LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102221\
Data File : BM032673.D
Acq On : 22 Oct 2021 13:43
Operator : CG/JU
Sample : M4300-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TH-CS

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-BM100221.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM032673.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.131	384	390	406	rBV	4200077	6097653	71.88%	7.765%
2	6.754	658	666	680	rBV	3925936	6286652	74.11%	8.006%
3	7.543	793	800	811	rBV	918707	1414277	16.67%	1.801%
4	8.701	989	997	1009	rBV	2669873	4176346	49.23%	5.318%
5	10.113	1231	1237	1251	rBV	540881	841839	9.92%	1.072%
6	10.331	1266	1274	1279	rBV	1220546	1996664	23.54%	2.543%
7	10.378	1279	1282	1293	rVB	313818	489346	5.77%	0.623%
8	12.001	1551	1558	1567	rBV	148549	242734	2.86%	0.309%
9	12.225	1589	1596	1607	rVB	91264	146882	1.73%	0.187%
10	12.819	1689	1697	1709	rBV	5695409	8483355	100.00%	10.803%
11	13.519	1809	1816	1821	rBV	67897	118774	1.40%	0.151%
12	13.919	1880	1884	1893	rBV2	62008	100859	1.19%	0.128%
13	14.201	1923	1932	1938	rBV	1687740	2457164	28.96%	3.129%
14	14.266	1938	1943	1950	rVB	268435	381730	4.50%	0.486%
15	14.601	1994	2000	2010	rBV	239887	368589	4.34%	0.469%
16	15.248	2105	2110	2123	rVB	411637	595429	7.02%	0.758%
17	15.548	2156	2161	2171	rVB	71414	116952	1.38%	0.149%
18	15.695	2180	2186	2195	rBV	3969267	5751002	67.79%	7.324%
19	16.254	2269	2281	2286	rBV3	56930	129376	1.53%	0.165%
20	16.760	2363	2367	2377	rVB	114400	181179	2.14%	0.231%
21	16.936	2391	2397	2401	rBV	1765301	2553686	30.10%	3.252%
22	16.977	2401	2404	2411	rVV	2075994	2822180	33.27%	3.594%
23	17.065	2411	2419	2425	rVV	527165	790889	9.32%	1.007%
24	17.336	2461	2465	2470	rBV	160970	217461	2.56%	0.277%
25	17.807	2541	2545	2548	rBV	196679	284212	3.35%	0.362%
26	17.842	2548	2551	2562	rVV2	458777	932672	10.99%	1.188%
27	17.936	2563	2567	2572	rVV	104237	154108	1.82%	0.196%
28	18.007	2573	2579	2582	rVV3	349878	608402	7.17%	0.775%
29	18.036	2582	2584	2590	rVB	138297	180548	2.13%	0.230%
30	18.307	2626	2630	2634	rBV	149712	200072	2.36%	0.255%
31	18.348	2634	2637	2648	rVB2	55050	90290	1.06%	0.115%
32	18.736	2698	2703	2707	rBV	121980	202838	2.39%	0.258%
33	18.871	2722	2726	2734	rBV2	66722	134509	1.59%	0.171%
34	18.995	2742	2747	2752	rBV	2489163	3164086	37.30%	4.029%
35	19.359	2799	2809	2818	rBV	1872523	3149422	37.12%	4.011%
36	19.436	2818	2822	2828	rVB2	93829	163569	1.93%	0.208%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102221\
Data File : BM032673.D
Acq On : 22 Oct 2021 13:43
Operator : CG/JU
Sample : M4300-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TH-CS

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-BM100221.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	19.565	2836	2844	2849	rBV	6204165	7873486	92.81%	10.027%
38	19.689	2859	2865	2871	rBV2	139134	333806	3.93%	0.425%
39	19.854	2890	2893	2899	rVB	342048	470888	5.55%	0.600%
40	19.954	2906	2910	2914	rBV	300874	397436	4.68%	0.506%
41	20.012	2916	2920	2924	rVB2	162835	244400	2.88%	0.311%
42	20.154	2941	2944	2948	rBV	99931	117061	1.38%	0.149%
43	20.201	2949	2952	2956	rVB	92080	116749	1.38%	0.149%
44	20.601	3017	3020	3026	rVB	96482	134661	1.59%	0.171%
45	20.765	3045	3048	3051	rBV	142132	157416	1.86%	0.200%
46	20.824	3052	3058	3066	rVV4	575314	985421	11.62%	1.255%
47	21.030	3091	3093	3097	rVB	134743	136368	1.61%	0.174%
48	21.112	3101	3107	3111	rVV2	1853204	3542888	41.76%	4.512%
49	21.153	3111	3114	3124	rVB	969910	1224827	14.44%	1.560%
50	21.271	3131	3134	3139	rBV	238781	291821	3.44%	0.372%
51	21.642	3193	3197	3202	rBV2	373375	670086	7.90%	0.853%
52	22.624	3359	3364	3369	rBV	862830	1868515	22.03%	2.379%
53	23.071	3437	3440	3449	rVB	499106	869584	10.25%	1.107%
54	23.159	3451	3455	3461	rVB	764335	1239936	14.62%	1.579%
55	23.253	3466	3471	3476	rBV2	1087402	1824530	21.51%	2.323%

