LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040623\
Data File : BG057020.D
Acq On : 6 Apr 2023 20:26
Operator : CG/JU
Sample : 02126-03 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RS-C

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-BG033023.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057020.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.442	318	324	331	rBV	44620	76316	17.24%	1.758%
2	5.924	400	406	414	rBB	117175	193426	43.70%	4.456%
3	7.545	674	682	691	rBV	123957	214544	48.47%	4.942%
4	8.409	821	829	836	rBB	72196	125385	28.33%	2.888%
5	9.584	1021	1029	1039	rBB	72546	128590	29.05%	2.962%
6	11.252	1306	1313	1320	rBV	96028	168822	38.14%	3.889%
7	13.649	1713	1721	1728	rVB	205000	308271	69.64%	7.102%
8	14.759	1906	1910	1919	rVB	2688	4588	1.04%	0.106%
9	15.023	1947	1955	1961	rBV	158687	244199	55.17%	5.626%
10	16.357	2179	2182	2187	rVB3	3175	4449	1.01%	0.102%
11	16.498	2200	2206	2214	rBV	160067	244627	55.26%	5.635%
12	17.761	2415	2421	2425	rBV	185557	285523	64.50%	6.578%
13	17.802	2425	2428	2436	rVB	41625	58855	13.30%	1.356%
14	17.896	2438	2444	2447	rBV2	6864	12086	2.73%	0.278%
15	18.160	2485	2489	2493	rVB2	4614	7588	1.71%	0.175%
16	18.201	2493	2496	2502	rVB3	3103	4693	1.06%	0.108%
17	18.595	2559	2563	2566	rBV2	25286	35041	7.92%	0.807%
18	18.677	2573	2577	2582	rVB2	14654	22220	5.02%	0.512%
19	18.748	2587	2589	2595	rVB5	3934	6237	1.41%	0.144%
20	18.824	2595	2602	2605	rBV3	13728	30700	6.94%	0.707%
21	19.012	2632	2634	2639	rVB6	5213	5211	1.18%	0.120%
22	19.106	2646	2650	2655	rBV4	8143	13105	2.96%	0.302%
23	19.159	2655	2659	2664	rVB5	10194	15403	3.48%	0.355%
24	19.406	2698	2701	2703	rBV4	5215	5505	1.24%	0.127%
25	19.523	2717	2721	2725	rVB5	13343	17603	3.98%	0.406%
26	19.676	2742	2747	2750	rVB7	8612	15020	3.39%	0.346%
27	19.787	2761	2766	2771	rVB	140914	199728	45.12%	4.601%
28	19.840	2773	2775	2778	rVB4	5924	4971	1.12%	0.115%
29	20.028	2804	2807	2808	rBV3	5468	5462	1.23%	0.126%
30	20.116	2817	2822	2823	rBV	22436	32080	7.25%	0.739%
31	20.152	2823	2828	2834	rVB	139154	214414	48.44%	4.939%
32	20.216	2834	2839	2842	rBV5	16247	25023	5.65%	0.576%
33	20.328	2852	2858	2863	rBV	347208	442662	100.00%	10.198%
34	20.463	2878	2881	2888	rVB3	14491	32661	7.38%	0.752%
35	20.516	2888	2890	2891	rBV2	7892	6411	1.45%	0.148%
36	21.420	3042	3044	3050	rVB3	16240	25263	5.71%	0.582%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040623\
Data File : BG057020.D
Acq On : 6 Apr 2023 20:26
Operator : CG/JU
Sample : 02126-03 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RS-C

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-BG033023.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	21.638	3078	3081	3084	rBV3	16742	18104	4.09%	0.417%
38	22.084	3148	3157	3161	rBV2	173558	417129	94.23%	9.609%
39	22.131	3162	3165	3171	rVB	65058	101069	22.83%	2.328%
40	24.493	3559	3567	3575	rBV2	49603	189935	42.91%	4.375%
41	25.450	3725	3730	3741	rVB2	45282	137029	30.96%	3.157%
42	25.626	3753	3760	3770	rVB2	81944	240928	54.43%	5.550%

