LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102623\
Data File : BM042459.D
Acq On : 26 Oct 2023 19:09
Operator : MA/JU
Sample : 05010-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
343

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_M\Methods\8270-BM102123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM042459.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.075	313	321	328	rBV	530383	724881	12.70%	1.256%
2	5.522	390	397	410	rBV	2696399	3849872	67.48%	6.671%
3	7.151	665	674	686	rBV	2545530	4124661	72.29%	7.147%
4	7.992	811	817	829	rVB	773261	1189504	20.85%	2.061%
5	9.192	1012	1021	1032	rBV	1659263	2672853	46.85%	4.631%
6	10.816	1288	1297	1304	rBV	989348	1625822	28.50%	2.817%
7	13.263	1706	1713	1725	rVB	3378453	4970491	87.12%	8.613%
8	13.480	1745	1750	1758	rVB	47712	75348	1.32%	0.131%
9	14.368	1896	1901	1908	rBV	33099	61337	1.08%	0.106%
10	14.639	1940	1947	1953	rBV	1406051	2006056	35.16%	3.476%
11	14.704	1953	1958	1965	rVB	54963	84941	1.49%	0.147%
12	15.686	2119	2125	2130	rVB	48118	71858	1.26%	0.125%
13	16.127	2192	2200	2211	rBV	2729008	3927964	68.84%	6.806%
14	17.209	2380	2384	2392	rVB	36410	64322	1.13%	0.111%
15	17.392	2405	2415	2418	rBV	1549672	2219605	38.90%	3.846%
16	17.433	2418	2422	2429	rVB	772349	1070232	18.76%	1.854%
17	17.521	2429	2437	2446	rBV	240635	388096	6.80%	0.672%
18	17.809	2476	2486	2492	rBV2	73161	141611	2.48%	0.245%
19	18.115	2533	2538	2544	rBV6	31948	57719	1.01%	0.100%
20	18.239	2553	2559	2567	rBV2	1385958	1995111	34.97%	3.457%
21	18.309	2567	2571	2580	rVB2	122409	219360	3.84%	0.380%
22	18.392	2581	2585	2590	rVB	45113	65961	1.16%	0.114%
23	18.462	2590	2597	2600	rBV2	203463	329668	5.78%	0.571%
24	18.762	2644	2648	2651	rBV	58630	78554	1.38%	0.136%
25	18.821	2654	2658	2664	rVB	86998	118313	2.07%	0.205%
26	19.327	2740	2744	2749	rVB	70511	87663	1.54%	0.152%
27	19.445	2758	2764	2770	rVB	2526882	3262964	57.19%	5.654%
28	19.509	2770	2775	2787	rBV2	723698	1130616	19.82%	1.959%
29	19.692	2803	2806	2813	rVB	69593	111814	1.96%	0.194%
30	19.774	2814	2820	2822	rBV2	282410	471325	8.26%	0.817%
31	19.809	2822	2826	2832	rVV	2138452	2659873	46.62%	4.609%
32	19.868	2833	2836	2841	rVB	59717	81507	1.43%	0.141%
33	19.998	2852	2858	2865	rBV	4614796	5705533	100.00%	9.886%
34	20.056	2866	2868	2873	rVV	65427	85279	1.49%	0.148%
35	20.121	2874	2879	2886	rVB4	98735	214031	3.75%	0.371%
36	20.256	2897	2902	2905	rBV6	77774	160315	2.81%	0.278%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102623\
Data File : BM042459.D
Acq On : 26 Oct 2023 19:09
Operator : MA/JU
Sample : 05010-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 343

