LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF062117\
Data File : BF096088.D
Acq On : 21 Jun 2017 17:10
Operator : SJ/MA
Sample : I3736-08
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G14-1.5-3

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-BF060517.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	1.551	9	11	59	rVB	853529	2039885	100.00%	11.796%
2	4.475	504	508	535	rBV	52909	165057	8.09%	0.954%
3	5.186	625	629	668	rBV	569215	1471809	72.15%	8.511%
4	6.863	910	914	925	rBV	693986	1320907	64.75%	7.638%
5	6.951	925	929	951	rVB	1033953	1857644	91.07%	10.742%
6	7.286	982	986	999	rBV	305814	427856	20.97%	2.474%
7	7.527	1022	1027	1043	rBV	850931	1234268	60.51%	7.137%
8	8.210	1139	1143	1174	rBV	608043	991739	48.62%	5.735%
9	9.321	1328	1332	1345	rBV	403323	588041	28.83%	3.400%
10	9.421	1345	1349	1358	rVB2	17807	31054	1.52%	0.180%
11	10.410	1512	1517	1525	rVB	33406	40683	1.99%	0.235%
12	11.098	1629	1634	1654	rVB	1263926	1673927	82.06%	9.680%
13	11.327	1668	1673	1678	rVB	21450	27578	1.35%	0.159%
14	11.798	1747	1753	1764	rBV	113578	179247	8.79%	1.037%
15	12.139	1806	1811	1817	rBV2	490857	644264	31.58%	3.726%
16	12.186	1817	1819	1823	rVB2	26950	29847	1.46%	0.173%
17	12.998	1952	1957	1961	rBV	25388	30917	1.52%	0.179%
18	13.439	2027	2032	2054	rBV	518906	829669	40.67%	4.798%
19	13.721	2075	2080	2085	rBV	46313	80541	3.95%	0.466%
20	13.768	2085	2088	2095	rVB2	31185	58234	2.85%	0.337%
21	14.533	2214	2218	2223	rBV	459778	602870	29.55%	3.486%
22	15.351	2353	2357	2361	rBV	24173	25774	1.26%	0.149%
23	15.392	2361	2364	2371	rVB	30240	41967	2.06%	0.243%
24	15.562	2387	2393	2397	rVV4	64084	87138	4.27%	0.504%
25	15.798	2430	2433	2440	rBV6	13073	22279	1.09%	0.129%
26	16.162	2489	2495	2498	rBV2	23740	29912	1.47%	0.173%
27	16.368	2527	2530	2536	rVB	27086	34709	1.70%	0.201%
28	16.674	2577	2582	2587	rBV2	50479	74143	3.63%	0.429%
29	16.768	2591	2598	2601	rBV2	27715	40606	1.99%	0.235%
30	16.915	2618	2623	2630	rVB	920607	1110612	54.44%	6.422%
31	17.721	2756	2760	2766	rVB2	38597	44830	2.20%	0.259%
32	18.174	2833	2837	2844	rBV2	90595	141130	6.92%	0.816%
33	18.268	2848	2853	2858	rBV	424650	519143	25.45%	3.002%
34	18.780	2937	2940	2944	rVB5	19907	23954	1.17%	0.139%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF062117\
Data File : BF096088.D
Acq On : 21 Jun 2017 17:10
Operator : SJ/MA
Sample : I3736-08
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G14-1.5-3

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-BF060517.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	19.303	3025	3029	3033	rBV	82984	106957	5.24%	0.618%
36	19.450	3051	3054	3057	rBV5	13119	21319	1.05%	0.123%
37	19.544	3066	3070	3073	rBV	26562	37492	1.84%	0.217%
38	19.703	3093	3097	3099	rBV3	17191	26310	1.29%	0.152%
39	19.891	3127	3129	3132	rBV	20302	21880	1.07%	0.127%
40	19.938	3133	3137	3143	rVV	375810	476569	23.36%	2.756%
41	20.374	3208	3211	3214	rBV4	26514	34233	1.68%	0.198%
42	20.497	3230	3232	3237	rVB5	13911	22608	1.11%	0.131%
43	20.550	3237	3241	3244	rBV6	14902	23623	1.16%	0.137%

