LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG110116\
Data File : BG024623.D
Acq On : 2 Nov 2016 11:30
Operator : UM/SJ
Sample : H5500-05
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 14B(1-4)-COMP

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_G\METHODS\8270-BG102516.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	3.737	149	153	160	rBV4	30834	61074	2.04%	0.302%
2	5.335	420	425	431	rBV3	30450	55729	1.86%	0.276%
3	5.799	498	504	510	rBV3	45991	81258	2.71%	0.402%
4	7.409	772	778	779	rBV3	53932	92040	3.07%	0.456%
5	7.421	779	780	786	rVB3	41281	55491	1.85%	0.275%
6	7.791	835	843	850	rVB3	93832	178929	5.97%	0.886%
7	8.267	917	924	932	rBV	495679	884449	29.52%	4.380%
8	8.596	974	980	985	rVB3	127117	233006	7.78%	1.154%
9	9.442	1116	1124	1133	rVB	137451	253133	8.45%	1.254%
10	11.093	1396	1405	1413	rBV2	612899	1171268	39.09%	5.801%
11	13.508	1809	1816	1822	rBV2	292011	476234	15.89%	2.359%
12	13.737	1849	1855	1864	rVB4	34438	67631	2.26%	0.335%
13	14.319	1946	1954	1960	rBV	605920	892774	29.79%	4.421%
14	14.736	2017	2025	2030	rBV2	49678	73948	2.47%	0.366%
15	14.883	2042	2050	2057	rBV	1043628	1656911	55.29%	8.206%
16	15.347	2124	2129	2132	rBV3	26896	36176	1.21%	0.179%
17	15.676	2181	2185	2192	rVB	125825	166678	5.56%	0.825%
18	16.087	2247	2255	2258	rBV7	41690	82980	2.77%	0.411%
19	16.305	2285	2292	2295	rVB5	20189	41551	1.39%	0.206%
20	16.363	2295	2302	2310	rBV4	112695	209591	6.99%	1.038%
21	16.540	2327	2332	2344	rVB	151259	280861	9.37%	1.391%
22	16.875	2385	2389	2393	rBV5	21810	34443	1.15%	0.171%
23	16.998	2404	2410	2414	rBV8	16913	35607	1.19%	0.176%
24	17.327	2462	2466	2471	rBV2	85757	109696	3.66%	0.543%
25	17.380	2471	2475	2483	rBV9	25140	59764	1.99%	0.296%
26	17.627	2510	2517	2528	rBV	1268117	2087053	69.65%	10.336%
27	17.962	2566	2574	2584	rBV	517047	877370	29.28%	4.345%
28	18.067	2588	2592	2600	rVB2	49121	80174	2.68%	0.397%
29	18.467	2656	2660	2665	rBV3	84971	123486	4.12%	0.612%
30	18.549	2671	2674	2681	rVB3	26295	31563	1.05%	0.156%
31	18.749	2705	2708	2712	rBV6	25090	37640	1.26%	0.186%
32	19.313	2798	2804	2813	rBV	928742	1399587	46.71%	6.931%
33	19.401	2817	2819	2822	rVB4	25727	31207	1.04%	0.155%
34	19.724	2871	2874	2880	rBV7	44807	78649	2.62%	0.390%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG110116\
Data File : BG024623.D
Acq On : 2 Nov 2016 11:30
Operator : UM/SJ
Sample : H5500-05
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 14B(1-4)-COMP

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_G\METHODS\8270-BG102516.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	19.947	2907	2912	2915	rBV3	72278	103245	3.45%	0.511%
36	20.200	2950	2955	2960	rVB2	319698	439668	14.67%	2.177%
37	20.470	2995	3001	3005	rBV	191246	262482	8.76%	1.300%
38	20.623	3023	3027	3029	rBV5	20782	30746	1.03%	0.152%
39	20.811	3054	3059	3062	rBV4	86483	127163	4.24%	0.630%
40	20.929	3077	3079	3081	rBV3	27063	30503	1.02%	0.151%
41	20.970	3083	3086	3090	rVV2	191572	236398	7.89%	1.171%
42	21.499	3171	3176	3188	rVB2	374221	660889	22.06%	3.273%
43	21.757	3215	3220	3226	rBV3	91460	150242	5.01%	0.744%
44	21.916	3240	3247	3256	rVB	1607302	2909923	97.11%	14.411%
45	22.862	3404	3408	3413	rVB7	33048	54927	1.83%	0.272%
46	23.009	3430	3433	3437	rBV6	27283	38748	1.29%	0.192%
47	23.226	3469	3470	3477	rVB7	25674	33208	1.11%	0.164%
48	23.637	3539	3540	3550	rVB8	44186	79227	2.64%	0.392%
49	25.347	3818	3831	3844	rVV2	956914	2996522	100.00%	14.840%