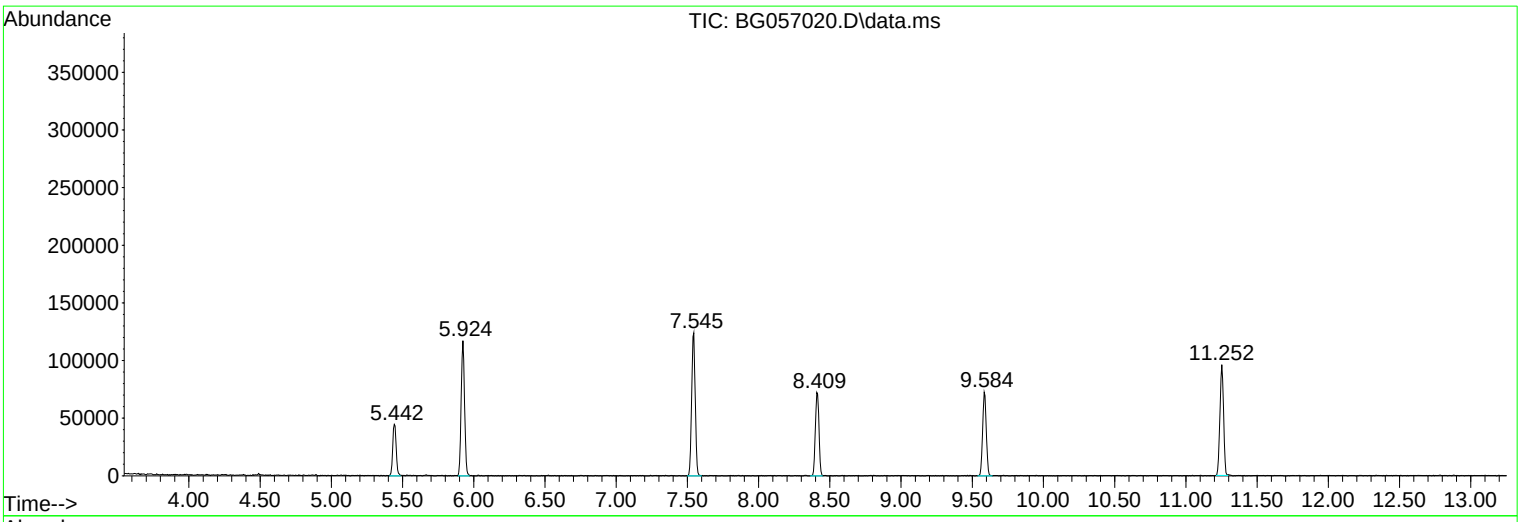
Sum of corrected areas: 4340876

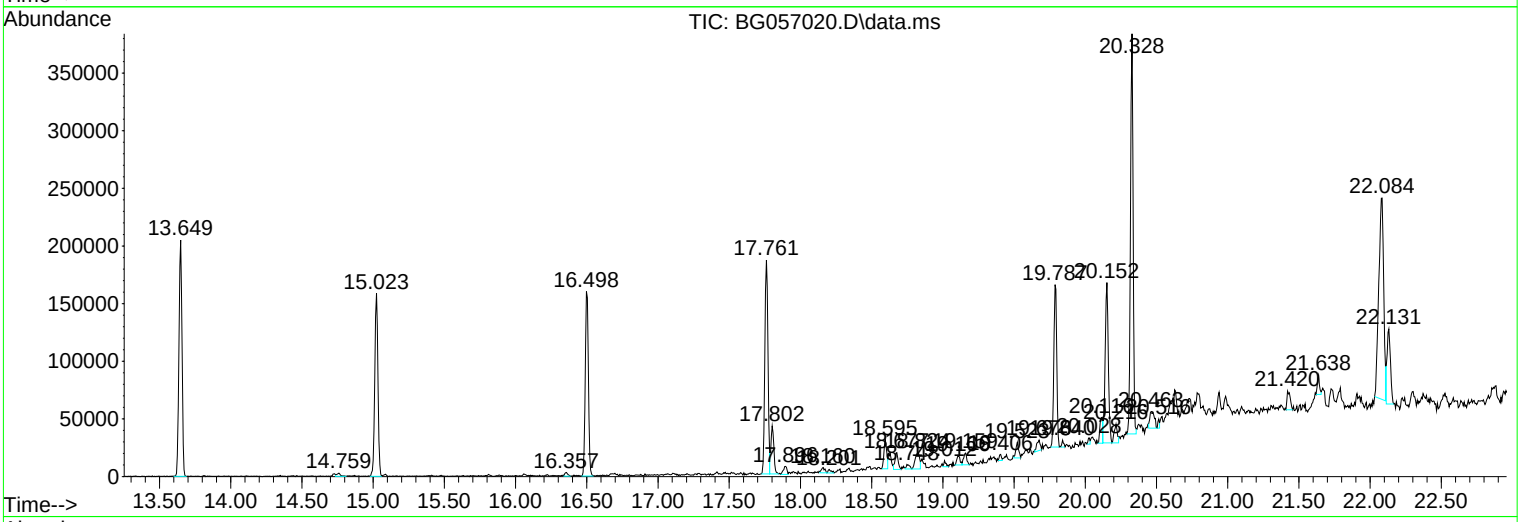
Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040623\
Data File : BG057020.D
Acq On : 6 Apr 2023 20:26
Operator : CG/JU
Sample : 02126-03 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