Sum of corrected areas: 17293225

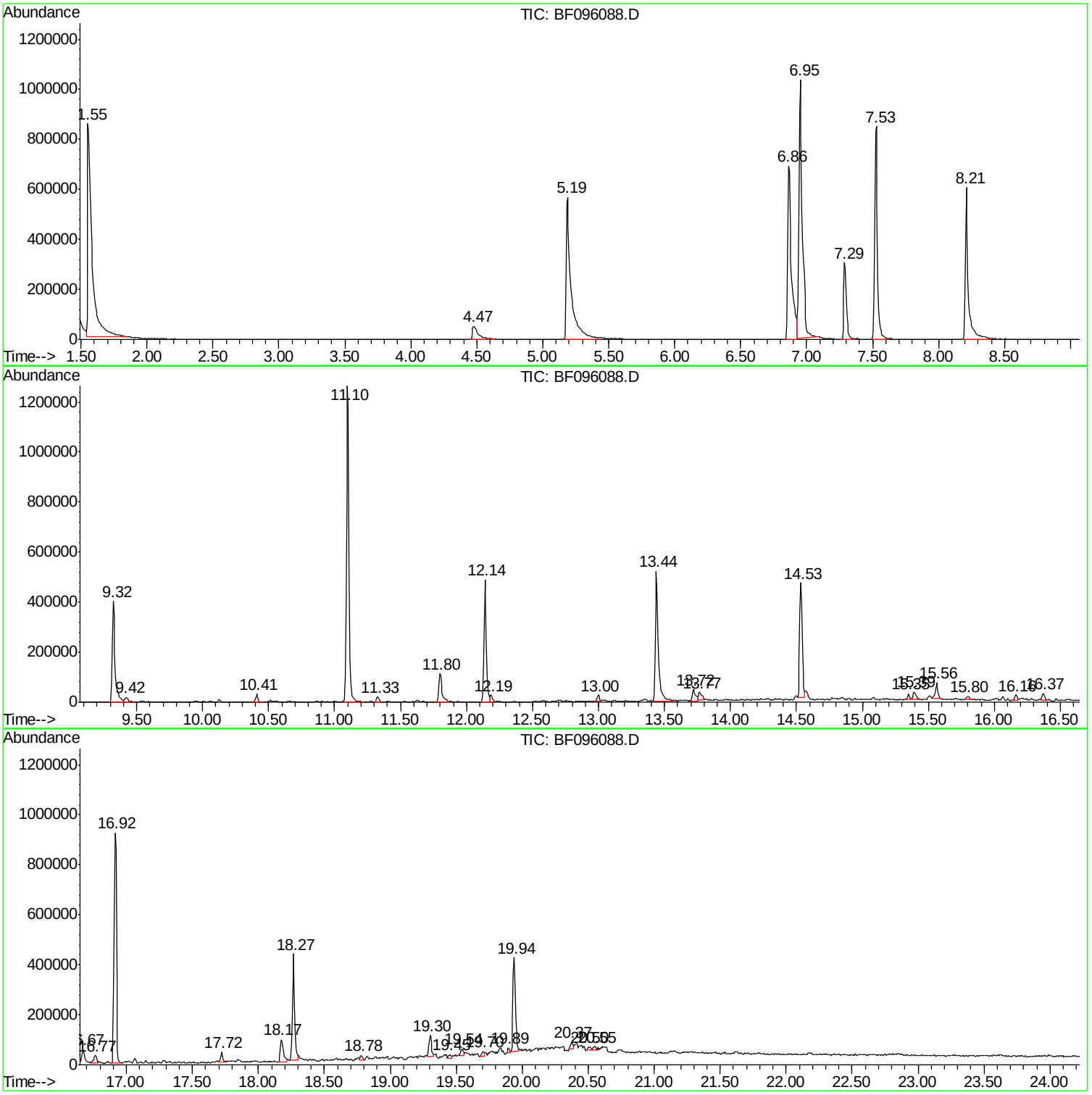
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF062117\
Data File : BF096088.D
Acq On : 21 Jun 2017 17:10
Operator : SJ/MA
Sample : I3736-08
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G14-1.5-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.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\BF062117\
Data File : BF096088.D
Acq On : 21 Jun 2017 17:10
Operator : SJ/MA
Sample : I3736-08
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G14-1.5-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

