LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070216\
Data File : BF088623.D
Acq On : 2 Jul 2016 18:08
Operator : UM/SJ
Sample : H3847-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : R5-B1(0-11)C

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-BF063016.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	1.861	21	24	34	rVB	68748	138241	5.63%	0.615%
2	3.016	122	125	143	rBV	94917	226629	9.24%	1.009%
3	4.284	233	236	239	rVB	43401	55352	2.26%	0.246%
4	4.959	292	295	299	rVB	187134	237987	9.70%	1.059%
5	5.381	330	332	335	rBV	1722931	2343233	95.49%	10.430%
6	6.422	421	423	426	rVB	1687352	2453908	100.00%	10.922%
7	6.559	432	435	437	rBV	2540480	2302925	93.85%	10.250%
8	6.787	453	455	458	rVB	558362	649603	26.47%	2.891%
9	6.947	467	469	472	rVB	1928118	1768809	72.08%	7.873%
10	7.359	502	505	507	rBV	1664445	1698965	69.24%	7.562%
11	7.450	511	513	517	rBB	25617	28371	1.16%	0.126%
12	8.079	565	568	570	rBV	1116738	921557	37.55%	4.102%
13	9.153	660	662	665	rVB	2352221	2262639	92.21%	10.071%
14	9.553	695	697	699	rBV	744783	678168	27.64%	3.018%
15	9.828	719	721	724	rVB	1045014	903128	36.80%	4.020%
16	10.273	759	760	762	rVB	41861	29002	1.18%	0.129%
17	10.616	787	790	792	rBV	1245957	1352681	55.12%	6.021%
18	10.719	797	799	800	rBV2	48585	51039	2.08%	0.227%
19	10.742	800	801	806	rVB	49558	52847	2.15%	0.235%
20	11.188	838	840	842	rBV	107928	107875	4.40%	0.480%
21	11.302	848	850	853	rVB	733961	720904	29.38%	3.209%
22	11.371	853	856	860	rVB3	33343	67775	2.76%	0.302%
23	11.542	869	871	875	rVB2	45853	64697	2.64%	0.288%
24	11.611	875	877	880	rVB	64375	83015	3.38%	0.369%
25	11.839	896	897	899	rBV	35524	40270	1.64%	0.179%
26	12.514	954	956	958	rBV	28026	32177	1.31%	0.143%
27	12.731	972	975	978	rBV3	20297	37205	1.52%	0.166%
28	12.891	986	989	991	rBV	1732602	1535846	62.59%	6.836%
29	13.794	1066	1068	1072	rBV2	97127	118917	4.85%	0.529%
30	13.931	1078	1080	1082	rBV	715630	655438	26.71%	2.917%
31	14.434	1121	1124	1128	rBV4	10114	30266	1.23%	0.135%
32	14.788	1152	1155	1157	rVB	81334	79140	3.23%	0.352%
33	14.937	1165	1168	1172	rBV	21376	56722	2.31%	0.252%
34	15.325	1199	1202	1205	rBV	515843	616681	25.13%	2.745%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070216\
Data File : BF088623.D
Acq On : 2 Jul 2016 18:08
Operator : UM/SJ
Sample : H3847-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : R5-B1(0-11)C

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-BF063016.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	16.251	1281	1283	1292	rVB4	11744	32924	1.34%	0.147%
36	17.748	1411	1414	1420	rVB5	11115	32413	1.32%	0.144%

