LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF053017\
Data File : BF095550.D
Acq On : 30 May 2017 23:05
Operator : SJ/MA
Sample : I3302-08
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM12-COMP-6-18

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	5.090	532	536	553	rBV	68647	166918	7.13%	0.833%
2	5.707	637	641	673	rBV	689814	1928014	82.38%	9.625%
3	7.289	907	910	925	rBV	678493	1648179	70.42%	8.228%
4	7.407	925	930	953	rVB	1268814	2340489	100.00%	11.685%
5	7.737	982	986	998	rBV	398903	490231	20.95%	2.447%
6	7.972	1021	1026	1046	rBV	1231968	1559805	66.64%	7.787%
7	8.642	1136	1140	1168	rBV	462140	1104971	47.21%	5.516%
8	9.766	1326	1331	1351	rBV	277666	630577	26.94%	3.148%
9	11.530	1626	1631	1658	rBV	1116150	2046097	87.42%	10.215%
10	12.242	1747	1752	1769	rBV	111214	232837	9.95%	1.162%
11	12.601	1808	1813	1834	rBV2	321072	610376	26.08%	3.047%
12	13.424	1948	1953	1958	rBV	32942	39739	1.70%	0.198%
13	13.901	2029	2034	2051	rBV	464162	927688	39.64%	4.631%
14	14.195	2080	2084	2087	rBV	31957	36137	1.54%	0.180%
15	15.001	2216	2221	2224	rVV	335383	449408	19.20%	2.244%
16	15.036	2224	2227	2240	rVV	208020	391185	16.71%	1.953%
17	15.130	2240	2243	2254	rVB2	38893	75849	3.24%	0.379%
18	15.789	2351	2355	2359	rBV2	22958	28358	1.21%	0.142%
19	15.836	2359	2363	2371	rVV2	28046	43743	1.87%	0.218%
20	15.954	2377	2383	2399	rVB6	59876	170481	7.28%	0.851%
21	16.783	2519	2524	2537	rBV	368151	473527	20.23%	2.364%
22	17.083	2571	2575	2584	rVB	344361	452623	19.34%	2.260%
23	17.312	2610	2614	2624	rVV	1222638	1507165	64.40%	7.524%
24	17.406	2624	2630	2638	rVB7	20298	46584	1.99%	0.233%
25	17.548	2651	2654	2660	rVB	39949	50388	2.15%	0.252%
26	17.636	2665	2669	2673	rBV	29595	37319	1.59%	0.186%
27	17.689	2673	2678	2683	rBV3	31952	55979	2.39%	0.279%
28	18.248	2769	2773	2779	rVB2	18700	25121	1.07%	0.125%
29	18.353	2786	2791	2793	rBV	21885	26954	1.15%	0.135%
30	18.383	2793	2796	2800	rVB2	25902	28882	1.23%	0.144%
31	18.553	2822	2825	2833	rVB6	26442	51889	2.22%	0.259%
32	18.671	2840	2845	2849	rBV2	492094	777459	33.22%	3.881%
33	18.706	2849	2851	2863	rVV2	144278	241137	10.30%	1.204%
34	18.801	2863	2867	2872	rVV2	31316	51263	2.19%	0.256%

LSC Area Percent Report

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Acq On : 30 May 2017 23:05
Operator : SJ/MA
Sample : I3302-08
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM12-COMP-6-18

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	18.959	2892	2894	2901	rVV7	16062	25033	1.07%	0.125%
36	19.183	2929	2932	2936	rVB2	23887	27404	1.17%	0.137%
37	19.336	2955	2958	2961	rBV4	13158	23584	1.01%	0.118%
38	19.783	3031	3034	3038	rBV3	46137	60349	2.58%	0.301%
39	19.947	3058	3062	3065	rBV	134647	195141	8.34%	0.974%
40	20.065	3078	3082	3086	rBV2	38064	63704	2.72%	0.318%
41	20.242	3108	3112	3117	rBV	76291	89124	3.81%	0.445%
42	20.300	3119	3122	3127	rVB	92666	112241	4.80%	0.560%
43	20.353	3127	3131	3140	rBV	295731	436894	18.67%	2.181%
44	20.789	3203	3205	3210	rBV6	19763	32469	1.39%	0.162%
45	21.718	3356	3363	3371	rBV5	71576	166164	7.10%	0.830%
46	22.094	3423	3427	3433	rVB3	23713	50866	2.17%	0.254%