Sum of corrected areas: 20191842

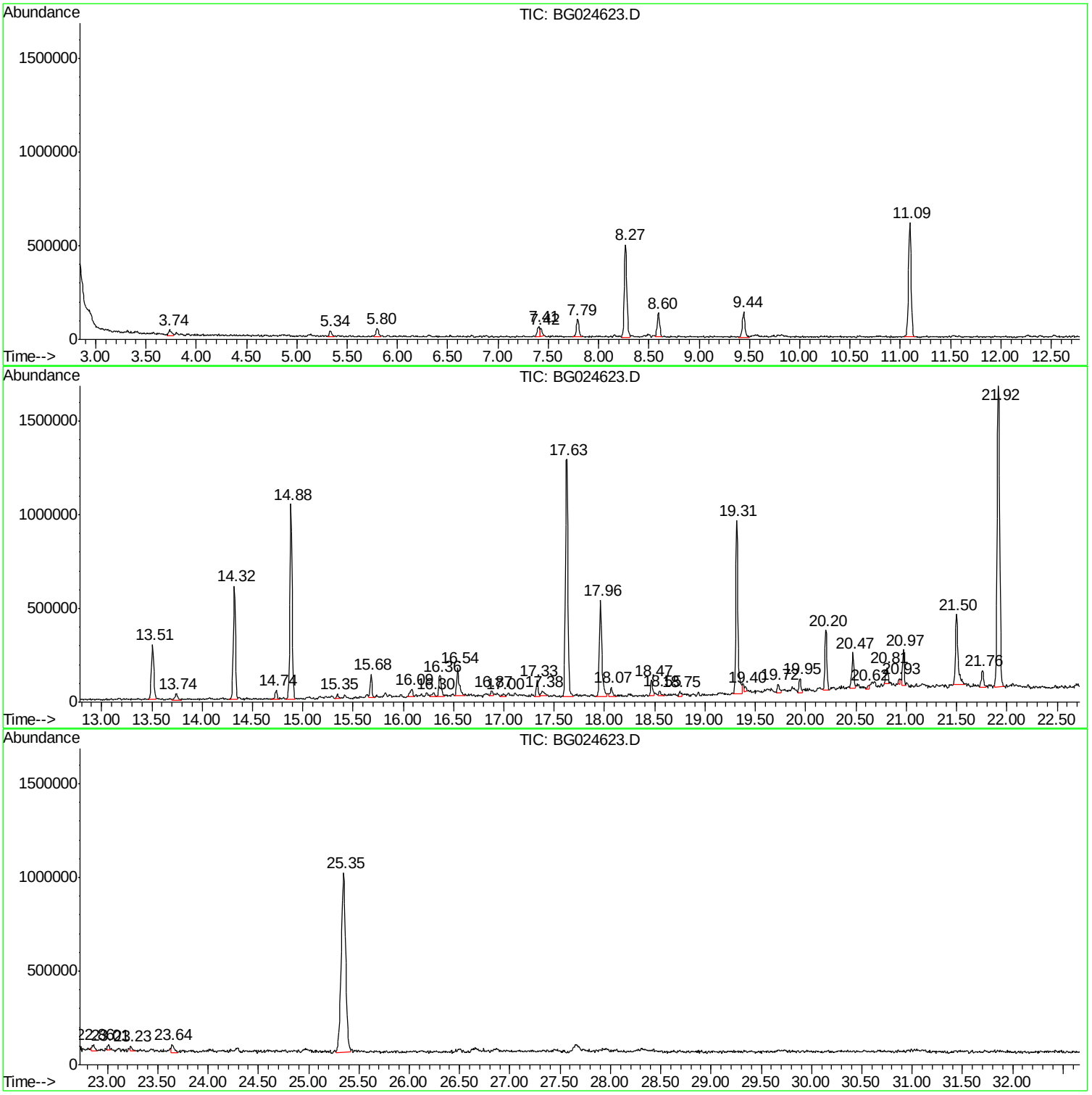
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA G\DATA\BG110116\
Data File : BG024623.D
Acq On : 2 Nov 2016 11:30
Operator : UM/SJ
Sample : H5500-05
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 14B(1-4)-COMP

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.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 G\DATA\BG110116\
Data File : BG024623.D
Acq On : 2 Nov 2016 11:30
Operator : UM/SJ
Sample : H5500-05
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 14B(1-4)-COMP

