

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050224\
 Data File : BG061091.D
 Acq On : 2 May 2024 13:21
 Operator : MA/JU
 Sample : P2330-13 2X
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 G-2(0.5-1.5)

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-BG043024.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG061091.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.152	23	28	36	rVB2	15532	24477	2.60%	0.351%
2	5.525	425	432	442	rVB	206056	334636	35.56%	4.804%
3	7.106	694	701	711	rBV	232999	392709	41.73%	5.638%
4	7.934	834	842	849	rBV	112104	184862	19.64%	2.654%
5	9.086	1030	1038	1045	rBV	151218	264261	28.08%	3.794%
6	10.731	1311	1318	1330	rVB	147474	259634	27.59%	3.727%
7	13.187	1729	1736	1741	rBV	412500	635094	67.49%	9.117%
8	14.562	1964	1970	1977	rBV	238249	362360	38.51%	5.202%
9	14.785	2000	2008	2015	rVB6	5124	12793	1.36%	0.184%
10	16.054	2218	2224	2233	rBV	346453	538017	57.17%	7.724%
11	17.312	2430	2438	2442	rBV	288637	433385	46.06%	6.222%
12	17.353	2442	2445	2451	rVB	83686	112780	11.98%	1.619%
13	17.447	2457	2461	2465	rVB2	16577	23592	2.51%	0.339%
14	17.893	2530	2537	2543	rBV9	7056	16032	1.70%	0.230%
15	18.211	2582	2591	2593	rBV4	66107	112380	11.94%	1.613%
16	18.316	2604	2609	2614	rBV4	10438	19069	2.03%	0.274%
17	18.381	2614	2620	2623	rVV3	31327	56739	6.03%	0.815%
18	18.416	2624	2626	2631	rVB2	18140	21973	2.34%	0.315%
19	18.681	2668	2671	2675	rBV2	16846	26654	2.83%	0.383%
20	18.722	2676	2678	2683	rVB6	11427	15023	1.60%	0.216%
21	18.980	2719	2722	2726	rBV3	14205	17041	1.81%	0.245%
22	19.110	2739	2744	2747	rBV	27571	42914	4.56%	0.616%
23	19.151	2747	2751	2752	rBV3	11853	13385	1.42%	0.192%
24	19.239	2762	2766	2772	rBV7	16581	30703	3.26%	0.441%
25	19.368	2782	2788	2794	rBV	223936	333841	35.48%	4.793%
26	19.427	2794	2798	2802	rBV7	14888	22103	2.35%	0.317%
27	19.609	2825	2829	2833	rBV3	12706	21920	2.33%	0.315%
28	19.726	2840	2849	2858	rVB	206130	347706	36.95%	4.992%
29	19.797	2858	2861	2866	rBV2	16137	28213	3.00%	0.405%
30	19.926	2878	2883	2889	rBV	701520	941014	100.00%	13.509%
31	20.050	2900	2904	2905	rBV4	19321	23710	2.52%	0.340%
32	20.220	2930	2933	2940	rVB5	33980	56571	6.01%	0.812%
33	20.320	2947	2950	2954	rVB	24030	27935	2.97%	0.401%
34	20.379	2956	2960	2963	rVV3	31958	49601	5.27%	0.712%
35	20.567	2989	2992	2995	rBV3	24009	27729	2.95%	0.398%
36	21.131	3086	3088	3089	rBV2	19306	15097	1.60%	0.217%

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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_G\Methods\8270-BG043024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	21.248	3104	3108	3111	rBV4	44979	68081	7.23%	0.977%
38	21.565	3155	3162	3167	rBV3	315762	683214	72.60%	9.808%
39	21.613	3168	3170	3179	rVB	114848	169400	18.00%	2.432%
40	24.691	3690	3694	3703	rVB2	84328	199219	21.17%	2.860%

