LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042621\
Data File : BM029653.D
Acq On : 26 Apr 2021 17:12
Operator : CG/JU
Sample : M2170-13
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : CN-1

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-BM042121.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM029653.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.216	388	396	411	rBV	1008061	1488424	37.98%	4.358%
2	6.804	656	666	683	rBV	966579	1571310	40.09%	4.600%
3	7.616	798	804	813	rBV	252828	411550	10.50%	1.205%
4	8.775	993	1001	1013	rBV	598024	1002991	25.59%	2.936%
5	10.398	1265	1277	1283	rBV	327945	555791	14.18%	1.627%
6	10.445	1283	1285	1291	rVB	30369	47232	1.21%	0.138%
7	12.886	1693	1700	1707	rBV	1648848	2443958	62.36%	7.155%
8	13.586	1813	1819	1823	rBV2	29447	45921	1.17%	0.134%
9	13.727	1839	1843	1852	rVB	43685	69721	1.78%	0.204%
10	13.986	1880	1887	1892	rBV2	47523	77332	1.97%	0.226%
11	14.121	1903	1910	1915	rBV2	25407	57495	1.47%	0.168%
12	14.269	1927	1935	1941	rBV	524166	784864	20.03%	2.298%
13	14.327	1941	1945	1953	rVB	70405	114948	2.93%	0.337%
14	14.668	1998	2003	2012	rBV	45547	76842	1.96%	0.225%
15	15.315	2108	2113	2122	rBV	76414	112800	2.88%	0.330%
16	15.763	2182	2189	2197	rBV	1492305	2136104	54.50%	6.254%
17	15.998	2224	2229	2236	rVB7	28082	52752	1.35%	0.154%
18	16.427	2298	2302	2307	rBV7	24806	40330	1.03%	0.118%
19	16.668	2339	2343	2350	rVB2	29412	49386	1.26%	0.145%
20	16.762	2353	2359	2361	rBV4	25393	54624	1.39%	0.160%
21	16.833	2367	2371	2379	rVB	46925	84638	2.16%	0.248%
22	17.009	2396	2401	2405	rBV	635210	951052	24.27%	2.784%
23	17.057	2405	2409	2415	rVB	830274	1151278	29.38%	3.371%
24	17.145	2420	2424	2429	rVV	218770	306982	7.83%	0.899%
25	17.204	2430	2434	2441	rVB2	30868	51090	1.30%	0.150%
26	17.415	2462	2470	2474	rBV2	71368	141485	3.61%	0.414%
27	17.527	2486	2489	2495	rVB3	29169	40358	1.03%	0.118%
28	17.886	2545	2550	2552	rBV	105972	136795	3.49%	0.400%
29	17.921	2552	2556	2564	rVV2	408249	717334	18.30%	2.100%
30	18.015	2568	2572	2577	rVV	80825	127995	3.27%	0.375%
31	18.080	2577	2583	2587	rVV2	181144	335168	8.55%	0.981%
32	18.115	2587	2589	2596	rVB	83903	110351	2.82%	0.323%
33	18.392	2632	2636	2639	rBV	71354	91205	2.33%	0.267%
34	18.433	2640	2643	2650	rVB	43492	64148	1.64%	0.188%
35	18.639	2675	2678	2682	rVB	36450	43129	1.10%	0.126%
36	18.809	2703	2707	2711	rBV	54880	91011	2.32%	0.266%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042621\
Data File : BM029653.D
Acq On : 26 Apr 2021 17:12
Operator : CG/JU
Sample : M2170-13
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : CN-1

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-BM042121.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	18.951	2727	2731	2739	rBV	63982	102799	2.62%	0.301%
38	19.074	2746	2752	2760	rBV	1673113	2289639	58.42%	6.703%
39	19.203	2771	2774	2781	rBV4	123727	191054	4.87%	0.559%
40	19.439	2804	2814	2822	rBV	1442101	2414548	61.61%	7.069%
41	19.509	2823	2826	2832	rVB2	64155	106701	2.72%	0.312%
42	19.645	2842	2849	2854	rBV	3234939	3919201	100.00%	11.474%
43	19.933	2895	2898	2902	rVB	224261	285490	7.28%	0.836%
44	20.033	2912	2915	2919	rBV	134964	156066	3.98%	0.457%
45	20.345	2965	2968	2973	rVB	174235	209548	5.35%	0.614%
46	20.886	3057	3060	3062	rBV	112010	116108	2.96%	0.340%
47	20.921	3062	3066	3072	rVV2	625889	818531	20.89%	2.396%
48	21.192	3106	3112	3116	rBV3	1332135	2578701	65.80%	7.550%
49	21.233	3116	3119	3127	rVB	780311	1018100	25.98%	2.981%
50	22.733	3370	3374	3379	rBV	741303	1475931	37.66%	4.321%
51	23.203	3450	3454	3461	rVB	397739	716745	18.29%	2.098%
52	23.291	3464	3469	3475	rVB	640526	1134058	28.94%	3.320%
53	23.386	3481	3485	3491	rBV2	586265	984444	25.12%	2.882%