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

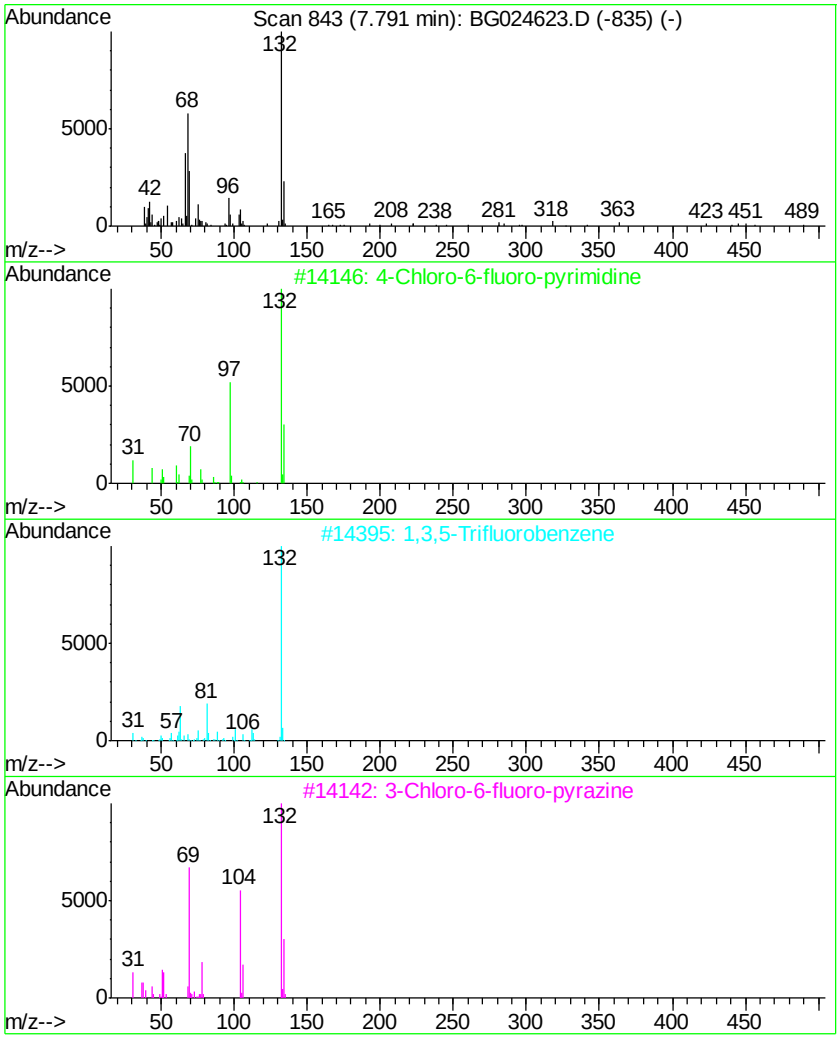
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

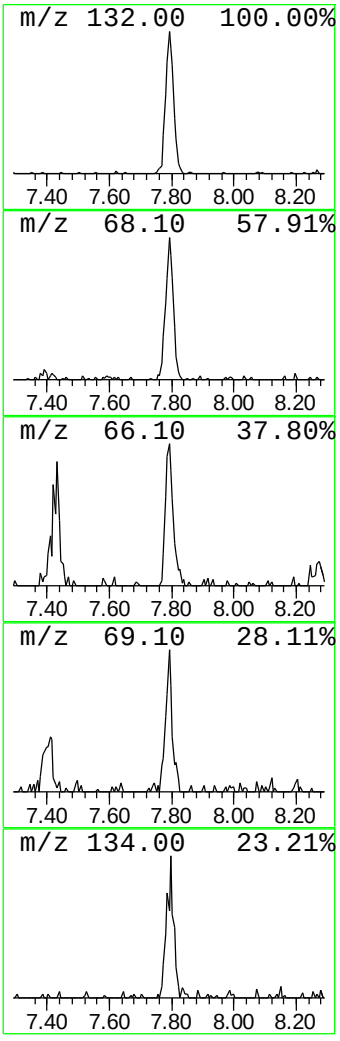
****

Peak Number 1 unknown7.79 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.79	4.05 ng	178929	1,4-Dichlorobenzene-d4	8.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	16
2	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	14
3	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	12
4	3H-1,2-Dithiol-3-one, 5-methyl-	132	C4H4OS2	003620-08-4	10
5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10





Data Path : Z:\HPCHEM1\BNA G\DATA\BG110116\
Data File : BG024623.D
Acq On : 2 Nov 2016 11:30
Operator : UM/SJ
Sample : H5500-05
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 14B(1-4)-COMP

