LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF050617\
Data File : BF094970.D
Acq On : 8 May 2017 5:42
Operator : SJ/MA
Sample : I2947-14
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-05-0-2.0

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:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.031	522	526	540	rBV	106759	202082	8.90%	0.972%
2	5.660	629	633	658	rBV	1189915	1877509	82.68%	9.030%
3	7.254	900	904	920	rBV	1353258	2007034	88.38%	9.653%
4	7.378	920	925	942	rVB	1699627	2270857	100.00%	10.921%
5	7.719	979	983	991	rBV	496162	563421	24.81%	2.710%
6	7.954	1018	1023	1035	rBV	1339130	1623588	71.50%	7.808%
7	8.619	1131	1136	1157	rBV	882109	1275258	56.16%	6.133%
8	9.742	1322	1327	1340	rBV	486934	707840	31.17%	3.404%
9	11.513	1623	1628	1646	rBV	1642662	2041909	89.92%	9.820%
10	12.207	1739	1746	1757	rBV	231670	307170	13.53%	1.477%
11	12.348	1766	1770	1777	rBV2	29539	38004	1.67%	0.183%
12	12.571	1803	1808	1825	rBV2	558551	843533	37.15%	4.057%
13	13.413	1946	1951	1957	rBV	37932	43982	1.94%	0.212%
14	13.865	2022	2028	2042	rBV	803704	1263302	55.63%	6.076%
15	14.183	2078	2082	2085	rBV	31992	37753	1.66%	0.182%
16	14.971	2211	2216	2230	rVB	561427	774418	34.10%	3.724%
17	15.936	2377	2380	2391	rVB2	64270	102909	4.53%	0.495%
18	16.554	2480	2485	2489	rBV	20692	25932	1.14%	0.125%
19	16.712	2509	2512	2515	rBV	29827	30821	1.36%	0.148%
20	16.753	2515	2519	2525	rBV	146238	175442	7.73%	0.844%
21	16.889	2538	2542	2549	rBV2	18992	24379	1.07%	0.117%
22	17.053	2566	2570	2577	rVB	170763	204871	9.02%	0.985%
23	17.142	2580	2585	2589	rBV3	46903	49485	2.18%	0.238%
24	17.295	2606	2611	2618	rVV	1389856	1537288	67.70%	7.393%
25	17.371	2618	2624	2632	rVB3	18715	32324	1.42%	0.155%
26	17.483	2639	2643	2646	rBV3	18604	32786	1.44%	0.158%
27	17.518	2646	2649	2654	rVB2	27983	36001	1.59%	0.173%
28	17.648	2668	2671	2674	rVV2	24059	31613	1.39%	0.152%
29	17.683	2674	2677	2681	rVB	48340	51413	2.26%	0.247%
30	17.765	2686	2691	2695	rVB	19630	22932	1.01%	0.110%
31	18.065	2738	2742	2747	rBV4	33890	40195	1.77%	0.193%
32	18.636	2833	2839	2843	rBV2	576291	763197	33.61%	3.671%
33	18.671	2843	2845	2854	rVB2	111563	161592	7.12%	0.777%
34	18.859	2873	2877	2885	rBV6	11178	23778	1.05%	0.114%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF050617\
Data File : BF094970.D
Acq On : 8 May 2017 5:42
Operator : SJ/MA
Sample : I2947-14
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-05-0-2.0

