LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032723\
Data File : BM039172.D
Acq On : 27 Mar 2023 22:24
Operator : CG/JU
Sample : O2021-15 2X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
JPP-46B-032023

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-BM030823.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM039172.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.034	292	297	308	rVB	746157	1019812	13.50%	1.387%
2	5.504	371	377	389	rVB	1865297	2651886	35.10%	3.606%
3	7.116	639	651	665	rBV	1750707	2719512	36.00%	3.698%
4	7.945	785	792	802	rBV	1105536	1690832	22.38%	2.299%
5	9.116	983	991	999	rBV	1041681	1686086	22.32%	2.292%
6	10.757	1261	1270	1277	rBV	1361124	2329631	30.83%	3.167%
7	13.215	1681	1688	1700	rBV	2601127	3652657	48.35%	4.966%
8	14.315	1868	1875	1882	rBV2	62898	102037	1.35%	0.139%
9	14.592	1912	1922	1928	rBV	2107306	2974780	39.37%	4.045%
10	14.657	1928	1933	1940	rVB	111694	175395	2.32%	0.238%
11	14.992	1985	1990	1998	rVB2	50850	92187	1.22%	0.125%
12	15.633	2095	2099	2104	rVB	82496	112913	1.49%	0.154%
13	15.945	2146	2152	2157	rVB2	112520	193404	2.56%	0.263%
14	16.080	2169	2175	2182	rBV	2032543	2853558	37.77%	3.880%
15	16.309	2207	2214	2221	rVB5	59685	140884	1.86%	0.192%
16	16.868	2302	2309	2312	rBV3	44554	84123	1.11%	0.114%
17	16.992	2326	2330	2335	rVB2	70174	103550	1.37%	0.141%
18	17.086	2339	2346	2350	rBV6	65477	129035	1.71%	0.175%
19	17.156	2355	2358	2367	rVB	75229	121465	1.61%	0.165%
20	17.339	2383	2389	2393	rBV	2460686	3551280	47.00%	4.828%
21	17.380	2393	2396	2403	rVV	1594320	2050554	27.14%	2.788%
22	17.468	2407	2411	2416	rVV	412903	563105	7.45%	0.766%
23	17.527	2417	2421	2426	rVB3	42078	85579	1.13%	0.116%
24	18.233	2534	2541	2544	rBV2	697365	1323153	17.51%	1.799%
25	18.262	2544	2546	2552	rVV	465876	617753	8.18%	0.840%
26	18.345	2556	2560	2565	rVV	185637	284195	3.76%	0.386%
27	18.409	2566	2571	2575	rVV2	454052	844771	11.18%	1.149%
28	18.445	2575	2577	2582	rVB	228977	278410	3.69%	0.379%
29	18.709	2619	2622	2626	rVV	212322	301561	3.99%	0.410%
30	18.756	2627	2630	2635	rVB2	152015	219036	2.90%	0.298%
31	18.956	2662	2664	2669	rVB	98680	118191	1.56%	0.161%
32	19.133	2689	2694	2699	rBV2	234312	483666	6.40%	0.658%
33	19.274	2714	2718	2725	rBV2	221359	383967	5.08%	0.522%
34	19.392	2733	2738	2744	rBV	3879708	5391822	71.37%	7.331%
35	19.503	2753	2757	2762	rBV2	388262	622094	8.23%	0.846%
36	19.727	2791	2795	2796	rBV	691407	833597	11.03%	1.133%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032723\
Data File : BM039172.D
Acq On : 27 Mar 2023 22:24
Operator : CG/JU
Sample : O2021-15 2X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
JPP-46B-032023

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-BM030823.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	19.756	2796	2800	2808	rVV	4079077	5554349	73.52%	7.552%
38	19.827	2809	2812	2818	rVB3	187010	318935	4.22%	0.434%
39	19.956	2829	2834	2838	rVB	4401498	5143537	68.08%	6.993%
40	20.250	2881	2884	2889	rVB2	515248	691465	9.15%	0.940%
41	20.350	2898	2901	2905	rBV2	285451	311797	4.13%	0.424%
42	21.515	3093	3099	3103	rBV2	3824988	7555168	100.00%	10.272%
43	21.556	3103	3106	3115	rVB	2115858	2894939	38.32%	3.936%
44	23.209	3382	3387	3392	rBV	1734350	3962032	52.44%	5.387%
45	23.838	3490	3494	3502	rVB	1703408	3249320	43.01%	4.418%
46	23.950	3508	3513	3518	rVB	1700735	3080566	40.77%	4.188%