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

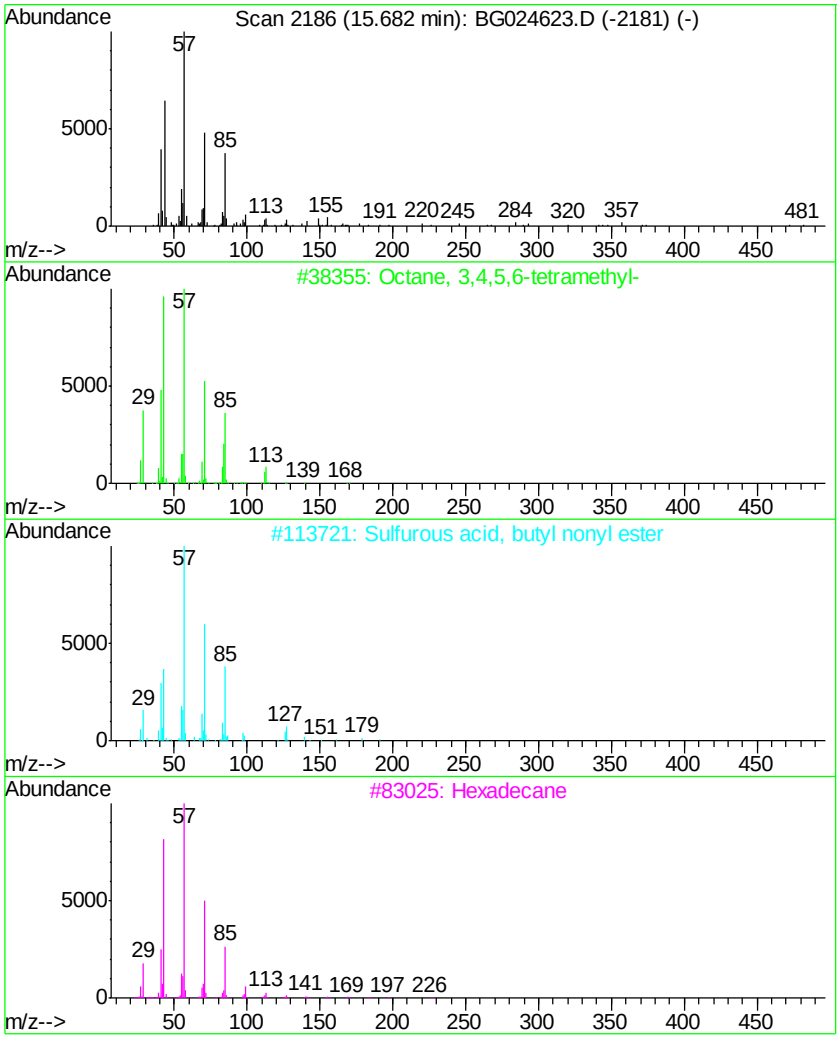
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

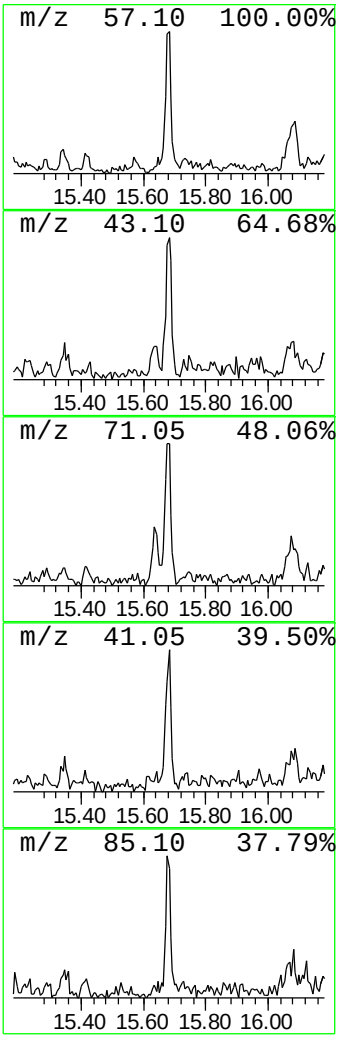
****

Peak Number 3 Octane, 3,4,5,6-tetramethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.68	2.01 ng	166678	Acenaphthene-d10	14.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 3,4,5,6-tetramethyl-	170	C12H26	062185-21-1	72
2	Sulfurous acid, butyl nonyl ester	264	C13H28O3S	1000309-17-6	72
3	Hexadecane	226	C16H34	000544-76-3	50
4	Tetradecane	198	C14H30	000629-59-4	47
5	Sulfurous acid, nonyl 2-propyl e...	250	C12H26O3S	1000309-12-0	43





Data Path : Z:\HPCHEM1\BNA G\DATA\BG110116\
Data File : BG024623.D
Acq On : 2 Nov 2016 11:30
Operator : UM/SJ
Sample : H5500-05
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 14B(1-4)-COMP

