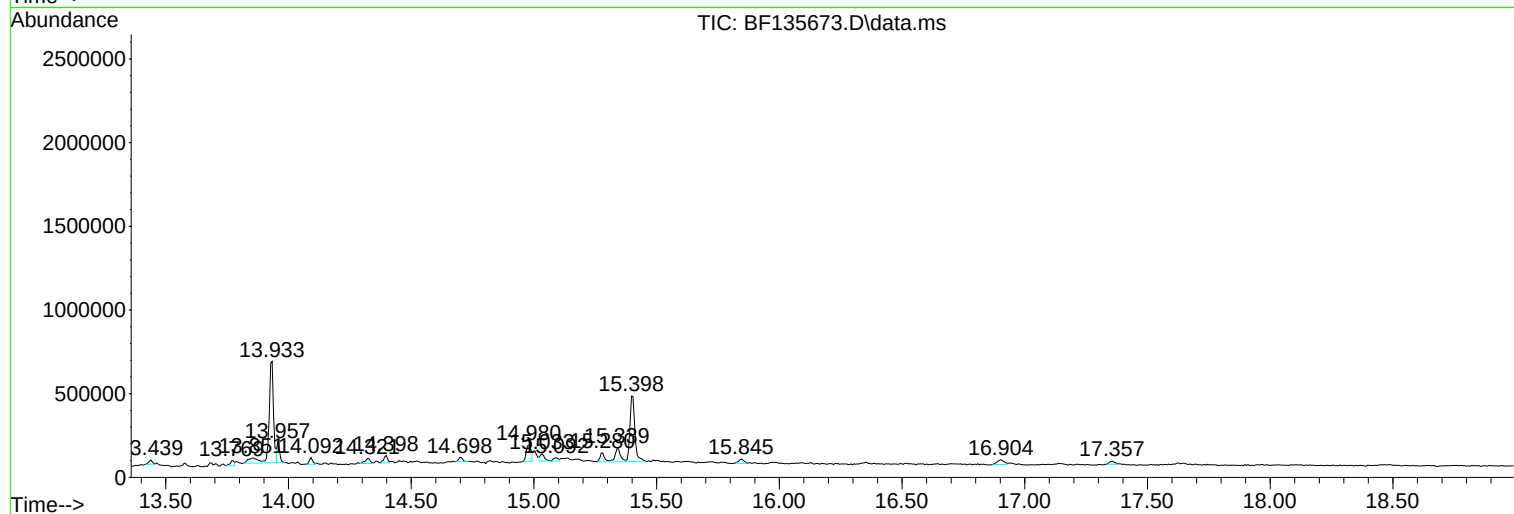
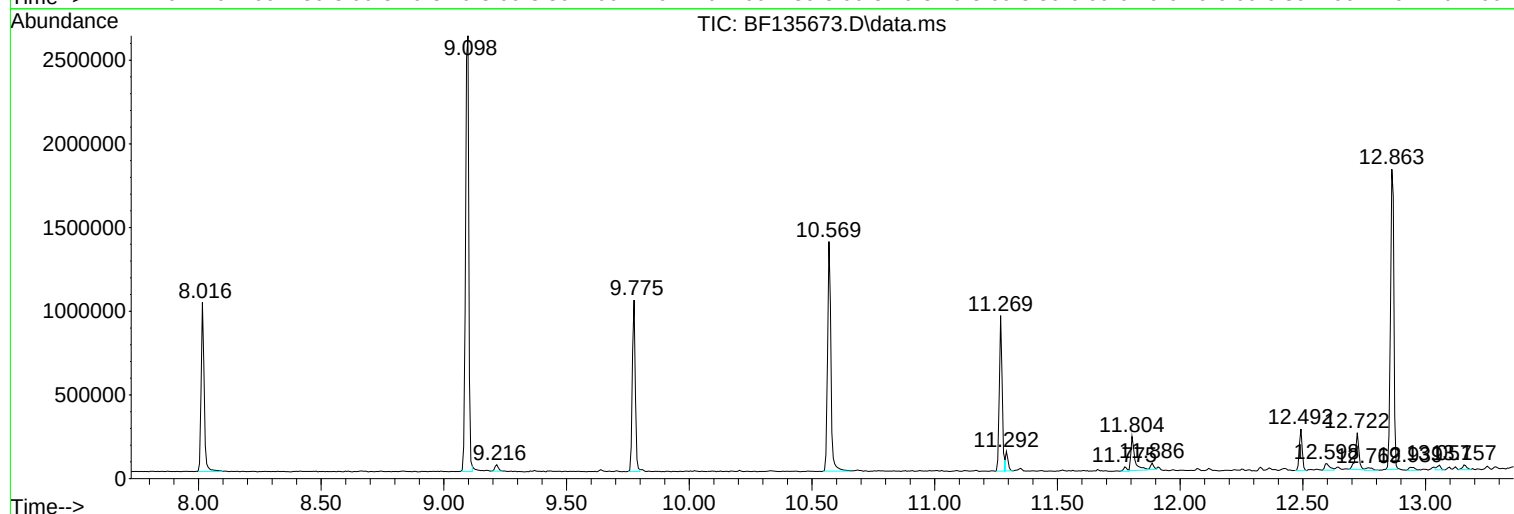
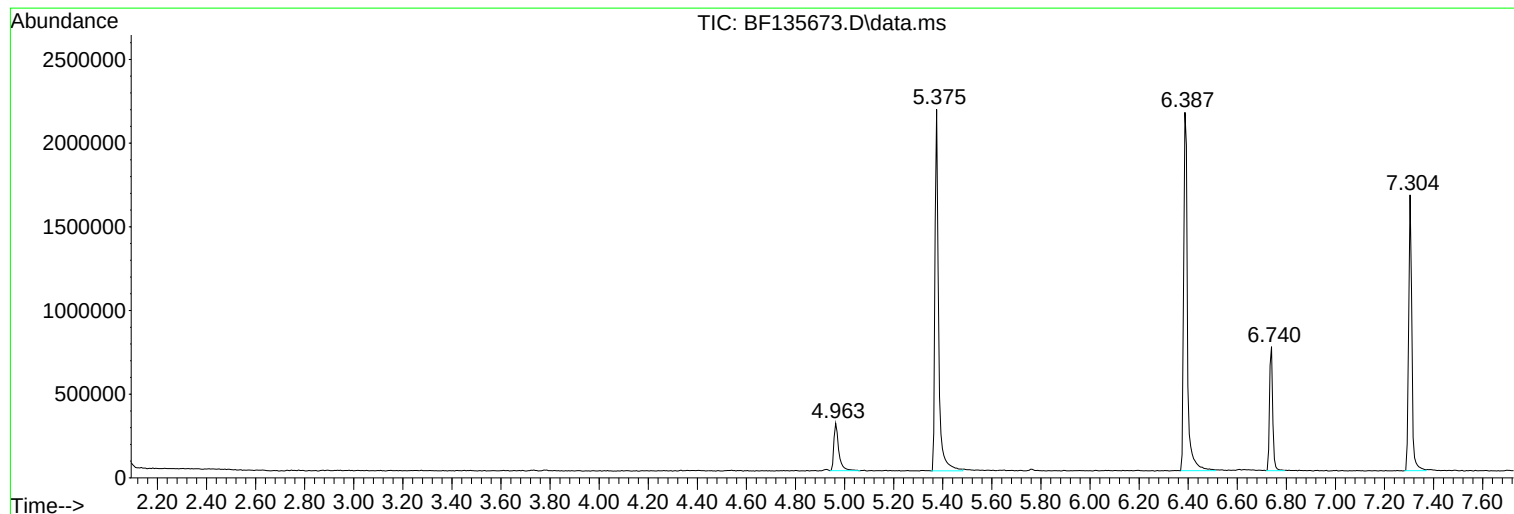
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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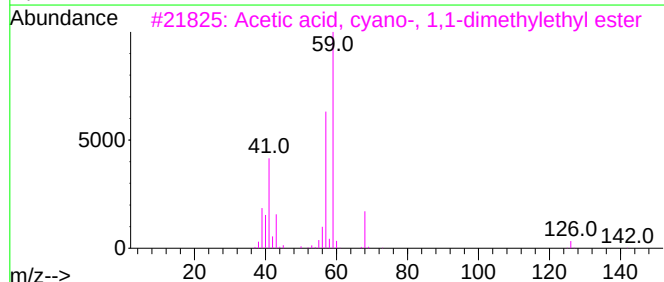
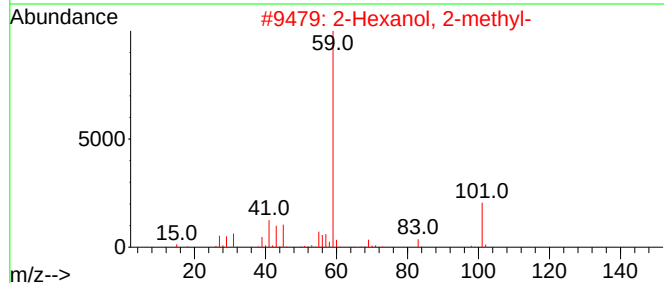
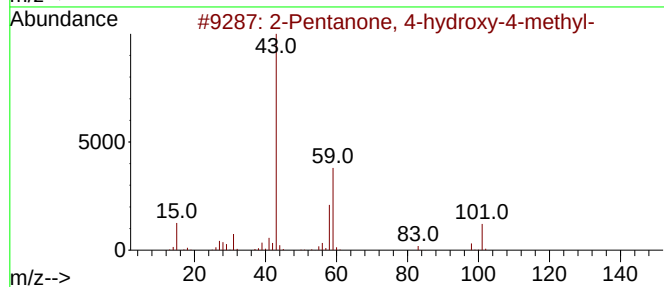
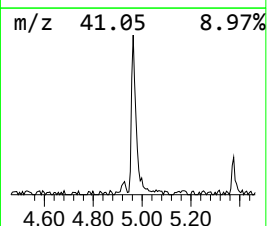
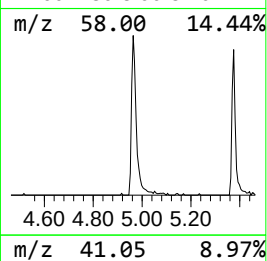
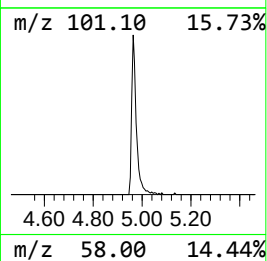
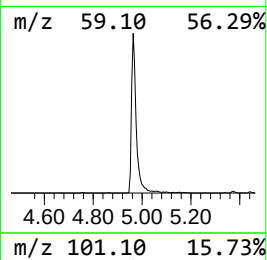
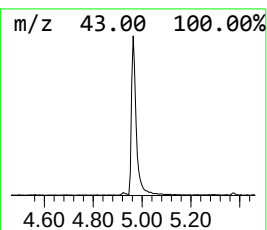
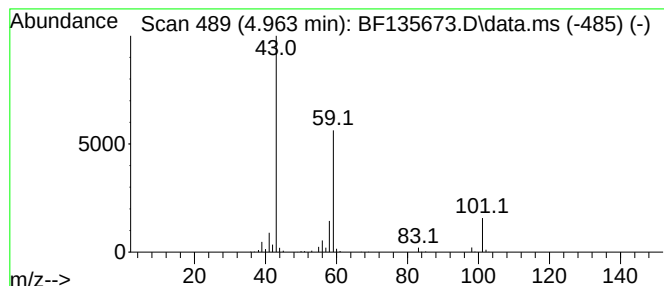
Instrument :
BNA_F