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_M\Methods\8270-BM102123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	20.297	2906	2909	2913	rVB	168716	211060	3.70%	0.366%
38	20.398	2922	2926	2929	rBV2	128189	160418	2.81%	0.278%
39	20.592	2956	2959	2962	rBV	69222	82669	1.45%	0.143%
40	21.045	3033	3036	3043	rBV	104033	158161	2.77%	0.274%
41	21.227	3061	3067	3074	rBV4	484394	978589	17.15%	1.696%
42	21.286	3074	3077	3082	rVV2	130193	207518	3.64%	0.360%
43	21.433	3099	3102	3104	rBV	88873	103173	1.81%	0.179%
44	21.568	3118	3125	3129	rBV2	1537579	3043141	53.34%	5.273%
45	21.609	3129	3132	3137	rVB	766816	916592	16.06%	1.588%
46	21.727	3149	3152	3159	rVB	206130	256067	4.49%	0.444%
47	23.268	3407	3414	3420	rBV	738094	1986205	34.81%	3.442%
48	23.809	3501	3506	3516	rVB	451868	921281	16.15%	1.596%
49	23.921	3520	3525	3532	rVB	601861	1141877	20.01%	1.979%
50	24.033	3538	3544	3550	rBV	721727	1438569	25.21%	2.493%

Sum of corrected areas: 57710380

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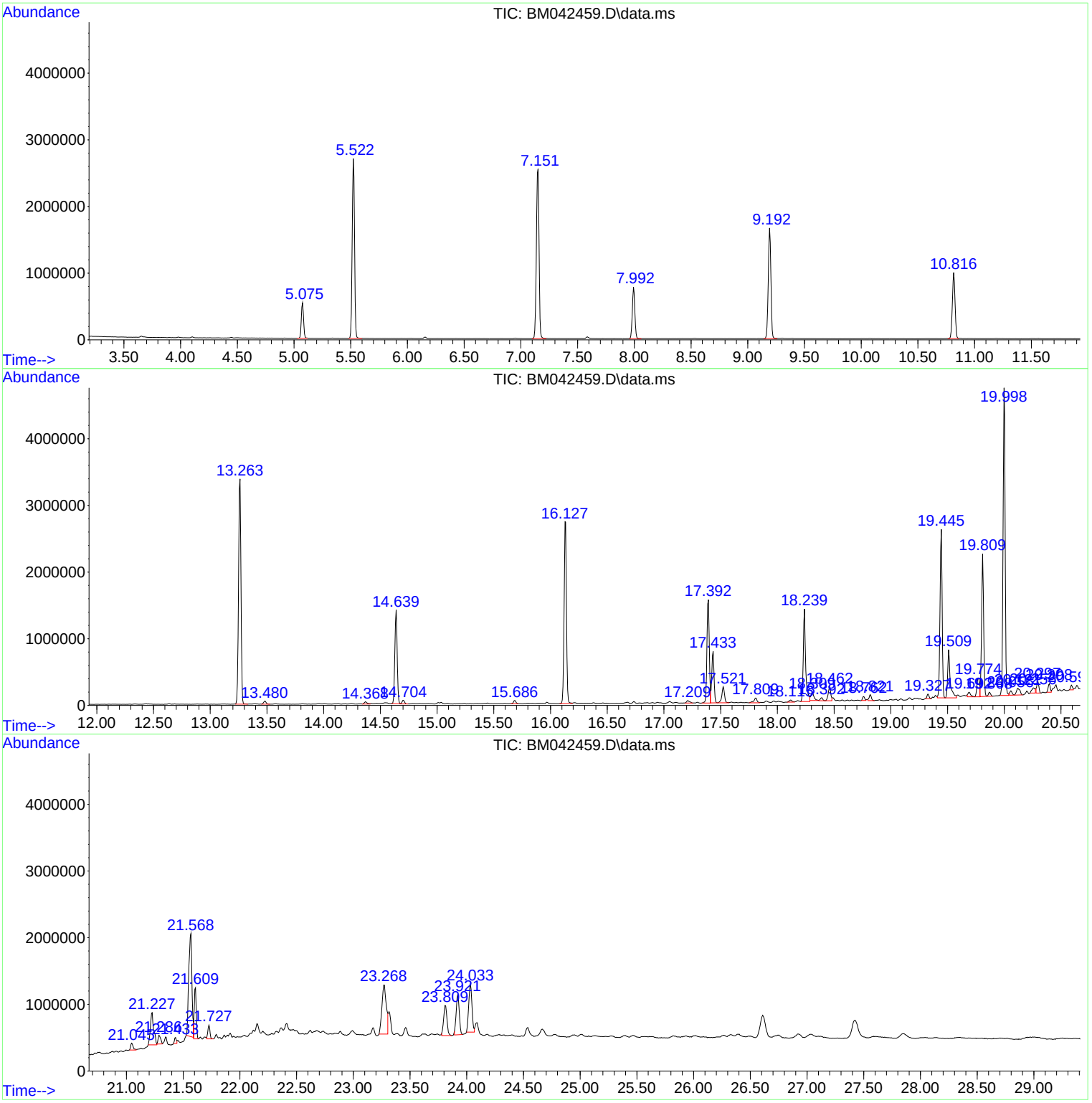
Sample : 05010-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
343