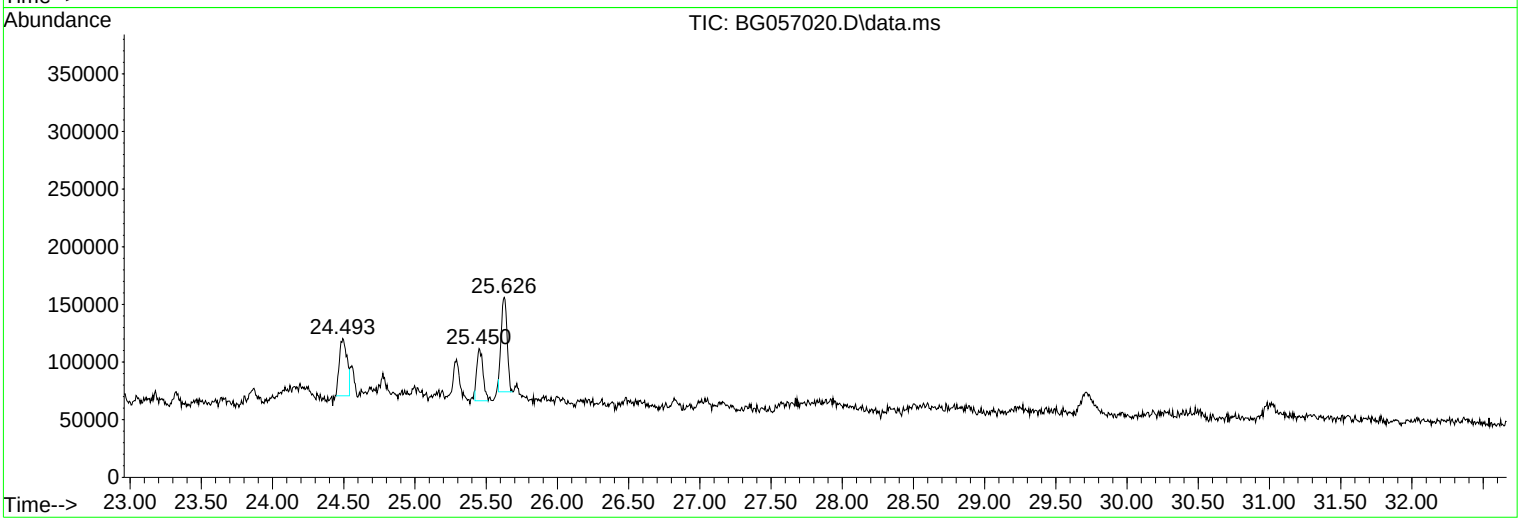
Instrument :
BNA_G
ClientSampleId :
RS-C