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:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	19.147	2920	2926	2929	rBV2	28158	38406	1.69%	0.185%
36	19.765	3029	3031	3035	rVB	23830	23482	1.03%	0.113%
37	19.900	3049	3054	3057	rBV	141160	200528	8.83%	0.964%
38	19.930	3057	3059	3064	rVB	61647	71954	3.17%	0.346%
39	20.012	3070	3073	3077	rBV	25326	30149	1.33%	0.145%
40	20.053	3077	3080	3084	rVB3	23182	24772	1.09%	0.119%
41	20.189	3099	3103	3107	rBV	95815	105668	4.65%	0.508%
42	20.247	3109	3113	3118	rVV	119793	123908	5.46%	0.596%
43	20.300	3118	3122	3131	rVV	454012	536399	23.62%	2.580%
44	20.394	3136	3138	3143	rVB5	17506	25043	1.10%	0.120%
45	21.194	3271	3274	3279	rBV5	15946	28525	1.26%	0.137%
46	21.600	3339	3343	3353	rVB2	57395	109676	4.83%	0.527%
47	21.694	3353	3359	3365	rVB8	13282	29674	1.31%	0.143%
48	21.806	3373	3378	3383	rBV8	13106	26057	1.15%	0.125%
49	21.983	3402	3408	3415	rBV2	41171	87709	3.86%	0.422%
50	23.741	3700	3707	3719	rVB9	39796	106058	4.67%	0.510%

Sum of corrected areas: 20792626

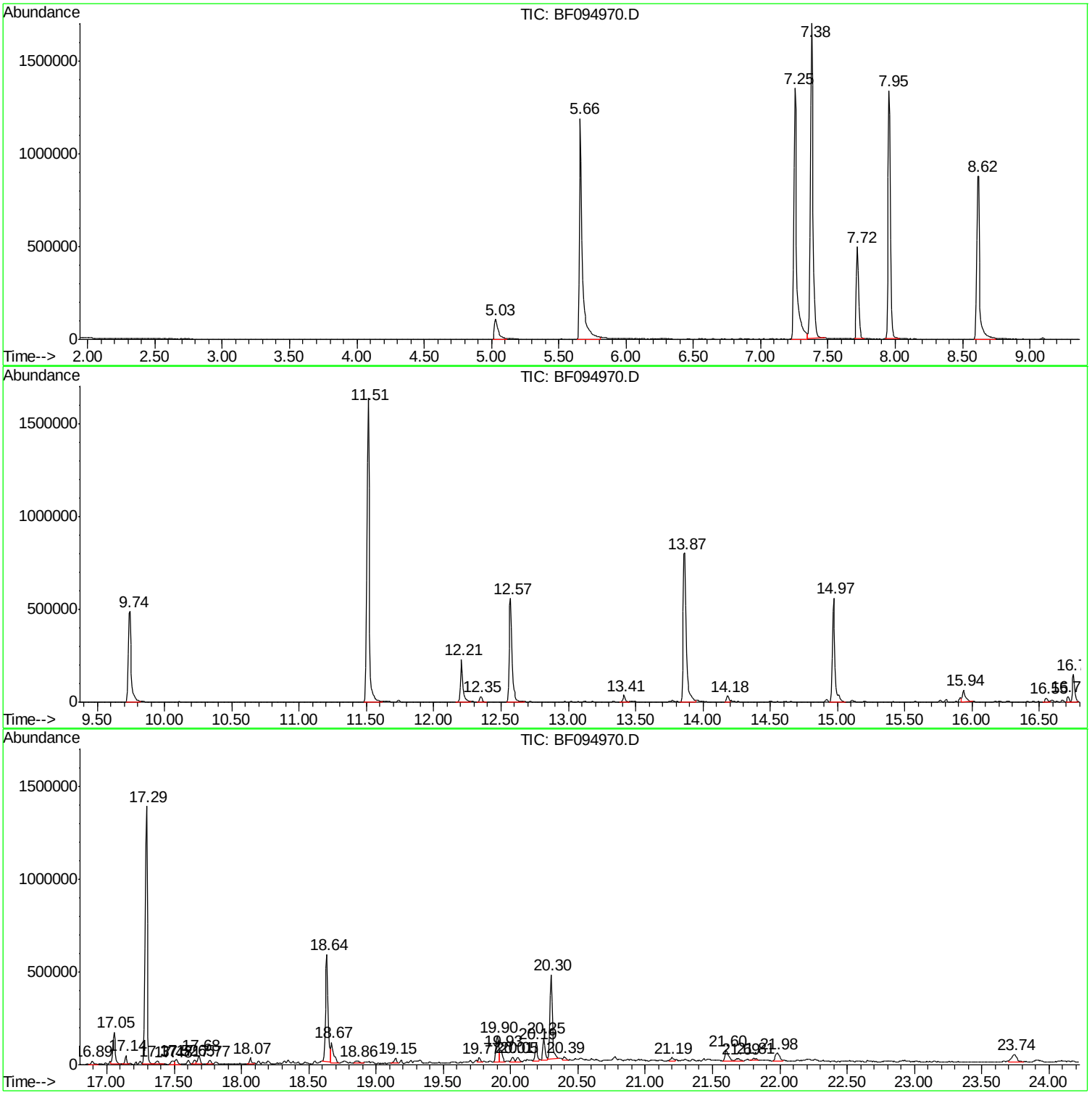
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF050617\
Data File : BF094970.D
Acq On : 8 May 2017 5:42
Operator : SJ/MA
Sample : I2947-14
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-05-0-2.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF050617\
Data File : BF094970.D
Acq On : 8 May 2017 5:42
Operator : SJ/MA
Sample : I2947-14
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-05-0-2.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