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102123.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_M\Data\BM102623\
Data File : BM042459.D
Acq On : 26 Oct 2023 19:09
Operator : MA/JU
Sample : 05010-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
343

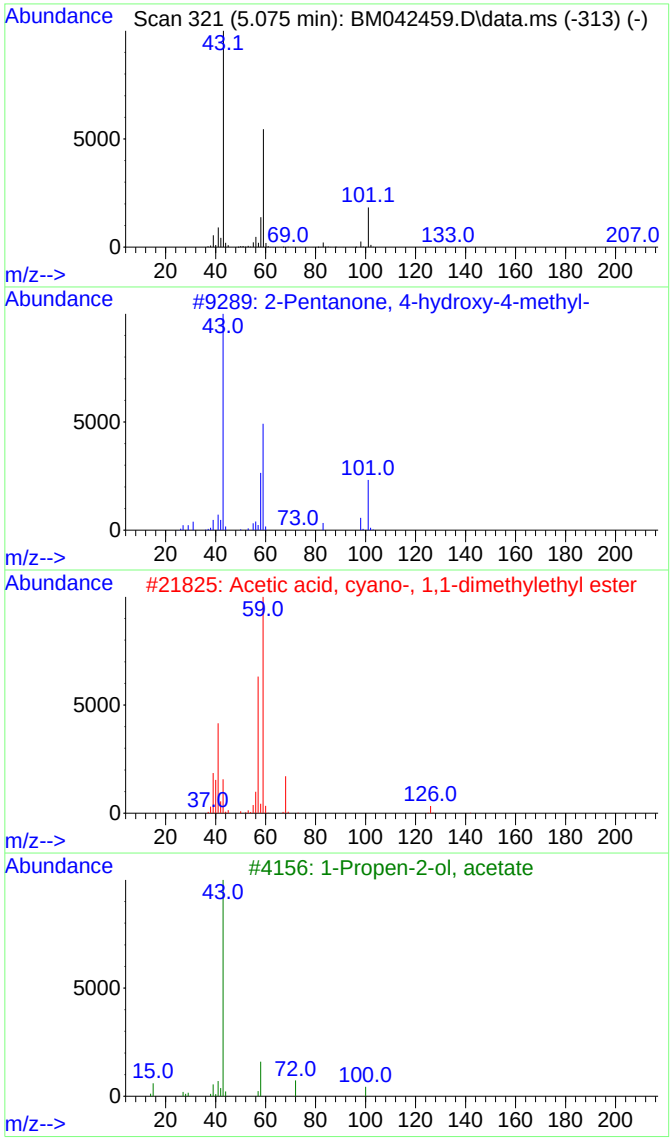
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

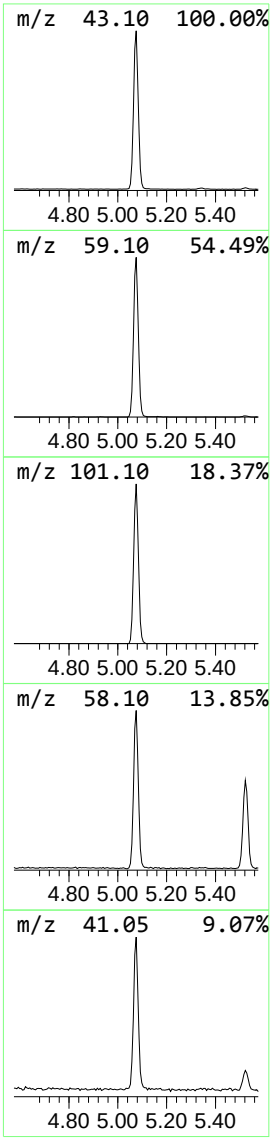
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.075	12.19 ng	724881	1,4-Dichlorobenzene-d4	7.992

