LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM060122\
Data File : BM035348.D
Acq On : 01 Jun 2022 15:49
Operator : CG/JU
Sample : N3107-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MS-6

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-BM052722.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM035348.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.445	395	401	418	rBV	1667399	2518101	49.96%	5.692%
2	7.045	664	673	690	rBV	1721642	2748619	54.53%	6.213%
3	7.863	803	812	820	rBV	488403	793649	15.75%	1.794%
4	9.022	1001	1009	1021	rBV	1041016	1756431	34.85%	3.970%
5	10.663	1280	1288	1294	rBV	623798	1068535	21.20%	2.415%
6	13.127	1700	1707	1719	rBV	3027727	4345676	86.22%	9.822%
7	14.504	1932	1941	1947	rBV	950566	1411227	28.00%	3.190%
8	14.563	1947	1951	1960	rVB	44365	77324	1.53%	0.175%
9	14.904	2002	2009	2017	rBV2	24865	51355	1.02%	0.116%
10	15.551	2114	2119	2125	rVB	42052	61286	1.22%	0.139%
11	15.992	2187	2194	2211	rBV	2191684	3181985	63.13%	7.192%
12	16.904	2344	2349	2356	rVB2	36066	58809	1.17%	0.133%
13	17.004	2359	2366	2372	rVV4	40704	88181	1.75%	0.199%
14	17.062	2372	2376	2386	rVB	47901	81070	1.61%	0.183%
15	17.245	2401	2407	2411	rBV	1103604	1587364	31.49%	3.588%
16	17.286	2411	2414	2421	rVV	1005317	1415028	28.07%	3.198%
17	17.380	2425	2430	2436	rVB	213786	315888	6.27%	0.714%
18	17.651	2469	2476	2482	rBV2	111622	186631	3.70%	0.422%
19	18.127	2552	2557	2558	rBV	122420	159152	3.16%	0.360%
20	18.151	2558	2561	2564	rBV	216569	290307	5.76%	0.656%
21	18.256	2575	2579	2584	rVB	53019	79296	1.57%	0.179%
22	18.321	2584	2590	2594	rVV2	184386	340596	6.76%	0.770%
23	18.356	2594	2596	2602	rVB	94626	114090	2.26%	0.258%
24	18.627	2638	2642	2645	rBV	98448	126830	2.52%	0.287%
25	18.668	2645	2649	2655	rVB	93040	134780	2.67%	0.305%
26	19.045	2709	2713	2716	rBV2	58396	82295	1.63%	0.186%
27	19.186	2733	2737	2744	rVB2	83236	128177	2.54%	0.290%
28	19.303	2752	2757	2763	rBV	1913103	2536118	50.32%	5.732%
29	19.362	2764	2767	2771	rVB2	101755	124917	2.48%	0.282%
30	19.427	2775	2778	2786	rVB2	190703	278508	5.53%	0.629%
31	19.668	2809	2819	2828	rBV	1623102	2593689	51.46%	5.862%
32	19.739	2828	2831	2836	rVV2	72456	104267	2.07%	0.236%
33	19.874	2847	2854	2858	rBV	4271170	5040321	100.00%	11.392%
34	20.003	2870	2876	2881	rVB3	97481	226888	4.50%	0.513%
35	20.162	2900	2903	2910	rVB	228924	315193	6.25%	0.712%
36	20.262	2917	2920	2924	rBV	110785	137872	2.74%	0.312%

LSC Area Percent Report

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Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
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ClientSampleId :
MS-6

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-BM052722.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	20.321	2927	2930	2934	rVB2	124601	172863	3.43%	0.391%
38	20.509	2959	2962	2966	rVB2	100487	128012	2.54%	0.289%
39	21.115	3062	3065	3067	rBV	131401	139829	2.77%	0.316%
40	21.150	3067	3071	3077	rVB3	275779	421578	8.36%	0.953%
41	21.344	3102	3104	3108	rVB	152221	166353	3.30%	0.376%
42	21.427	3112	3118	3122	rVV3	1597061	3135879	62.22%	7.088%
43	21.468	3122	3125	3135	rVB	911071	1243567	24.67%	2.811%
44	23.080	3394	3399	3405	rBV	815320	1768203	35.08%	3.997%
45	23.691	3499	3503	3511	rVB	568094	1094296	21.71%	2.473%
46	23.797	3516	3521	3527	rVB2	773083	1412108	28.02%	3.192%