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG033023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040623\
Data File : BG057020.D
Acq On : 6 Apr 2023 20:26
Operator : CG/JU
Sample : 02126-03 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RS-C

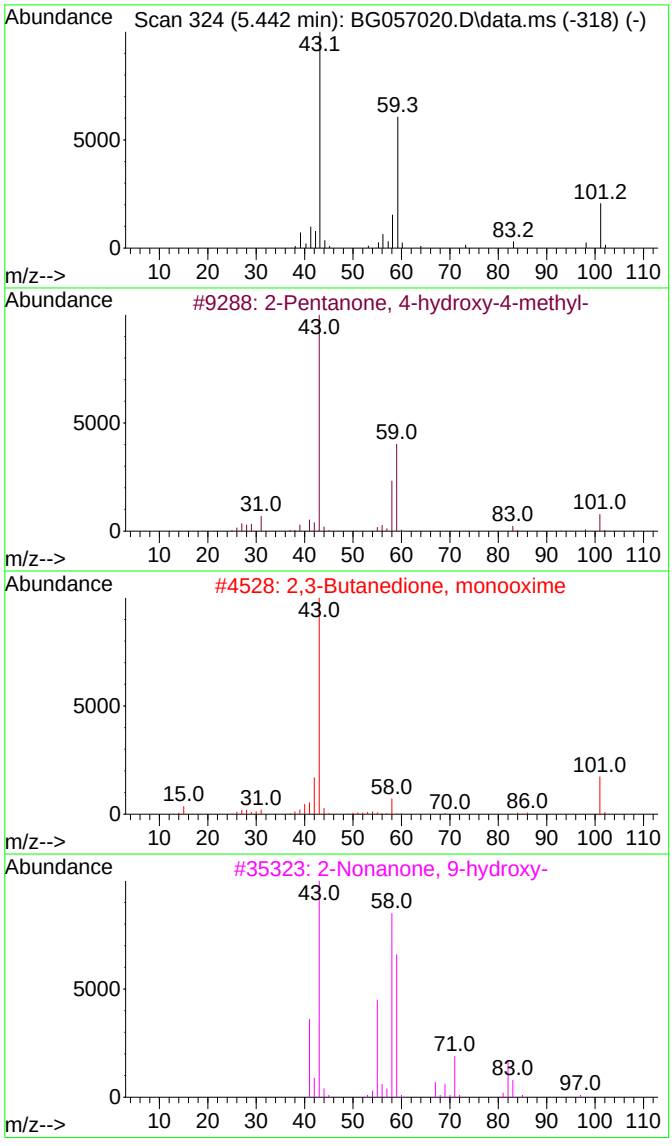
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG033023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

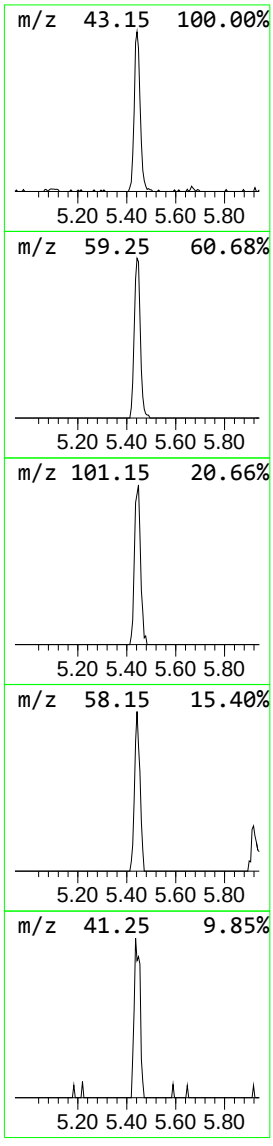
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.442	12.17 ng	76316	1,4-Dichlorobenzene-d4	8.409

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	38
3	2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	28
4	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	25
5	1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040623\
Data File : BG057020.D
Acq On : 6 Apr 2023 20:26
Operator : CG/JU
Sample : 02126-03 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RS-C

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG033023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