Sum of corrected areas: 22467349

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070216\
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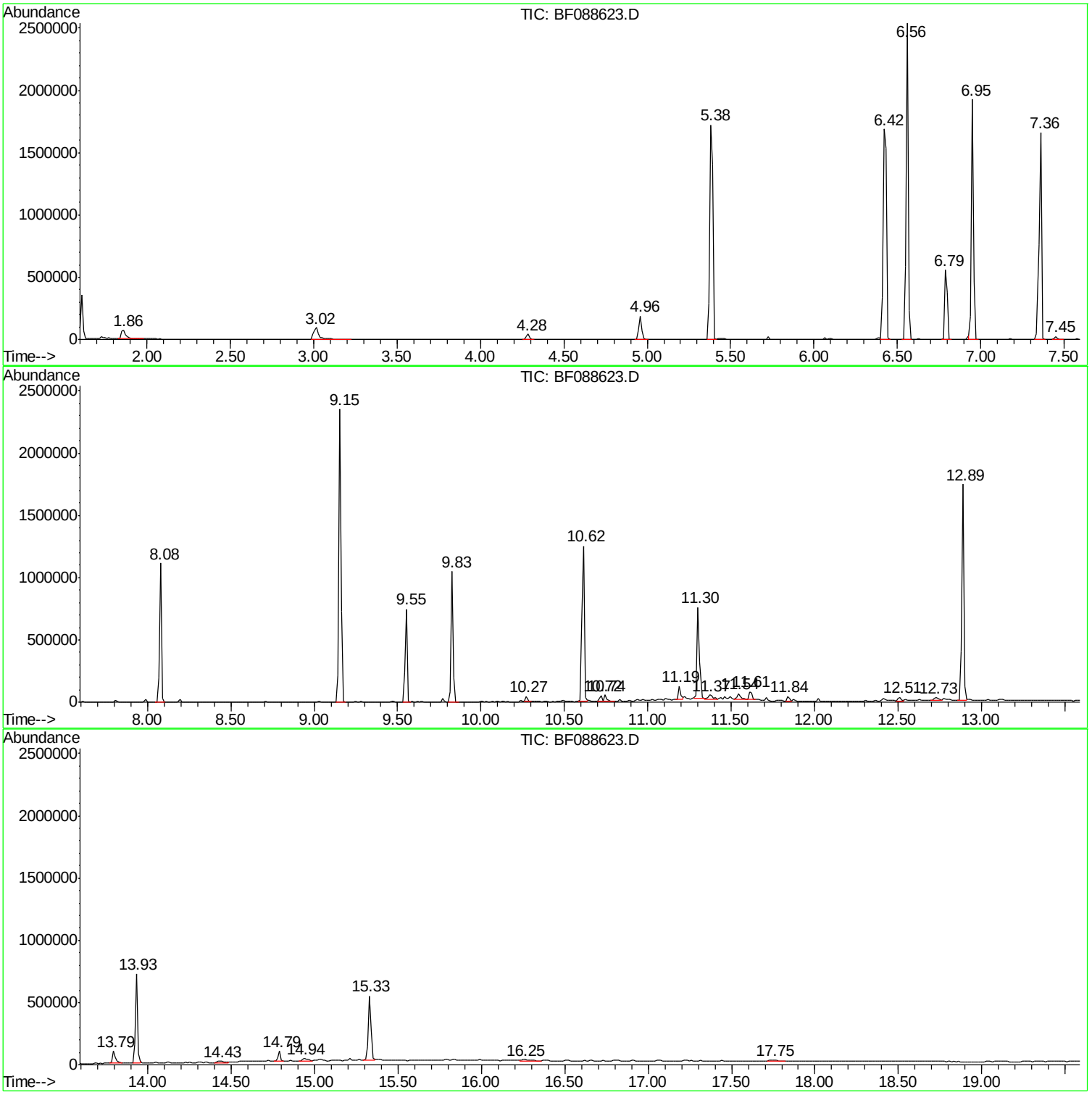
Operator : UM/SJ
Sample : H3847-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
R5-B1(0-11)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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\BF070216\
Data File : BF088623.D
Acq On : 2 Jul 2016 18:08
Operator : UM/SJ
Sample : H3847-01
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Instrument : BNA_F
ClientSampleId : R5-B1(0-11)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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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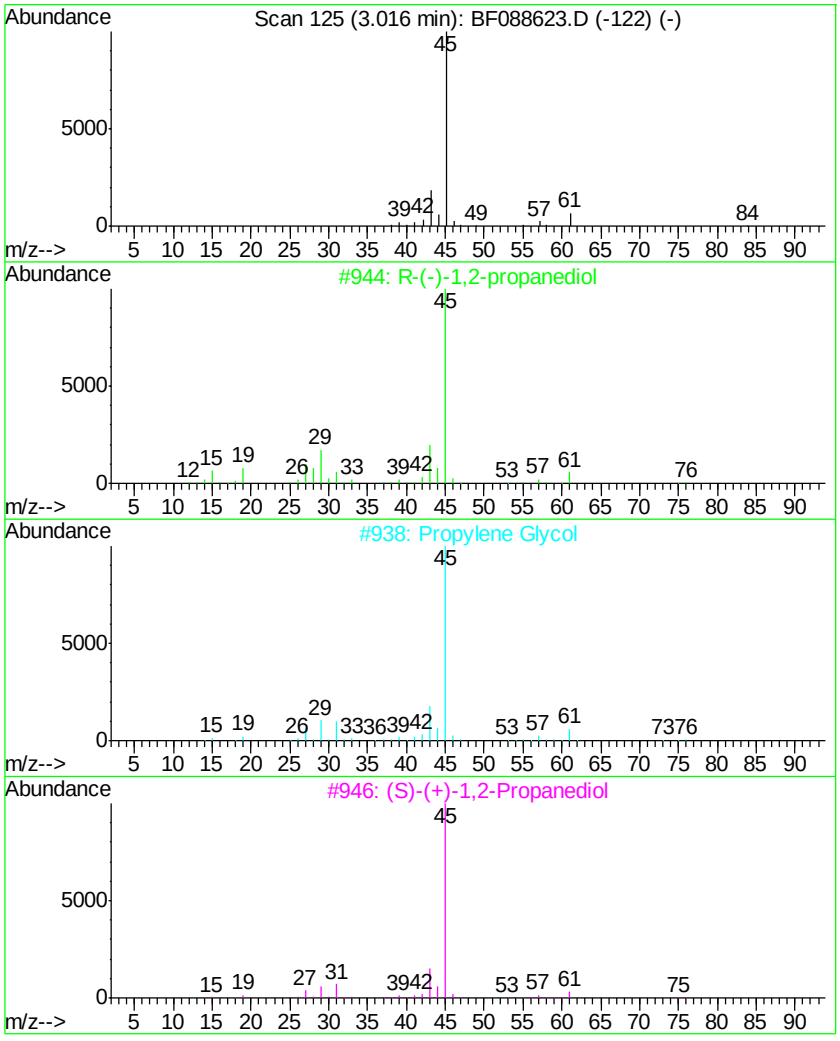
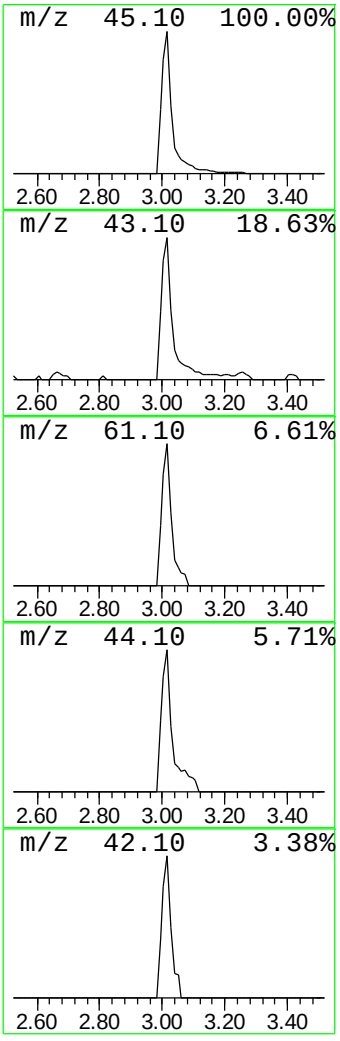
Peak Number 2 unknown3.02 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.02	6.98 ng	226629	1,4-Dichlorobenzene-d4	6.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	43
2	Propylene Glycol	76	C3H8O2	000057-55-6	43
3	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	43
4	2-Butanol	74	C4H10O	000078-92-2	9
5	Isopropyl Alcohol	60	C3H8O	000067-63-0	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070216\
Data File : BF088623.D
Acq On : 2 Jul 2016 18:08
Operator : UM/SJ
Sample : H3847-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : R5-B1(0-11)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