Sum of corrected areas: 44243143

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Instrument :
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ClientSampleId :
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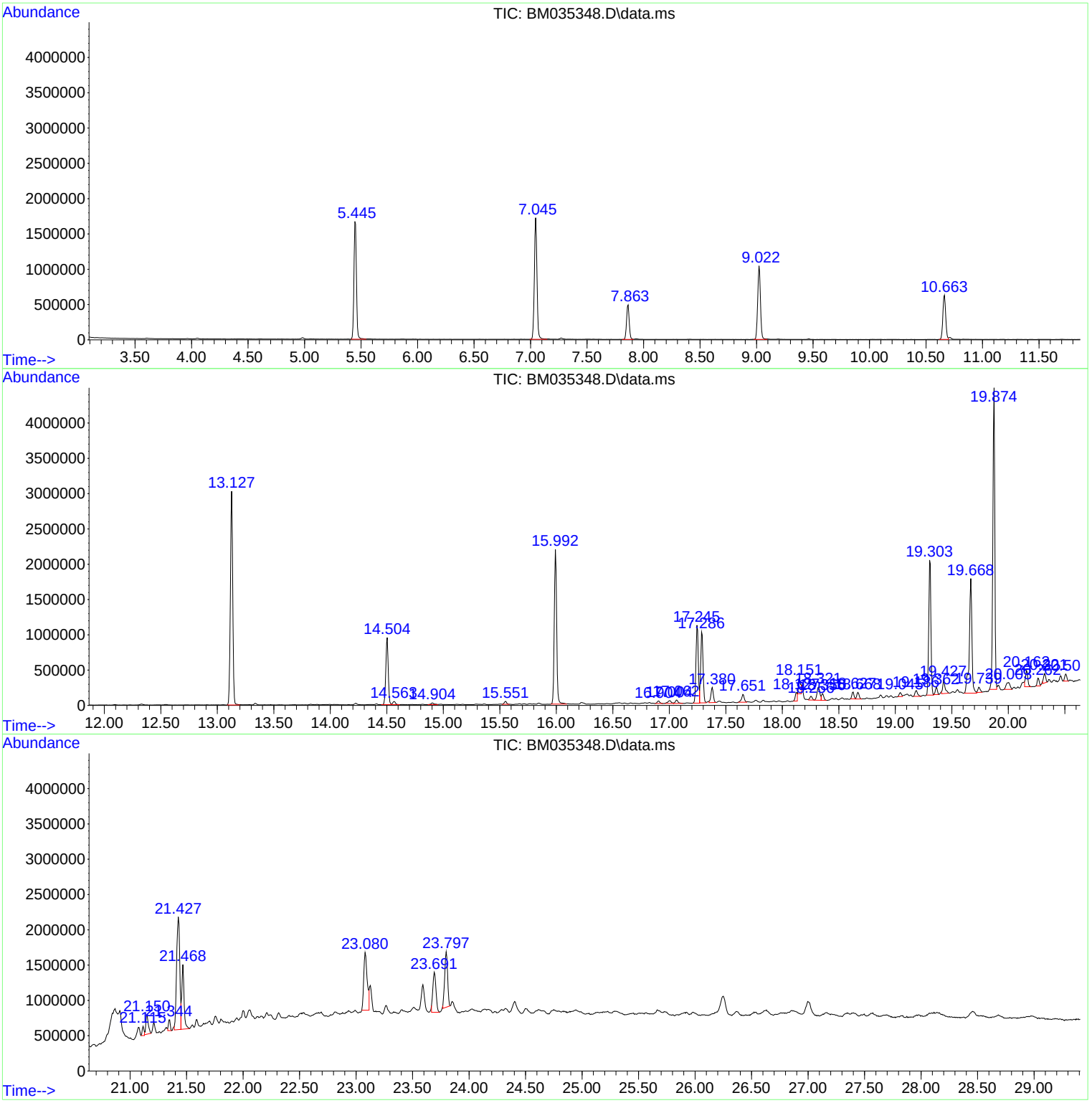
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM060122\
Data File : BM035348.D
Acq On : 01 Jun 2022 15:49
Operator : CG/JU
Sample : N3107-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MS-6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