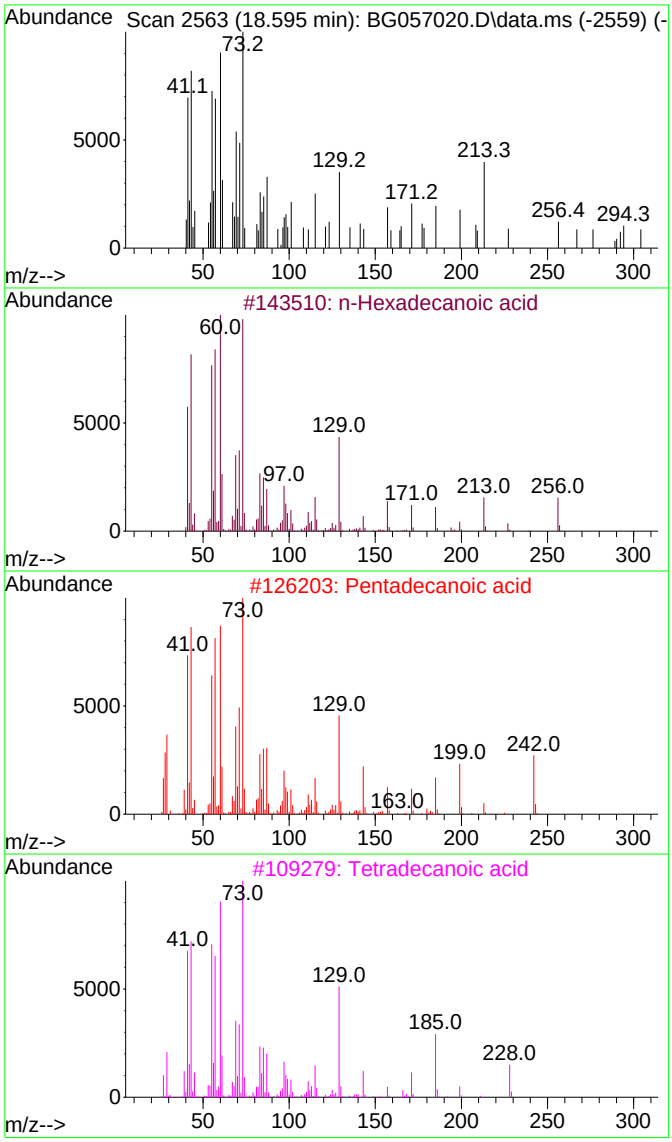
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

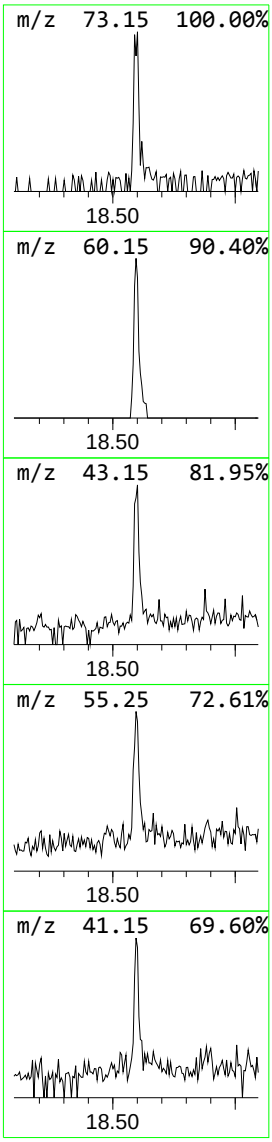
****

Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.595	2.45 ng	35041	Phenanthrene-d10	17.761

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	92
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	53
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	49
4	Tridecanoic acid	214	C13H26O2	000638-53-9	49
5	Dodecanoic acid	200	C12H24O2	000143-07-7	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040623\
Data File : BG057020.D
Acq On : 6 Apr 2023 20:26
Operator : CG/JU
Sample : 02126-03 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RS-C

