

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111723\
 Data File : BG059753.D
 Acq On : 18 Nov 2023 7:11
 Operator : MA/JU
 Sample : 05311-01
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_G
 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_G\Methods\8270-BG111623.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG059753.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.831	407	416	423	rBV	292661	449300	18.13%	4.049%
2	7.459	686	693	702	rBV2	334842	579818	23.40%	5.225%
3	8.340	833	843	848	rBV3	97555	161696	6.52%	1.457%
4	9.533	1040	1046	1055	rBV	213045	390637	15.76%	3.520%
5	11.190	1320	1328	1333	rBV	130708	237190	9.57%	2.137%
6	13.593	1728	1737	1746	rBV	636088	979178	39.51%	8.823%
7	14.968	1965	1971	1977	rVB2	227561	351367	14.18%	3.166%
8	16.448	2216	2223	2232	rBV	586111	913504	36.86%	8.232%
9	17.717	2432	2439	2444	rBV	471808	729752	29.45%	6.576%
10	17.759	2444	2446	2450	rVB2	51743	69177	2.79%	0.623%
11	17.853	2459	2462	2469	rBV3	17994	30713	1.24%	0.277%
12	18.528	2571	2577	2581	rBV4	100574	140686	5.68%	1.268%
13	18.628	2591	2594	2601	rVB4	27022	43814	1.77%	0.395%
14	18.769	2613	2618	2623	rBV6	29248	64717	2.61%	0.583%
15	18.810	2623	2625	2630	rVB6	22201	27277	1.10%	0.246%
16	19.069	2663	2669	2675	rBV8	27830	57099	2.30%	0.515%
17	19.468	2734	2737	2744	rBV8	41778	69307	2.80%	0.625%
18	19.627	2762	2764	2769	rVB5	24792	38265	1.54%	0.345%
19	19.750	2780	2785	2789	rBV	182591	268763	10.85%	2.422%
20	19.791	2789	2792	2796	rVB4	43008	48178	1.94%	0.434%
21	20.079	2834	2841	2843	rBV5	28604	60662	2.45%	0.547%
22	20.115	2843	2847	2852	rVB	194100	278841	11.25%	2.513%
23	20.291	2871	2877	2882	rBV	2028716	2478179	100.00%	22.331%
24	20.426	2895	2900	2904	rBV8	29306	45473	1.83%	0.410%
25	20.591	2926	2928	2933	rVB4	35742	44369	1.79%	0.400%
26	20.696	2938	2946	2948	rBV8	21925	51048	2.06%	0.460%
27	20.755	2952	2956	2959	rVB4	26549	40108	1.62%	0.361%
28	20.896	2976	2980	2984	rVV6	27969	34512	1.39%	0.311%
29	20.943	2986	2988	2992	rVB5	23343	30217	1.22%	0.272%
