LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051917\
Data File : BF095286.D
Acq On : 20 May 2017 3:32
Operator : SJ/MA
Sample : I3202-10 5X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-10COMP

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	2.155	35	37	46	rVB4	3503	7287	1.07%	0.103%
2	5.096	533	537	548	rBV	29728	72757	10.70%	1.025%
3	5.766	648	651	666	rBV2	55157	192896	28.37%	2.717%
4	7.342	915	919	932	rBV2	64778	205047	30.16%	2.888%
5	7.442	932	936	954	rVB	152290	364025	53.55%	5.128%
6	7.760	986	990	1008	rBV	365920	478407	70.37%	6.739%
7	7.995	1026	1030	1045	rBV	192979	282569	41.56%	3.980%
8	8.678	1143	1146	1166	rBV	53759	160025	23.54%	2.254%
9	9.778	1329	1333	1352	rBV	383106	633094	93.13%	8.918%
10	11.554	1631	1635	1649	rBV	236582	391933	57.65%	5.521%
11	11.648	1649	1651	1656	rVB3	7372	10127	1.49%	0.143%
12	12.095	1723	1727	1732	rVV3	5613	9360	1.38%	0.132%
13	12.142	1732	1735	1739	rVB2	7489	8235	1.21%	0.116%
14	12.266	1749	1756	1767	rBV2	20981	49093	7.22%	0.692%
15	12.407	1775	1780	1786	rVV2	4180	8547	1.26%	0.120%
16	12.472	1786	1791	1796	rVB3	7180	11140	1.64%	0.157%
17	12.613	1811	1815	1823	rBV2	371485	548996	80.76%	7.734%
18	12.989	1873	1879	1887	rBV4	9357	20562	3.02%	0.290%
19	13.054	1887	1890	1895	rVB2	7456	9998	1.47%	0.141%
20	13.160	1904	1908	1913	rVB5	7917	13625	2.00%	0.192%
21	13.448	1952	1957	1961	rBV3	10276	14852	2.18%	0.209%
22	13.524	1964	1970	1977	rVV4	10301	19750	2.91%	0.278%
23	13.607	1979	1984	1989	rBV5	4730	9481	1.39%	0.134%
24	13.807	2011	2018	2025	rBV5	8220	17189	2.53%	0.242%
25	13.930	2035	2039	2048	rBV2	44589	89519	13.17%	1.261%
26	14.142	2071	2075	2081	rVB5	4982	8028	1.18%	0.113%
27	14.218	2083	2088	2090	rBV2	12337	15523	2.28%	0.219%
28	14.242	2090	2092	2098	rVB5	8915	15059	2.22%	0.212%
29	14.642	2156	2160	2164	rBV3	7422	11499	1.69%	0.162%
30	14.865	2194	2198	2201	rVB2	6219	7434	1.09%	0.105%
31	14.954	2208	2213	2216	rBV4	10450	13242	1.95%	0.187%
32	15.018	2216	2224	2228	rVV	300199	419794	61.75%	5.914%
33	15.054	2228	2230	2240	rVV	124675	196169	28.86%	2.763%
34	15.148	2242	2246	2257	rVB	24739	43415	6.39%	0.612%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051917\
Data File : BF095286.D
Acq On : 20 May 2017 3:32
Operator : SJ/MA
Sample : I3202-10 5X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-10COMP