Sum of corrected areas: 34156058

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Operator : CG/JU
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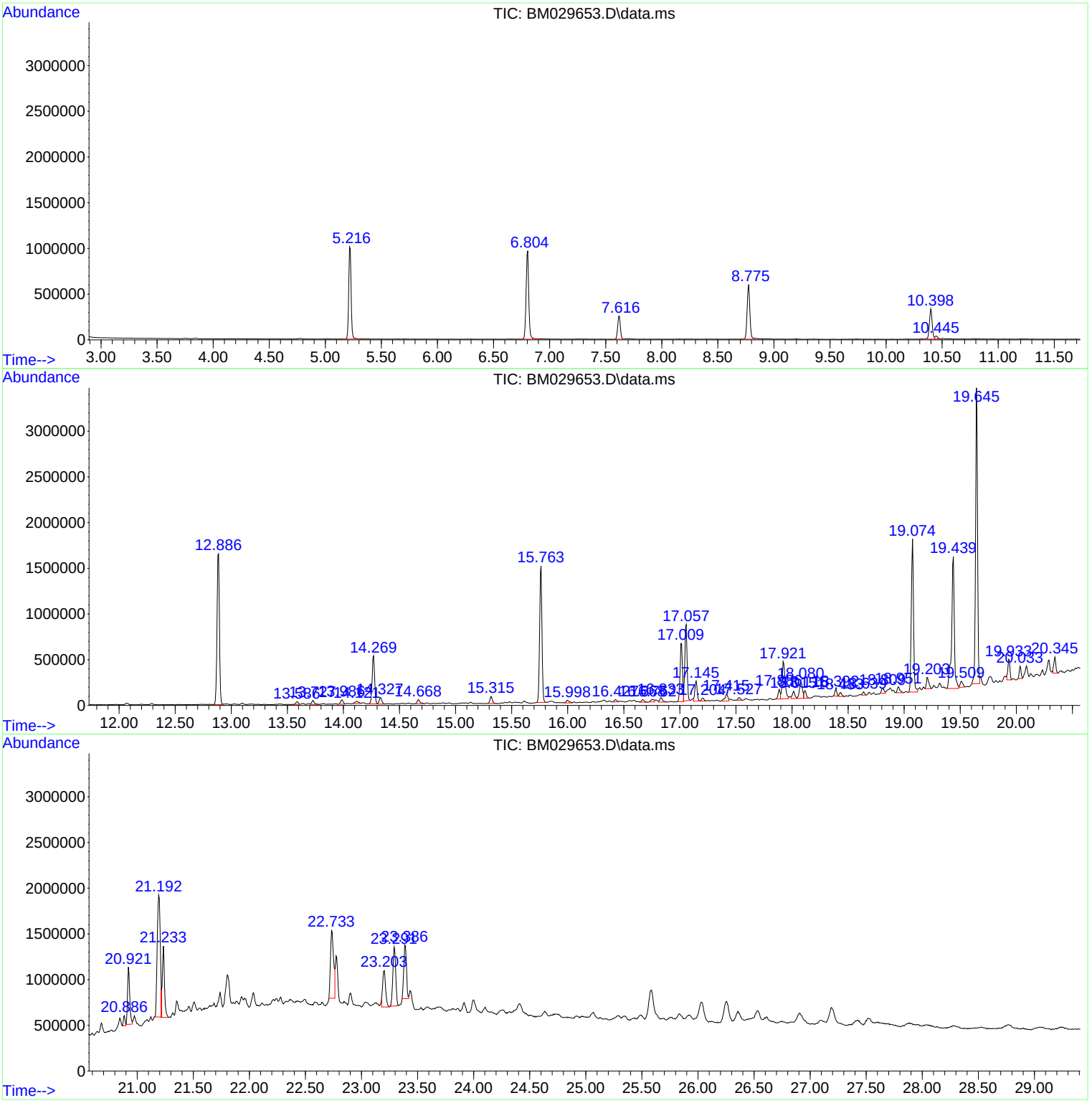
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
CN-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042621\
Data File : BM029653.D
Acq On : 26 Apr 2021 17:12
Operator : CG/JU
Sample : M2170-13
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
CN-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

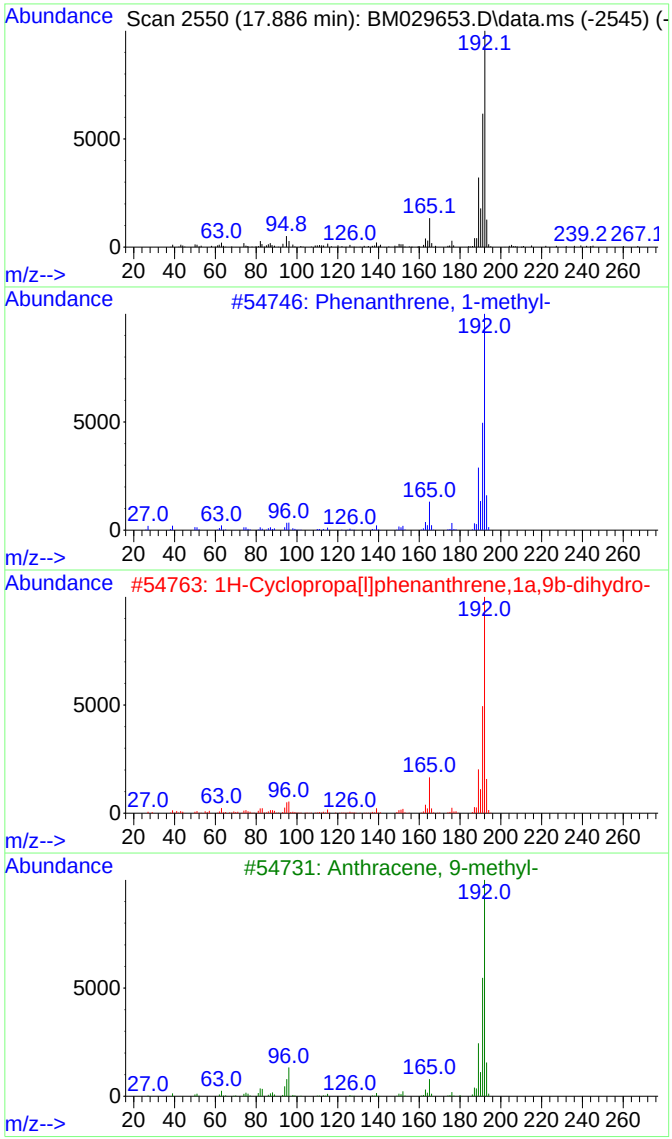
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

