

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040821\
 Data File : BG048640.D
 Acq On : 8 Apr 2021 15:34
 Operator : CG/JU
 Sample : M1951-04
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SW-2

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_G\METHODS\8270-BG033021.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG048640.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.635	384	391	400	rBV	252998	409400	17.04%	4.799%
2	7.239	658	664	676	rVB2	193817	355255	14.79%	4.164%
3	8.091	800	809	815	rBV	79836	136325	5.67%	1.598%
4	9.260	1000	1008	1015	rBV	286541	521992	21.73%	6.119%
5	10.911	1282	1289	1296	rBV	100068	182942	7.62%	2.144%
6	13.361	1699	1706	1717	rBV	801397	1227123	51.08%	14.385%
7	14.183	1838	1846	1856	rBV	30195	46863	1.95%	0.549%
8	14.742	1935	1941	1949	rBV	161577	262068	10.91%	3.072%
9	16.234	2186	2195	2206	rBV	880440	1410157	58.70%	16.530%
10	17.491	2403	2409	2417	rBV	249976	404702	16.85%	4.744%
11	18.384	2555	2561	2564	rBV7	15697	32905	1.37%	0.386%
12	19.137	2685	2689	2693	rVB2	21918	25917	1.08%	0.304%
13	19.648	2771	2776	2782	rBV6	31247	58604	2.44%	0.687%
14	20.106	2847	2854	2860	rBV	1828140	2402239	100.00%	28.160%
15	20.882	2982	2986	2992	rBV9	11901	24540	1.02%	0.288%
16	21.410	3071	3076	3086	rBV3	76668	163232	6.79%	1.913%
17	21.792	3134	3141	3151	rBV2	246942	442592	18.42%	5.188%
18	25.129	3699	3709	3723	rBV2	126528	423907	17.65%	4.969%

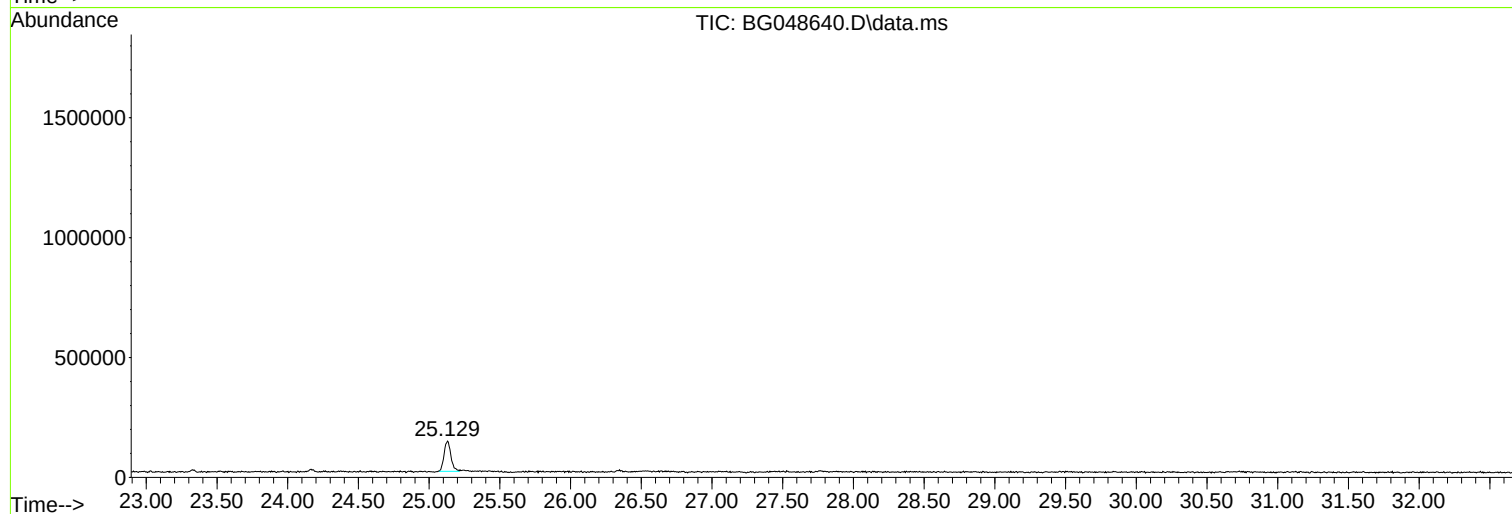
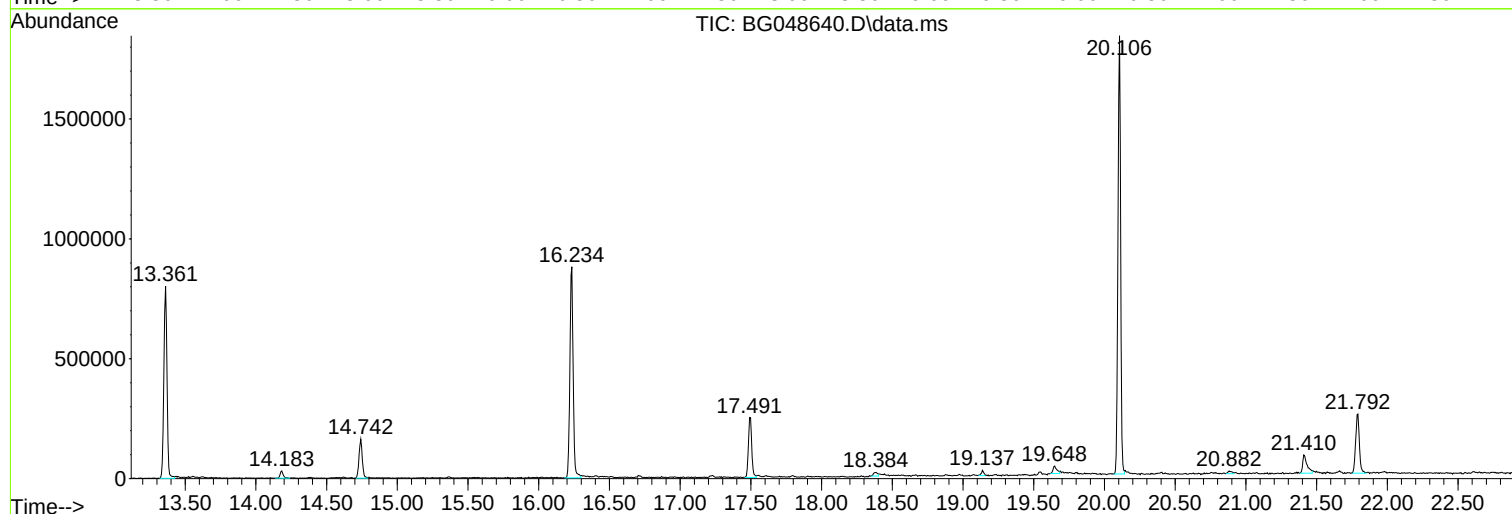
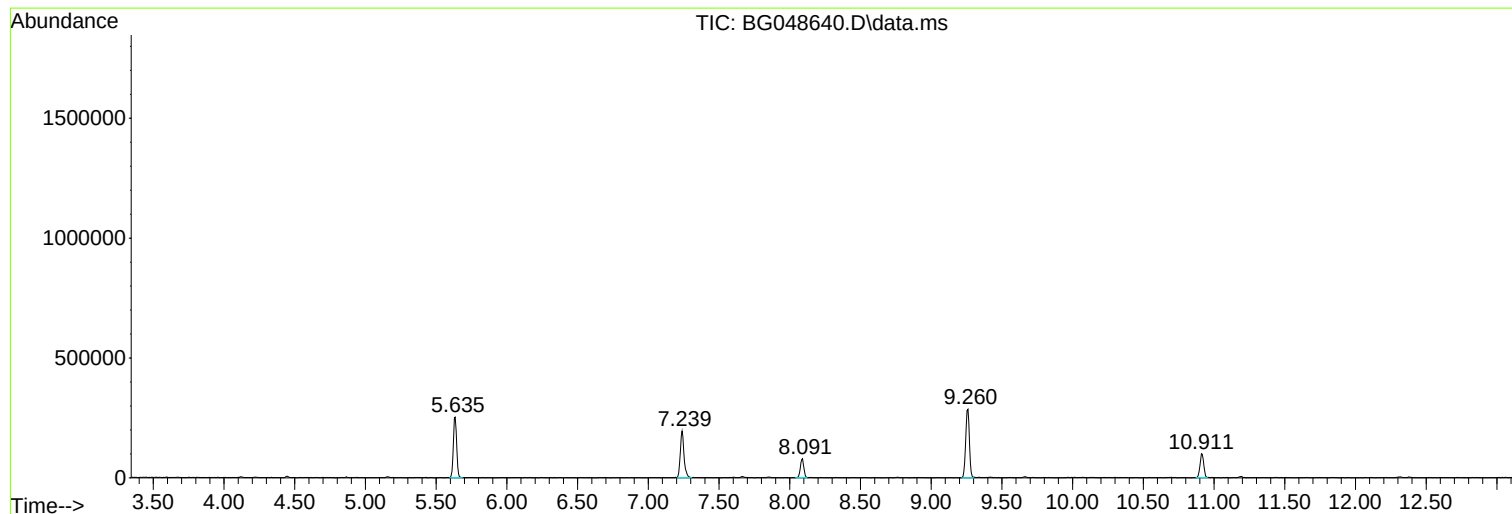
Sum of corrected areas: 8530763

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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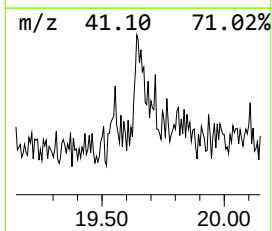
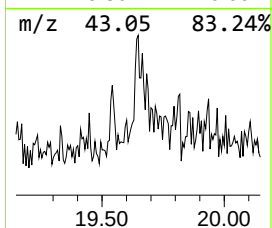
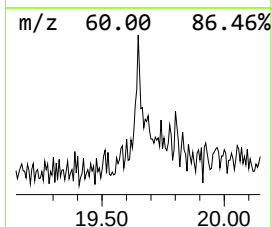