Sum of corrected areas: 73548589

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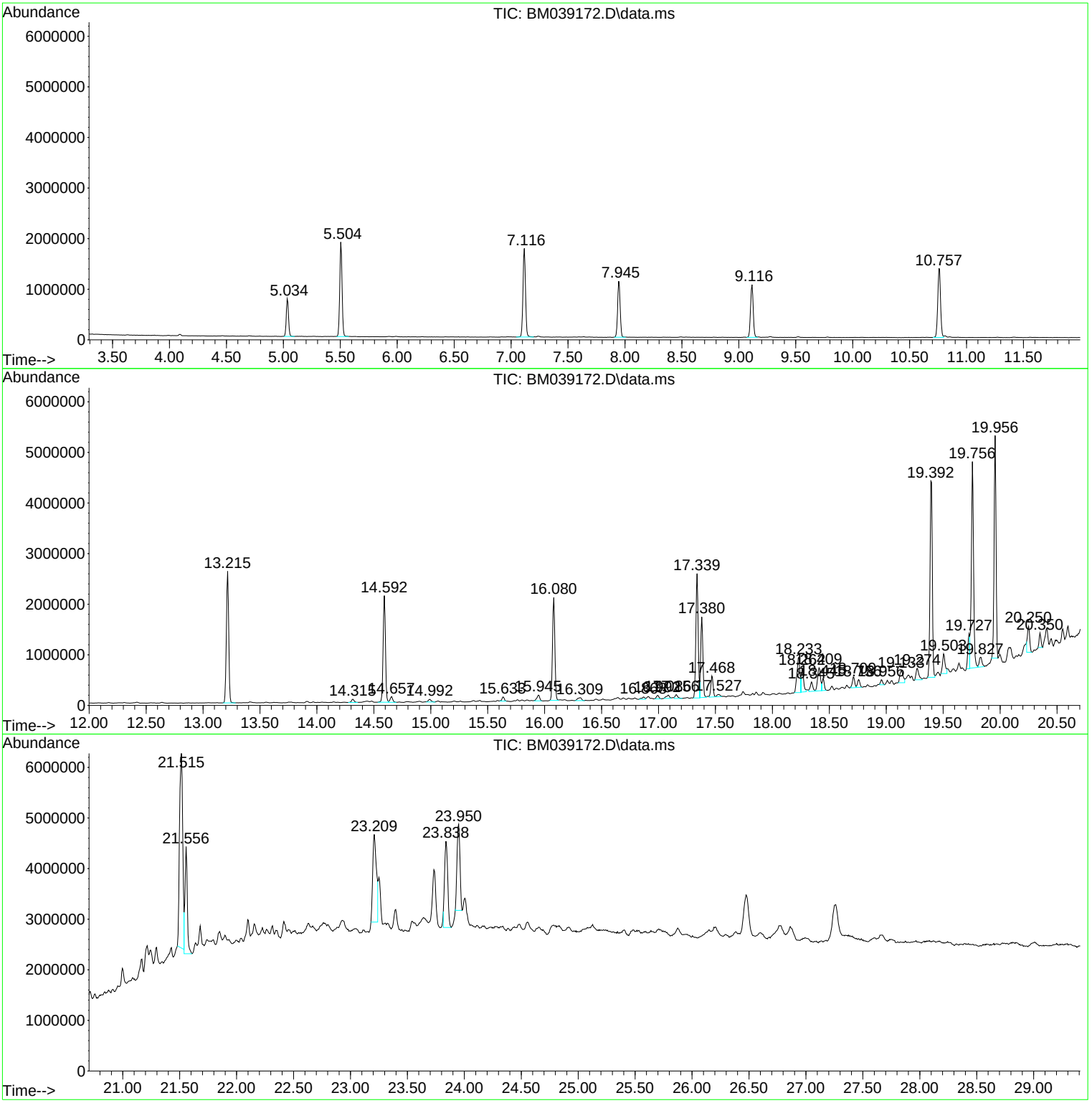
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
JPP-46B-032023