Sum of corrected areas: 78525625

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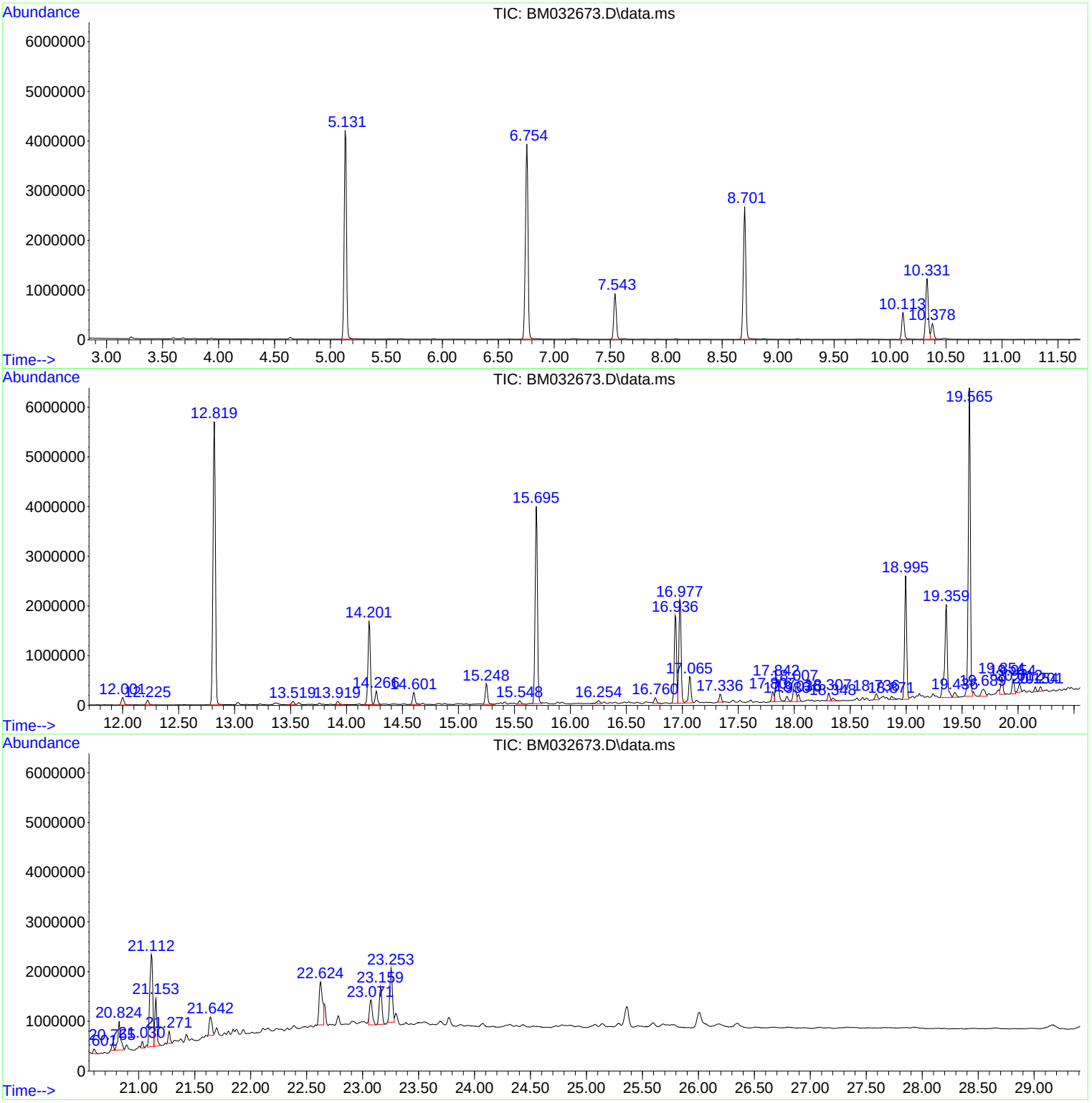
Data File : BM032673.D
Acq On : 22 Oct 2021 13:43
Operator : CG/JU
Sample : M4300-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TH-CS

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM100221.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\BM102221\
Data File : BM032673.D
Acq On : 22 Oct 2021 13:43
Operator : CG/JU
Sample : M4300-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TH-CS

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM100221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

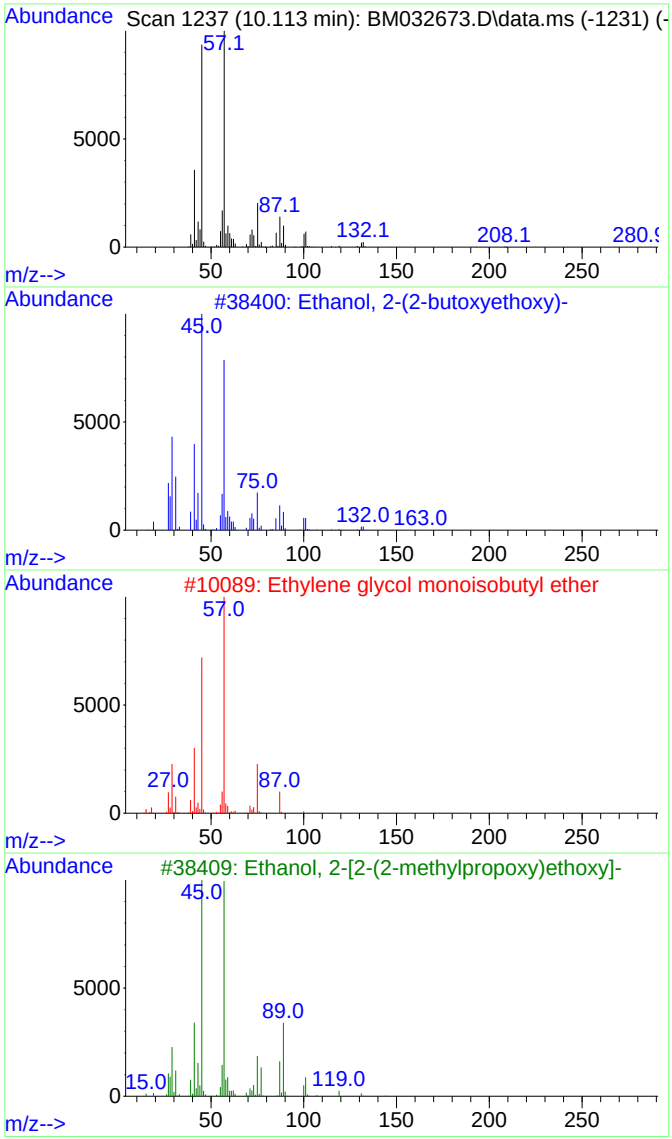
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