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

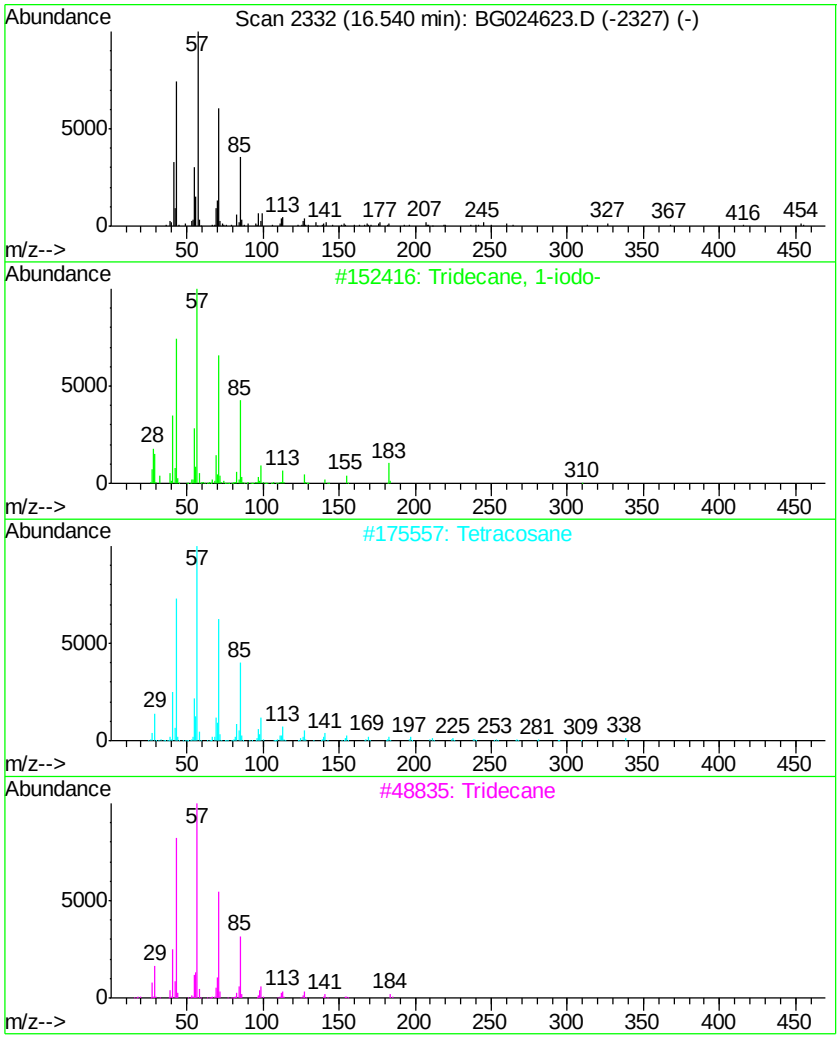
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

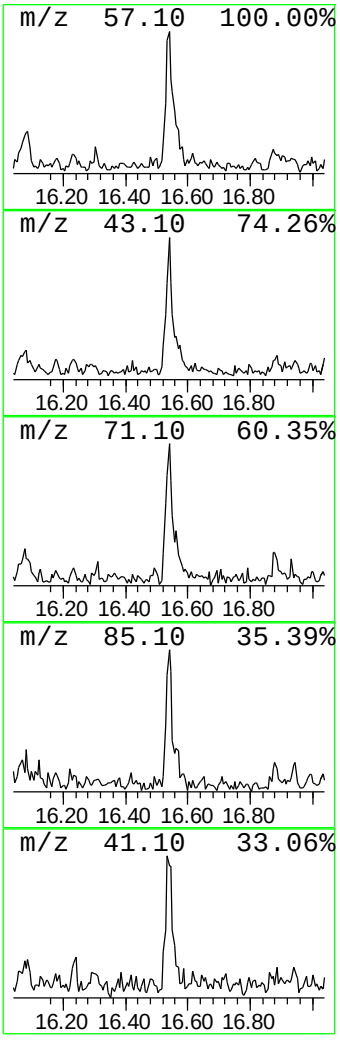
****

Peak Number 4 Tridecane, 1-iodo- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.54	2.69 ng	280861	Phenanthrene-d10	17.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	80
2	Tetracosane	338	C24H50	000646-31-1	80
3	Tridecane	184	C13H28	000629-50-5	80
4	Heptadecane	240	C17H36	000629-78-7	74
5	Dodecane	170	C12H26	000112-40-3	72





Data Path : Z:\HPCHEM1\BNA G\DATA\BG110116\
Data File : BG024623.D
Acq On : 2 Nov 2016 11:30
Operator : UM/SJ
Sample : H5500-05
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 14B(1-4)-COMP