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102623\
Data File : BM042459.D
Acq On : 26 Oct 2023 19:09
Operator : MA/JU
Sample : 05010-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
343

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

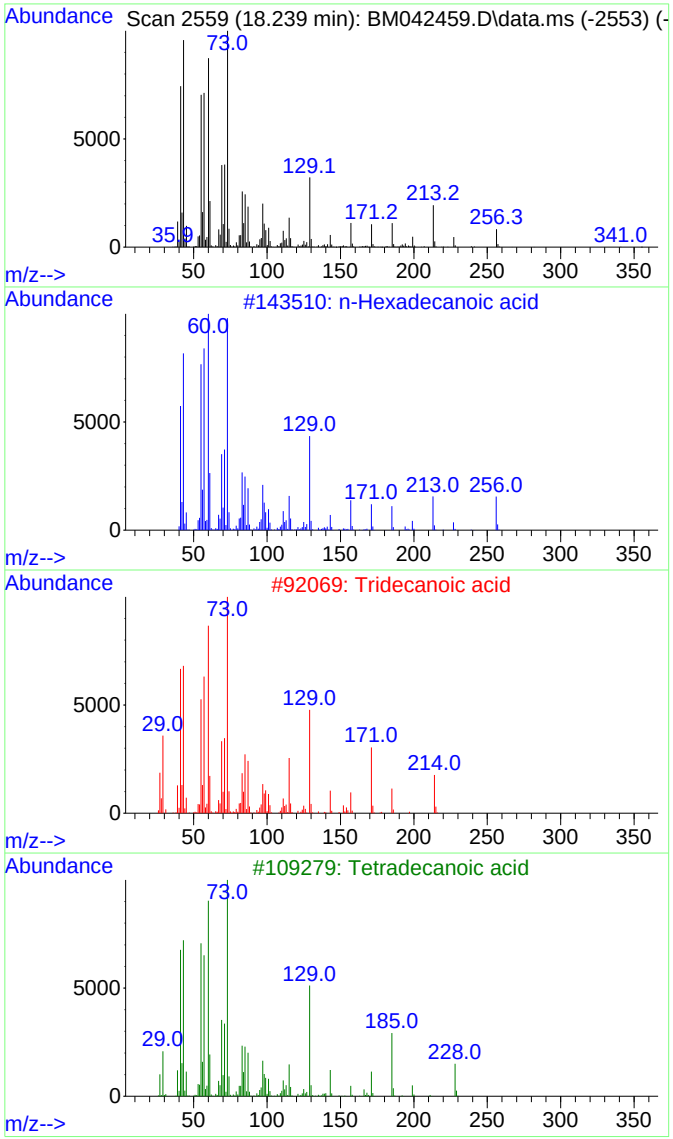
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

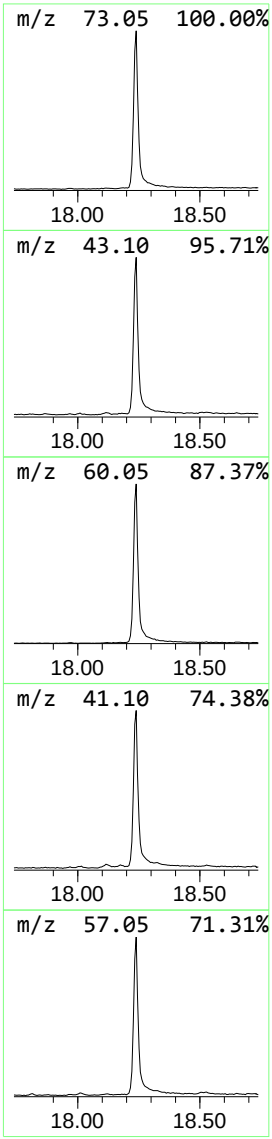
****

Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.239	17.98 ng	1995110	Phenanthrene-d10	17.392

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	95
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	55





