LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052223\
Data File : BG057510.D
Acq On : 23 May 2023 2:13
Operator : CG/JU
Sample : 02847-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TR-04-051823

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-BG042723.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057510.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.388	310	315	322	rBV	18163	29216	2.35%	0.335%
2	5.875	391	398	408	rBV	307161	520030	41.83%	5.954%
3	7.502	667	675	691	rVB	317733	577202	46.42%	6.609%
4	8.354	814	820	828	rVB	89733	145092	11.67%	1.661%
5	9.535	1014	1021	1034	rVB	201710	368931	29.67%	4.224%
6	11.191	1296	1303	1310	rVV	110377	193610	15.57%	2.217%
7	12.355	1494	1501	1506	rBV3	10610	16727	1.35%	0.192%
8	12.543	1528	1533	1537	rBV3	8488	12681	1.02%	0.145%
9	13.060	1613	1621	1626	rVB6	8629	17006	1.37%	0.195%
10	13.594	1705	1712	1719	rVB	577779	875230	70.39%	10.021%
11	13.759	1731	1740	1745	rBV3	11849	19799	1.59%	0.227%
12	14.816	1914	1920	1925	rVB2	11795	17156	1.38%	0.196%
13	14.969	1936	1946	1953	rVB	171116	274842	22.11%	3.147%
14	15.756	2075	2080	2085	rVB2	13751	21180	1.70%	0.243%
15	16.302	2168	2173	2179	rVB	58623	86166	6.93%	0.987%
16	16.449	2192	2198	2205	rBV	408433	630741	50.73%	7.222%
17	16.614	2221	2226	2229	rBV2	14132	20108	1.62%	0.230%
18	17.401	2357	2360	2366	rBV2	12590	16596	1.33%	0.190%
19	17.706	2406	2412	2417	rBV	214007	334727	26.92%	3.833%
20	17.747	2417	2419	2425	rVB	42130	53412	4.30%	0.612%
21	17.841	2430	2435	2439	rBV2	9870	16651	1.34%	0.191%
22	18.147	2483	2487	2492	rVB	11136	16352	1.32%	0.187%
23	18.317	2507	2516	2522	rVB	130858	169707	13.65%	1.943%
24	18.546	2550	2555	2564	rBV4	53896	108652	8.74%	1.244%
25	18.623	2564	2568	2575	rVV	19017	31165	2.51%	0.357%
26	18.775	2586	2594	2597	rVV4	22313	45268	3.64%	0.518%
27	18.816	2599	2601	2606	rVB	11781	15764	1.27%	0.180%
28	18.975	2620	2628	2630	rBV8	7190	15577	1.25%	0.178%
29	19.057	2638	2642	2646	rBV2	8597	12483	1.00%	0.143%
30	19.116	2648	2652	2658	rVB7	10454	18016	1.45%	0.206%
31	19.445	2703	2708	2710	rBV	583754	728578	58.60%	8.342%
32	19.474	2710	2713	2724	rVB2	298406	446676	35.93%	5.114%
33	19.598	2731	2734	2742	rBV2	65725	79934	6.43%	0.915%
34	19.739	2753	2758	2764	rVB	114586	164618	13.24%	1.885%
35	20.062	2809	2813	2815	rBV2	20476	31619	2.54%	0.362%
36	20.103	2815	2820	2826	rVV	119135	173813	13.98%	1.990%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052223\
Data File : BG057510.D
Acq On : 23 May 2023 2:13
Operator : CG/JU
Sample : 02847-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TR-04-051823

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-BG042723.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	20.162	2826	2830	2836	rVB5	11868	17915	1.44%	0.205%
38	20.279	2844	2850	2855	rBV	937071	1243338	100.00%	14.236%
39	20.579	2899	2901	2908	rVB	25476	34861	2.80%	0.399%
40	20.679	2915	2918	2922	rVB	23274	28695	2.31%	0.329%
41	20.878	2950	2952	2957	rBV2	11336	15492	1.25%	0.177%
42	21.572	3066	3070	3083	rVB6	43241	108144	8.70%	1.238%
43	22.012	3136	3145	3151	rBV2	211420	486472	39.13%	5.570%
44	22.065	3151	3154	3161	rVB	48150	82407	6.63%	0.944%
45	24.397	3545	3551	3560	rBV	40829	123063	9.90%	1.409%
46	25.513	3734	3741	3751	rVB	102340	287936	23.16%	3.297%