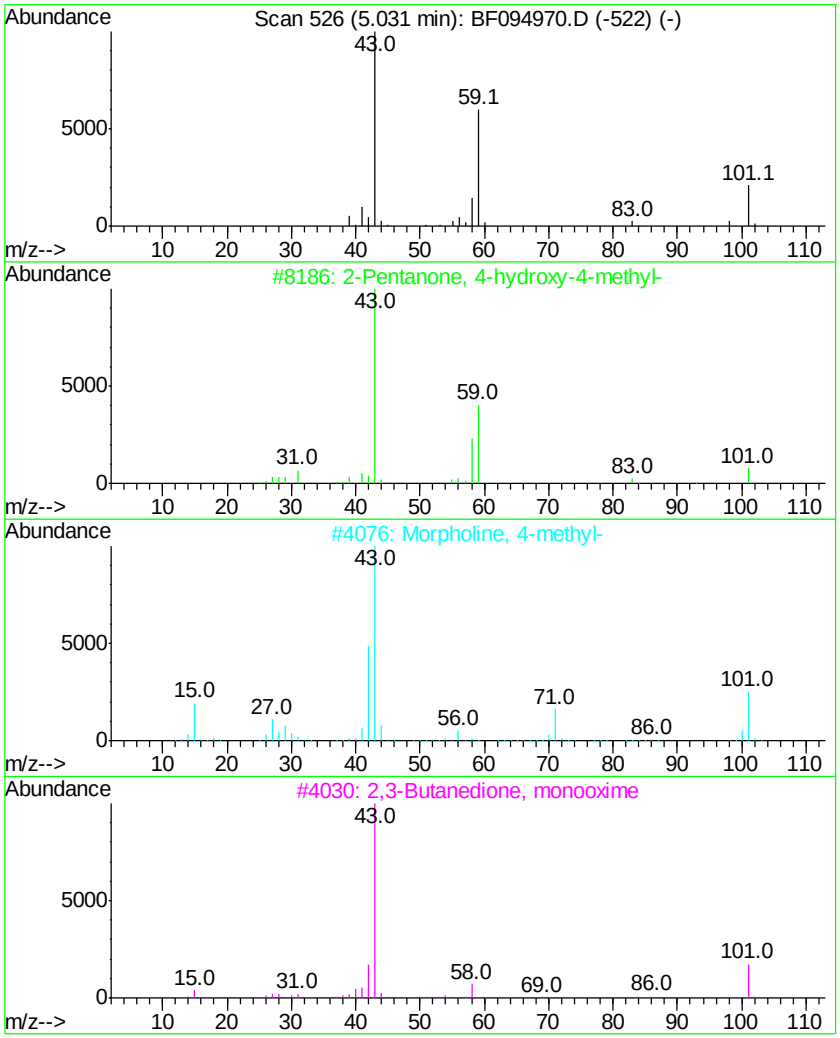
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