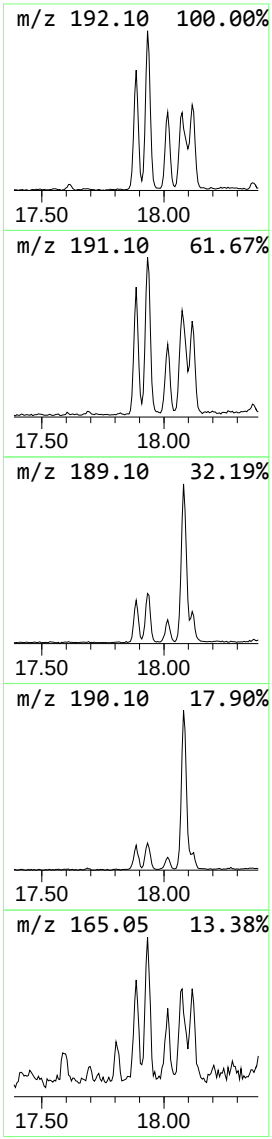
****

Peak Number 1 Phenanthrene, 1-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.886	2.88 ng	136795	Phenanthrene-d10	17.009

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	95
2	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	95
3	Anthracene, 9-methyl-	192	C15H12	000779-02-2	93
4	Anthracene, 2-methyl-	192	C15H12	000613-12-7	91
5	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042621\
Data File : BM029653.D
Acq On : 26 Apr 2021 17:12
Operator : CG/JU
Sample : M2170-13
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
CN-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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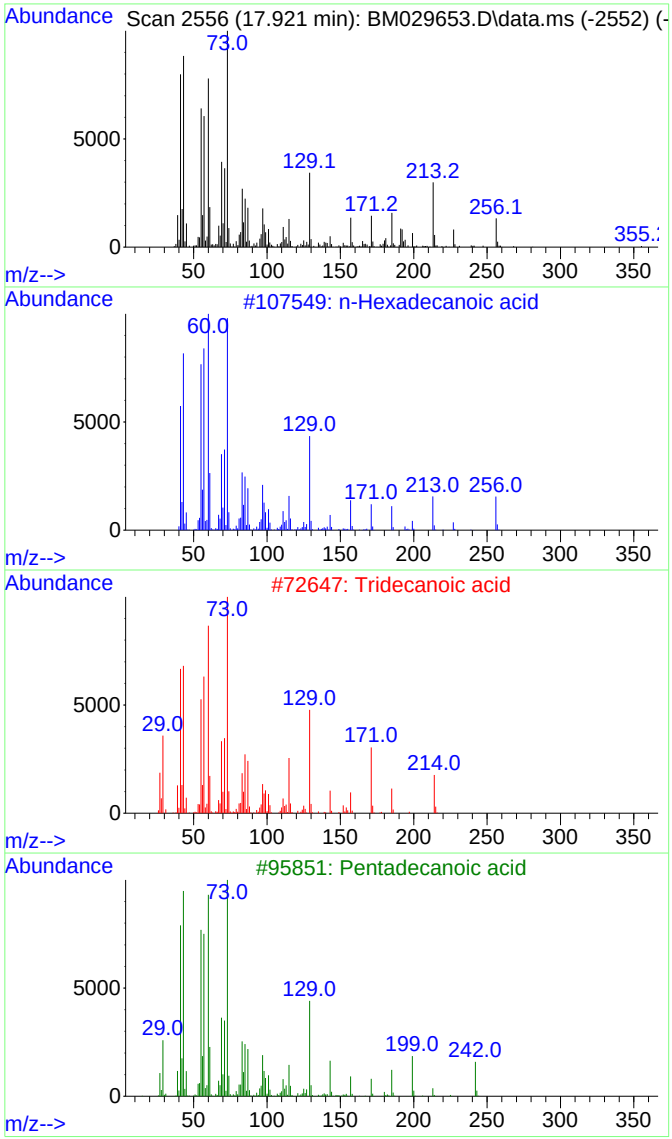
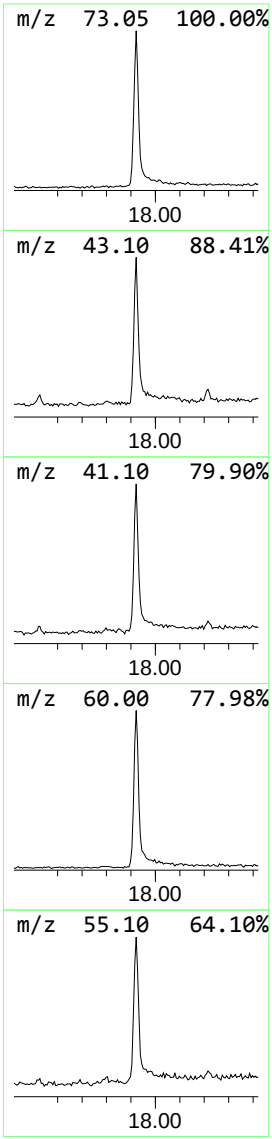
Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.921	15.09 ng	717334	Phenanthrene-d10	17.009

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	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4	Octadecanoic acid	284	C18H36O2	000057-11-4	70
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042621\
Data File : BM029653.D
Acq On : 26 Apr 2021 17:12
Operator : CG/JU
Sample : M2170-13
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : CN-1