30	21.390	3059	3064	3071	rVB9	34208	73767	2.98%	0.665%
31	21.578	3091	3096	3102	rBV7	93625	161891	6.53%	1.459%
32	21.631	3103	3105	3110	rVB6	24736	27466	1.11%	0.247%
33	21.742	3121	3124	3131	rVB8	30664	56472	2.28%	0.509%
34	21.813	3132	3136	3138	rBV5	17532	26622	1.07%	0.240%
35	22.042	3167	3175	3180	rBV2	394329	827200	33.38%	7.454%
36	22.095	3180	3184	3190	rVB	90940	158195	6.38%	1.426%

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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-BG111623.M
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37	22.253	3209	3211	3216	rBV6	15155	26192	1.06%	0.236%
38	22.829	3305	3309	3314	rVB5	21899	36189	1.46%	0.326%
39	24.010	3508	3510	3513	rBV4	21186	26911	1.09%	0.242%
40	24.457	3580	3586	3587	rBV6	70672	106665	4.30%	0.961%
41	25.279	3721	3726	3727	rBV4	37716	60004	2.42%	0.541%
42	25.432	3747	3752	3753	rBV5	48618	56522	2.28%	0.509%
43	25.632	3776	3786	3797	rBV2	210898	711135	28.70%	6.408%
44	26.948	4008	4010	4015	rBV6	14362	28423	1.15%	0.256%

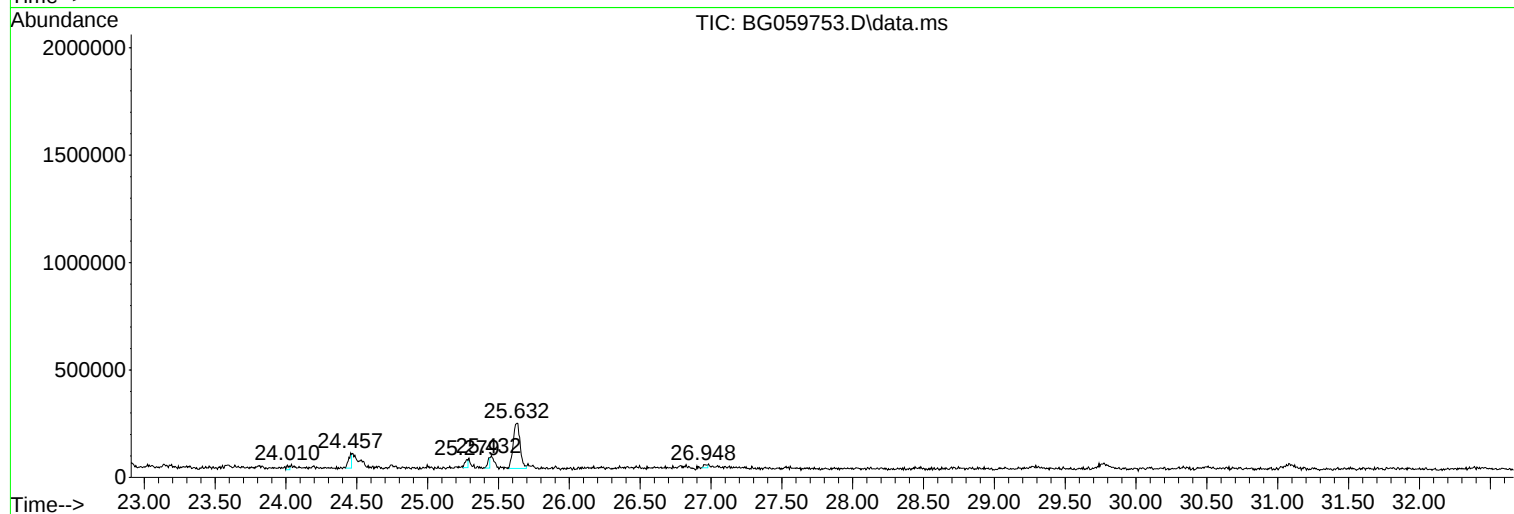