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM030823.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\BM032723\
Data File : BM039172.D
Acq On : 27 Mar 2023 22:24
Operator : CG/JU
Sample : 02021-15 2X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
JPP-46B-032023

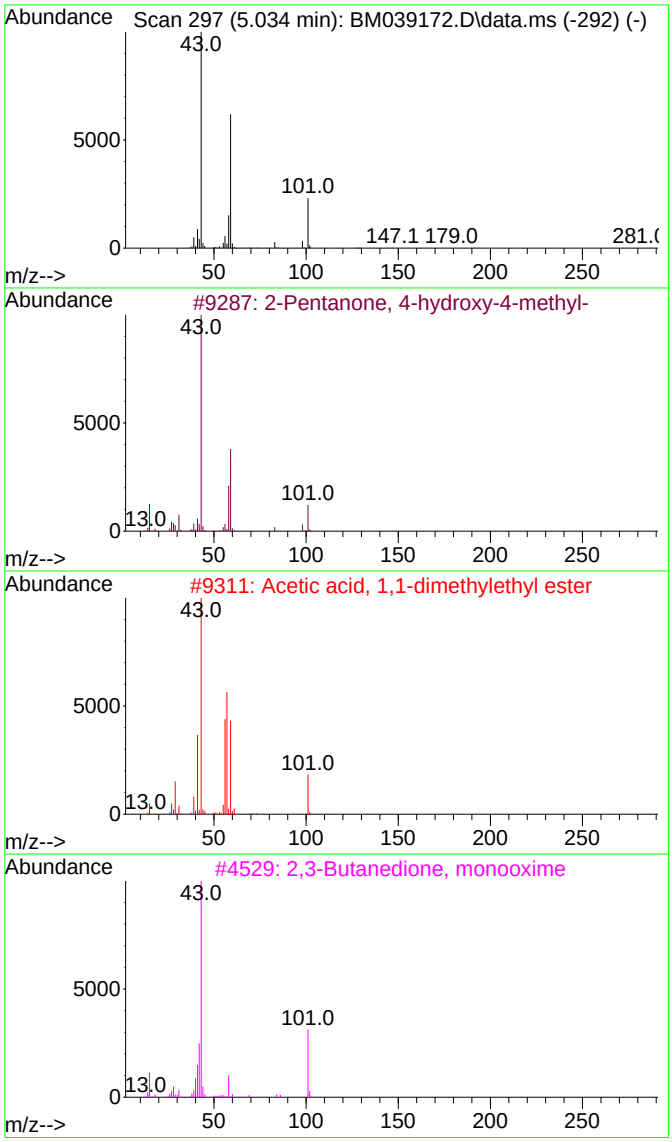
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM030823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

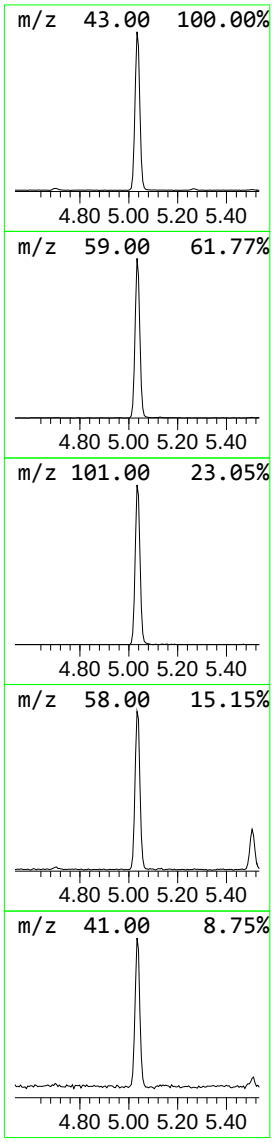
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.034	12.06 ng	1019810	1,4-Dichlorobenzene-d4	7.945

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032723\
Data File : BM039172.D
Acq On : 27 Mar 2023 22:24
Operator : CG/JU
Sample : 02021-15 2X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
JPP-46B-032023

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM030823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