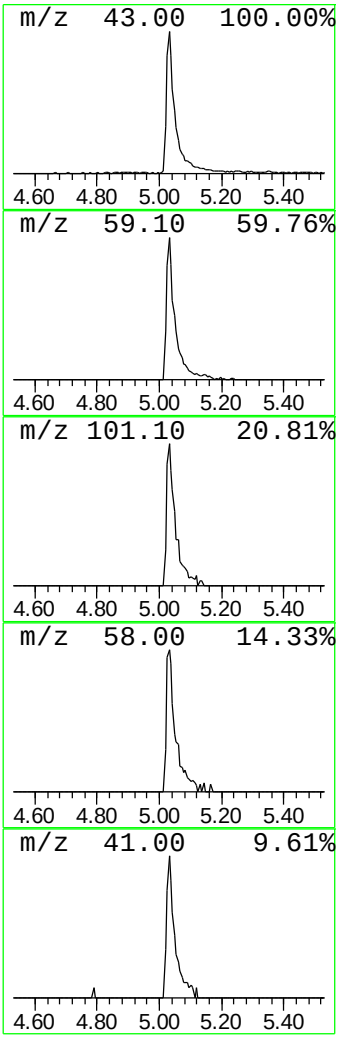
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.03	7.17 ng	202082	1,4-Dichlorobenzene-d4	7.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	9
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF050617\
Data File : BF094970.D
Acq On : 8 May 2017 5:42
Operator : SJ/MA
Sample : I2947-14
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-05-0-2.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

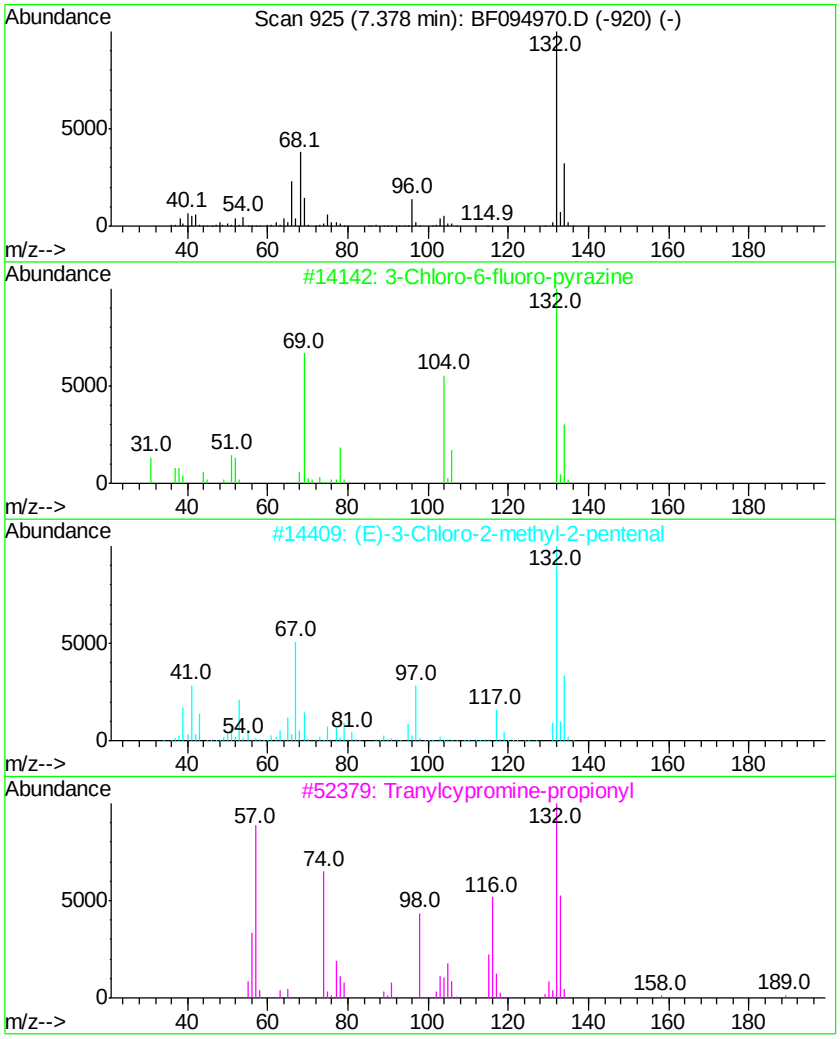
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