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102623\
Data File : BM042459.D
Acq On : 26 Oct 2023 19:09
Operator : MA/JU
Sample : 05010-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
343

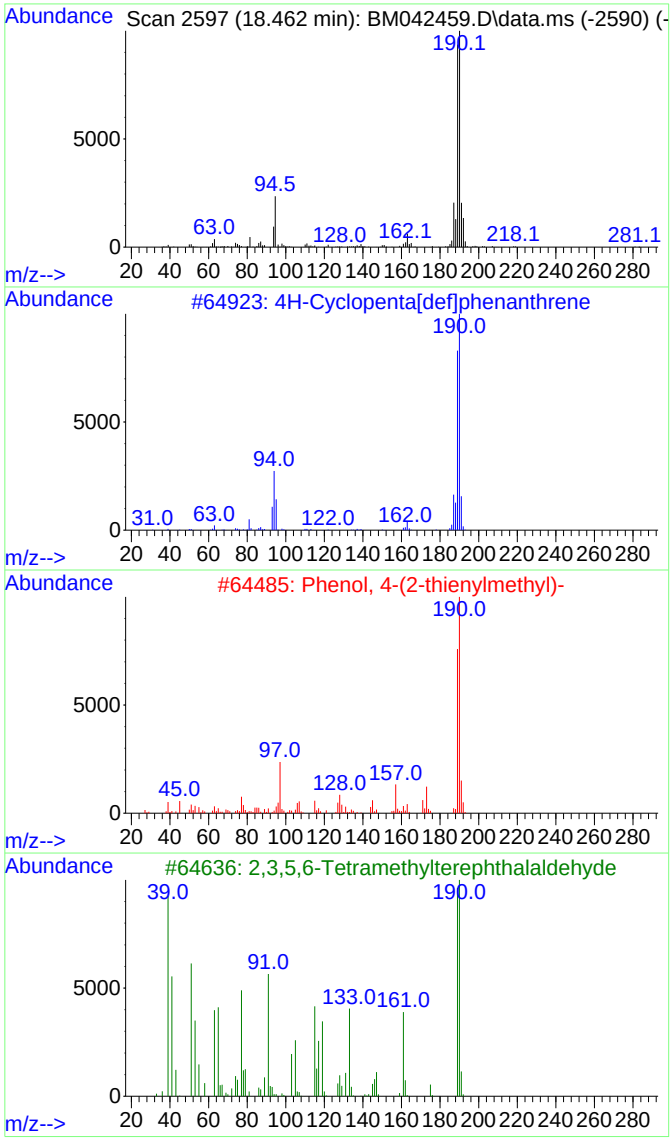
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

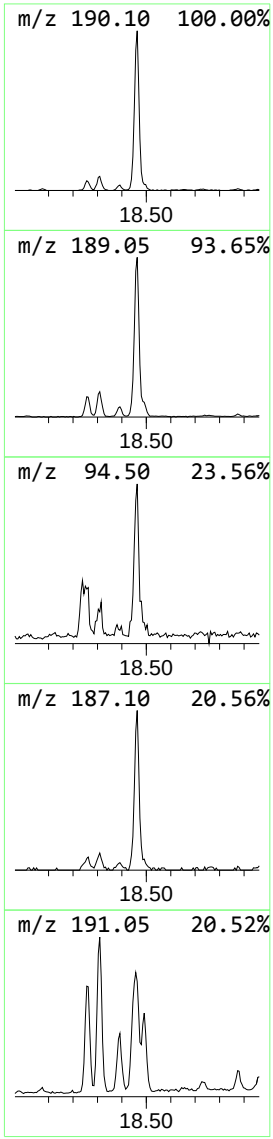
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 4H-Cyclopenta[def]phenanthrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.462	2.97 ng	329668	Phenanthrene-d10	17.392

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	96
2	Phenol, 4-(2-thienylmethyl)-	190	C11H10OS	091680-55-6	59
3	2,3,5,6-Tetramethylterephthalald...	190	C12H14O2	007072-01-7	50
4	Methyl diselenide	190	C2H6Se2	007101-31-7	45
5	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	45





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102623\
Data File : BM042459.D
Acq On : 26 Oct 2023 19:09
Operator : MA/JU
Sample : 05010-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
343