Sum of corrected areas: 20030345

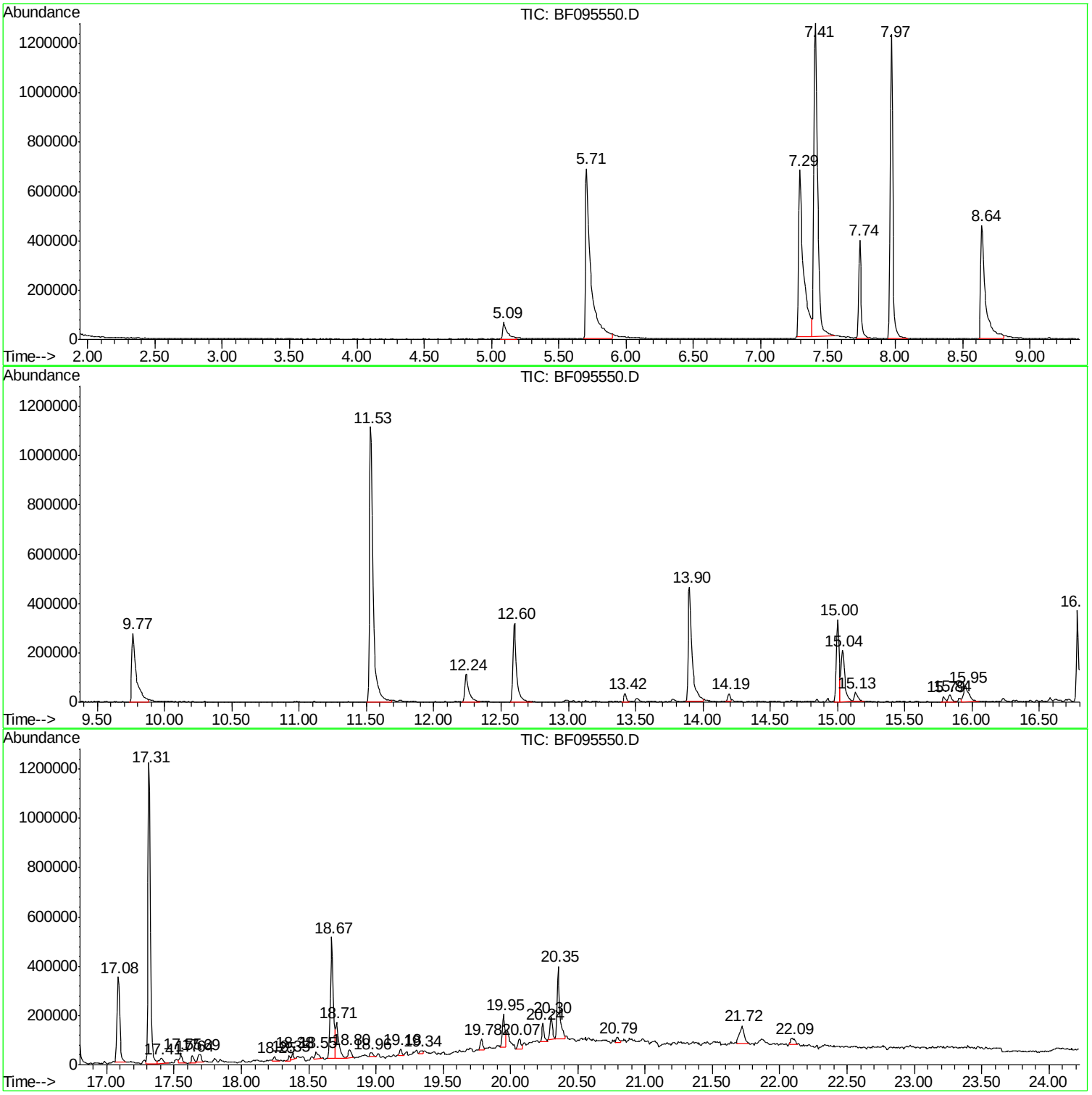
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF053017\
Data File : BF095550.D
Acq On : 30 May 2017 23:05
Operator : SJ/MA
Sample : I3302-08
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NM12-COMP-6-18

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF053017\
Data File : BF095550.D
Acq On : 30 May 2017 23:05
Operator : SJ/MA
Sample : I3302-08
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM12-COMP-6-18