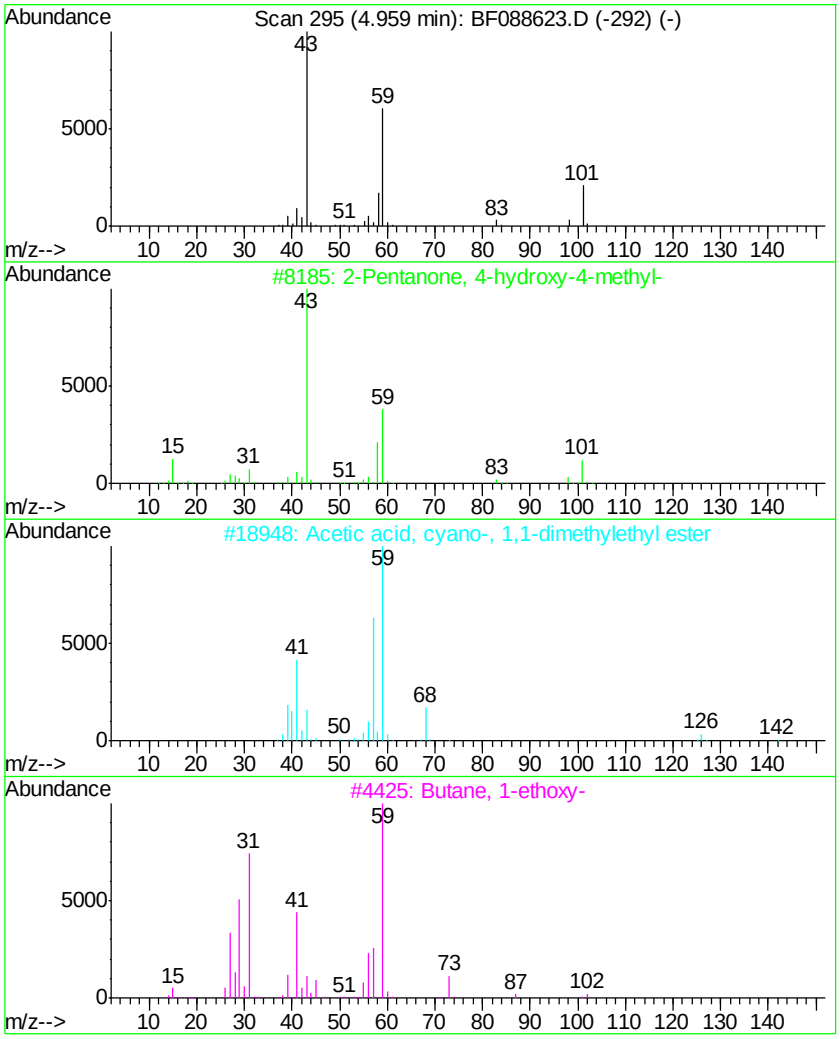
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