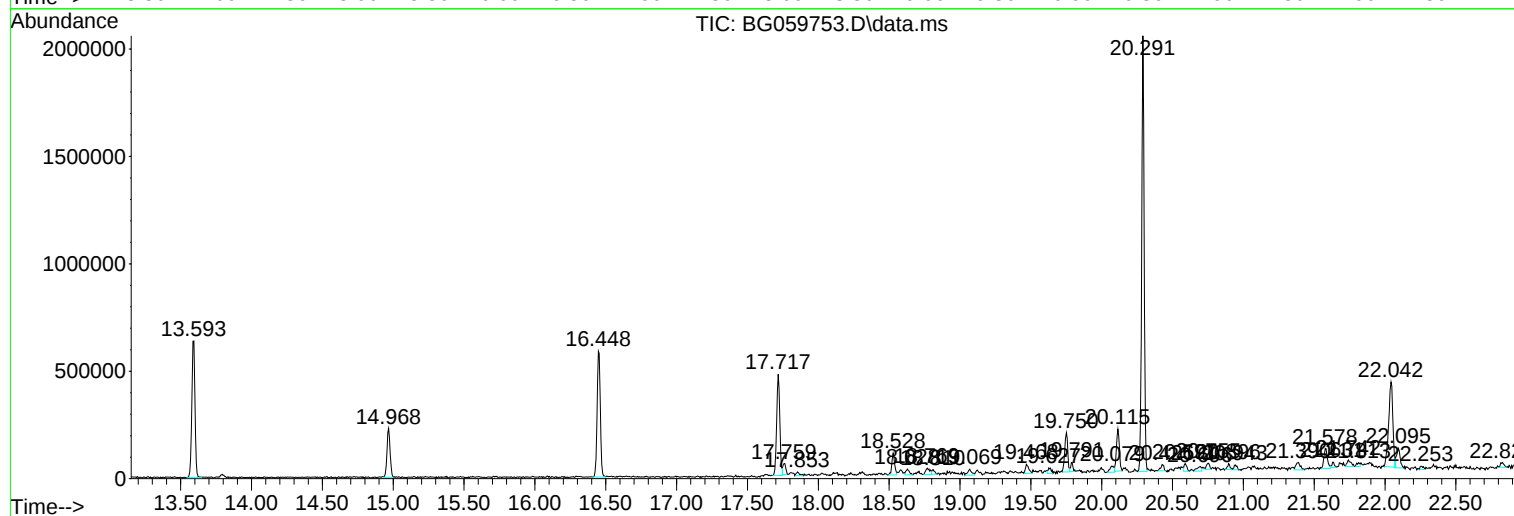
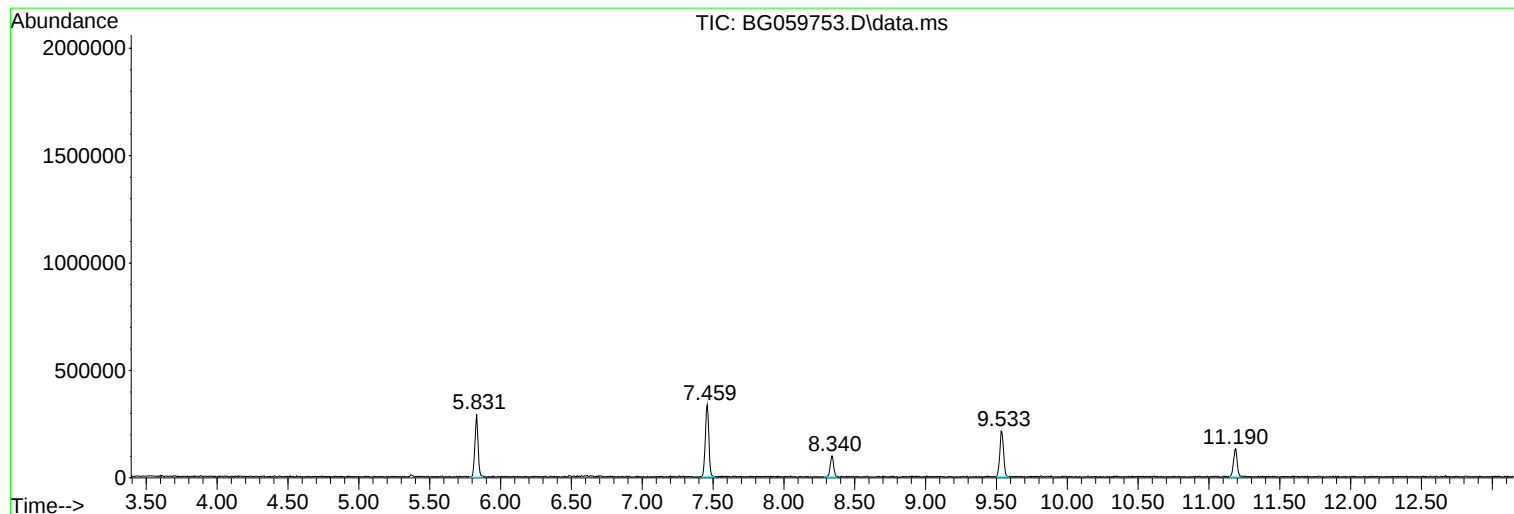
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Operator : MA/JU
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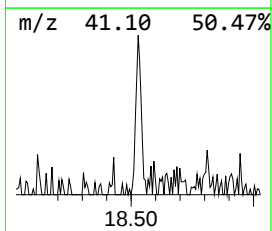
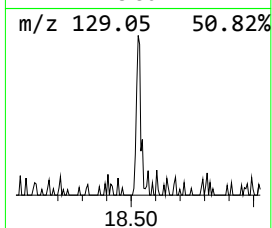
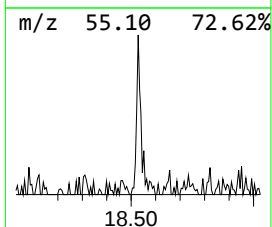
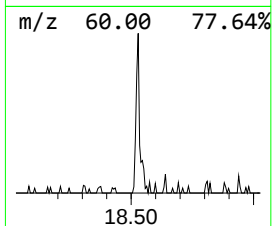
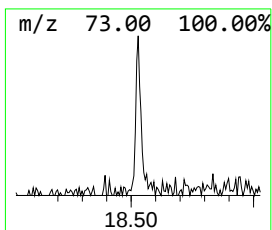
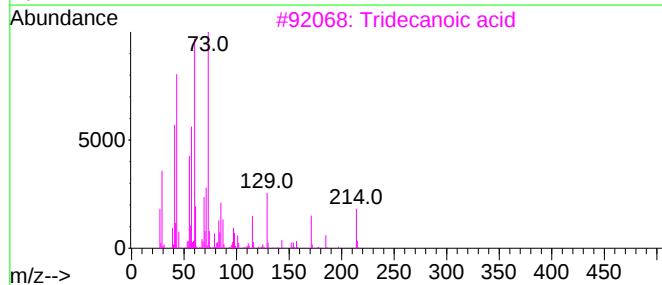
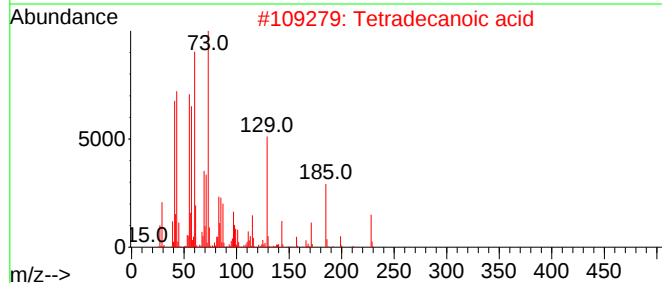
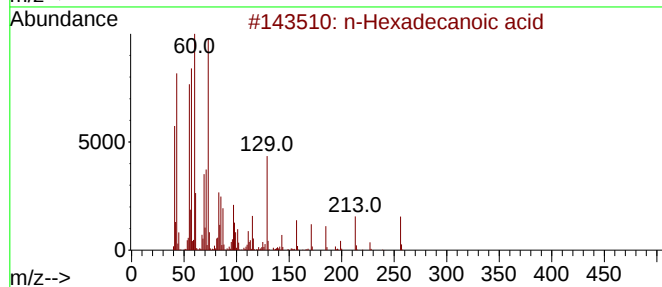
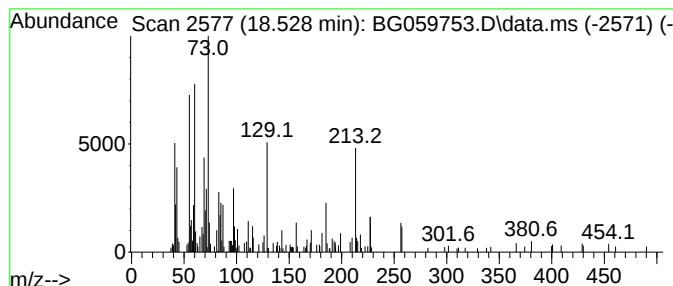
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.528	3.86 ng	140686	Phenanthrene-d10	17.717

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	60
3			Tridecanoic acid	214	C13H26O2	000638-53-9	46
4			Undecanoic acid	186	C11H22O2	000112-37-8	46
5			Pyrrole-2-carboxylic acid, 4-(1-...	339	C19H30ClNO2	1000295-53-6	38



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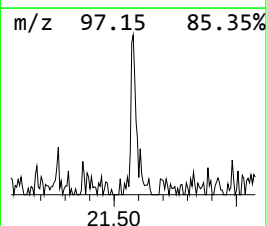