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

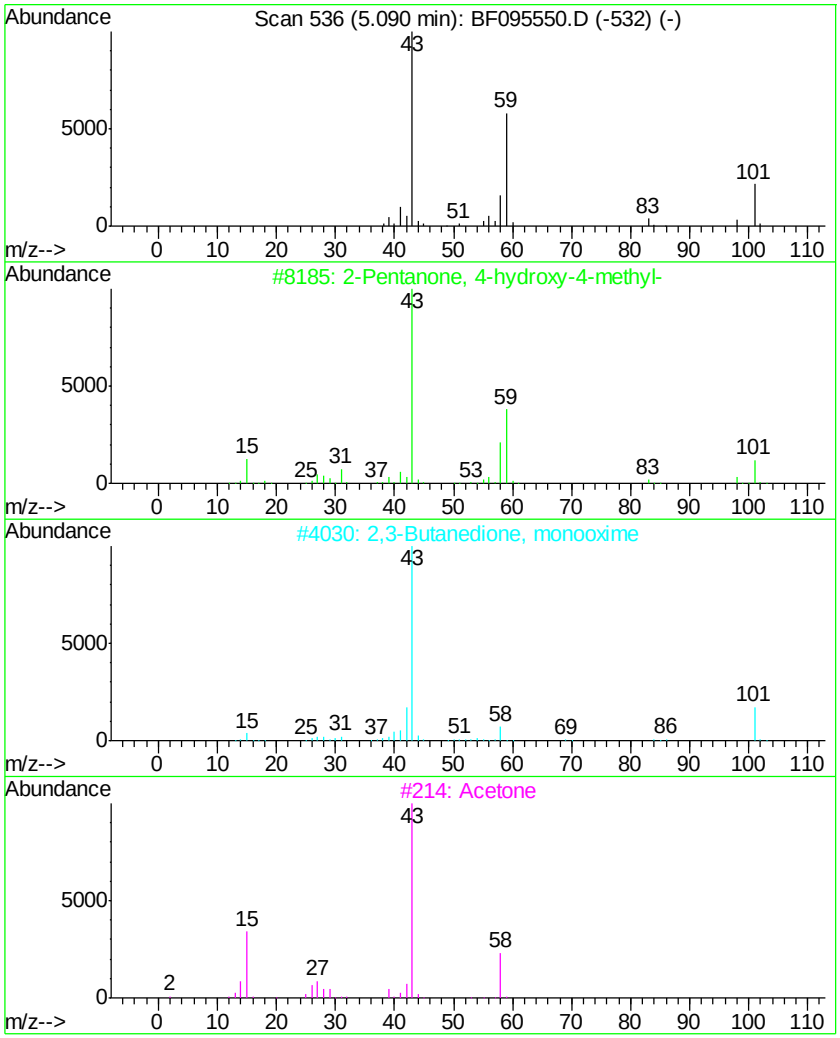
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

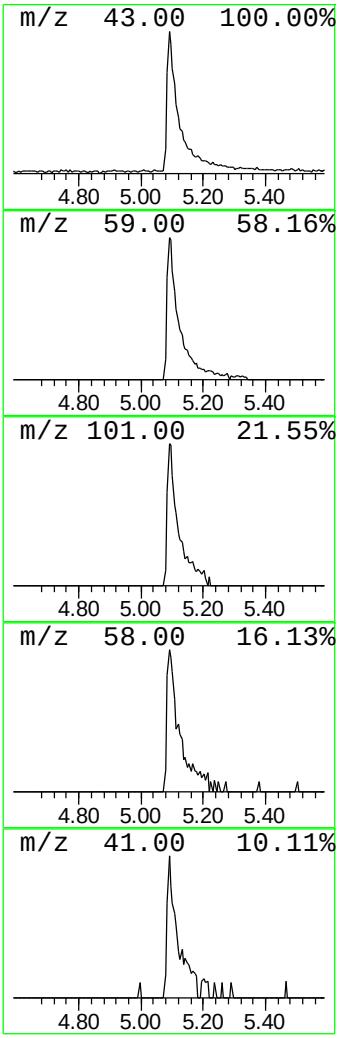
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.09	6.81 ng	166918	1,4-Dichlorobenzene-d4	7.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	12
3	Acetone	58	C3H6O	000067-64-1	10
4	5-Hexen-2-one	98	C6H10O	000109-49-9	10
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF053017\
Data File : BF095550.D
Acq On : 30 May 2017 23:05
Operator : SJ/MA
Sample : I3302-08
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM12-COMP-6-18