Sum of corrected areas: 8733648

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052223\
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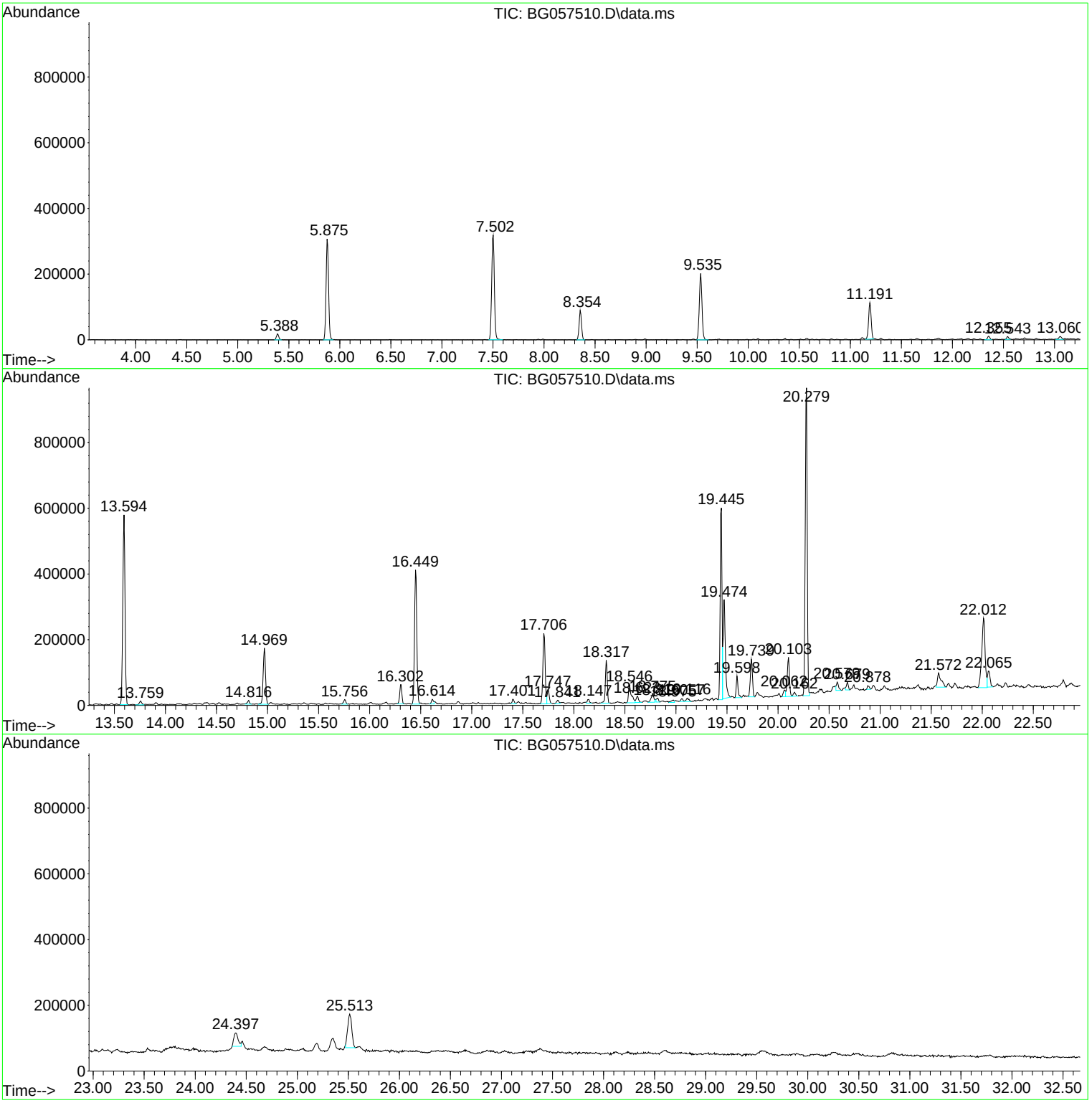
Acq On : 23 May 2023 2:13
Operator : CG/JU
Sample : 02847-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TR-04-051823

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042723.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\BG052223\
Data File : BG057510.D
Acq On : 23 May 2023 2:13
Operator : CG/JU
Sample : 02847-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TR-04-051823

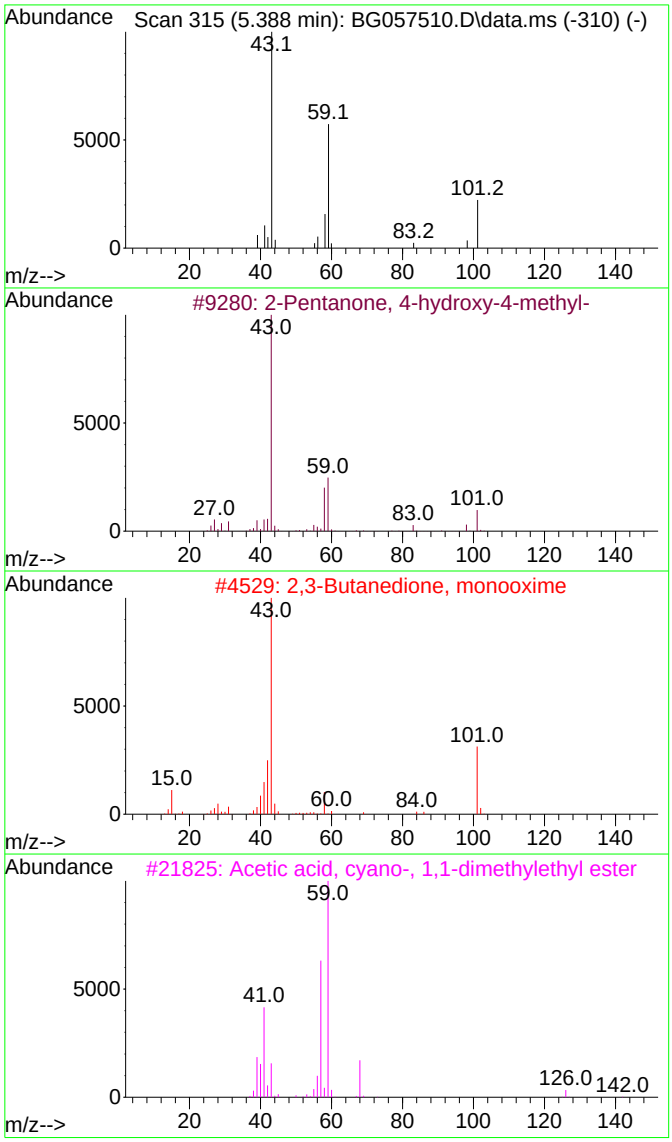
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