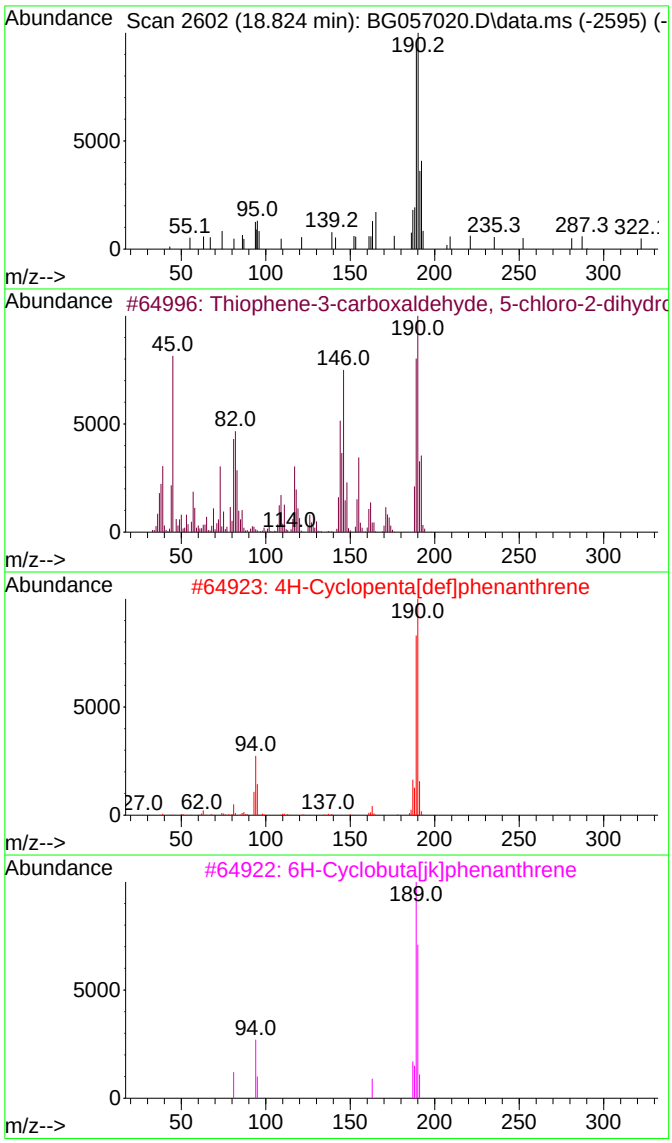
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG033023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

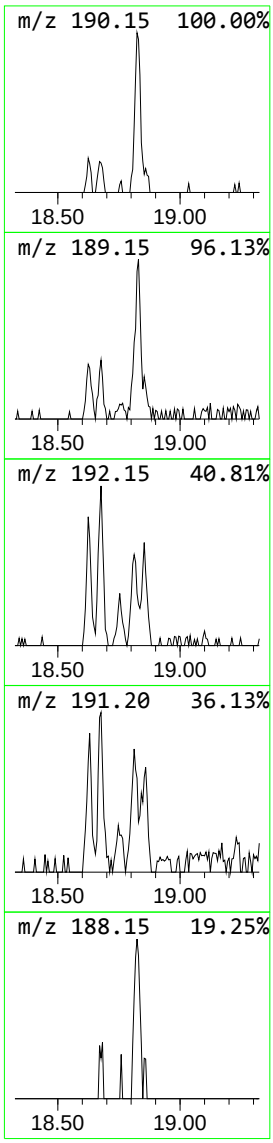
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Thiophene-3-carboxaldehyde,... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.824	2.15 ng	30700	Phenanthrene-d10	17.761

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	72
2	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	58
3	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	52
4	1H-Pyrazole-4-carboxaldehyde, 1-...	190	C10H7FN2O	1000338-05-6	47
5	Cyclopenta[c]pyran-4-carboxylic ...	190	C11H10O3	063785-74-0	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040623\
Data File : BG057020.D
Acq On : 6 Apr 2023 20:26
Operator : CG/JU
Sample : 02126-03 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RS-C

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG033023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-...	5.442	12.2	ng	76316	1	8.409	125385	20.0
n-Hexadecanoic ...	18.595	2.5	ng	35041	4	17.761	285523	20.0
Thiophene-3-car...	18.824	2.1	ng	30700	4	17.761	285523	20.0