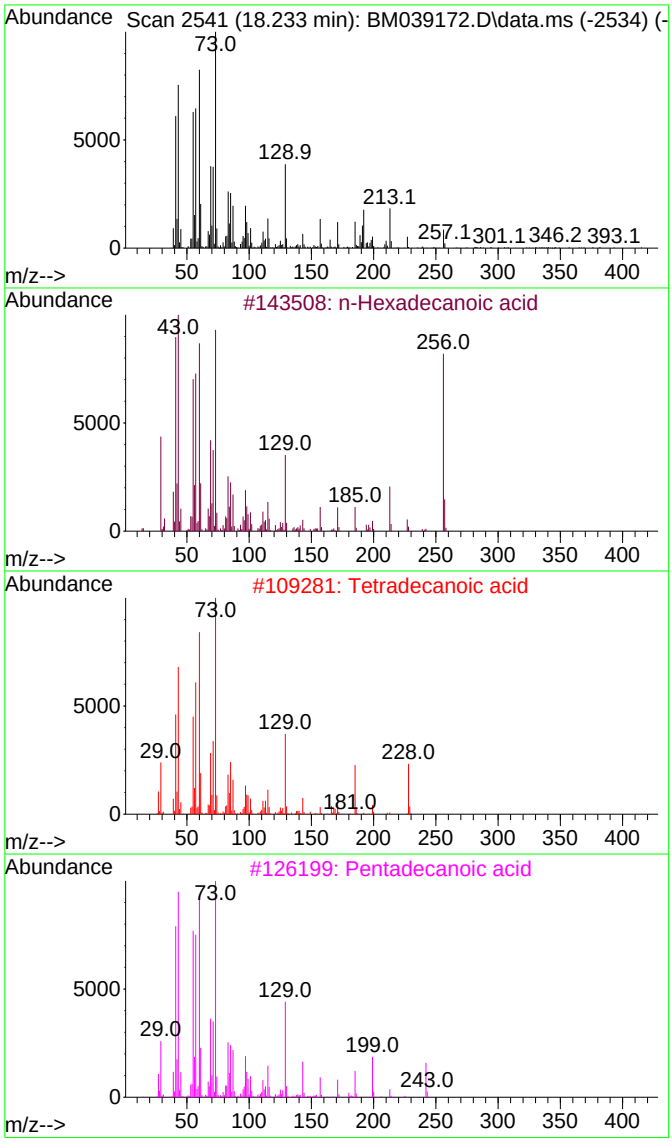
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

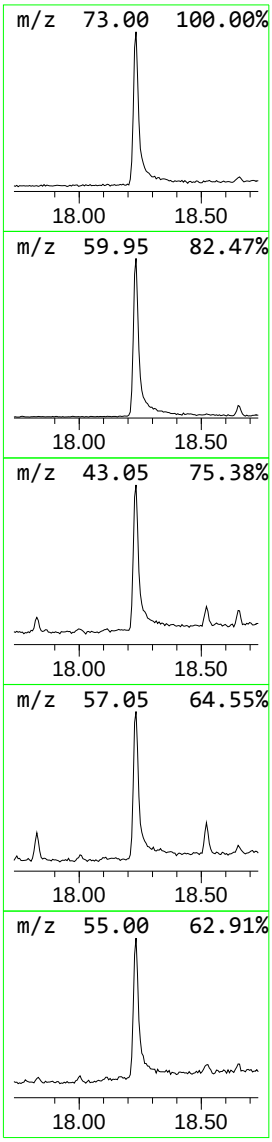
****

Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.233	7.45 ng	1323150	Phenanthrene-d10	17.339

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4	Tridecanoic acid	214	C13H26O2	000638-53-9	91
5	Octadecanoic acid	284	C18H36O2	000057-11-4	81





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Data File : BM039172.D
Acq On : 27 Mar 2023 22:24
Operator : CG/JU
Sample : 02021-15 2X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
JPP-46B-032023

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM030823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