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	15.242	2257	2262	2266	rBV7	3783	7742	1.14%	0.109%
36	15.454	2295	2298	2304	rBV6	5880	12061	1.77%	0.170%
37	15.607	2320	2324	2330	rBV4	8898	11678	1.72%	0.165%
38	15.807	2354	2358	2361	rBV	19550	24805	3.65%	0.349%
39	15.848	2361	2365	2370	rVB2	22694	33727	4.96%	0.475%
40	15.918	2373	2377	2379	rVV3	7882	10068	1.48%	0.142%
41	15.954	2379	2383	2387	rVV2	31310	52210	7.68%	0.735%
42	15.995	2387	2390	2396	rVB3	19412	31603	4.65%	0.445%
43	16.148	2413	2416	2422	rVB5	7763	13985	2.06%	0.197%
44	16.201	2422	2425	2428	rBV3	9749	11508	1.69%	0.162%
45	16.254	2428	2434	2436	rBV2	15090	23246	3.42%	0.327%
46	16.418	2459	2462	2466	rVB6	7081	8686	1.28%	0.122%
47	16.495	2472	2475	2477	rBV3	12519	10377	1.53%	0.146%
48	16.595	2489	2492	2496	rBV	34489	46540	6.85%	0.656%
49	16.636	2496	2499	2500	rVV3	14499	18442	2.71%	0.260%
50	16.671	2503	2505	2508	rVV4	9962	9846	1.45%	0.139%
51	16.724	2509	2514	2516	rVV5	13882	23222	3.42%	0.327%
52	16.748	2516	2518	2523	rVV5	14675	16571	2.44%	0.233%
53	16.795	2523	2526	2537	rVB	243209	331276	48.73%	4.667%
54	16.895	2541	2543	2546	rVV4	10508	10313	1.52%	0.145%
55	17.001	2558	2561	2564	rBV	12382	14743	2.17%	0.208%
56	17.030	2564	2566	2567	rBV2	9754	7421	1.09%	0.105%
57	17.101	2574	2578	2586	rVB	215908	277676	40.85%	3.912%
58	17.212	2594	2597	2600	rBV5	12440	14724	2.17%	0.207%
59	17.254	2602	2604	2606	rVB3	12640	7890	1.16%	0.111%
60	17.295	2608	2611	2614	rVV3	11472	14066	2.07%	0.198%
61	17.330	2614	2617	2626	rVV	237944	306572	45.10%	4.319%
62	17.495	2642	2645	2646	rBV3	10649	10861	1.60%	0.153%
63	17.654	2669	2672	2676	rVV2	18330	22768	3.35%	0.321%
64	17.712	2677	2682	2686	rVV3	24476	47946	7.05%	0.675%
65	17.818	2697	2700	2702	rVB	18990	15443	2.27%	0.218%
66	17.854	2704	2706	2708	rBV2	13879	13621	2.00%	0.192%
67	17.895	2711	2713	2716	rVV4	14263	12523	1.84%	0.176%
68	18.059	2737	2741	2743	rBV5	18164	29383	4.32%	0.414%
69	18.253	2772	2774	2777	rBV4	15806	19825	2.92%	0.279%
70	18.401	2796	2799	2802	rVB2	27122	26424	3.89%	0.372%
71	18.689	2842	2848	2852	rBV2	455142	679826	100.00%	9.577%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051917\
Data File : BF095286.D
Acq On : 20 May 2017 3:32
Operator : SJ/MA
Sample : I3202-10 5X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-10COMP

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

72	18.983	2895	2898	2901	rBV3	38240	42355	6.23%	0.597%
73	19.959	3062	3064	3068	rVB	68693	79494	11.69%	1.120%
74	20.365	3130	3133	3142	rVB	273510	388754	57.18%	5.476%