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

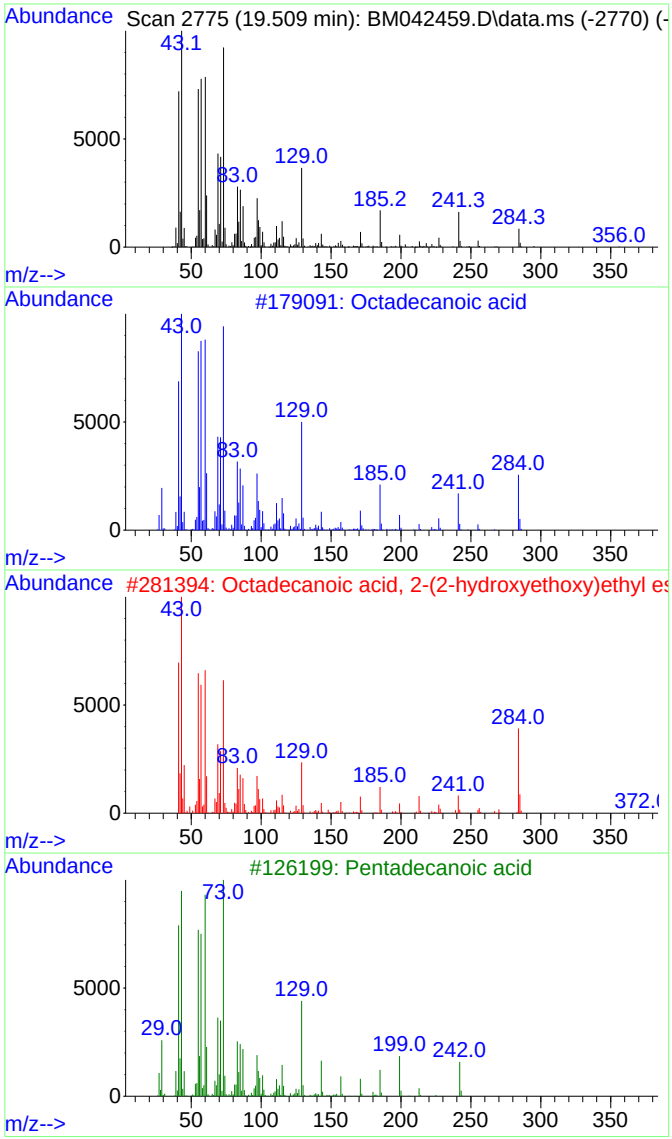
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

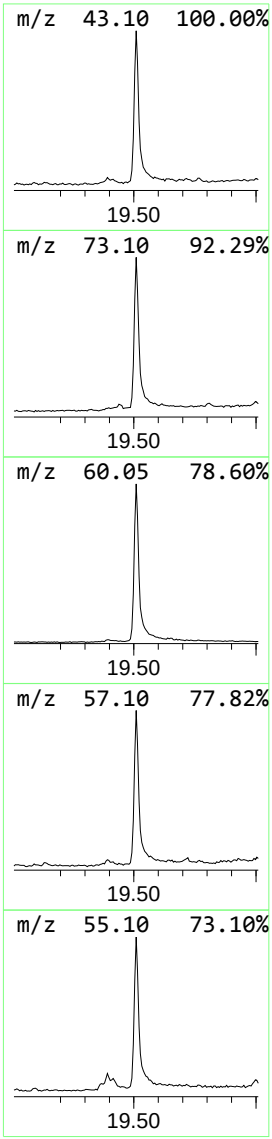
****

Peak Number 4 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.509	7.43 ng	1130620	Chrysene-d12	21.568

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	n-Decanoic acid	172	C10H20O2	000334-48-5	62





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102623\
Data File : BM042459.D
Acq On : 26 Oct 2023 19:09
Operator : MA/JU
Sample : 05010-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
343