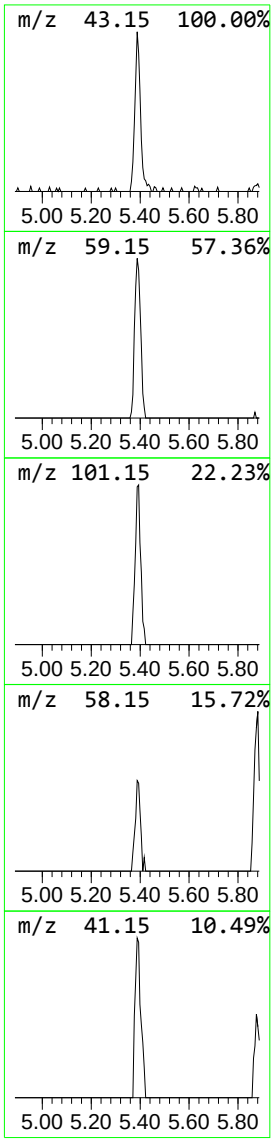
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.388	4.03 ng	29216	1,4-Dichlorobenzene-d4	8.354

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	9
4	3-Octanol	130	C8H18O	000589-98-0	9
5	2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052223\
Data File : BG057510.D
Acq On : 23 May 2023 2:13
Operator : CG/JU
Sample : 02847-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TR-04-051823

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

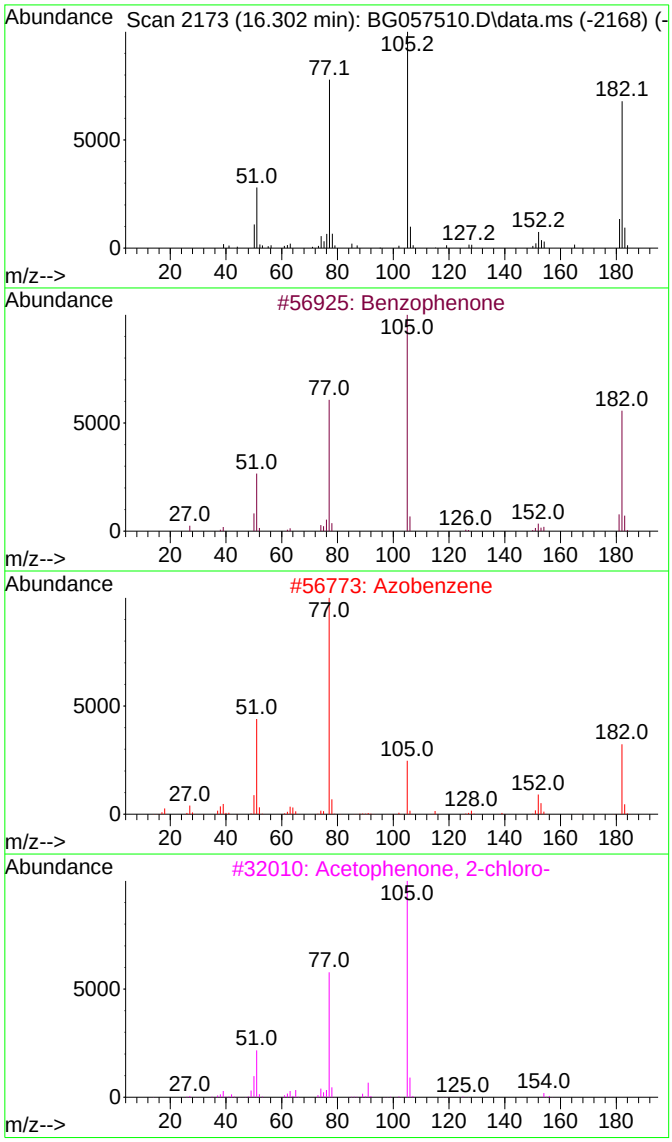
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

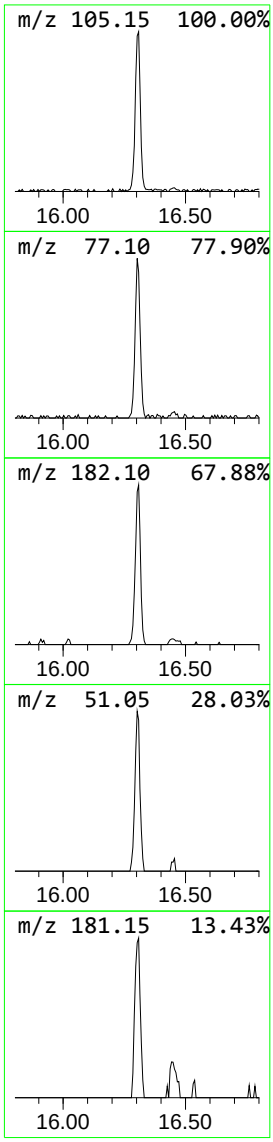
****

Peak Number 2 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.302	6.27 ng	86166	Acenaphthene-d10	14.969

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	Azobenzene	182	C12H10N2	000103-33-3	53
3	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	52
4	Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	52
5	Benzoylformic acid	150	C8H6O3	000611-73-4	52





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052223\
Data File : BG057510.D
Acq On : 23 May 2023 2:13
Operator : CG/JU
Sample : 02847-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TR-04-051823