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

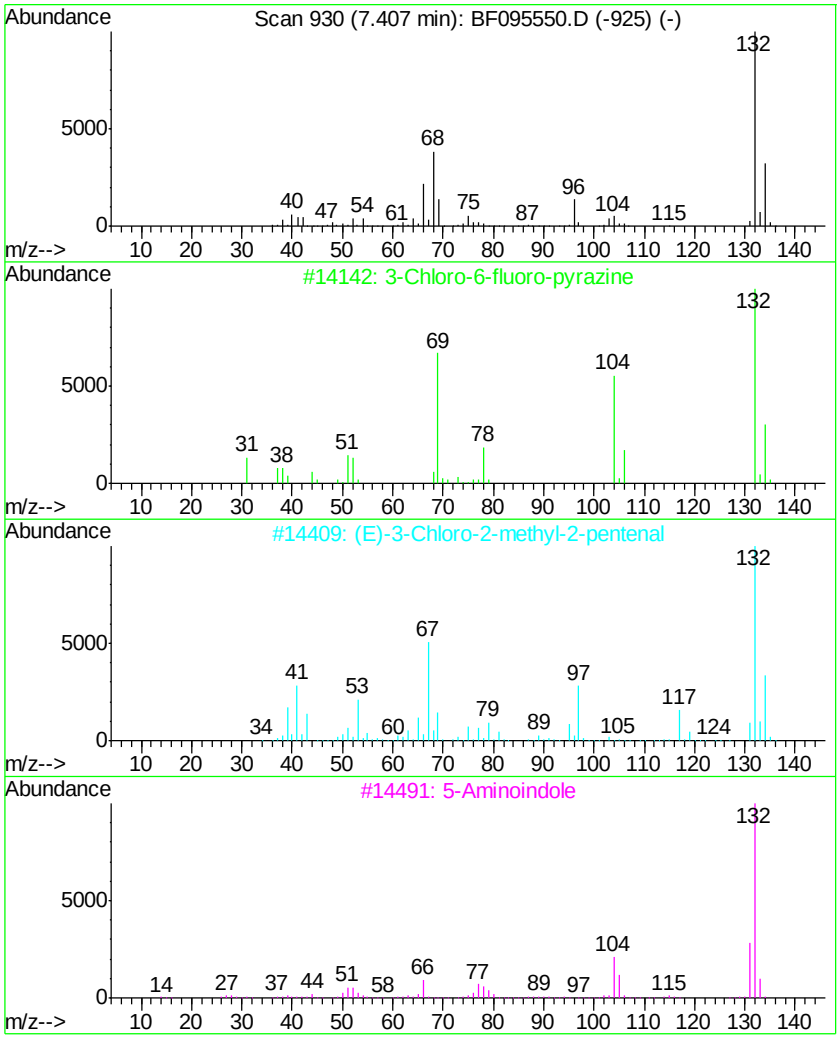
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

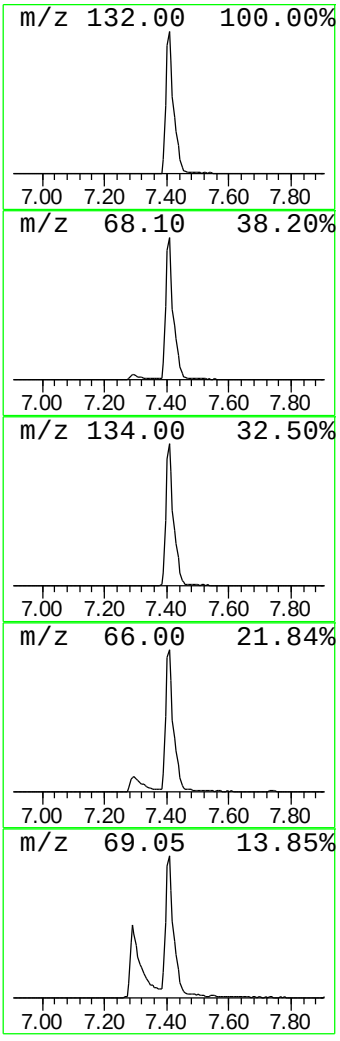
****

Peak Number 2 unknown7.41 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.41	95.49 ng	2340490	1,4-Dichlorobenzene-d4	7.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	30
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF053017\
Data File : BF095550.D
Acq On : 30 May 2017 23:05
Operator : SJ/MA
Sample : I3302-08
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM12-COMP-6-18