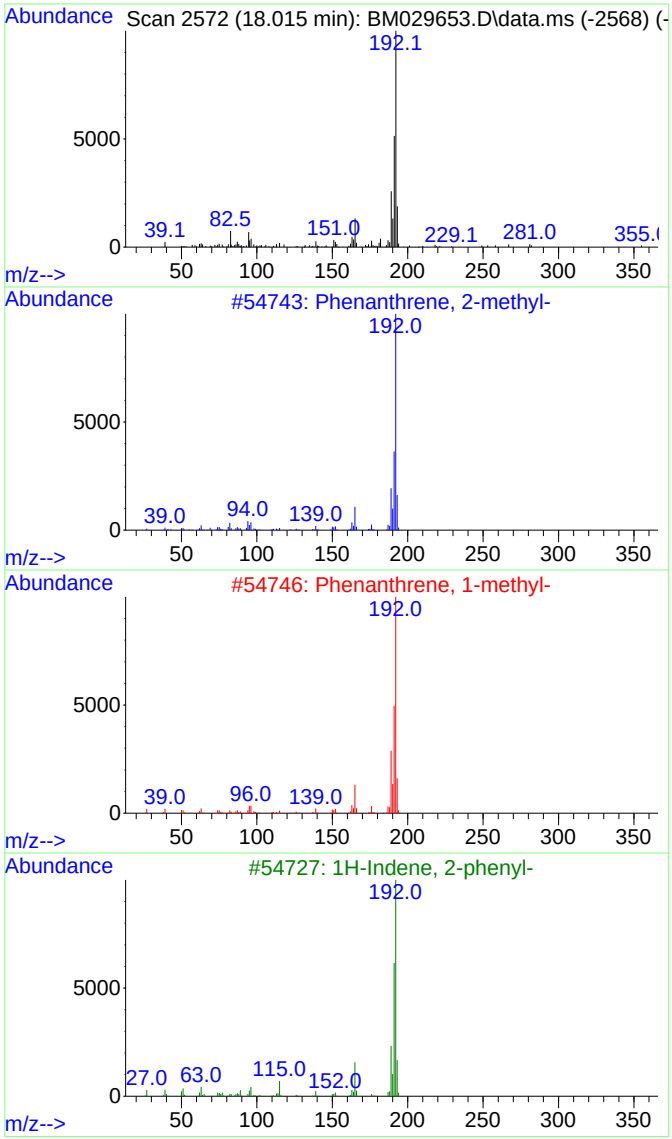
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

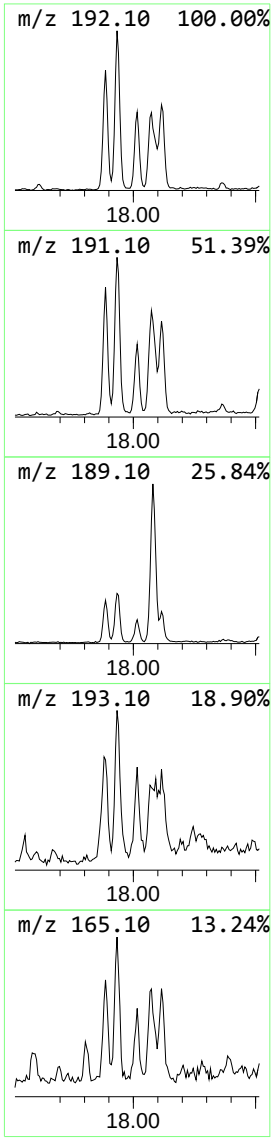
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Phenanthrene, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.015	2.69 ng	127995	Phenanthrene-d10	17.009

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	96
2	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	96
3	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	95
4	Anthracene, 2-methyl-	192	C15H12	000613-12-7	94
5	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	93





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042621\
Data File : BM029653.D
Acq On : 26 Apr 2021 17:12
Operator : CG/JU
Sample : M2170-13
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : CN-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

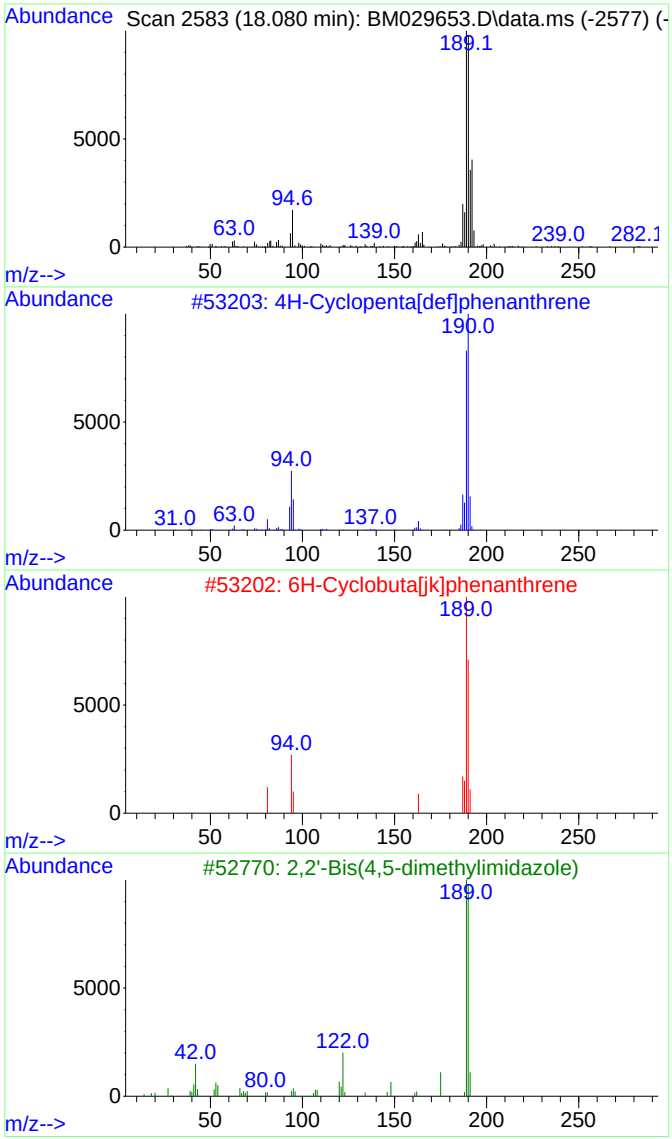
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