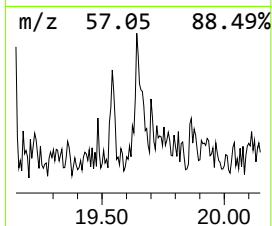
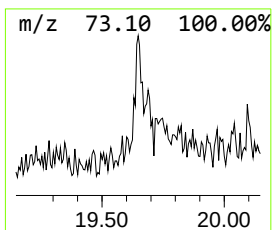
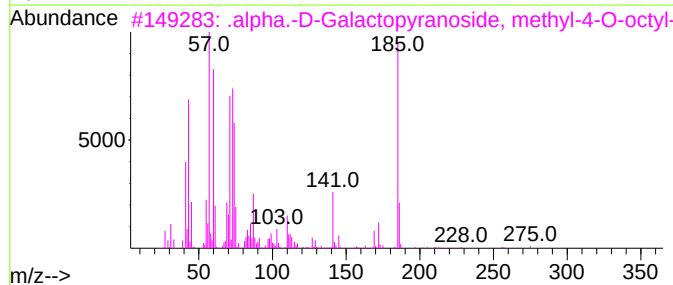
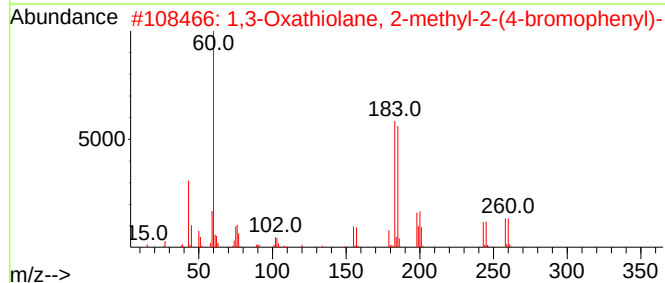
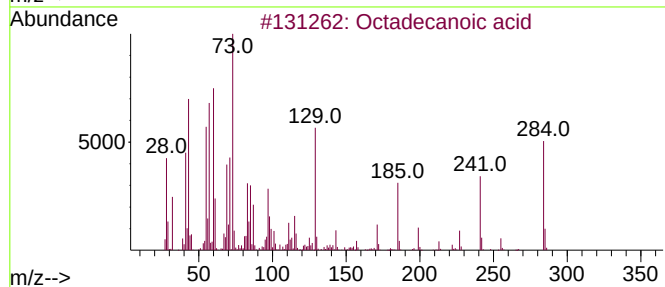
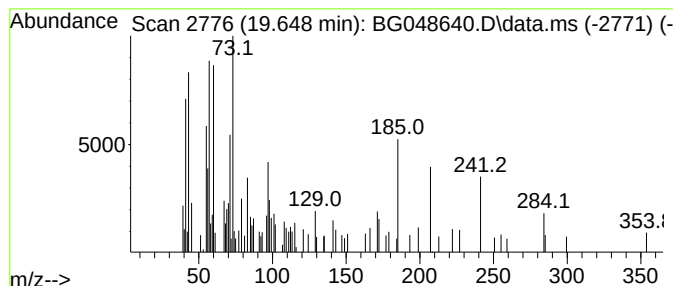
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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Peak Number 1 unknown19.64 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.648	2.65 ng	58604	Chrysene-d12	21.792	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	47
2	1,3-Oxathiolane, 2-methyl-2-(4-b...	258	C10H11BrOS	1000115-94-9	27
3	.alpha.-D-Galactopyranoside, met...	306	C15H30O6	1000157-05-0	25
4	n-Decanoic acid	172	C10H20O2	000334-48-5	18
5	Octane, 1-(ethenylthio)-	172	C10H20S	042779-08-8	14



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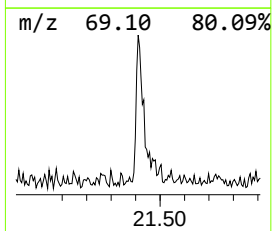
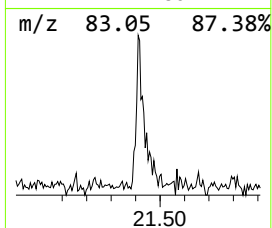