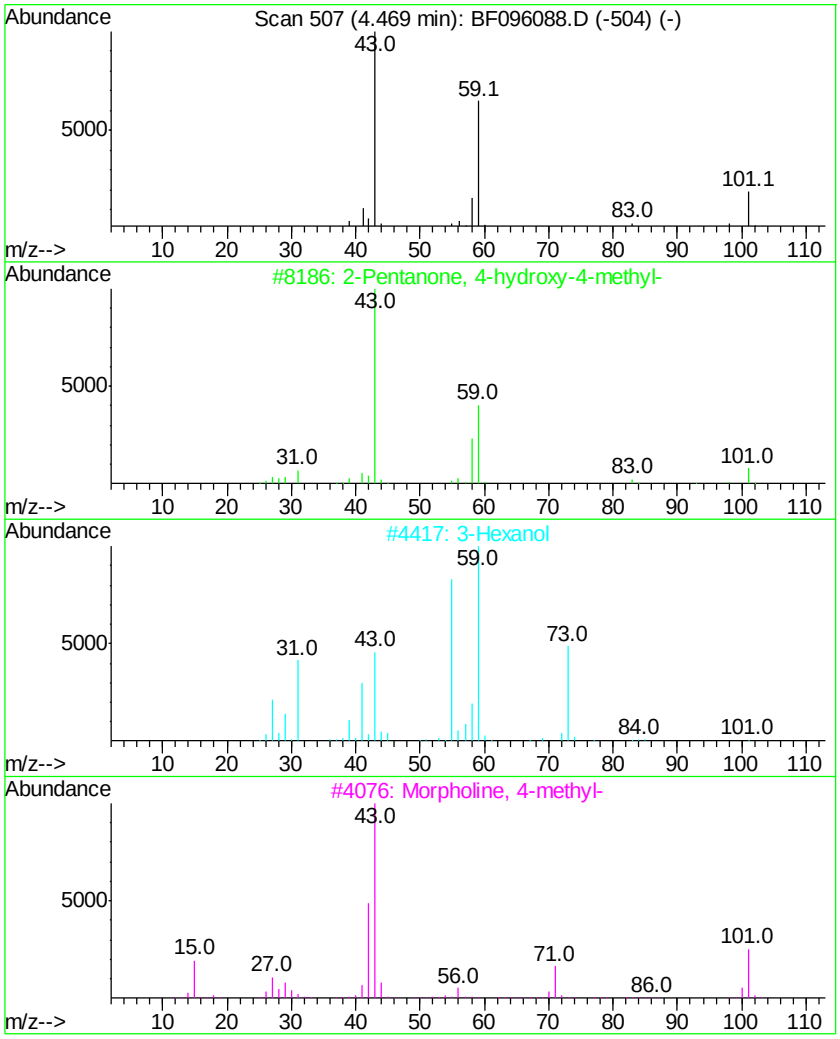
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

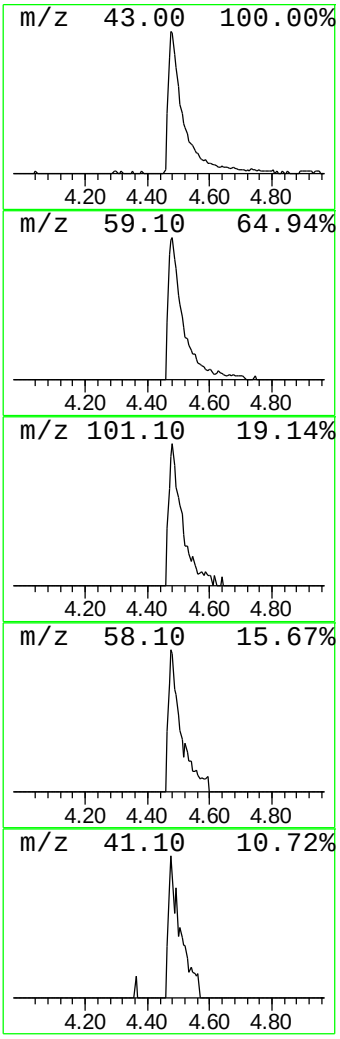
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.47	7.72 ng	165057	1,4-Dichlorobenzene-d4	7.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	42
2	3-Hexanol	102	C6H14O	000623-37-0	33
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF062117\
Data File : BF096088.D
Acq On : 21 Jun 2017 17:10
Operator : SJ/MA
Sample : I3736-08
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G14-1.5-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