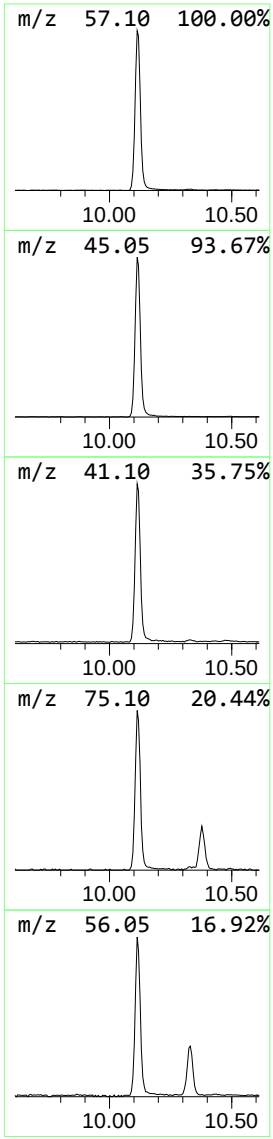
****

Peak Number 1 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.113	8.43 ng	841839	Naphthalene-d8	10.331

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
3	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
4	Di-sec-Butyl ether	130	C8H18O	006863-58-7	50
5	Methoxyacetic acid, 2-butyl ester	146	C7H14O3	070159-90-9	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102221\
Data File : BM032673.D
Acq On : 22 Oct 2021 13:43
Operator : CG/JU
Sample : M4300-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TH-CS

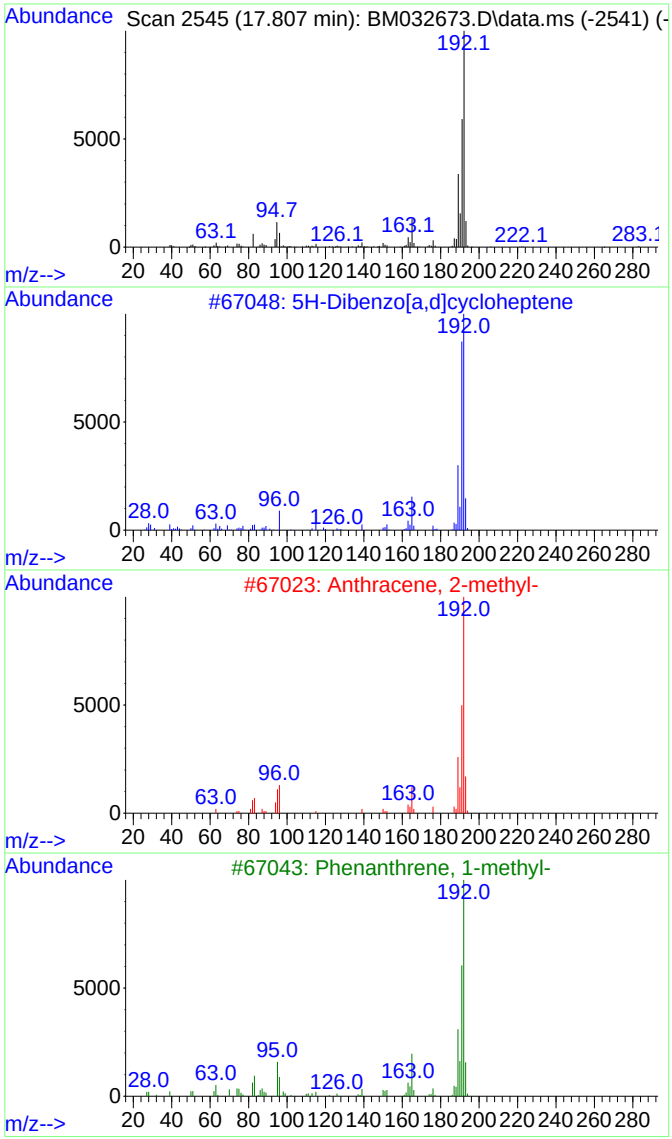
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM100221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

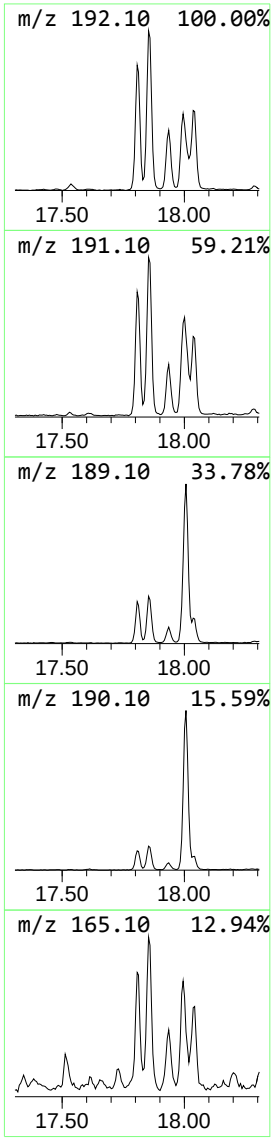
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 5H-Dibenzo[a,d]cycloheptene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.807	2.23 ng	284212	Phenanthrene-d10	16.936

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	94
2	Anthracene, 2-methyl-	192	C15H12	000613-12-7	93
3	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	91
4	Anthracene, 9-methyl-	192	C15H12	000779-02-2	91
5	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102221\
Data File : BM032673.D
Acq On : 22 Oct 2021 13:43
Operator : CG/JU
Sample : M4300-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TH-CS