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

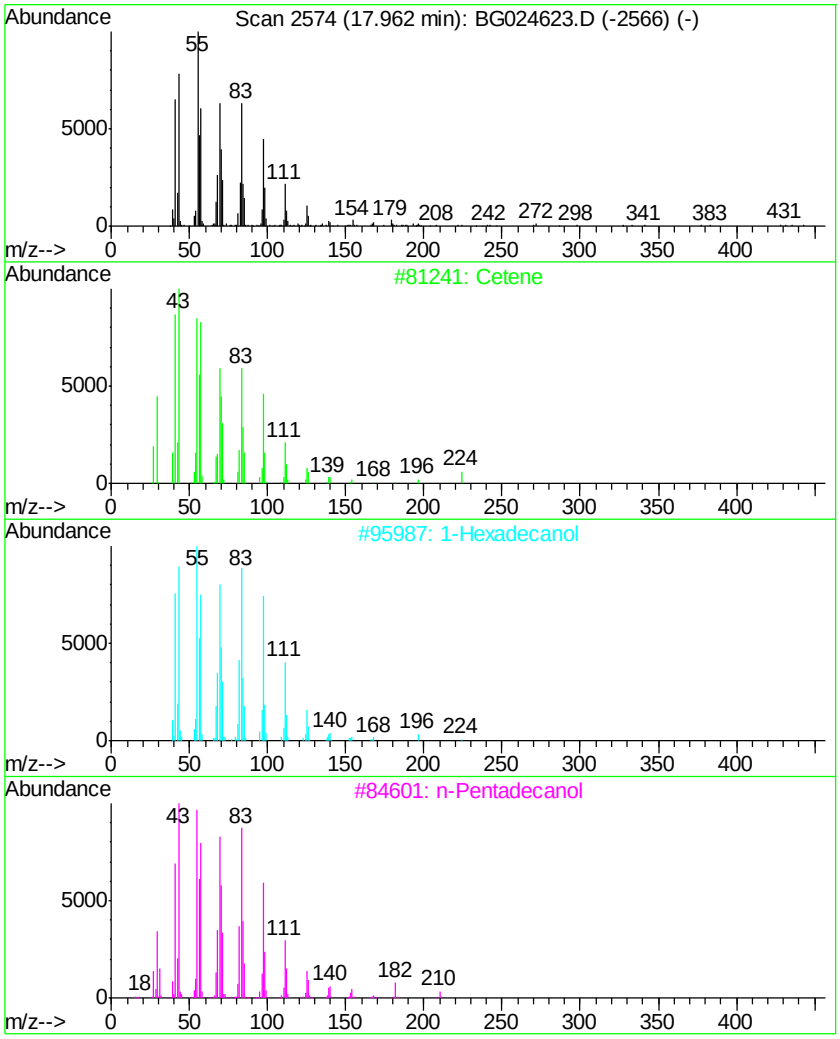
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

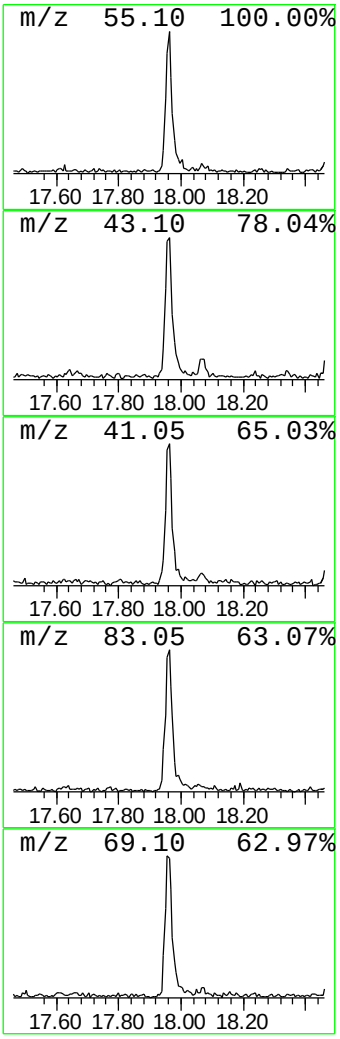
****

Peak Number 5 Cetene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.96	8.41 ng	877370	Phenanthrene-d10	17.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cetene	224	C16H32	000629-73-2	96
2	1-Hexadecanol	242	C16H34O	036653-82-4	91
3	n-Pentadecanol	228	C15H32O	000629-76-5	91
4	Cyclohexadecane	224	C16H32	000295-65-8	91
5	n-Heptadecanol-1	256	C17H36O	001454-85-9	91





Data Path : Z:\HPCHEM1\BNA G\DATA\BG110116\
Data File : BG024623.D
Acq On : 2 Nov 2016 11:30
Operator : UM/SJ
Sample : H5500-05
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 14B(1-4)-COMP