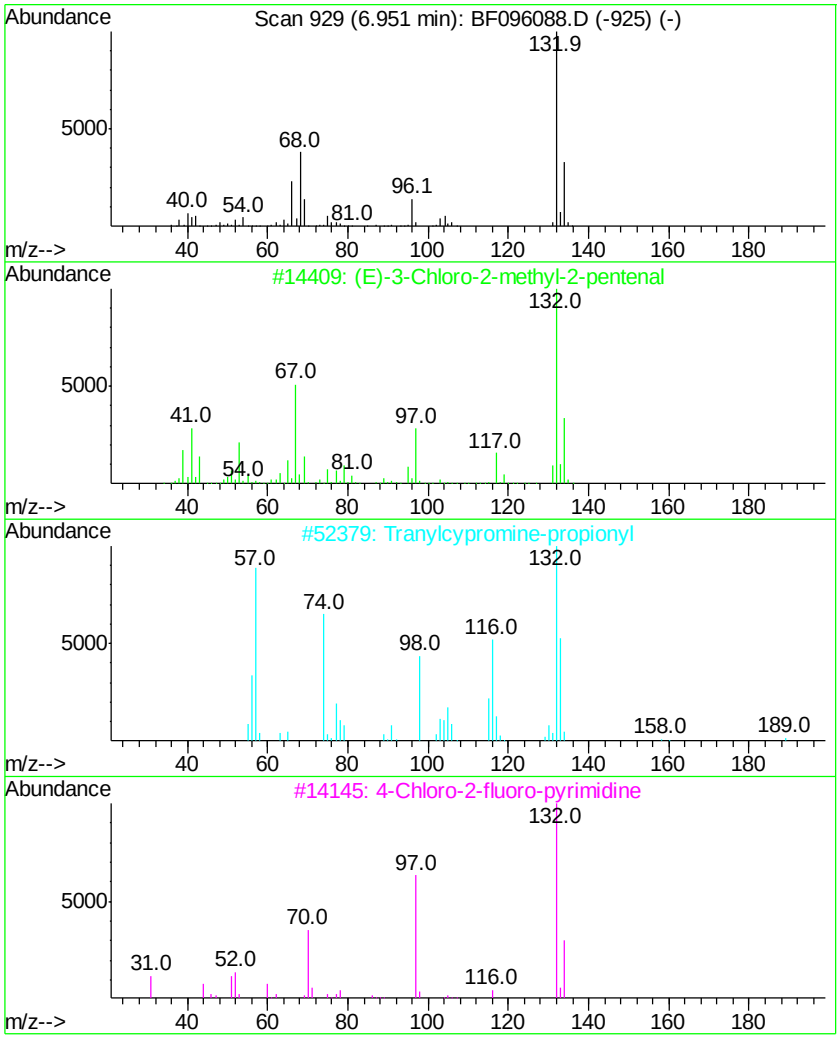
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

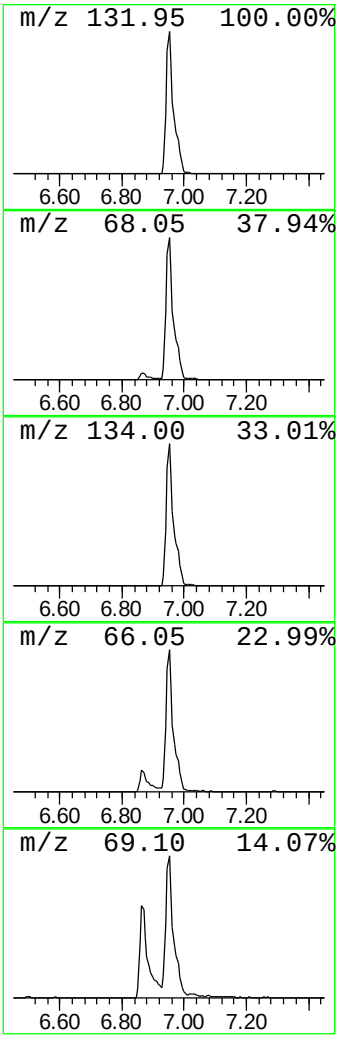
****

Peak Number 3 unknown6.95 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.95	86.84 ng	1857640	1,4-Dichlorobenzene-d4	7.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9
5	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF062117\
Data File : BF096088.D
Acq On : 21 Jun 2017 17:10
Operator : SJ/MA
Sample : I3736-08
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G14-1.5-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