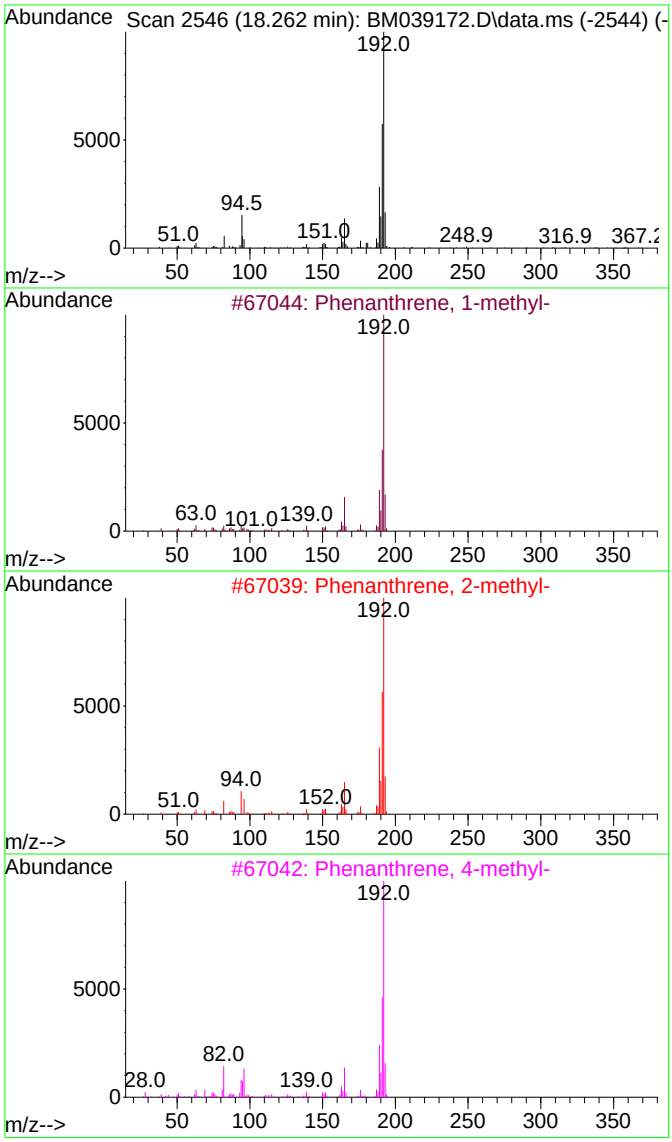
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

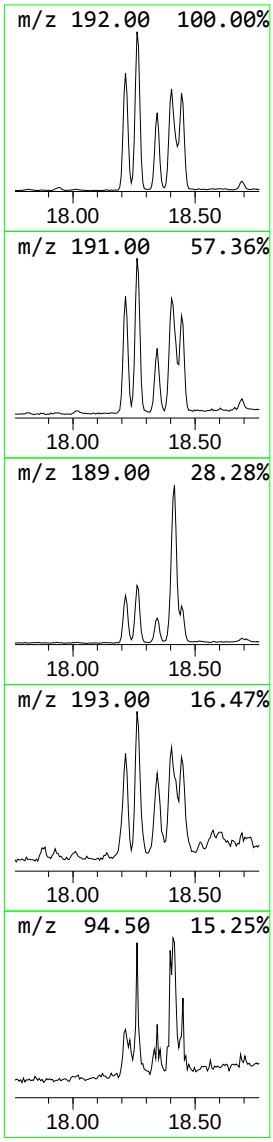
****

Peak Number 3 Phenanthrene, 1-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.262	3.48 ng	617753	Phenanthrene-d10	17.339

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	95
2	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	95
3	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	93
4	Anthracene, 1-methyl-	192	C15H12	000610-48-0	91
5	Anthracene, 2-methyl-	192	C15H12	000613-12-7	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032723\
Data File : BM039172.D
Acq On : 27 Mar 2023 22:24
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Sample : 02021-15 2X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
JPP-46B-032023