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

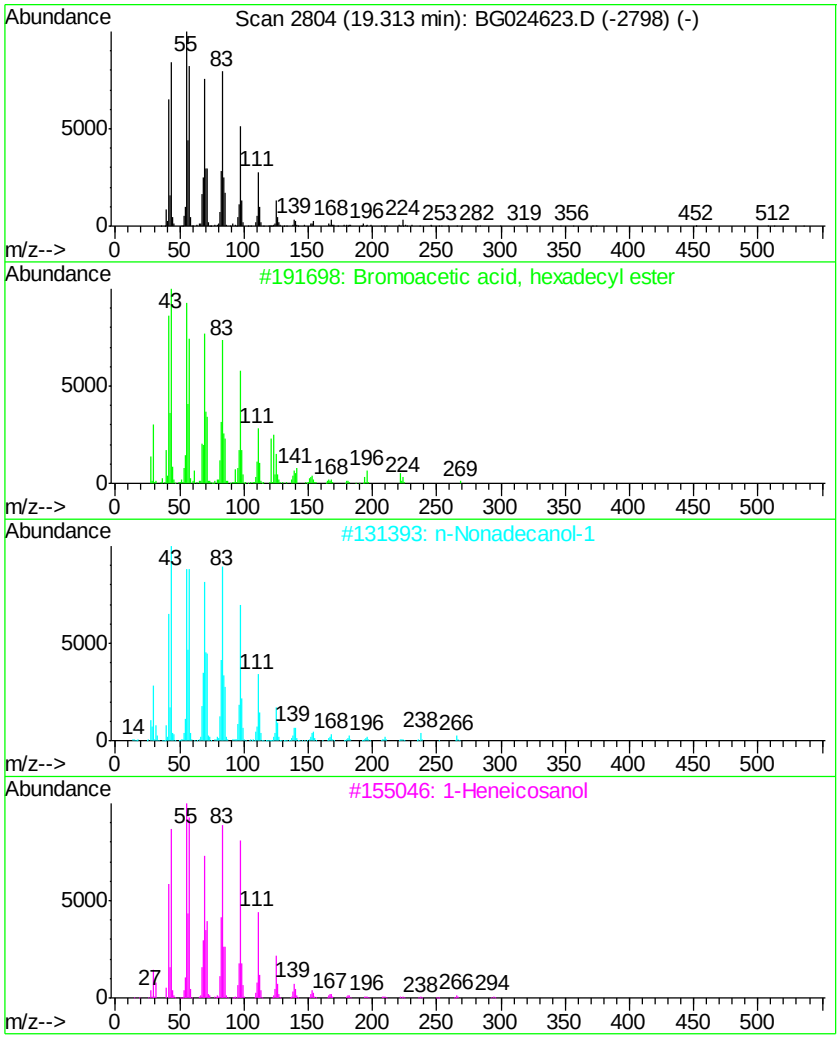
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

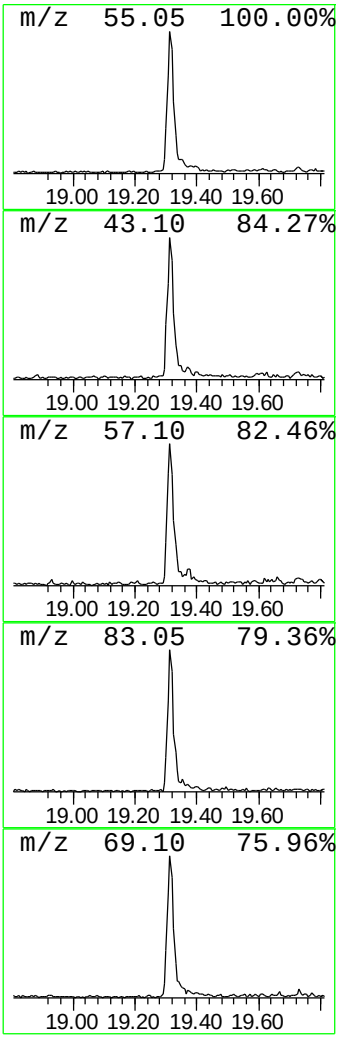
****

Peak Number 6 Bromoacetic acid, hexadecyl... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.31	13.41 ng	1399590	Phenanthrene-d10	17.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	94
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	94
3	1-Heneicosanol	312	C21H44O	015594-90-8	94
4	n-Heptadecanol-1	256	C17H36O	001454-85-9	91
5	Pentafluoropropionic acid, 4-hex...	388	C19H33F5O2	1000283-04-1	91





Data Path : Z:\HPCHEM1\BNA G\DATA\BG110116\
Data File : BG024623.D
Acq On : 2 Nov 2016 11:30
Operator : UM/SJ
Sample : H5500-05
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 14B(1-4)-COMP