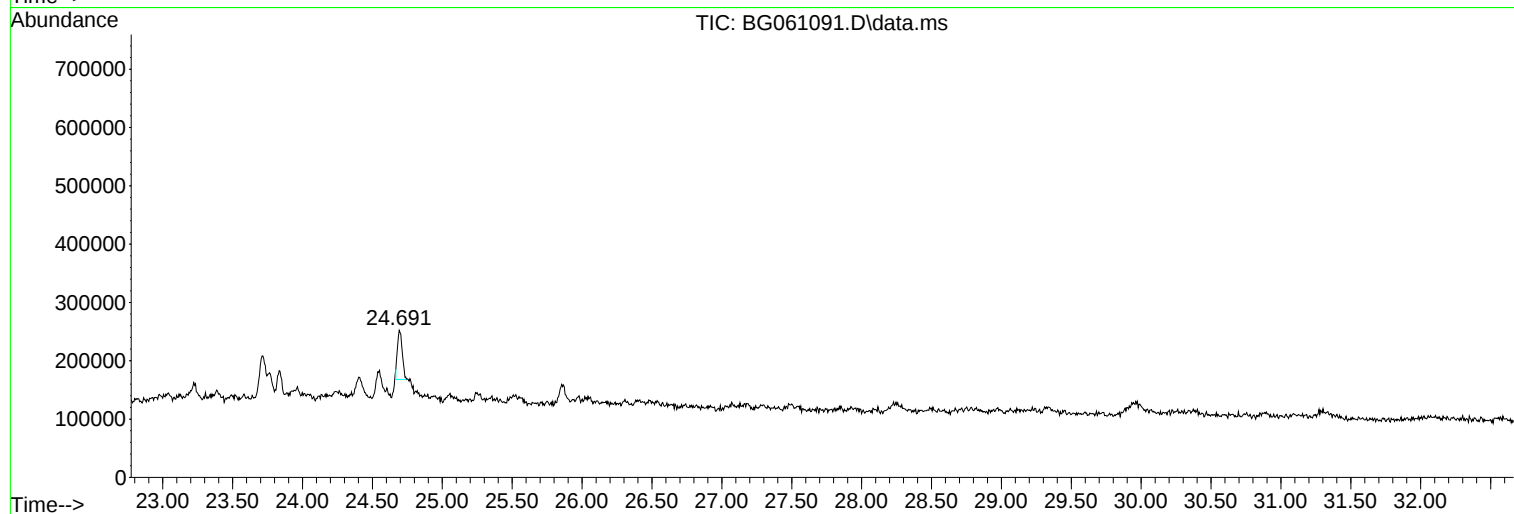
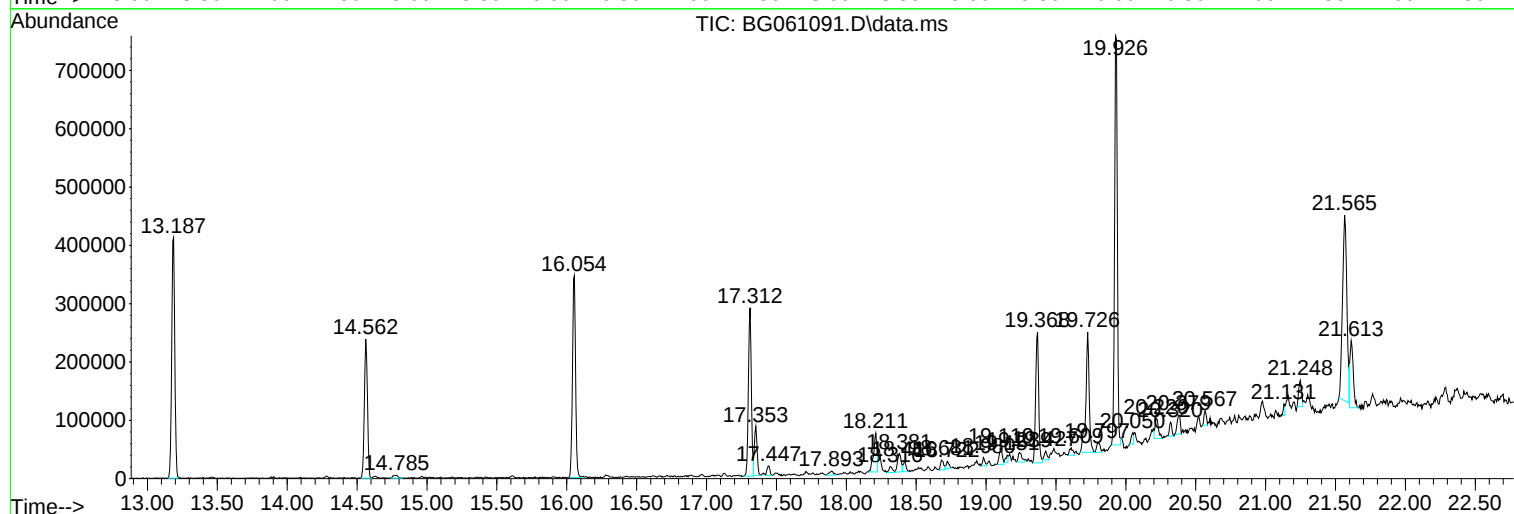