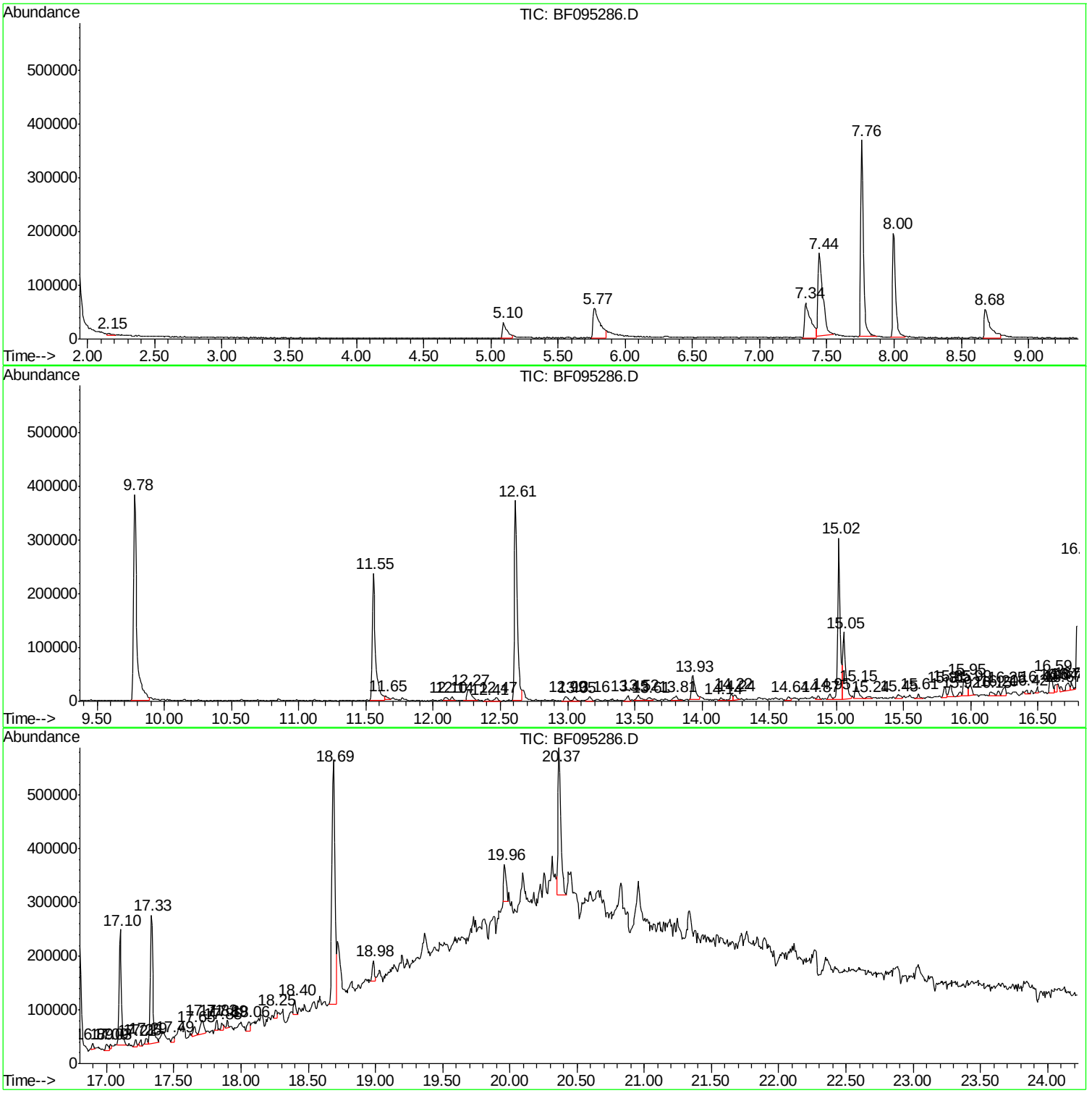
Sum of corrected areas: 7098898

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051917\
Data File : BF095286.D
Acq On : 20 May 2017 3:32
Operator : SJ/MA
Sample : I3202-10 5X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-10COMP

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\BF051917\
Data File : BF095286.D
Acq On : 20 May 2017 3:32
Operator : SJ/MA
Sample : I3202-10 5X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-10COMP

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

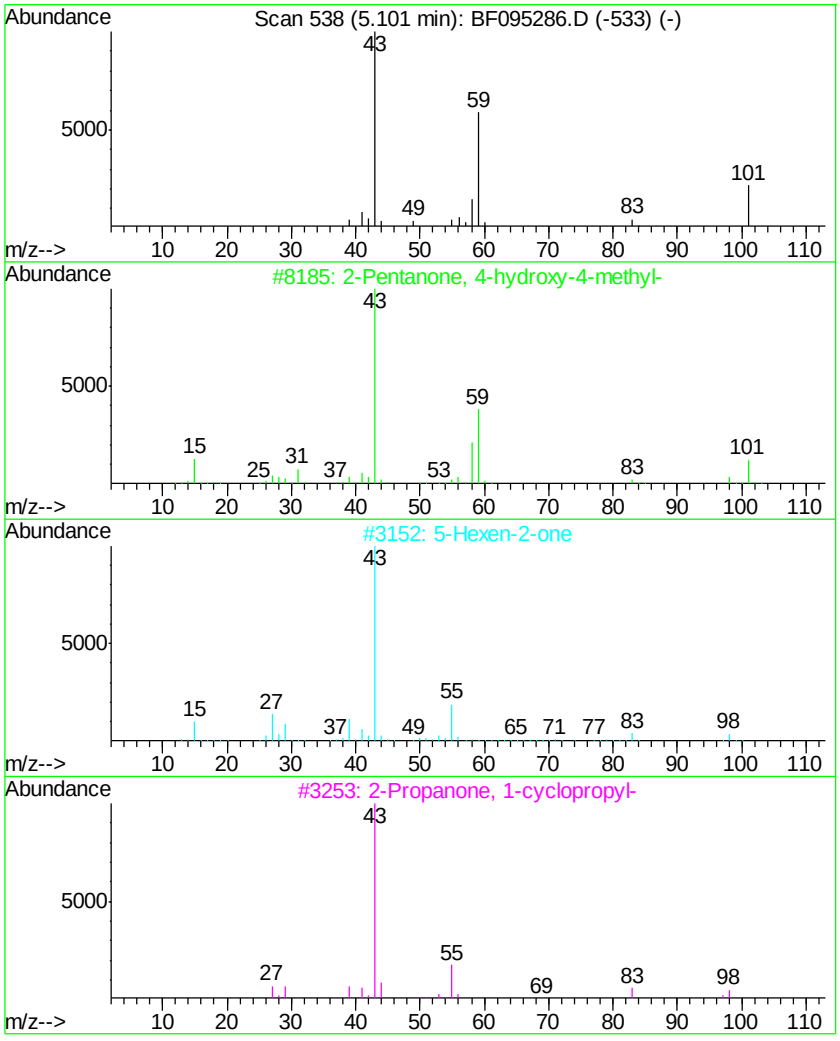
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