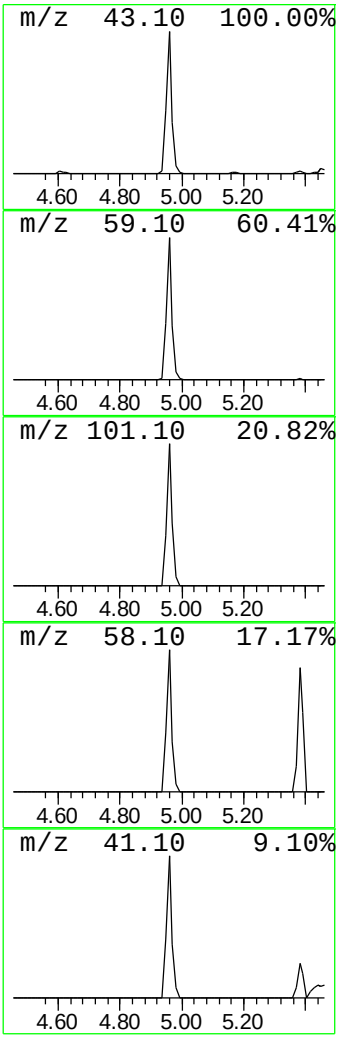
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.96	7.33 ng	237987	1,4-Dichlorobenzene-d4	6.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070216\
Data File : BF088623.D
Acq On : 2 Jul 2016 18:08
Operator : UM/SJ
Sample : H3847-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : R5-B1(0-11)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