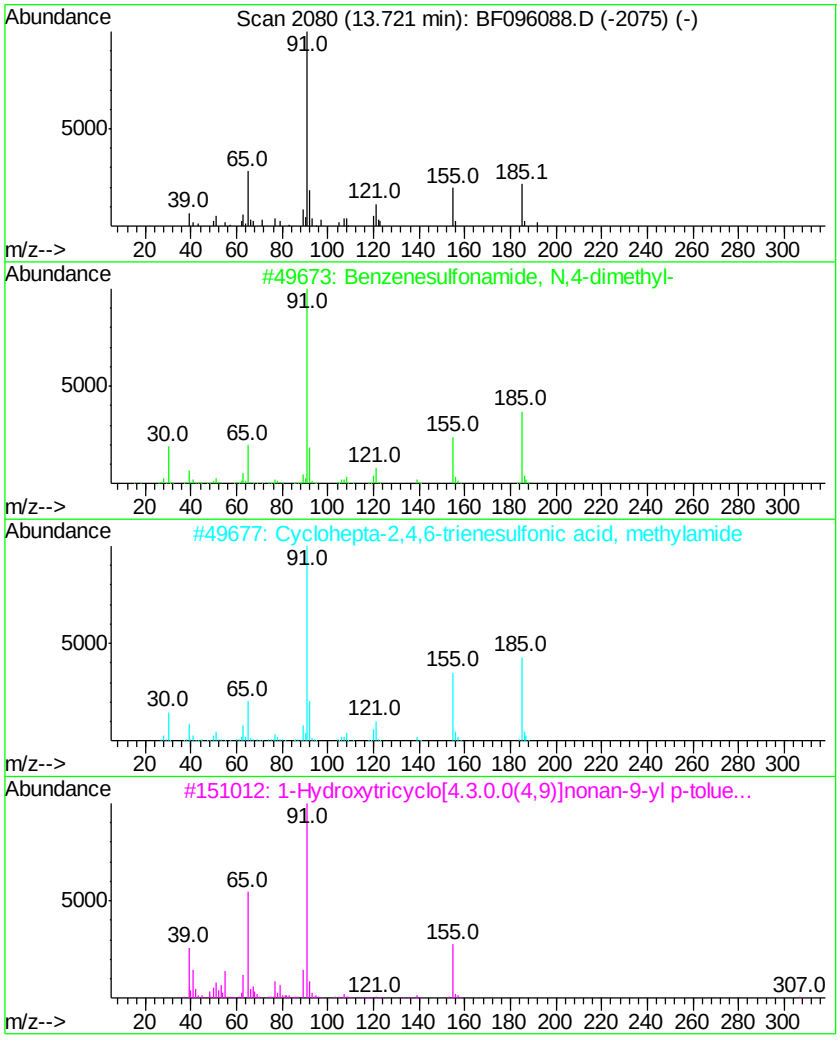
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

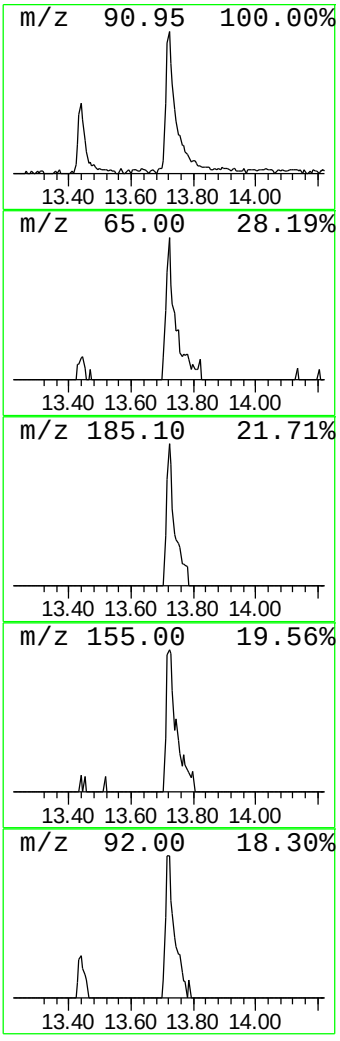
****

Peak Number 5 Benzenesulfonamide, N,4-dim... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	2.67 ng	80541	Phenanthrene-d10	14.53

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenesulfonamide, N,4-dimethyl-	185	C8H11NO2S	000640-61-9	83
2	Cyclohepta-2,4,6-trienesulfonic ...	185	C8H11NO2S	1000187-28-7	58
3	1-Hydroxytricyclo[4.3.0.0(4,9)]n...	308	C16H20O4S	201992-83-8	50
4	Ethyl(E/Z)-.alpha.-cyano-4-nitro...	416	C19H16N2O7S	1000287-26-8	50
5	4-Toluenesulfonylmethyl isocyanide	195	C9H9NO2S	036635-61-7	50





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF062117\
Data File : BF096088.D
Acq On : 21 Jun 2017 17:10
Operator : SJ/MA
Sample : I3736-08
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G14-1.5-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