ClientSampleId :
TP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.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 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
4.963	11.45 ng	383047	1,4-Dichlorobenzene-d4	6.740	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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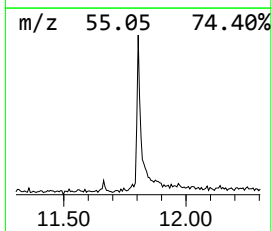
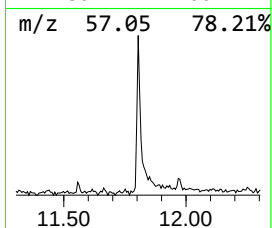
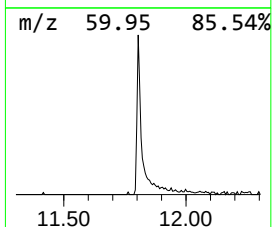
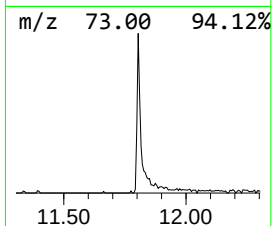
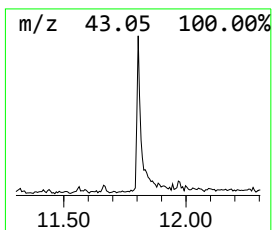
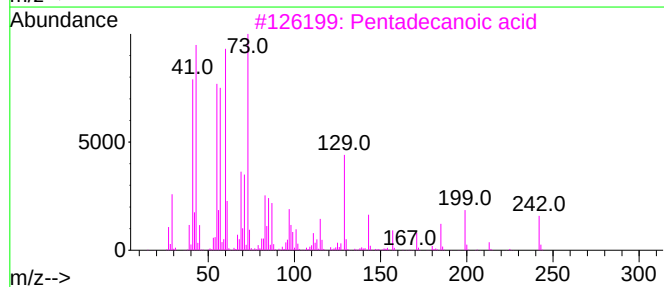
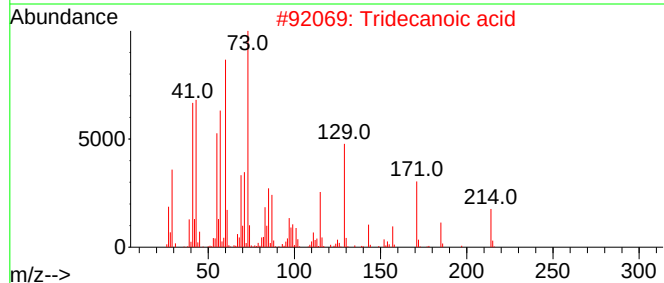