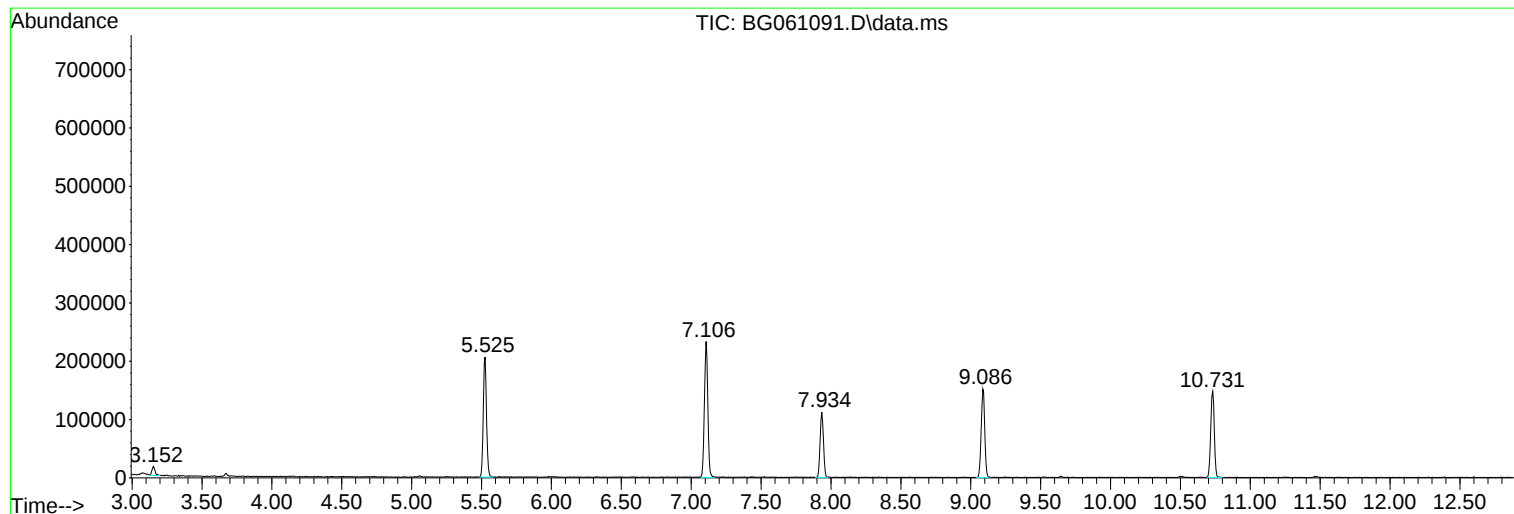
Sum of corrected areas: 6965867