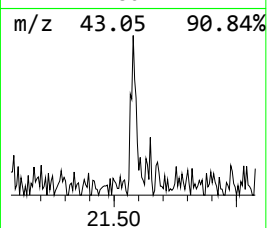
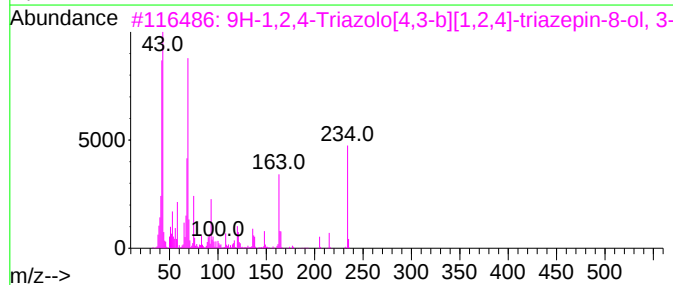
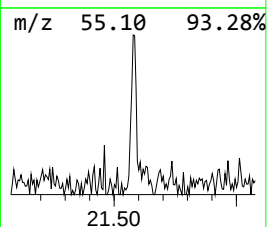
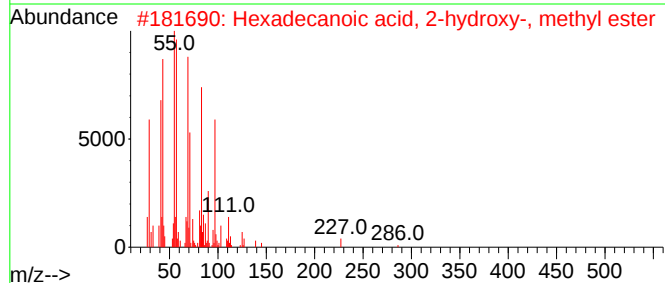
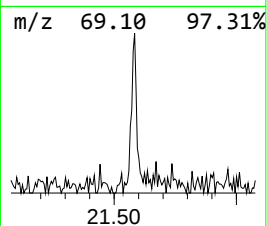
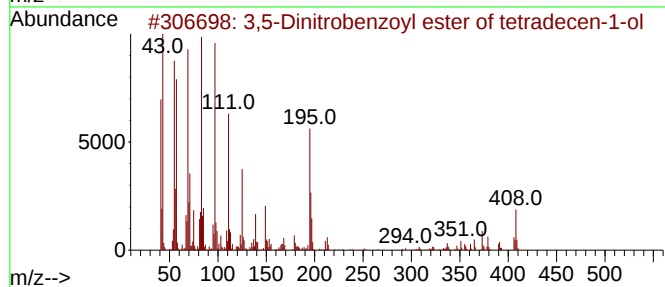
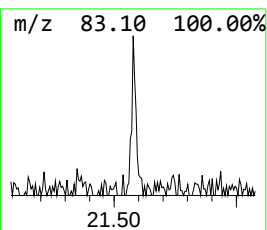
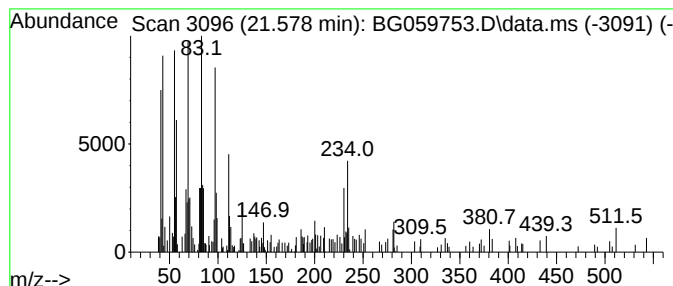
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown21.578 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.578	3.91 ng	161891	Chrysene-d12	22.042

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,5-Dinitrobenzoyl ester of tetr...	408	C21H32N2O6	094999-94-7	45	
2	Hexadecanoic acid, 2-hydroxy-, m...	286	C17H34O3	016742-51-1	33	
3	9H-1,2,4-Triazolo[4,3-b][1,2,4]-...	234	C6H5F3N6O	294875-48-2	14	
4	Methyl 2-hydroxydodecanoate	230	C13H26O3	051067-85-7	10	
5	5-Hexen-3-one	98	C6H10O	024253-30-3	9	



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Hexadecanoic ...	18.528	3.9	ng	140686	4	17.717	729752	20.0
unknown21.578	21.578	3.9	ng	161891	5	22.042	827200	20.0