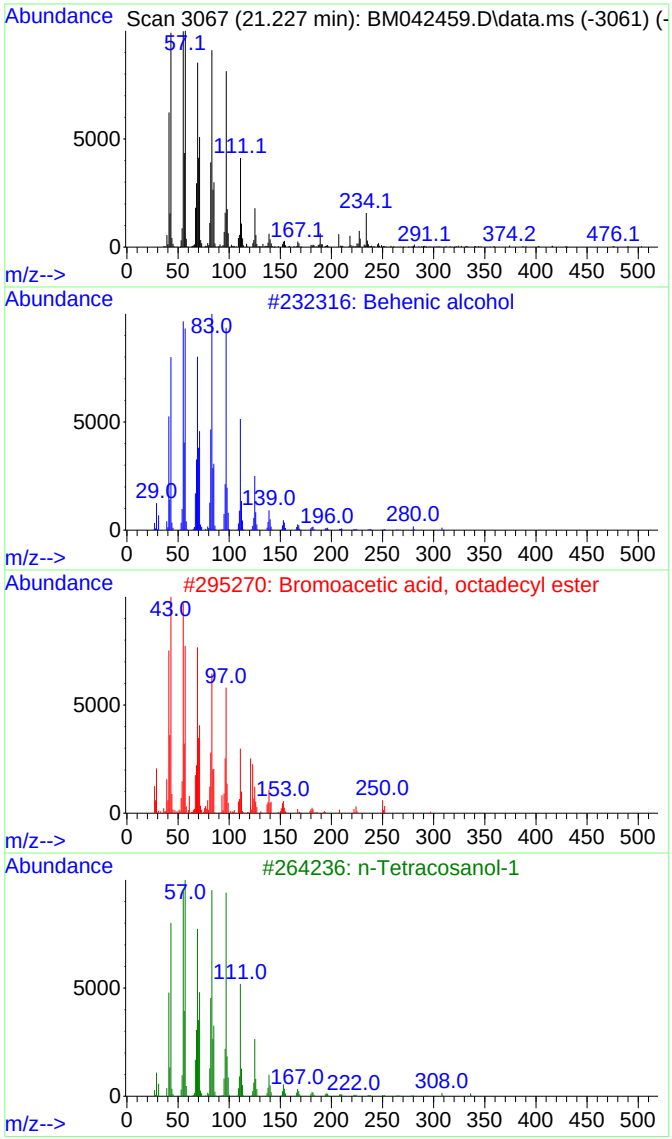
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

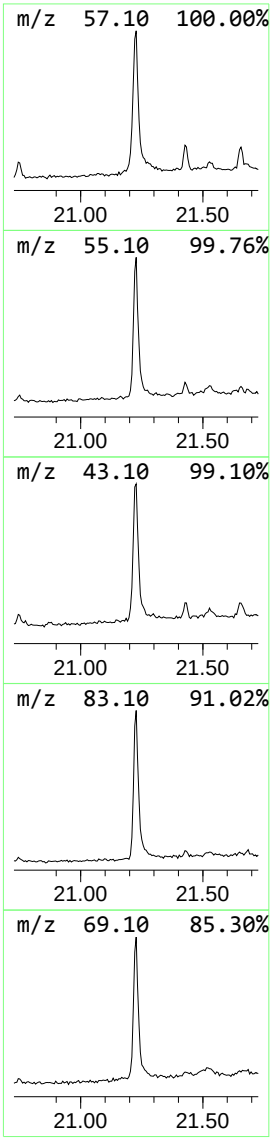
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Behenic alcohol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.227	6.43 ng	978589	Chrysene-d12	21.568

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	94
2	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	94
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	93
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	93
5	1-Tetracosene	336	C24H48	010192-32-2	93





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Data File : BM042459.D
Acq On : 26 Oct 2023 19:09
Operator : MA/JU
Sample : 05010-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