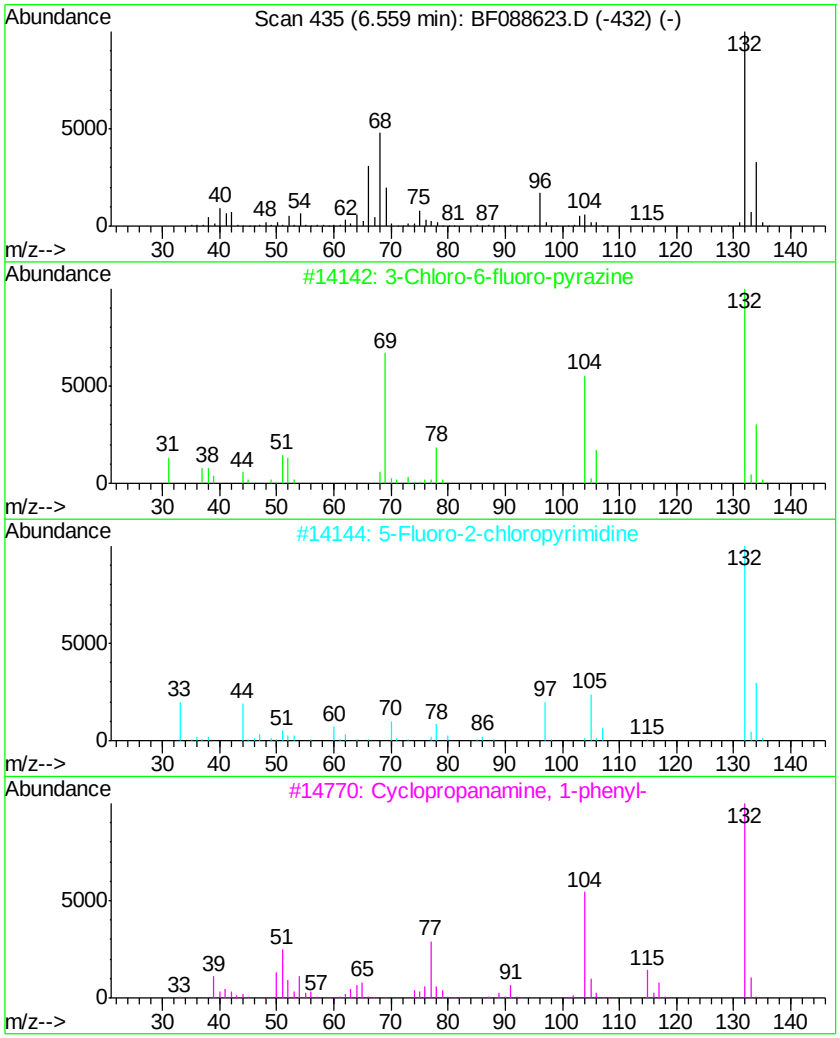
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