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G-2(0.5-1.5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.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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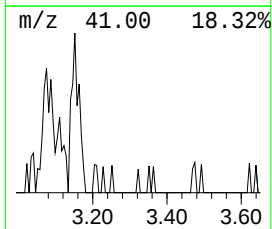
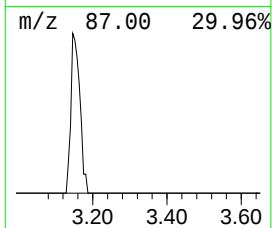
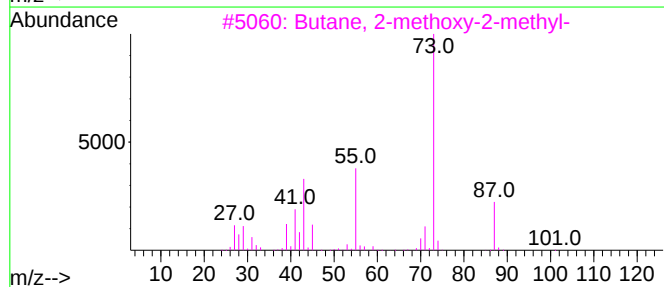
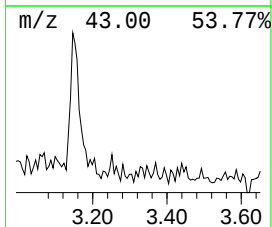
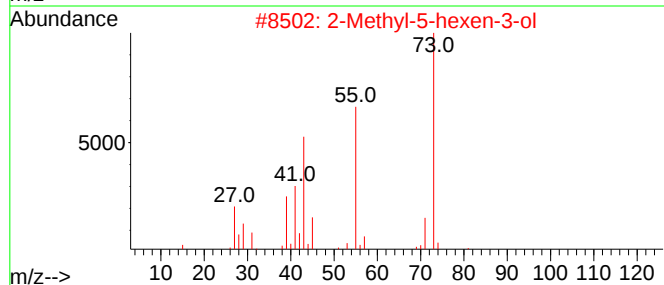
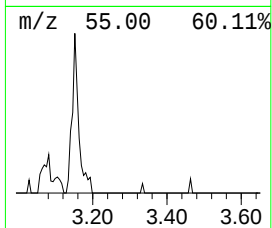
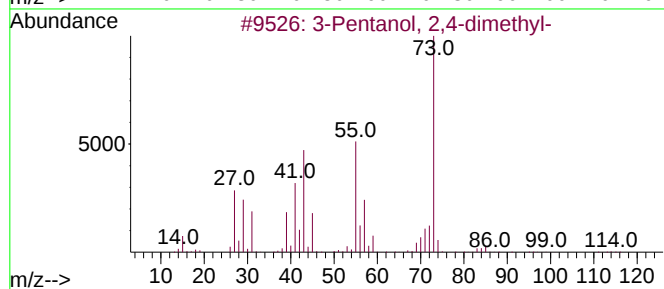
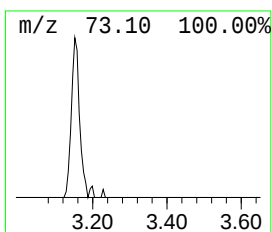
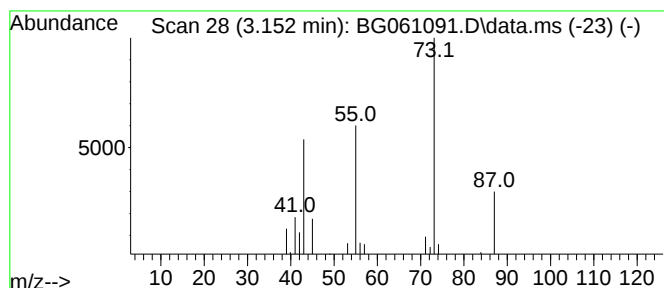
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown3.152 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.152	2.65 ng	24477	1,4-Dichlorobenzene-d4	7.934