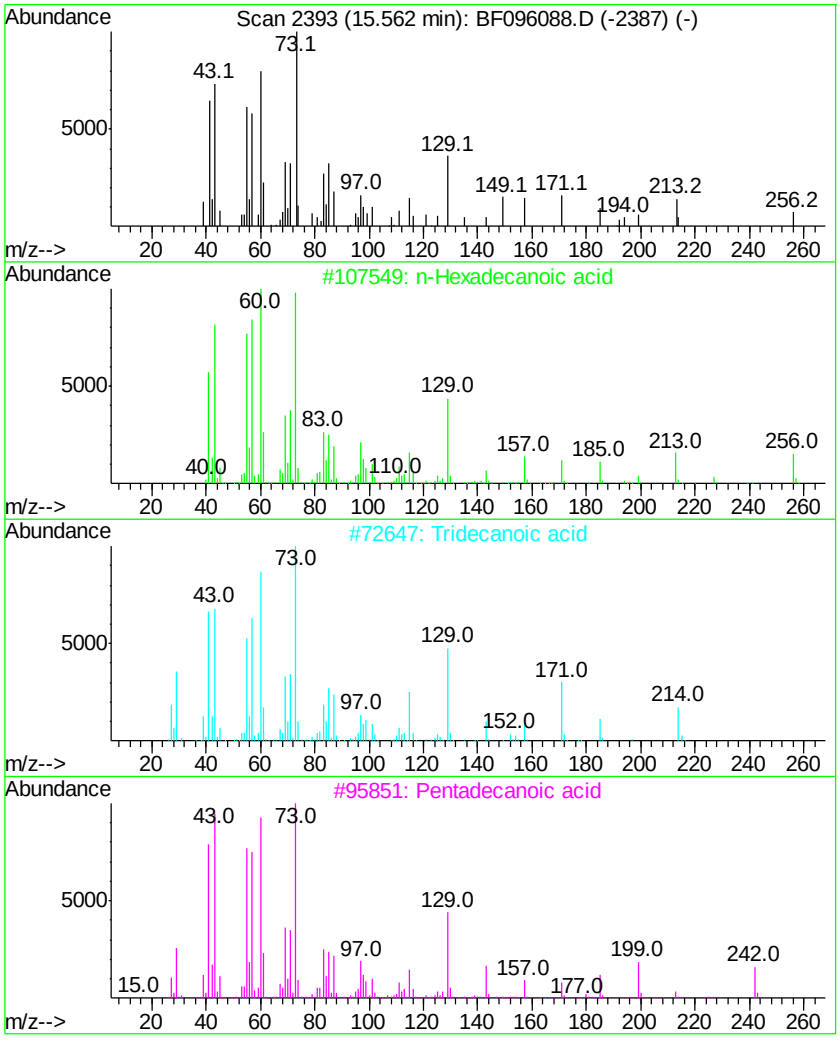
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

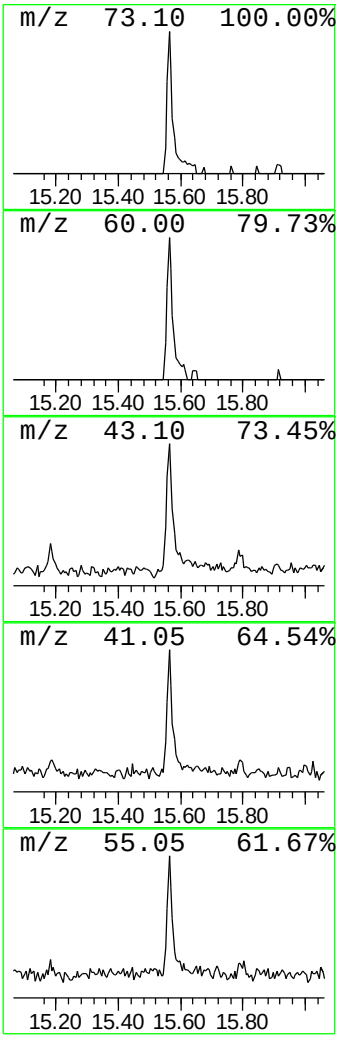
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.56	2.89 ng	87138	Phenanthrene-d10	14.53

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Dodecanoic acid	200	C12H24O2	000143-07-7	59





Data Path : Z:\HPCHEM1\BNA F\DATA\BF062117\
Data File : BF096088.D
Acq On : 21 Jun 2017 17:10
Operator : SJ/MA
Sample : I3736-08
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G14-1.5-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