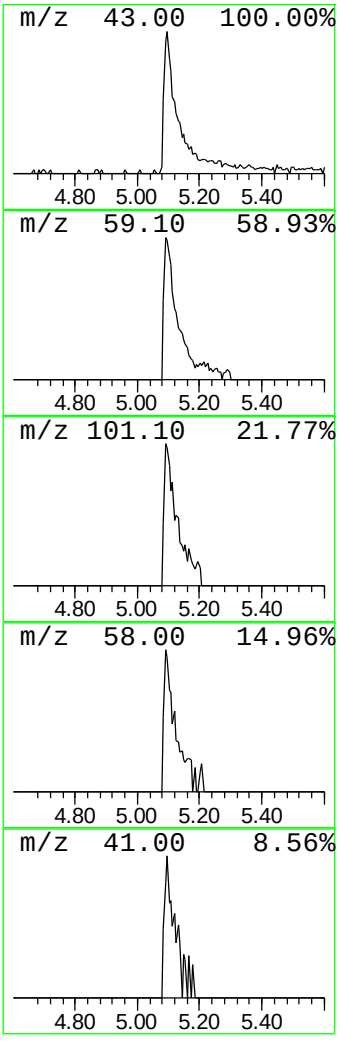
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	3.04 ng	72757	1,4-Dichlorobenzene-d4	7.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	5-Hexen-2-one	98	C6H10O	000109-49-9	12
3	2-Propanone, 1-cyclopropyl-	98	C6H10O	004160-75-2	9
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
5	2-Heptanone, 7,7-dichloro-	182	C7H12Cl2O	066241-43-8	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051917\
Data File : BF095286.D
Acq On : 20 May 2017 3:32
Operator : SJ/MA
Sample : I3202-10 5X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-10COMP

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

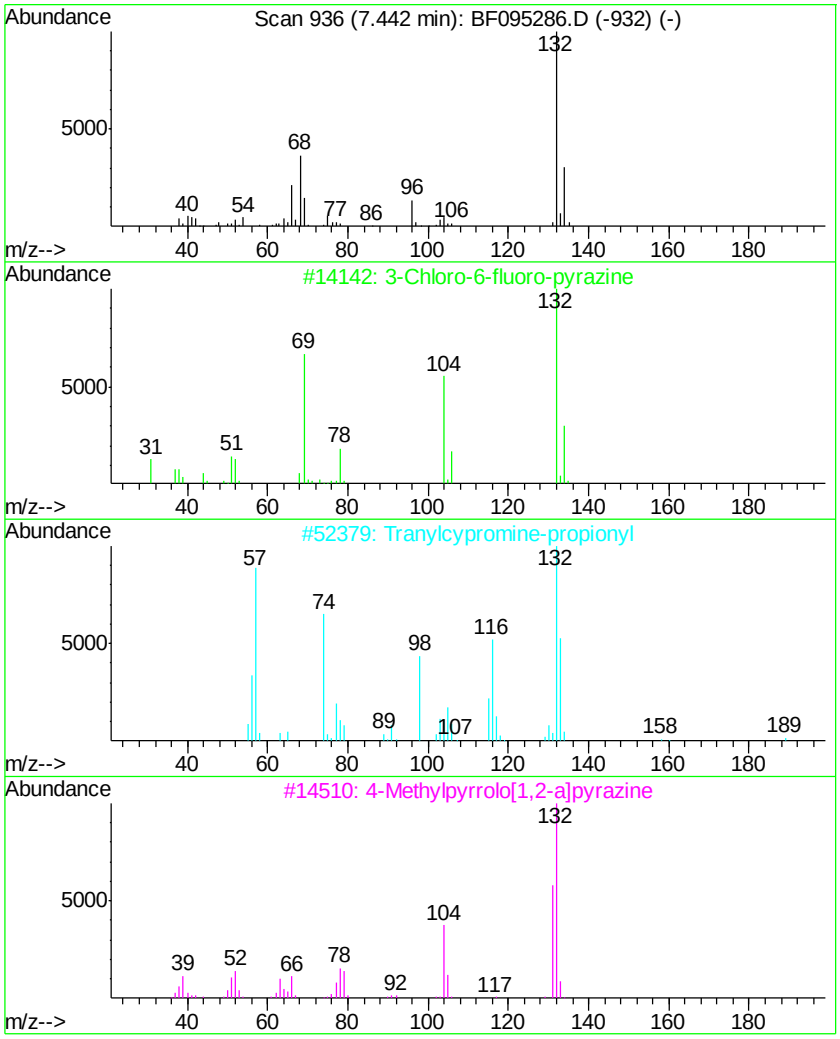
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