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	42	
2	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	25	
3	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	25	
4	1-Hepten-4-ol	114	C7H14O	003521-91-3	12	
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9	



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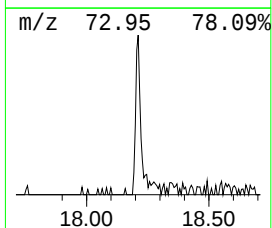
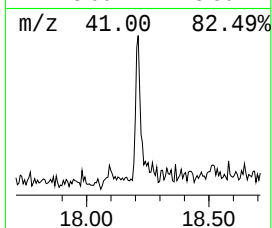
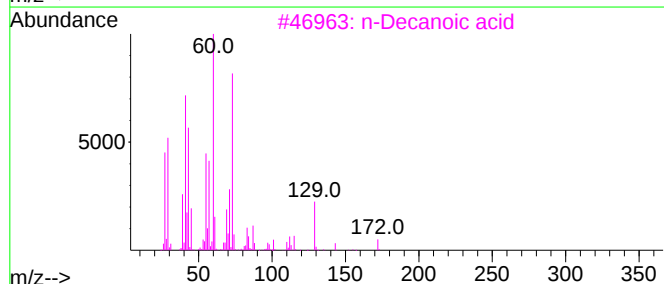
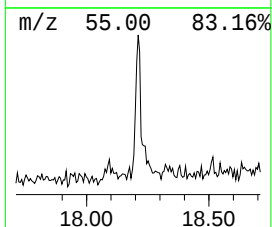
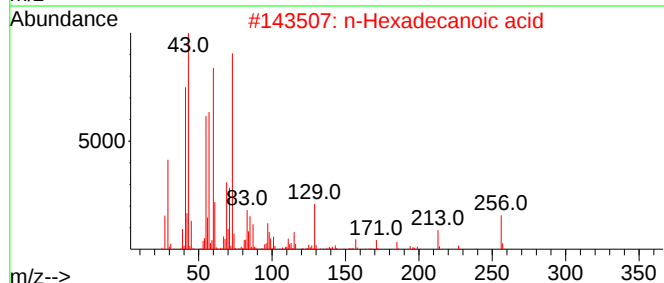
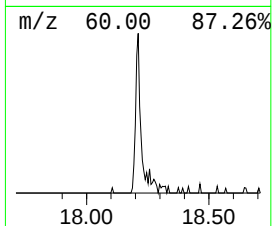
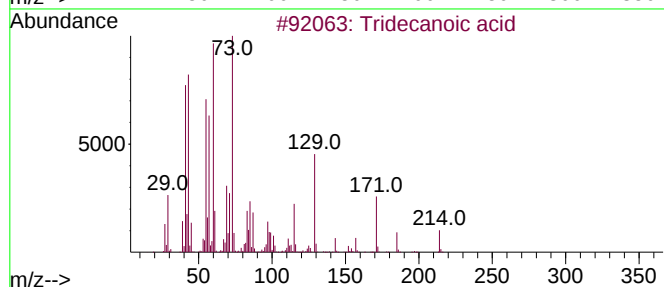
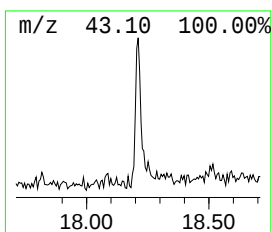
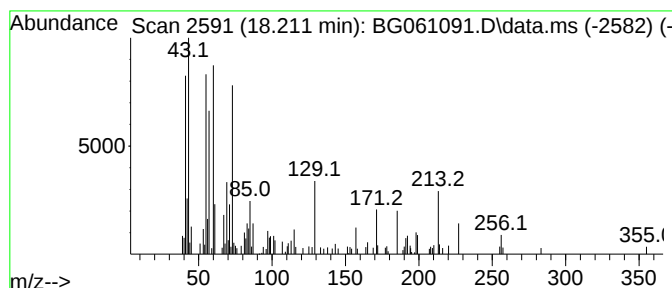
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Tridecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.211	5.19 ng	112380	Phenanthrene-d10	17.312

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecanoic acid	214	C13H26O2	000638-53-9	64
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	50
3			n-Decanoic acid	172	C10H20O2	000334-48-5	45
4			Nonanoic acid	158	C9H18O2	000112-05-0	43
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	35