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM100221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

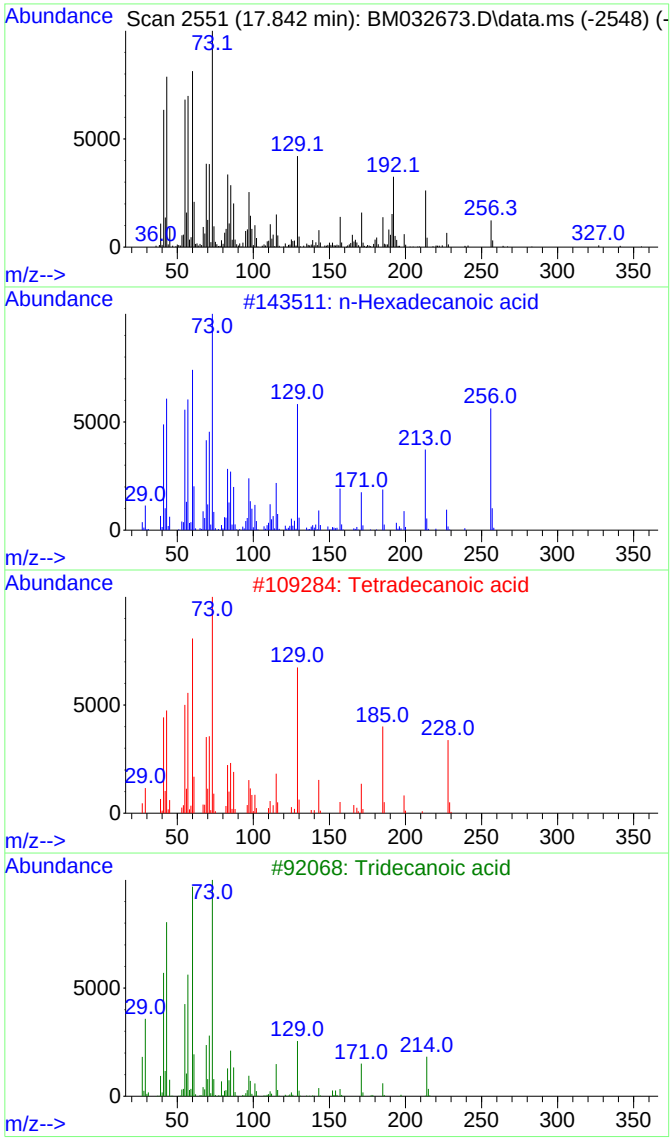
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

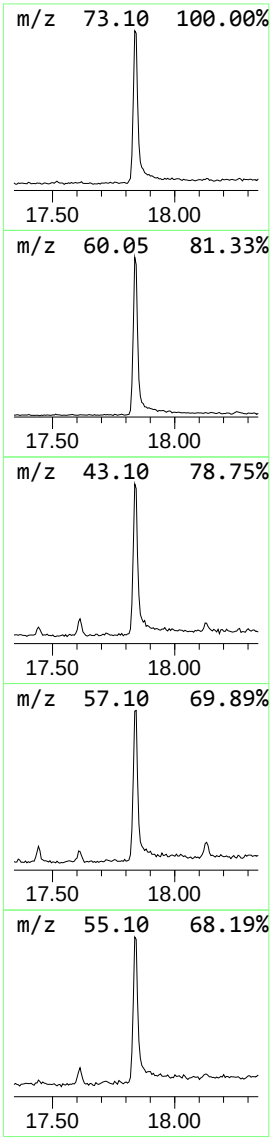
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.842	7.30 ng	932672	Phenanthrene-d10	16.936

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	Tridecanoic acid	214	C13H26O2	000638-53-9	86
4	Octadecanoic acid	284	C18H36O2	000057-11-4	83
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	81





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102221\
Data File : BM032673.D
Acq On : 22 Oct 2021 13:43
Operator : CG/JU
Sample : M4300-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TH-CS

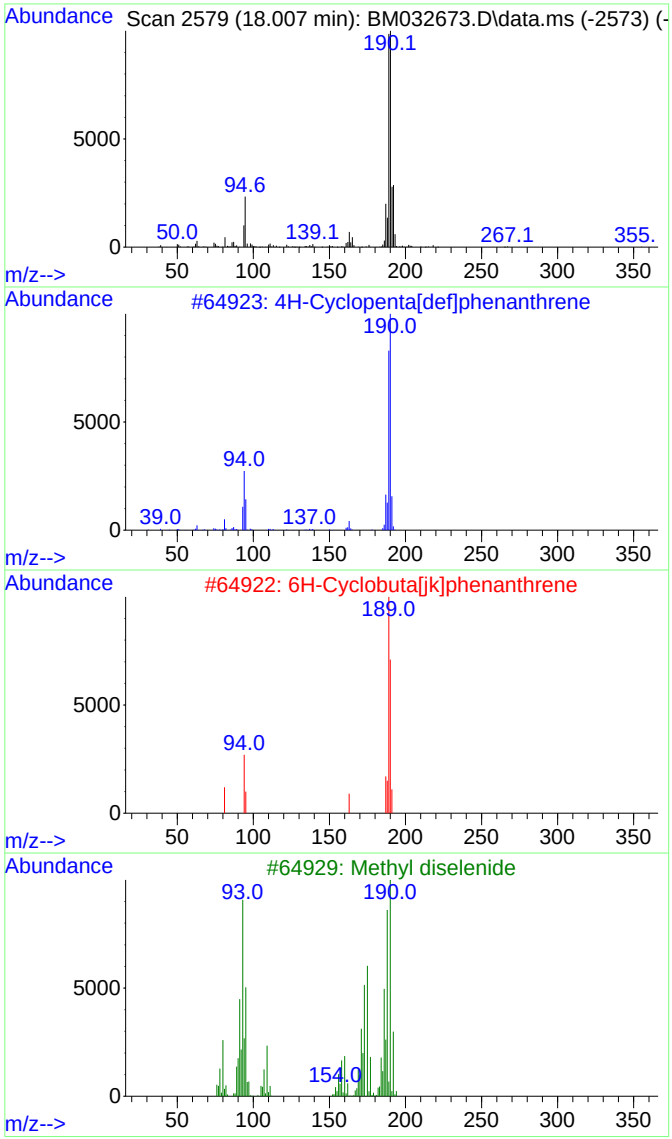
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM100221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