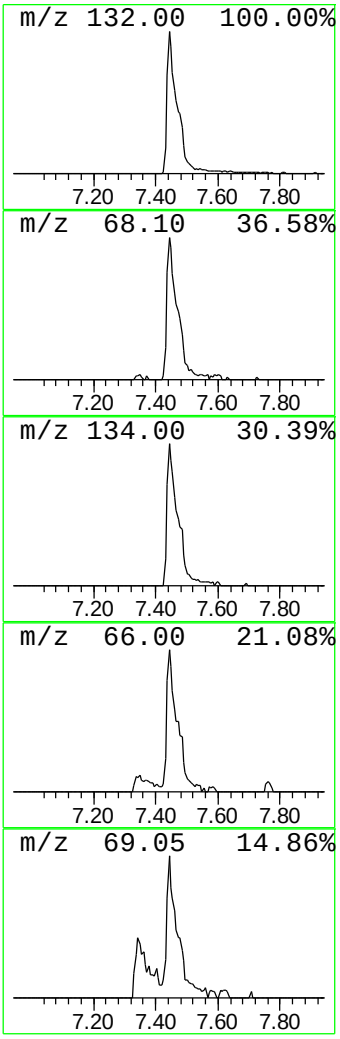
****

Peak Number 2 unknown7.44 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.44	15.22 ng	364025	1,4-Dichlorobenzene-d4	7.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051917\
Data File : BF095286.D
Acq On : 20 May 2017 3:32
Operator : SJ/MA
Sample : I3202-10 5X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-10COMP

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

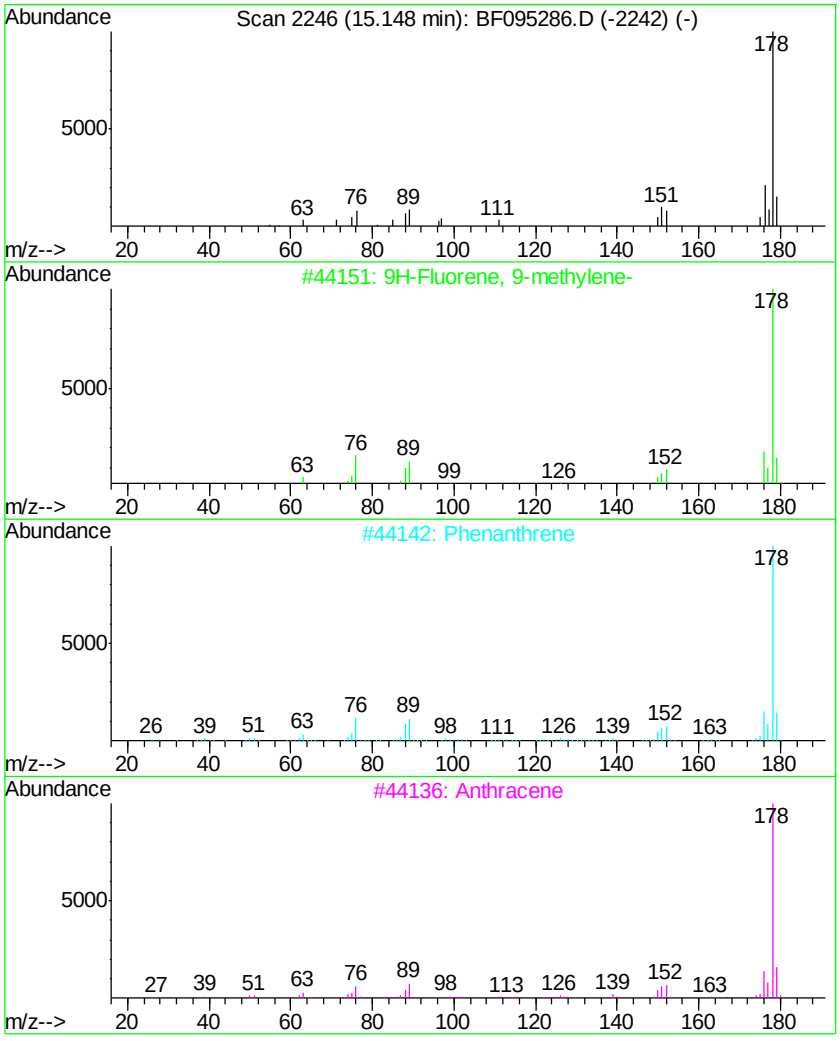
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