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

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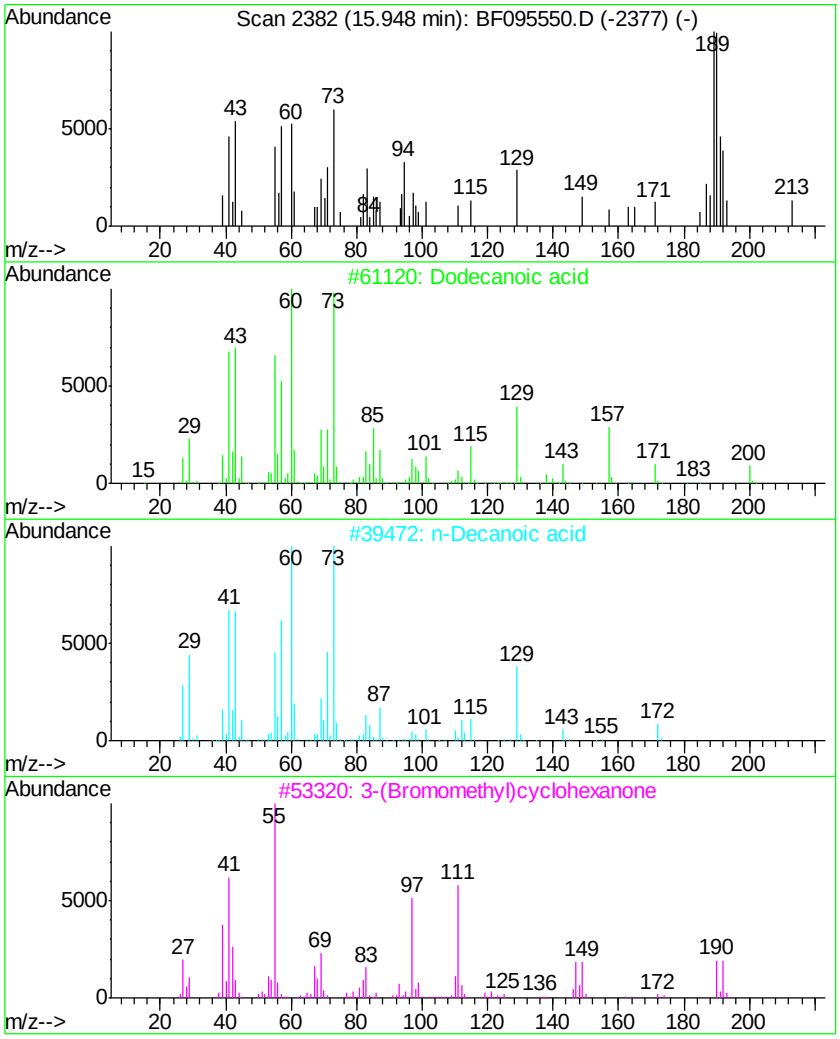
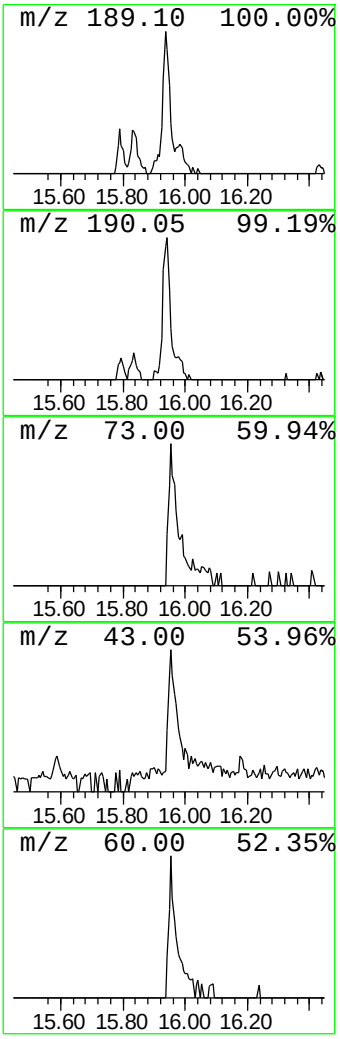
Peak Number 4 unknown15.95 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.95	7.59 ng	170481	Phenanthrene-d10	15.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid	200	C12H24O2	000143-07-7	22
2	n-Decanoic acid	172	C10H20O2	000334-48-5	22
3	3-(Bromomethyl)cyclohexanone	190	C7H11BrO	168278-83-9	22
4	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	22
5	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	14





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF053017\
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Sample : I3302-08
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM12-COMP-6-18