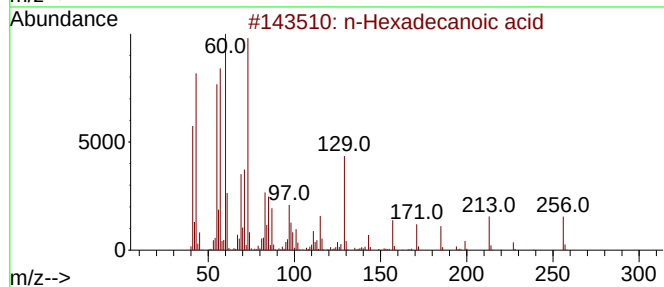
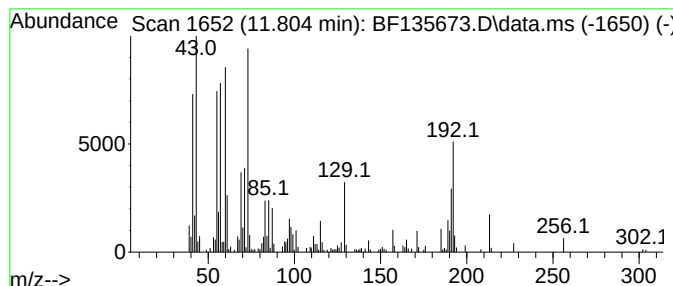
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.804	5.87 ng	225362	Phenanthrene-d10	11.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2			Tridecanoic acid	214	C13H26O2	000638-53-9	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4			Octadecanoic acid	284	C18H36O2	000057-11-4	43
5			Nonanoic acid	158	C9H18O2	000112-05-0	38



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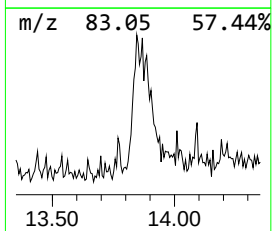
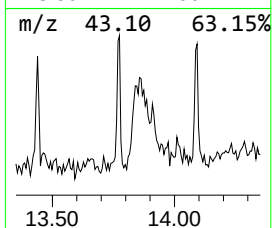
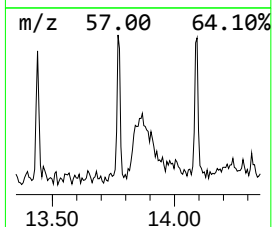
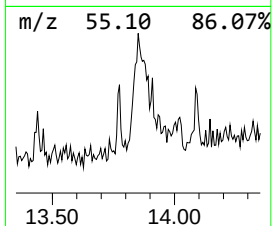