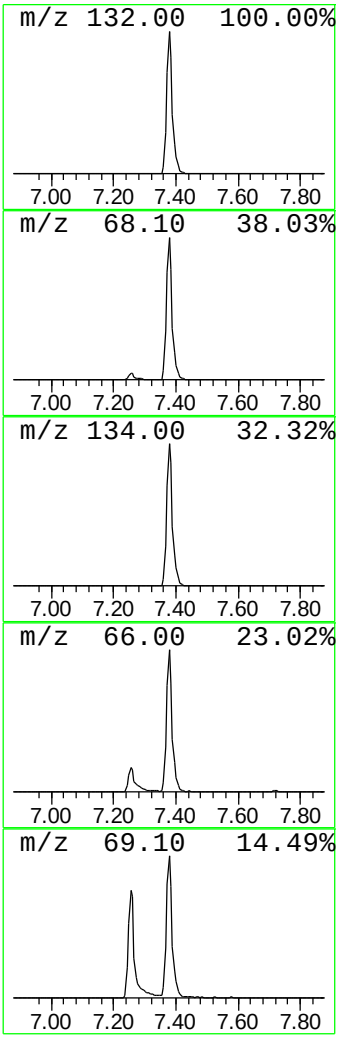
****

Peak Number 2 unknown7.38 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.38	80.61 ng	2270860	1,4-Dichlorobenzene-d4	7.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF050617\
Data File : BF094970.D
Acq On : 8 May 2017 5:42
Operator : SJ/MA
Sample : I2947-14
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-05-0-2.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

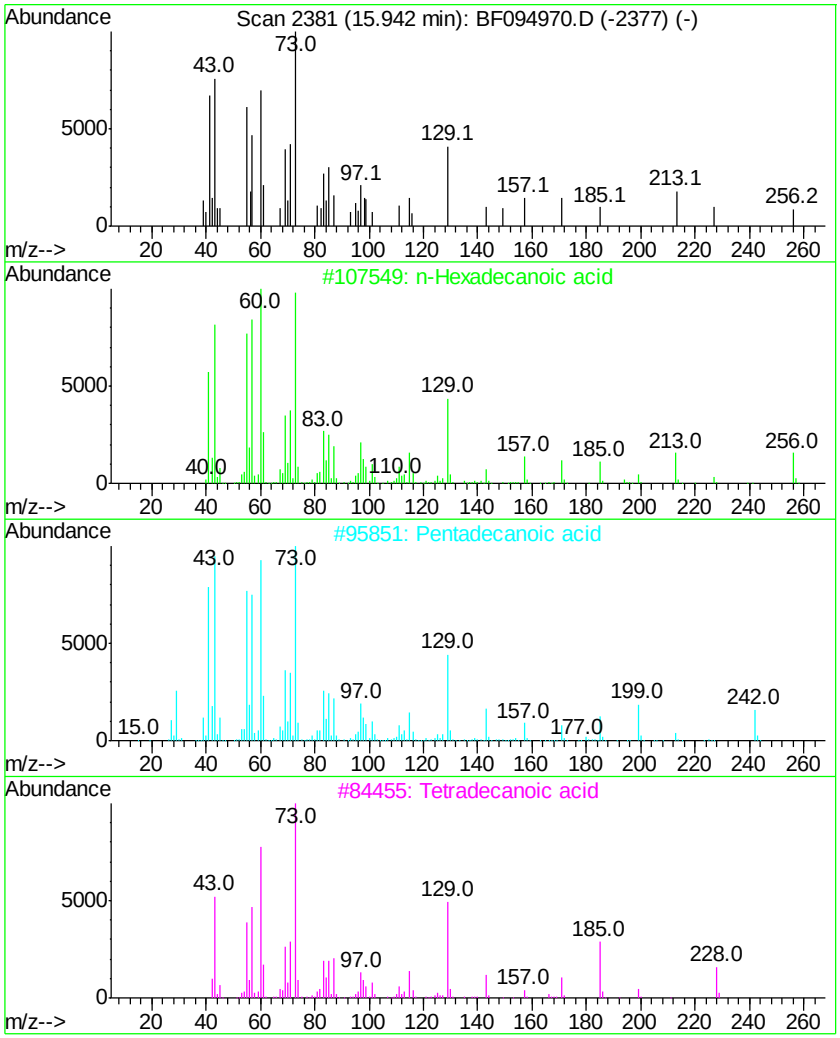
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