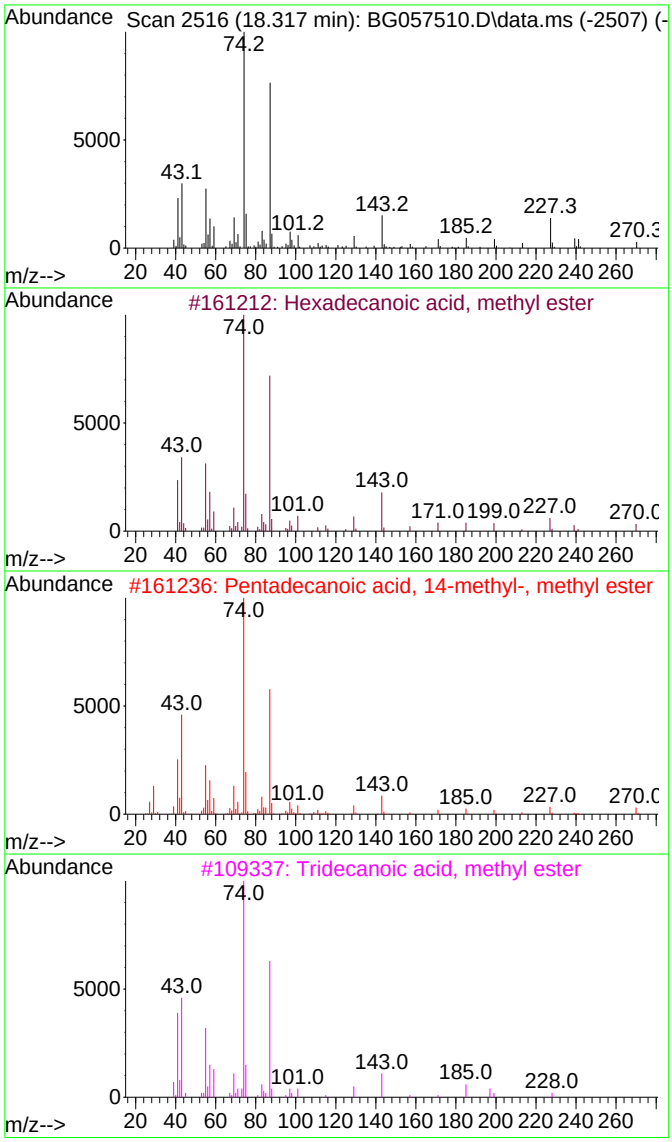
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

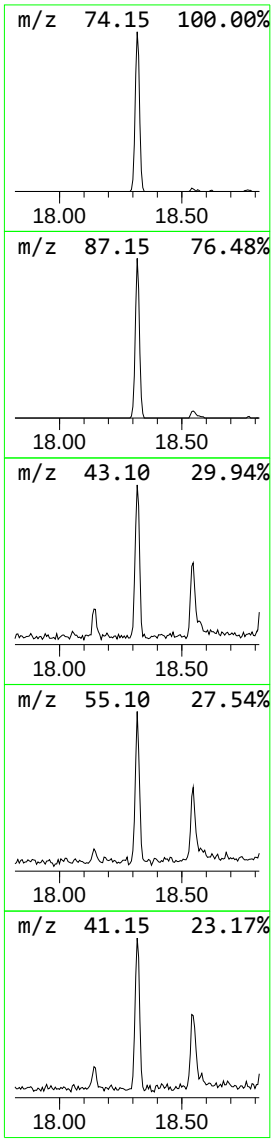
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Hexadecanoic acid, methyl e... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.317	10.14 ng	169707	Phenanthrene-d10	17.706

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	93
3	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	91
4	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86
5	Methyl tetradecanoate	242	C15H30O2	000124-10-7	83





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052223\
Data File : BG057510.D
Acq On : 23 May 2023 2:13
Operator : CG/JU
Sample : 02847-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TR-04-051823

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

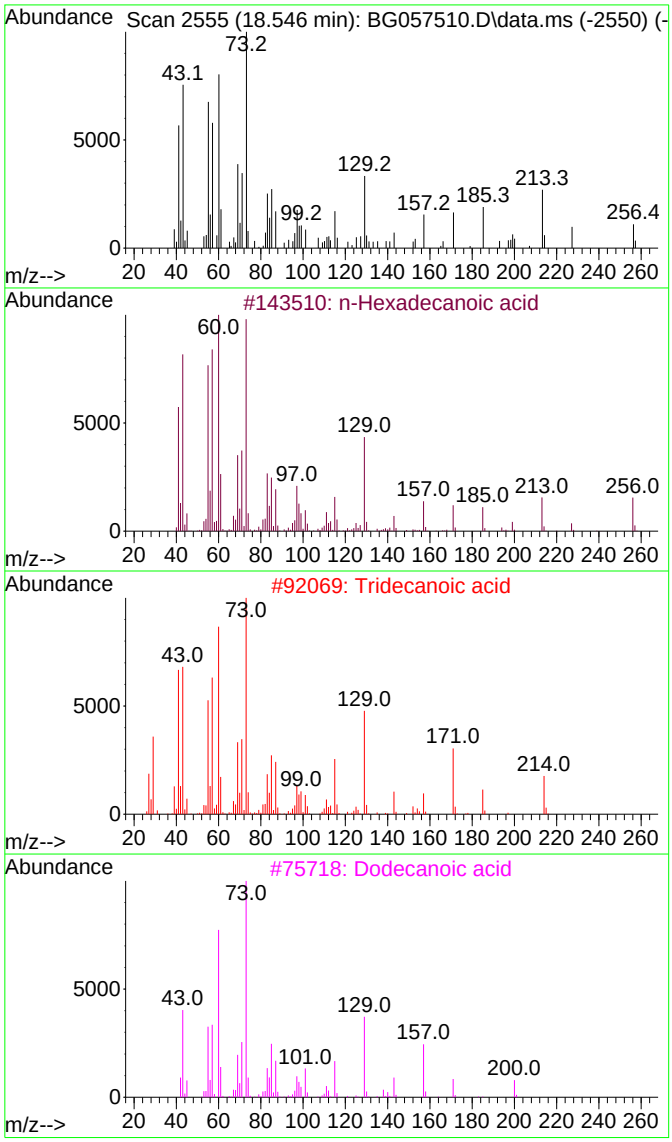
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