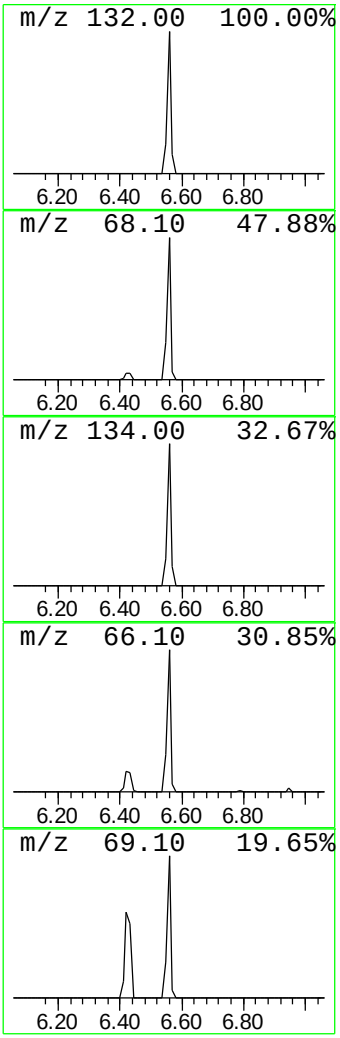
****

Peak Number 4 unknown6.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	70.90 ng	2302930	1,4-Dichlorobenzene-d4	6.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070216\
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Acq On : 2 Jul 2016 18:08
Operator : UM/SJ
Sample : H3847-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : R5-B1(0-11)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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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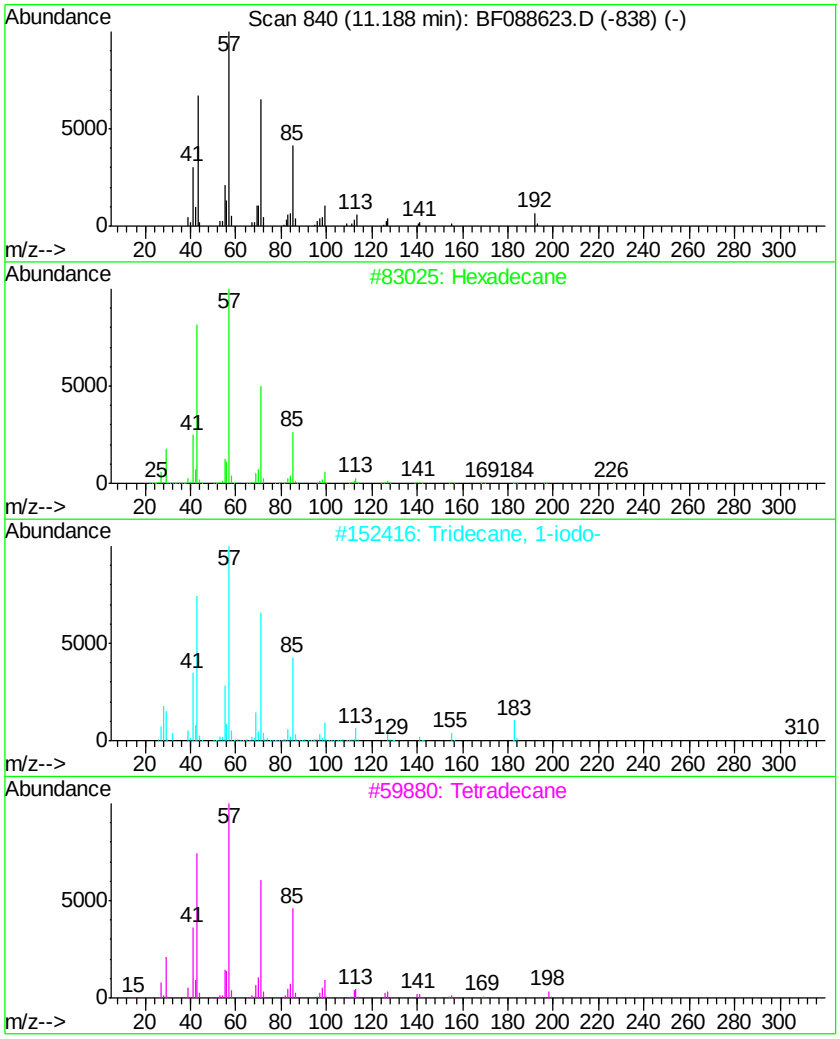
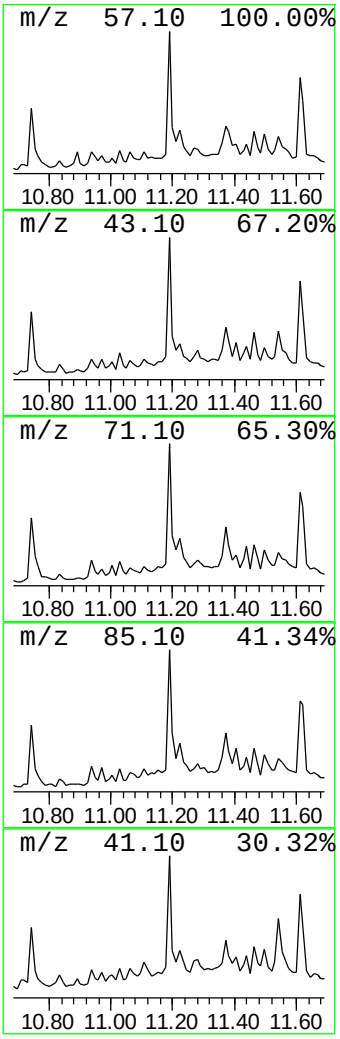
Peak Number 6 Hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.19	2.99 ng	107875	Phenanthrene-d10	11.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	90
2	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	87
3	Tetradecane	198	C14H30	000629-59-4	87
4	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	86
5	Sulfurous acid, 2-propyl tetrade...	320	C17H36O3S	1000309-12-5	86





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Misc :
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Instrument : BNA_F
ClientSampleId : R5-B1(0-11)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

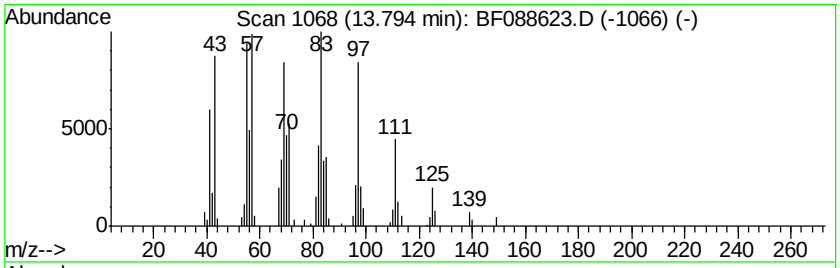
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