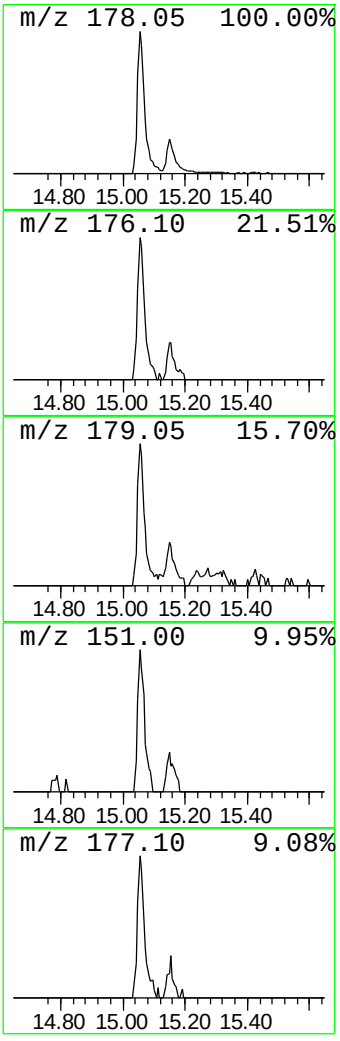
****

Peak Number 4 9H-Fluorene, 9-methylene- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.15	2.07 ng	43415	Phenanthrene-d10	15.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9H-Fluorene, 9-methylene-	178	C14H10	004425-82-5	81
2	Phenanthrene	178	C14H10	000085-01-8	74
3	Anthracene	178	C14H10	000120-12-7	74
4	2-Cyclopropen-1-one, 2,3-diphenyl-	206	C15H10O	000886-38-4	74
5	Diphenylacetylene	178	C14H10	000501-65-5	72





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051917\
Data File : BF095286.D
Acq On : 20 May 2017 3:32
Operator : SJ/MA
Sample : I3202-10 5X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-10COMP