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

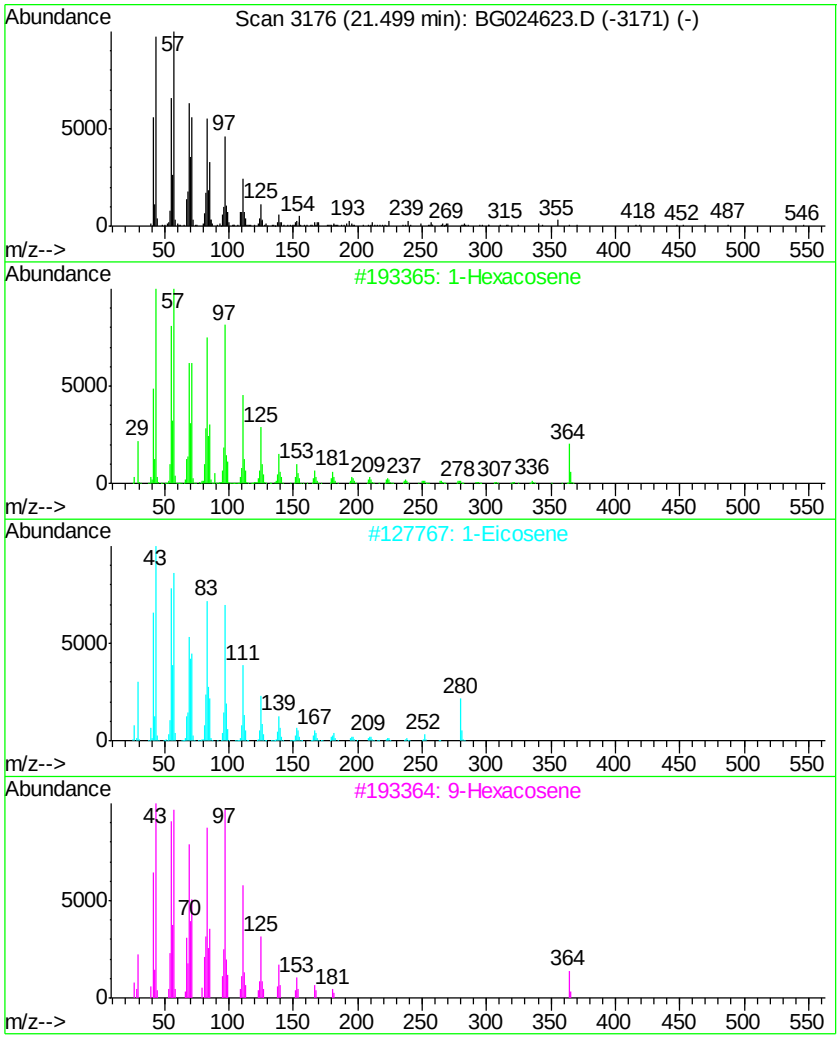
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

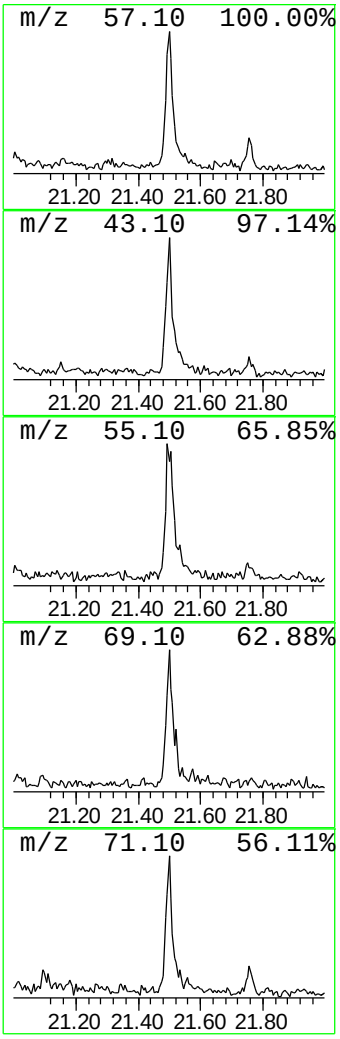
****

Peak Number 7 1-Hexacosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.50	4.54 ng	660889	Chrysene-d12	21.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosene	364	C26H52	018835-33-1	98
2	1-Eicosene	280	C20H40	003452-07-1	95
3	9-Hexacosene	364	C26H52	071502-22-2	93
4	Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	91
5	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG110116\
Data File : BG024623.D
Acq On : 2 Nov 2016 11:30
Operator : UM/SJ
Sample : H5500-05
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 14B(1-4)-COMP

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.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
unknown7.79	7.79	4.0	ng	178929	1	8.27	884449	20.0
Octane, 3,4,5,6-t...	15.68	2.0	ng	166678	3	14.88	1656910	20.0
Tridecane, 1-iodo-	16.54	2.7	ng	280861	4	17.62	2087050	20.0
Cetene	17.96	8.4	ng	877370	4	17.62	2087050	20.0
Bromoacetic acid,...	19.31	13.4	ng	1399590	4	17.62	2087050	20.0
1-Hexacosene	21.50	4.5	ng	660889	5	21.92	2909920	20.0