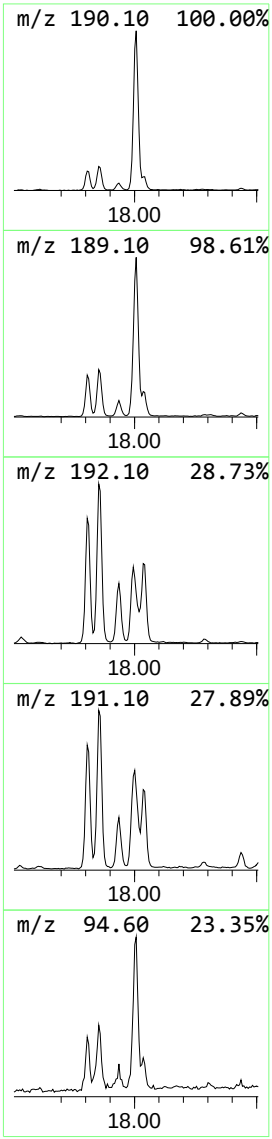
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.007	4.76 ng	608402	Phenanthrene-d10	16.936

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	94
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	50
3	Methyl diselenide	190	C2H6Se2	007101-31-7	46
4	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	45
5	2,4(1H,3H)-Pyrimidinedione, 5-br...	190	C4H3BrN2O2	000051-20-7	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102221\
Data File : BM032673.D
Acq On : 22 Oct 2021 13:43
Operator : CG/JU
Sample : M4300-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TH-CS

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM100221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

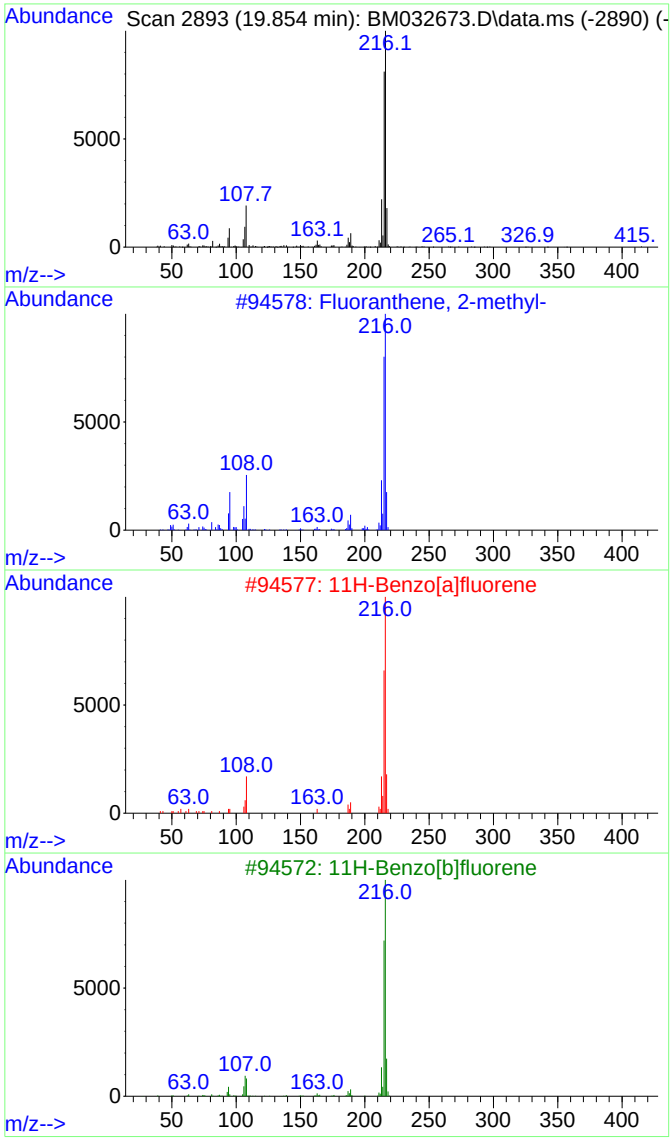
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

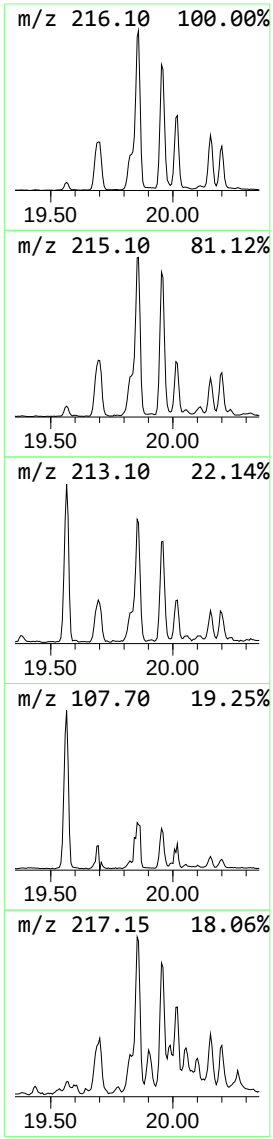
****

Peak Number 5 Fluoranthene, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.854	2.66 ng	470888	Chrysene-d12	21.118