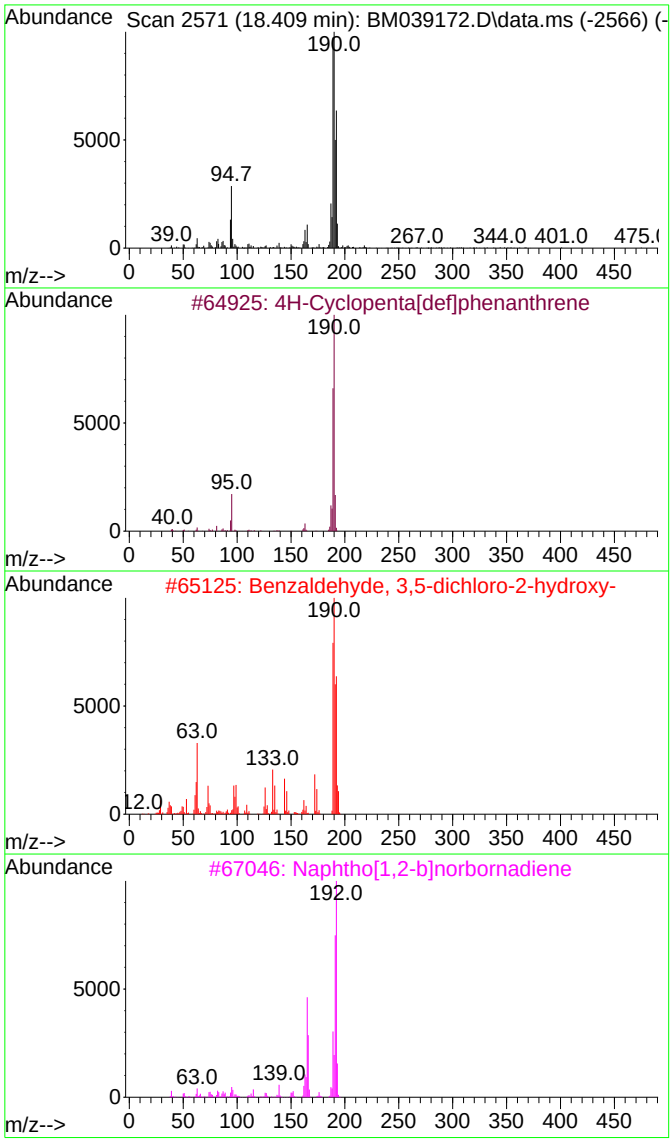
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM030823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

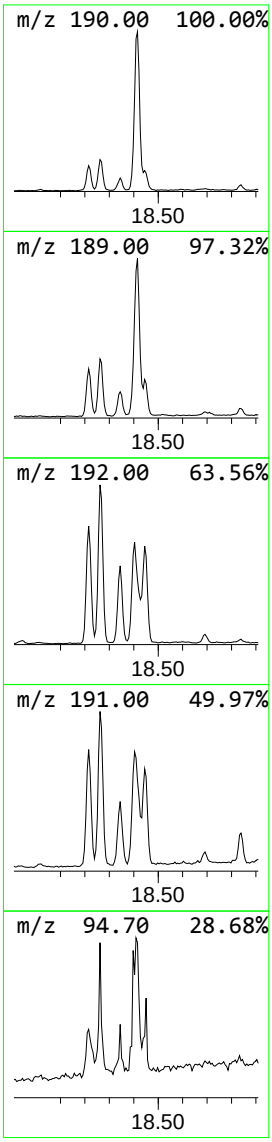
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.409	4.76 ng	844771	Phenanthrene-d10	17.339

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	70
2	Benzaldehyde, 3,5-dichloro-2-hyd...	190	C7H4Cl2O2	000090-60-8	64
3	Naphtho[1,2-b]norbornadiene	192	C15H12	1000210-14-8	42
4	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	38
5	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	30





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032723\
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Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
JPP-46B-032023

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM030823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