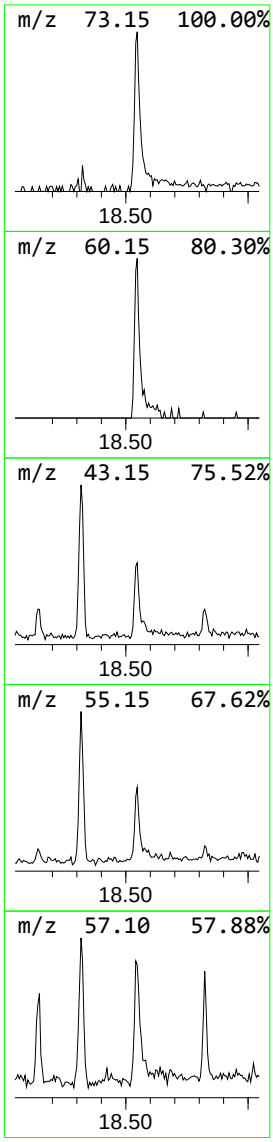
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.546	6.49 ng	108652	Phenanthrene-d10	17.706

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	97
3	Dodecanoic acid	200	C12H24O2	000143-07-7	86
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	68
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	68





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052223\
Data File : BG057510.D
Acq On : 23 May 2023 2:13
Operator : CG/JU
Sample : 02847-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TR-04-051823

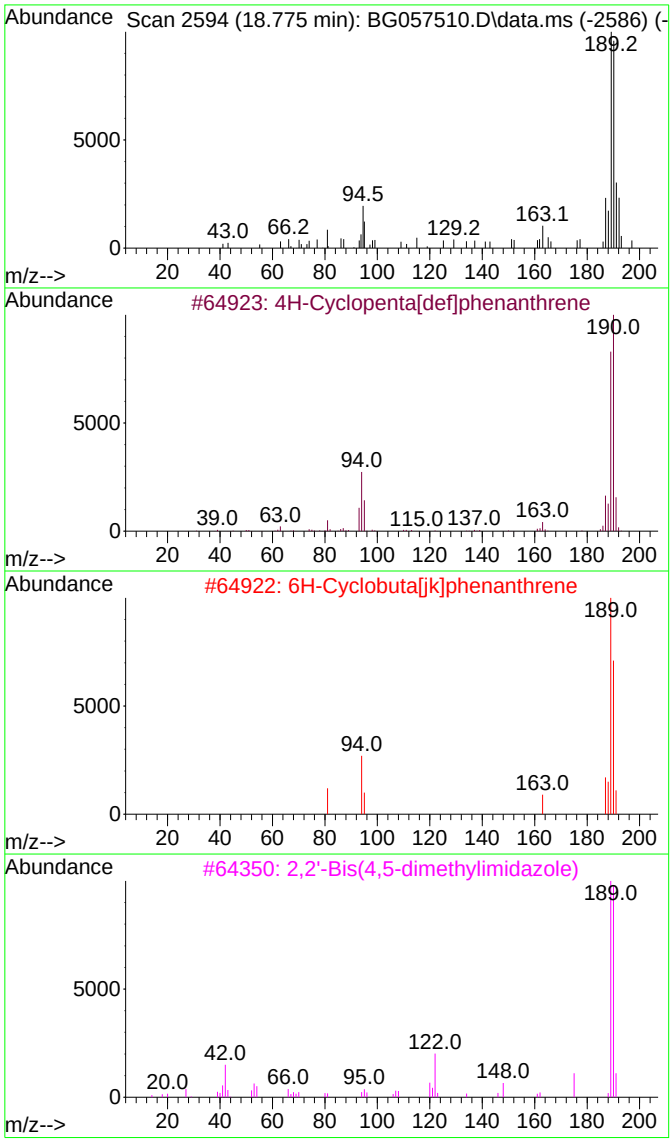
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

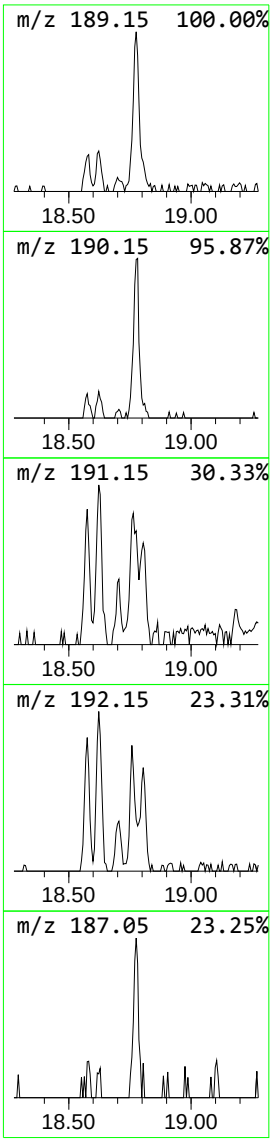
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.775	2.70 ng	45268	Phenanthrene-d10	17.706

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	87
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	83
3	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	50
4	2-Chloro-1-(2-propynyl)-1H-benzi...	190	C10H7ClN2	080276-19-3	43
5	5,8-Quinoxalinediol, 2,3-dimethyl-	190	C10H10N2O2	007698-00-2	27





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052223\
Data File : BG057510.D
Acq On : 23 May 2023 2:13
Operator : CG/JU
Sample : 02847-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TR-04-051823