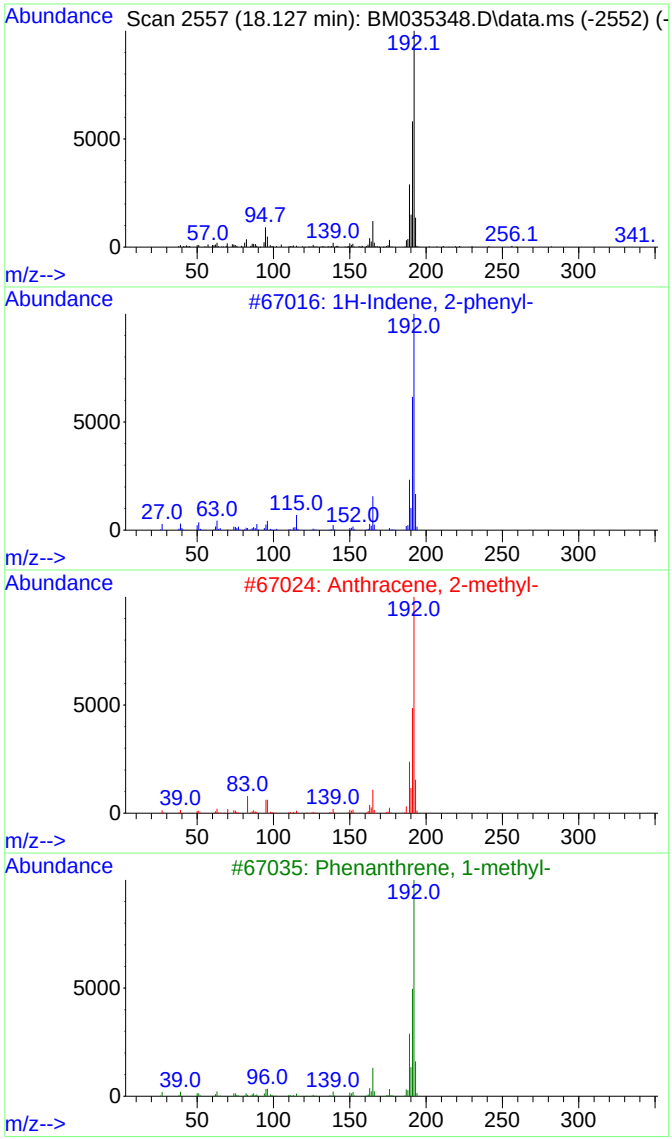
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

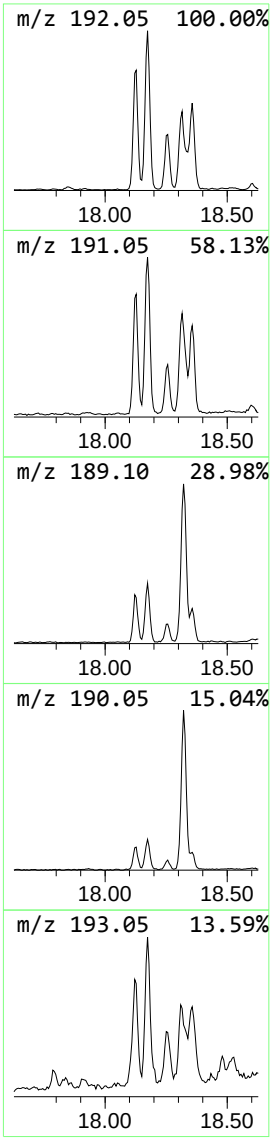
****

Peak Number 1 1H-Indene, 2-phenyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.127	2.01 ng	159152	Phenanthrene-d10	17.245

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	91
2	Anthracene, 2-methyl-	192	C15H12	000613-12-7	91
3	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	91
4	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	91
5	Anthracene, 1-methyl-	192	C15H12	000610-48-0	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM060122\
Data File : BM035348.D
Acq On : 01 Jun 2022 15:49
Operator : CG/JU
Sample : N3107-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MS-6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