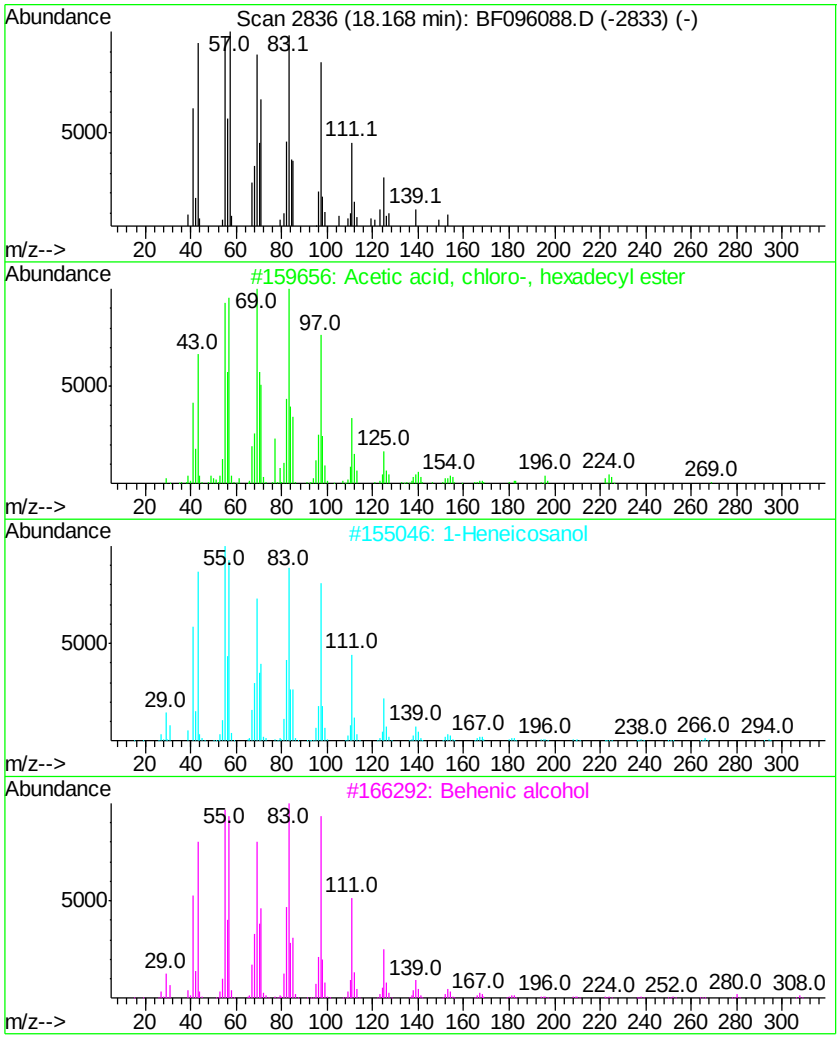
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

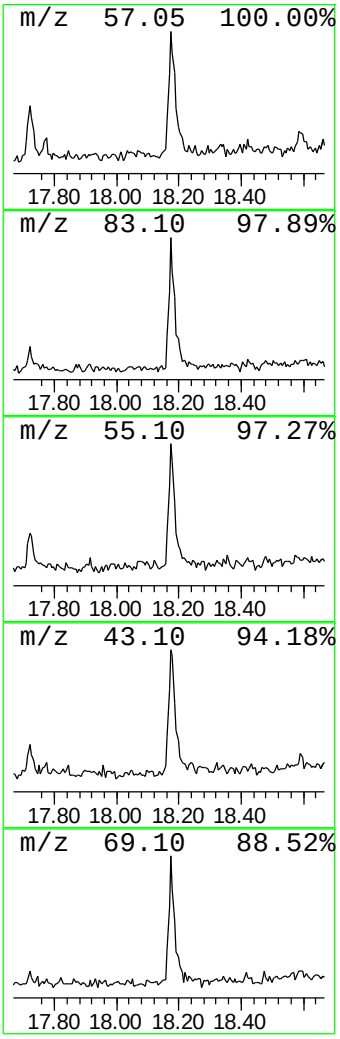
****

Peak Number 8 Acetic acid, chloro-, hexad... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.17	5.44 ng	141130	Chrysene-d12	18.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, chloro-, hexadecyl ...	318	C18H35ClO2	052132-58-8	94
2	1-Heneicosanol	312	C21H44O	015594-90-8	94
3	Behenic alcohol	326	C22H46O	000661-19-8	93
4	Pentafluoropropionic acid, tride...	346	C16H27F5O2	959261-22-4	91
5	Carbonic acid, tetradecyl 2,2,2-...	388	C17H31Cl3O3	1000314-56-0	91





Data Path : Z:\HPCHEM1\BNA F\DATA\BF062117\
Data File : BF096088.D
Acq On : 21 Jun 2017 17:10
Operator : SJ/MA
Sample : I3736-08
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G14-1.5-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