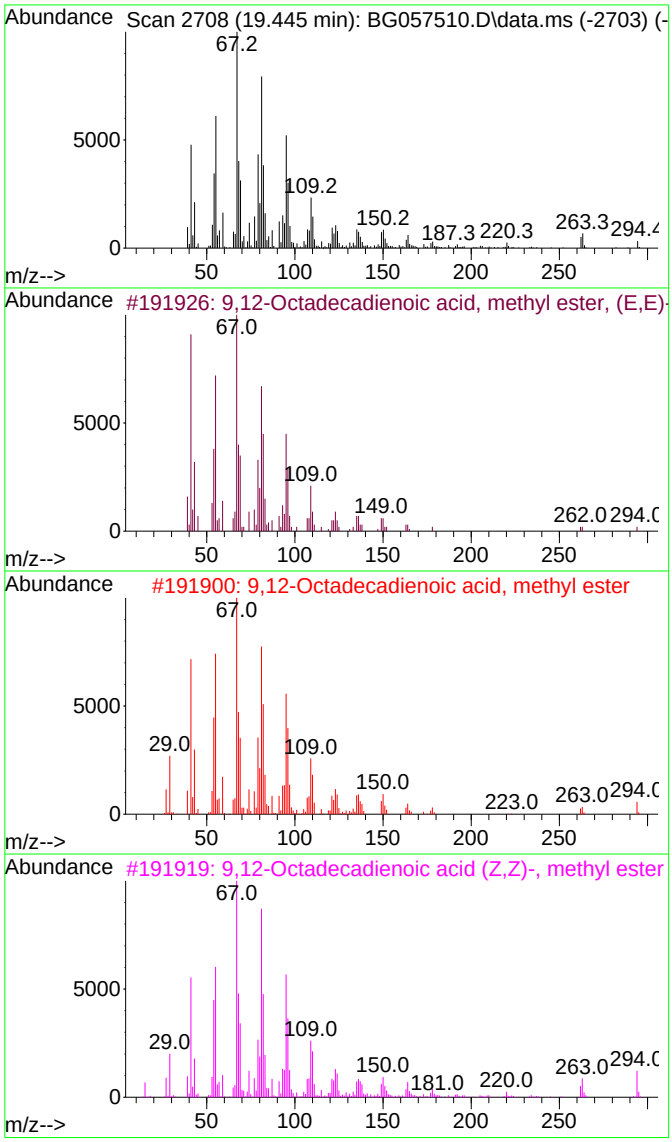
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

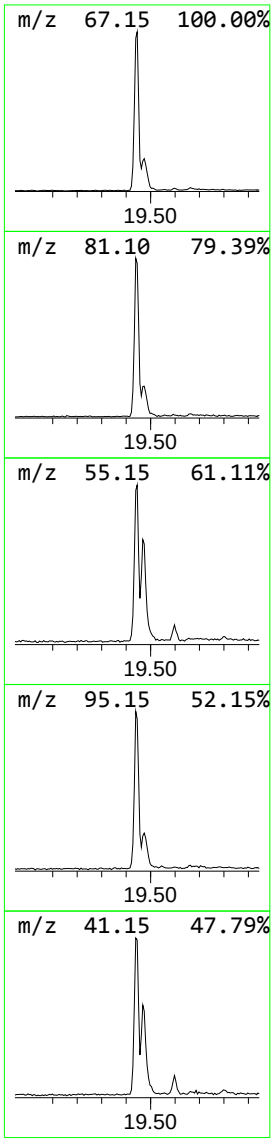
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 9,12-Octadecadienoic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.445	43.53 ng	728578	Phenanthrene-d10	17.706

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
2	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
3	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	98
4	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	98
5	Methyl 10-trans,12-cis-octadecad...	294	C19H34O2	1000336-44-2	93





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052223\
Data File : BG057510.D
Acq On : 23 May 2023 2:13
Operator : CG/JU
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Instrument :
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ClientSampleId :
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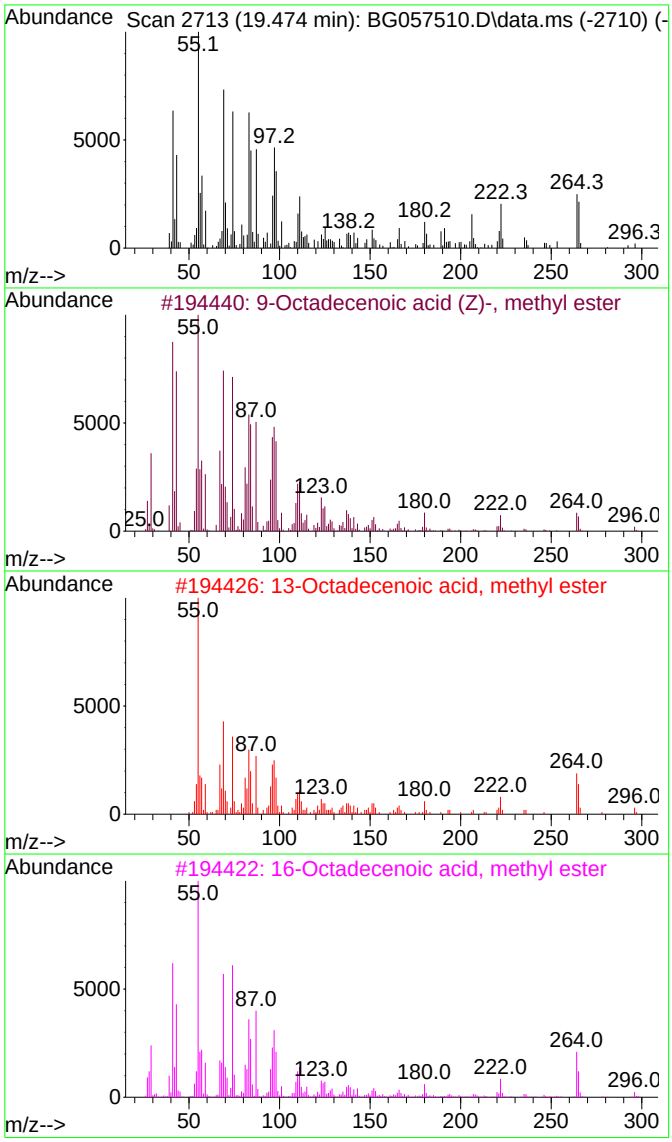
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