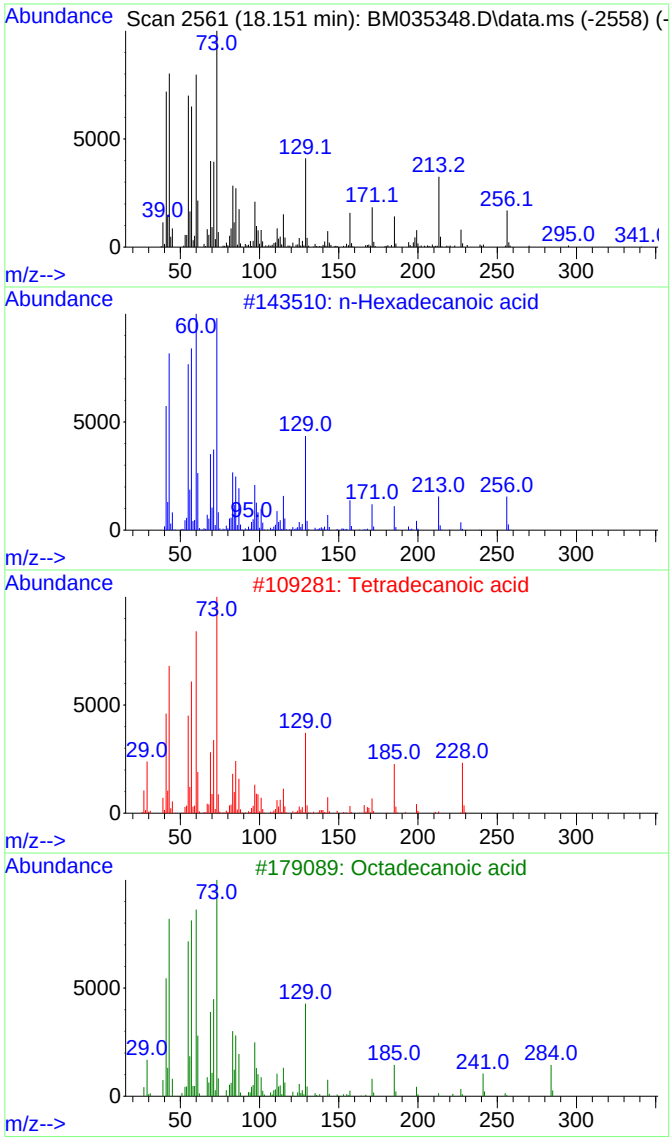
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

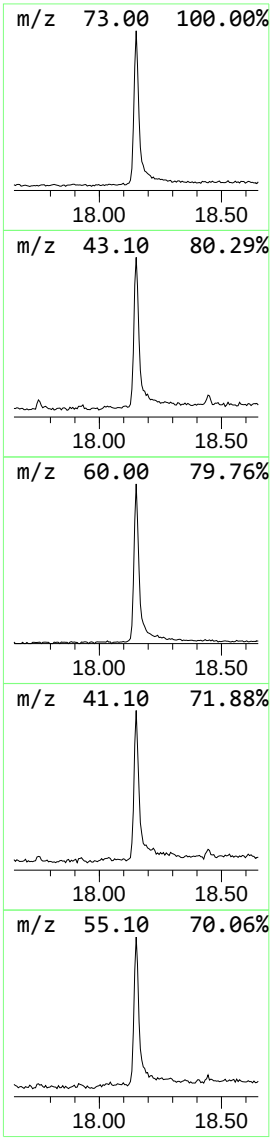
****

Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.151	3.66 ng	290307	Phenanthrene-d10	17.245

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	Octadecanoic acid	284	C18H36O2	000057-11-4	87
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5	Tridecanoic acid	214	C13H26O2	000638-53-9	70





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM060122\
Data File : BM035348.D
Acq On : 01 Jun 2022 15:49
Operator : CG/JU
Sample : N3107-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MS-6