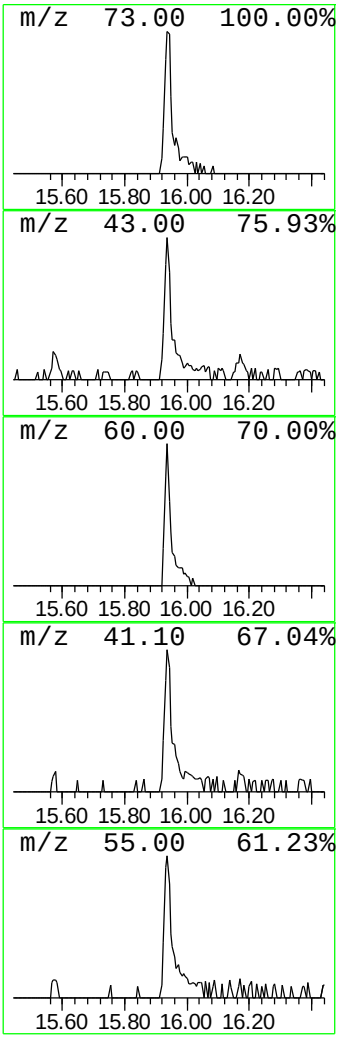
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.94	2.66 ng	102909	Phenanthrene-d10	14.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	59
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	53
4	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	18
5	Oxalic acid, dodecyl propyl ester	300	C17H32O4	1000309-26-5	14





Data Path : Z:\HPCHEM1\BNA F\DATA\BF050617\
Data File : BF094970.D
Acq On : 8 May 2017 5:42
Operator : SJ/MA
Sample : I2947-14
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-05-0-2.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

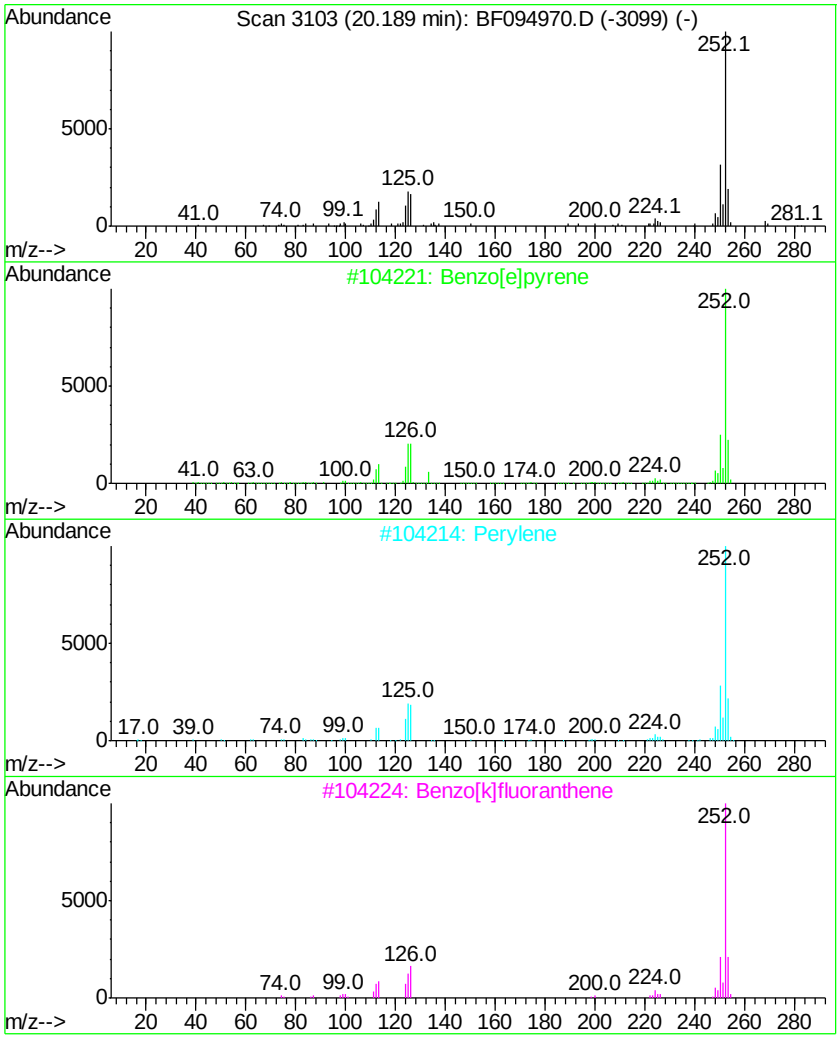
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