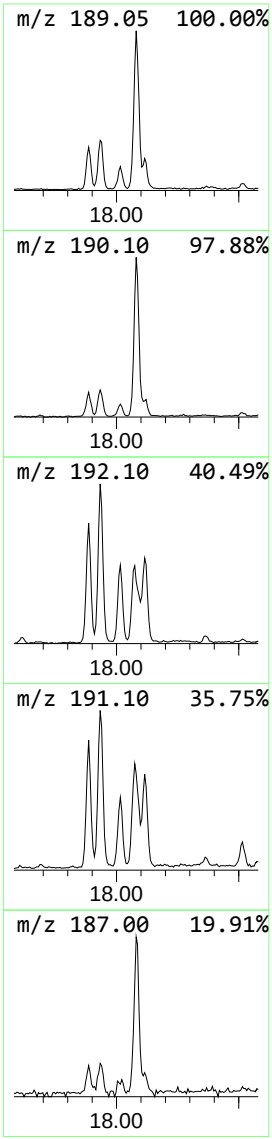
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.080	7.05 ng	335168	Phenanthrene-d10	17.009

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	81
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	59
3	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	47
4	2,3,5,6-Tetramethylterephthalald...	190	C12H14O2	007072-01-7	47
5	Methyl diselenide	190	C2H6Se2	007101-31-7	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042621\
Data File : BM029653.D
Acq On : 26 Apr 2021 17:12
Operator : CG/JU
Sample : M2170-13
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : CN-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

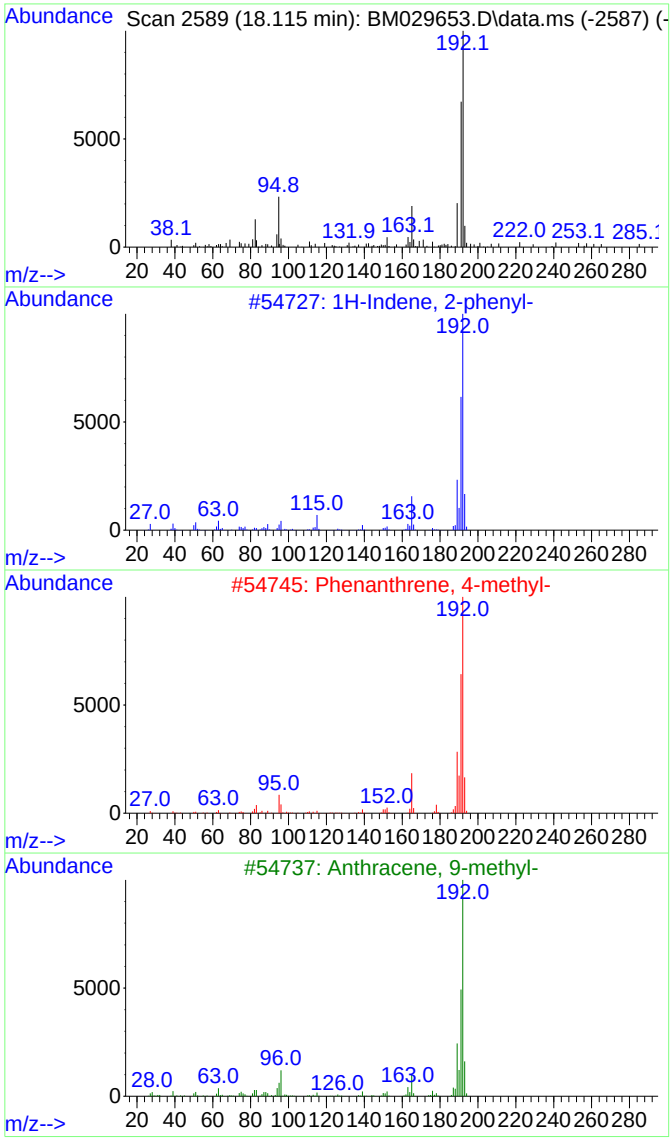
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

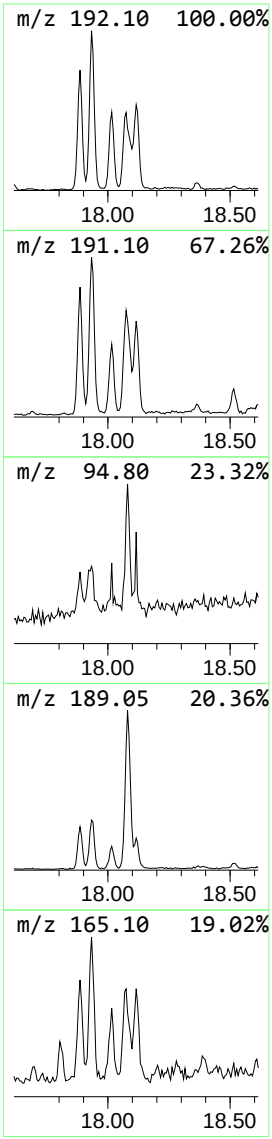
****

Peak Number 5 1H-Indene, 2-phenyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.115	2.32 ng	110351	Phenanthrene-d10	17.009

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	64
2	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	62
3	Anthracene, 9-methyl-	192	C15H12	000779-02-2	58
4	Benzene, 1,1'-(2-cyclopropen-1-y...	192	C15H12	022825-21-4	53
5	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	53