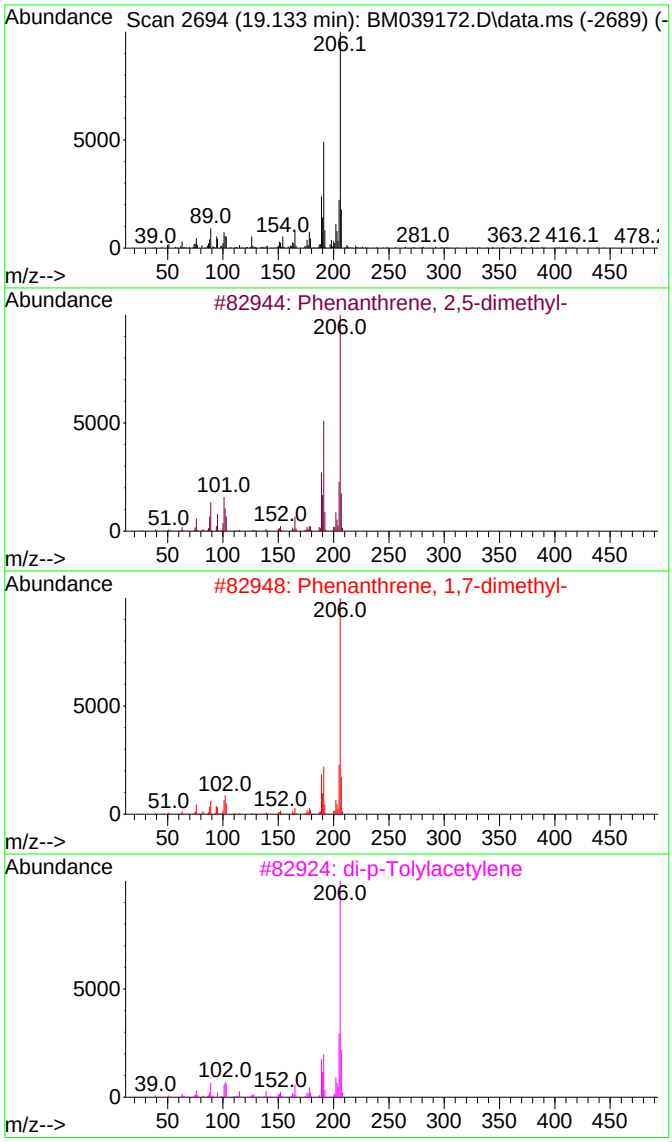
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

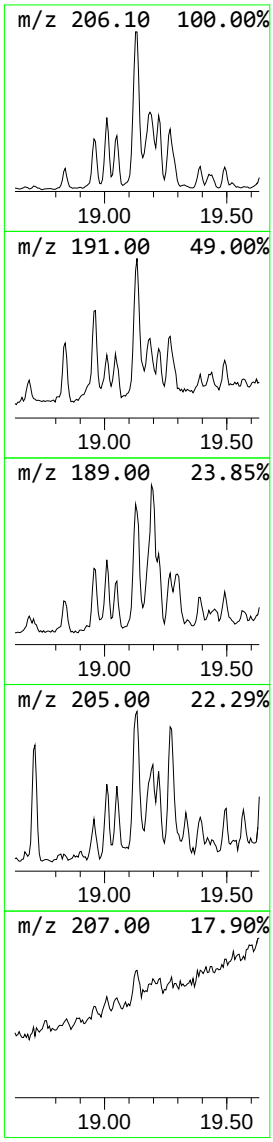
****

Peak Number 5 Phenanthrene, 2,5-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.133	2.72 ng	483666	Phenanthrene-d10	17.339

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	98
2	Phenanthrene, 1,7-dimethyl-	206	C16H14	000483-87-4	93
3	di-p-Tolylacetylene	206	C16H14	002789-88-0	92
4	Phenanthrene, 2,3-dimethyl-	206	C16H14	003674-65-5	91
5	9,10-Dimethylanthracene	206	C16H14	000781-43-1	91





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Misc :
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM030823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