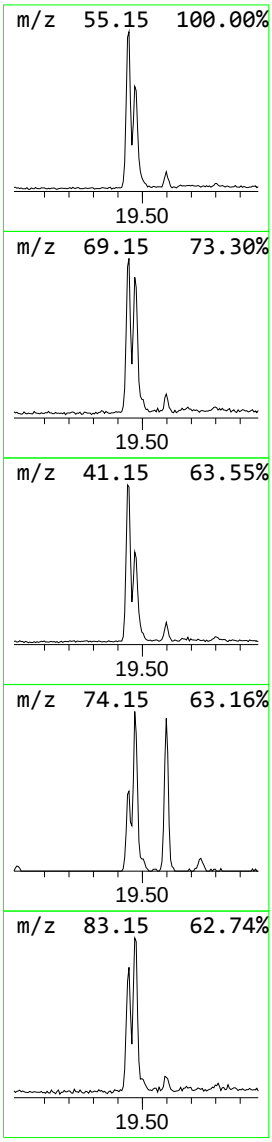
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 9-Octadecenoic acid (Z)-, m... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.474	26.69 ng	446676	Phenanthrene-d10	17.706

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	90
2	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	70
3	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	70
4	12-Octadecenoic acid, methyl ester	296	C19H36O2	056554-46-2	47
5	3-Octadecenoic acid, methyl ester	296	C19H36O2	056599-33-8	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052223\
Data File : BG057510.D
Acq On : 23 May 2023 2:13
Operator : CG/JU
Sample : 02847-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TR-04-051823

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

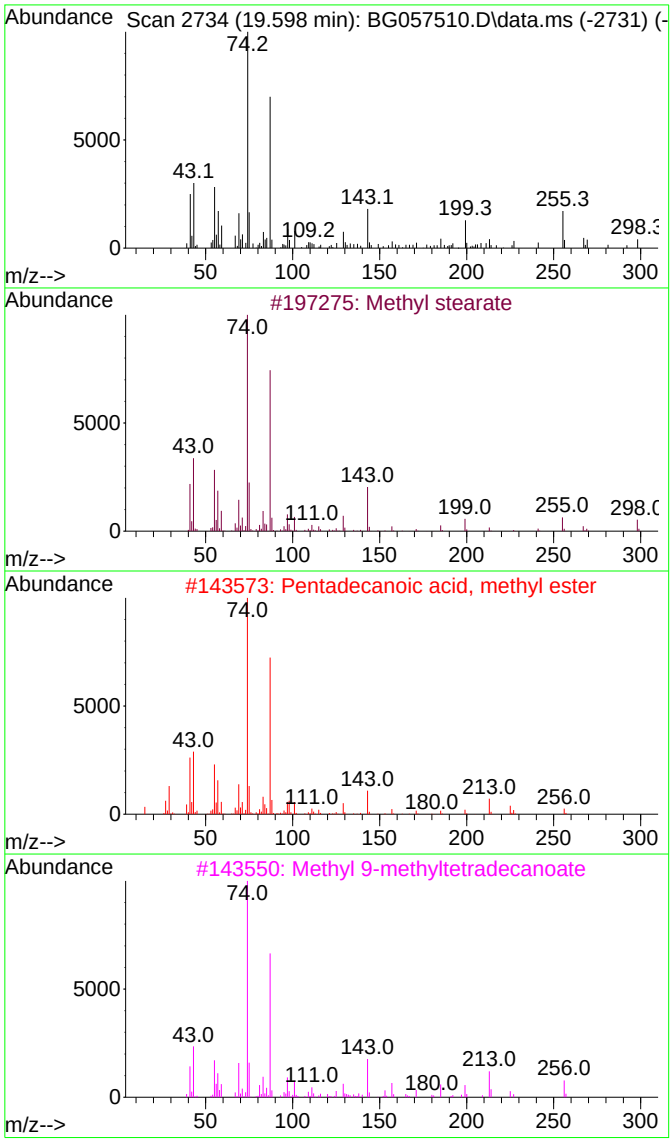
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

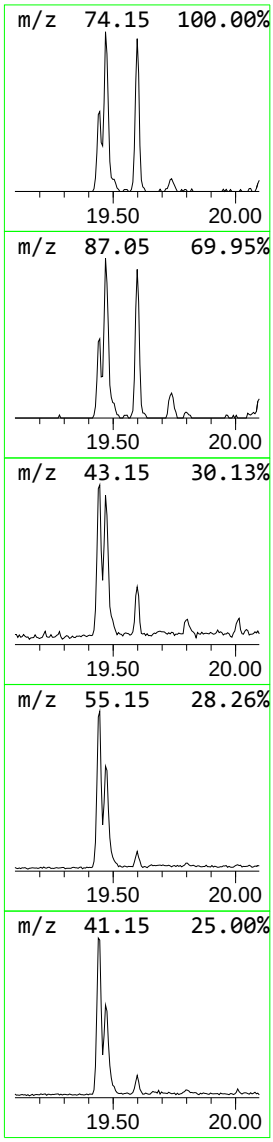
****

Peak Number 8 Methyl stearate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.598	4.78 ng	79934	Phenanthrene-d10	17.706