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	93
2	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	91
3	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	87
4	Pyrene, 1-methyl-	216	C17H12	002381-21-7	87
5	7H-Benzo[c]fluorene	216	C17H12	000205-12-9	72





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Data File : BM032673.D
Acq On : 22 Oct 2021 13:43
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Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TH-CS

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM100221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

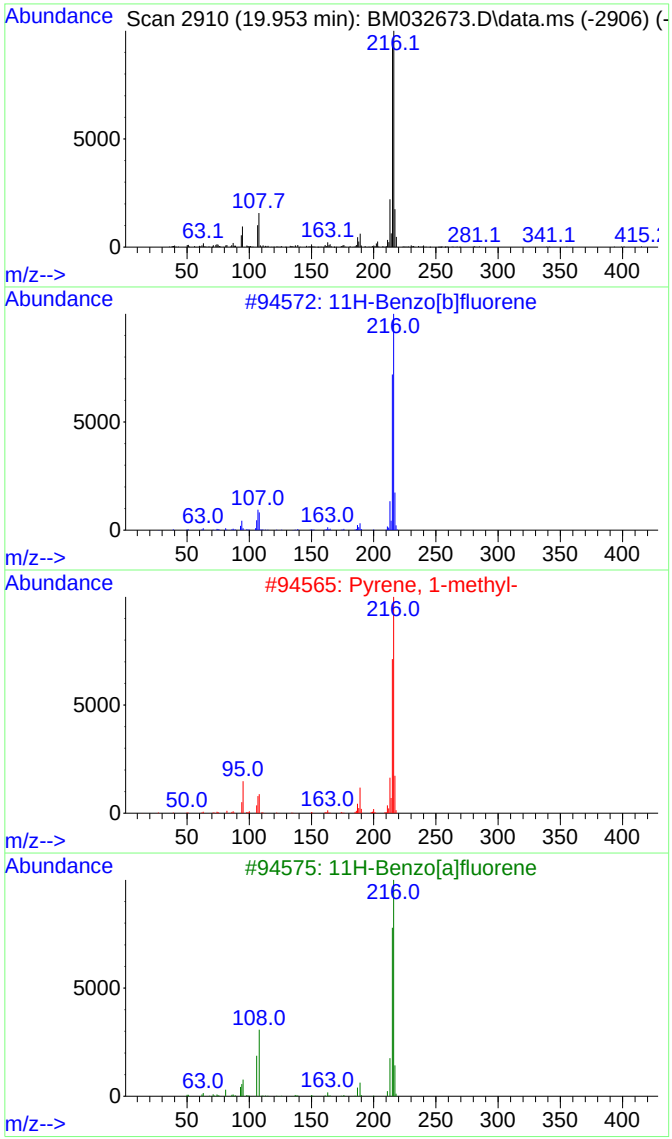
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

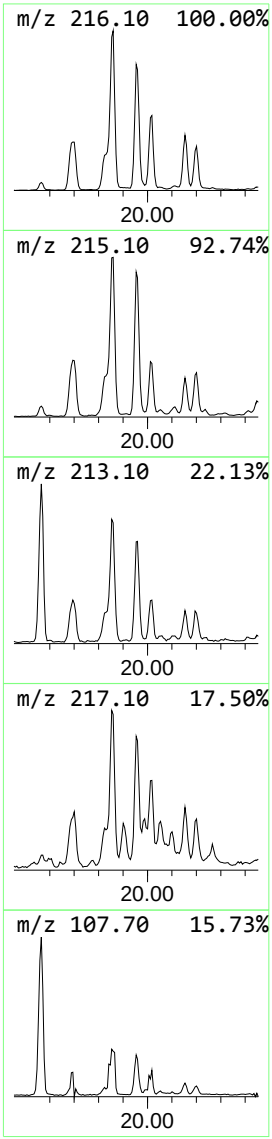
****

Peak Number 6 11H-Benzo[b]fluorene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.953	2.24 ng	397436	Chrysene-d12	21.118

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	96
2	Pyrene, 1-methyl-	216	C17H12	002381-21-7	93
3	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	91
4	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	81
5	Pyrene, 2-methyl-	216	C17H12	003442-78-2	60





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102221\
Data File : BM032673.D
Acq On : 22 Oct 2021 13:43
Operator : CG/JU
Sample : M4300-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TH-CS

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM100221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

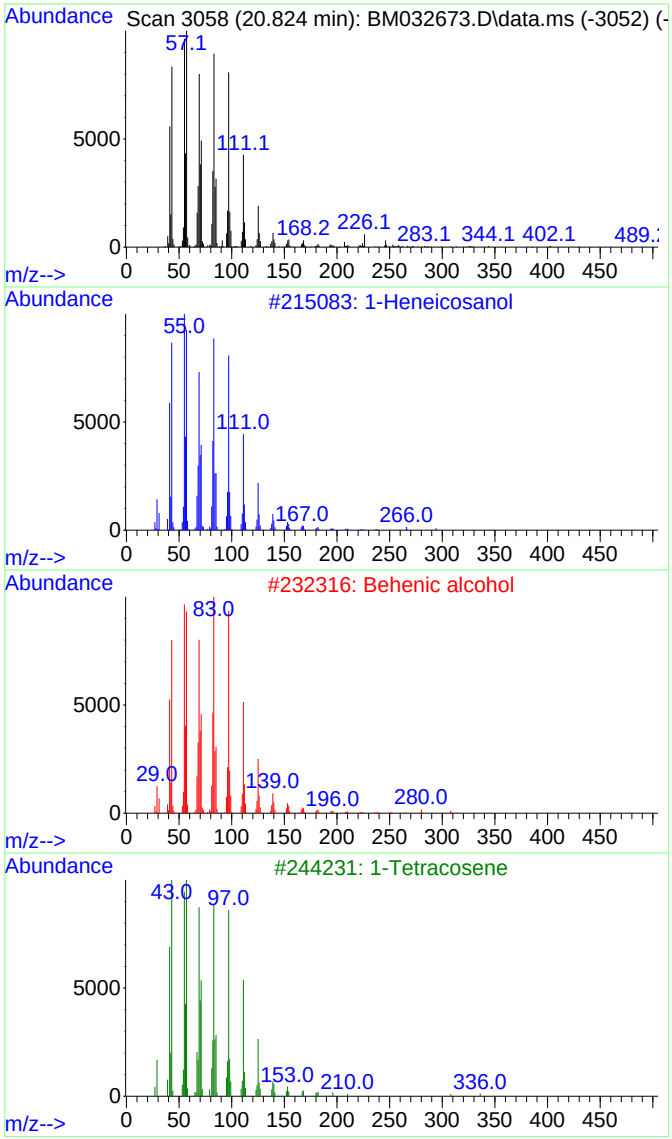
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