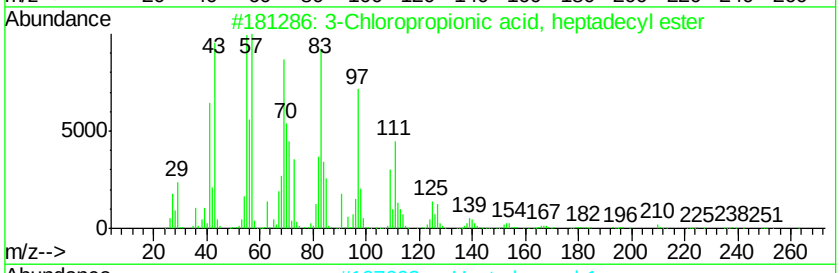
****

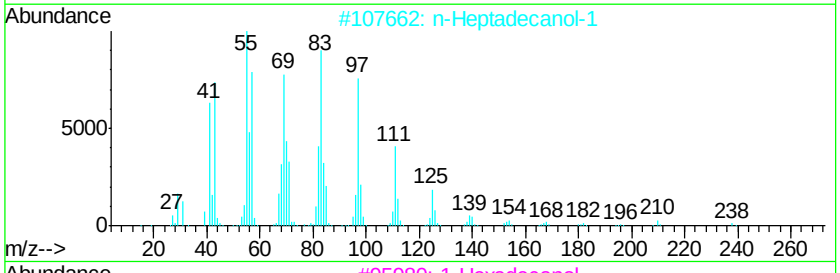
Peak Number 8 3-Chloropropionic acid, hep... Concentration Rank 6

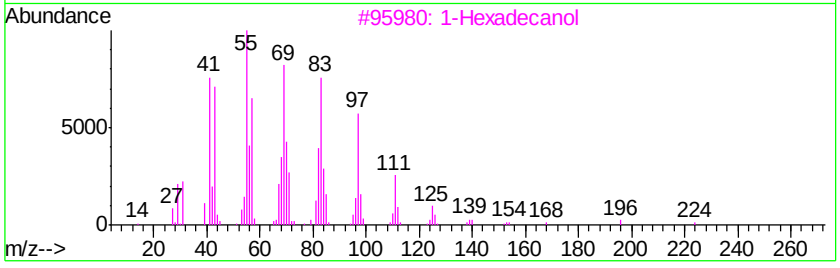
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.79	3.63 ng	118917	Chrysene-d12	13.93

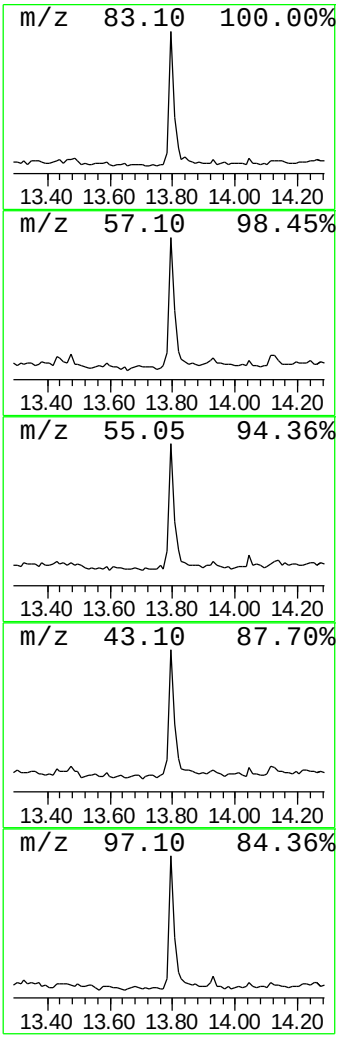
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	91
2	n-Heptadecanol-1	256	C17H36O	001454-85-9	91
3	1-Hexadecanol	242	C16H34O	036653-82-4	91
4	3-Eicosene, (E)-	280	C20H40	074685-33-9	90
5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	90











Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070216\
Data File : BF088623.D
Acq On : 2 Jul 2016 18:08
Operator : UM/SJ
Sample : H3847-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : R5-B1(0-11)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