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Data File : BM029653.D
Acq On : 26 Apr 2021 17:12
Operator : CG/JU
Sample : M2170-13
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
CN-1

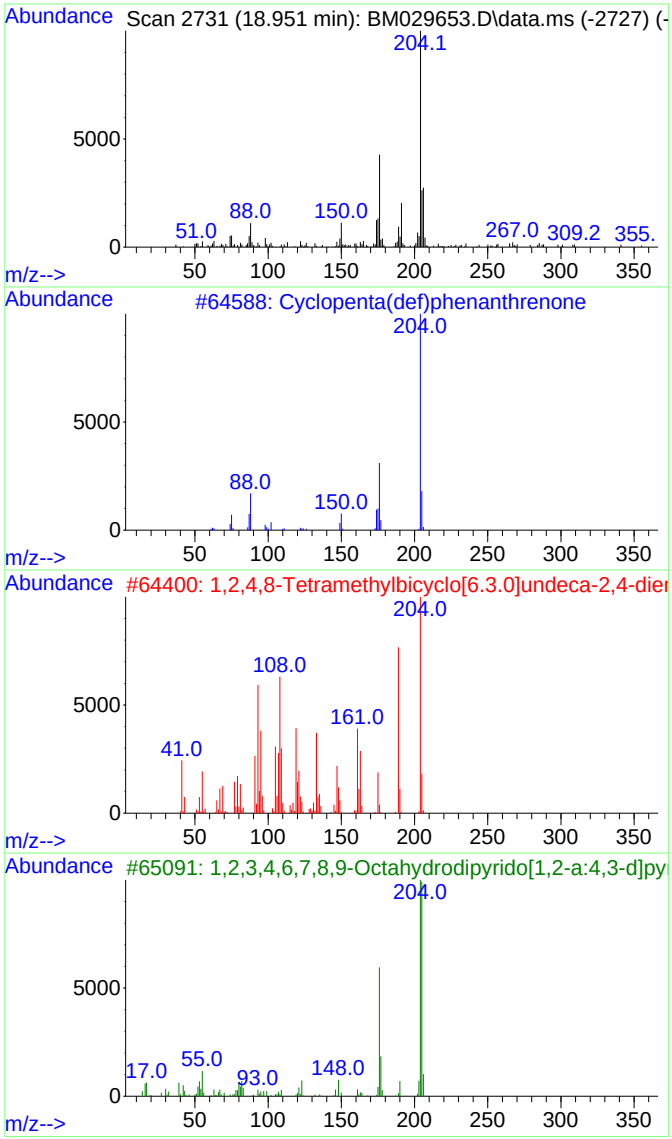
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

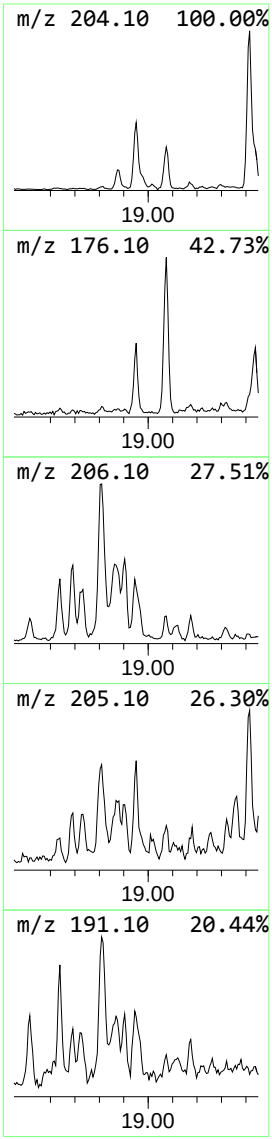
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Cyclopenta(def)phenanthrenone Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.951	2.16 ng	102799	Phenanthrene-d10	17.009

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopenta(def)phenanthrenone	204	C15H8O	005737-13-3	68
2	1,2,4,8-Tetramethylbicyclo[6.3.0...	204	C15H24	137235-51-9	41
3	1,2,3,4,6,7,8,9-Octahydrodipyrid...	205	C11H15N3O	111303-60-7	37
4	[1,1'-Biphenyl]-2,2'-dicarbonitrile	204	C14H8N2	004341-02-0	37
5	[1,1'-Biphenyl]-4,4'-dicarbonitrile	204	C14H8N2	001591-30-6	37





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042621\
Data File : BM029653.D
Acq On : 26 Apr 2021 17:12
Operator : CG/JU
Sample : M2170-13
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : CN-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

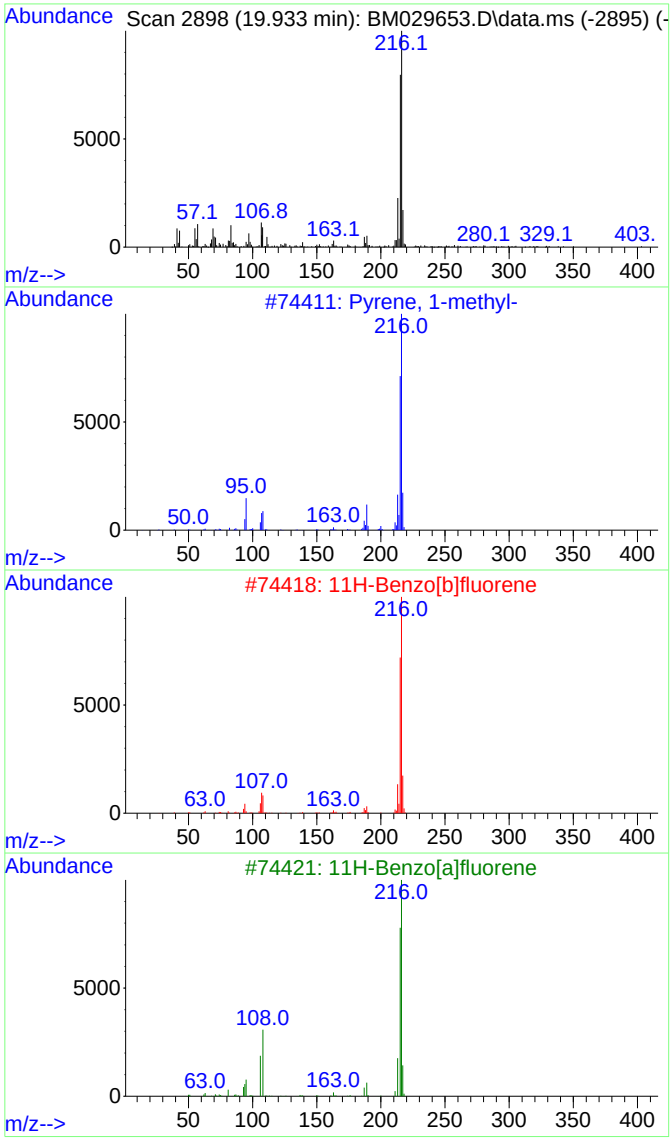
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