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

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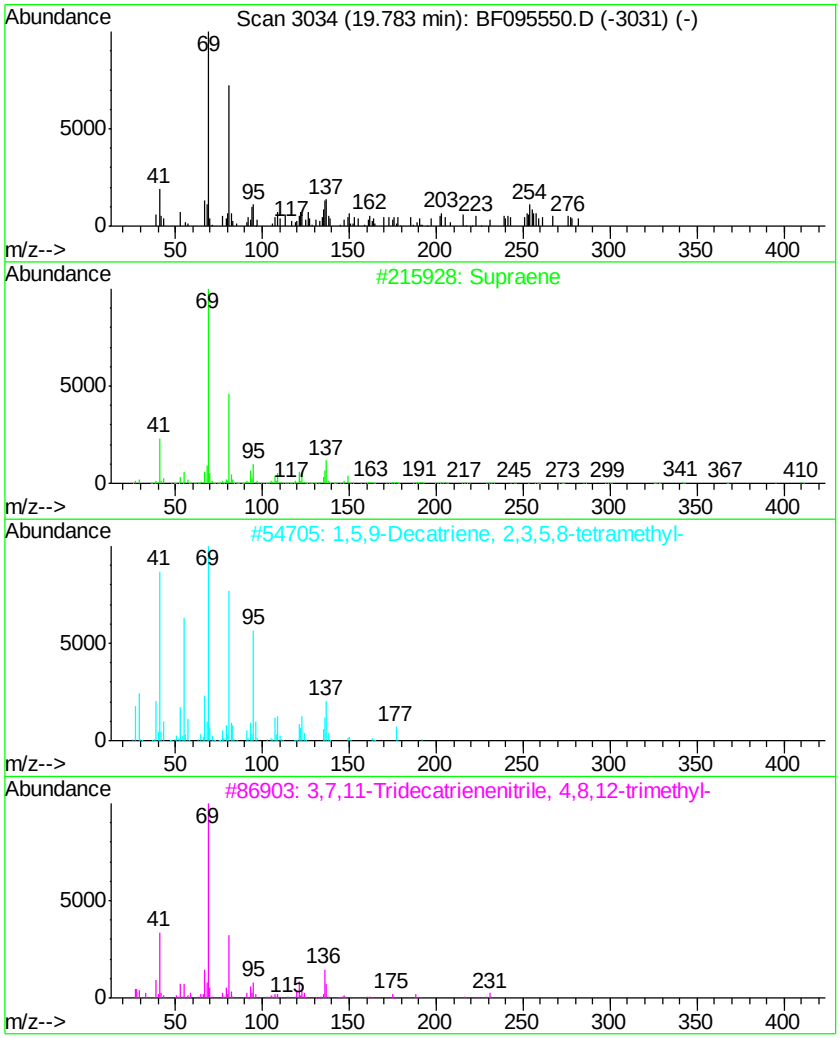
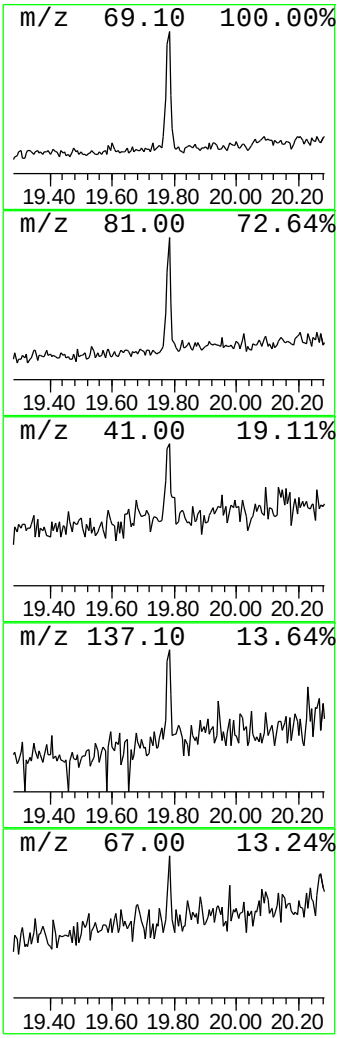
Peak Number 5 unknown19.78 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.78	2.76 ng	60349	Perylene-d12	20.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	49
2	1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	49
3	3,7,11-Tridecatrienenitrile, 4,8...	231	C16H25N	006006-01-5	49
4	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	47
5	2,6,10-Dodecatrien-1-ol, 3,7,11-...	264	C17H28O2	004128-17-0	47





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Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM12-COMP-6-18