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

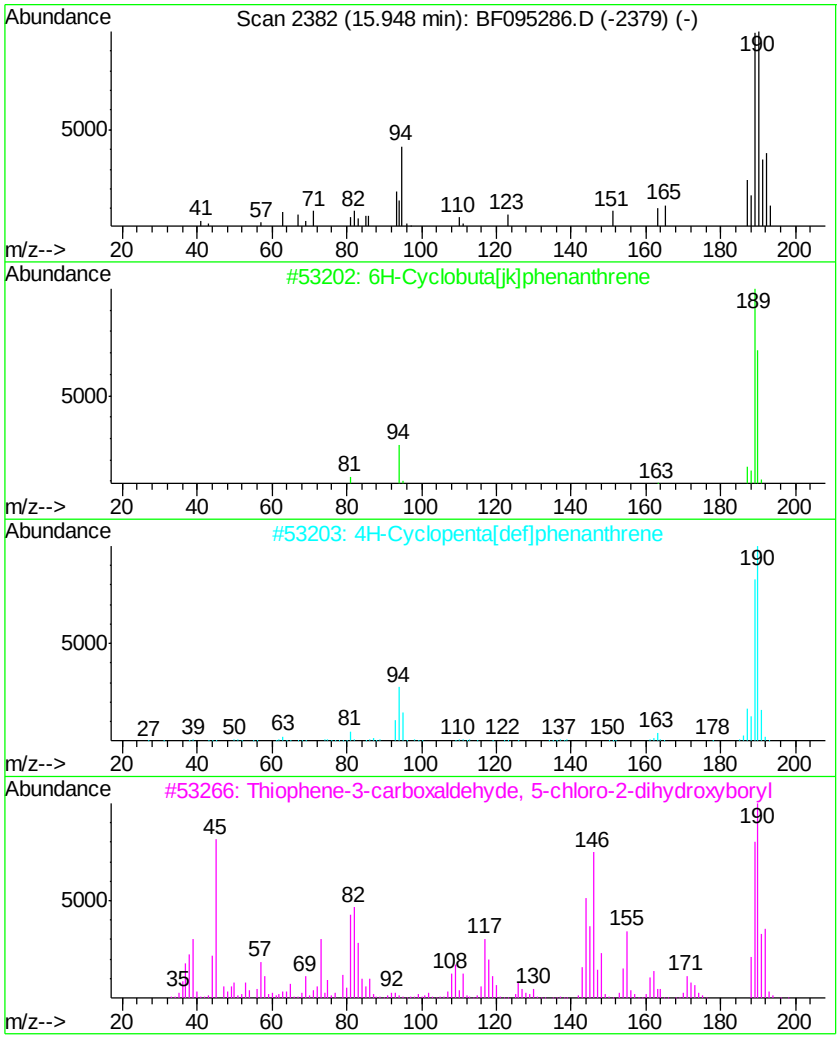
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

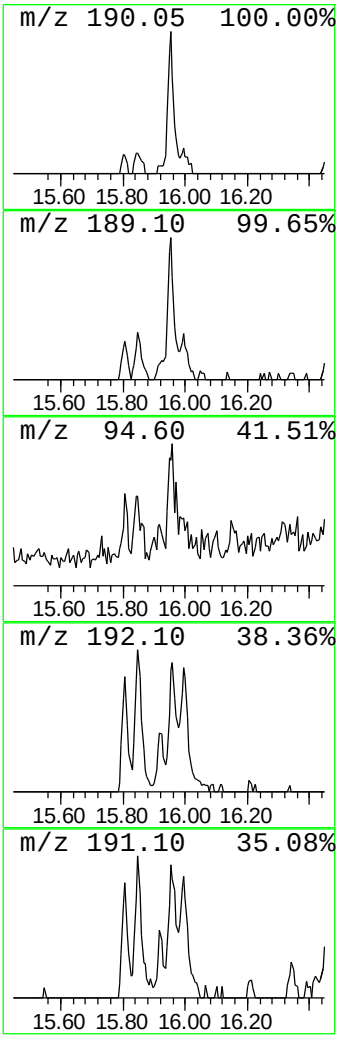
****

Peak Number 5 6H-Cyclobuta[jk]phenanthrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.95	2.49 ng	52210	Phenanthrene-d10	15.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	58
2	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	58
3	Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	50
4	Methyl diselenide	190	C2H6Se2	007101-31-7	27
5	Benzene, 1,1'-(1,2-propadienylid...	192	C15H12	014251-57-1	22





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051917\
Data File : BF095286.D
Acq On : 20 May 2017 3:32
Operator : SJ/MA
Sample : I3202-10 5X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-10COMP