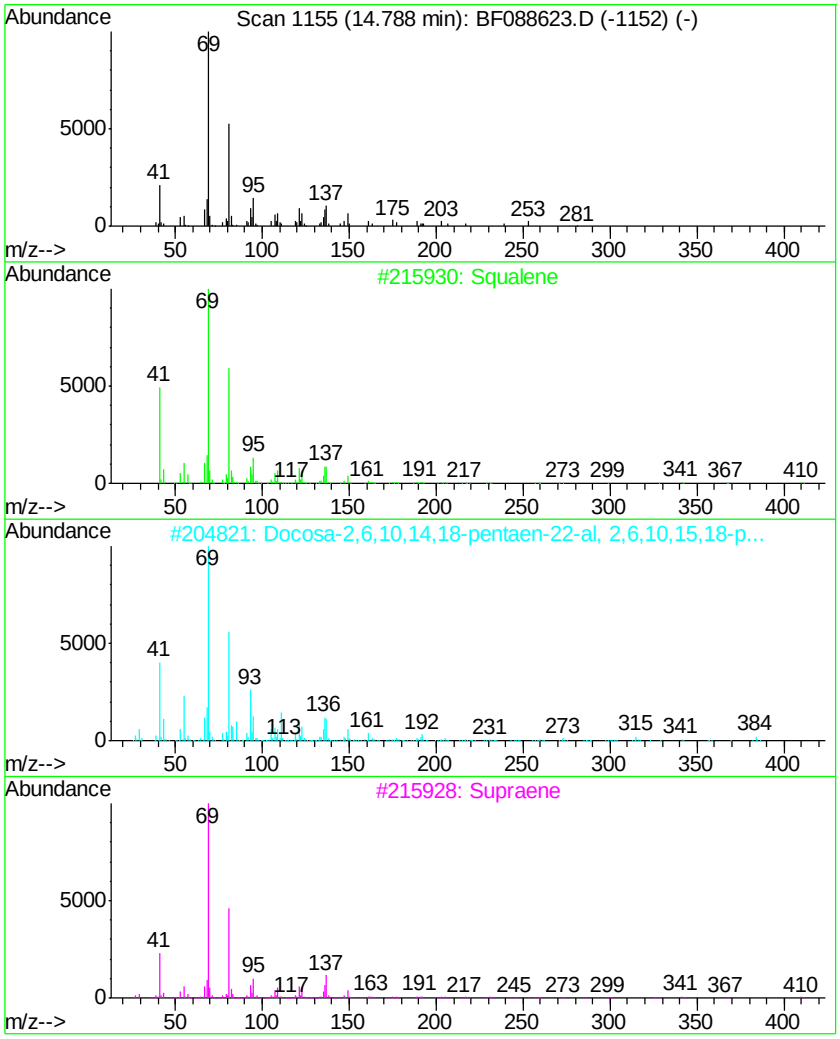
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

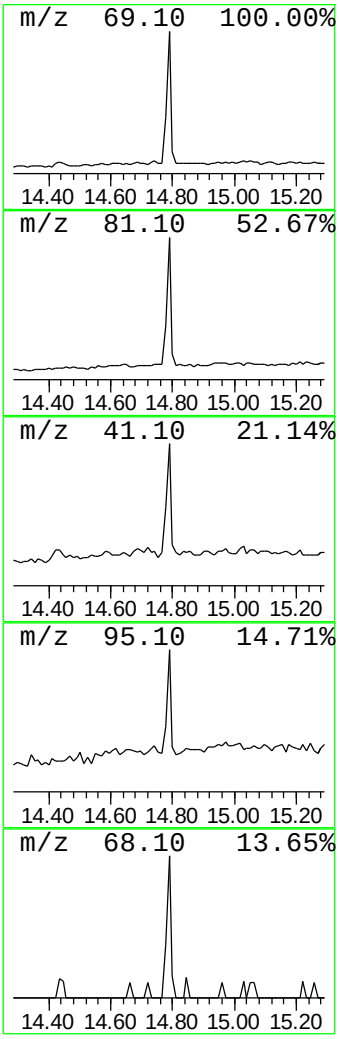
****

Peak Number 9 Squalene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.79	2.57 ng	79140	Perylene-d12	15.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	91
2	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	90
3	Supraene	410	C30H50	007683-64-9	87
4	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	80
5	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070216\
Data File : BF088623.D
Acq On : 2 Jul 2016 18:08
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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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
unknown3.02	3.02	7.0	ng	226629	1	6.79	649603	20.0
2-Pentanone, 4-hy...	4.96	7.3	ng	237987	1	6.79	649603	20.0
unknown6.56	6.56	70.9	ng	2302930	1	6.79	649603	20.0
Hexadecane	11.19	3.0	ng	107875	4	11.30	720904	20.0
3-Chloropropionic...	13.79	3.6	ng	118917	5	13.93	655438	20.0
Squalene	14.79	2.6	ng	79140	6	15.33	616681	20.0