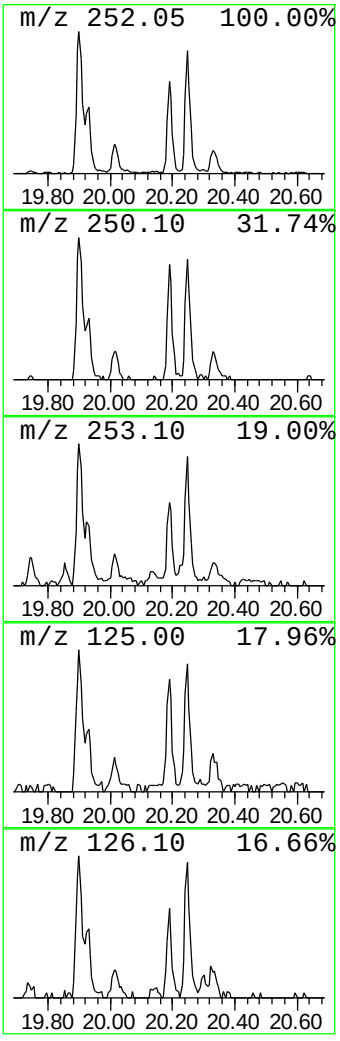
****

Peak Number 5 Benzo[e]pyrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.19	3.94 ng	105668	Perylene-d12	20.30

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	98
4	Benzo[a]pyrene	252	C20H12	000050-32-8	96
5	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	95





Data Path : Z:\HPCHEM1\BNA F\DATA\BF050617\
Data File : BF094970.D
Acq On : 8 May 2017 5:42
Operator : SJ/MA
Sample : I2947-14
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-05-0-2.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