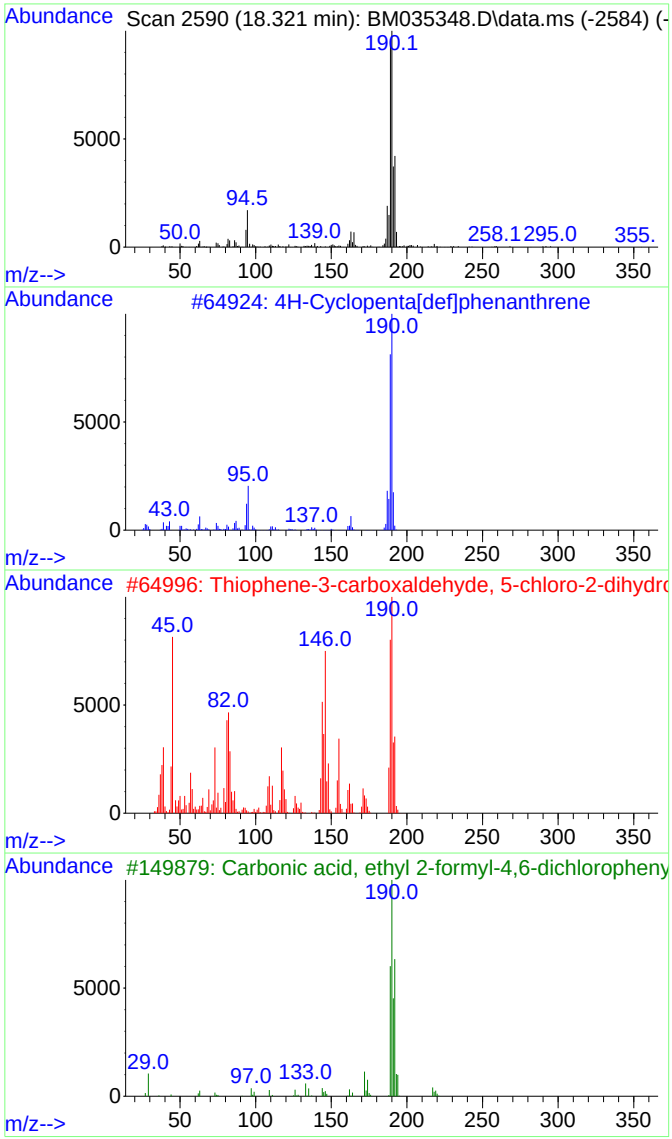
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

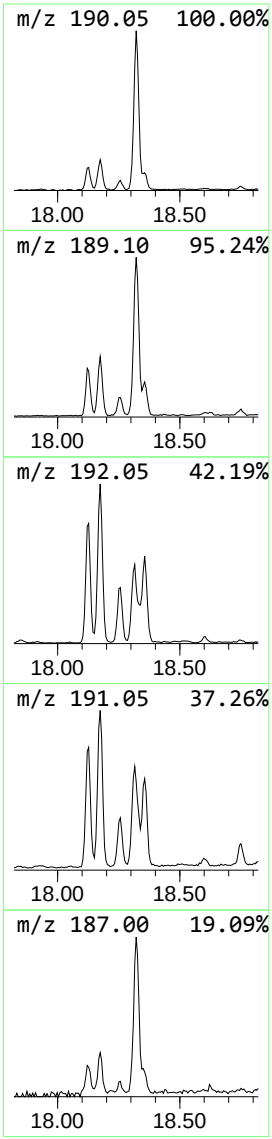
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 4H-Cyclopenta[def]phenanthrene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.321	4.29 ng	340596	Phenanthrene-d10	17.245

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	70
2	Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	53
3	Carbonic acid, ethyl 2-formyl-4,...	262	C10H8Cl2O4	1000331-34-4	50
4	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	45
5	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	40