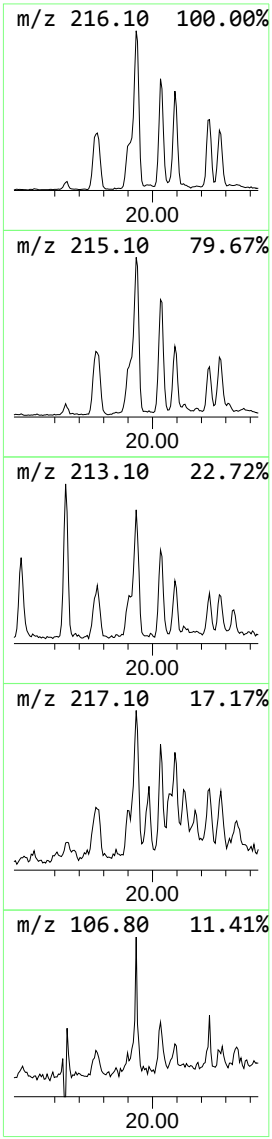
****

Peak Number 7 Pyrene, 1-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.933	2.21 ng	285490	Chrysene-d12	21.198

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 1-methyl-	216	C17H12	002381-21-7	91
2	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	87
3	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	87
4	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	83
5	7H-Benzo[c]fluorene	216	C17H12	000205-12-9	81





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042621\
Data File : BM029653.D
Acq On : 26 Apr 2021 17:12
Operator : CG/JU
Sample : M2170-13
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
CN-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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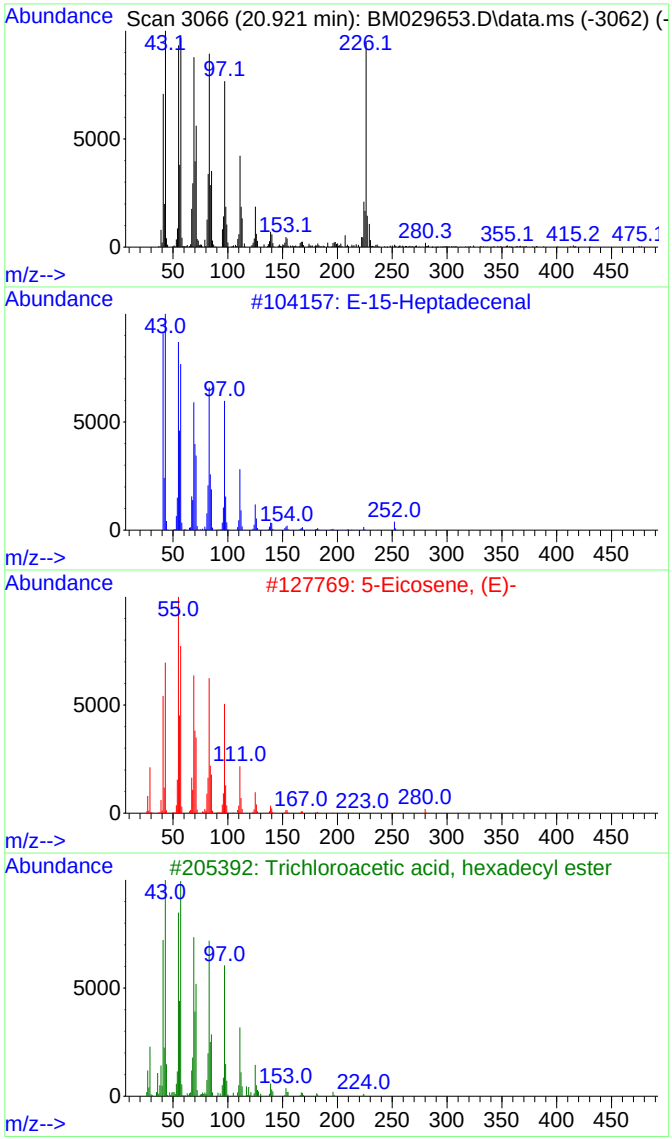
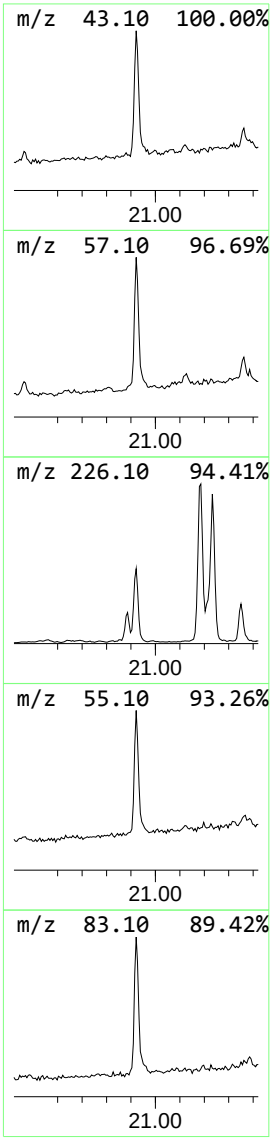
Peak Number 8 E-15-Heptadecenal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.921	6.35 ng	818531	Chrysene-d12	21.198