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

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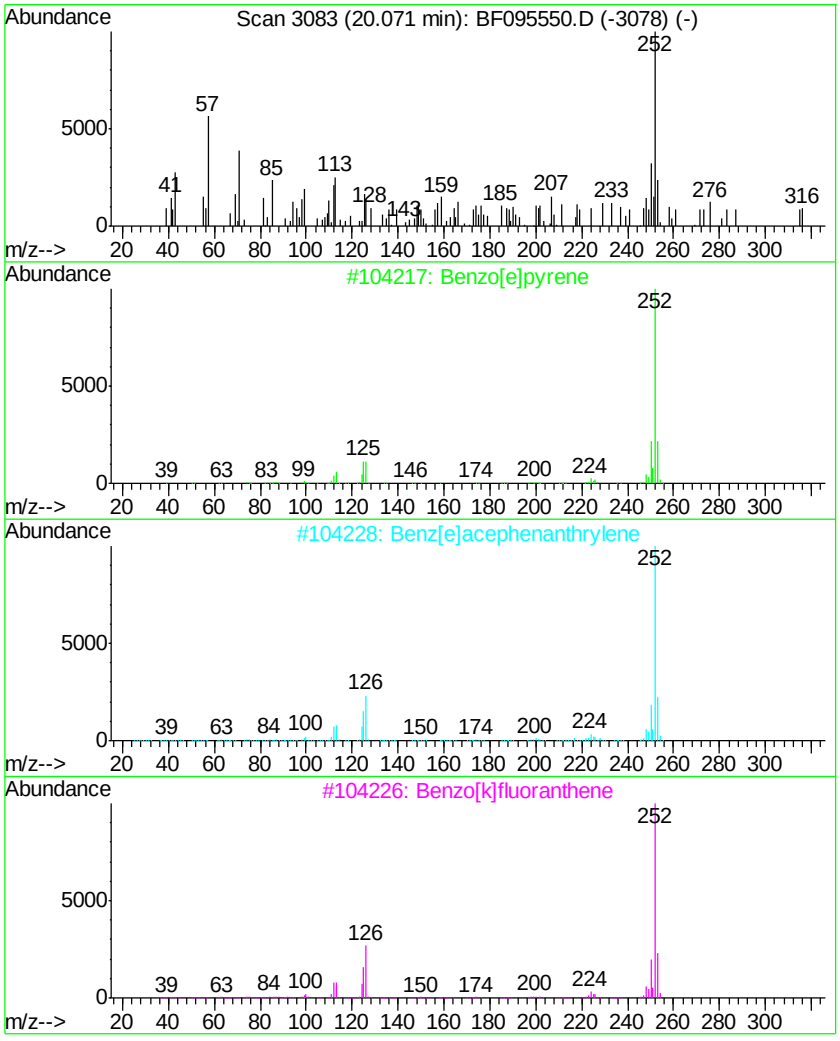
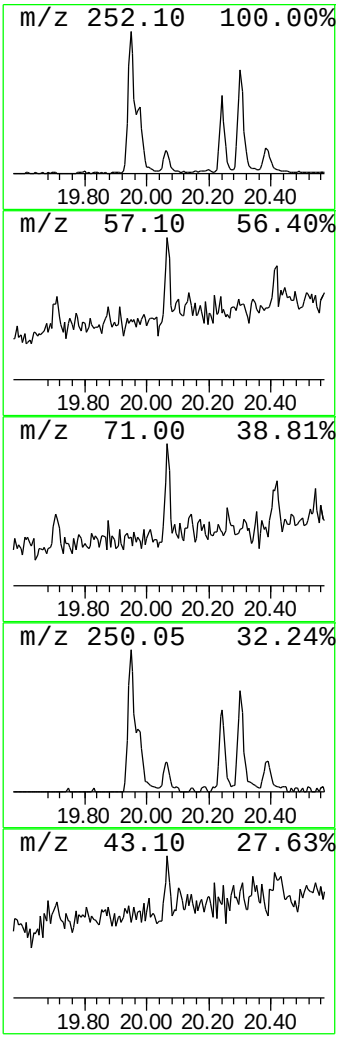
Peak Number 6 Benzo[e]pyrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.07	2.92 ng	63704	Perylene-d12	20.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	64
2	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	52
3	Benzo[k]fluoranthene	252	C20H12	000207-08-9	52
4	Benzo[a]pyrene	252	C20H12	000050-32-8	52
5	Perylene	252	C20H12	000198-55-0	52





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Operator : SJ/MA
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ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM12-COMP-6-18