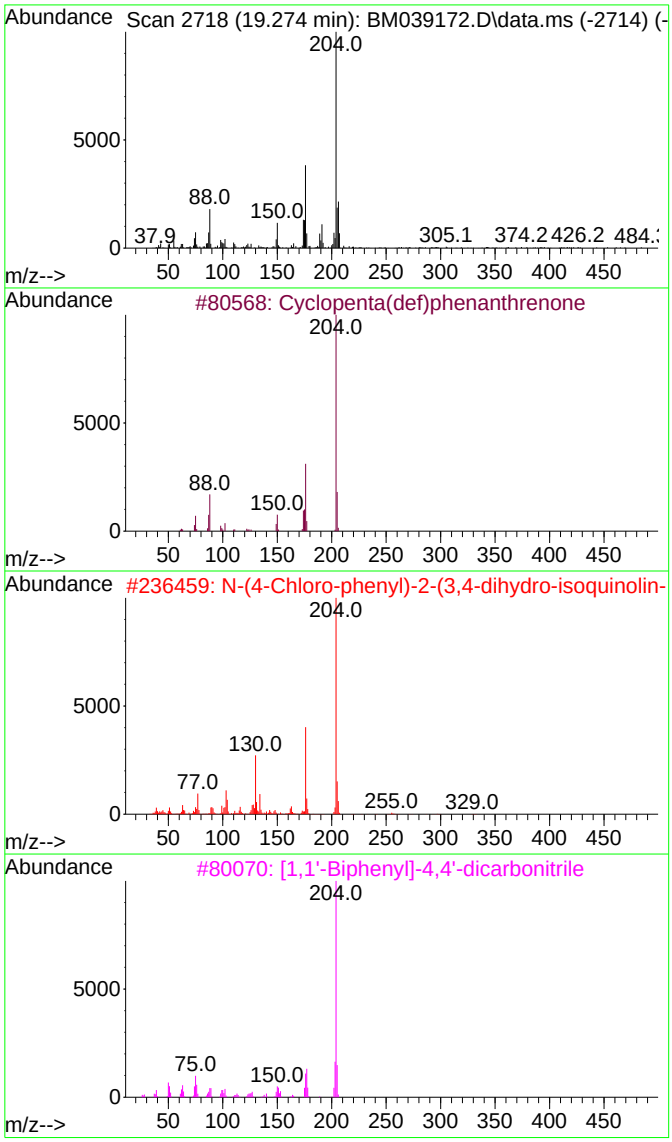
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

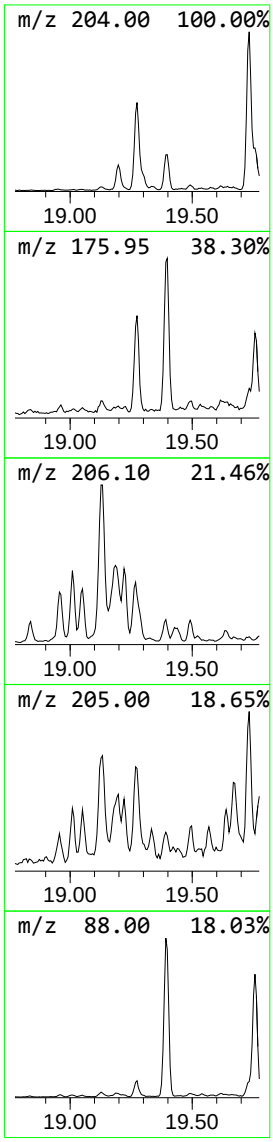
****

Peak Number 6 Cyclopenta(def)phenanthrenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.274	2.16 ng	383967	Phenanthrene-d10	17.339

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopenta(def)phenanthrenone	204	C15H8O	005737-13-3	98
2	N-(4-Chloro-phenyl)-2-(3,4-dihyd...	330	C17H15ClN2OS	1010296-34-3	50
3	[1,1'-Biphenyl]-4,4'-dicarbonitrile	204	C14H8N2	001591-30-6	47
4	[1,1'-Biphenyl]-2-ol, 5-chloro-	204	C12H9ClO	000607-12-5	43
5	Dihydrofuranno(3,2-H)homochromanone	204	C12H12O3	057052-85-4	43





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032723\
Data File : BM039172.D
Acq On : 27 Mar 2023 22:24
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Misc :
ALS Vial : 18 Sample Multiplier: 1

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BNA_M
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM030823.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-...	5.034	12.1	ng	1019810	1	7.945	1690830	20.0
n-Hexadecanoic ...	18.233	7.5	ng	1323150	4	17.339	3551280	20.0
Phenanthrene, 1...	18.262	3.5	ng	617753	4	17.339	3551280	20.0
4H-Cyclopenta[d...	18.409	4.8	ng	844771	4	17.339	3551280	20.0
Phenanthrene, 2...	19.133	2.7	ng	483666	4	17.339	3551280	20.0
Cyclopenta(def)...	19.274	2.2	ng	383967	4	17.339	3551280	20.0