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	E-15-Heptadecenal	252	C17H32O	1000130-97-9	95
2	5-Eicosene, (E)-	280	C20H40	074685-30-6	95
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	93
4	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	90
5	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042621\
Data File : BM029653.D
Acq On : 26 Apr 2021 17:12
Operator : CG/JU
Sample : M2170-13
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
CN-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

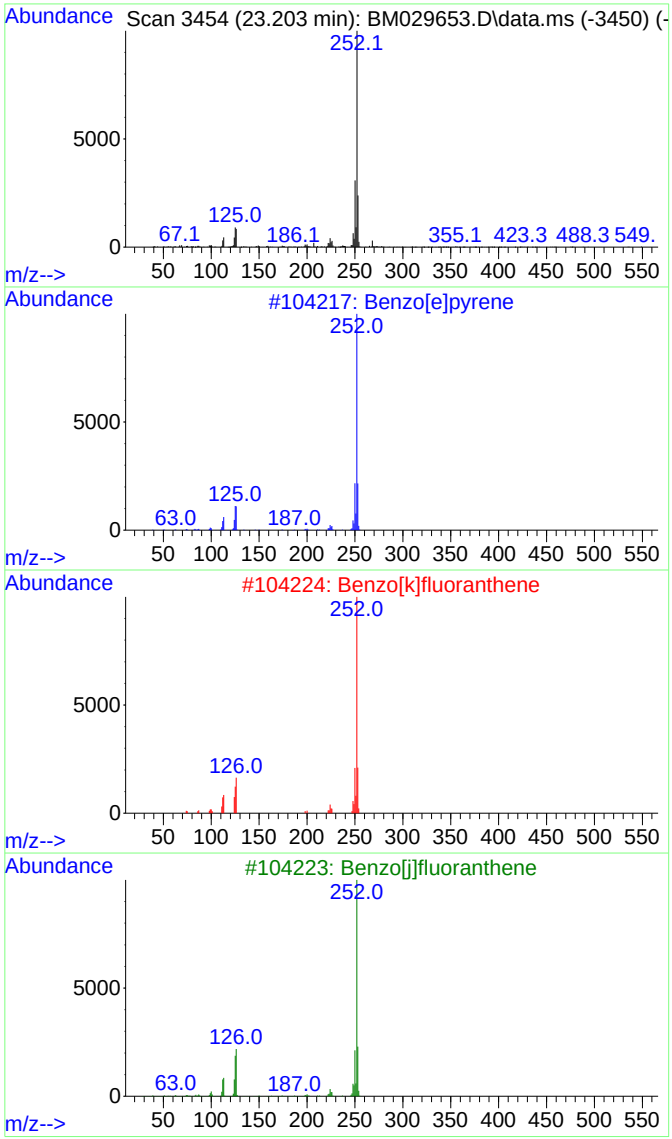
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

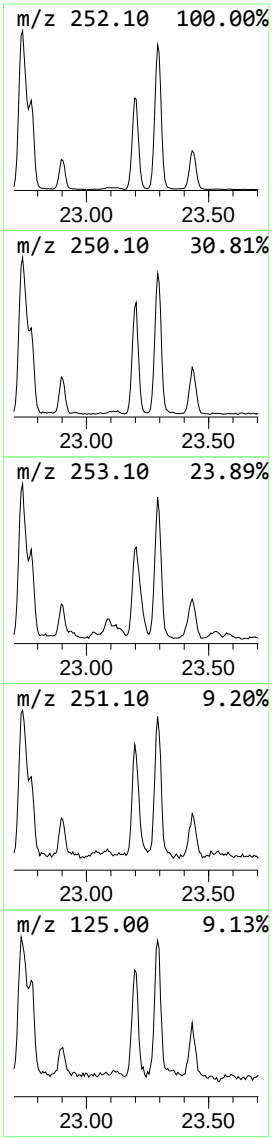
****

Peak Number 9 Benzo[e]pyrene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.203	14.56 ng	716745	Perylene-d12	23.391

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	95
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	95
3	Benzo[j]fluoranthene	252	C20H12	000205-82-3	94
4	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	93
5	Benzo[a]pyrene	252	C20H12	000050-32-8	93





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042621\
Data File : BM029653.D
Acq On : 26 Apr 2021 17:12
Operator : CG/JU
Sample : M2170-13
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : CN-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Phenanthrene, 1...	17.886	2.9	ng	136795	4	17.009	951052	20.0
n-Hexadecanoic ...	17.921	15.1	ng	717334	4	17.009	951052	20.0
Phenanthrene, 2...	18.015	2.7	ng	127995	4	17.009	951052	20.0
4H-Cyclopenta[d...	18.080	7.0	ng	335168	4	17.009	951052	20.0
1H-Indene, 2-ph...	18.115	2.3	ng	110351	4	17.009	951052	20.0
Cyclopenta(def)...	18.951	2.2	ng	102799	4	17.009	951052	20.0
Pyrene, 1-methyl-	19.933	2.2	ng	285490	5	21.198	2578700	20.0
E-15-Heptadecenal	20.921	6.3	ng	818531	5	21.198	2578700	20.0
Benzo[e]pyrene	23.203	14.6	ng	716745	6	23.391	984444	20.0