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Data File : BM035348.D
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Operator : CG/JU
Sample : N3107-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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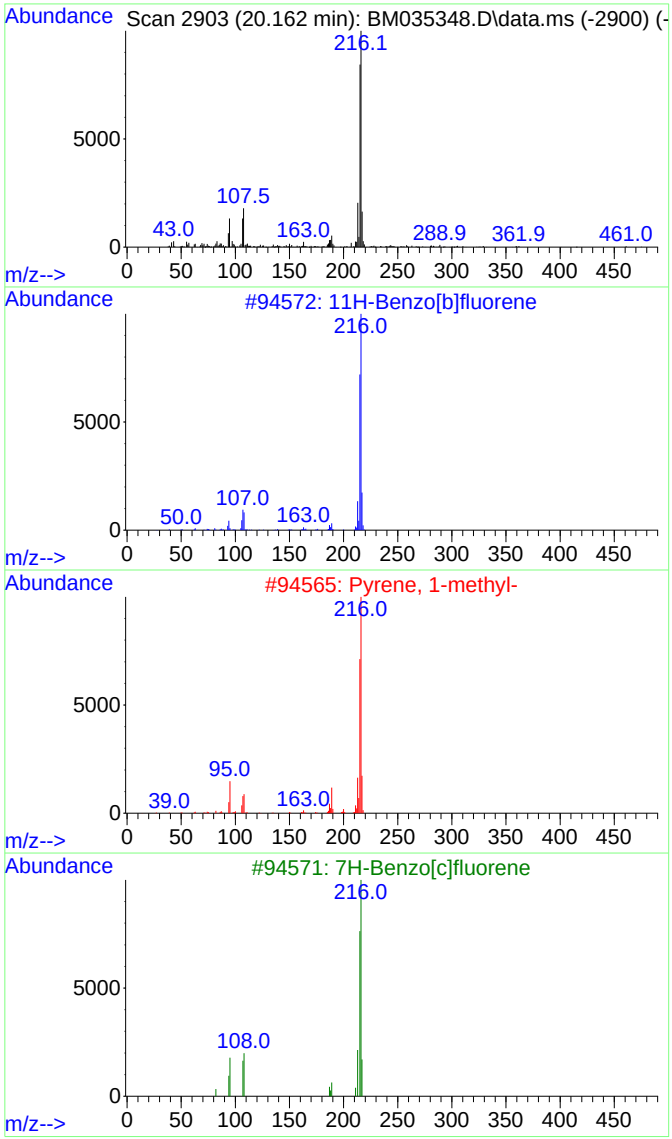
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

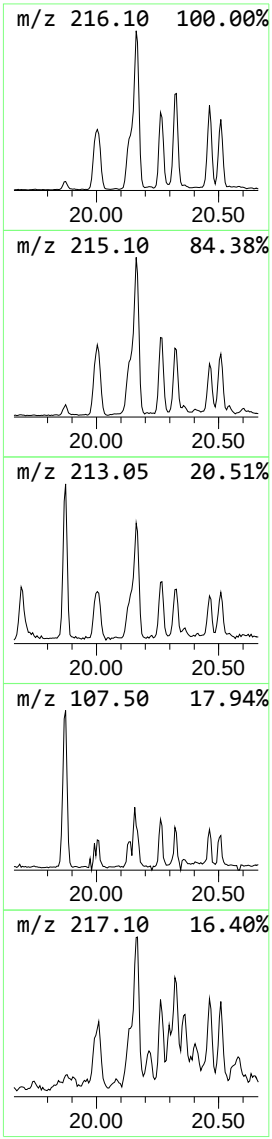
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 11H-Benzo[b]fluorene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.162	2.01 ng	315193	Chrysene-d12	21.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	90
2	Pyrene, 1-methyl-	216	C17H12	002381-21-7	83
3	7H-Benzo[c]fluorene	216	C17H12	000205-12-9	72
4	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	72
5	Pyrene, 2-methyl-	216	C17H12	003442-78-2	62





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM060122\
Data File : BM035348.D
Acq On : 01 Jun 2022 15:49
Operator : CG/JU
Sample : N3107-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MS-6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