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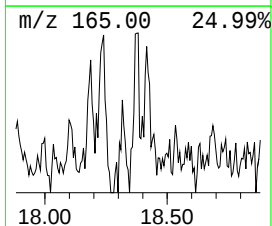
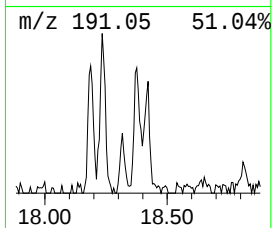
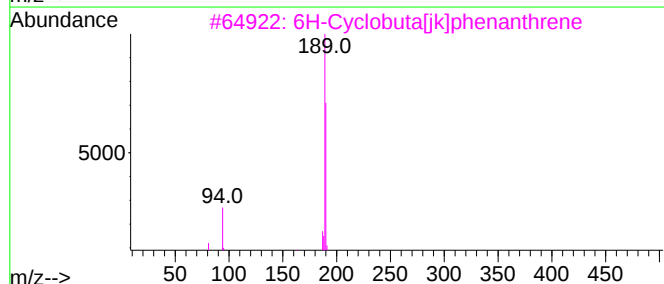
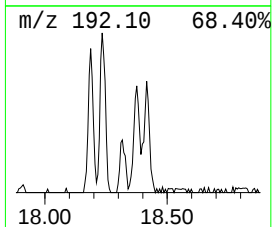
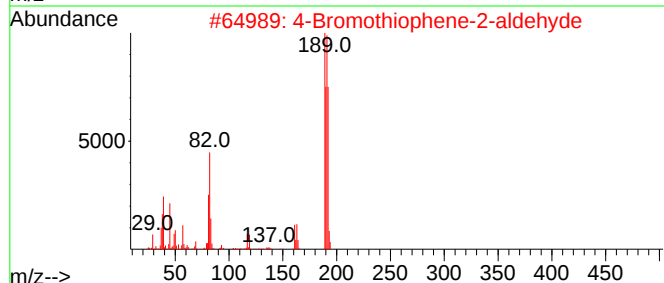
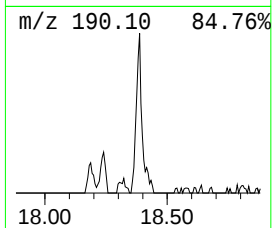
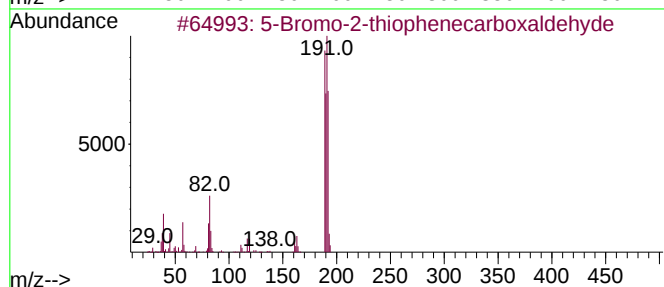
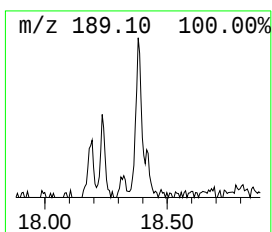
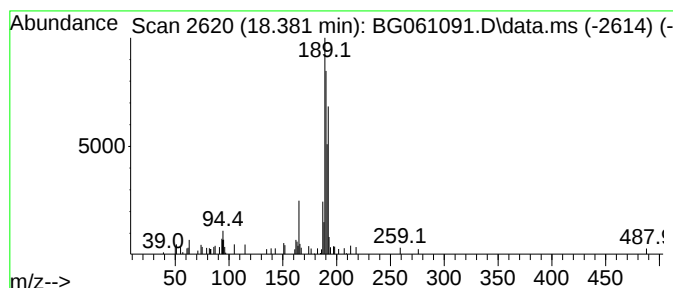
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 5-Bromo-2-thiophenecarboxal... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.381	2.62 ng	56739	Phenanthrene-d10	17.312

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		5-Bromo-2-thiophenecarboxaldehyde	190	C5H3BrOS	004701-17-1	50
2		4-Bromothiophene-2-aldehyde	190	C5H3BrOS	018791-75-8	50
3		6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	47
4		1H-Pyrazole-4-carboxaldehyde, 1-...	190	C10H7FN2O	1000338-05-6	46
5		4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	38



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown3.152	3.152	2.6	ng	24477	1	7.934	184862	20.0
Tridecanoic acid	18.211	5.2	ng	112380	4	17.312	433385	20.0
5-Bromo-2-thiop...	18.381	2.6	ng	56739	4	17.312	433385	20.0