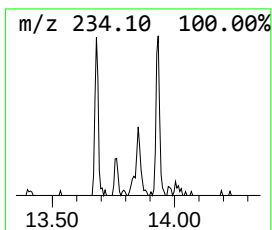
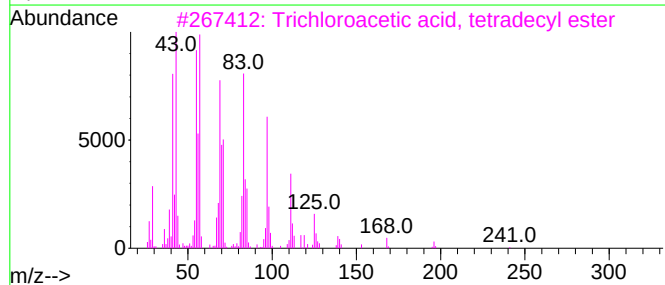
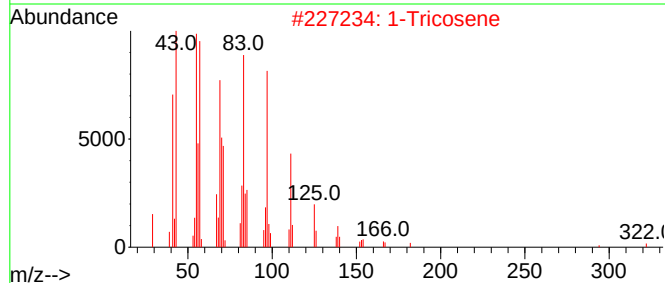
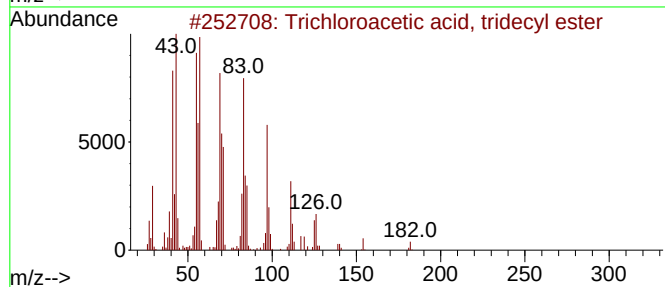
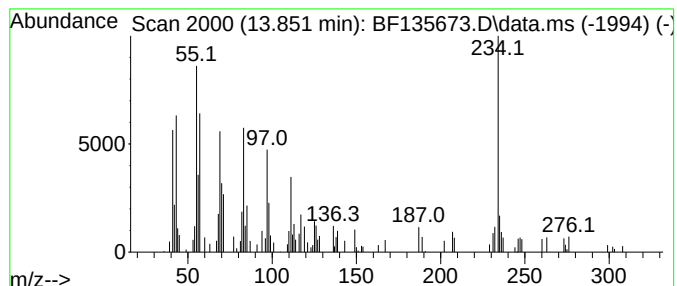
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown13.851 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.851	2.47 ng	90091	Chrysene-d12	13.933	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, tridecyl e...	344	C15H27Cl3O2	074339-51-8	46
2	1-Tricosene	322	C23H46	018835-32-0	45
3	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	45
4	10-Heneicosene (c,t)	294	C21H42	095008-11-0	43