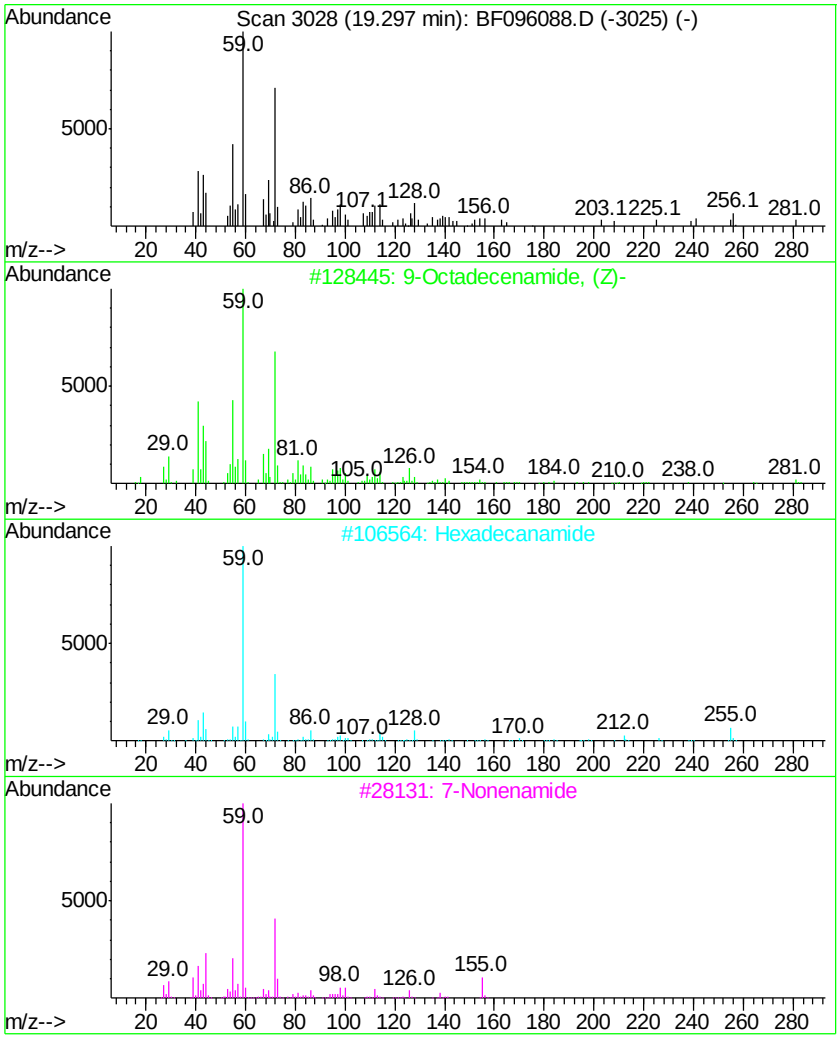
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

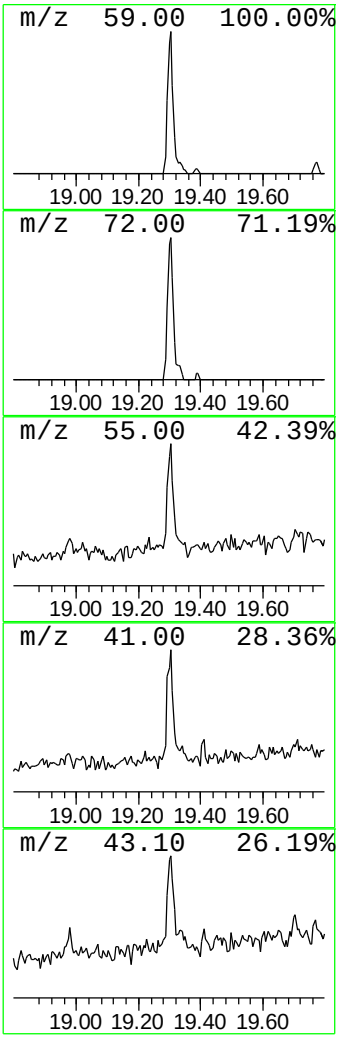
****

Peak Number 9 9-Octadecenamide, (Z)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.30	4.49 ng	106957	Perylene-d12	19.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	90
2	Hexadecanamide	255	C16H33NO	000629-54-9	76
3	7-Nonenamide	155	C9H17NO	090949-53-4	53
4	d-Glucosamine	179	C6H13NO5	000090-77-7	47
5	Tetradecanamide	227	C14H29NO	000638-58-4	42





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062117\
Data File : BF096088.D
Acq On : 21 Jun 2017 17:10
Operator : SJ/MA
Sample : I3736-08
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G14-1.5-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.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...	4.47	7.7	ng	165057	1	7.29	427856	20.0
unknown6.95	6.95	86.8	ng	1857640	1	7.29	427856	20.0
Benzenesulfonamid...	13.72	2.7	ng	80541	4	14.53	602870	20.0
n-Hexadecanoic acid	15.56	2.9	ng	87138	4	14.53	602870	20.0
Acetic acid, chlo...	18.17	5.4	ng	141130	5	18.27	519143	20.0
9-Octadecenamide,...	19.30	4.5	ng	106957	6	19.94	476569	20.0