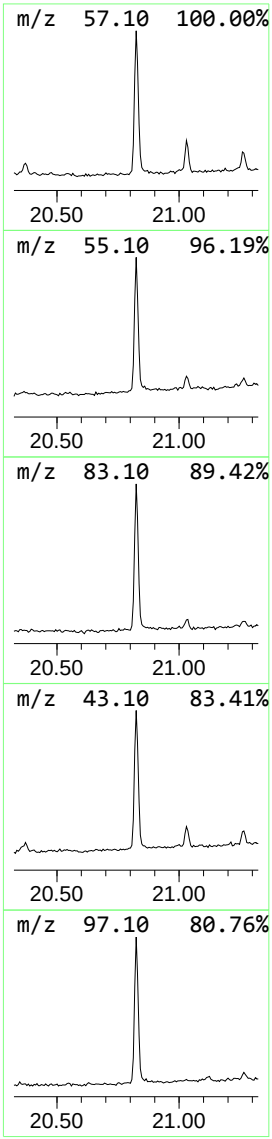
****

Peak Number 7 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.824	5.56 ng	985421	Chrysene-d12	21.118

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Behenic alcohol	326	C22H46O	000661-19-8	94
3	1-Tetracosene	336	C24H48	010192-32-2	94
4	Pentacos-1-ene	350	C25H50	016980-85-1	94
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	94





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102221\
Data File : BM032673.D
Acq On : 22 Oct 2021 13:43
Operator : CG/JU
Sample : M4300-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TH-CS

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM100221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

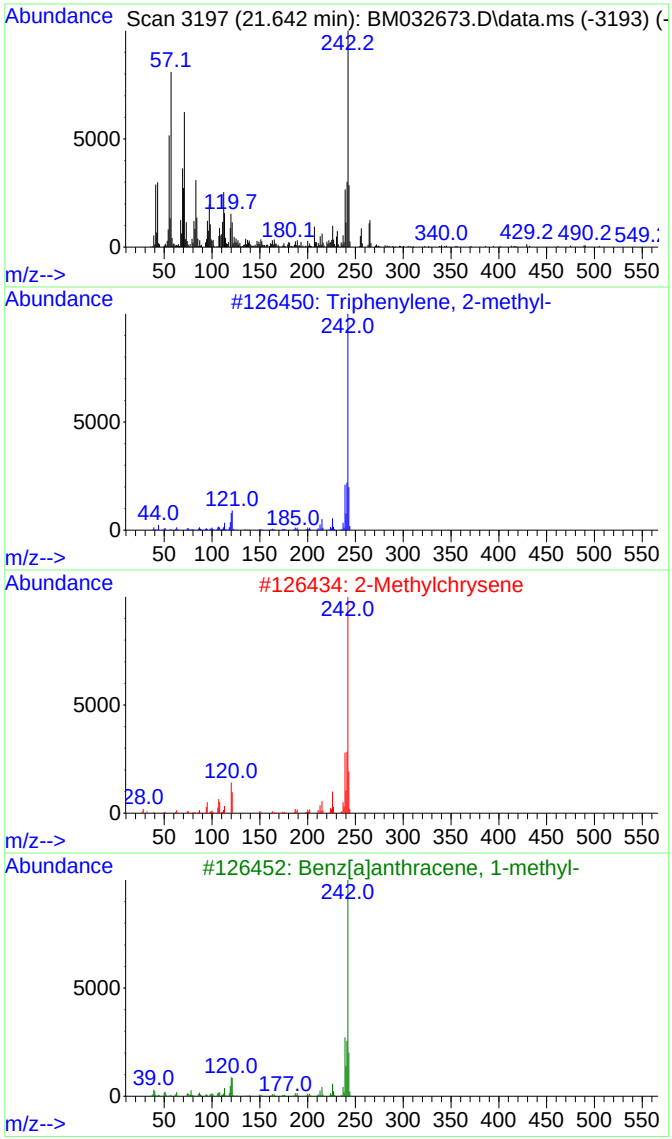
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

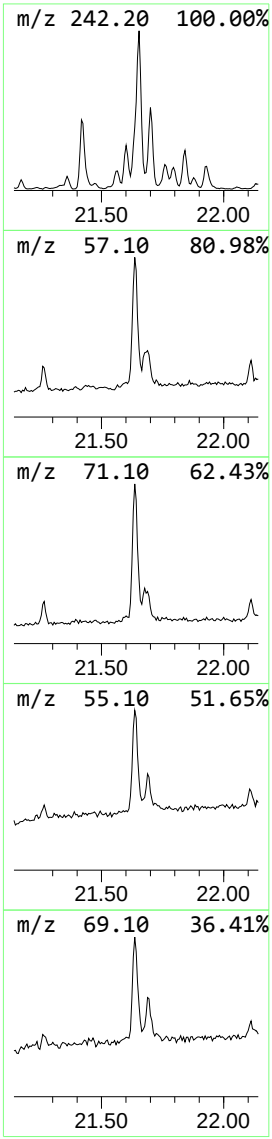
****

Peak Number 8 Triphenylene, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.642	3.78 ng	670086	Chrysene-d12	21.118