5	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	42



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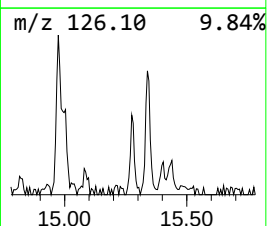
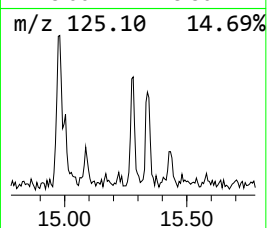
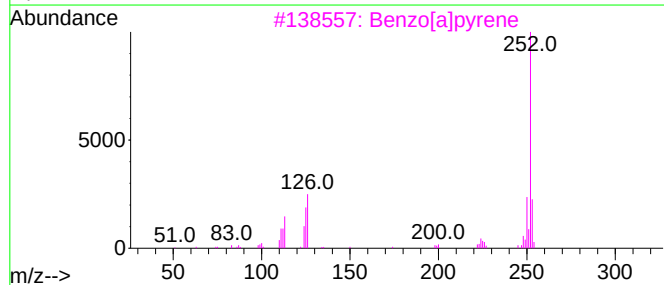
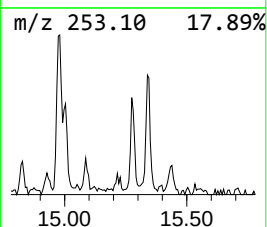
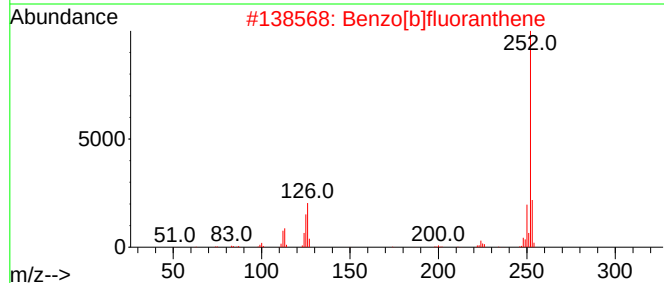
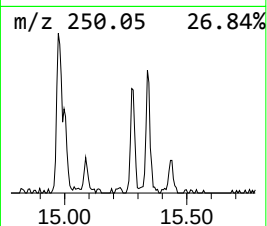
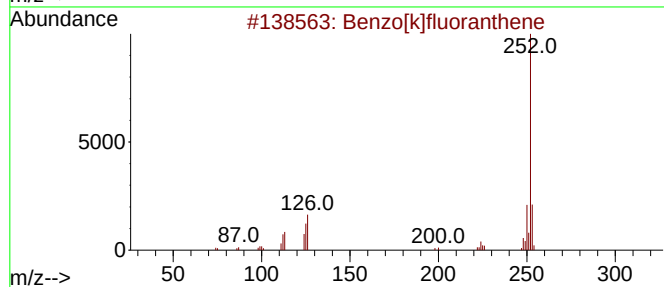
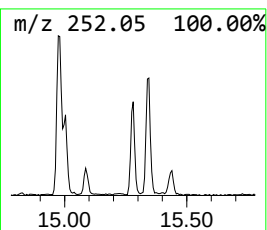
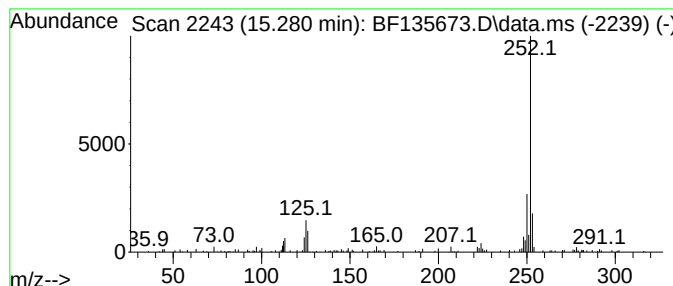
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Benzo[e]pyrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.280	2.61 ng	72129	Perylene-d12	15.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[k]fluoranthene	252	C20H12	000207-08-9	90
2			Benzo[b]fluoranthene	252	C20H12	000205-99-2	89
3			Benzo[a]pyrene	252	C20H12	000050-32-8	89
4			Benzo[e]pyrene	252	C20H12	000192-97-2	89
5			Benzo[j]fluoranthene	252	C20H12	000205-82-3	89



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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-...	4.963	11.4	ng	383047	1	6.740	668881	20.0
n-Hexadecanoic ...	11.804	5.9	ng	225362	4	11.269	767362	20.0
unknown13.851	13.851	2.5	ng	90091	5	13.933	728564	20.0
Benzo[e]pyrene	15.280	2.6	ng	72129	6	15.398	551905	20.0