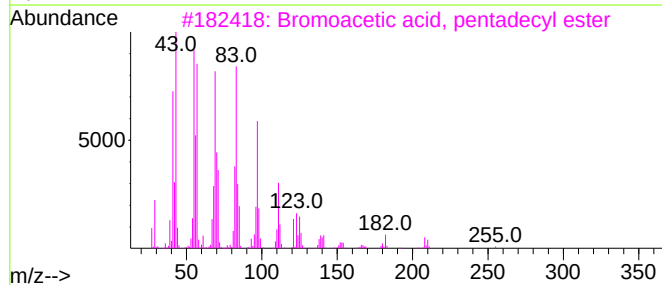
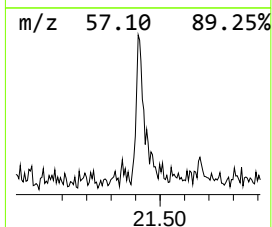
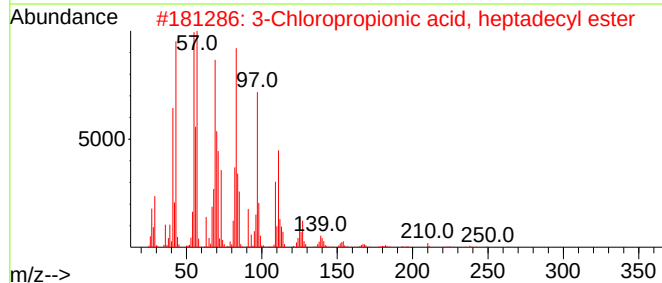
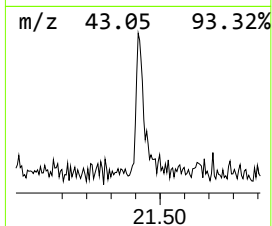
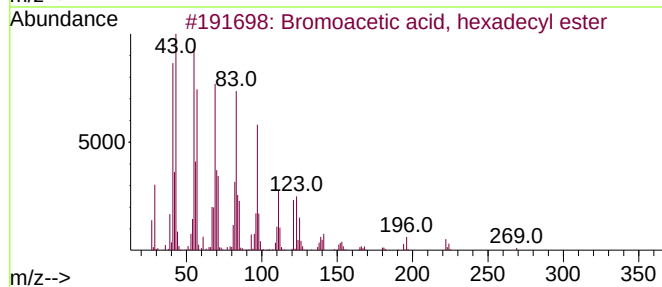
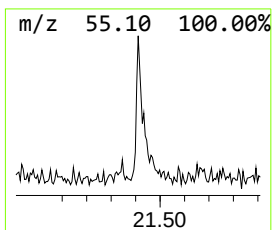
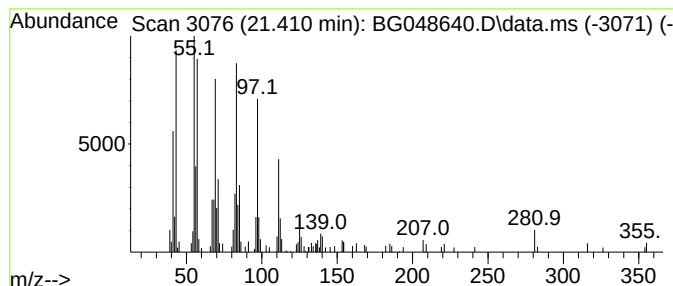
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Peak Number 2 Bromoacetic acid, hexadecyl... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.410	7.38 ng	163232	Chrysene-d12	21.792

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	87
2			3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	83
3			Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	83
4			17-Pentatriacontene	491	C35H70	006971-40-0	83
5			10-Heneicosene (c,t)	294	C21H42	095008-11-0	64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown19.64	19.648	2.6	ng	58604	5	21.792	442592	20.0
Bromoacetic aci...	21.410	7.4	ng	163232	5	21.792	442592	20.0