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

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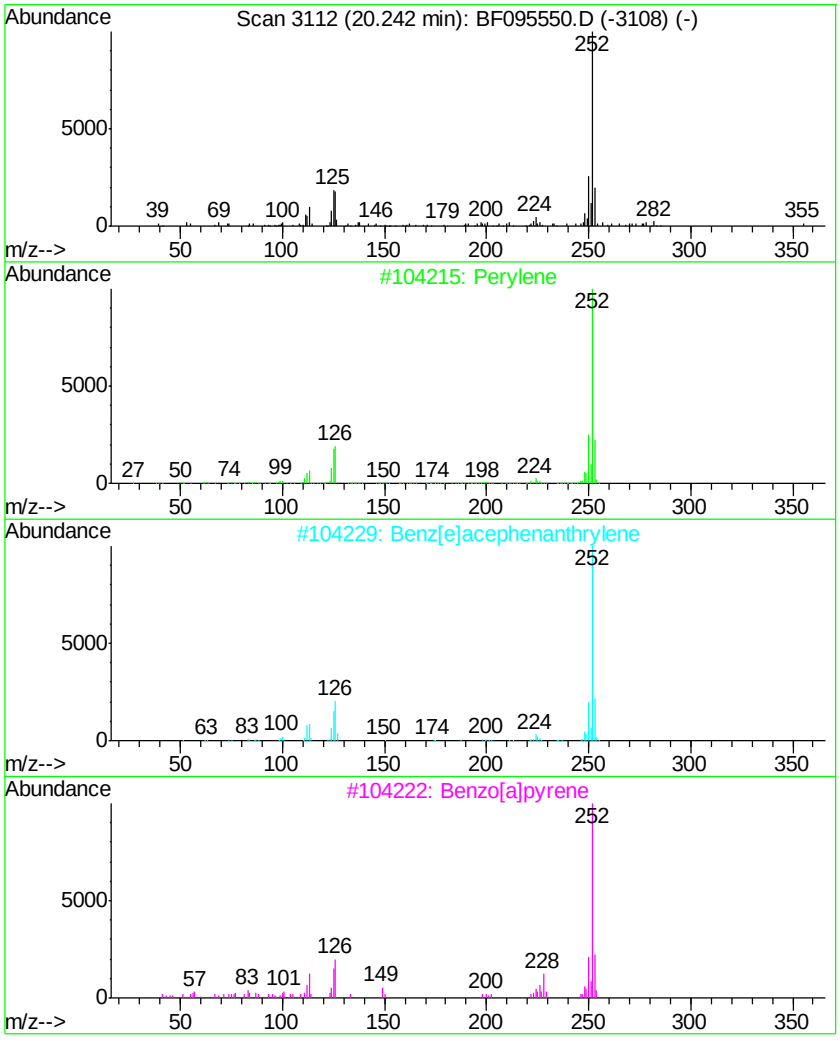
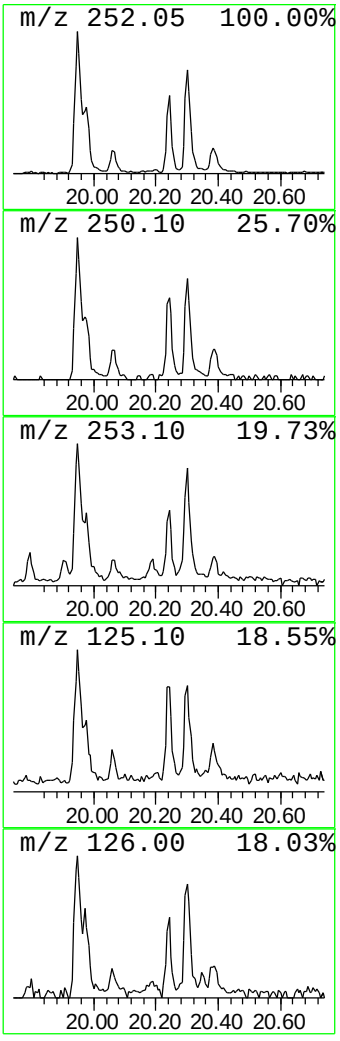
Peak Number 7 Perylene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.24	4.08 ng	89124	Perylene-d12	20.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Perylene	252	C20H12	000198-55-0	97
2	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	93
3	Benzo[a]pyrene	252	C20H12	000050-32-8	91
4	Benzo[j]fluoranthene	252	C20H12	000205-82-3	90
5	Benzo[e]pyrene	252	C20H12	000192-97-2	87





Tentatively Identified Compound (LSC) summary

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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...	5.09	6.8	ng	166918	1	7.74	490231	20.0
unknown7.41	7.41	95.5	ng	2340490	1	7.74	490231	20.0
unknown15.95	15.95	7.6	ng	170481	4	15.00	449408	20.0
unknown19.78	19.78	2.8	ng	60349	6	20.35	436894	20.0
Benzo[e]pyrene	20.07	2.9	ng	63704	6	20.35	436894	20.0
Perylene	20.24	4.1	ng	89124	6	20.35	436894	20.0