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylene, 2-methyl-	242	C19H14	001705-84-6	95
2	2-Methylchrysene	242	C19H14	003351-32-4	94
3	Benz[a]anthracene, 1-methyl-	242	C19H14	002498-77-3	94
4	Chrysene, 1-methyl-	242	C19H14	003351-28-8	92
5	Chrysene, 3-methyl-	242	C19H14	003351-31-3	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102221\
Data File : BM032673.D
Acq On : 22 Oct 2021 13:43
Operator : CG/JU
Sample : M4300-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TH-CS

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM100221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

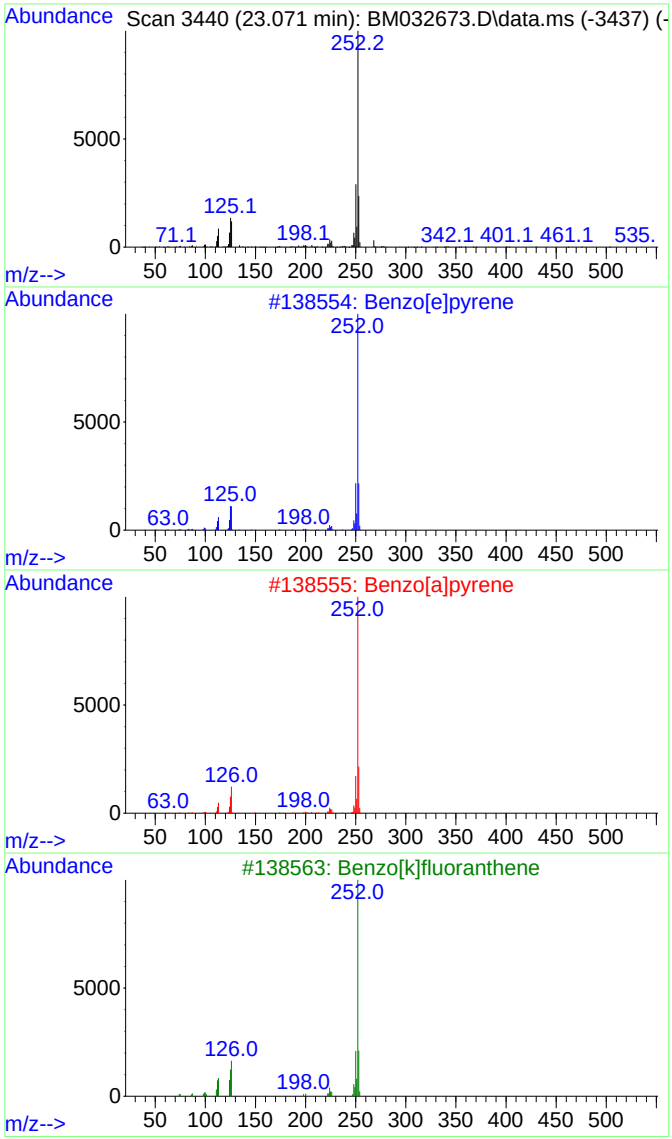
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

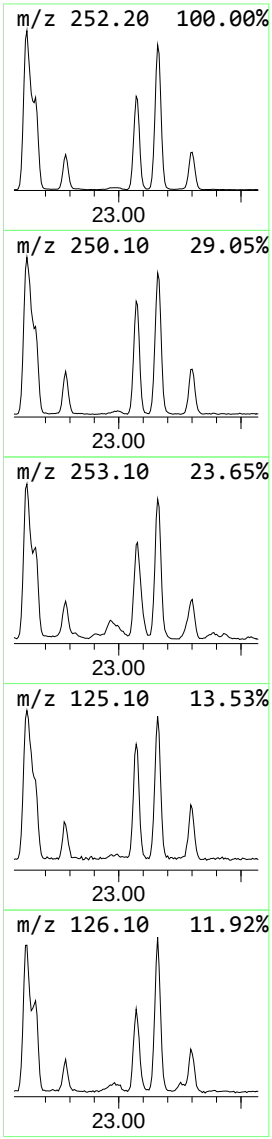
****

Peak Number 9 Benzo[e]pyrene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.071	9.53 ng	869584	Perylene-d12	23.253

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	99
2	Benzo[a]pyrene	252	C20H12	000050-32-8	98
3	Benzo[k]fluoranthene	252	C20H12	000207-08-9	97
4	Benzo[b]fluoranthene	252	C20H12	000205-99-2	94
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102221\
Data File : BM032673.D
Acq On : 22 Oct 2021 13:43
Operator : CG/JU
Sample : M4300-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TH-CS

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM100221.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
Ethanol, 2-(2-b...	10.113	8.4	ng	841839	2	10.331	1996660	20.0
5H-Dibenzo[a,d]...	17.807	2.2	ng	284212	4	16.936	2553690	20.0
n-Hexadecanoic ...	17.842	7.3	ng	932672	4	16.936	2553690	20.0
4H-Cyclopenta[d...	18.007	4.8	ng	608402	4	16.936	2553690	20.0
Fluoranthene, 2...	19.854	2.7	ng	470888	5	21.118	3542890	20.0
11H-Benzo[b]flu...	19.953	2.2	ng	397436	5	21.118	3542890	20.0
1-Heneicosanol	20.824	5.6	ng	985421	5	21.118	3542890	20.0
Triphenylene, 2...	21.642	3.8	ng	670086	5	21.118	3542890	20.0
Benzo[e]pyrene	23.071	9.5	ng	869584	6	23.253	1824530	20.0