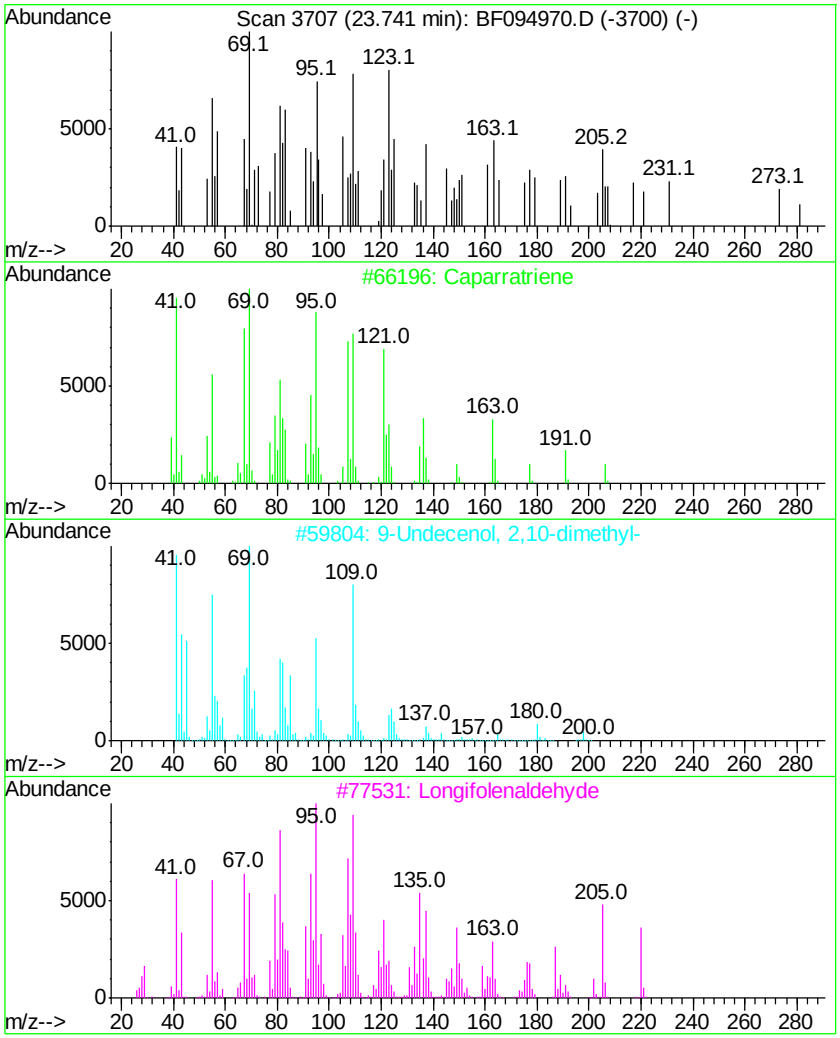
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

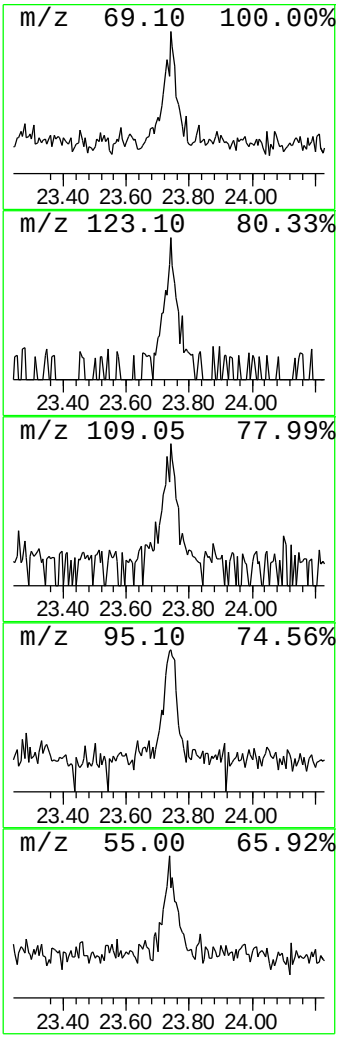
****

Peak Number 6 unknown23.74 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.74	3.95 ng	106058	Perylene-d12	20.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Caparratriene	206	C15H26	1000374-08-7	43
2	9-Undecenol, 2,10-dimethyl-	198	C13H26O	1000131-86-0	38
3	Longifolenaldehyde	220	C15H24O	019890-84-7	35
4	2,10-Dodecadien-1-ol, 3,7,11-tri...	224	C15H28O	020576-57-2	35
5	6-Octen-1-ol, 3,7-dimethyl-, (R)-	156	C10H20O	001117-61-9	27





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050617\
Data File : BF094970.D
Acq On : 8 May 2017 5:42
Operator : SJ/MA
Sample : I2947-14
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-05-0-2.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.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
2-Pentanone, 4-hy...	5.03	7.2	ng	202082	1	7.72	563421	20.0
unknown7.38	7.38	80.6	ng	2270860	1	7.72	563421	20.0
n-Hexadecanoic acid	15.94	2.7	ng	102909	4	14.97	774418	20.0
Benzo[e]pyrene	20.19	3.9	ng	105668	6	20.30	536399	20.0
unknown23.74	23.74	4.0	ng	106058	6	20.30	536399	20.0