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl stearate	298	C19H38O2	000112-61-8	91
2	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	90
3	Methyl 9-methyltetradecanoate	256	C16H32O2	213617-69-7	81
4	Tridecanoic acid, 12-methyl-, me...	242	C15H30O2	005129-58-8	74
5	2-Methyloctadecanoic acid	298	C19H38O2	007217-83-6	74





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052223\
Data File : BG057510.D
Acq On : 23 May 2023 2:13
Operator : CG/JU
Sample : 02847-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TR-04-051823

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

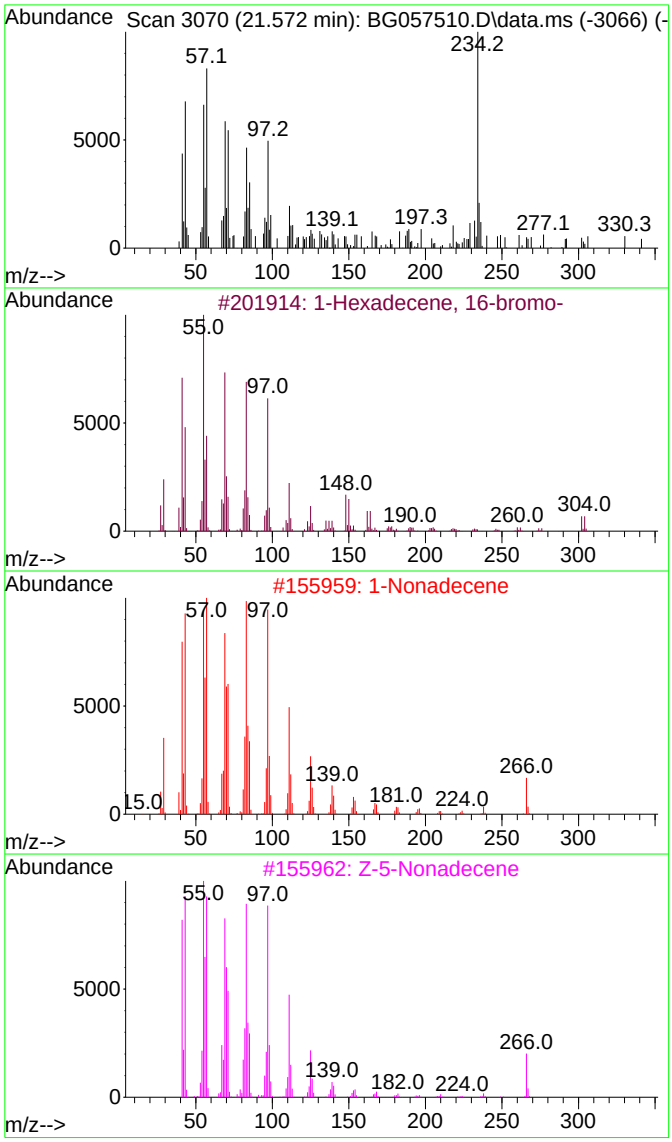
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

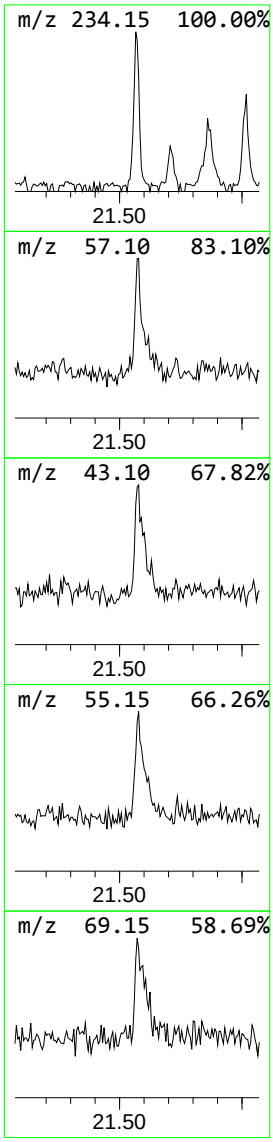
****

Peak Number 9 1-Hexadecene, 16-bromo- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.572	4.45 ng	108144	Chrysene-d12	22.012

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexadecene, 16-bromo-	302	C16H31Br	118625-56-2	52
2	1-Nonadecene	266	C19H38	018435-45-5	46
3	Z-5-Nonadecene	266	C19H38	1000131-11-8	46
4	1-Octadecene	252	C18H36	000112-88-9	46
5	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	45





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052223\
Data File : BG057510.D
Acq On : 23 May 2023 2:13
Operator : CG/JU
Sample : 02847-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TR-04-051823

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042723.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-...	5.388	4.0	ng	29216	1	8.354	145092	20.0
Benzophenone	16.302	6.3	ng	86166	3	14.969	274842	20.0
Hexadecanoic ac...	18.317	10.1	ng	169707	4	17.706	334727	20.0
n-Hexadecanoic ...	18.546	6.5	ng	108652	4	17.706	334727	20.0
4H-Cyclopenta[d...	18.775	2.7	ng	45268	4	17.706	334727	20.0
9,12-Octadecadi...	19.445	43.5	ng	728578	4	17.706	334727	20.0
9-Octadecenoic ...	19.474	26.7	ng	446676	4	17.706	334727	20.0
Methyl stearate	19.598	4.8	ng	79934	4	17.706	334727	20.0
1-Hexadecene, 1...	21.572	4.5	ng	108144	5	22.012	486472	20.0