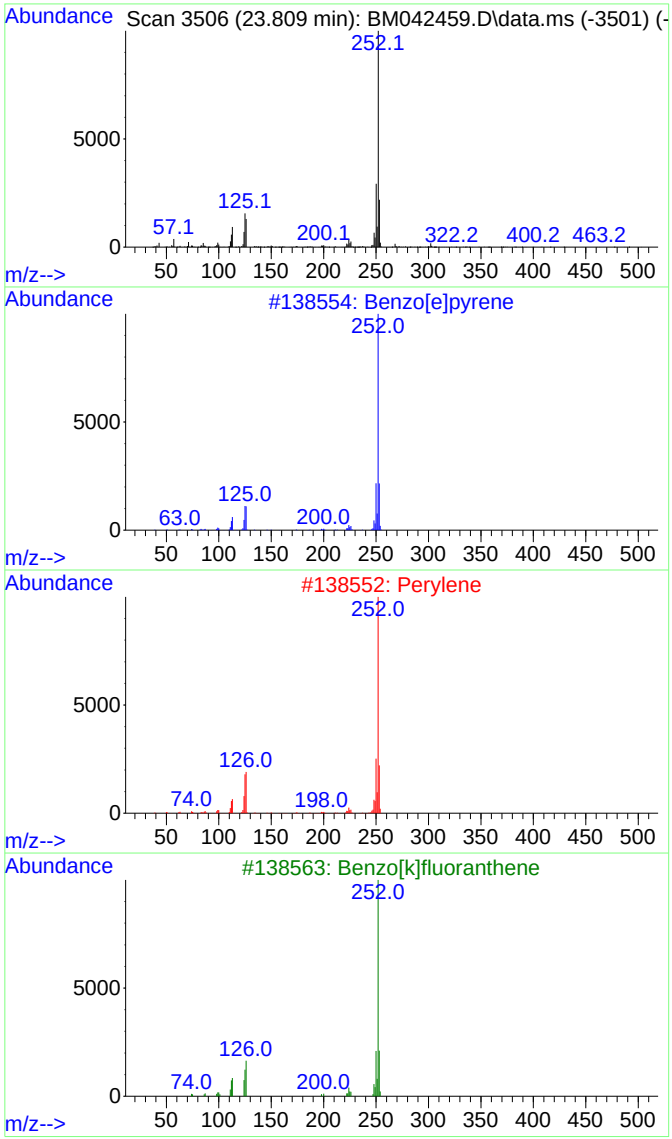
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

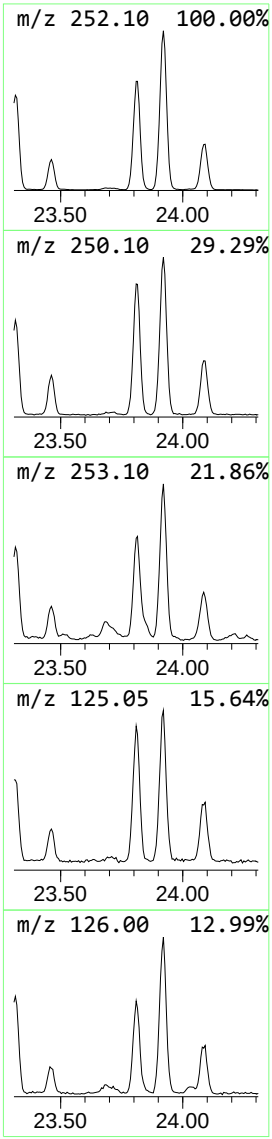
****

Peak Number 6 Benzo[e]pyrene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.809	12.81 ng	921281	Perylene-d12	24.033

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	99
2	Perylene	252	C20H12	000198-55-0	98
3	Benzo[k]fluoranthene	252	C20H12	000207-08-9	96
4	Benzo[b]fluoranthene	252	C20H12	000205-99-2	96
5	Benzo[a]pyrene	252	C20H12	000050-32-8	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102623\
Data File : BM042459.D
Acq On : 26 Oct 2023 19:09
Operator : MA/JU
Sample : 05010-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
343

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102123.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-...	5.075	12.2	ng	724881	1	7.992	1189500	20.0
n-Hexadecanoic ...	18.239	18.0	ng	1995110	4	17.392	2219610	20.0
4H-Cyclopenta[d...	18.462	3.0	ng	329668	4	17.392	2219610	20.0
Octadecanoic acid	19.509	7.4	ng	1130620	5	21.568	3043140	20.0
Behenic alcohol	21.227	6.4	ng	978589	5	21.568	3043140	20.0
Benzo[e]pyrene	23.809	12.8	ng	921281	6	24.033	1438570	20.0