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

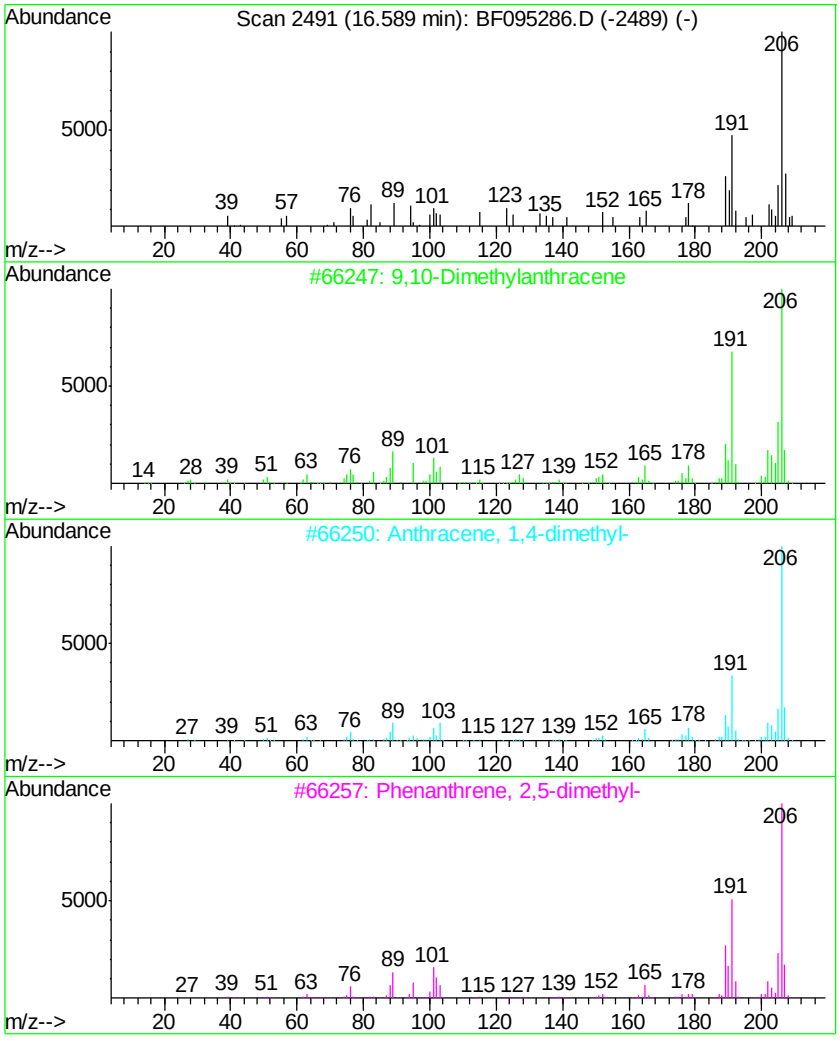
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

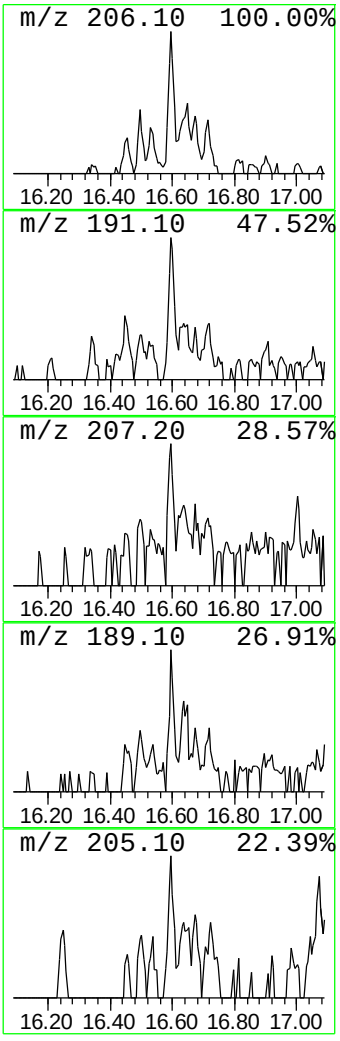
****

Peak Number 6 9,10-Dimethylanthracene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.59	2.22 ng	46540	Phenanthrene-d10	15.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,10-Dimethylanthracene	206	C16H14	000781-43-1	95
2	Anthracene, 1,4-dimethyl-	206	C16H14	000781-92-0	95
3	Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	91
4	di-p-Tolylacetylene	206	C16H14	002789-88-0	90
5	Phenanthrene, 3,6-dimethyl-	206	C16H14	001576-67-6	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051917\
Data File : BF095286.D
Acq On : 20 May 2017 3:32
Operator : SJ/MA
Sample : I3202-10 5X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-10COMP

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...	5.10	3.0	ng	72757	1	7.76	478407	20.0
unknown7.44	7.44	15.2	ng	364025	1	7.76	478407	20.0
9H-Fluorene, 9-me...	15.15	2.1	ng	43415	4	15.02	419794	20.0
6H-Cyclobuta[jk]p...	15.95	2.5	ng	52210	4	15.02	419794	20.0
9,10-Dimethylanth...	16.59	2.2	ng	46540	4	15.02	419794	20.0