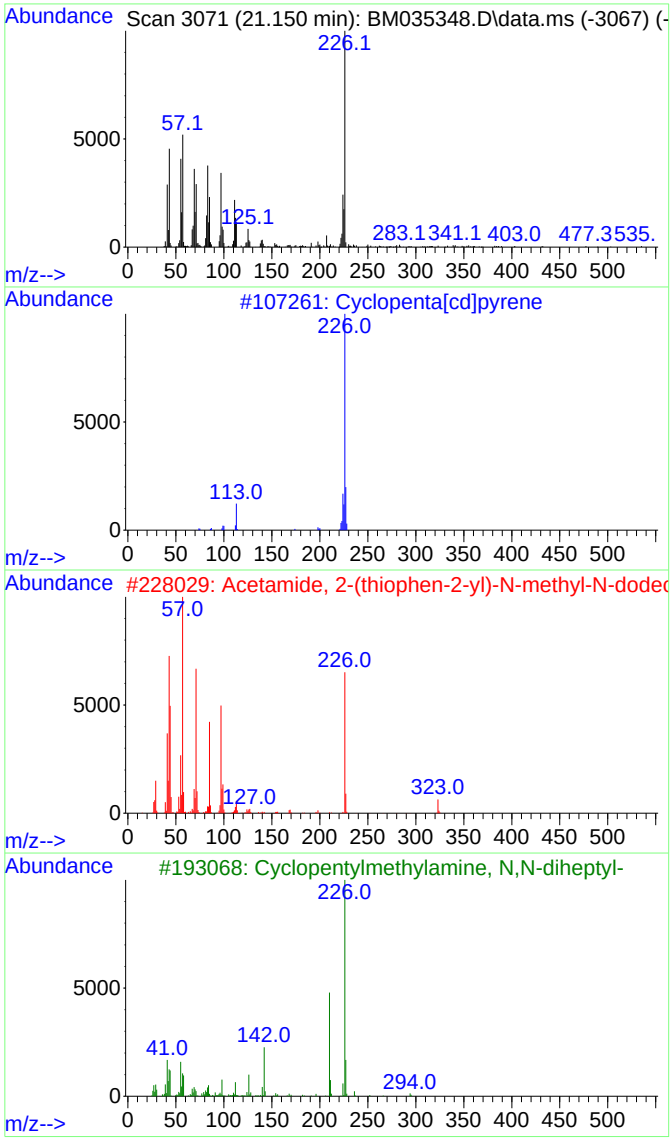
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

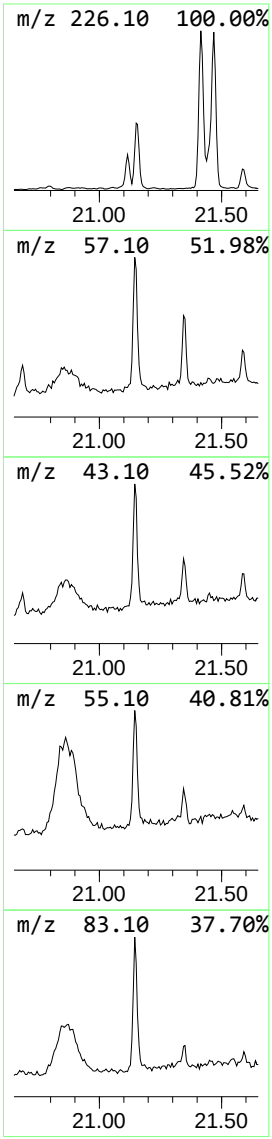
****

Peak Number 5 unknown21.150 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.150	2.69 ng	421578	Chrysene-d12	21.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopenta[cd]pyrene	226	C18H10	027208-37-3	46
2	Acetamide, 2-(thiophen-2-yl)-N-m...	323	C19H33NOS	1000421-20-9	40
3	Cyclopentylmethylamine, N,N-dihe...	295	C20H41N	1000310-50-0	25
4	Pentadecafluorooctanoic acid, he...	638	C24H33F15O2	1000406-04-6	25
5	Diheptylisobutylamine	269	C18H39N	1000310-32-0	23





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM060122\
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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
1H-Indene, 2-ph...	18.127	2.0	ng	159152	4	17.245	1587360	20.0
n-Hexadecanoic ...	18.151	3.7	ng	290307	4	17.245	1587360	20.0
4H-Cyclopenta[d...	18.321	4.3	ng	340596	4	17.245	1587360	20.0
11H-Benzo[b]flu...	20.162	2.0	ng	315193	5	21.433	3135880	20.0
unknown21.150	21.150	2.7	ng	421578	5	21.433	3135880	20.0